PHOTOTOXIC TARGET LIPID MODEL FOR PREDICTING THE TOXICITY OF POLYCYCLIC AROMATIC HYDROCARBONS AND PETROLEUM TO AQUATIC LIFE

by

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ABSTRACT

The objective of this doctoral dissertation is to develop a model to predict the phototoxicity of petroleum and petroleum components to aquatic organisms. Petroleum contains polycyclic aromatic hydrocarbons (PAHs), alkylated PAHs and heterocyclic PAHs some of which absorb light in the ultraviolet light (UV) and visible (VIS) regions. The result is increased photo-enhanced toxicity, by a factor of two to greater than 1000 in the presence of light.

The PAHs in petroleum differ in their properties, such as octanol-water partitioning coefficients and molar absorption spectra, and each may exhibit phototoxicity. It is inefficient and impractical to conduct toxicity tests on all the chemicals and all the organisms of concern. Even if the testing was undertaken, it is not clear how to interpret the results and use them for phototoxic risk assessments where light conditions and time of exposure vary. Accordingly, there has been a considerable effort expended to develop models to predict the phototoxicity of PAHs to the aquatic organisms. In each of the previous modeling frameworks various combination of the underlying factors in phototoxicity were incorporated to varying degrees. However, no model included all elements in a unified modeling framework such that the model can be applicable to all PAHs, PAH mixtures, organisms, and light exposure conditions.

In this dissertation, a phototoxic target lipid model (PTLM) is developed to predict phototoxicity of single PAHs measured either as median lethal concentration (LC50) at a fixed duration of exposure or median lethal time (LT50) at a fixed concentration. The model accounts for differences in the physical and chemical

properties of PAHs and test species sensitivities, as well as variations in light characteristics, such as length of exposure, and the light source irradiance spectrum and intensity. The PTLM is based on the narcotic target lipid model (NTLM) of PAHs. Both models rely on the assumption that mortality occurs when the toxicant concentration in the target lipid of the organism reaches a threshold concentration. The model is calibrated using 333 observations of LC50s and LT50s for 20 individual PAHs, 15 test species, and various UV light exposure conditions and times ranging from 1 hour to 100 hours. The LC50 concentrations range from less than 0.1 to greater that 10^4 μg/L. The model has two fitting parameters that are shown to be constant across PAHs and organisms. The compound specific parameters incorporated in the PTLM are the octanol-water partition coefficient and molar absorption coefficient. The critical target lipid body burden is the only organism specific parameter. The root mean square error (RMSE) of prediction for log(LC50) and log(LT50) are 0.473 and 0.382, respectively. Other phototoxic components of petroleum include alkylated PAHs (APAHs) and benzothiophenes. The PTLM is validated by predicting the observed phototoxic LT50 and LC50 of those chemicals exposed to four different species under different light conditions with RMSE = 0.478. The results support the PTLM capability to predict the phototoxicity of single PAHs for organisms with a wide range of sensitivity and for various light exposure conditions.

Modeling the phototoxicity of mixtures is accomplished by using the toxic unit (TU) approach and TU additivity. The model is validated by predicting the phototoxicity of the binary and ternary mixtures of three PAHs, pyrene, anthracene, and fluoranthene exposed to *Americamysis bahia* and *Menidia beryllina.* The

comparison between the observed and predicted phototoxicity for the mixtures results in RMSE = 0.274.

The PTLM is applied to predict petroleum phototoxicity of the water accommodated fraction for three field collected oil samples, MASS (neat oil), CTC (moderately weathered oil), and Juniper (heavily weathered oil) exposed to four aquatic species indigenous to the Gulf of Mexico, *M. beryllina*, *A. bahia*, *Cyprinodon variegatus*, and *Fundulus grandis* using natural or simulated solar radiation. For cases in which no phototoxicity was observed, the PTLM predictions are correct in over 70% of the cases (10 out of 14 predictions). When toxicity was observed the RMSE = 0.321.

Chapter 1

INTRODUCTION

1.1 Motivation

Crude oils and refined petroleum products are complex mixtures with many components, including polycyclic aromatic hydrocarbons (PAHs), alkylated PAHs (APAHs), and heterocyclic PAHs [1-3]. Toxicity of petroleum released to the aquatic environment is increased by exposure to solar radiation. PAHs are known to exhibit photo-enhanced toxicity, showing a factor of two to greater than 1000 increase in toxicity in the presence of light in the ultraviolet (UV) and visible (VIS) regions [4-9]. Phototoxicity is expressed either as the concentration of the chemical require to cause 50% morality (PLC50) at a fixed duration of exposure or the time at which 50% morality occurs at a fixed concentration (PLT50).

The individual PAHs present in petroleum number in the hundreds to thousands of the parent and alkylated compounds. They differ in their properties such as octanol-water partitioning coefficients and spectral absorption coefficients. Performing toxicity tests on that many chemicals is impractical. Even if they were performed, it is not clear how to use the results for risk assessments purpose when light conditions and time of exposure vary. Therefore, a model to predict the phototoxicity of PAHs and PAH mixtures to aquatic organisms is required.

Studies have been done on modeling the phototoxicity of PAHs to aquatic organisms [10-17]. These modeling efforts often were applied to a single organism including, *Artemia salina* nauplii [10], *Daphnia magna* [11], *Pimephales promelas* [4],

Lumbriculus variegatus [13], *Lemna gibba* [15], and *Scenedesmus vacuolatus* [16]. Chemical dependent factors that contribute to phototoxicity that were considered included molar absorption spectrum [12-14,17] and bioconcentration factor [10,12]. For studies that developed models to predict phototoxicity for more than one PAH, a relative potency activity (RPA) was introduced to account for the PAHs different photodynamic potentials [10,11,16,17]. However, the RPAs for a specific PAH were not consistent across the studies because the RPA is a function of species sensitivities and light exposure conditions and duration.

In summary, each of the previous models incorporated the underlying factors that determine the phototoxicity to varying extents: properties of the PAHs (spectral molar absorption) [10,11,15,16], incident light (intensity, spectral irradiance, and duration) [10,11,15,16], and tissue PAH concentration [11,13,14,16,17]. However, no study presented a model that included all these components such that the model can predict the phototoxicity to an organism without including an empirical RPA or similar normalization. Additionally, the difference in species sensitivity was not considered in any of the models limiting their scope of application to one organism.

Therefore, developing a predictive model applicable to many aquatic organisms, PAHs, and light conditions would be of significant improvement in predicting the phototoxicity of PAHs and subsequently risk assessment of petroleum phototoxicity. Chapter 2 provides a comprehensive review of state of the art of modeling PAH phototoxicity.

1.2 Research Goals

The overall objective of this doctoral dissertation is to develop a model to predict the phototoxicity of petroleum and petroleum components to aquatic

organisms. Since PAHs are the primary phototoxic components of petroleum, the first task is to develop a predictive model for single PAHs phototoxicity.

In Chapter 3, a phototoxic target lipid model (PTLM) is developed to predict phototoxicity of single PAHs measured either as median lethal concentration (LC50) at a fixed duration of exposure, or median lethal time (LT50) at a fixed exposure concentration. The model is able to account for the differences in the physical and chemical properties of PAHs, the test species sensitivities, and variations in light source characteristics, intensity, and length of exposure. The PTLM is based on the narcotic target lipid model (NTLM) of PAHs [18]. Both models are based on the assumption that mortality occurs when the toxicant concentration in the target lipid of the organism reaches a threshold concentration. The PTLM is applied to 333 experimental LC50 and LT50 data, for 20 individual PAHs, 15 organisms exposed to natural and simulated solar radiation and different UV light sources for light exposure times varying from less than 1 hour to 100 hours. The LC50 concentrations span from less than 0.1 to greater than 10^4 μg/L. The model has only two fitting parameters which are constant across PAHs and organisms. The root mean square error of prediction for log(LC50) and log(LT50) are 0.473 and 0.382, respectively. The results indicate that the PTLM can predict the phototoxicity of single PAHs over a wide range of exposure conditions to many organisms with a wide range of sensitivity.

Similar to parent PAHs, APAHs and heterocyclic aromatic hydrocarbons, including dibenzothiophene, that are present in petroleum exhibit photo-enhanced toxicity. Accordingly, the PTLM ability to predict phototoxicity of these constituents is examined. In Chapter 4, the predicted and observed PLC50s are compared for 10 APAHs, as well as dibenzothiophene and acridine for four different organisms,

Americamysis bahia, *Rhepoxynius abronius*, *Daphnia magna*, and *Pimephales promelas* resulting the RMSE = 0.483.

Additionally, as these compounds occur as mixtures in petroleum, the PTLM application to the prediction of phototoxicity of mixtures also is investigated in Chapter 4. The toxicity of a chemical in a mixture is predicted using toxic units (TU) [19-23], which is the ratio of the concentration of the chemical in the exposre medium to the effect concentration in that medium (LC50). Assuming TU additivity, the total toxic unit for a mixture is calculated as the sum of the TU of all the toxic components in the mixture.

Initially the phototoxicity of binary and ternary mixtures of PAHs is investigated. The phototoxic units (PTU) of the components are calculated using the PTLM and summed to predict the total PTU of the mixture. The validity of PTLM to predict phototoxicity of mixtures is tested comparing the predicted versus observed PTUs for binary and ternary combinations of pyrene, anthracene, and fluoranthene exposed to *A. bahia* and *Menidia beryllina.* The comparison resulted in RMSE = 0.291 demonstrating that PTLM can be applied to predict phototoxity of PAHs in the mixture. Also, comparing the observed mortalities at the corresponding predicted PTUs for the mixtures reproduces the observed dose-response within the usual uncertainty supporting the additivity assumption and the model predictive ability for mixtures [20].

Finally, the PTLM is used to predict phototoxicity of petroleum in terms of water accommodated fraction (PLC50 (%WAF)). Validation is performed for three petroleum samples, MASS (neat oil), CTC (moderately weathered oil), and Juniper (heavily weathered oil) collected during the Deep Water Horizon oil spill and exposed

to four species indigenous to the Gulf of Mexico, *M. beryllina*, *A. bahia*, *Cyprinodon variegatus,* and *Fundulus grandis*. The oil samples were exposed to *M. beryllina* and *A. bahia* under natural radiation for all three types of oil. For CTC oil, additional artificial radiation exposure experiments were conducted for these two organisms. *C. variegatus* and *F. grandis* were exposed to only artificial radiation. Narcotic toxicity of the oil samples were also predicted applying NTLM and toxic unit additivity. For cases in which no phototoxicity was observed, the PTLM predictions are correct in over 70% of the cases (10 out of 14 predictions). When toxicity was observed, the RMSE = 0.321.

Chapter 2

A CRITICAL REVIEW OF MODELS OF POLYCYCLIC AROMATIC HYDROCARBONS PHOTOTOXICITY

Polycyclic aromatic hydrocarbons (PAHs) are known to exhibit photo-induced toxicity. PAHs number hundreds to thousands of the parent and substituted compounds in the environment and developing a predictive model applicable to a wide variety of PAHs and organisms is a necessary precursor to environmental risk assessments. There has been evolutionary progress in phototoxicity modeling since 1977. In this chapter, a comprehensive review of the models developed to predict phototoxicity of PAHs is presented. The contributions of the models to the state of the art are discussed. The models are also compared in terms of their scope of applicability to different organisms, PAHs, endpoints (median lethal time and median lethal concertation), and light conditions.

2.1 Introduction

Polycyclic aromatic hydrocarbons (PAHs) are organic compounds composed of carbon and hydrogen atoms grouped into at least two condensed aromatic rings. They are a ubiquitous class of environmental contaminants [24-26] and are of particular concern in the aquatic environment because they are introduced into surface waters by urban and industrial runoff, oil spills, and aerial (atmospheric) deposition [27]. Most PAHs are toxic only at concentrations large enough to exert baseline narcotic toxicity [5,25,28]. Environmental factors such as solar radiation, however, can considerably increase the toxicity of some PAHs. This important subset of PAHs

can absorb light in ultraviolet (UV) and visible (VIS) wavelengths resulting in the generation of reactive species that increases their toxicity.

The photo-enhanced toxicity of PAHs has been known since 1928 [29]. Later, the adverse effects of PAH sensitizers in mammalian models in the presence of UV have been observed [30,31]. The occurrence, mechanism of action, and predictability of PAH phototoxicity to various organisms have been reported, including bacteria [32,33], crustacea [10,11,34-36], fish [4,12], worms [13,14], the aquatic plant *Lemna gibba* [15], and algae [13,37,38]. Comprehensive reviews of these studies are presented by Arfsten et al. [7], Diamond [27], and Giesy et al. [39].

The individual PAHs present in almost every contaminated site number hundreds to thousands of the parent and substituted compounds. They differ in their properties such as octanol-water partitioning coefficients and spectral absorption coefficients. It is infeasible to perform toxicity tests on that many chemicals and even if it were undertaken, it would not be clear how to interpret the results and utilize them in risk evaluations where light conditions and time of light exposure vary. Therefore, a considerable effort has been expended in developing models to predict the phototoxicity of PAHs to aquatic organisms. This chapter presents a comprehensive review of the available models.

2.2 Morgan and Warshawsky (1977)

Morgan and Warshawsky [10] exposed *Artemia salina* nauplii to PAHs and UV light at a single wavelength (366 nm). The average number of *A. salina* nauplii immobilized per sample (ANI) was predicted as a function of the amount of light absorbed by the nauplii, I_a (quanta), as follows:

$$\frac{d(\text{ANI})}{dt} = \phi_I I_a \tag{2-1}$$

where ϕ_I is the quantum yield for immobilization and t is time (min). The Beer-Lambert law was applied to calculate I_a as a function of the incident light intensity on nauplii (I_o), molar absorption of the sensitizer at 366 nm (ε), the path length of the nauplii (l), the fraction of available sensitizer absorbed by the nauplii (α), and concentration of the sensitizer placed in solution with nauplii (C). Integrating Equation 2-1 yields:

$$\text{ANI} = (I_o l \alpha \phi_I)(2.303 \varepsilon C t) + B \tag{2-2}$$

where B is a constant of integration. Performing a linear regression of ANI versus (2.303 ε C t) resulted in a linear correlation with the slope of ($I_o l \alpha \phi_I$). The results for benz[c]acridine and benzo[a]pyrene shown in Figure 2-1 (termed the immobilization curves).

To overcome the difficulties of quantifying the parameters I_o, l, α, and ϕ_I, a relative photodynamic activity (RPA) was defined by dividing the slope of the immobilization curve ($I_o l \alpha \phi_I$) for each PAH by the slope of a reference compound ($I_o l \alpha' \phi'_I$), chosen to be benzo[c]acridine. The RPAs reported for 41 PAHs are listed in Table 2-1 for two different incubation times, 2 and 22 (h).

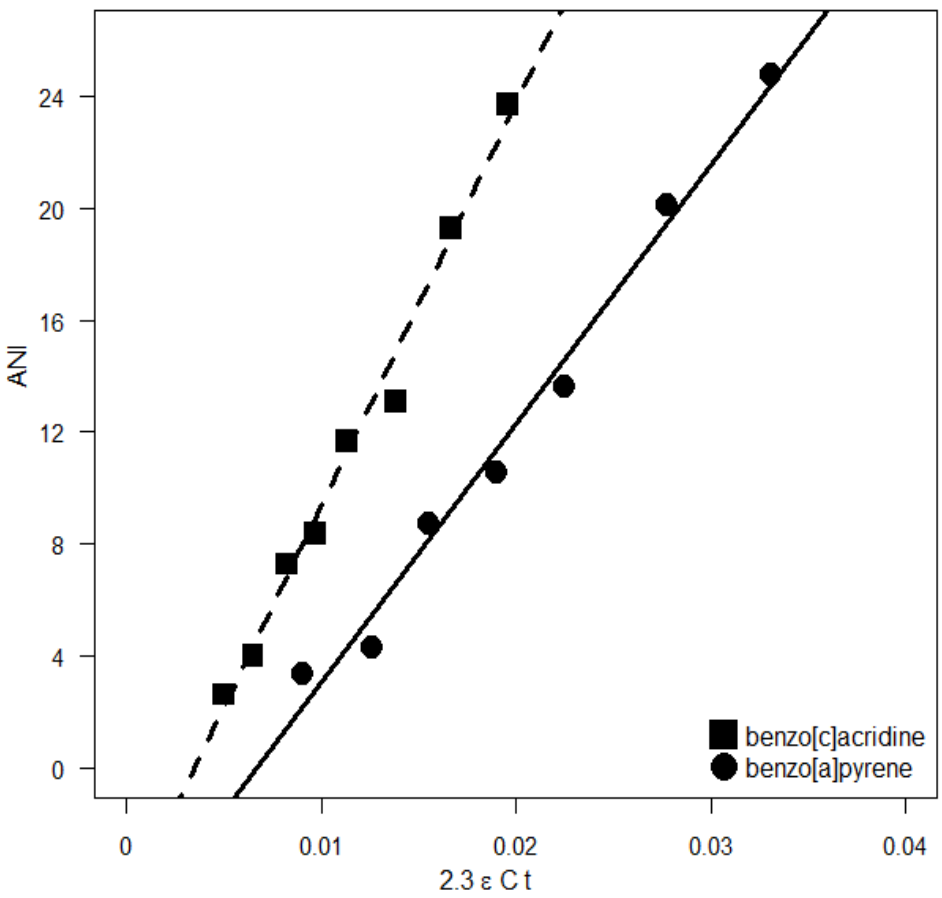

Figure 2-1. Average number of *Artemia Salina* nauplii immobilized (ANI) as a function of (2.3 ε C t). Benzo[*c*]acridine (square symbols with dashed line), C = 85.7 nM; benzo[*a*]pyrene (circles with solid line), C = 22 nM. The slopes determine $I_o l \alpha \phi_I$ [10].

Table 2-1. Relative photodynamic activities (RPA) of carcinogenic and noncarcinogenic PAHs in *Artemia salina* nauplii [10].

PAH	RPA[a] 2 h	RPA[a] 22 h
Benzo[*a*]anthracene	9.8	
Benzo[*c*]phenanthrene	2	4.7
11H-Benzo[*a*]carbazole	1.2	4.4
Dibenzo[*a,j*]acridine	2.2	0.11
Benzo[*a*]pyrene	0.55	2.3
7H-Dibenzo[*c,g*]carbazole	0.23	2.3
Benzo[*e*]acephenanthrylene	0.14	3.3
Benzo[*k*]fluoranthene	0.08	0.01
Dibenzo[*a,h*]anthracene	0	0
Dibenzo[*a,e*]aceanthrylene	0.1	
Benzo[*r,s,t*]pentaphene	0.02	
Dibenzo[*h,r,s,t*]pentaphene	0	
Acridine	0.02	
Phenazine	0.003	
Benzo[*c*]acridine	1	1
Pyrene	0.72	
Chrysene	0.2	
Fluoranthene	0.15	
Benzo[*a*]acridine	0.06	0.63
Benzo[*g,h,i*]fluoranthene	0.96	0.007
Dibenzo[*a,c*]phenazine	0.33	1.3
Benzo[*e*]pyrene	0.19	0.37
Benzo[*b*]triphenylene	0.12	0.16
Perylene	0.04	
Dibenzo[*g,p*]chrysene	0.21	0.19
Rubicene	0	
Pyanthrene	0	
Diindeno[1,2,3-*c,d*-3,2,1-lm]-perylene	0	

The work pointed out the importance of quantifying the amount of light absorbed by the photosensitizer and introduced the concept of phototoxic potential of the sensitizer. The use of an RPA to normalize the toxicity of different PAHs is common to many subsequent models.

2.3 Newsted and Giesy (1987)

Newsted and Giesy [11] utilized the formulation introduced by Morgan and Warshawsky [10] starting with a similar differential equation (Equation 2-1). However, rather than using a single-wavelength light source, a source with a distribution of wavelengths was employed. The light intensity absorbed by the organism (I_a) was replaced by the average number of quanta absorbed $\bar{A}$ (μJ/s/cm^2)

$$\bar{A} = (1/n)\sum_{\lambda}^{n}[(I_\lambda T_\lambda)(\varepsilon_\lambda b C_a)] \qquad (2\text{-}3)$$

where n = the number of wavelengths used in the summation, λ is wavelength (nm), I_λ = the irradiation intensity of the light source (μJ/s/cm^2), T_λ = the optical transmittance of the organism (%/100), ε_λ = the molar absorption coefficient of the PAH (L/mol/cm), b = the path length of the organism (cm), and C_a = the concentration of the PAH in the organism (mmol/g). Substituting $\bar{A}$, replacing ANI with percent mortality (M), and integrating the differential Equation 2-1 yields

$$M = \bar{A}\phi t + B \qquad (2\text{-}4)$$

where ϕ = the potency (percent mortality × cm^2/μJ), t = time (s), and B is the integration constant. The linear relationship in Equation 2-4 was used to determine ϕ for each PAH from the slope of M vs. t (i.e., $\bar{A}\phi$). The value of ϕ obtained for each chemical was normalized by the ϕ of benzo[b]anthracene to determine the RPAs for 16 PAHs (Table 2-2).

Table 2-2. Median lethal times (LT50), potency (ϕ), relative photodynamic activities (RPA), and median lethal times adjusted to a constant PAH concentration (ALT50) for *Daphnia magna* exposed to 16 PAHs [11].

PAH	LT50 (min)	ϕ	RPA	ALT50 (min)
Anthracene	298.5	4.6×10^{-3}	1.06	289.5
Benzo[*a*]pyrene	266.5	8.4×10^{-3}	1.83	268.7
Dibenzo[*a,h*]anthracene	185	4.9×10^{-3}	1.13	276.9
Fluoranthene	648.9	1.8×10^{-3}	0.42	648.8
Pyrene	208.6	7.2×10^{-3}	1.64	205.7
Benzo[*a*]anthracene	750.6	2.0×10^{-3}	0.45	334.3
Benzo[*e*]pyrene	915.8	9.6×10^{-4}	0.22	888.6
Benzo[*a*]fluorine	1376.7	7.9×10^{-4}	0.18	1494.1
Benzo[*b*]fluorine	1344.1	6.0×10^{-4}	0.14	1436.8
Acridine	53.8	2.2×10^{-2}	5.05	53.2
Benzo[*k*]fluoranthene	780.4	1.3×10^{-4}	0.3	770.3
Benzanthrone	323	3.7×10^{-3}	0.85	331.1
Chrysene	1438.8	2.0×10^{-3}	0.44	348
Perylene	1099.7	5.9×10^{-4}	0.13	466
Benzo[*b*]anthracene	985.5	4.3×10^{-3}	1	775
Benzo[*g,h,i*]perylene	828.9	6.3×10^{-3}	1.45	227.1

The exposure time required to produce 50% mortality (LT50s) for various PAHs were obtained by exposing *Daphnia magna* to a simulated sunlight light source. The adjusted LT50s (ALT50s) were scaled to represent a constant concentration of the

PAH in *D. magna* (Table 2-2). Multiple linear regression models were developed using photophysical and physiochemical parameters (singlet energy, triplet energy, singlet-triplet splitting energy, molecular connectivity, etc.). The models using triplet energy were the most accurate descriptors of the phototoxicity found in this study. The best model obtained (R^2 = 0.686) for LT50 (min) was a four-variable quantitative structure-activity relationship (QSAR)

$$\begin{aligned} \mathrm{LT50} = {} & 506.576\ (\mathrm{TP}) - 3.823(\mathrm{ES}) - 4.414\ (\mathrm{ET}) \\ & - 187.460\ (\mathrm{ABSO}) + 2447.864 \end{aligned} \tag{2-5}$$

where TP = phosphorescence lifetime (s), ES = the singlet energy (kJ/mol), ET = the triplet energy (kJ/mol), and ABSO stands for the total electromagnetic energy absorbed. For the ALT50 (min), the best fit was (R^2 = 0.545)

$$\begin{aligned} \mathrm{ALT50} = {} & 386.288\ (\mathrm{TP}) - 8.417\ (\mathrm{ES}) - 794.222\ (\mathrm{MC2}) \\ & + 544.739\ (\mathrm{MC1}) + 3118.160 \end{aligned} \tag{2-6}$$

where MC2 and MC1 represent the second-order and the first-order molecular connectivity, respectively. The plots of LT50 and ALT50 vs ET are shown in Figure 2-2, top and bottom panel, respectively. Table 2-3 provides the list the PAHs in Figure 2-2 indicated by numbers.

The major improvements made by Newsted and Giesy [11] were accounting for the light absorption at all the wavelengths in the light source (Equation 2-4), and using the organism tissue concentration rather than the aqueous concertation as a measure of the PAH dose.

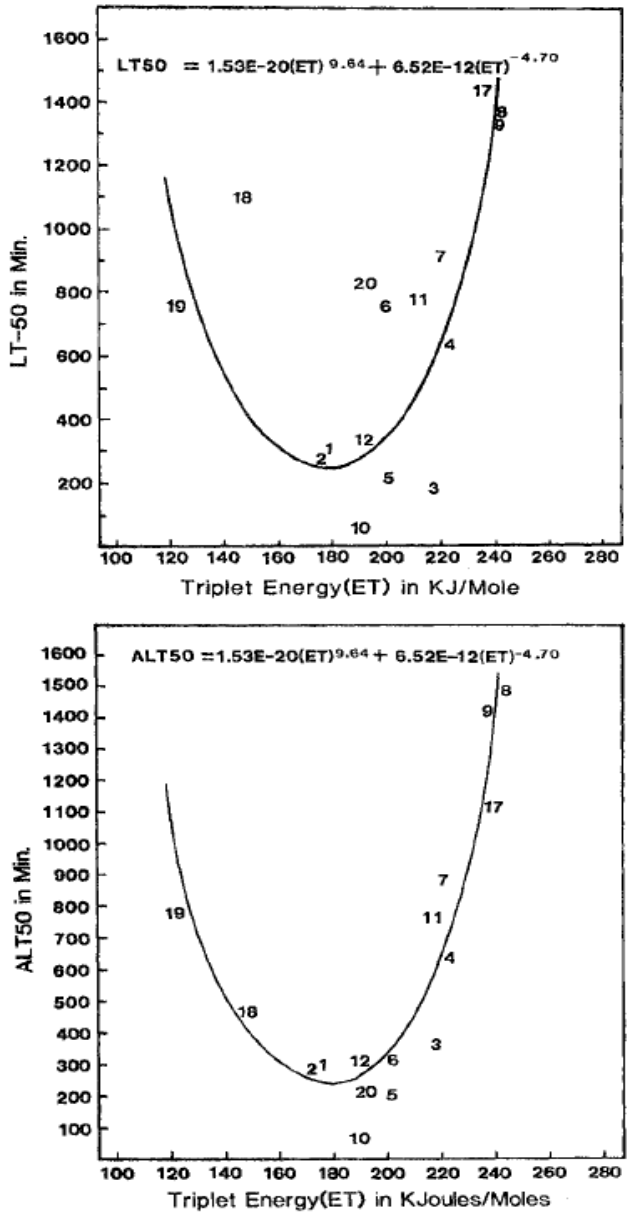

Figure 2-2. Top: Median lethal time (LT50) as a function of lowest triplet energy. Bottom: Adjusted median lethal time (ALT50) as a function of lowest triplet energy. The PAHs are identified by numbers for which the corresponding names are indicated in Table 2-3 [11].

Table 2-3. List of PAHs in Figure 2-2 [11].

Number	Compound
1	Anthracene
2	Benzo[*a*]pyrene
3	Dibenzo[*a*,*h*]anthracene
4	Fluoranthene
5	Pyrene
6	Benzo[*a*]anthracene
7	Benzo[*e*]pyrene
8	Benzo[*a*]fluorene
9	Benro[*b*]fluorene
10	Acridine
11	Benzo[*k*]fluoranthene
12	Benzanthrone
13	Phenanthrene
14	Fluorene
15	Carbazole
16	Triphenylene
17	Chrysene
18	Perylene
19	Benzo[*b*]anthracene
20	Benzo[*g*,*h*,*i*]perylene

2.4 Mekenyan et al. (1994)

Mekenyan et al. [40] suggested that the parabolic relationship (Figure 2-2) observed for the PAHs in *D. magna* studied by Newsted and Giesy [11] was a consequence of two factors that influences photo-enhanced toxicity: internal (structural) factors (e.g. light absorption and compound stability) and the external factors (e.g. UV exposure intensity and energy). An analysis of the relationships between these factors and the PAH's HOMO-LUMO gap, the difference in energy between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), convinced the authors that the HOMO-LUMO gap of PAHs was a suitable predictor of PAH phototoxicity. Using the data from PAHs

phototoxicity to *D. magna* reported by Newsted and Giesy [11], Mekenyan et al. [40] proposed that PAHs exhibiting phototoxicity were consistently within HOMO–LUMO gap "window" of 7.2 ± 0.4 (eV).

The QSARs derived using the data from Newsted and Giesy [11], required the initial classification of PAHs as stable and unstable under the test conditions. For the stable PAHs, Equations 2-7 and 2-8 were established to relate ALT50 (min) to the HOMO-LUMO gaps, $\Delta E_{\text{HOMO-LUMO}}^{\text{PM3}}$ (eV) and $\Delta E_{\text{HOMO-LUMO}}^{\text{AM1}}$ (eV), which were calculated using the semi-empirical quantum chemical methods, PM3 and AM1, respectively.

$$\log(1/\text{ALT50}) = 2.473(\pm 1.021) - 0.687(\pm 0.132)\Delta E_{\text{HOMO-LUMO}}^{\text{PM3}} \quad (2\text{-}7)$$

$$\log(1/\text{ALT50}) = 2.369(\pm 0.994) - 0.674(\pm 0.128)\Delta E_{\text{HOMO-LUMO}}^{\text{AM1}} \quad (2\text{-}8)$$

For the unstable PAHs, the following equations were proposed to predict phototoxicity of PAHs to *D. magna*

$$\log(1/\text{ALT50}) = -11.40(\pm 0.577) + 1.306(\pm 0.084)\Delta E_{\text{HOMO-LUMO}}^{\text{PM3}} \quad (2\text{-}9)$$

$$\log(1/\text{ALT50}) = -10.18(\pm 0.524) + 1.128(\pm 0.076)\Delta E_{\text{HOMO-LUMO}}^{\text{AM1}} \quad (2\text{-}10)$$

The results are presented in Table 2-4. The phototoxic response in *D. magna* versus HOMO-LUMO gap is illustrated in Figure 2-3. Non-phototoxic compounds such as phenanthrene, triphenylene, carbazole, and fluorene appeared on the right side of the curve near the baseline. The strongly phototoxic compounds such as benzo[*a*]pyrene, anthracene, and pyrene appeared in the middle of the curve at 7.2 ±

0.4 (eV). Compounds falling on the left side of the curve were considered less phototoxic or non-phototoxic.

This study developed an approach that related phototoxicity of PAHs to their intrinsic molecular properties that can be computed from their chemical structures. The approach can be used in the absence of empirical data to classify the PAHs into toxic or non-toxic groups. What remained to be done was to find the reason that this relationship succeeded.

Table 2-4. Observed and calculated toxicities of 28 PAHs in relation to HOMO–LUMO Gap (data are presented in Figure 2-3) [40].

		HOMO-LUMO Gap[a]	
PAH	log(1/ALT50)	PM3	AM1
Anthracene	-2.46	7.279	7.284
Benzo[*a*]pyrene	-2.43	6.817	6.812
Dibenzo[*a,h*]anthracene	-2.44	7.458	7.452
Fluoranthene	-2.81	7.68	7.701
Pyrene	-2.31	7.239	7.239
Benzo[*a*]anthracene	-2.52	7.395	7.392
Benzo[*e*]pyrene	-2.95	7.365	7.362
Benzo[*a*]fluorene	-3.17	7.846	7.804
Benzo[*b*]fluorene	-3.16	7.974	7.986
Acridine	-1.73	7.402	7.531
Benzo[*k*]fluoranthene	-2.89	7.382	7.389
Benzanthrone	-2.52	7.455	7.427
Phenanthrene	-3.2	8.202	8.207
Fluorene	-3.2	8.507	8.493
Carbazole	-3.2	8.191	8.309
Triphenylene	-3.2	8.215	8.204
Chrysene	-2.54	7.713	7.693
Perylene	-2.67	6.712	6.7
Benzo[*b*]anthracene	-2.89	6.517	6.517
Benzo[*g,h,i*]perylene	-2.36	6.971	6.957
Coronene[b]	-2.27, -2.33, -2.34, -2.38	6.907	6.967
Dibenzo[*a,j*]anthracene[b]	-2.36, -2.43	7.035	7.119
Benzo[*b*]chrysene[b]	-2.75, -2.89	6.519	6.606
Benzo[*b*]triphenylene[b]	-2.40, -2.46	7.088	7.163
Benzene[b]	-3.00, -3.06	7.958	8.052
Naphthalene[b]	<-3.2	10.06	10.164
Dibenzo[*b,i*]anthracene[b]	<-3.2	5.328	5.386
Benzo[*a*]chrysene[b]	-2.40, -2.48	7.097	7.203

[a]HOMO–LUMO gap calculations were performed using two different quantum chemical techniques.

[b]Toxicity (log(1/LT50)) was estimated using the HOMO-LUMO gap model. For some compounds, toxicity was estimated using more than one HOMO-LUMO gap model.

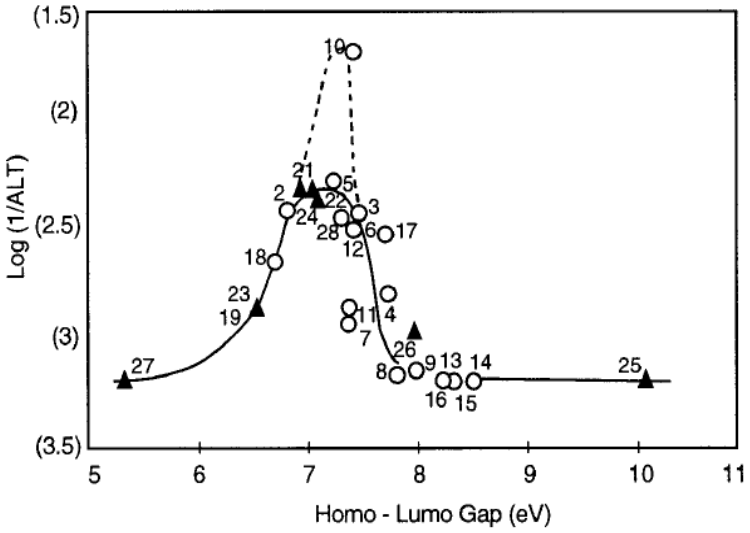

Figure 2-3. Variation of toxicity (log(1/ALT50)) with HOMO–LUMO gap. The solid triangles denote the predicted toxicity values for PAHs 21–28 in Table 2-4 [40].

2.5 Veith et al. (1995)

The HOMO–LUMO gap analysis introduced by Mekenyan et al. [40] was further extended by Veith et al.'s [41] investigation of substituents effects on phototoxicity of PAHs. The observations showed alkyl and hydroxyl substituents did not have significant effects on the HOMO–LUMO gap of PAHs, while nitro, alkane, and chloro substitution on PAHs altered the HOMO–LUMO gap. Veith et al. [41]

defined a new window of 7.75 ± 0.25 (eV) to identify phototoxic substituted PAHs derivatives.

2.6 Oris and Giesy (1985)

Oris and Giesy [12] compared the experimental LT50 data from *Lepomis macrochirus* exposure to anthracene using a laboratory lamp simulating solar irradiance to the LT50 values predicted using the Bunsen–Roscoe law (BRL) of reciprocity. The BRL states that for a fixed concentration of the sensitizer –anthracene in this study– there is a linear relationship between the biological effect and the product of light intensity and the reaction time [42]. The experiments were conducted for varying light intensities and anthracene aqueous concentrations. The relationship between the experimentally determined log(LT50 × UV intensity) and the corresponding anthracene aqueous concentrations did not produce the expected common slope and intercept (Figure 2-4). A comparison of predicted and observed LT50s revealed that the model consistently over-predicted toxicity at high UV intensities (filled triangles in Figure 2-4) and under-predicted toxicity at low UV intensities (filled circles in Figure 2-4).

Although they found an apparent inconsistency between the expected linear relationship and the experimental results, the BRL was brought to future researchers' attention and used in subsequent attempts to model PAHs phototoxicity.

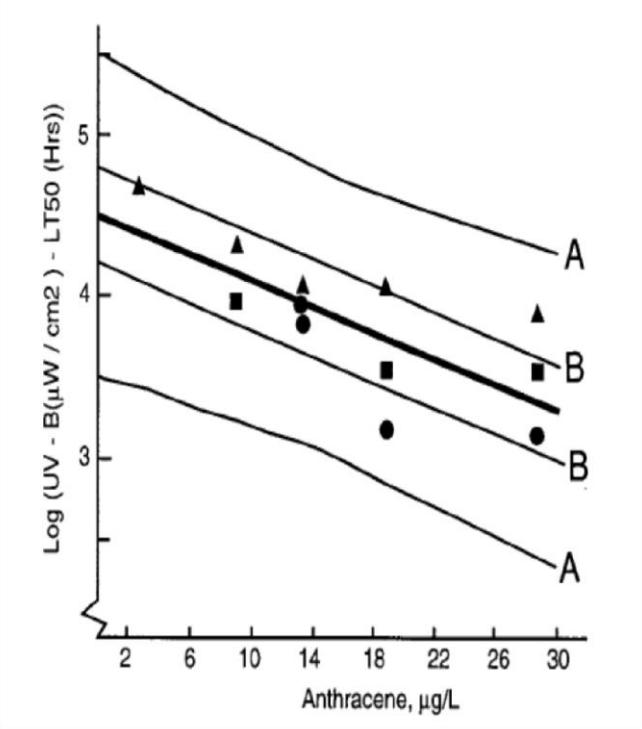

Figure 2-4. Correlation between the product of UV light intensity and median lethal time versus anthracene concentration in water for continuous simulated sunlight exposures. Experiments were conducted at ▲ 170 mW/cm^2, ■ 70 mW/cm^2, and ● 14.8 mW/cm^2 UVB. A and B lines represent the continuous confidence bands around the regression for the 95th and 90th percentile, respectively [12].

2.7 Ankley et al. (1995)

Ankley et al. [13] applied the BRL to *Lumbriculus variegatus* co-exposed to UV light and the PAHs fluoranthene [13], anthracene [14], and pyrene [14]. Whereas Oris and Giesy [12] used the aqueous PAH concentrations, Ankley et al. [13,14] used the measured tissue concentrations of the PAHs in the organism. The experimentally

determined log(LT50)s were correlated to the measured log(initial residue × UV intensity) = log(R_oI)

$$\log(\mathrm{LT50}) = -\log(R_oI) + \log(\frac{D_L}{k}) \qquad (2\text{-}11)$$

where LT50 is in h, R_o = concentration of chemical in tissue (μg/g wet wt), I = incident light intensity (μW/cm^2), D_L = lethal damage, and k = a rate constant for accrual of damage (g cm^2 h μg^{-1} μW^{-1}). The equation predicts the slope of -1 and a constant quantity for the intercept log(D_L/k).

Additionally, the BRL application appeared in further studies utilizing the same method to predict phototoxicity of fluoranthene to *Pimephales promelas* [43], as well as fluoranthene [44], anthracene, and pyrene [45] to *Utterbackia imbecillis*. The slopes and intercepts obtained fitting the model (Equation 2-11) to the experimental data are provided in Table 2-5. The slopes ranged from -0.768 to -1.105. The variation among the intercepts was from 3.190 to 5.728.

Table 2-5. Slopes and intercepts obtained by linear regression of the median time to death and (light intensity×initial tissue concentration) for different PAHs and organisms.

PAH	Organism	Slope	Intercept	R^2	References
Fluoranthene	*Lumbriculus variegatus*	-0.768	4.263	0.928	[13]
Anthracene	*Lumbriculus variegatus*	-1.074	4.889	0.927	[14]
Pyrene	*Lumbriculus variegatus*	-0.751	3.772	0.876	[14]
Fluoranthene	*Pimephales promelas*	-1.105	5.728	0.698	[43]
Fluoranthene	*Utterbackia imbecillis*	-0.840	3.510	0.883	[44]
Anthracene	*Utterbackia imbecillis*	-0.850	3.190	0.883	[45]
Pyrene	*Utterbackia imbecillis*	-0.960	3.620	0.749	[45]

2.8 Krylov et al. (1997)

Krylov et al. [15] and Huang et al. [46] developed a QSAR to explain phototoxicity of 16 PAHs to *L. gibba* under simulated solar radiation on the basis of photosensitization reactions and direct toxicity of the photo modification products. To estimate the portion of toxicity due to photosensitization reactions, the toxicity of the parent PAHs was considered, whereas toxicity of the photomodified PAHs was determined by irradiating the test solution prior to incubation. For all experiments, the chemical exposure concentration was 2 mg/L. Toxicity of the intact and photomodified PAHs was determined as diminished leaf production, expressed as Y =

$\ln(N_t/N_c)$, where N_t is the number of leaves in the sample treated with a given PAH and N_c is the number of leaves in the control at time, t. Y was calculated for each 2-d time interval during the 8-d test. Toxicity of each PAH was expressed as the corresponding Y normalized to that of anthracene indicated as Y^n and was correlated with two constants: a photosensitization factor (PSF) and a photomodification factor (PMF). PSF was calculated for each PAH [46]

$$\mathrm{PSF} = [C_{\mathrm{L}}]^n \varphi^n J^n \tag{2-12}$$

where $[C_{\mathrm{L}}]^n$ = plant uptake of PAH (μmol/g fresh weight), φ^n = the quantum yield for triplet-state formation, and J^n = absorption of the simulated sunlight. The superscript n indicates that the values are normalized to those of anthracene. For the light absorption calculation, Krylov et al. [15] introduced the following formulation

$$J = \int_{\lambda_{\min}}^{\lambda_{\max}} I(\lambda)\varepsilon(\lambda)d\lambda \tag{2-13}$$

where $\lambda_{\min}$ and $\lambda_{\max}$ = the lower and upper limits of the wavelength range (nm), respectively, $I(\lambda)$ = the photon irradiance rate (μmol/m^2/s), and $\varepsilon(\lambda)$ = the molar absorption coefficient (L/mol/cm) at wavelength λ (nm). The triplet-state quantum yields were experimental quantities obtained from the literature [47-50]. PMF accounted for photomodification and was defined by Equation 2-14

$$\mathrm{PMF} = k_m^n T_{\mathrm{pm}}^n \tag{2-14}$$

where k_m^n = the normalized exponential decay rate constant based on half-life (h^{-1}) and T_{pm}^n = the inhibition of growth of *L. gibba* exposed to 2 mg/L of fully modified PAH

normalized to that of anthracene [15]. Linear regression was performed to correlate normalized toxicity, Y^n, to the PSFs and PMFs (R^2 = 0.850)

$$Y^n = 1.3 + 0.09\log(\text{PSF}) + 0.2\log(\text{PMF}) \quad (2\text{-}15)$$

The authors pointed out the importance of the overlap between the spectral irradiance of the light source and the molar absorbance spectrum of compound in phototoxicity. They presented the formula to calculate the light absorption in the range of wavelength that the overlap takes place (Equation 2-13).

2.9 Grote et al. (2005)

A model using the equation proposed by Ankley et al. [13] (Equation 2-11) was developed by Grote et al. [16] for the green alga *Scenedesmus vacuolatus* with the following modifications. Unlike the approach used by Ankley et al. [13,14] in which the endpoint of interest was LT50, the light exposure duration, Grote et al. [16] kept the duration of exposure t (h) constant and found the ED50 concentration as the measure of toxicity. Accordingly, the tissue concentration, R_o, in Equation 2-11 was replaced by the median effective dose, ED50 (nmol/L), which is the tissue concentration at which 50% mortality occurs after t = 24 (h). The critical level of damage (D_L) was replaced by the level of damage of cellular functions required to produce 50% of inhibition of reproduction ($D_{I50\%}$). Another modification made by Grote et al. [16] was replacing the incident light (I_o) with the absorbed light, J, introduced by Krylov et al. [15] (Equation 2-13). J was expressed in the unit of (μE/mol/s). Applying these replacements, Equation 2-11 becomes

$$\left(\frac{D_L}{k\ \mathrm{LT50}}\right)\left(\frac{1}{R\ I_o}\right) = \left(\frac{D_{I50\%}}{k\ t}\right)\left(\frac{1}{\mathrm{ED50}\ J}\right) = 1 \qquad (2\text{-}16)$$

where $C = (k\ t/D_{I50\%})$ was considered as a constant. The equation can be written as

$$\log(\mathrm{ED50}) = -\log(J) - \log(C) \qquad (2\text{-}17)$$

The model predicts that log(ED50) should vary with log(J) with the slope = -1. The data for nine PAHs are presented in Figure 2-5. The test chemicals were exposed to three light sources: simulated sunlight, standard growth light, and UV-filtered light that correspond to the three different data points for each PAH. The slopes appeared to be quite similar with average slope = -0.51 ± 0.09 (-0.412 to -0.678). However, the intercepts varied more significantly ranging from -0.363 to -2.152 (Table 2-6).

Table 2-6. Slope and intercept for linear regression of log(ED50) and log(J) for nine PAHs [16].

PAH	a[a] slope	b[a] y-axis intercept	R^2
Anthracene	-0.678	-2.152	0.931
benzo[*a*]pyrene	-0.496	-1.188	0.997
benzo[*g,h,i*]fluoranthene	-0.48	-1.452	0.984
Fluoranthene	-0.496	-1.273	0.987
indeno[1,2,3-*c,d*]pyrene	-0.412	-0.363	0.938
Pyrene	-0.492	-1.233	0.999

[a]Data were fitted using the following equation: log(ED50) = a log (J) + b.

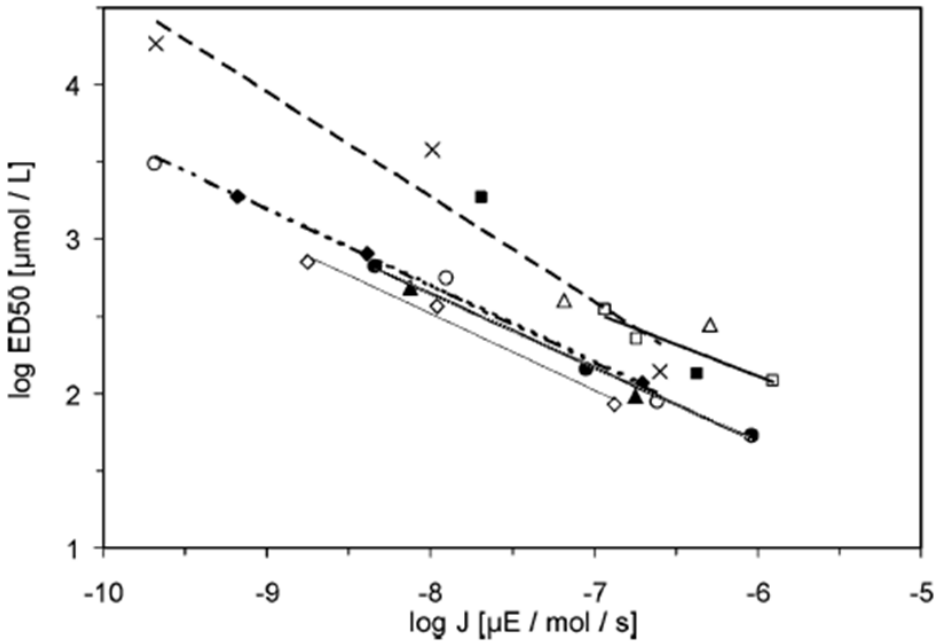

Figure 2-5. Relationship between log(ED50) and log(*J*) for the investigated PAHs exhibiting phototoxicity. Regressions results are presented in Table 2-6; anthracene (×), benzo[*a*]pyrene (●), benzo[*a*]anthracene (▲), fluoranthene (O), pyrene (♦), benzo[*b*]fluoranthene (■), benzo[*k*]fluoranthene (Δ), indeno[1,2,3-*c*,*d*]pyrene (□), and benzo[*g*,*h*,*i*]fluoranthene (◊)[16].

To accommodate the varying intercepts, a relative phototoxic efficacy (RPE) was defined to represent the different phototoxic potency of PAHs. The RPEs were obtained empirically for the nine PAHs. They were treated as nine unknowns and estimated using a linear regression of log(ED50)s with a common slope and intercept.

$$\log(ED50) = -0.54 \log(J \ RPE) - 1.805 \qquad (2\text{-}18)$$

Figure 2-6 presents the results. The slope (-0.54) was comparable to the median slope of the individual compounds (i.e. -0.51).

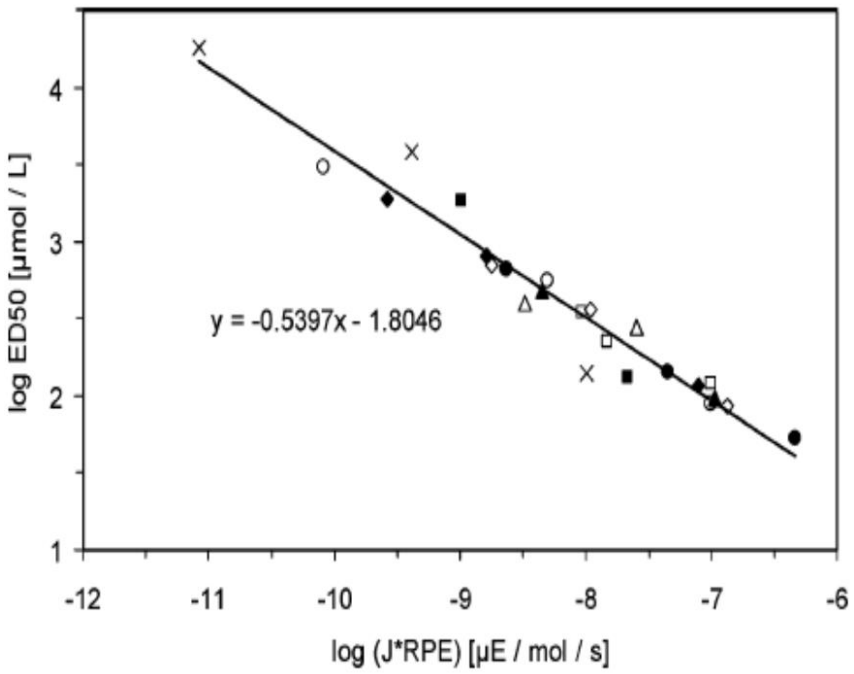

Figure 2-6. Regression through the data set in Figure 2-5. PAHs are shown with different symbols as anthracene (×), benzo[*a*]pyrene (●), benzo[*a*]anthracene (▲), fluoranthene (O), pyrene (♦), benzo[*b*]fluoranthene (■), benzo[*k*]fluoranthene (Δ), indeno[1,2,3-*c,d*]pyrene (□), and benzo[*g,h,i*]fluoranthene (◊)[16].

An important modification made by Grote et al. [16] to the BRL was using the absorbed light rather than the incident light in the modeling framework. Additionally, fixing the light exposure time at 24 (h) and determining the median lethal concentration to be predicted using the BRL introduced a fixed time of exposure which corresponds to determining an LC50 rather than an LT50 as done previously. A fairly constant slope of -0.510 was achieved in this study suggesting that the correlation between the phototoxic concentration and the irradiance intensity on a log-log scale is less than unity.

2.10 Sellin Jeffries et al. (2013)

Sellin Jeffries et al. [17] also developed a model based on the BRL. The experimental data from the literature for various PAHs, test organisms, and lighting conditions were used as inputs. The total phototoxic PAH equivalents ($t_p\,PAH_{eq}$) calculated using:

$$t_pPAH_{eq} = \Sigma([PAH]_i \times RPA_i) \tag{2-19}$$

where t_pPAH_{eq} = total phototoxic PAH equivalents (μM/g), $[PAH]_i$ = the whole-body concentration of PAH_i (μM/g), and RPA_i = the photodynamic activity of PAH_i relative to anthracene quantified as follow:

$$RPA_i = \frac{(LT50_i)^{-1}}{(LT50_{anthracene})^{-1}} \tag{2-20}$$

The approach to RPA determination was based on the observed LT50s [11] associated with exposing the PAHs to one specific organism (*D. magna*) and light source (solar simulating light source spectrum used by Newsted and Giesy [11]). The resulting model is a polynomial regression.

$$\log(\frac{1}{LT50}) = -0.13\ (\log(I_{UVA} \times t_pPAH_{eq}))^2 + 1.13\ (\log(I_{UVA} \times t_pPAH_{eq})) - 2.09 \tag{2-21}$$

The comparison to the experimental data is shown in Figure 2-7.

This model introduced the phototoxic PAH equivalent (Equation 2-19) which incorporates the PAH concentration in organism tissue and its relative photodynamic activity.

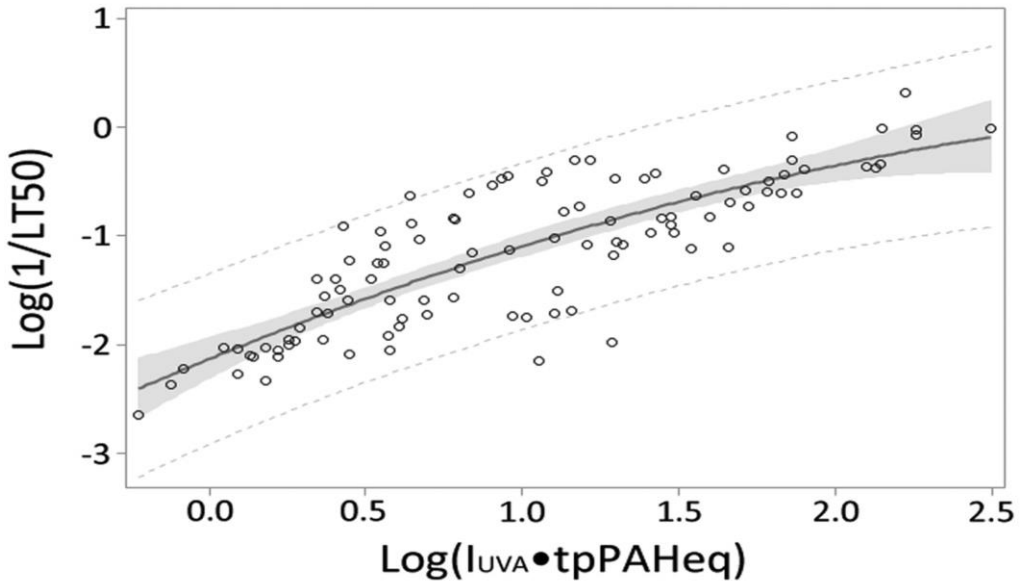

Figure 2-7. Polynomial regression showing the fitted polynomial (Equation 2-21) through the experimental data ($p < 0.001$, $R^2 = 0.69$) [17].

2.11 Conclusions

The modeling efforts to predict phototoxicity of PAHs that have been developed incorporate various of the underlying factors that affect phototoxicity. The factors include PAH budy burden, light absorption, and chemical phototoxic potency. Table 2-7 provides a listing of the characteristics of the models proposed for PAHs phototoxicity prediction and the factors accounted for in each model. It illustrates how the modeling efforts have evolved and how they have dealt with light exposure, internal versus aqueous concentrations, and species sensitivities. In the studies that dealt with more than one PAH, RPAs were introduced. The RPAs determined for each PAH and test species in different studies are presented in Table 2-8 and Figure 2-8. The differences are due to factors other that the chemical specific or species specific properties, i.e. the light source spectral irradiance and its interaction with the PAH molar absorbance, the

varying exposure times, and the use of either LC50s or LT50s. Also it is not clear how RPAs would be determined for PAHs or species that have not been tested.

It appears that no model included all elements affecting phototoxicity in a unified framework that can predict the observed phototoxicity to an organism without including an empirical RPA or similar normalization. Additionally, the difference in species sensitivity is not considered in any of the models, which limits their domain of application to one organism.

Therefore, developing a predictive model addressing these issues of relative sensitivitity of PAHs and exposure conditions that is applicable to many aquatic organisms, PAHs, and light conditions would be of significant improvement in predicting the phototoxicity of PAHs. A comprehensive model is presented in Chapter 3.

Table 2-7. List of the PAHs phototoxicity models in the literature.

	Modeling elements								
Phototoxicity model	**$\varepsilon(\lambda)$[a]**	**$I(\lambda)$[b]**	**Light exposure time**	**Prediction**	**BCF[i]**	**Species sensitivity[j]**	**Chemical potency[l]**	**No. of PAHs**	**No. of species**
Morgan and Warshawsky, 1977 [10]	✓	Monochromatic light (366 nm)	✓	ANI[c] Rate	✓		RPA[m]	28	1
Newsted and Giesy, 1987 [11]	✓	UV	✓	QSAR[d]	✓		RPA[m]	16	1
Mekenyan et al., 1994 [40]		UV		QSAR[e]			HOMO-LUMO gap	28	1
Oris and Giesy, 1985 [12]		UV	✓	LT50[f]				1	1
Ankley et al., 1995 [13]		UVA	✓	LT50[f]	✓			3[o]	1
Krylov et al., 1997 [15]	✓	UV+VIS		QSAR[g]				16	1
Grote et al., 2005 [13]	✓	UV+VIS	✓	LC50[h]	✓		RPE[n]	9	1
Jeffries et al., 2013 [17]		UVA	✓	LT50[f]		RPA[k]	RPA[k]	18	4

[a]Chemical molar absorption coefficient

[b]Irradiation spectrum

[c]Average number of *Artemia salina* nauplii immobilized

[d]Quantitative structure activity relationship model developed to predict the LT50 using the empirical physiochemical parameters

[e]QSAR to predict LT50 based on HOMO-LUMO gap

[f]Lethal time at 50% mortality

[g]QSAR to calculate photosensitization constant and a photomodification constant

[h]Lethal concentration at 50% mortality

[i]Bioconcentration factor

[j]Factor accounting for the difference between organisms sensitivities

[k]$RPA = (LT50_{PAHi})^{-1}/(LT50_{Anthracene})^{-1}$

[g]QSAR to calculate photosensitization constant and a photomodification constant

[h]Lethal concentration at 50% mortality

[i]Bioconcentration factor

[j]Factor accounting for the difference between organisms sensitivities

[k]$RPA = (LT50_{PAHi})^{-1}/(LT50_{Anthracene})^{-1}$

[l]Chemical toxicity potency accounting for differing chemicals properties

[m]Potency (rate of mortality per unit time per unit of absorbed irradiance) relative to that of the reference compound (benzo[*b*]anthracene)

[n]Relative phototoxic efficacy calculated as coefficients for each PAH to fix the varying intercepts into a common intercept

[o]Regression analyses were done for each PAHs separately so that chemical potency correction was not performed

Table 2-8. Estimated relative phototoxic efficacy (RPE), relative phototoxic activity (RPA), and relative phototoxic factor (RPF) values for photo-induced toxicity of the investigated PAHs [16].

PAH	RPE *Scenedesmus vacuolatus* [16]	RPA *Artemia Salina* nauplii [10]	RPA *Daphnia magna* [11]	RPF *Pimephales promelas* [4,10,11]
anthracene	0.04		1.019	21.5
benzo[*a*]anthracene	0.6	9.8	0.45	16.4
benzo[*a*]pyrene	0.5	0.55	1.83	1
benzo[*b*]fluoranthene	0.05			
benzo[*g,h,i*]fluoranthene	1	0.96		
benzo[*g,h,i*]perylene	≤ 0.02	0.02	1.45	
benzo[*k*]fluoranthene	0.05	0.08	0.3	
chrysene	≤ 0.0004	0.2	0.44	
fluoranthene	0.4	0.15	0.42	
indeno[1,2,3-*c,d*]pyrene	0.08	0.19		
perylene	≤ 0.00002	0.04	0.13	
phenanthrene	≤ 0.03		Not measured	
pyrene	0.4	0.72	1.64	100.1

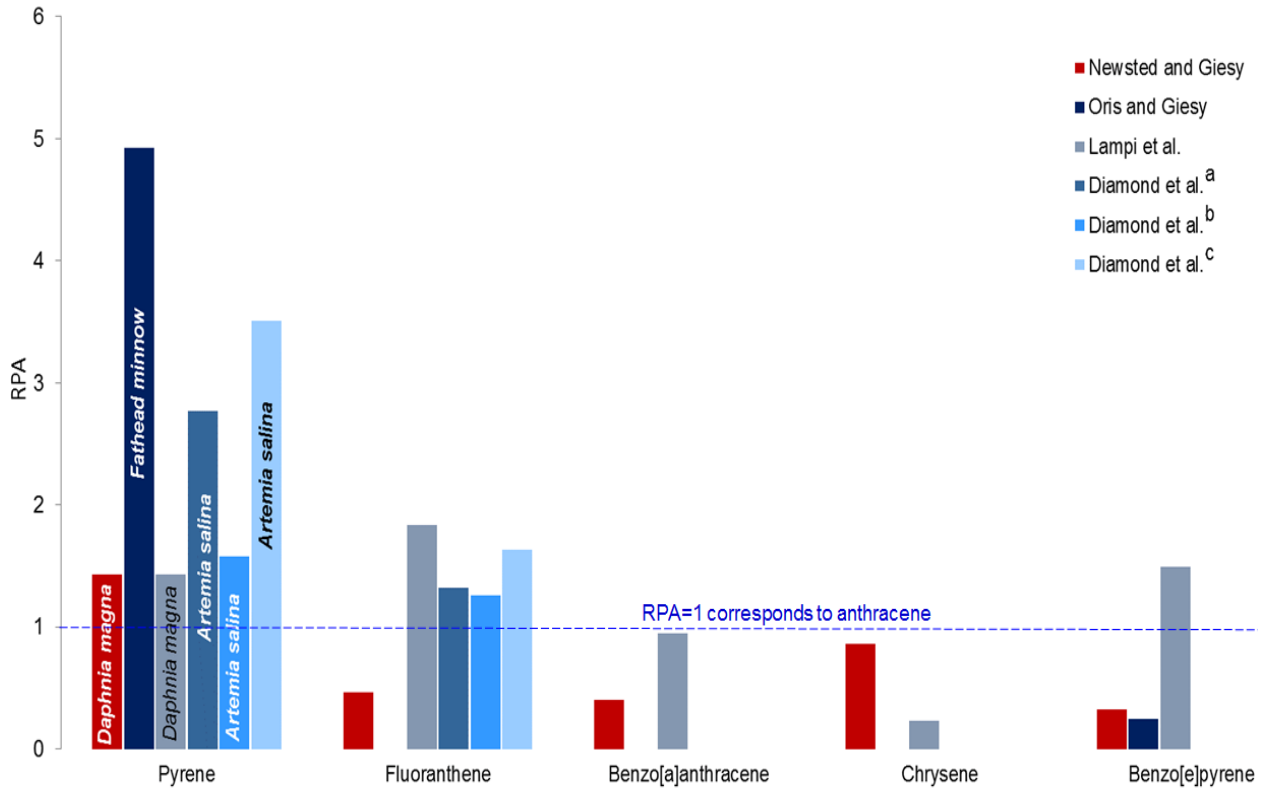

Figure 2-8. Graphical comparison of the RPAs listed in Table 2-8. Organisms are color-coded and are indicated in the bar plots. RPA are calculated based on the experimental LT50s presented in Newstead and Giesy [11], Oris and Giesy [4], Lampi et al. [70], and Diamond et al. [68] described in the legend; Diamond et al. with superscripts a, b, and c correspond to light conditions, UV lamp with no filter, with silica glass filter, and c with KCr filter, respectively.

Chapter 3

PHOTOTOXIC TARGET LIPID MODEL OF SINGLE POLYCYCLIC AROMATIC HYDROCARBONS

A phototoxic target lipid model (PTLM) is developed to predict phototoxicity of individual polycyclic aromatic hydrocarbons (PAHs) measured either as median lethal concentration (LC50) or median lethal time (LT50) for a 50% toxic response. The model is able to account for the differences in the physical/chemical properties of PAHs, test species sensitivities, and variations in light source characteristics, intensity, and length of exposure. The PTLM is based on the narcotic target lipid model (NTLM) of PAHs. Both models rely on the assumption that mortality occurs when the toxicant concentration in the target lipid of the organism reaches a threshold concentration. The PTLM is applied to observed LC50s and LT50s for 20 individual PAHs, 15 test species, including arthropods, fishes, amphibians, annelids, mollusks, and algae, exposed to simulated solar and various UV light sources, for exposure times varying from less than 1 (h) to 100 (h), a total of 333 observations. The LC50 concentrations range from less than 0.1 μg/L to greater that 10^4 μg/L. The model has two fitting parameters that are constant and apply to all PAHs and organisms. The root mean square error of prediction for log(LC50) and log(LT50) are 0.473 and 0.382, respectively. The results indicate that the PTLM can predict the phototoxicity of single PAHs over a wide range of exposure conditions and to organisms with a wide range of sensitivities.

3.1 Introduction

Phototoxicity is the toxicity exhibited by a chemical in the presence of certain wavelengths of light. Phototoxic polycyclic aromatic hydrocarbons (PAHs) absorb light in the ultraviolet (UV) and to some extent in the visible (VIS) region. The effect of light absorption on the toxicity of PAHs has been reported since the late 1920s [29]. Subsequently, the toxic effect of PAHs sensitizers in mammalian models in the presence of UV light was recognized [30,31], resulting in the study of the occurrence, mechanism of action, and predictability of phototoxicity of PAHs to various organisms. Arfsten et al. [7], Diamond [27], and Giesy et al. [39] present comprehensive reviews describing toxicological interactions between PAHs and light.

There are a limited number of studies that predict the phototoxicity of PAHs to aquatic organisms. Morgan and Warshawsky [10] investigated the photodynamic immobilization of *Artemia salina* nauplii co-exposed to 41 PAHs and monochromatic UV light. The rate of immobilization was determined to be proportional to the amount of light absorbed by the compound with a proportionality constant ϕ_i for a compound *i*, which was termed the "quantum yield for immobilization". The relative photodynamic activity (RPA) was defined as the ratio of ϕ_i to that of a reference compound ϕ_0 (benz[*c*]acridine). Newsted and Giesy [11] and Oris and Giesy [4] investigated the photo-enhanced toxicity of PAHs and their relative potencies to *Daphnia magna* and *Pimephales promelas* larvae, respectively. Potency (Φ) was defined as a rate of mortality per unit time per unit of absorbed irradiance [4,11]. The relative potency factor (RPF) for each PAH was defined as the ratio of its potency factor to the potency factor for the reference compounds benzo[*b*]anthracene [11] and benzo[*a*]pyrene [4]. This was similar to the method used by Morgan and Warshawsky [10] to calculate RPA, except that the estimated internal PAH concentrations were

used rather than the ambient water concentrations. Mekenyan et al. [40] reanalyzed the data presented by Newsted and Giesy [11] and found that PAHs exhibiting photo-enhanced toxicity to *D. magna* exhibited a HOMO-LUMO (highest occupied molecular orbital energy-lowest unoccupied molecular orbital energy) window of 7.2 ± 0.4 eV and proposed using the gap as an indicator of PAH phototoxicity in *D. magna*.

Veith et al. [41] studied the substituents effects on HOMO–LUMO gap of PAHs. Alkyl and hydroxyl substituents did not change the HOMO–LUMO gap of PAHs significantly, whereas nitro, alkane, and chloro substitution on PAHs had considerable effects on the HOMO–LUMO gap. A window of 7.75 ± 0.25 eV was suggested by Veith et al. [41] for the substituted PAHs as their phototoxicity indicator.

Oris and Giesy [12] developed a model for the phototoxicity of anthracene to *Lepomis spp* at varying light intensities and aqueous concentrations using the Bunsen–Roscoe law (BRL) of reciprocity. The BRL states that for a fixed concentration of the sensitizer –in this case anthracene– a biological effect is proportional to the product of light intensity and reaction time [42]. Regression analysis of the experimentally determined log(LT50 × UV intensity) versus the log of the corresponding anthracene aqueous concentration did not produce the common slope and intercept that was expected. The applicability of the BRL to PAHs phototoxicity was rejected due to the variability of slopes and intercepts. Ankley et al. applied the BRL to *Lumbriculus variegatus* co-exposed to UV light and fluoranthene [13], anthracene, or pyrene [14]. The experimentally determined log(LT50) values were proportional to the log(initial residue× UV intensity) using measured tissue residues of PAHs in the organism, contrary to the aqueous concentration used in the model by Oris and Giesy [12].

Ankley et al. [12,13] reported considerable variations among the slopes and intercepts for the three PAHs tested, whereas BRL predicted common slope of -1.0.

Krylov et al. [15] and Huang et al. [46] developed a quantitative structure–activity relationship (QSAR) model to explain the toxicity of 16 PAHs to *Lemna gibba* under simulated solar radiation on the basis of photosensitization reactions and direct toxicity of the photomodification products. To estimate the component of toxicity due to photosensitization reactions, the toxicity of the parent PAHs was used. The toxicity of the photomodified PAHs was determined by irradiating the test solution prior to incubation. A photosensitization factor (PSF) and a photomodification factor (PMF) were calculated for each PAH investigated [46]. The sums of the PSF and PMF were correlated to a measure of relative toxicity that was calculated from the growth rate inhibition induced by exposure to 2 mg/L of each PAH. However, this concentration was above the water solubility of the PAHs of interest. The possible shortcomings of predictions based on the measurements in supersaturated solutions and mechanisms to cope with issues of PAHs water solubility and the associated toxicity are discussed below.

Grote et al. [16] developed a predictive phototoxicity model for the green alga *Scenedesmus vacuolatus* by modifying the model previously developed by Ankley et al. [13]. The tissue concentration was replaced by the median effective dose (ED50) which is the concentration in the tissue corresponding to 50% mortality. Another modification was replacing the incident UV intensity with a measure of UV absorption, *J*, which had been introduced by Krylov et al. [51]. The model linearly correlated log(ED50) to log(*J*) for different PAHs. The average slope was -0.51 ± 0.09 (varying from -0.412 to -0.678). However, the intercepts varied significantly for each

PAH ranging from -0.363 to -2.152. A relative phototoxic efficacy (RPE) was defined to accommodate the varying intercepts and to describe the distinct behavior of different compounds. The factors quantifying the efficacy for each compound was computed individually such that the factors when multiplied by *J* caused the varying intercepts to converge to a common value. The reported RPE for each compound was calculated by dividing the factor fitted for the compound by that of the reference compound benzo[*g,h,i*]fluoranthene. The RPE values found by Grote et al. [16] were different from those reported for *A. salina* [10], *D.magna* [11], or *P. promelas* [4]. This observation suggests that the relative potency values are organism dependent and the models developed previously are applicable only to the specific organisms tested.

Sellin Jeffries et al. [17] also developed a model based on the BRL. The experimental data from the literature for various PAHs, test organisms, and lighting conditions were combined to correlate $(LT50)^{-1}$ with the product of the UVA light intensity (I_{UVA}) and total phototoxic PAH equivalents $t_pPAH_{eq}=\Sigma([PAH]_i \times RPA_i)$, where $[PAH]_i$ is the whole-body concentration of PAH_i (μM/g) and RPA_i is the photodynamic activity of PAH_i relative to anthracene, $RPA_i = \frac{(LT50_i)^{-1}}{(LT50_{anthracene})^{-1}}$. The resulting RPAs varied by species and irradiance spectra of the light sources used to obtain the LT50s. Therefore, RPAs were not found to be a consistent metric for characterizing the phototoxicity potential of individual PAHs.

Each of the models described above incorporated factors that influence phototoxicity to varying degrees: properties of the PAHs (molar absorption spectra), incident light (intensity and spectral irradiance), tissue PAH concentration, and exposure duration. However, no model included all these components in a unified framework that can predict the observed phototoxicity to an organism without

including an empirical RPA or similar normalization. Additionally, the difference in species sensitivity is not considered in any of the models.

The objective of this chapter is to present a phototoxicity model based on the target lipid model of PAH toxicity [18] that accounts for all these factors in order to predict LC50s and LT50s. The model is applied to data for 20 PAHs, 15 organisms, and different light exposure conditions. In particular the model can predict both the LC50 and LT50 within the same framework.

3.2 Phototoxicity Modeling for Individual PAHs

3.2.1 Bioconcentration of PAHs

Early observations of PAH phototoxicity established that chemical concentrations inside the organism have a pivotal role in determining the extent of phototoxicity [31,52,53]. Several experiments demonstrated that irradiation of the exposure media prior to addition of the organisms did not increase the observed toxicity, while increasing the length of the PAH uptake period prior to UV irradiation did increase the toxicity suggesting that photoactivated toxicity occurred within the organism, rather than in the exposure media [31,52,53]. Accordingly, the subsequent models of the phototoxic process used the concentration of PAHs in the organism tissue as a measure of the dose [10,11,13,14,16,20]. This requires a method for determining or estimating the concentration of PAHs in the organism.

The narcotic target lipid model (NTLM) [18] employs the lipid-water partition coefficient K_{LW} to compute the organism concentration

$$C_{\mathrm{L}} = K_{\mathrm{LW}} C_{\mathrm{W}} \tag{3-1}$$

where C_L = the concentration of the chemical in the lipid fraction of the organism (mol chemical/kg lipid), K_{LW} = the lipid- water partition coefficient (L/kg lipid), and C_W = the aqueous concentration of the chemical (mol chemical/L).

3.2.2 Baseline Narcosis

The phototoxicity model is based on the NTLM of baseline narcosis. When the chemical concentration in water, denoted by NLC50 produces 50% mortality in the absence of exposure to light – the "N" is used to denote narcotic toxicity (i.e. the toxicity without exposure to light) – the chemical concentration in the organism target lipid is equal to the narcotic critical target lipid body burden (CTLBB), C^*_{LN}

$$C^*_{LN} = K_{LW}\text{NLC50} \tag{3-2}$$

or

$$\log(\text{NLC50}) = \log(C^*_{LN}) - \log(K_{LW}) \tag{3-3}$$

where the superscript * denotes the concentration at which the toxic endpoint occurs. The NTLM [18,23] predicts narcotic toxicity using Equation 3-4 in which the lipid-water partition coefficient is replaced with an estimation equation

$$\log(\text{NLC50}) = -0.936\log(K_{OW}) + \log(C^*_{LN}) + \Delta c \tag{3-4}$$

where K_{OW} = the octanol-water partition coefficient (L/kg octanol), C^*_{LN} = the narcotic CTLBB (mmol chemical/kg octanol), and Δc accounts for a chemical class correction (log(mmol/L)) required for using $\log(K_{OW})$ to predict $\log(K_{LW})$ as discussed below.

There are two critical assumptions that underlie the NTLM:

(1) The lipid-water partition coefficient, $\log(K_{LW})$, estimated using the slope of the log(NLC50) versus the $\log(K_{OW})$ regression, is constant for all species That is, the target lipid where the toxic effect occurs has the same target lipid-water partition coefficient in all aquatic organisms.

(2) The species sensitivity as determined by the CTLBB concentration is specific to the organism but is the same for any narcotic chemical. This follows from the experimentally demonstrated additivity of narcotic toxic units [18].

These assumptions were validated by comparisons of observed and predicted NLC50s for 156 chemicals, including halogenated and nonhalogenated aliphatic and aromatic hydrocarbons, PAHs, alcohols, ethers, furans, and ketones, and for 47 species, including fish, amphibians,arthropods, mollusks, polychaetes, coelenterates, and protozoans [18,23]. The CTLBB has been determined for 47 aquatic [23] and five algal species [54].

It has been demonstrated that PAHs are toxic via the narcotic mode of action [23] and their toxicity in the dark can be predicted using the NTLM. The chemical class correction, Δc, was determined to be -0.352 for PAHs [23]. It was later found that this correction does not imply that PAHs are more toxic than baseline narcotics, but rather that the chemical class correction, Δc, corrects the relationship between the lipid-water partition coefficient K_{LW} (Equation 3-1) and K_{OW} in Equation 3-4 for the various classes of chemicals [55].

3.2.3 Light Absorption

Upon exposure to light, PAHs inside the organism absorb light from the UVB, UVA, and a portion of the visible spectrum. The amount of absorbed light at each

wavelength depends on the product of the absorption spectrum of the PAH and the irradiance spectrum of the light [51]. Figure 3-1A presents molar absorption coefficient spectra for four PAHs, fluoranthene, anthracene, phenanthrene, and chrysene and the solar radiation spectrum. The extent to which there is an overlap of the molar absorption coefficient and solar radiation spectra is shown in Figure 3-1B which presents the action spectrum = molar absorption coefficient spectrum × the irradiance spectrum, which is the quantity of the light that is absorbed.

The dependence of PAH toxicity on the amount of light absorbed is shown in Figure 3-2 which presents the toxicity to *D. magna* for four PAHs exposed to simulated solar radiation. For phenanthrene with little molar absorption of solar radiation (Figure 3-1A), there is no change in toxicity in the presence of light (red bars) as opposed to the absence of light (gray bars). Chrysene shows intermediate absorption and there is approximately one order of magnitude increase in toxicity in the presence of light. For the compounds such as fluoranthene and anthracene that exhibit high molar absorption in the UVB and UVA spectral regions, the ratio of the toxicity in the presence to the absence of light can be as large as two orders of magnitude. Interestingly, even though phenanthrene and anthracene are isomers and exert essentially equal narcotic toxicity, the difference in their light absorption properties (i.e. spectral molar absorption coefficient) leads to a considerable gap between their observed phototoxicity as shown in Figure 3-2.

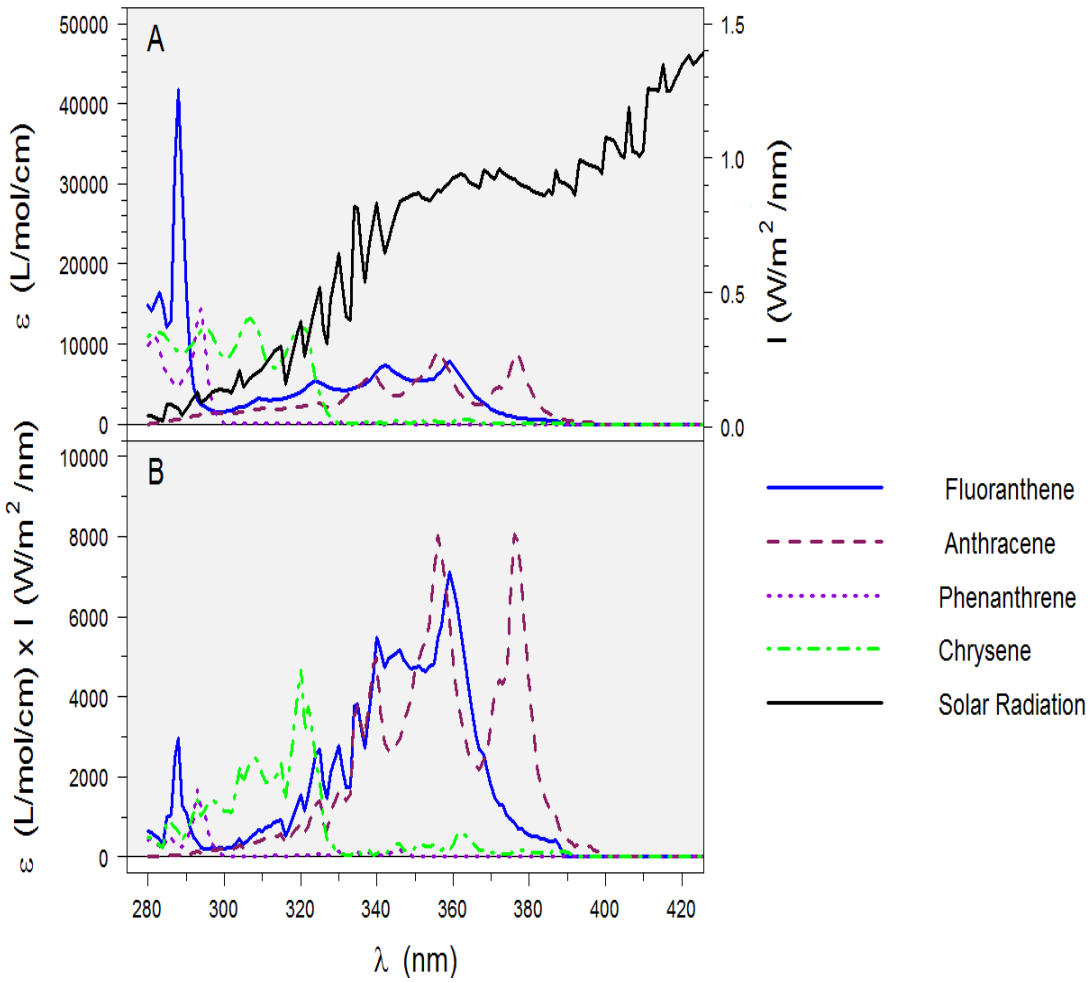

Figure 3-1. A: Molar absorption coefficient spectra (ε (λ)) [56] of four PAHs (fluoranthene, anthracene, phenanthrene, and chrysene; and solar radiation spectrum (I (λ)) [87]; on the primary and secondary axes, respectively, versus wavelength λ. B: Action spectra = product of molar absorption coefficient and solar radiation spectra. The area under each curve is the quantity of light energy absorbed by each PAH.

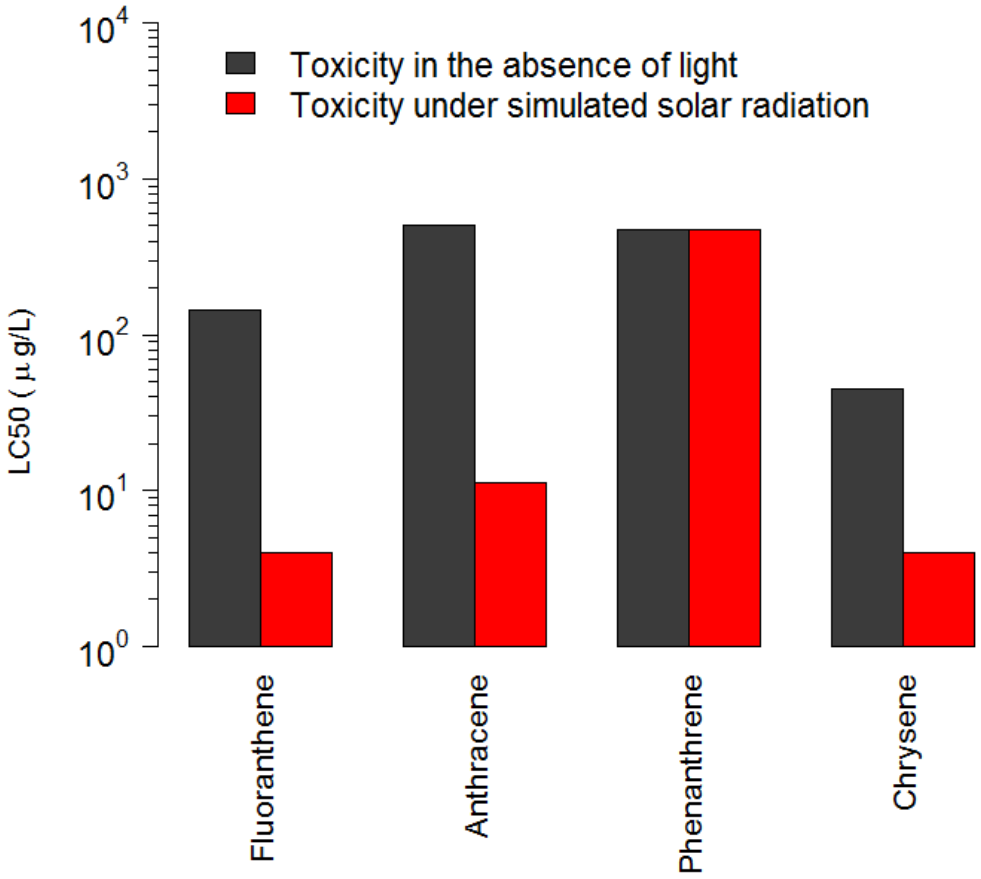

Figure 3-2. The effect of simulated sunlight absorption (Figure 3-1) on the toxicity to *Daphnia magna* for four PAHs, fluoranthene, anthracene, phenanthrene, and chrysene. The toxicity data under simulated solar radiation are from [36]. Toxicity for dark exposure are calculated using the NTLM (Equation 3-4).

The total amount of absorbed light is quantified by the integral of the product of the spectra of the incident light intensity and the molar absorption coefficient of a

compound. The most useful form of this integral expresses the amount of light energy absorbed in terms of moles of photons absorbed per mole of PAH

$$P_{abs} = \int_{\lambda_1}^{\lambda_2} I_o(\lambda)\left(\frac{\lambda}{N_A hc}\right) T_{\exp}\varepsilon(\lambda)d\lambda \qquad (3\text{-}5)$$

where P_{abs} denotes number of photons absorbed by the PAH (mole photon/mole PAH), λ is the wavelength (nm), $I_o(\lambda)$ indicates the incident light intensity (W/m^2/nm) at wavelength λ, N_A = the Avogadro number (6.022×10^{23}) , h = the Planck's constant (6.626×10^{-34} (J.s)), c = the speed of light (2.998×10^8 (m/s)), T_{exp} = time of exposure to the light (s), and $\varepsilon(\lambda)$ = the molar absorption coefficient (L/mol/cm) of the PAH at wavelength λ (nm). The term ($\lambda/N_A\, h.c$) converts the incident light $I_o(\lambda)$ in units of W/m^2/nm to moles photons/m^3/s which, when multiplied by the exposure time T_{exp} (s), yields the total moles of incident photons per m^3 absorbed at the end of the exposure time. It is important to note that the dose of light energy can be expressed as moles of photons absorbed per mole of PAH rather than the less useful energy units. We shall see subsequently that P_{abs} plays a central role in the PTLM.

3.2.4 Reactive Excited Species Formation

As discussed previously, in Section 3.2.1, it was observed that photo-enhanced toxicity occurred within the organism, rather than in the exposure media [31,52,53], where the light absorbed by PAHs initiates photochemical reactions. Briefly, as currently understood, the phototoxic action pathway includes two types of reaction mechanisms: photosensitization and photomodification. Photosensitization is initiated when a PAH absorbs a photon, which elevates the PAH to an excited singlet state. The excited singlet-state PAH can undergo intersystem crossing to form the excited triplet

state. The triplet PAH can transfer energy to triplet oxygen and decay back to the ground state PAH. Energy transfer to triplet oxygen can lead to reactive oxygen species (ROS) formation [6,57]. ROS has been accepted as the agent responsible for the oxidative damage and lipid peroxidation in the organisms [57,58]. The second mechanism, photomodification, results in the formation of new toxic products, usually via oxidation of the PAHs [6,11,15,36,59]. Studies have suggested that photomodification can play a significant role in PAH phototoxicity [15,46].

Previous models of PAHs phototoxicity were primarily based on photosensitization reactions [10,11,40] with the toxic species assumed to be ROS. However, direct experimental evidence suggesting that the formation of ROS is the sole cause of phototoxicity has not been reported. Since either ROS (photosensitization) or photomodified PAHs (photomodification) present in the lipid can cause toxicity, the toxic reactant will be denoted as RTS (reactive toxic species).

3.3 PTLM Formulation

3.3.1 RTS Formation in Target Lipid

The concentration of photons absorbed by the PAH in the lipid fraction of the organism, C_{LP}, can be computed as the product of the ratio of moles of photons absorbed per mole of PAH, P_{abs} (mol photon/mol PAH) (Equation 3-5), and the PAH concentration in target lipid, C_{LN} (mol PAH/kg lipid)

$$C_{LP} = P_{abs} C_{LN} \tag{3-6}$$

where C_{LN} = PAHs concentration in the target lipid (mol PAH/kg lipid). and C_{LP} = the concentration of photons absorbed in organism target lipid (mol photon/kg lipid). The concentration of RTS produced can be computed by specifying the quantum yield of

RTS formation, Φ_{RTS}, which is defined as the ratio of moles of RTS produced in the lipid fraction per mole of photons absorbed:

$$\Phi_{RTS} = \frac{C_{LRTS}}{C_{LP}} \tag{3-7}$$

Therefore the concentration of RTS in the lipid fraction (mol RTS/kg lipid) is

$$C_{LRTS} = \Phi_{RTS} C_{LP} \tag{3-8}$$

or, substituting the concentration of photons absorbed in the lipid fraction (C_{LP}) with the PAH target lipid concentration using Equation 3-6 yields

$$C_{LRTS} = \Phi_{RTS} P_{abs} C_{LN} \tag{3-9}$$

Finally, using Equation 3-1 to relate the target lipid concentration to the aqueous concentration yields

$$C_{LRTS} = \Phi_{RTS} P_{abs} K_{LW} C_{W} \tag{3-10}$$

This equation is analogous to Equation 3-1, the basis for the target lipid model of narcosis toxicity. This analogy will be pursued in the formulation of the phototoxic target lipid model.

3.4 Phototoxic Target Lipid Model (PTLM)

3.4.1 Reactive Toxic Species Effect

The PAH body burdens predicted from the TLM were found to be comparable to the measured concentrations in extracted lipid [19]. The observation suggested that there is a correlation between concentrations of PAHs in the lipid tissues and the observed adverse effect. The TLM is based on the assumption that mortality occurs when the

chemical concentration in the target lipid reaches a threshold concentration [18,23]. An analogy can be drawn between the target lipid narcotic and the target lipid phototoxic modes of action. At 50% mortality, the relationship between the narcotic LC50 and the critical target lipid body burden is given by Equation 3-2**.** Similarly, at 50% mortality, the concentration of RTS in target lipid is the RTS critical target lipid body burden (C^*_{LRTS}) and the corresponding aqueous LC50 concentration of the PAH that produces the critical concentration of RTS in the lipid is denoted by RLC50, where "R" denotes the toxicity due to the reactive toxic species. Consequently, Equation 3-10 yields

$$C^*_{\mathrm{LRTS}} = \Phi_{\mathrm{RTS}} P_{\mathrm{abs}} K_{\mathrm{LW}} \mathrm{RLC50} \tag{3-11}$$

where C^*_{LRTS} = RTS critical lipid body burden (mol RTS/kg lipid). RLC50 = aqueous concentration of the PAH (mol PAH/L).

The connection between the narcotic TLM and the phototoxic reactive species is made using Equation 3-2 for the lipid-water partition coefficient in Equation 3-11 to yield

$$C^*_{\mathrm{LRTS}} = \Phi_{\mathrm{RTS}} P_{\mathrm{abs}} \left(\frac{C^*_{\mathrm{LN}}}{\mathrm{NLC50}} \right) \mathrm{RLC50} \tag{3-12}$$

Equation 3-12 can be rearranged to define the ratio of the phototoxic reactive species LC50 (RLC50) relative to the narcotic LC50 (NLC50)

$$\left(\frac{\mathrm{RLC50}}{\mathrm{NLC50}} \right) = (\Phi_{\mathrm{RTS}} P_{\mathrm{abs}})^{-1} \left(\frac{C^*_{\mathrm{LRTS}}}{C^*_{\mathrm{LN}}} \right) \tag{3-13}$$

The expression $\left(\frac{C^*_{\mathrm{LRTS}}}{C^*_{\mathrm{LN}}} \right)$ represents the sensitivity of the organisms to RTS toxicity relative to narcosis toxicity. It is convenient to define the ratio as

$$R^* \equiv \left(\frac{C^*_{\text{LRTS}}}{C^*_{\text{LN}}} \right) \tag{3-14}$$

where R^* = ratio of critical body burdens (mol RTS/mol PAH). Therefore, Equation 3-14 becomes

$$\left(\frac{\text{RLC50}}{\text{NLC50}} \right) = \frac{R^*}{\Phi_{\text{RTS}} P_{\text{abs}}} \tag{3-15}$$

Equation 3-15 states that the ratio of the phototoxic reactive species LC50 to the narcotic LC50 is inversely related to the RTS production in lipid ($\Phi_{\text{RTS}} P_{\text{abs}}$) and directly related to ratio of critical body burdens (R^*). This is the basic equation used in the PTLM for predicting the toxicity due to reactive toxic species (RLC50).

3.4.2 Reactive Toxic Species and Narcotic PAHs

The toxic components in phototoxicity are both the unexcited PAH and RTS since both are present in the target lipid. The toxicity of individual components in a mixture depends on the mode of action of each component. If the mode of action is the same, then toxic units (TU) can be used to compute the resulting toxicity [60]. The TU is defined as the ratio of the measured concentration of a chemical in a medium (e.g. water) to the corresponding effect concentration in that medium (e.g. LC50) [20,60]. Therefore, the toxic unit for the RTS-related toxicity (TU_{R}) and the narcotic toxicity (TU_{N}) are

$$\text{TU}_{\text{R}} = \frac{C_{\text{PAH,W}}}{\text{RLC50}} \tag{3-16}$$

and

$$\text{TU}_{\text{N}} = \frac{C_{\text{PAH,W}}}{\text{NLC50}} \tag{3-17}$$

where $C_{PAH,W}$ = aqueous PAH concentration (mol PAH/L), TU_R and TU_N = toxic units associated with the reactive species toxicity and the narcotic toxicity, respectively. Toxic unit additivity is assumed since the toxic mechanism for both the reactive species and narcosis occur in the lipid of the cell membrane and cause alteration of lipid properties [61-64]. Therefore, the total phototoxic toxic unit, TU_P , is the sum of the reactive species and narcotic toxic units

$$TU_P = TU_R + TU_N \tag{3-18}$$

It remains to compute the PAH aqueous concentration that causes 50% mortality ($C^*_{PAH,W}$) which is equal to the phototoxic LC50, indicated as PLC50. It is that concentration at which the total toxic unit concentration is unity [24]. That is, at 50% mortality:

$$C^*_{PAH,W} = PLC50 \tag{3-19}$$

and

$$TU_R + TU_N = 1 \tag{3-20}$$

Combining Equations 3-16 through 3-20 yields

$$(PLC50)^{-1} = (RLC50)^{-1} + (NLC50)^{-1} \tag{3-21}$$

Rearranging Equation 3-21 yields

$$\frac{PLC50}{NLC50} = \frac{1}{1+\left(\frac{RLC50}{NLC50}\right)^{-1}} \tag{3-22}$$

Combining Equations 3-15 and 3-22 yields

$$\frac{PLC50}{NLC50} = \frac{1}{1+\left(\frac{\Phi_{RTS} P_{abs}}{R^*}\right)} \tag{3-23}$$

Equation 3-23 is the final form of the PTLM. It contains three terms: the quantity of photons absorbed (Equation 3-5), the quantum yield that determines the quantity of

reactive toxic species produced by excited PAH (Equation 3-7), and the ratio of the critical body burden for phototoxicity to narcosis toxicity (Equation 3-14). It states that when no photons absorption takes place ($P_{abs} = 0$), PLC50 = NLC50. That is, no phototoxic effect is observed and the PAH acts as a narcotic. However, if $P_{abs} > 0$, then PLC50 is less than NLC50 and phototoxicity is occurring. What remains to determine is whether Equation 3-23 in fact can predict both the observed ratios of PLC50 to NLC50, as well as PLC50 itself.

3.4.3 Phototoxic LC50 and LT50 Data

A phototoxic database for individual PAH was compiled from the available literature sources [4,9,11-14,34-38,43,65-73]. A total of 15 freshwater and marine species including arthropods (insect and crustacean), fishes, amphibians, annelids, invertebrates, mollusks, and algae are represented. There are 20 PAHs and various light sources and light exposure durations. The species and chemicals used in the PTLM development are presented in Table 1. A complete list of the 333 individual observations are listed in Table A.1 (Appendix A.1).

Table 3-1. List of organisms and PAHs used in the PTLM modeling.

Species[a]		Compounds[b]	
M. Liliana	*L. variegatus*	FLA	PHE
S. capricornutum	*F. grandis*	ANT	NAP
D. magna	*A. salina*	PYR	FLU
L. macrochirus	*P. pugio*	B*a*P	ACN
M. lateralis	*R. abronius*	B*a*A	B*b*FU
M. bahia		D*a*A	PER
O. mykiss		CHR	BAN
P. promelas		B*g*P	B*b*FL
M. beryllina		B*b*A	B*k*FL
C. variegatus		B*e*P	B*a*FU

[a]Abbreviations for organisms: *M. Liliana = Macomona liliana; S. capricornutum = Selenastrum capricornutum; D. magna = Daphnia magna; L. macrochirus = Lepomis macrochirus; M. lateralis = Mulinia lateralis; M. bahia = Mysidopsis bahia; O. mykiss = Oncorhynchus mykiss; P. promelas = Pimephales promelas; M. beryllina = Menidia beryllina; C. variegatus = Cyprinodon variegatus; L. variegatus = Lumbriculus variegatus; F. grandis = Fundulus grandis; A. salina = Artemia salina; P. pugio = Palaemonetes pugio; R. abronius = Rhepoxynius abronius.*

[b]Abbreviations for polycyclic aromatic hydrocarbons (PAHs): FLA = fluoranthene; ANT = anthracene; PYR = pyrene; B*a*P = benzo[*a*]pyrene; B*a*A = benzo[*a*]anthracene; D*a*A = dibenzo[*a,h*]anthracene; CHR = chrysene; B*g*P = benzo[*g,h,i*]perylene; B*b*A = benzo[*b*]anthracene; B*e*P = benzo[*e*]pyrene; PHE = phenanthrene; NAP = naphthalene; FLU = fluorene; ACN = acenaphthene; BbFU = benzo[*b*]fluorene; PER = perylene; BAN = bezanthrone; BbFL = benzo[*b*]fluoranthene; BkFL = benzo[*k*]fluoranthene; BaFU = benzo[*a*]fluorene.

The toxic endpoint was reported as either the LC50 at a fixed length of exposure (48 or 96 hours of exposure) or as the LT50 at a fixed PAH concentration. The PTLM can accommodate both types of data. Table A.2 provides the endpoint type and the light regime (periodic or continuous) for each observation. For phototoxic LC50s (PLC50s), the total time of light exposure is T_{exp} in Equation 3-5, e.g. T_{exp} = 32 (h) for a 48-h LC50 with a 16:8 h light:dark photoperiod. For the phototoxic time-to-death data (PLT50s), the reported PLT50 values are the total light exposure time (T_{exp} = PLT50) which is the model prediction, while the corresponding aqueous concentrations at which this time to death occurs is the PLC50, for which the exposure PAH concentration is substituted. To emphasize the type of the phototoxic data being considered, the phototoxic LC50s associated with time to death data, T_{exp} , is denoted by PLT50 in Equation 3-5, that is:

$$P_{abs} = \int_{\lambda_1}^{\lambda_2} I_o(\lambda)(\lambda / N_A hc)(\text{PLT50})\varepsilon(\lambda)d\lambda \tag{3-24}$$

3.4.4 Narcotic LC50 Data

In order to predict the PLC50 or PLT50, the NLC50 concentration is required (Equation 3-23). It is predicted using the NTLM without recourse to the phototoxic data. Thus the NLC50 is a pure prediction. Also, since the observed NLC50, usually as a dark control, was not provided for the majority of studies, using the NTLM for all data allows a consistent approach. Therefore, NTLM predictions are preferred over the experimental NLC50s. The octanol-water partition coefficients and CTLBBs used for the NTLM predictions are provided in Tables A.3 and A.4, respectively.

If the CTLBB was not available for a species in the data base, the LC50 in the dark control experiment reported by the authors was used. This was the case for only one observation associated with *Macomona liliana* [69]. With this one exception, the NLC50 concentration is predicted using the NTLM.

3.4.5 PAHs Solubility Data

For chemicals where the reported PLC50 exceeded the aqueous solubility of the compound, *S*, it is assumed that the concentrations at which organisms were exposed is the aqueous solubility. That is, if PLC50 > *S*, then, for those cases, PLC50 = *S*. PAH solubilities are calculated using

$$\log(S) = -1.414\log(K_{OW}) + 7.102 \tag{3-25}$$

where *S* is the solid solubility (μmol/L) [23]. The K_{ow}s used to calculate water solubilities are included in Table A.3.

3.4.6 Molar Absorption Coefficient Spectra

The absorbance spectra, quantified by the molar absorption coefficient, $\varepsilon(\lambda)$, were obtained from the literature. The absorbance is measured in an organic solvent since the PAHs are not soluble enough in water. Most spectra were measured in cyclohexane [56]. Fluorene, benzo[*a*]fluorene, benzo[*b*]fluorene, perylene, benzanthrone, and acenaphthene [74] were measured in ethanol and the solvent for the benzo[*b*]anthracene spectrum was benzene [74]. The $\varepsilon(\lambda)$ data are presented at the intervals of 1 nm in Tables A.5-a and A.5-b for the PAHs used in the PTLM model development.

A comparison of the effect of the solvent used to measure the light absorption by PAHs, presented in Appendix A.2 (Figure A.1), indicates no significant differences. This suggests that using $\varepsilon(\lambda)$ measured in organic solvents for which $\varepsilon(\lambda)$ is available in the literature, will provide acceptable estimates of P_{abs}. The integral (Equation 3-5) was calculated as a summation of the product of $I(\lambda)$ and $\varepsilon(\lambda)$ at the intervals of 1(nm).

3.4.7 Light Irradiance Spectra

For each phototoxicity observation, the associated irradiance spectrum of the light source ($I(\lambda)$) was extracted from the reference when provided by the authors. Otherwise, it was acquired from the spectrum published by the manufacturer of the light source. A total of ten spectra were included in the database. The light source corresponding to each observation is presented in Table A.1. Additionally, Tables A.6-a and A.6-b present $I(\lambda)$ at intervals of 1 (nm) for the light sources. It is possible the actual light intensities exposed to the organisms are likely to undergo some attenuation in the exposure chambers. It is assumed that this is not a significant loss of incident radiation.

3.4.8 RTS Production

The dose (Equation 3-11) requires the quantum yield: the ratio of toxic species produced per photon absorbed, Φ_{RTS}. This quantity is dependent on the PAH's properties. It has previously been proposed to use a quantum yield of toxicity [4,10,11,16], to describe the distinct behavior of different PAHs. In these studies, Φ_{RTS} is understood to be analogous to the quantum yield defined in photochemistry, i.e. the capacity of a compound to elucidate a specific effect relative to the absorbed dose of

radiation. Depending on the bioassay and the test species used, different magnitudes of quantum yields were found for the quantum yields of single PAHs [4,10,11,16].

In order to proceed, it is assumed that Φ_{RTS} is constant for all PAHs considered below. The suitability of this assumption is tested and discussed below in the statistical analyses section (section3.6).

3.4.9 Estimation of PTLM Parameters

The parameter R^* is defined as the ratio of the RTS critical body burden to the narcotic critical body burden, $R^* = \left(\frac{C^*_{LRTS}}{C^*_{LN}} \right)$. A fundamental assumption in the NTLM is that C^*_{LN} is the same for any narcotic chemical. It quantifies the species sensitivity to narcotic toxicity. Since the site of action of phototoxicity is assumed to be the target lipid, it is also assumed that C^*_{LRTS} is the same for any phototoxic chemical. Since both C^*_{LN} and C^*_{LRTS} are the same for all PAHs, so also is R^*. This assumption is also tested below in the statistical analysis section.

At this stage of development, the PTLM has two constants R^* and Φ_{RTS}. However, it has been found that the slope of log(PLC50) versus log(irradiance intensity) is less than unity [16]. Therefore, a third parameter, *a*, is needed for Equation 3-23

$$\frac{\text{PLC50}}{\text{NLC50}} = \frac{1}{1+\left(\frac{P_{abs}{}^{a}}{\left(R^*/\Phi_{RTS} \right)} \right)} \tag{3-26}$$

where the notation PLC50 indicates that both types of phototoxicity data, PLC50s from phototoxic LC50 and LT50 endpoints, are included in the modeling framework. Since both parameters R^* and Φ_{RTS} are assumed to be constant across the chemicals and species, so is their ratio $\left(R^*/\Phi_{RTS} \right)$, they can be combined into a single constant,

R'^{*}, where $R'^{*} = \left(R^{*}/\Phi_{RTS}\right)$ expressed in mol RTS/mol PAH which results in Equation 3-27.

$$\frac{\text{PLC50}}{\text{NLC50}} = \frac{1}{1+\left(\frac{P_{\text{abs}}{}^{a}}{R'^{*}}\right)} \tag{3-27}$$

For each observation with species k and PAH j, the $\text{PLC50}_{k,j}$ for that species–PAH pair is computed as

$$\frac{\text{PLC50}_{k,j}}{\text{NLC50}_{k,j}} = \frac{1}{1+\left(\frac{P_{\text{abs},j}{}^{a}}{R'^{*}}\right)} \tag{3-28}$$

where $k = 1, \ldots, N_s$ and $j = 1, \ldots, N_c$ corresponding to the $N_s = 15$ species and $N_c = 20$ PAHs, respectively. The species dependency of the PTLM is introduced by the $\text{NLC50}_{k,j}$, while the PAH, light source, and exposure time is accounted for by $P_{\text{abs},j}$. The model parameters: a, and R'^{*}, and their standard errors (SE) are computed using the R program nonlinear regression package: nls [75].

3.5 Results and Discussion

The model (Equation 3-28) is fitted using the experimental data summarized in Table A.1. A total of 333 data points comprising 20 PAHs and 15 species are compiled in the dataset. The PTLM model parameters, a and R'^{*}, as well as the respective standard errors (SEs) are tabulated in Table 3-2.

Table 3-2. Nonlinear regression estimated parameters and standard errors (SE)

PTLM parameters	a	R'^{*}
Estimate	0.426	0.511
SE	0.037	0.097

The PTLM model is capable of predicting both LC50 and LT50 data. This greatly expands the quantity of data that can be analyzed using the PTLM. For notational simplicity, both types of data are referred to as PLC50 in the derivation above. Computational examples for PLC50 can be found in Appendix A.3. The experimental PLC50s obtained directly from the reported aqueous concentrations at 50% mortality (labeled "PLC50") are shown in Figures 3-3A and 3-3C distinguished by different colors for different organisms and chemicals, respectively. The experimental PLC50s corresponding to the reported phototoxic LT50 data (labeled "PLT50") are shown in Figure 3-3B (in which different colors indicate different organisms) and Figure 3-3D (color-coded for different chemicals). The plots contain all the experimental data in the database. The data that produced residuals greater than one order of magnitude (shown with the plus symbols in the plots) were considered outliers and were not included in the nonlinear regression calculations. However, they are included in Figure 3-3. A total of 13 data points were eliminated from the regression, decreasing the number of data points to 320 associated with 20 PAHs and 15 species. Note that no chemicals and species were eliminated by removal of the outliers. The lines show the model fit using Equation 3-28. The dashed lines represent one order of magnitude uncertainties.

The experimental PLC50s and PLT50s data are also compared with the PTLM prediction in Figure A.2 through Figure A.5 in Appendix A.4. Each panel presents the similar comparison grouped by chemical (Figure A.2), by organism (Figure A.3), by the reference reporting the experimental data (Figure A.4), and by the light source used in the experiment (Figure A.5). These comparisons can be used to analyze for biases in the model predictions, for example, the model prediction for a specific organism is always biased high or low. No consistent biases are evident.

The objective for the phototoxic model is to predict the phototoxic concentration for each species and each PAH for the conditions of the experiment. Since the narcotic LC50 (NLC50) is a predicted concentration using the NTLM (Equation 3-4), it is also part of the model framework. Therefore the PTLM equation to predict PLC50 is

$$\mathrm{PLC50} = \frac{\mathrm{NLC50}}{1 + \left(\frac{P_{\mathrm{abs}}{}^{a}}{R'^{*}} \right)} \tag{3-29}$$

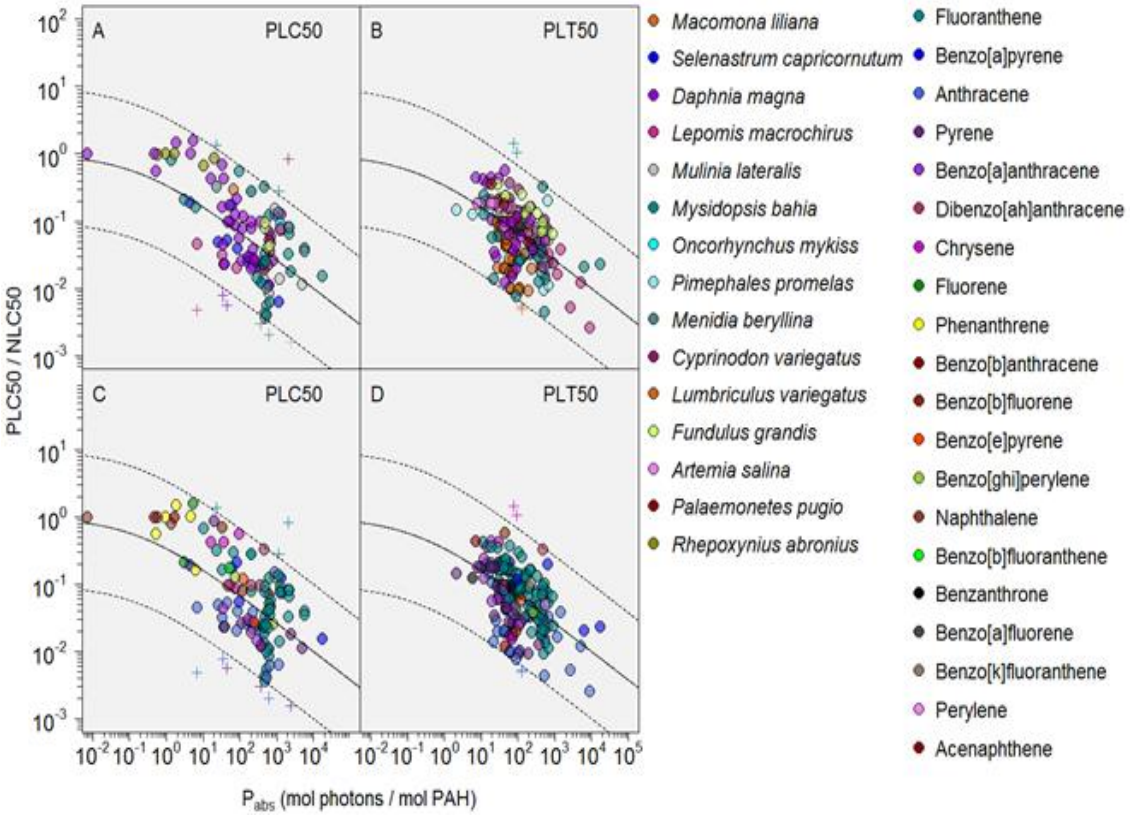

Figure 3-3. Ratio of PLC50s to NLC50s predicted by NTLM (Equation 3-4). A and C: PLC50s are obtained directly from the reported aqueous concentrations at 50% mortality (labeled PLC50). B and D: the experimental PLC50s corresponding to the reported phototoxic LT50 data (labeled PLT50). Organisms are color coded in panels A and B and described in the left legend. Chemicals are differentiated by colors (described in the right legend) in panels C and D. The solid lines show the PTLM model fit (Equation 3-27). The dashed lines represent one order of magnitude uncertainties. The outliers are indicated by plus symbols. Note that panels A and C contain the same set of phototoxic LC50 data, (A) is color coded for organisms (B) is color coded for chemicals. Similarly, panels B and D are the same set of phototoxic LT50 data (B) is color coded for organism and (D) is color coded for chemicals.

Figures 3-4A-D compare PLC50s predicted using Equation 3-29 to the observed PLC50s. The observed PLC50s for LC50-based data are shown in Figures 3-4A and 3-4C, while observed PLC50s associated with the LT50 endpoints are shown in Figures 3-4B and 3-4D. In Figures 3-4A and 3-4B, different colors indicate different organisms, whereas in Figures 3-4C and 3-4D different chemicals are color-coded. Data with residuals greater than one order of magnitude are shown with plus symbols. The diagonal line indicates perfect agreement of the experimental data with the predicted values and the dashed lines represent one order of magnitude uncertainties in the prediction. The root mean square error of the prediction, RMSE, is calculated using Equation 3-30 where *n* indicates the number of data

$$\text{RMSE} = \sqrt{\frac{1}{n}\left(\sum_{j=1}^{n}(\log(\text{PLC50})_{\text{predicted}} - \log(\text{PLC50})_{\text{observed}})^2\right)} \qquad (3\text{-}30)$$

The RMSE of the LC50-based data = 0.473 (n = 120), while RMSE associated with the LT50-based data = 0.382 (n = 213). The RMSE of prediction for the entire data (including both LC50-based and LT50-based data) = 0.416 (n = 333). Note that all data, including the outliers, are included in the RMSEs calculation. The NTLM yielded RMSE = 0.416 (n = 148) for NLC50 prediction of PAHs [23]. Interestingly, the PTLM yielded comparable RMSEs to that of NTLM indicating that they both offer the same level of quality in prediction. For both models less than approximately 5% of data exceed factor of 10 error.

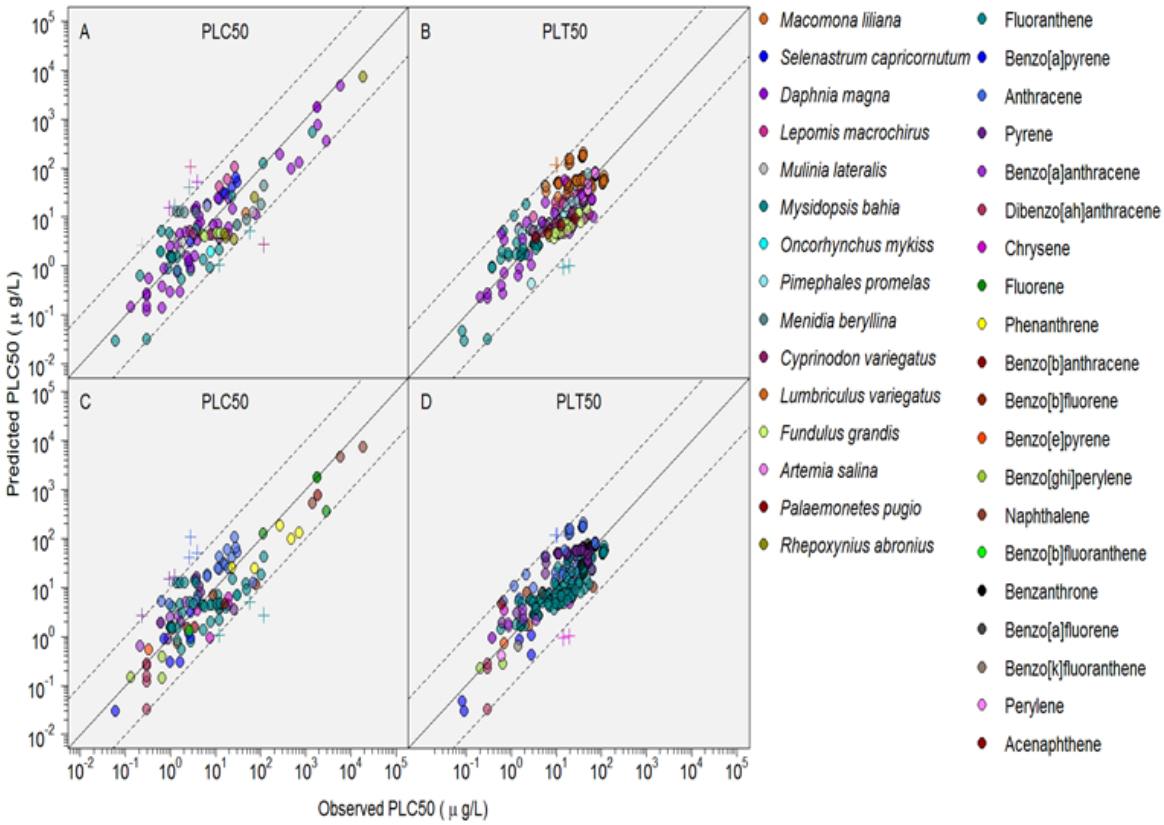

Figure 3-4. Predicted PLC50 (µg/L) (Equation 3-29) versus observed PLC50 (µg/L). A and C: PLC50s are obtained directly from the reported aqueous concentrations at 50% mortality (labeled PLC50). B and D: the experimental PLC50s corresponding to the reported phototoxic LT50 data (labeled PLT50). The solid diagonal lines indicate perfect agreement between predicted and observed PLC50s. The dashed lines represent one order of magnitude uncertainties. The outliers are indicated by plus symbols. Note that panels A and C contain the same set of phototoxic LC50 data; A is color coded for organisms B is color coded for chemicals. Similarly, panels B and D are the same set of phototoxic LT50 data; B is color coded for organism and D is color coded for chemicals.

3.6 Statistical Analysis

The relatively low standard errors of the fitted parameters $a = 0.426 \pm 0.037$ and $R'^{*} = 0.511 \pm 0.097$, indicates that both parameters are estimated with high

confidence. Two assumptions have been made in order to simplify the model to the point that only these parameters are necessary. They are that the quantum yield for moles of reactive toxic species produced to moles of photon absorbed, Φ_{RTS}, is constant for all PAHs and the ratio of critical body burden for phototoxicity to narcosis toxicity, R'^{*}, is constant for all species. Unfortunately, it is not possible to validate these assumptions directly since Φ_{RTS} and R^{*} occur as a ratio in the model

$$R'^{*} = \frac{R^{*}}{\Phi_{RTS}} \tag{3-31}$$

Figure 3-5 is a boxplot of log of residuals for individual PAHs sorted by increasing $\log(K_{OW})$. Log of residuals are calculated as log(predicted PLC50) – log(observed PLC50). The width of each box is proportional to the square root of the number of data points for each PAH. For the PAHs with the most data, anthracene and pyrene, appear to be biased high (predicted > observed), whereas fluoranthene is biased slightly low. However the magnitude of the biases is relatively small: median residuals are a few tenths of a log unit, and it is not possible to know if this is also due to a species specific effect that is correlated to the PAHs involved.

A similar boxplot of residuals for individual organisms sorted by increasing CTLBB (decreasing organism sensitivity) is provided in Figure 3-6. Again there are variations but no species with a very large bias and the boxplot exhibits no specific trend for the median of the residuals versus the species sensitivities.

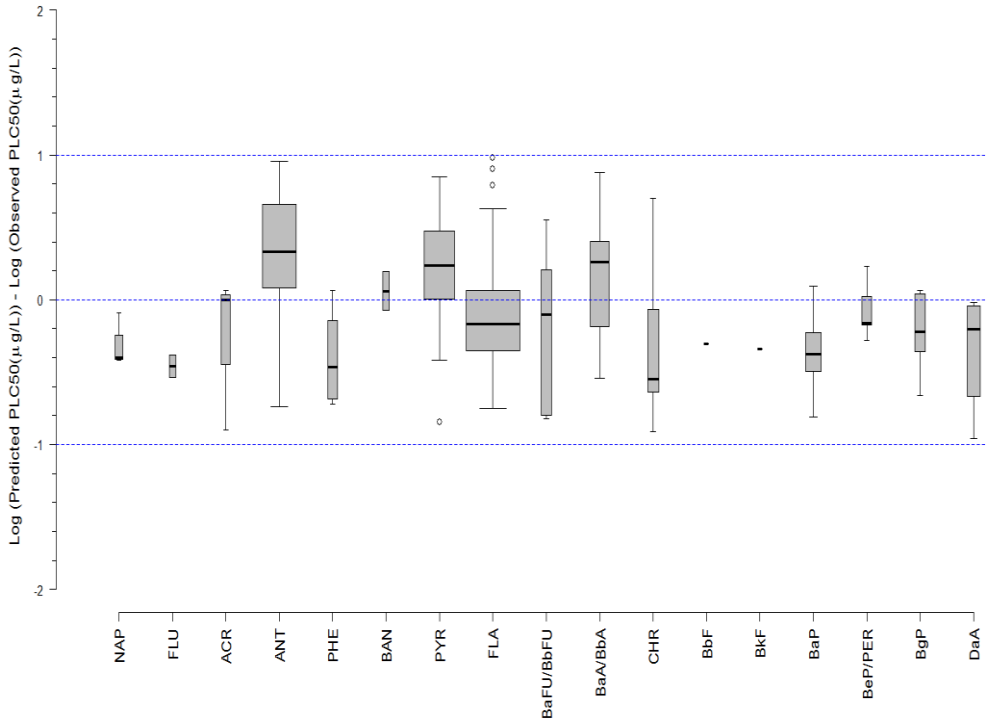

Figure 3-5. Boxplot of residuals for 20 PAHs used for the PTLM model calibration. Residuals (y-axis) are calculated as log(Predicted PLC50 (µg/L)) – log(Observed PLC50 (µg/L)). Width of each box is proportional to the square root of number of data points for each chemical. The boxes are sorted by the octanol-water partition coefficients from low to high. The chemicals with the same octanol-water partition coefficients are located at the same points on the x-axis.

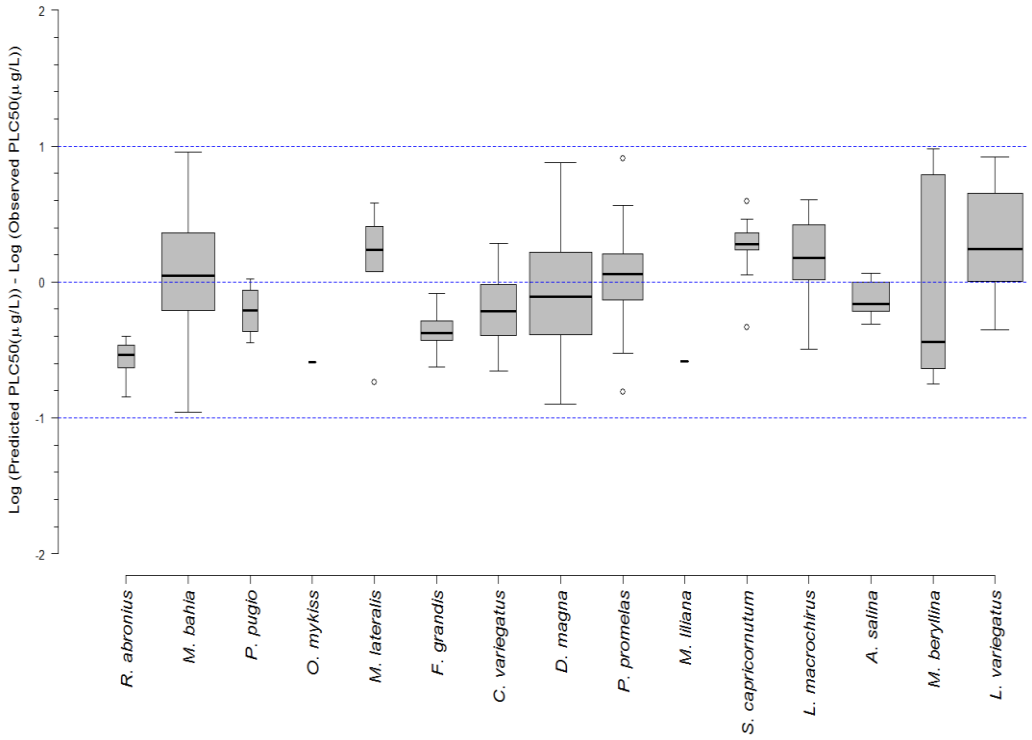

Figure 3-6. Boxplot of residuals for 15 organisms used for the PTLM model calibration. Residuals (y-axis) are calculated as log(Predicted PLC50 (µg/L)) – log(Observed PLC50 (µg/L)). Width of each box is proportional to the square root of number of data points for each organism. The boxes are sorted by increasing critical target lipid body burden, CTLBB, corresponding to decreasing organism sensitivity.

In an attempt to provide an analysis of the magnitude of the improvement that could be derived from chemical specific or species specific model parameters, the following analysis has been performed. The medians for each PAH (PAH-specific medians) were subtracted from the corresponding residuals. The new predicted PLC50s based on the PAH-specific medians were compared with the observed PLC50s resulting in a RMSE of 0.347, which improved the predictions by17%. Similarly, with organism-specific medians subtracted from the associated residuals, the RMSE of the prediction became equal to 0.374, which decreased the error only 10%. This suggests that errors in the model prediction are not due entirely to the model simplifications but are also due to other random or uncontrolled features in the experiments.

Additional analyses of the residuals can be found in Appendix A.5. The residuals are plotted against the factors related to photo-enhanced toxicity, including the intensity of irradiance (P_{abs} / T_{exp}) and the photons absorbed (P_{abs}) in Figures A.6 and A.7, respectively. The plots show no trends with respect to light intensity and the photons absorbed indicating the lack of bias toward these parameters.

With regard to the light exposure duration, T_{exp} , the quantities range from 0.1 (h) to over 100 (h) with 269 (h) and 485 (h) for two data points. Residual plots versus light exposure time are shown in Figure A.8 and separated based on the light regime for continuous irradiation, as well as periodic irradiation associated with 48-h and 96-h PLC50s.

Perhaps the most interesting and puzzling result of this modeling analysis is the fact that the toxicity decreases not as the unity power of the photon dose, but rather at a markedly lower rate with an exponent $a = 0.426 \pm 0.037$. The fact that the model prediction is not biased by the length of light exposure or the magnitude of the light

intensity suggests that another factor is operating that produces this less than proportional relationship between toxicity and photo dose. This is an area that would profit from further investigation.

3.7 Conclusions

The PTLM model is capable of predicting the phototoxicity of PAHs measured as either LC50 or LT50. It accounts for the differences in the chemical and physical properties of PAHs, test species sensitivities, and light sources spectra, intensity and duration. The validation is performed using 333 data including 120 LC50 and 213 LT50 toxicity endpoints associated with 20 PAHs, 15 organisms, and 10 light sources. The model has two fitting parameters and does not rely on relative measures of toxicity, e.g. RPAs, determined from the experiments. The factors accounting for the chemical properties in the modeling framework (octanol-water partition coefficient and the molar absorption coefficient) can be estimated from the compound structure. The organism specific factor in the PTLM is the target lipid model, CTLBB, which is available in the TLM database for The CTLBB has been determined for 47 aquatic [23] and five algal species [54].

The motivation for the development of PTLM was to apply it to mixtures of PAHs in petroleum. The next chapter presents the results.

Chapter 4

PHOTOTOXIC TARGET LIPID MODEL VALIDATION: PREDICTING PHOTOTOXICITY OF ALKYLATED PAHS, MIXTURES, AND NEAT AND WEATHERED PETROLEUM

The toxicity of petroleum increases considerably when exposed to solar radiation. It occurs when certain components in the mixture, including polycyclic aromatic hydrocarbons (PAHs) absorb light in ultraviolet and visible portions of the solar radiation spectrum. A phototoxic target lipid model (PTLM), previously developed in Chapter 3 to predict phototoxicity of single PAHs, is validated in this chapter for 12 compounds that are components of petroleum, including alkylated PAHs and dibenzothiophene, exposed to four species *Americamysis bahia*, *Rhepoxynius abronius*, *Daphnia magna*, and *Pimephales promelas*. The PTLM is also used to the predict phototoxicity of binary and ternary mixtures of three PAHs: pyrene, anthracene, and fluoranthene exposed to *A.bahia* and *Menidia beryllina*. Finally, it is used to predict the toxicity of water accommodated fractions of neat and naturally weathered Macondo crude oil samples collected from the Deepwater Horizon oil spill sites. The oil samples were exposed to the Gulf of Mexico species, including *A.bahia, M.beryllina, Cyprinodon variegatus,* and *Fundulus grandis* under natural and simulated solar radiation. The results support the applicability of the PTLM for predicting phototoxicity of petroleum.

4.1 Introduction

More than 200 million gallons of crude oil were released from the Macondo Well in the Gulf of Mexico during the 2010 Deepwater Horizon oil spill [76,77]. Crude oil is a complex mixture of many components, including straight-chain alkanes (n-alkanes or n-paraffins), branched alkanes (isoalkanes or isoparaffins), cyclicoalkanes (cycloparaffins), and aromatics [3]. The petroleum that flowed from the Macondo well during the Deep Water Horizon oil spill contained approximately 3.9% polycyclic aromatic hydrocarbons (PAHs) by weight resulting in an estimated 2.10×10^{10} g of PAHs released during the oil spill [78]. PAHs are known to exhibit photo-enhanced toxicity, with a factor of two to greater than 1000 enhancement in toxicity in the presence of ultraviolet (UV) and visible (VIS) light [4-9]. Alkylated PAHs (APAHs) and heterocyclic aromatic hydrocarbons (e.g. dibenzothiophene) present in petroleum in substantial concentrations also exhibit photo-enhanced toxicity.

The objective of this chapter is to predict the toxicity of neat and naturally weathered Macondo crude oils to species indigenous to the Gulf of Mexico, including the mysid shrimp (*Americamysis bahia*), inland silverside (*Menidia beryllina*), sheepshead minnow (*Cyprinodon variegatus*), and Gulf killifish (*Fundulus grandis*). In addition, phototoxicity of major components of petroleum including APAHs, as well as binary and ternary mixtures of PAHs are also predicted. The predictions are made using the phototoxic target lipid model (PTLM) developed in Chapter 3.

4.2 Narcotic Target Lipid Model

In the absence of light, the components of petroleum exhibit a narcotic toxicity mode of action that can be predicted using the narcotic target lipid model (NTLM) [18,21,23]:

$$\log(\text{NLC50}) = -0.936\log(K_{\text{OW}}) + \log(C^{*}_{\text{LN}}) + \Delta c \qquad (4\text{-}1)$$

where NLC50 = aqueous concentration at 50% mortality (mmol/L), K_{OW} = octanol-water partition coefficient (L/kg octanol), C^{*}_{LN} = critical target lipid body burden CTLBB (mmol chemical/kg octanol), the concentration in the target lipid that causes 50% mortality, and Δc = chemical class correction (log (mmol/L) for target lipid-water partitioning. It is assumed that all the components of the petroleum mixture exhibit a narcotic mode of action, which has been validated by an extensive data analysis and more recent applications [18,20,23,28,79-81].

4.3 Phototoxic Target Lipid Model

To predict phototoxicity of single PAHs, a phototoxic target lipid model (PTLM) has been developed in Chapter 3. The PTLM predicts the increase in toxicity relative to the narcotic toxicity

$$\frac{\text{PLC50}}{\text{NLC50}} = \frac{1}{1+\left(\frac{P_{\text{abs}}}{R'^{*}}\right)^{a}} \qquad (4\text{-}2)$$

where PLC50 = aqueous concentration that produces 50% mortality (μg/L) in the presence of light (phototoxicity), NLC50 = narcotic LC50 (Equation 4-1). P_{abs} (mol photon/mol PAH) = quantity of energy absorbed by the PAHs, a and R'^{*} are the equation constants (0.426 ± 0.037 and 0.511 ± 0.097, respectively). P_{abs} is obtained from the spectral intensity of the incident radiation and the molar absorption coefficient of the PAH

$$P_{abs} = \int_{\lambda_1}^{\lambda_2} I_o(\lambda)\left(\frac{\lambda}{N_A hc}\right) T_{exp}\varepsilon(\lambda)d\lambda \quad (4\text{-}3)$$

where λ is the wavelength (nm), $I_o(\lambda)$ = incident light intensity (W/m^2/nm) at wavelength λ, N_A = Avogadro number (6.02×10^{23}), h = Planck's constant (6.63×10^{-34}J s), c = the speed of light (2.30×10^8 m/s), T_{exp} = time of exposure to the light (s), and $\varepsilon(\lambda)$ = molar absorption coefficient (L/mol/cm) of the PAH at wavelength λ (nm). The term $(\frac{\lambda}{N_A hc})$ converts the incident light $I_o(\lambda)$ in units of (W/m^2/nm) to (moles photons/m^3/s) which when multiplied by time T_{exp} (s) yields moles of incident photons per m^3 during the light exposure time.

The PTLM is validated in Chapter 3 for 333 toxicity experiments for 20 PAHs and 15 species including arthropods, fishes, amphibians, annelids, mollusks, and algae, as well as 10 different light sources and exposure durations from 0.2 to about 485 hours. The toxic endpoints were reported as either the LC50 concentration for a fixed length of exposure (48 or 96 hours of exposure) or as the LT50, the time at which 50% mortality occurred, at a fixed concentration. The PTLM can predict either LC50s or LT50s. An LC50 is predicted using Equations 4-2 and 4-3 with T_{exp} = time of light exposure employed in the experiment. For an LT50 determined at a fixed concentration, the PLC50 is set to the fixed concentration in Equation 4-2 and T_{exp} = LT50 is computed from Equation 4-3.

The root mean square error (RMSE) quantifies the error between predicted and observed LC50s.

$$\text{RMSE} = \sqrt{\frac{1}{n}\left(\sum_{j=1}^{n}(\log(\text{PLC50})_{\text{predicted}} - \log(\text{PLC50})_{\text{observed}})^2\right)} \quad (4\text{-}4)$$

where n = number of data points. For the LC50 data, RMSE = 0.473 and for the LT50 data RMSE = 0.382. The RMSE of prediction for the entire data set = 0.416.

4.4 Alkylated PAHs and Other Phototoxic Chemicals

Crude oils and refined petroleum products contain alkylated PAHs (APAH), in particular the alkylated homologues of naphthalene, phenanthrene, fluorene, and chrysene, and heterocyclic PAHs, e.g. benzothiophenes. APAHs usually occur in significantly higher concentrations than their corresponding unsubstituted parent PAHs [1,2]. Similar to PAHs, APAHs and heterocyclic aromatic hydrocarbons present in petroleum can absorb light in UV and visible portions of solar radiation and cause an increase in the toxicity of petroleum. The applicability of the PTLM to predict phototoxicity of these constituents of petroleum is examined next.

4.4.1 Predicting Phototoxicity of APAHs and other Phototoxic Chemicals

Validation of the PTLM to predict phototoxicity of APAHs and phototoxic chemicals other than PAHs is performed using experimental data for 10 APAHs, dibenzothiophene, and acridine exposed to four different organisms, *A. bahia*, *Rhepoxynius abronius*, *Daphnia magna*, and *Pimephales promelas* [4,8,11,34]. The detailed procedure to predict PLC50 of a compound using PTLM is provided in Appendix A.3. The octanol-water partition coefficients, K_{OW}, required in Equation 4-1 are computed from SPARC (Sparc Performs Automated Reasoning in Chemistry) [82] and presented in Table B.3. The narcotic CTLBBs for *R. abronius*, *D. magna*, and *P. promelas* are from the values provided in the literature [23] (Table A.4 in Appendix A.1). For *A. bahia*, the CTLBB is estimated using Equation 4-1 and the observed NLC50 (Table B.1 in Appendix B.1) for an exposure to fluoranthene in the dark [88].

The molar absorption coefficients available in the literature for the compounds are provided Tables B.2-a and B.2-b in Appendix B.2. Table B.3 provides a list of the assumed molar absorption coefficients as the parameter is available for a limited number of APAHs and benzothiophenes in the literature.

The predicted and observed PLC50s are compared in Figure 4-1. The detailed information is provided in Table B.4 in Appendix B.3. Data associated with LC50s and LT50s are shown with square and diamond symbols, respectively. An alternate presentation (Figure B.1) denotes the organisms with different symbols.

Comparison between the predicted and experimentally observed PLC50 for APHAs and other phototoxic compounds, including dibenzothiophene, yields a RMSE = 0.478 (Figures 4-1) that is comparable to the RMSE = 0.416 for PAHs analyzed in Chapter 3. This result suggests that the PTLM can predict the phototoxicity of the components of petroleum without further experimental data.

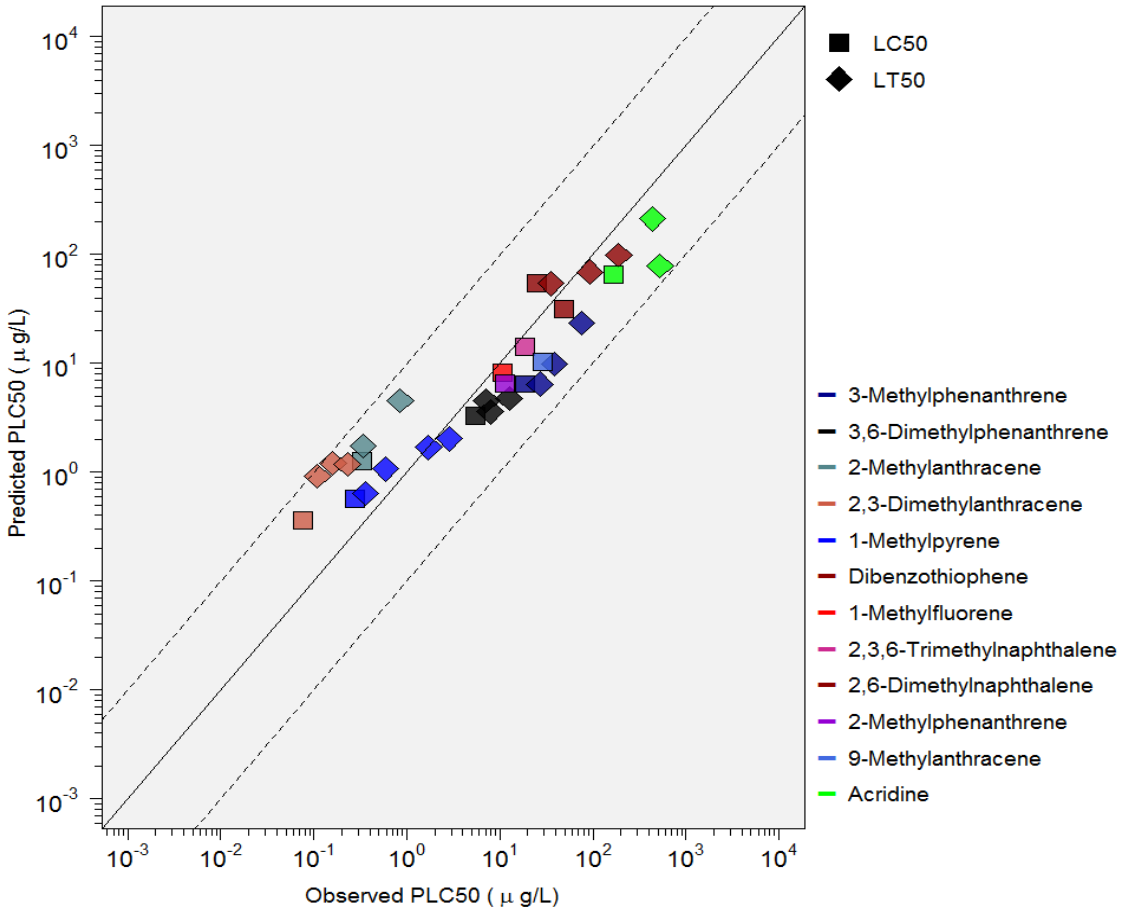

Figure 4-1. Predicted PLC50 (µg/L) (Equation 4-2) versus observed PLC50 (µg/L) for APAHs and other phototoxic chemicals. The experimental PLC50s corresponding to the reported phototoxic LT50 data (labeled PLT50) are shown with diamond symbols, while data obtained directly from the reported aqueous concentrations at 50% mortality (labeled PLC50) are shown with square symbols. Chemical are color-coded as described in the legend. The solid diagonal lines indicate perfect agreement between predicted and observed PLC50s. The dashed lines represent one order of magnitude uncertainties. RMSE = 0.478.

4.5 Mixtures

The PAHs occur as mixtures in petroleum. Therefore, a method is required to predict the toxicity of mixtures using the toxicity of the individual PAHs. The toxicity of mixtures is modeled employing toxic units [19-23]. A toxic unit (TU) is defined as the ratio of the concentration in a medium to the effect concentration in that medium. Thus, aqueous narcotic toxic unit is defined as

$$\mathrm{NTU}_i = \frac{C_{\mathrm{W},i}}{\mathrm{NLC50}_i} \tag{4-5}$$

where the subscript *i* denotes the individual chemicals, $C_{\mathrm{W},i}$ = the aqueous concentration (μg/L), and $\mathrm{NLC50}_i$ = narcotic LC50 (Equation 4-1). Similarly, the aqueous phototoxic unit PTU_i is

$$\mathrm{PTU}_i = \frac{C_{\mathrm{W},i}}{\mathrm{PLC50}_i} \tag{4-6}$$

where $\mathrm{PLC50}_i$ = phototoxic LC50 (Equation 4-3). It has been demonstrated for narcotics in general and for PAHs in particular that the toxicity of mixtures can be estimated using toxic units [19-23,83]. Therefore, the NTLM and the additivity of TUs can be used to predict the toxicity of mixtures of the components of petroleum. Experimental data from PAHs mixtures and crude oil are used to examine whether TU additivity applies to phototoxic TUs as well.

Narcotic toxicity and phototoxicity of a mixture is computed as the sum of the individuals NTUs and PTUs, respectively (Equations 4-7 and 4-8).

$$\mathrm{NTU} = \sum_{i=1}^{n} \mathrm{NTU}_i \tag{4-7}$$

$$\mathrm{PTU} = \sum_{i=1}^{n} \mathrm{PTU}_i \tag{4-8}$$

At 50% mortality, the total TU of the mixture is equal to unity. Mortalities less and greater than 50% are expected below and above TU = 1, respectively.

4.5.1 Mixtures Phototoxicity Prediction and Validation

The ability of PTLM to predict phototoxicity of PAHs in the mixtures and the additivity assumption are tested by comparing the predictions to the observations for mixtures of PAHs. The data are for *A. bahia* and *M. beryllina* exposed to binary and ternary mixtures of pyrene, anthracene, and fluoranthene. In phototoxicity bioassays, the LC50s were reported for the organisms placed in complete darkness for a 24-h chemical loading period, followed by 12-h exposure to SolarConstant 1200 lamp. Further details on the experimental conditions and data associated with the mixtures experiments are provided in Table B.5 in Appendix B.4 [88].

Predicted and experimental PTUs for *A. bahia* and *M. beryllina* exposed to binary and ternary mixtures of pyrene, anthracene, and fluoranthene are compared in Figure 4-2 (data in Table B.5). The diagonal solid line indicates perfect prediction and the dashed lines represent one order of magnitude uncertainties. The detailed procedures to predict phototoxicity of a mixture is described in Appendix B.5. The comparison resulted in RMSE = 0.291 that is significantly smaller than the RMSE = 0.473 for LC50 predictions found in Chapter 3. However, the comparison between the predicted and observed PTUs for *A. bahia* (the circles in Figure 4-2) indicate that the predicted PTUs are consistently lower than the observations. This underprediction in phototoxicity is observed for all combinations of the PAHs in the mixtures suggesting that the underprediction is related to the CTLBB for *A. bahia*, the only organism specific parameter in the PTLM. The CTLBB is estimated using the observed NLC50 for the organism exposed to fluoranthene (Table B.1). CTLBB are usually estimated using at least three LC50s [18]. Although the single observed NLC50 is the most accurate basis available to calculate the species sensitivity for 3-d old *A. bahia*, the resulting CTLBB appears to be higher than that suggested by the mixture experiments.

Additional NLC50 using other PAHs would be required to estimate a more reliable CTLBB for *A. bahia*.

A more detailed analysis of the mixture data is presented in Figure 4-3, the observed dose response: observed mortality on the y-axis at the corresponding predicted PTUs on the x-axis. The vertical solid line is the predicted PTU for 50% mortality and the two parallel dashed lines indicate one order of magnitude uncertainties in the prediction. The experimental data for the observed mortalities and the associated PTUs are presented in Table B.4. The model reproduces the observed dose response for binary and ternary mixtures of pyrene, anthracene, and fluoranthene exposed to *M .beryllina* and supports the observation that the CTLBB for *A .bahia* higher than a value consistent with these data.

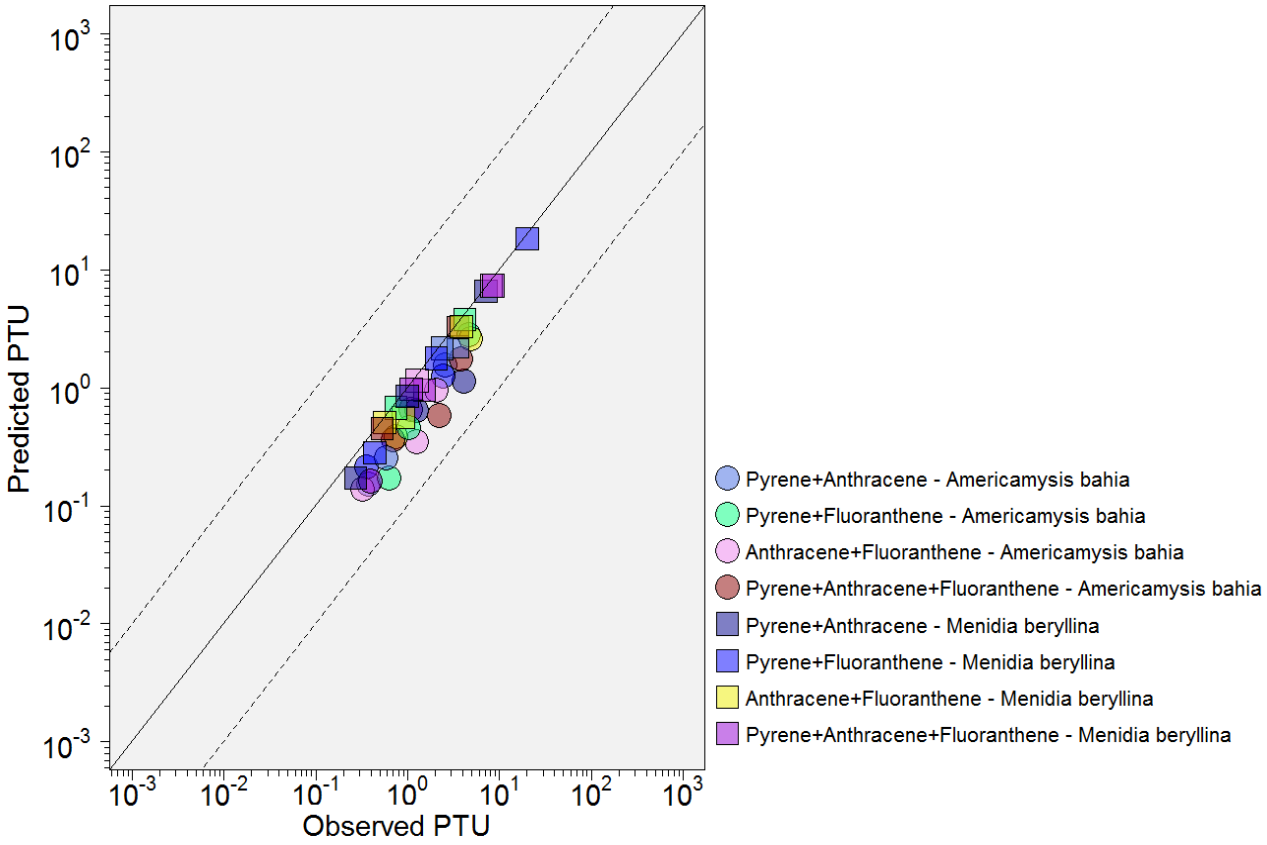

Figure 4-2. Predicted vs. experimental PTUs for binary and ternary mixtures of PAHs pyrene, anthracene, and fluoranthene distinguished by the colors listed in the legend. Solid line represents 1:1 agreement, dashed lines represent ± an order of magnitude errors. RMSE = 0.274. Data associated with *Americamysis bahia* and *Menidia beryllina* are shown with circle and square symbols, respectively.

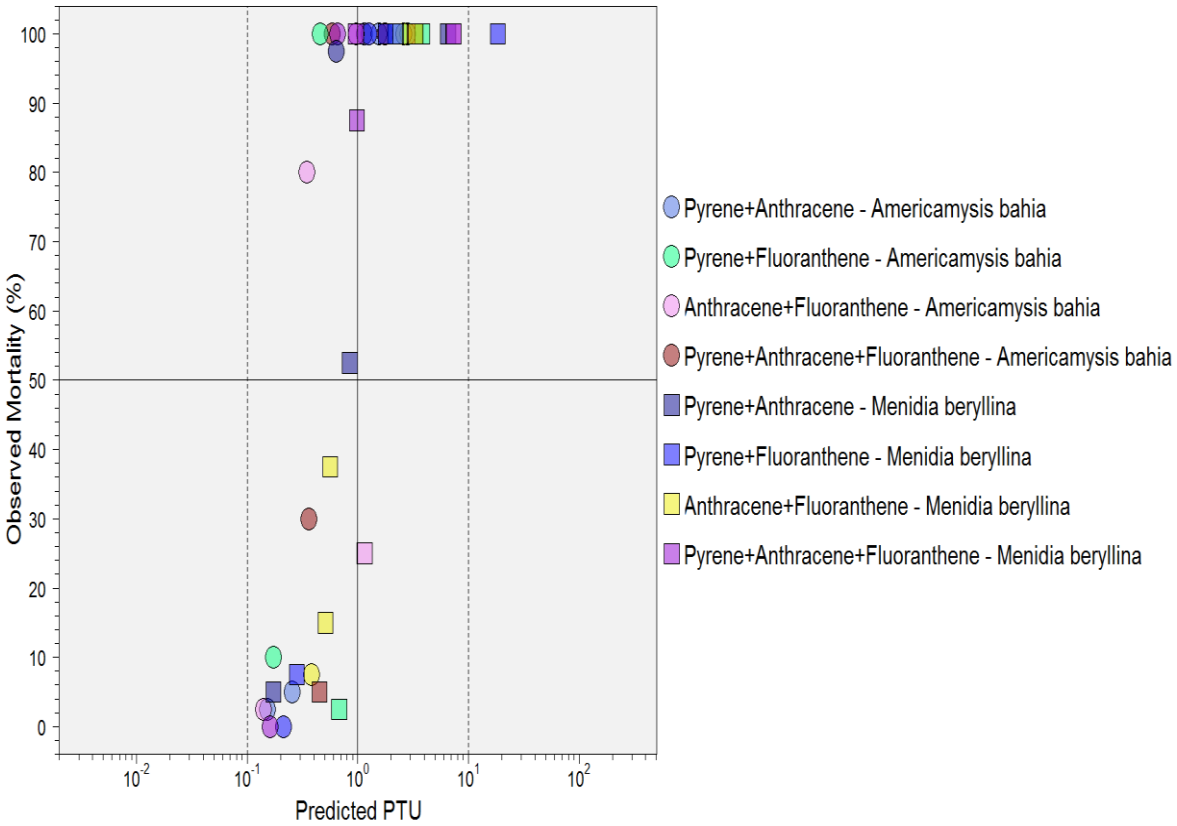

Figure 4-3. Observed mortality vs. the corresponding predicted PTUs for binary and ternary mixtures of PAHs pyrene, anthracene, and fluoranthene distinguished by colors in the legend. Solid vertical line represent PTU = 1 and the horizontal line indicates 50% mortality. The dashed line represent ± one order of magnitude variations. Data associated with *Americamysis bahia* and *Menidia beryllina* are shown with circle and square symbols, respectively.

4.6 Toxicity of Petroleum Water Accomodated Fraction

The complex nature and limited aqueous solubility of the components of crude oil and related petroleum products poses challenges for evaluating the aquatic toxicity of these substances [84]. The commonly used approach to assess toxicity of petroleum is to test the water-accommodated fraction (WAF). The WAF is made by equilibrating an oil–water mixture 10 L clear glass aspirator bottles with a bottom dispensing port. Bottles were initially filled with 8 L of filtered saltwater (~20% headspace) and oil samples were then added at a loading rate of 1 gram of oil per liter of seawater followed by mixing for 20 hours, and then allowing to settle for 4 hours for phase separation before collecting samples for testing [88]. The WAF is tested in closed exposure vessels containing the test organism, with no headspace to prevent volatilization of the more volatile hydrocarbon components [84].

To test the toxicity of the WAF, it is diluted with uncontaminated water to achieve various dilutions resulting in different exposure concentrations of the WAF solutions, denoted as C_{exp} (%WAF). Concentration of the oil mixture in terms of %WAF and the dilution factors DF at which the mixture is diluted are related via

$$C_{\text{exp}}(\%\text{WAF}) = 100\times\text{DF} \tag{4-9}$$

For example, DF = 1, 1/4, and 1/16 correspond to the C_{exp} = 100% WAF, 25% WAF, and 6.25% WAF, respectively. The organisms are exposed to different WAF concentrations. The results are expressed as a lethal or effective concentration C_{exp} (%WAF) that causes an adverse effect (e.g. 50% mortality) to the exposed organism after a specified period of exposure.

4.6.1 Predicting Narcotic Toxicity and Phototoxicity of Petroleum WAF

Predicting phototoxicity of petroleum requires predicting both the narcotic and phototoxicity of all components *j* present in the WAF solution at concentration $C_{w,i}$ (μg/L). It can be calculated using the composition of the petroleum and the aqueous solubility of the components [85]. For each component the expected dissolved concentration can be estimated as its aqueous solubility × the mole fraction in the mixture (Raoult's Law). However, for mixtures of chemicals that are solids as single compounds and liquids as mixtures, such as those in petroleum, the subcooled liquid solubility, i.e. the solubility of the component if it were a liquid at the temperature of interest, is used [23]. Also, it appears that, for chemicals with higher K_{OW}s, they do not contribute to the toxicity of the mixture. In this regard, only the TUs for components with $\log(K_{OW}) \leq 5.3$ are included in the total TU. This cutoff was established by examining the toxicity of single PAHs [20] and the toxicity of WAFs from various types of petroleum.

Total narcotic and phototoxic TUs (NTU and PTU respectively) of a mixture of petroleum components are estimated using Equation 4-7 and 4-8, respectively. If the experiments produce the DF at which 50% effect is observed, e.g. DF = 0.25 causes 50% mortality, the TU in that WAF is 1/DF = 4 TU. The predicted TU is obtained by summing the TUs for each PAH in the WAF up to $\log(K_{OW}) = 5.3$, the toxicity cutoff [20, 80].

Computational procedures and examples for quantitative prediction of narcotic toxicity and phototoxicity of petroleum are presented in Appendix B.9.

4.6.2 Petroleum Narcotic Toxicity and Phototoxicity Validation

Petroleum narcotic toxicity and phototoxicity predictions are validated using the experimental toxicity data for WAFs of Macondo crude oil samples collected during the Deep Water Horizon oil spill. For petroleum phototoxicity assessment, three field collected oils were tested: neat MASS oil from the Massachusetts barge was collected directly from a sub-surface containment system at the MC-252 wellhead before the well was capped on July 15, 2010. Moderately weathered CTC oil was recovered from the CTC02404 barge on July 29, 2010 by skimming the surface of Gulf of Mexico waters. The further weathered Juniper oil was recovered from the Gulf of Mexico by skimming the surface approximately 25 miles northwest of the MC-252 wellhead by the Coastguard cutter "Juniper" and then sampled from the vessel on July 19, 2010 [88]. Weathering removes the more soluble chemicals with lower log(K_{OW}) which are more soluble compounds that have higher toxic potentials [21]. Observations also confirm that weathering lowers the toxicity of petroleum (see references in [21]).

Figure 4-4 presents the toxic unit contributions for MASS, CTC, and Juniper oil WAFs for the top 10 phototoxic components. The notation C1-naphthalene indicates that this is the total concentration of all substituted naphthalene compounds with a one carbon containing substuent, which can be a methyl group in any position. C2-naphthalene is the total concentration of the substituted naphthalenes for which the substitution is either two methyl groups or one ethyl group in any positions. The reason for this grouping of compounds is the inability of the analytical technique to separate each of these substituted compounds as they co-elute. The left and right column are individual NTU_is and PTU_is, and cumulative NTUs and PTUs, respectively. Note that in progressing from neat oil to the moderately and heavily

weathered oils (from the top to the bottom panels), the narcotic and phototoxic units decrease indicating that the toxicity of the oils decrease with increasing the degree of weathering. This is due to the relationship between subcooled liquid solubility and toxicity of PAHs [21]. The complete chemical compositions and concentrations for all oil samples are provided in Appendix B.7.

Perhaps the most surprising result is that nearly all of the components in the list are methylated PAHs. This is not due to their increased phototoxicity compared to the parent compound but rather their higher abundance relative to the unsubstituted parent.

The oils were exposed to four species indigenous to the Gulf of Mexico, including *A. bahia*, *M. beryllina, C. variegatus*, and *F. grandis*. Dark, natural sunlight, and solar simulated light exposure studies were conducted with the exposure concentrations of 100%, 25%, and 6.25% WAF. The CTLBBs are calculated from the observed NLC50s. Table B.1 provides the estimated CTLBBs for these species.

The molar absorption coefficients available in the literature and the corresponding references are presented in Tables B.2-a and B.2-b in Appendix B. Due to the limitation in the availability of molar absorption coefficient for APAHs and benzothiophenes, molar absoprtions of the chemicals with the closest chemical structure are used. Table B.3 provides the molar absorptions for the chemicals for which their molar absorption was not available in the literature.

The observed and predicted NLC50 and PLC50 for the three oils exposed to four species indigenous to the Gulf of Mexico with diverse sensitivities (Table B.2) are presented in Tables B.5 and B.6. The observations for which 50% mortality could not be achieved even at the maximum exposure concentration of oil $C_{exp} = 100$

(%WAF) are indicated as ">100" implying that the WAF for that oil was not toxic to the test organism. The quantitative comparison between the predicted and observed LC50s can only be made for experiments that produced an LC50 ≤ 100%. Figure 4-5 presents the comparison. The RMSE = 0.321 which is again smaller than the results for single compounds. A portion of this improvement is due to the fact that the CTLBBs are calculated from the observed NLC50s for dark exposure. This removes the error associated with predicting the CTLBB from the NTLM.

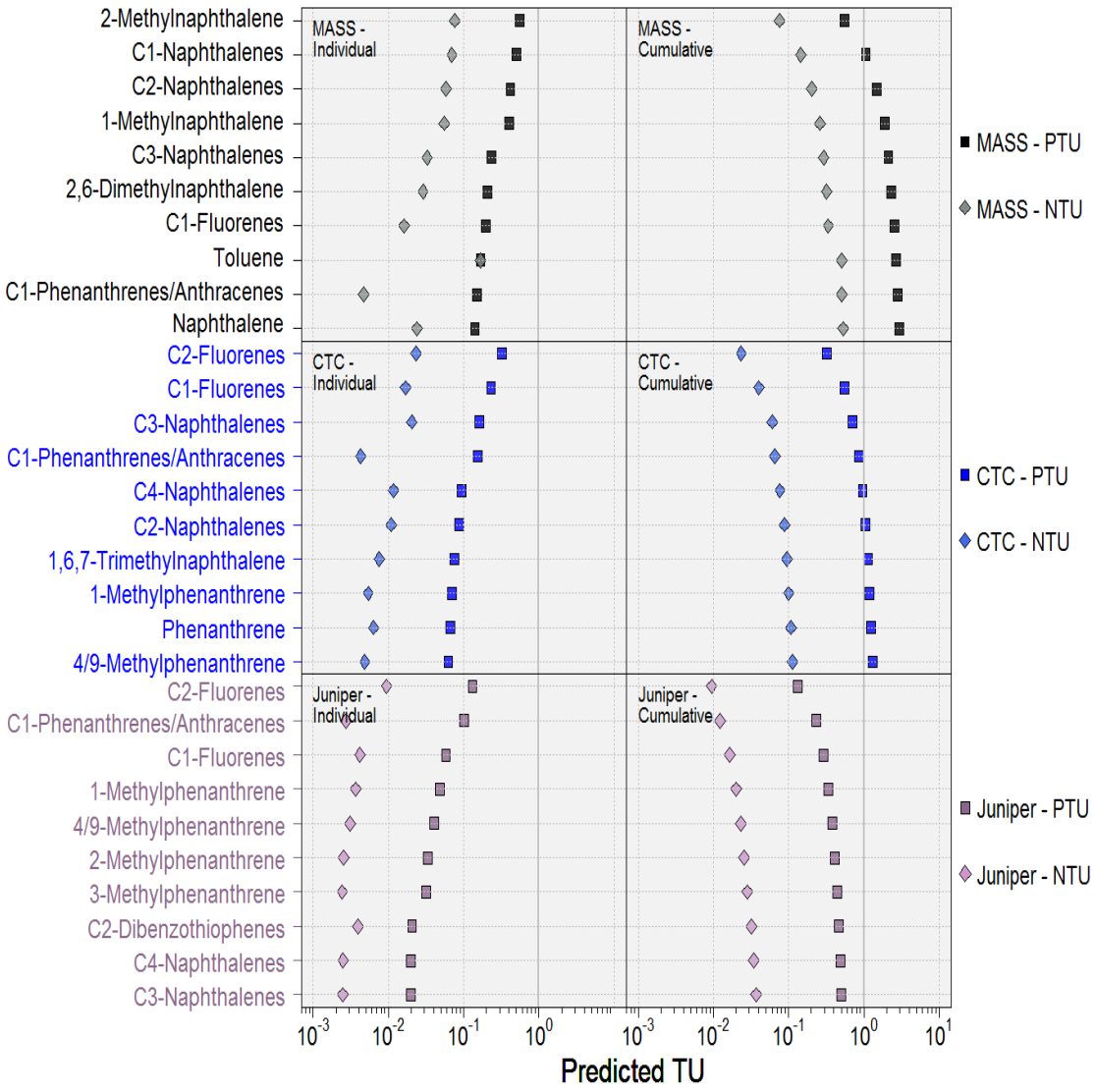

Figure 4-4. Predicted narcotic toxic units (NTU) and phototoxic units (PTU) for the top 10 phototoxic components of MASS, CTC, and Juniper oils ordered from high PTU to low PTU. Left and right panels show individual and cumulative toxic units for narcotic and phototoxic effects, respectively. C1-PAH, C2-PAH, and C3-PAH indicate degree of alkyl substitution (see text for details). The solid verical lines indicate TU = 1.

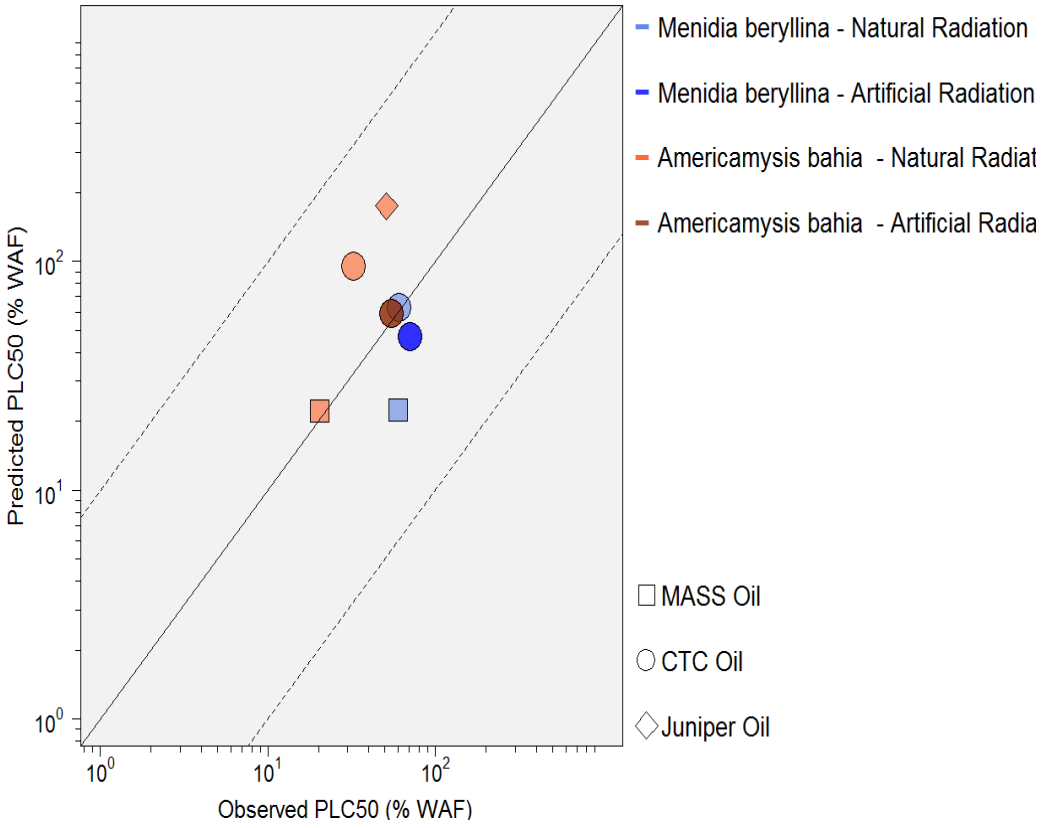

Figure 4-5. Predicted vs. experimental PLC50s (%WAF). Solid line represents 1:1 agreement, dashed lines represent ± an order of magnitude errors. RMSE = 0.321. Three types of oil, MASS (neat), CTC (moderately weathered) and Juniper (heavily weathered) are shown with different symbols described in the legend. The test organisms are identified by the color listed in the legend.

A comprehensive comparison between the observations and predictions for petroleum narcotic toxicity and phototoxicity are presented in Figure 4-6. The associated data are provided in Tables B.5 and B.6. The predictions of narcotic toxicity agree with the observations for CTC and Juniper, which were not narcotically toxic. MASS was narcoticly toxic to the organisms *M. beryllina* and *A. bahia* and was predicted to be either toxic or very close to toxic. (Table B.5).

Natural and artificial sources of light were observed to cause increase in toxicity of all three oils. The cases for which the LC50 was less than 100% are compared in Figure 4-5. Only one miss prediction occurred: Jupiter WAF exposed to *A. bahia* was observed to be toxic but predicted to be non-toxic (the prediction was that the LC50 was >100% WAF).

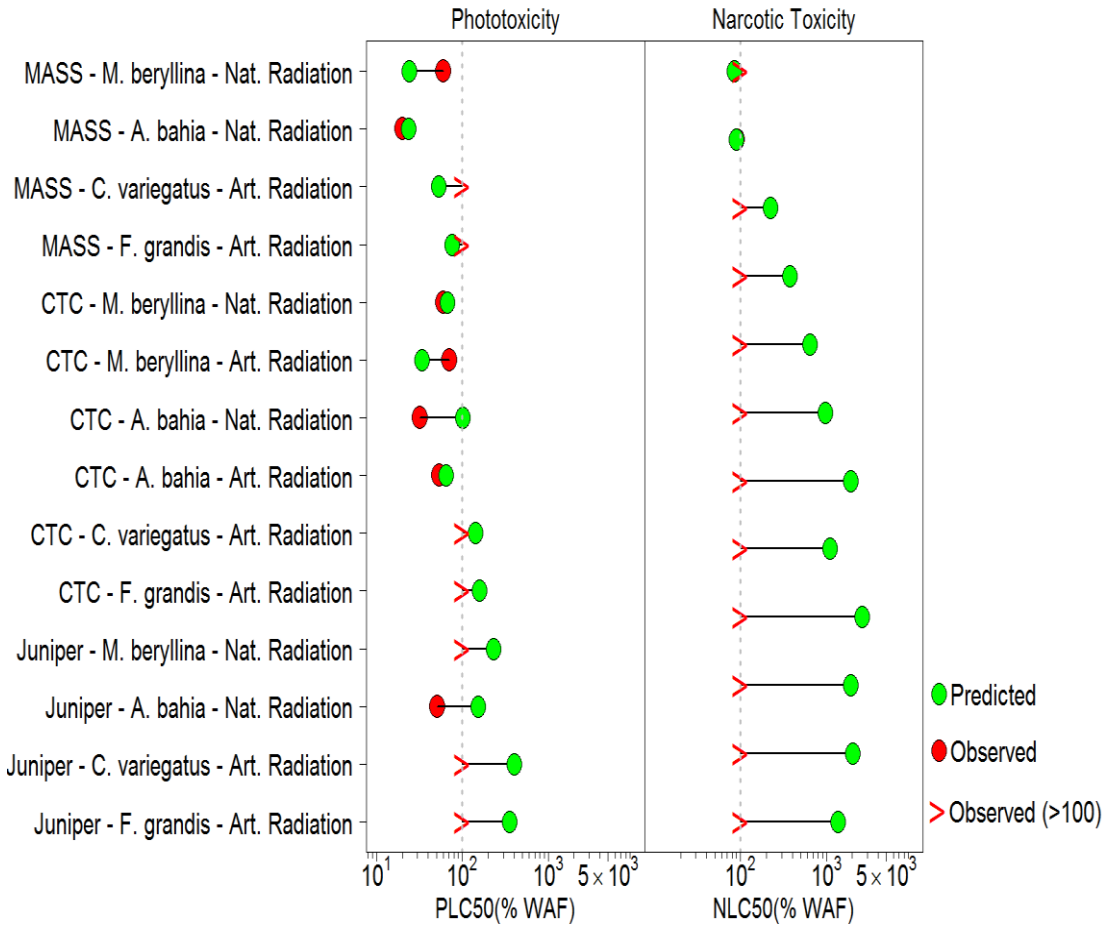

Figure 4-6. Dot plots comparing the predictions to the observations for phototoxicity (left panel) and narcotic toxicity (right panels). The organisms and the oil types are shown on y-axis and the x-axes show the corresponding PLC50s and NLC50s in terms of %WAF. Green and red dots represent the predicted and observed values, respectively. The quantities reported as ">100%" are indicated as ">" and plotted at 100%. These are the cases for which less than 50% mortality was observed. *Americamysis bahia*, *Menidia beryllina*, *Cyprinodon variegatus*, and *Fundulus grandis* are abbreviations for *A. bahia*, *M. beryllina*, *C. variegatus*, and *F. grandis.* Nat. and Art. Radiation on the y-axis indicate natural and solar radiation, respectively.

4.7 Conclusions

The PTLM that was calibrated in the previous chapter with 20 single unsubstituted PAHs and 15 species, was utilized in this chapter to predict the phototoxicity of individual alkylated PAHs (APAHs) and other phototoxic chemicals including dibenzothiophene and acridine. The RMSE = 0.478 obtained for 12 chemicals and four species is comparable to the RMSE = 0.416 for the PAHs analyzed in Chapter 3. This result suggests that the PTLM can predict the phototoxicity of the alkylated components of petroleum without further experimental data.

The comparison of predicted and observed PTUs for *A. bahia* and *M. beryllina* exposed to binary and ternary mixtures of pyrene, anthracene, and fluoranthene, resulted in RMSE = 0.274, suggesting that the PTLM can successfully predict the toxicity of mixtures. The RMSE = 0.321 for predicted phototoxicity of MASS, CTC, and Juniper samples of neat and weathered Macondo crude oil when both observed and predicted LC50s were <100% WAF dilutions. For the cases when either predicted or observed LC50 was >100%, the results were correctly predicted for 13 of the 14 cases for narcotic toxicity, and for 11 of the 14 cases for phototoxicity. In summary, the PTLM appears to have the same predictive ability for mixtures as it does for single compounds. This supports the use of toxic unit additions as the model for assessing the toxicity of PAH mixtures for phototoxicity.

Chapter 5

CONCLUSIONS & RECOMMENDATIONS

In this doctoral dissertation, a phototoxic target lipid model (PTLM) is developed to predict phototoxicity of single PAHs. The model can predict the phototoxicity in terms of median lethal concentration (LC50) or median lethal time (LT50). The model is based on the narcotic target lipid model (NTLM) of PAHs. Both models rely on the assumption that mortality occurs when the toxicant concentration in the target lipid of the organism reaches a critical concentration. The PTLM predicts phototoxicity as a function of the narcotic toxicity and moles of photons absorbed per mole of chemical in the target lipid. The model has two fitting parameters that apply to all chemicals and species, as well as light exposure types, intensities, and duration of exposure. The PTLM accounts for the differences in species sensitivities by predicting the increase in toxicity relative to that predicted by the NTLM for each species. The NTLM species dependent parameter is the critical target lipid body burden. The PTLM has no additional species dependent parameters. The chemical properties required are the molar absorption coefficient for the PTLM and the octanol-water partition coefficient for the NTLM.

Validation of the PTLM is performed using 333 experimental LC50 and LT50 data comprising 20 PAHs and 15 test species, including arthropods, fishes, amphibians, annelids, mollusks, and algae, with simulated solar and various UV light sources for exposure times spanning from less than 1 hour to 100 hours. The root mean square error of prediction for log(LC50) and log(LT50) are 0.473 and 0.382,

respectively. The results demonstrate that the PTLM can predict the phototoxicity of single PAHs over a wide range of exposure conditions and to a broad selection of organisms. Analysis of the residuals indicate that the model prediction is not biased with respect to species sensitivity, octanol-water partition coefficient of chemicals, or light exposure duration and intensity.

The applicability of the PTLM to predict the phototoxicity of other phototoxic components of petroleum is examined using alkalyted PAHs and phototoxic compounds other than PAHs, including dibenzothiophene and acridine. The comparison between the the PTLM predictions and the observations have an RMSE = 0.478 that is comparable to the RMSE = 0.416 for unsubstituted PAHs.

The prediction of the phototoxicity of petroleum mixtures utilized the toxic unit approach which is also used in the NTLM. The method is applied to binary and ternary mixtures of three PAHs, pyrene, anthracene, and fluoranthene exposed to *Americamysis bahia*, *Menidia beryllina* under simulated solar radiation. The PTUs predicted with the method are compared to the experimental PTUs for the binary and ternary mixtures resulting in RMSE = 0.274. These observations support the applicability of toxic unit additions for mixture phototoxicity prediction.

These mixture studies were followed by predicting the phototoxicity for water accommodated fractions (WAFs) of Macondo crude oil samples collected during the Deep Water Horizon oil spill. Three field collected oils were tested: MASS (neat), CTC (moderately weathered), and Juniper (heavily weathered). The RMSE = 0.321 for predicted phototoxicity of MASS, CTC, and Juniper samples of neat and weathered Macondo crude oil when both observed and predicted LC50s were <100% WAF dilutions. For the cases when either predicted or observed LC50 was >100% the

results were correctly predicted for 13 of the 14 cases for narcotic toxicity, and for 11 of the 14 cases for phototoxicity.

The results discussed above suggest that PTLM is capable of predicting phototoxicity of PAHs and other phototoxic components of petroleum to a wide range of aquatic organisms under various illumination conditions. However, there remain interesting and unanswered questions.

(1) In the PTLM formulation, the toxicity decreases not as the unity exponent of the logarithm of the photon dose as was expected, but rather at a considerably slower rate with an exponent $a = 0.426 \pm 0.037$. The mechanism responsible for this nonlinear dependence on the dose metric is an interesting and important question.

(2) The PTLM predicts continuous decrease in the PLC50 as the exposure time increases (Equation 2-28). Analysis of the residuals versus the exposure time did not indicate the PTLM breakdown at $T_{\exp}$ ranging from less than1 (h) to 100 (h). However, this cannot be true indefinitely since as the duration of light exposure continues to increase the PTLM continues to decrease and the PLC50 decreases to very low concentrations. Clearly this decrease cannot continue indefinitely. This suggests that another mechanism, perhaps a repair mechanism is operating. For the available data, the model prediction is not biased relative to the length of light exposure or the magnitude of the light intensity. Therefore, whatever the mechanism is, it is not involved in the short term acute phototoxicity of PAHs. Future work needs to provide some modification for longer exposure times.

(3) The PTLM predicts LC50s and LT50s, for which mortality is the toxic effect. It would be interesting to examine if there are sublethal effect corresponding to longer exposures. The NTLM can predict PAH chronic and sublethal effects using an

acute to chronic ratio. If the same were true for phototoxic effects, it would be an important additional useful tool in assessing the risk of petroleum exposure.

From the regulatory point of view, the PTLM presented in this dissertation would be a critical component of a risk assessment of petroleum in freshwater and marine ecosystems. For application to actual field situations, the risk assessment requires incorporating several large-scale field efforts, including assessing shoreline and wildlife oiling, as well as petroleum constituents and solar radiation intensity attenuation in water column. It would be interesting and useful to apply these factors to which the requisite data are available.

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Appendix A

PHOTOTOXIC TARGET LIPID MODEL OF SINGLE POLYCYCLIC AROMATIC HYDROCARBONS

A1. Experimental Data Used for the PTLM Model Formulation

a. **Table A.1.** General experimental data used to develop the PTLM model.

b. **Table A.2.** Irradiance intensities corresponding to the experimental data in Table A.1.

c. **Table A.3**. Octanol-water partition coefficient, molecular weight, and water solubilities of 20 PAHs of used in PTLM development.

d. **Table A.4**. Assumed critical target lipid body burdens for the species of interest.

e. **Table A5-a.** Molar absorption spectra ($\varepsilon(\lambda)$) at different wavelength λ (nm).

f. **Table A5-b.** Molar absorption spectra ($\varepsilon(\lambda)$) at different wavelength λ (nm).

g. **Table A6-a.** Irradiance spectra ($I(\lambda)$) for the light sources used in the experimental data presented in Table A.1 at 1 (nm) wavelength (λ) intervals.

h. **Table A6-b.** Irradiance spectra ($I(\lambda)$) used by Diamond et al [68].

A.2. Comparison between PAHs Photon Absorption in Solvent Octanol and other Solvents

a. **Figure A.1**. P_{abs} calculated based on PAHs $\varepsilon(\lambda)$ measured in octanol shown on y axis vs. those calculated based on $\varepsilon(\lambda)$ measured in cyclohexane or ethanol (x axis).

A.3. Computational Example

a. **NLC50 calculation**
b. **Light absorption**
c. **Dimensional analysis**
d. **P_{abs} calculation example**
e. **PLC50 calculation**

A.4. Diagnostic Plots

a. **Figure A.2.** Diagnostic plot showing PLC50/NLC50 vs. P_{abs} separated by the chemicals.
b. **Figure A.3.** Diagnostic plot showing PLC50/NLC50 vs. P_{abs} separated by the organisms.
c. **Figure A.4.** Diagnostic plot showing PLC50/NLC50 vs. P_{abs} separated by the references.
d. **Figure A.5.** Diagnostic plot showing PLC50/NLC50 vs. P_{abs} separated by the light sources.

A.5. Residuals Analysis

a. **Figure A.6.** Plot of log of residuals for PLC50 vs. the irradiance (P_{abs}/T_{exp}).

b. **Figure A.7.** Plot of log of residuals for PLC50 vs. P_{abs}

c. **Figure A.8.** Plot of log of residuals for PLC50 vs. T_{exp}

A.1 Experimental Data Used for PTLM Model Formulation.

Table A.1. General experimental data used to develop the PTLM model.

Reference	PLC50 (µg/L)	PAH [a]	Organism [b]	NLC50 (µg/L)	End point	Light source	T_{exp} (h)	P_{abs} (mol photon/mol chem)
[69]	46.000	FLA	*M. liliana*	153.000[c]	96 h EC50	Ultra-Vitalux lamp	1.000	67.639
[37]	2.523	BaP	*S. capricornutum*	14.459	96 h LC50[g]	Black light	16.000	61.342
[37]	2.782	BaP	*S. capricornutum*	14.459	96 h LC50 [g]	Cool-White light	16.000	4.257
[38]	14.500	ANT	*S. capricornutum*	566.101	96 h LC50 [g]	GE F40 BLB blacklight	4.000	159.322
[38]	22.600	ANT	*S. capricornutum*	566.101	96 h LC50 [g]	GE F40 BLB blacklight	4.000	84.555
[38]	30.100	ANT	*S. capricornutum*	566.101	96 h LC50 [g]	GE F40 BLB blacklight	4.000	45.401
[38]	27.800	ANT	*S. capricornutum*	566.101	96 h LC50 [g]	GE F40 BLB blacklight	4.000	26.033
[38]	3.600	ANT	*S. capricornutum*	566.101	96 h LC50 [g]	GE F40 BLB blacklight	28.000	1115.251
[38]	6.400	ANT	*S. capricornutum*	566.101	96 h LC50 [g]	GE F40 BLB blacklight	28.000	591.885
[38]	12.200	ANT	*S. capricornutum*	566.101	96 h LC50 [g]	GE F40 BLB blacklight	28.000	317.810
[38]	16.100	ANT	*S. capricornutum*	566.101	96 h LC50 [g]	GE F40 BLB blacklight	28.000	182.230
[36]	3.985	FLA	*D. magna*	143.903	48 h EC50	SSR II[d]	32.000	229.066
[36]	11.373	FLA	*D. magna*	143.903	48 h EC50	SSR II[d] – UVB Filtered	32.000	207.401
[36]	0.981	BaP	*D. magna*	12.975	48 h EC50	SSR II[d]	32.000	1361.739

[36]	1.625	BaP	*D. magna*	12.975	48 h EC50	SSR II[d] – UVB Filtered	32.000	1300.725
[36]	11.191	ANT	*D. magna*	507.986	48 h EC50	SSR II[d]	32.000	220.018
[36]	19.696	ANT	*D. magna*	507.986	48 h EC50	SSR II[d] – UVB Filtered	32.000	222.474
[36]	4.581	PYR	*D. magna*	165.19	48 h EC50	SSR II[d]	32.000	225.859
[36]	4.328	PYR	*D. magna*	165.186	48 h EC50	SSR II[d] – UVB Filtered	32.000	110.317
[36]	0.959	BaA	*D. magna*	49.216	48 h EC50	SSR II[d]	32.000	197.869
[36]	1.482	BaA	*D. magna*	49.216	48 h EC50	SSR II[d] – UVB Filtered	32.000	163.827
[36]	0.295	DaA	*D. magna*	3.033	48 h EC50	SSR II[d]	32.000	348.207
[36]	0.295	DaA	*D. magna*	3.033	48 h EC50	SSR II[d] – UVB Filtered	32.000	203.063
[36]	3.972	CHR	*D. magna*	45.346	48 h EC50	SSR II[d]	32.000	74.373
[36]	19.375	CHR	*D. magna*	45.346	48 h EC50	SSR II[d] – UVB Filtered	32.000	16.311
[36]	2842.020	FLU	*D. magna*	1787.109	48 h EC50	SSR II[d]	32.000	5.217
[36]	1787.109	FLU	*D. magna*	1787.109	48 h EC50	SSR II[d] – UVB Filtered	32.000	0.000
[36]	477.656	PHE	*D. magna*	468.120	48 h EC50	SSR II[d]	32.000	4.567
[36]	699.219	PHE	*D. magna*	468.120	48 h EC50	SSR II[d] – UVB Filtered	32.000	1.792
[36]	2.329	BbA	*D. magna*	49.216	48 h EC50	SSR II[d]	32.000	674.984
[36]	3.445	BbA	*D. magna*	49.216	48 h EC50	SSR II[d] – UVB Filtered	32.000	614.501
[36]	8.911	BbFU	*D. magna*	111.371	48 h EC50	SSR II[d]	32.000	114.873
[36]	77.372	BbFU	*D. magna*	111.371	48 h EC50	SSR II[d] – UVB Filtered	32.000	32.320
[36]	0.325	BeP	*D. magna*	11.954	48 h EC50	SSR II[d]	32.000	247.265
[36]	1.428	BeP	*D. magna*	11.954	48 h EC50	SSR II[d] – UVB Filtered	32.000	119.201
[36]	0.645	BgP	*D. magna*	5.083	48 h EC50	SSR II[d]	32.000	888.704

[36]	0.133	BgP	*D. magna*	5.083	48 h EC50	SSR II[d] – UVB Filtered	32.000	798.651
[12]	26.470	ANT	*L. macrochirus*	576.570	96 h LC50	SSR I[e]	8.000	6.962
[12]	18.230	ANT	*L. macrochirus*	576.570	96 h LC50	SSR I[e]	8.000	32.928
[12]	11.920	ANT	*L. macrochirus*	576.570	96 h LC50	SSR I[e]	8.000	79.969
[12]	2.780	ANT	*L. macrochirus*	576.570	96 h LC50	SSR I[e]	8.000	6.962
[34]	1.600	FLA	*D. magna*	143.903	48 h LC50	Qpanel	24.000	621.464
[34]	7.700	FLA	*O. mykiss*	82.427	96 h LC50	Qpanel	48.000	1242.928
[34]	12.200	FLA	*P. promelas*	152.430	96 h LC50	Qpanel	48.000	1242.928
[34]	12.300	FLA	*L. macrochirus*	163.332	96 h LC50	Qpanel	48.000	1242.928
[34]	1.400	FLA	*M. bahia*	42.763	96 h LC50	Qpanel	48.000	2080.254
[34]	30.000	FLA	*M. beryllina*	363.974	96 h LC50	Qpanel	48.000	2080.254
[34]	117.903	FLA	*C. variegatus*	141.602	96 h LC50	Qpanel	48.000	2080.254
[34]	58.000	FLA	*M. bahia*	42.763	96 h LC50	Qpanel	48.000	22.450
[34]	12.000	FLA	*M. bahia*	42.763	96 h LC50	Qpanel	48.000	205.261
[34]	12.000	FLA	*M. bahia*	42.763	96 h LC50	Qpanel	48.000	1154.593
[34]	2.800	FLA	*M. bahia*	42.763	96 h LC50	Qpanel	48.000	2168.069
[34]	1.700	FLA	*M. bahia*	42.763	96 h LC50	Qpanel	48.000	5734.480
[34]	117.903	FLA	*M. beryllina*	363.974	96 h LC50	Qpanel	48.000	22.450
[34]	103.000	FLA	*M. beryllina*	363.974	96 h LC50	Qpanel	48.000	205.261
[34]	49.000	FLA	*M. beryllina*	363.974	96 h LC50	Qpanel	48.000	1154.593
[34]	30.000	FLA	*M. beryllina*	363.974	96 h LC50	Qpanel	48.000	2168.069
[34]	13.000	FLA	*M. beryllina*	363.974	96 h LC50	Qpanel	48.000	5734.480

[34]	1.090	FLA	*M. lateralis*	127.858	48 h LC50	Qpanel	32.000	604.182
[34]	5.320	FLA	*M. bahia*	42.763	48 h LC50	Qpanel	32.00	604.182
[34]	1.800	FLA	*M. lateralis*	127.858	96 h LC50	Qpanel	64.00	1208.365
[34]	6.470	ANT	*M. lateralis*	451.348	48 h LC50	Qpanel	32.00	434.140
[34]	3.600	ANT	*M. bahia*	150.956	48 h LC50	Qpanel	32.000	434.140
[34]	68.900	ANT	*M. lateralis*	451.348	96 h LC50	Qpanel	64.000	868.280
[34]	0.230	PYR	*M. lateralis*	146.769	48 h LC50	Qpanel	32.000	2400.849
[34]	0.890	PYR	*M. bahia*	49.088	48 h LC50	Qpanel	32.000	2400.849
[34]	1.680	PYR	*M. lateralis*	146.769	96 h LC50	Qpanel	64.000	4801.699
[71]	0.970	FLA	*M. bahia*	32.20	48 h EC50	SolarConstant 1200	12.000	430.072
[71]	1.090	FLA	*M. bahia*	32.20	48 h EC50	SolarConstant 1200	12.000	427.132
[71]	0.990	FLA	*M. bahia*	32.20	48 h EC50	SolarConstant 1200	12.000	452.894
[71]	1.400	FLA	*M. bahia*	32.20	48 h EC50	SolarConstant 1200	12.000	475.779
[71]	1.340	FLA	*M. beryllina*	363.974	48 h EC50	SolarConstant 1200	12.000	486.804
[71]	1.600	FLA	*M. beryllina*	363.974	48 h EC50	SolarConstant 1200	12.000	485.967
[71]	2.020	FLA	*M. beryllina*	363.974	48 h EC50	SolarConstant 1200	12.000	522.160
[71]	3.670	FLA	*M. beryllina*	363.974	48 h EC50	SolarConstant 1200	12.000	519.862
[71]	2.680	FLA	*C. variegatus*	141.602	48 h EC50	SolarConstant 1200	12.000	458.064
[71]	3.170	FLA	*C. variegatus*	141.602	48 h EC50	SolarConstant 1200	12.000	594.398
[71]	5.040	FLA	*C. variegatus*	141.602	48 h EC50	SolarConstant 1200	12.000	642.667
[71]	8.300	FLA	*C. variegatus*	141.602	48 h EC50	SolarConstant 1200	12.000	678.533
[71]	7.390	FLA	*C. variegatus*	141.602	48 h EC50	SolarConstant 1200	12.000	629.110

[71]	5.340	FLA	*F. grandis*	132.456	48 h EC50	SolarConstant 1200	12.000	562.182
[71]	5.670	FLA	*F. grandis*	132.456	48 h EC50	SolarConstant 1200	12.000	655.649
[71]	10.300	FLA	*F. grandis*	132.456	48 h EC50	SolarConstant 1200	12.000	476.086
[71]	12.500	FLA	*F. grandis*	132.456	48 h EC50	SolarConstant 1200	12.000	469.121
[71]	0.952	ANT	*M. bahia*	150.956	48 h EC50	SolarConstant 1200	12.000	657.316
[71]	2.607	ANT	*M. beryllina*	1284.848	48 h EC50	SolarConstant 1200	12.000	610.511
[71]	0.603	PYR	*M. bahia*	49.088	48 h EC50	SolarConstant 1200	12.000	366.627
[71]	1.248	PYR	*M. beryllina*	417.805	48 h EC50	SolarConstant 1200	12.000	363.901
[71]	1.070	FLA	*M. bahia*	42.763	48 h EC50	SolarConstant 1200	12.000	491.446
[71]	0.620	ANT	*M. bahia*	150.956	48 h EC50	SolarConstant 1200	12.000	517.273
[71]	0.600	PYR	*M. bahia*	49.088	48 h EC50	SolarConstant 1200	12.000	366.979
[71]	0.060	BaP	*M. bahia*	3.856	48 h EC50	SolarConstant 1200	12.000	17528.155
[71]	0.210	BaA	*M. bahia*	14.625	48 h EC50	SolarConstant 1200	12.000	282.730
[71]	0.295	DaA	*M. bahia*	0.901	48 h EC50	SolarConstant 1200	12.000	460.429
[71]	7.570	CHR	*M. bahia*	13.475	48 h EC50	SolarConstant 1200	12.000	93.490
[71]	22.800	PHE	*M. bahia*	139.109	48 h EC50	SolarConstant 1200	12.000	6.333
[71]	1415.000	NAP	*M. bahia*	1750.806	48 h EC50	SolarConstant 1200	12.000	1.389
[71]	111.300	FLU	*M. bahia*	531.069	48 h EC50	SolarConstant 1200	12.000	3.004
[35]	3.355	FLA	*D. magna*	143.903	24 h LC50	Qpanel	2.000	37.083
[35]	0.719	BaP	*D. magna*	12.975	24 h LC50	Qpanel	2.000	92.512
[35]	3.958	ANT	*D. magna*	507.986	24 h LC50	Qpanel	2.000	34.561
[35]	0.928	PYR	*D. magna*	165.186	24 h LC50	Qpanel	2.000	44.519

[35]	2.177	BaA	*D. magna*	49.216	24 h LC50	Qpanel	2.000	33.662
[35]	0.295	DaA	*D. magna*	3.033	24 h LC50	Qpanel	2.000	53.841
[35]	NT	CHR	*D. magna*	45.346	24 h LC50	Qpanel	2.000	37.083
[35]	NT	FLU	*D. magna*	1787.109	24 h LC50	Qpanel	2.000	0.000
[35]	263.672	PHE	*D. magna*	468.117	24 h LC50	Qpanel	2.000	0.517
[35]	NT	NAP	*D. magna*	5891.666	24 h LC50	Qpanel	2.000	0.007
[35]	0.645	BgP	*D. magna*	5.083	24 h LC50	Qpanel	2.000	72.584
[35]	1854.832	ACN	*D. magna*	1854.832	24 h LC50	Qpanel	2.000	0.4593
[34]	23.435	FLA	*D. magna*	143.903	24 h LC50	Qpanel	2.000	32.072
[34]	2.782	BaP	*D. magna*	12.975	24 h LC50	Qpanel	2.000	80.010
[34]	3.833	PYR	*D. magna*	165.186	24 h LC50	Qpanel	2.000	38.503
[34]	0.295	DaA	*D. magna*	3.033	24 h LC50	Qpanel	2.000	46.565
[34]	2.613	BbF	*D. magna*	15.024	24 h LC50	Qpanel	2.000	52.197
[72]	5.000	FLA	*P. promelas*	152.430	LT50	SSR I[e]	40.800	192.751
[72]	15.000	FLA	*P. promelas*	152.430	LT50	SSR I[e]	14.100	66.613
[70]	60.678	FLA	*D. magna*	143.90	ET50	SSR II[d]	1.580	10.963
[70]	2.782	BaP	*D. magna*	12.98	ET50	SSR II[d]	2.457	60.394
[70]	53.460	ANT	*D. magna*	507.99	ET50	SSR II[d]	2.893	19.340
[70]	60.678	PYR	*D. magna*	165.19	ET50	SSR II[d]	2.022	14.269
[70]	21.927	BaA	*D. magna*	49.22	ET50	SSR II[d]	3.065	18.952
[70]	0.295	DaA	*D. magna*	3.03	ET50	SSR II[d]	7.093	77.186
[70]	19.375	CHR	*D. magna*	45.35	ET50	SSR II[d]	12.738	29.606

[70]	21.927	BbA	*D. magna*	143.903	ET50	SSR II[d]	6.158	7.151
[70]	64.883	BbFU	*D. magna*	12.975	ET50	SSR II[d]	12.125	43.526
[70]	2.458	BgP	*D. magna*	507.986	ET50	SSR II[d]	1.937	14.329
[70]	0.645	BgP	*D. magna*	165.186	ET50	SSR II[d]	7.575	160.603
[70]	3.066	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	269.713	2696.072
[70]	9.310	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	125.292	515.705
[70]	9.461	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	115.380	1153.351
[70]	13.583	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	485.510	422.514
[70]	13.603	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	126.853	522.133
[70]	13.624	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	65.467	654.412
[70]	18.932	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	100.512	87.470
[70]	19.012	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	50.265	206.891
[70]	19.123	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	66.778	667.516
[70]	28.751	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	94.061	81.856
[70]	28.806	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	53.395	219.777
[12]	28.885	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	50.556	505.361
[12]	1.500	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	66.570	9052.633
[10]	7.000	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	37.830	5144.376
[12]	22.000	ANT	*L. macrochirus*	576.570	LT50	SSR I[e]	10.450	1421.061
[4]	2.782	BaP	*P. promelas*	13.744	LT50	SSR I[e]	40.050	639.995
[4]	5.400	ANT	*P. promelas*	538.086	LT50	SSR I[e]	15.750	61.958
[4]	25.600	PYR	*P. promelas*	174.974	LT50	SSR I[e]	3.200	2.162

[4]	1.800	BaA	*P. promelas*	52.133	LT50	SSR I^{e}	65.090	167.614
[4]	49.500	BAN	*P. promelas*	393.620	LT50	SSR I^{e}	0.830	5.671
[4]	1.451	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	101.578	499.850
[4]	1.731	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	133.555	657.204
[4]	2.620	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	92.460	454.981
[4]	2.667	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	86.359	424.960
[4]	3.182	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	104.641	514.923
[4]	4.258	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	76.532	376.603
[4]	4.305	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	95.242	468.670
[4]	5.475	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	52.287	257.298
[4]	5.522	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	59.134	290.989
[4]	6.832	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	46.323	227.947
[4]	10.201	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	16.249	79.959
[4]	10.248	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	17.399	85.619
[4]	11.745	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	62.992	309.974
[4]	12.728	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	106.021	521.714
[4]	14.178	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	19.514	96.026
[4]	17.033	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	5.886	28.962
[4]	21.899	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	17.680	86.999
[4]	22.133	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	3.249	15.986
[4]	29.854	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	2.675	13.162
[4]	33.223	FLA	*P. promelas*	152.430	LT50	SSR I^{e}	7.287	35.857

[13]	17.632	FLA	*L. variegatus*	547.181	LT50	Qpanel	88.0277	147.777
[13]	10.695	FLA	*L. variegatus*	547.181	LT50	Qpanel	62.2128	234.445
[13]	53.092	FLA	*L. variegatus*	547.181	LT50	Qpanel	41.2417	34.307
[13]	55.409	FLA	*L. variegatus*	547.181	LT50	Qpanel	33.2486	27.658
[13]	34.141	FLA	*L. variegatus*	547.181	LT50	Qpanel	37.1373	62.344
[13]	17.781	FLA	*L. variegatus*	547.181	LT50	Qpanel	23.6081	88.966
[13]	40.441	FLA	*L. variegatus*	547.181	LT50	Qpanel	18.6221	31.262
[13]	19.989	FLA	*L. variegatus*	547.181	LT50	Qpanel	18.2644	68.828
[13]	106.484	FLA	*L. variegatus*	547.181	LT50	Qpanel	61.751	51.368
[13]	53.272	FLA	*L. variegatus*	547.181	LT50	Qpanel	28.3768	47.638
[13]	112.689	FLA	*L. variegatus*	547.181	LT50	Qpanel	22.6283	18.824
[13]	60.539	FLA	*L. variegatus*	547.181	LT50	Qpanel	51.0072	85.629
[13]	117.903	FLA	*L. variegatus*	547.181	LT50	Qpanel	38.6106	32.119
[13]	40.571	FLA	*L. variegatus*	547.181	LT50	Qpanel	37.0818	139.740
[13]	107.117	FLA	*L. variegatus*	547.181	LT50	Qpanel	22.5923	37.927
[13]	112.256	FLA	*L. variegatus*	547.181	LT50	Qpanel	16.6132	27.890
[13]	53.329	FLA	*L. variegatus*	547.181	LT50	Qpanel	14.7323	55.518
[13]	60.548	FLA	*L. variegatus*	547.181	LT50	Qpanel	17.0308	64.179
[13]	106.012	FLA	*L. variegatus*	547.181	LT50	Qpanel	11.3574	42.800
[13]	112.515	FLA	*L. variegatus*	547.181	LT50	Qpanel	10.0437	37.849
[14]	36.928	ANT	*L. variegatus*	1931.580	LT50	Qpanel	64.5231	50.024
[14]	18.591	ANT	*L. variegatus*	1931.580	LT50	Qpanel	72.0892	112.790

[14]	38.533	ANT	*L. variegatus*	1931.580	LT50	Qpanel	62.281	48.286
[14]	19.921	ANT	*L. variegatus*	1931.580	LT50	Qpanel	69.803	109.213
[14]	9.641	ANT	*L. variegatus*	1931.580	LT50	Qpanel	35.878	126.009
[14]	10.385	ANT	*L. variegatus*	1931.580	LT50	Qpanel	36.4158	127.898
[14]	37.917	ANT	*L. variegatus*	1931.580	LT50	Qpanel	26.9708	42.198
[14]	39.155	ANT	*L. variegatus*	1931.580	LT50	Qpanel	18.2173	28.503
[14]	18.840	ANT	*L. variegatus*	1931.580	LT50	Qpanel	17.4474	61.278
[14]	20.028	ANT	*L. variegatus*	1931.580	LT50	Qpanel	16.9859	59.657
[14]	38.102	ANT	*L. variegatus*	1931.580	LT50	Qpanel	13.4364	47.191
[14]	39.548	ANT	*L. variegatus*	1931.580	LT50	Qpanel	12.1354	42.622
[14]	5.891	PYR	*L. variegatus*	628.109	LT50	Qpanel	94.4578	190.381
[14]	17.151	PYR	*L. variegatus*	628.109	LT50	Qpanel	69.3516	69.264
[14]	10.636	PYR	*L. variegatus*	628.109	LT50	Qpanel	31.6287	63.748
[14]	11.228	PYR	*L. variegatus*	628.109	LT50	Qpanel	29.6764	59.813
[14]	5.931	PYR	*L. variegatus*	628.109	LT50	Qpanel	22.2811	100.808
[14]	27.708	PYR	*L. variegatus*	628.109	LT50	Qpanel	46.522	46.463
[14]	33.998	PYR	*L. variegatus*	628.109	LT50	Qpanel	42.9206	42.866
[14]	17.612	PYR	*L. variegatus*	628.109	LT50	Qpanel	38.3301	77.255
[14]	39.378	PYR	*L. variegatus*	628.109	LT50	Qpanel	30.3051	30.267
[14]	10.748	PYR	*L. variegatus*	628.109	LT50	Qpanel	16.1152	72.911
[14]	11.354	PYR	*L. variegatus*	628.109	LT50	Qpanel	16.0892	72.794
[14]	26.664	PYR	*L. variegatus*	628.109	LT50	Qpanel	23.4213	47.206

[14]	27.905	PYR	*L. variegatus*	628.109	LT50	Qpanel	23.1011	46.561
[14]	59.585	PYR	*L. variegatus*	628.109	LT50	Qpanel	26.8813	26.847
[14]	34.443	PYR	*L. variegatus*	628.109	LT50	Qpanel	24.1277	48.630
[14]	39.499	PYR	*L. variegatus*	628.109	LT50	Qpanel	15.8169	31.879
[14]	17.630	PYR	*L. variegatus*	628.109	LT50	Qpanel	12.3877	56.047
[14]	54.373	PYR	*L. variegatus*	628.109	LT50	Qpanel	15.7988	31.843
[14]	60.511	PYR	*L. variegatus*	628.109	LT50	Qpanel	18.8966	38.086
[14]	28.051	PYR	*L. variegatus*	628.109	LT50	Qpanel	11.0174	49.847
[14]	34.908	PYR	*L. variegatus*	628.109	LT50	Qpanel	10.5461	47.714
[14]	40.571	PYR	*L. variegatus*	628.109	LT50	Qpanel	10.2418	46.338
[14]	55.729	PYR	*L. variegatus*	628.109	LT50	Qpanel	8.3865	37.944
[14]	61.892	PYR	*L. variegatus*	628.109	LT50	Qpanel	8.29164	37.514
[71]	1.730	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	9.090	325.780
[71]	3.430	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	2.050	73.471
[71]	1.610	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	10.200	363.063
[71]	3.030	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	2.890	102.868
[71]	1.270	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	9.100	343.445
[71]	3.160	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	2.890	109.072
[71]	2.080	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	8.970	355.645
[71]	3.980	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	3.080	122.117
[71]	0.590	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	4.000	548.873
[71]	1.650	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	1.980	271.692

[71]	3.460	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	0.760	104.286
[71]	2.990	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	12.000	458.064
[71]	6.140	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	6.190	236.285
[71]	11.400	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	3.220	122.914
[71]	22.400	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	1.390	53.059
[71]	4.790	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	9.710	480.967
[71]	9.580	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	3.760	186.245
[71]	19.800	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	2.170	107.487
[71]	9.860	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	5.880	314.907
[71]	20.500	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	3.060	163.880
[71]	12.800	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	9.370	529.821
[71]	23.400	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	3.890	219.958
[71]	10.800	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	12.000	629.110
[71]	19.200	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	3.500	183.491
[71]	42.500	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	1.940	101.706
[71]	52.900	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	1.120	58.717
[71]	3.380	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	4.000	895.775
[71]	6.990	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	1.830	409.817
[71]	12.900	FLA	*C. variegatus*	141.602	LT50	SolarConstant 1200	0.900	201.549
[71]	7.320	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	12.000	562.182
[71]	15.400	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	3.240	151.789
[71]	7.020	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	12.000	655.649

[71]	17.500	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	2.960	161.727
[71]	30.400	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	0.810	44.256
[71]	46.800	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	0.500	27.319
[71]	10.500	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	12.000	476.086
[71]	21.600	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	5.400	214.239
[71]	32.000	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	1.190	47.212
[71]	12.600	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	12.000	466.523
[71]	34.000	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	3.280	127.516
[71]	8.720	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	4.000	879.103
[71]	17.300	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	1.530	336.257
[71]	9.310	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	4.000	455.699
[71]	19.800	FLA	*F. grandis*	132.456	LT50	SolarConstant 1200	0.980	111.646
[71]	1.610	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	10.200	417.729
[71]	0.670	ANT	*M. bahia*	150.956	LT50	SolarConstant 1200	12.000	517.273
[71]	0.630	PYR	*M. bahia*	49.088	LT50	SolarConstant 1200	12.000	366.979
[71]	0.090	BaP	*M. bahia*	3.856	LT50	SolarConstant 1200	12.000	17528.155
[71]	0.370	BaA	*M. bahia*	14.625	LT50	SolarConstant 1200	4.470	105.317
[71]	0.295	DaA	*M. bahia*	0.901	LT50	SolarConstant 1200	12.000	460.429
[71]	14.200	CHR	*M. bahia*	13.475	LT50	SolarConstant 1200	12.000	93.490
[71]	3.870	FLA	*M. bahia*	42.763	LT50	SolarConstant 1200	2.890	118.357
[71]	1.160	ANT	*M. bahia*	150.956	LT50	SolarConstant 1200	2.100	90.523
[71]	1.330	PYR	*M. bahia*	49.088	LT50	SolarConstant 1200	3.870	118.351

[71]	0.080	BaP	*M. bahia*	3.856	LT50	SolarConstant 1200	4.260	6222.495
[71]	0.880	BaA	*M. bahia*	14.625	LT50	SolarConstant 1200	1.190	28.037
[71]	19.375	CHR	*M. bahia*	13.475	LT50	SolarConstant 1200	9.720	75.727
[71]	2.100	ANT	*M. bahia*	150.956	LT50	SolarConstant 1200	0.500	21.553
[71]	1.830	BaA	*M. bahia*	14.625	LT50	SolarConstant 1200	0.500	11.780
[71]	3.570	BaA	*M. bahia*	14.625	LT50	SolarConstant 1200	0.500	11.780
[71]	0.370	BaA	*M. bahia*	14.625	LT50	SolarConstant 1200	4.710	110.972
[71]	0.840	BaA	*M. bahia*	14.625	LT50	SolarConstant 1200	0.820	19.320
[68]	39.600	FLA	*A. salina*	242.142	LT50	Qpanel	0.588	54.765
[68]	39.600	FLA	*A. salina*	242.142	LT50	Qpanel	0.903	64.156
[68]	39.600	FLA	*A. salina*	242.142	LT50	Qpanel	1.278	55.892
[68]	39.600	FLA	*A. salina*	242.142	LT50	Qpanel	1.567	42.057
[68]	39.600	FLA	*A. salina*	242.142	LT50	Qpanel	1.352	49.315
[68]	39.600	FLA	*A. salina*	242.142	LT50	Qpanel	0.418	38.940
[68]	39.600	FLA	*A. salina*	242.142	LT50	Qpanel	0.652	28.909
[68]	39.600	FLA	*A. salina*	242.142	LT50	Qpanel	0.825	30.100
[68]	72.600	ANT	*A. salina*	854.775	LT50	Qpanel	0.678	60.780
[68]	72.600	ANT	*A. salina*	854.775	LT50	Qpanel	0.882	60.577
[68]	72.600	ANT	*A. salina*	854.775	LT50	Qpanel	1.200	51.556
[68]	72.600	ANT	*A. salina*	854.775	LT50	Qpanel	1.463	37.855
[68]	72.600	ANT	*A. salina*	854.775	LT50	Qpanel	1.140	45.408
[68]	72.600	ANT	*A. salina*	854.775	LT50	Qpanel	0.553	49.580

[68]	72.600	ANT	*A. salina*	854.775	LT50	Qpanel	1.063	42.970
[68]	72.600	ANT	*A. salina*	854.775	LT50	Qpanel	1.037	41.292
[68]	50.700	PYR	*A. salina*	277.955	LT50	Qpanel	0.220	23.403
[68]	50.700	PYR	*A. salina*	277.955	LT50	Qpanel	0.285	22.084
[68]	50.700	PYR	*A. salina*	277.955	LT50	Qpanel	0.568	24.946
[68]	50.700	PYR	*A. salina*	277.955	LT50	Qpanel	0.563	16.766
[68]	50.700	PYR	*A. salina*	277.955	LT50	Qpanel	0.808	9.415
[68]	50.700	PYR	*A. salina*	277.955	LT50	Qpanel	0.200	21.275
[68]	50.700	PYR	*A. salina*	277.955	LT50	Qpanel	0.303	18.195
[68]	50.700	PYR	*A. salina*	277.955	LT50	Qpanel	0.658	7.668
[73]	25.800	FLA	*P. pugio*	71.461	LT50	SSR I[e]	8.300	18.208
[73]	12.900	FLA	*P. pugio*	71.461	LT50	SSR I[e]	18.900	41.460
[73]	6.500	FLA	*P. pugio*	71.461	LT50	SSR I[e]	48.000	105.296
[73]	3.500	FLA	*P. pugio*	71.461	LT50	SSR I[e]	86.730	190.257
[11]	15.000	ANT	*D. magna*	507.986	LT50	Solar Radiation[f]	4.975	25.591
[11]	1.800	BaA	*D. magna*	49.216	LT50	Solar Radiation[f]	12.510	77.723
[11]	1.500	BAP	*D. magna*	12.975	LT50	Solar Radiation[f]	4.442	95.904
[11]	0.700	CHR	*D. magna*	45.346	LT50	Solar Radiation[f]	23.980	70.053
[11]	0.290	DaA	*D. magna*	3.033	LT50	Solar Radiation[f]	3.083	43.702
[11]	9.000	FLA	*D. magna*	143.903	LT50	Solar Radiation[f]	10.815	55.566
[11]	5.700	PYR	*D. magna*	165.186	LT50	Solar Radiation[f]	3.477	22.968
[11]	35.100	BAN	*D. magna*	371.601	LT50	Solar Radiation[f]	5.383	64.774

[11]	0.600	BbA	*D. magna*	49.216	LT50	Solar Radiation[f]	16.425	44.077
[11]	4.800	BaFU	*D. magna*	111.371	LT50	Solar Radiation[f]	22.945	90.516
[11]	2.200	BbFU	*D. magna*	111.371	LT50	Solar Radiation[f]	22.402	88.372
[11]	0.700	BeP	*D. magna*	11.954	LT50	Solar Radiation[f]	15.263	122.086
[11]	1.400	BkFL	*D. magna*	13.230	LT50	Solar Radiation[f]	13.007	222.644
[11]	0.600	PER	*D. magna*	11.955	LT50	Solar Radiation[f]	18.328	542.640
[11]	0.200	BgP	*D. magna*	5.083	LT50	Solar Radiation[f]	13.815	262.815
[65]	16.790	FLA	*R. abronius*	24.625	10 d LC50	Qpanel	1.000	10.093
[65]	24.952	PYR	*R. abronius*	28.464	10 d LC50	Qpanel	1.000	19.584
[65]	73.317	PNT	*R. abronius*	73.317	10 d LC50	Qpanel	1.000	0.933
[65]	15.700	ACN	*R. abronius*	15.700	10 d LC50	Qpanel	1.000	1.661
[65]	18563.249	NAP	*R. abronius*	18805.378	10 d LC50	Qpanel	1.000	0.583

[a]Abbreviations for polycyclic aromatic hydrocarbons (PAHs): FLA = fluoranthene; ANT = anthracene; PYR = pyrene; BaP = benzo[*a*]pyrene; BaA = benzo[*a*]anthracene; DaA = dibenzo[*a*,*h*]anthracene; CHR = chrysene; BgP = benzo[*g*,*h*,*i*]perylene; BbA = benzo[*b*]anthracene; BeP = benzo[*e*]pyrene; PHE = phenanthrene; NAP = naphthalene.; FLU = fluorene; ACN = acenaphthene; BbFU = benzo[*b*]fluorene; PER = perylene; BAN = bezanthrone; BbFL = benzo[*b*]fluoranthene; BkFL = benzo[*k*]fluoranthene; BaFU = benzo[*a*]fluorene.

[b]Abbreviations for organisms: *M. liliana = Macomona liliana; S. capricornutum = Selenastrum capricornutum; D. magna = Daphnia magna; L. macrochirus = Lepomis macrochirus; M.= Mulinia lateralis; M. bahia = Mysidopsis bahia; O. mykiss = Oncorhynchus mykiss; P. promelas = Pimephales promelas; M. beryllina = Menidia beryllina; C. variegatus = Cyprinodon variegatus; L. variegatus = Lumbriculus variegatus; F. grandis = Fundulus grandis ; A. salina = Artemia salina.; P. pugio = Palaemonetes pugio; R. abronius= Rhepoxynius abronius.*

[c]The CTLBB was not available, the LC50 in the dark control experiment reported by the author [69] was used as the NLC50.

[d]Standard CWF lamps were combined with RPR-3500 (UVA), and RPR-3000A (UVB) lamps (Southern New England Ultraviolet, Branford, CT, USA) to simulate solar radiation.

[e]Simulated solar radiation provided by James T. Oris through personal communication.

[f]A combination of Chroma F40C50 white (General Electric, Cleveland, OH) and FS40 ultraviolet (Westinghouse, Bloomfield, NJ) fluorescent bulbs was used to simulate solar radiation. The associated spectrum was not provided. Accordingly, solar radiation spectral variation was used as the light source spectrum.

[g]Test endpoint associated with inhibition to growth, otherwise survival.

Table A.2. Irradiance intensities corresponding to the experimental data in Table A.1.

Reference	Light source[a]	I_{UVB} ($\mu W/cm^2/nm$)	I_{UVA} ($\mu W/cm^2/nm$)	I_{VIS} ($\mu W/cm^2/nm$)	End point	T_{exp} (h)	Light exposure regime[e]
[69]	Ultra-Vitalux lamp	250	1300	0	96 h EC50	1	Continuous
[37]	Black light	0.037	22.634	0	96 h LC50[d]	16	Periodic
[37]	Cool-White light	0.080	2.719	0	96 h LC50[d]	16	Periodic
[38]	GE F40 BLB blacklight	0	765	0	96 h LC50[d]	4	Continuous
[38]	GE F40 BLB blacklight	0	406	0	96 h LC50[d]	4	Continuous
[38]	GE F40 BLB blacklight	0	218	0	96 h LC50[d]	4	Continuous
[38]	GE F40 BLB blacklight	0	125	0	96 h LC50[d]	4	Continuous
[38]	GE F40 BLB blacklight	0	765	0	96 h LC50[d]	28	Continuous
[38]	GE F40 BLB blacklight	0	406	0	96 h LC50[d]	28	Continuous
[38]	GE F40 BLB blacklight	0	218	0	96 h LC50[d]	28	Continuous
[38]	GE F40 BLB blacklight	0	125	0	96 h LC50[d]	28	Continuous
[36]	SSR II	0.45	4.400	61	48 h EC50	32	Periodic
[36]	SSR II– UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[36]	SSR II	0.45	4.400	61	48 h EC50	32	Periodic
[36]	SSR II – UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[36]	SSR II[a]	0.45	4.400	61	48 h EC50	32	Periodic
[36]	SSR II – UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[36]	SSR II	0.45	4.400	61	48 h EC50	32	Periodic

[36]	SSR II – UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[36]	SSR II	0.450	4.400	61	48 h EC50	32	Periodic
[36]	SSR II – UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[36,86]	SSR II	0.450	4.400	61	48 h EC50	32	Periodic
[36]	SSR II – UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[36]	SSR II	0.450	4.400	61	48 h EC50	32	Periodic
[36]	SSR II – UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[36]	SSR II	0.450	4.400	61	48 h EC50	32	Periodic
[36]	SSR II – UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[36]	SSR II	0.450	4.400	61	48 h EC50	32	Periodic
[36]	SSR II – UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[36]	SSR II	0.450	4.400	61	48 h EC50	32	Periodic
[36]	SSR II – UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[36]	SSR II	0.450	4.400	61	48 h EC50	32	Periodic
[36]	SSR II – UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[36]	SSR II	0.450	4.400	61	48 h EC50	32	Periodic
[36]	SSR II – UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[36]	SSR II	0.450	4.400	61	48 h EC50	32	Periodic
[36]	SSR II – UVB Filtered	0	4.600	56	48 h EC50	32	Periodic
[12]	SSR I	14.8	21.016	0	96 h LC50	8	Continuous
[12]	SSR I	70	99.400	0	96 h LC50	8	Continuous
[12]	SSR I	170	241.400	0	96 h LC50	8	Continuous

[12]	SSR I	14.800	21.016	0	96 h LC50	8	Continuous
[67]	Qpanel	71.5	473	0	48 h LC50	24	Periodic
[67]	Qpanel	71.5	473	0	96 h LC50	48	Periodic
[67]	Qpanel	71.500	473	0	96 h LC50	48	Periodic
[67]	Qpanel	71.500	473	0	96 h LC50	48	Periodic
[67]	Qpanel	88.500	594.500	0	96 h LC50	48	Periodic
[67]	Qpanel	88.500	594.500	0	96 h LC50	48	Periodic
[67]	Qpanel	88.500	594.500	0	96 h LC50	48	Periodic
[67]	Qpanel	0	7	0	96 h LC50	48	Periodic
[67]	Qpanel	0	64	0	96 h LC50	48	Periodic
[67]	Qpanel	0	360	0	96 h LC50	48	Periodic
[67]	Qpanel	0	676	0	96 h LC50	48	Periodic
[67]	Qpanel	0	1788	0	96 h LC50	48	Periodic
[67]	Qpanel	0	7	0	96 h LC50	48	Periodic
[67]	Qpanel	0	64	0	96 h LC50	48	Periodic
[67]	Qpanel	0	360	0	96 h LC50	48	Periodic
[67]	Qpanel	0	676	0	96 h LC50	48	Periodic
[67]	Qpanel	0	1788	0	96 h LC50	48	Periodic
[67]	Qpanel	71.5	473	0	48 h LC50	32.000	Periodic
[67]	Qpanel	71.5	473	0	48 h LC50	32.00	Periodic
[67]	Qpanel	71.5	473	0	96 h LC50	64.00	Periodic
[67]	Qpanel	71.5	473	0	48 h LC50	32.00	Periodic

[67]	Qpanel	88.5	594.5	0	48 h LC50	32.000	Periodic
[67]	Qpanel	88.5	594.5	0	96 h LC50	64.000	Periodic
[67]	Qpanel	88.5	594.5	0	48 h LC50	32.000	Periodic
[67]	Qpanel	0	7	0	48 h LC50	32.000	Periodic
[67]	Qpanel	0	64	0	96 h LC50	64.000	Periodic
[86]	SolarConstant 1200	35.700	778	2820	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	39.400	775	2740	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	32.800	793	3240	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	34.700	795	3720	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	39.500	802	3860	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	33.900	796	3950	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	32.800	803	4720	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	32.800	798	4710	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	30.600	787	3430	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	24.600	805	6420	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	23.200	790	7650	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	25.500	805	8310	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	23.600	784	7390	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	27.100	801	5700	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	25.200	801	7830	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	37.200	813	3550	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	37.200	799	3510	48 h EC50	12.000	Periodic

[86]	SolarConstant 1200	26.600	801	7773	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	29.800	803	6511	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	30.900	800	3970	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	29.900	798	6288	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	30.100	800	4080	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	30.500	803	4080	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	30.100	805	4450	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	28.700	806	4440	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	28.500	805	4450	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	30.500	802	3880	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	37.100	800	4340	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	30.100	806	4060	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	31.000	809	4150	48 h EC50	12.000	Periodic
[86]	SolarConstant 1200	30.100	805	4020	48 h EC50	12.000	Periodic
[35]	Qpanel	0	370	0	24 h LC50	2.000	Continuous
[35]	Qpanel	0	370	0	24 h LC50	2.000	Continuous
[35]	Qpanel	0	370	0	24 h LC50	2.000	Continuous
[35]	Qpanel	0	370	0	24 h LC50	2.000	Continuous
[35]	Qpanel	0	370	0	24 h LC50	2.000	Continuous
[35]	Qpanel	0	370	0	24 h LC50	2.000	Continuous
[35]	Qpanel	0	370	0	24 h LC50	2.000	Continuous
[35]	Qpanel	0	370	0	24 h LC50	2.000	Continuous

[35]	Qpanel	0	370	0	24 h LC50	2.000	Continuous
[35]	Qpanel	0	370	0	24 h LC50	2.000	Continuous
[35]	Qpanel	0	370	0	24 h LC50	2.000	Continuous
[35]	Qpanel	0	370	0	24 h LC50	2.000	Continuous
[34]	Qpanel	0	320	0	24 h LC50	2.000	Continuous
[34]	Qpanel	0	320	0	24 h LC50	2.000	Continuous
[34]	Qpanel	0	320	0	24 h LC50	2.000	Continuous
[34]	Qpanel	0	320	0	24 h LC50	2.000	Continuous
[34]	Qpanel	0	320	0	24 h LC50	2.000	Continuous
[72]	SSR I	2.560	134.600	0	LT50	40.800	Continuous
[72]	SSR I	2.560	134.600	0	LT50	14.100	Continuous
[70]	SSR II	0.45	4.4	61	ET50	1.580	Continuous
[70]	SSR II	0.45	4.4	61	ET50	2.457	Continuous
[70]	SSR II	0.45	4.4	61	ET50	2.893	Continuous
[70]	SSR II	0.45	4.4	61	ET50	2.022	Continuous
[70]	SSR II	0.45	4.4	61	ET50	3.065	Continuous
[70]	SSR II	0.45	4.4	61	ET50	7.093	Continuous
[70]	SSR II	0.45	4.4	61	ET50	12.738	Continuous
[70]	SSR II	0.45	4.4	61	ET50	6.158	Continuous
[70]	SSR II	0.45	4.4	61	ET50	12.125	Continuous
[70]	SSR II	0.45	4.4	61	ET50	1.937	Continuous
[70]	SSR II	0.45	4.4	61	ET50	7.575	Continuous

[12]	SSR I	170	241.4	0	LT50	269.713	Continuous
[12]	SSR I	70	99.4	0	LT50	125.292	Continuous
[12]	SSR I	170	241.4	0	LT50	115.380	Continuous
[12]	SSR I	14.8	21.016	0	LT50	485.510	Continuous
[12]	SSR I	70	99.4	0	LT50	126.853	Continuous
[12]	SSR I	170	241.4	0	LT50	65.467	Continuous
[12]	SSR I	14.8	21.016	0	LT50	100.512	Continuous
[12]	SSR I	70	99.4	0	LT50	50.265	Continuous
[12]	SSR I	170	241.4	0	LT50	66.778	Continuous
[12]	SSR I	14.8	21.016	0	LT50	94.061	Continuous
[12]	SSR I	70	99.4	0	LT50	53.395	Continuous
[12]	SSR I	170	241.4	0	LT50	50.556	Continuous
[12]	SSR I	400	3284	0	LT50	66.570	Continuous
[12]	SSR I	400	3284	0	LT50	37.830	Continuous
[12]	SSR I	400	3284	0	LT50	10.450	Continuous
[4]	SSR I	20	95	0	LT50	40.050	Continuous
[4]	SSR I	20	95	0	LT50	15.750	Continuous
[4]	SSR I	20	95	0	LT50	3.200	Continuous
[4]	SSR I	20	95	0	LT50	65.090	Continuous
[4]	SSR I	20	95	0	LT50	0.830	Continuous
[43]	SSR I	0	140.2	0	LT50	101.578	Continuous
[43]	SSR I	0	140.2	0	LT50	133.555	Continuous

[43]	SSR I	0	140.2	0	LT50	92.460	Continuous
[43]	SSR I	0	140.2	0	LT50	86.359	Continuous
[43]	SSR I	0	140.2	0	LT50	104.641	Continuous
[43]	SSR I	0	140.2	0	LT50	76.532	Continuous
[43]	SSR I	0	140.2	0	LT50	95.242	Continuous
[43]	SSR I	0	140.2	0	LT50	52.287	Continuous
[43]	SSR I	0	140.2	0	LT50	59.134	Continuous
[43]	SSR I	0	140.2	0	LT50	46.323	Continuous
[43]	SSR I	0	140.2	0	LT50	16.249	Continuous
[43]	SSR I	0	140.2	0	LT50	17.399	Continuous
[43]	SSR I	0	140.2	0	LT50	62.992	Continuous
[43]	SSR I	0	140.2	0	LT50	106.021	Continuous
[43]	SSR I	0	140.2	0	LT50	19.514	Continuous
[43]	SSR I	0	140.2	0	LT50	5.886	Continuous
[43]	SSR I	0	140.2	0	LT50	17.680	Continuous
[43]	SSR I	0	140.2	0	LT50	3.249	Continuous
[43]	SSR I	0	140.2	0	LT50	2.675	Continuous
[43]	SSR I	0	140.2	0	LT50	7.287	Continuous
[13]	Qpanel	0	33.5	0	LT50	88.0277	Continuous
[13]	Qpanel	0	75.2	0	LT50	62.2128	Continuous
[13]	Qpanel	0	16.6	0	LT50	41.2417	Continuous
[13]	Qpanel	0	16.6	0	LT50	33.2486	Continuous

[13]	Qpanel	0	33.5	0	LT50	37.1373	Continuous
[13]	Qpanel	0	75.2	0	LT50	23.6081	Continuous
[13]	Qpanel	0	33.5	0	LT50	18.6221	Continuous
[13]	Qpanel	0	75.2	0	LT50	18.2644	Continuous
[13]	Qpanel	0	16.6	0	LT50	61.751	Continuous
[13]	Qpanel	0	33.5	0	LT50	28.3768	Continuous
[13]	Qpanel	0	16.6	0	LT50	22.6283	Continuous
[13]	Qpanel	0	33.5	0	LT50	51.0072	Continuous
[13]	Qpanel	0	16.6	0	LT50	38.6106	Continuous
[13]	Qpanel	0	75.2	0	LT50	37.0818	Continuous
[13]	Qpanel	0	33.5	0	LT50	22.5923	Continuous
[13]	Qpanel	0	33.5	0	LT50	16.6132	Continuous
[13]	Qpanel	0	75.2	0	LT50	14.7323	Continuous
[13]	Qpanel	0	75.2	0	LT50	17.0308	Continuous
[13]	Qpanel	0	75.2	0	LT50	11.3574	Continuous
[13]	Qpanel	0	75.2	0	LT50	10.0437	Continuous
[14]	Qpanel	0	16.6	0	LT50	64.5231	Continuous
[14]	Qpanel	0	33.5	0	LT50	72.0892	Continuous
[14]	Qpanel	0	16.6	0	LT50	62.281	Continuous
[14]	Qpanel	0	33.5	0	LT50	69.803	Continuous
[14]	Qpanel	0	75.2	0	LT50	35.878	Continuous
[14]	Qpanel	0	75.2	0	LT50	36.4158	Continuous

[14]	Qpanel	0	33.5	0	LT50	26.9708	Continuous
[14]	Qpanel	0	33.5	0	LT50	18.2173	Continuous
[14]	Qpanel	0	75.2	0	LT50	17.4474	Continuous
[14]	Qpanel	0	75.2	0	LT50	16.9859	Continuous
[14]	Qpanel	0	75.2	0	LT50	13.4364	Continuous
[14]	Qpanel	0	75.2	0	LT50	12.1354	Continuous
[14]	Qpanel	0	33.5	0	LT50	94.4578	Continuous
[14]	Qpanel	0	16.6	0	LT50	69.3516	Continuous
[14]	Qpanel	0	33.5	0	LT50	31.6287	Continuous
[14]	Qpanel	0	33.5	0	LT50	29.6764	Continuous
[14]	Qpanel	0	75.2	0	LT50	22.2811	Continuous
[14]	Qpanel	0	16.6	0	LT50	46.522	Continuous
[14]	Qpanel	0	16.6	0	LT50	42.9206	Continuous
[14]	Qpanel	0	33.5	0	LT50	38.3301	Continuous
[14]	Qpanel	0	16.6	0	LT50	30.3051	Continuous
[14]	Qpanel	0	75.2	0	LT50	16.1152	Continuous
[14]	Qpanel	0	75.2	0	LT50	16.0892	Continuous
[14]	Qpanel	0	33.5	0	LT50	23.4213	Continuous
[14]	Qpanel	0	33.5	0	LT50	23.1011	Continuous
[14]	Qpanel	0	16.6	0	LT50	26.8813	Continuous
[14]	Qpanel	0	33.5	0	LT50	24.1277	Continuous
[14]	Qpanel	0	33.5	0	LT50	15.8169	Continuous

[14]	Qpanel	0	75.2	0	LT50	12.3877	Continuous
[14]	Qpanel	0	33.5	0	LT50	15.7988	Continuous
[14]	Qpanel	0	33.5	0	LT50	18.8966	Continuous
[14]	Qpanel	0	75.2	0	LT50	11.0174	Continuous
[14]	Qpanel	0	75.2	0	LT50	10.5461	Continuous
[14]	Qpanel	0	75.2	0	LT50	10.2418	Continuous
[14]	Qpanel	0	75.2	0	LT50	8.3865	Continuous
[14]	Qpanel	0	75.2	0	LT50	8.29164	Continuous
[86]	SolarConstant 1200	35.7	778	2820	LT50	9.090	Continuous
[86]	SolarConstant 1200	35.7	778	2820	LT50	2.050	Continuous
[86]	SolarConstant 1200	39.4	775	2740	LT50	10.200	Continuous
[86]	SolarConstant 1200	39.4	775	2740	LT50	2.890	Continuous
[86]	SolarConstant 1200	32.8	793	3240	LT50	9.100	Continuous
[86]	SolarConstant 1200	32.8	793	3240	LT50	2.890	Continuous
[86]	SolarConstant 1200	34.7	795	3720	LT50	8.970	Continuous
[86]	SolarConstant 1200	34.7	795	3720	LT50	3.080	Continuous
[86]	SolarConstant 1200	91.9	2263	17260	LT50	4.000	Continuous
[86]	SolarConstant 1200	91.9	2263	17260	LT50	1.980	Continuous
[86]	SolarConstant 1200	91.9	2263	17260	LT50	0.760	Continuous
[86]	SolarConstant 1200	30.6	787	3430	LT50	12.000	Continuous
[86]	SolarConstant 1200	30.6	787	3430	LT50	6.190	Continuous
[86]	SolarConstant 1200	30.6	787	3430	LT50	3.220	Continuous

[86]	SolarConstant 1200	30.6	787	3430	LT50	1.390	Continuous
[86]	SolarConstant 1200	24.6	805	6420	LT50	9.710	Continuous
[86]	SolarConstant 1200	24.6	805	6420	LT50	3.760	Continuous
[86]	SolarConstant 1200	24.6	805	6420	LT50	2.170	Continuous
[86]	SolarConstant 1200	23.2	790	7650	LT50	5.880	Continuous
[86]	SolarConstant 1200	23.2	790	7650	LT50	3.060	Continuous
[86]	SolarConstant 1200	25.5	805	8310	LT50	9.370	Continuous
[86]	SolarConstant 1200	25.5	805	8310	LT50	3.890	Continuous
[86]	SolarConstant 1200	23.6	784	7390	LT50	12.000	Continuous
[86]	SolarConstant 1200	23.6	784	7390	LT50	3.500	Continuous
[86]	SolarConstant 1200	23.6	784	7390	LT50	1.940	Continuous
[86]	SolarConstant 1200	23.6	784	7390	LT50	1.120	Continuous
[86]	SolarConstant 1200	61.9	2325	40550	LT50	4.000	Continuous
[86]	SolarConstant 1200	61.9	2325	40550	LT50	1.830	Continuous
[86]	SolarConstant 1200	61.9	2325	40550	LT50	0.900	Continuous
[86]	SolarConstant 1200	27.1	801	5700	LT50	12.000	Continuous
[86]	SolarConstant 1200	27.1	801	5700	LT50	3.240	Continuous
[86]	SolarConstant 1200	25.2	801	7830	LT50	12.000	Continuous
[86]	SolarConstant 1200	25.2	801	7830	LT50	2.960	Continuous
[86]	SolarConstant 1200	25.2	801	7830	LT50	0.810	Continuous
[86]	SolarConstant 1200	25.2	801	7830	LT50	0.500	Continuous
[86]	SolarConstant 1200	37.2	813	3550	LT50	12.000	Continuous

[86]	SolarConstant 1200	37.2	813	3550	LT50	5.400	Continuous
[86]	SolarConstant 1200	37.2	813	3550	LT50	1.190	Continuous
[86]	SolarConstant 1200	31.6	799	3510	LT50	12.000	Continuous
[86]	SolarConstant 1200	31.6	799	3510	LT50	3.280	Continuous
[86]	SolarConstant 1200	59.7	2298	39670	LT50	4.000	Continuous
[86]	SolarConstant 1200	59.7	2298	39670	LT50	1.530	Continuous
[86]	SolarConstant 1200	101.7	2308	10470	LT50	4.000	Continuous
[86]	SolarConstant 1200	30.5	803	4080	LT50	0.980	Continuous
[86]	SolarConstant 1200	30.5	803	4080	LT50	10.200	Continuous
[86]	SolarConstant 1200	30.5	803	4080	LT50	12.000	Continuous
[86]	SolarConstant 1200	30.1	805	4450	LT50	12.000	Continuous
[86]	SolarConstant 1200	30.1	805	4450	LT50	12.000	Continuous
[86]	SolarConstant 1200	30.1	800	4080	LT50	4.470	Continuous
[86]	SolarConstant 1200	28.7	806	4440	LT50	12.000	Continuous
[86]	SolarConstant 1200	28.5	805	4450	LT50	12.000	Continuous
[86]	SolarConstant 1200	30.5	802	3880	LT50	2.890	Continuous
[86]	SolarConstant 1200	37.1	800	4340	LT50	2.1	Continuous
[86]	SolarConstant 1200	30.1	800	4080	LT50	3.87	Continuous
[86]	SolarConstant 1200	28.7	806	4440	LT50	4.26	Continuous
[86]	SolarConstant 1200	28.5	805	4450	LT50	1.19	Continuous
[86]	SolarConstant 1200	37.1	800	4340	LT50	9.72	Continuous
[86]	SolarConstant 1200	28.5	805	4450	LT50	0.5	Continuous

[86]	SolarConstant 1200	28.5	805	4450	LT50	0.5	Continuous
[86]	SolarConstant 1200	28.5	805	4450	LT50	0.5	Continuous
[86]	SolarConstant 1200	28.5	805	4450	LT50	4.71	Continuous
[86]	SolarConstant 1200	35.7	778	2820	LT50	0.82	Continuous
[68]	Qpanel	0	1940	0	LT50	0.588	Continuous
[68]	Qpanel	0	1483	0	LT50	0.903	Continuous
[68]	Qpanel	0	923	0	LT50	1.278	Continuous
[68]	Qpanel	0	560	0	LT50	1.567	Continuous
[68]	Qpanel	0	810	0	LT50	1.352	Continuous
[68]	Qpanel	0	1940	0	LT50	0.418	Continuous
[68]	Qpanel	0	902	0	LT50	0.652	Continuous
[68]	Qpanel	0	810	0	LT50	0.825	Continuous
[68]	Qpanel	0	1940	0	LT50	0.678	Continuous
[68]	Qpanel	0	1483	0	LT50	0.882	Continuous
[68]	Qpanel	0	923	0	LT50	1.200	Continuous
[68]	Qpanel	0	560	0	LT50	1.463	Continuous
[68]	Qpanel	0	810	0	LT50	1.140	Continuous
[68]	Qpanel	0	1940	0	LT50	0.553	Continuous
[68]	Qpanel	0	902	0	LT50	1.063	Continuous
[68]	Qpanel	0	810	0	LT50	1.037	Continuous
[68]	Qpanel	0	1940	0	LT50	0.220	Continuous
[68]	Qpanel	0	1483	0	LT50	0.285	Continuous

[68]	Qpanel	0	923	0	LT50	0.568	Continuous
[68]	Qpanel	0	560	0	LT50	0.563	Continuous
[68]	Qpanel	0	810	0	LT50	0.808	Continuous
[68]	Qpanel	0	1940	0	LT50	0.2	Continuous
[68]	Qpanel	0	902	0	LT50	0.303	Continuous
[68]	Qpanel	0	810	0	LT50	0.658	Continuous
[73]	SSR I[b]	0	62.5	0	LT50	8.300	Continuous
[73]	SSR I[b]	0	62.5	0	LT50	18.900	Continuous
[73]	SSR I[b]	0	62.5	0	LT50	48.000	Continuous
[73]	SSR I[b]	0	62.5	0	LT50	86.730	Continuous
[11]	Solar Radiation	25	120	680	LT50	4.975	Continuous
[11]	Solar Radiation	25	120	680	LT50	12.510	Continuous
[11]	Solar Radiation	25	120	680	LT50	4.442	Continuous
[11]	Solar Radiation	25	120	680	LT50	23.980	Continuous
[11]	Solar Radiation	25	120	680	LT50	3.083	Continuous
[11]	Solar Radiation	25	120	680	LT50	10.815	Continuous
[11]	Solar Radiation	25	120	680	LT50	3.477	Continuous
[11]	Solar Radiation	25	120	680	LT50	5.383	Continuous
[11]	Solar Radiation	25	120	680	LT50	16.425	Continuous
[11]	Solar Radiation	25	120	680	LT50	22.945	Continuous
[11]	Solar Radiation	25	120	680	LT50	22.402	Continuous
[11]	Solar Radiation	25	120	680	LT50	15.263	Continuous

[11]	Solar Radiation	25	120	680	LT50	13.007	Continuous
[11]	Solar Radiation	25	120	680	LT50	18.328	Continuous
[11]	Solar Radiation	25	120	680	LT50	13.815	Continuous
[65]	Qpanel	60	156	0	10 d LC50	1	Continuous
[65]	Qpanel	60	156	0	10 d LC50	1	Continuous
[65]	Qpanel	60	156	0	10 d LC50	1	Continuous
[65]	Qpanel	60	156	0	10 d LC50	1	Continuous
[8]	Qpanel	128	279	0	10 d LC50	1	Continuous

[a]Ultra-Vitalux lamp: irradiation spectrum provided by Michael Ahrens through personal communication.

Black light and Cool-white light: irradiation spectrum provided in Cody et al. [37]

GE F40 BLB blacklight: irradiation spectrum provided in Gala and Giesy [38]

SSR II: solar simulated radiation irradiation spectrum provided in Lampi et al. [36]

SSR I: solar simulated radiation irradiation spectrum provided by James T. Oris through personal communication.

Qpanel lamp: irradiation spectrum provided in Diamond et al. [68]

SolarConstant 1200 lamp: irradiation spectrum provided in [86]

Solar radiation spectral variation was used as the light source spectrum for Newsted and Giesy [11] since the irradiance spectrum was not provided. Standard CWF lamps were combined with RPR-3500 (UVA), and RPR-3000A (UVB) lamps (Southern New England Ultraviolet, Branford, CT, USA) to simulate solar radiation. A combination of Chroma F40C50 white (General Electric, Cleveland, OH) and FS40 ultraviolet (Westinghouse, Bloomfield, NJ) fluorescent bulbs was used to simulate solar radiation.

Table A.3. Octanol-water partition coefficient, molecular weight, and water solubilities of 20 PAHs of used in PTLM development.

PAH[a]	log(K_{ow})[b]	Molecular weight (g/mol)
FLA	5.190	202.260
ANT	4.546	178.200
PYR	5.126	202.260
BaP	6.409	252.310
BaA	5.744	228.290
DaA	7.129	278.350
CHR	5.782	228.290
BgP	6.886	276.340
BbA	5.744	228.290
BeP	6.447	252.300
PHE	4.584	178.230
NAP	3.256	128.190
FLU	3.930	166.200
ACN	3.878	154.210
BbFU	5.340	216.277
PER	6.447	252.310
BAN	4.810	230.270
BbFL	6.341	252.320
BkFL	6.400	252.320
BaFU	5.340	216.277

Table A.4. Assumed critical target lipid body burdens for the species of interest.

Organism[a]	C^{*}_{LN} (μmol/g octanol)
M. liliana	122.637[b]
S. capricornutum	128.541 [c]
D. magna	115.345 [c]
L. macrochirus	130.918 [c]
M. lateralis	102.485 [c]
M. bahia	34.277 [c]
O. mykiss	66.069 [c]
P. promelas	122.180 [c]
M. beryllina	291.743 [c]
C. variegatus	113.501 [c]
L. variegatus	438.592 [c]
F. grandis	106.170 [c]
A. salina	194.089 [c]
P. pugio	57.280 [c]
R. abronius	31.189 [c]

[a] Abbreviations for organisms: *M. liliana = Macomona liliana; S. capricornutum = Selenastrum capricornutum; D. magna = Daphnia magna; L. macrochirus = Lepomis macrochirus; M.= Mulinia lateralis; M. bahia = Mysidopsis bahia; O. mykiss = Oncorhynchus mykiss; P. promelas = Pimephales promelas; M. beryllina = Menidia beryllina; C. variegatus = Cyprinodon variegatus; L. variegatus = Lumbriculus variegatus; F. grandis = Fundulus grandis ; A. salina = Artemia salina.; P. pugio = Palaemonetes pugio; R. abronius = Rhepoxynius abronius.*

Table A.5-a. Molar absorption spectra ($\varepsilon(\lambda)$) at wavelength intervals of λ =1 (nm).

λ (nm)	$\varepsilon^a(\lambda)$ (L/mol/cm)	$\varepsilon^b(\lambda)$ (L/mol/cm)	$\varepsilon^c(\lambda)$ (L/mol/cm)	$\varepsilon^d(\lambda)$ (L/mol/cm)	$\varepsilon^e(\lambda)$ (L/mol/cm)	$\varepsilon^f(\lambda)$ (L/mol/cm)	$\varepsilon^g(\lambda)$ (L/mol/cm)	$\varepsilon^h(\lambda)$ (L/mol/cm)	$\varepsilon^i(\lambda)$ (L/mol/cm)	$\varepsilon^j(\lambda)$ (L/mol/cm)
280	14867	9	4000	28152	47317	39952	11019	22909	104951	40886
281	14067	91	4000	30544	43415	39949	11072	23399	78948	32751
282	15323	173	4000	33905	41098	43362	11259	23400	78924	28846
283	16489	255	4000	40269	44512	52089	11393	24221	42764	26241
284	14886	338	4000	45750	56707	72776	11285	25071	38318	26236
285	12032	420	4000	47700	72195	84161	10777	26252	28824	28509
286	12930	502	4000	46739	86707	88521	9949	27488	27583	32408
287	32235	584	4000	42071	88781	87380	9467	29791	25265	36957
288	41800	667	4000	38108	87805	85003	9093	32660	19423	43620
289	29742	749	4000	32999	70122	82056	8986	36218	18586	57275
290	16344	831	4000	30625	55000	75978	9092	40629	15594	59711
291	8396	913	4195	29574	39146	69899	9653	44034	15589	50439
292	4559	995	4195	30113	29268	63631	10107	44545	16281	35313
293	3045	1078	4293	34005	25366	59639	10855	38811	17377	25392
294	2513	1160	4341	40105	14634	65141	11764	35815	18546	20672
295	2161	1242	4390	44349	11707	98356	11977	32672	23072	16441
296	1898	1324	4245	57596	9756	163461	11817	30497	24625	14485
297	1724	1324	4173	64400	8841	148651	10908	29129	24081	13669
298	1461	1324	4100	59821	7439	130614	9999	28799	24074	13178
299	1555	1397	5800	48621	8902	103655	8823	30154	23037	12524
300	1470	1322	7500	37601	9006	85238	8341	34217	13040	12195
301	1653	1343	8750	27636	7982	55432	8288	39730	8988	13167
302	1748	1365	9375	20407	6897	45557	8795	54805	4366	13976
303	1932	1443	10000	14150	4090	36631	9890	58719	3009	14623
304	2115	1465	11250	9749	3475	29793	10906	54811	2167	14782
305	2209	1568	11875	8210	3246	26942	12295	45090	1741	14779
306	2393	1782	12500	5973	3222	25989	13017	35837	1338	14612
307	2665	1777	12069	5364	3282	24277	13177	26893	1338	14446
308	2938	1773	11854	4928	3378	23038	12589	20414	1173	13955
309	3211	1851	11639	4228	3571	21609	11573	15675	1074	13789
310	3037	1954	11208	3976	3908	20848	9595	12176	1074	13947
311	3131	1951	10992	3812	4185	18754	7991	10249	826	14431
312	2957	1945	10777	3700	4317	17232	7429	8627	790	14916

313	3052	1831	11177	3559	4461	15900	7001	7691	685	15725
314	3056	1823	12255	3749	4563	14282	7081	6779	634	17348
315	3061	1928	13333	3929	4605	13234	7749	6255	607	19621
316	3244	2031	16448	3760	4485	13230	8818	5641	607	22544
317	3428	2055	18883	3509	4581	14175	10074	5327	581	25792
318	3522	2106	24713	3167	4340	15879	10795	4972	487	24162
319	3706	2126	29864	3131	4243	16446	11490	4641	446	21395
320	3979	2120	31621	3094	4231	17768	11837	4382	427	19440
321	4340	2307	28919	2839	4460	18335	11837	4138	408	16346
322	4792	2356	26216	2588	4652	19089	11489	3952	391	15530
323	5154	2677	23513	2729	4857	18040	8255	3775	358	14551
324	5516	2838	20811	2869	5447	16994	5502	3648	358	13735
325	5164	2668	18108	3054	5881	13951	3684	3648	328	13244
326	4990	2334	15405	3239	6314	12429	2561	3733	314	14865
327	4726	2221	12703	3781	6422	11096	1412	3953	300	17301
328	4464	2367	11351	3963	6422	9954	957	4285	275	18923
329	4379	2513	10000	4413	6386	9380	316	5033	275	19895
330	4294	2618	12136	4686	6240	10136	182	6189	257	26232
331	4210	3017	15930	4958	5952	11364	130	6785	251	32246
332	4215	3395	19044	5318	5747	14112	101	6261	251	40696
333	4398	3935	54082	5249	5554	14867	154	5393	241	29474
334	4581	4255	37291	5255	5108	16003	154	4592	220	21341
335	4675	4632	19300	5086	4987	15808	154	4047	211	13206
336	4859	4981	10101	4920	5086	14475	100	3650	206	6699
337	5043	5411	8000	4929	5276	13713	260	3486	193	4907
338	5405	5842	3896	5025	5456	10860	260	3608	193	3277
339	5856	6300	3130	5474	5998	9908	72	3956	193	2460
340	6576	5968	941	6099	6522	7671	99	4387	184	2132
341	7027	4928	879	6904	7070	6672	205	5036	184	1449
342	7300	4379	815	8148	7407	6291	152	5584	188	1221
343	7126	3829	753	9127	7184	5907	205	6410	201	1074
344	6774	3552	692	10241	6985	6088	258	7358	201	765
345	6421	3521	660	11176	6130	6656	418	8254	210	650
346	6158	3517	628	12245	6009	7222	391	9154	229	634
347	5805	3943	680	12960	5623	8167	204	9920	239	650
348	5631	4238	617	13053	5418	10249	150	10387	261	698
349	5457	4561	498	12804	4779	12335	177	10152	272	698
350	5462	5536	493	12194	4484	14418	257	9809	272	600
351	5467	5694	430	11847	4189	13844	363	8948	284	518
352	5471	6119	369	11151	3646	10994	363	8070	302	469
353	5476	6303	366	10457	3646	7380	309	7620	310	420
354	5660	7000	362	10109	3851	5669	309	7299	324	403
355	5575	8355	300	10298	4019	3197	362	7362	324	387
356	6206	9100	297	10570	4310	2055	201	7979	338	403
357	6568	8563	294	11990	4501	1671	201	8598	353	435

358	7288	7625	230	13499	4753	1097	255	9701	353	434
359	7829	6500	343	16952	5079	618	201	10758	353	434
360	7298	5296	340	18813	5253	139	334	11794	352	401
361	6765	4400	276	20678	4921	0	628	13079	368	352
362	6056	3741	244	22715	3873	130	627	15013	384	303
363	5256	3200	212	24312	2957	0	574	17432	402	270
364	4635	2800	150	26001	2900	0	520	19555	419	286
365	4015	2584	144	26184	2800	0	413	21936	457	302
366	3394	2501	82	25576	2426	0	306	25179	499	464
367	3041	2472	138	24879	2077	0	198	25181	544	610
368	2689	2549	192	23299	1667	0	172	23236	594	414
369	2246	2700	129	21454	1330	0	118	18897	620	349
370	1894	3720	66	17582	775	0	118	15725	648	267
371	1631	4385	122	15736	642	0	117	13390	691	218
372	1368	4623	118	13979	437	91	117	11938	738	169
373	1373	4568	71	13016	389	277	90	10401	771	136
374	1109	4858	23	12501	377	461	90	9167	770	120
375	1025	6672	19	12861	413	647	89	8756	705	87
376	940	8753	19	14545	424	644	116	8656	737	103
377	767	8617	19	17202	376	259	169	8960	675	53
378	772	7572	19	21535	320	0	182	9600	674	53
379	687	6101	19	24194	285	0	195	11019	645	53
380	602	4896	19	24819	243	0	142	12081	566	36
381	607	3600	19	26416	189	0	141	14189	591	36
382	611	2593	19	25984	146	0	141	15735	591	35
383	527	2110	19	26346	206	0	141	18062	603	35
384	531	1760	17	30594	363	0	141	19575	644	35
385	447	1400	14	30602	796	0	140	21708	673	18
386	452	1193	12	29639	772	223	167	26696	734	18
387	456	1058	10	27882	531	0	140	29605	813	17
388	283	760	7	21537	181	0	139	29948	913	65
389	10	651	5	15986	133	0	139	23802	1040	32
390	10	487	2	10876	72	0	112	12801	1185	32
391	10	404	0	7798	24	0	85	6806	1411	32
392	10	322	0	5953	0	0	31	4878	1474	32
393	10	293	0	5078	0	0	0	3967	1916	15
394	10	277	0	5176	0	188	0	3378	2065	15
395	10	261	0	4303	0	566	0	2876	1914	15
396	10	258	0	3343	0	752	0	2477	1832	15
397	10	175	0	2204	0	555	0	1696	1445	15
398	10	146	0	1245	0	0	0	777	1182	15
399	10	91	0	901	0	0	0	404	1131	15
400	10	9	0	819	0	0	0	299	908	15
401	0	0	0	0	0	0	0	227	0	0
402	0	0	0	0	0	0	0	225	0	0

403	0	0	0	0	0	0	0	241	0	0
404	0	0	0	0	0	0	0	289	0	0
405	0	0	0	0	0	0	0	394	0	0
406	0	0	0	0	0	0	0	538	0	0
407	0	0	0	0	0	0	0	491	0	0
408	0	0	0	0	0	0	0	227	0	0
409	0	0	0	0	0	0	0	171	0	0
410	0	0	0	0	0	0	0	149	0	0
411	0	0	0	0	0	0	0	112	0	0

[a] $\varepsilon(\lambda)$ for fluoranthene measured in solvent cyclohexane [56].

[b] $\varepsilon(\lambda)$ for anthracene measured in solvent cyclohexane [56].

[c] $\varepsilon(\lambda)$ for pyrene measured in solvent cyclohexane [56].

[d] $\varepsilon(\lambda)$ for benzo[*a*]pyrene measured in solvent cyclohexane [56].

[e] $\varepsilon(\lambda)$ for benzo[*a*]anthracene measured in solvent cyclohexane [56].

[f] $\varepsilon(\lambda)$ for Dibenzo[*a,h*]anthracene measured in solvent cyclohexane [56].

[g] $\varepsilon(\lambda)$ for chrysene measured in solvent cyclohexane [56].

[h] $\varepsilon(\lambda)$ for benzo[*g,h,i*]perylene measured in solvent cyclohexane [56].

[i] $\varepsilon(\lambda)$ for benzo[*b*]anthracene measured in solvent benzene [74]

[j] $\varepsilon(\lambda)$ for benzo[*e*]pyrene measured in solvent cyclohexane [56].

Table A.5-b. Molar absorption spectra ($\varepsilon(\lambda)$) at wavelength intervals of λ =1 (nm).

λ (nm)	$\varepsilon^a(\lambda)$ (L/mol/cm)	$\varepsilon^b(\lambda)$ (L/mol/cm)	$\varepsilon^c(\lambda)$ (L/mol/cm)	$\varepsilon^d(\lambda)$ (L/mol/cm)	$\varepsilon^e(\lambda)$ (L/mol/cm)	$\varepsilon^f(\lambda)$ (L/mol/cm)	$\varepsilon^g(\lambda)$ (L/mol/cm)	$\varepsilon^h(\lambda)$ (L/mol/cm)	$\varepsilon^i(\lambda)$ (L/mol/cm)	$\varepsilon^j(\lambda)$ (L/mol/cm)
280	9790	5789	5464	6066	8223	2153	7089	24257	16643	10200
281	10257	5122	4867	5990	8514	2081	7171	23636	18130	9988
282	11000	4724	4539	5847	9125	2011	7254	23464	19404	9590
283	9531	3618	4283	5708	10007	1966	7423	22753	21104	9578
284	7509	3876	4136	5832	11231	1900	7596	22041	24081	9567
285	6225	3878	4134	6028	11628	1815	7596	21151	24184	9750
286	5585	3774	4278	6090	10855	1774	7425	20170	24076	9641
287	4765	3934	4854	6223	9456	1715	7257	20625	22796	9727
288	4679	4100	5703	6505	9137	1638	6932	22964	22794	9910
289	5514	3777	6397	6724	9139	1602	6853	24763	23218	10092
290	6258	3117	6248	6792	9354	1566	6621	26294	24066	10281
291	7372	2369	5828	6707	9356	1496	6253	26660	26617	10067
292	8946	1704	5500	6399	9251	1446	6182	26038	27465	10059
293	12825	1160	5435	5968	8939	1397	6254	26403	30867	10046
294	14400	834	5308	5565	8738	1320	6327	25782	32993	10432
295	9934	679	4728	5190	8740	1261	6624	24174	35118	10425
296	4823	523	4212	4784	8843	1205	6778	21401	41499	10103
297	2523	397	4511	4513	9262	1165	6936	20509	44475	9619
298	1239	315	4722	4257	10158	1138	7179	21144	44898	9796
299	508	319	7487	4350	11270	1113	7263	22317	41491	9781
300	125	319	9533	4445	12794	1039	7432	25821	41064	9962
301	125	278	8591	4241	13871	1016	7604	30222	40636	9762
302	125	286	7652	3651	15567	960	7781	38030	38718	9752
303	125	294	5603	2835	16305	906	7963	40545	39354	9933
304	125	253	3183	2675	15574	856	8148	27281	39777	9171
305	125	227	1208	3029	13725	828	8337	17063	41052	9431
306	125	230	788	2991	12095	809	8434	10881	43603	9519
307	125	209	584	2575	11687	791	8532	8914	49132	8961
308	125	209	423	2142	11424	782	8435	7217	54662	9129
309	125	180	343	1761	11426	773	8436	6684	60192	9119
310	125	148	289	1587	12106	773	8151	5973	64870	9109
311	125	128	0	1447	12679	782	7876	5800	67847	9100

312	125	148	0	1349	13589	782	7698	5359	51248	9267
313	125	231	0	1273	14733	782	7524	5276	28267	9443
314	125	228	0	1214	15791	792	7396	5372	15924	9431
315	143	123	0	1172	17721	783	7106	5378	13794	9606
316	160	80	0	1068	19436	801	6866	5743	11664	9597
317	143	71	0	849	17935	801	6558	5750	10812	9775
318	125	58	0	765	15624	801	6337	5935	8681	9761
319	125	30	0	982	11452	810	5916	6031	8253	9653
320	125	21	0	1818	8995	810	5651	6127	8250	9173
321	125	20	0	1755	6369	829	5336	6314	8248	8649
322	125	22	0	1202	6372	858	4982	6409	7820	7099
323	158	15	0	655	7489	878	4545	6685	8243	6060
324	190	12	0	357	6910	899	4147	6780	7816	4006
325	158	0	0	184	5124	919	3656	6966	7600	3558
326	125	0	0	56	4782	941	3374	7063	7385	2920
327	125	0	0	0	3978	963	3043	7248	6957	2696
328	125	0	0	0	3125	985	2745	7435	6530	2489
329	173	0	0	0	2630	985	2714	7530	6528	2537
330	220	0	0	0	2483	1008	2365	7896	5673	2533
331	173	0	0	0	2512	1020	2234	8081	5671	2632
332	12	0	0	0	2484	1055	2234	8176	5669	2681
333	149	0	0	0	2091	1080	2234	8452	5241	2428
334	12	0	0	0	1700	1131	2286	8728	5239	1992
335	125	0	0	0	1398	1184	2339	8913	5235	1735
336	141	0	0	0	1662	1253	2449	9368	5234	1633
337	158	0	0	0	2759	1282	2477	9464	5232	1632
338	174	0	0	0	4373	1358	2564	9561	5230	1662
339	190	0	0	0	6323	1422	2624	9746	4800	1726
340	96	0	0	0	7096	1471	2685	9752	4798	1865
341	48	0	0	0	5769	1488	2779	9848	4794	1900
342	1	0	0	0	3135	1523	2748	10124	4792	1654
343	111	0	0	0	1263	1541	2748	10042	4365	1358
344	165	0	0	0	710	1559	2844	10048	4363	1148
345	193	0	0	0	340	1559	2911	10143	3936	1092
346	220	0	0	0	233	1577	3118	9970	3508	766
347	166	0	0	0	0	1613	3191	9886	3506	366
348	112	0	0	0	0	1632	3379	9893	3079	487
349	59	0	0	0	0	1709	3579	10169	2649	487
350	5	0	0	0	0	1809	3704	10265	2647	487

351	0	0	0	0	0	1851	3923	10451	3071	0
352	0	0	0	0	0	2052	4155	10280	3069	0
353	0	0	0	0	0	2173	4350	10284	3492	0
354	0	0	0	0	0	2173	4555	9663	3489	0
355	0	0	0	0	0	2354	4769	9310	2636	0
356	0	0	0	0	0	2551	4936	8688	3485	0
357	0	0	0	0	0	2795	5110	8336	4759	0
358	0	0	0	0	0	2960	5289	7984	6034	0
359	0	0	0	0	0	3206	5474	7990	7306	0
360	0	0	0	0	0	3434	5666	7908	7304	0
361	0	0	0	0	0	3636	5865	7734	6877	0
362	0	0	0	0	0	3807	6002	7561	6449	0
363	0	0	0	0	0	3985	6071	7299	5170	0
364	0	0	0	0	0	4220	6284	6946	4956	0
365	0	0	0	0	0	4469	6357	6773	3889	0
366	0	0	0	0	0	4572	6505	6511	4312	0
367	0	0	0	0	0	4679	6581	6428	3884	0
368	0	0	0	0	0	4733	6657	6705	4306	0
369	0	0	0	0	0	4788	6734	6709	4730	0
370	0	0	0	0	0	4844	6658	6984	5153	0
371	0	0	0	0	0	4900	6735	6452	5151	0
372	0	0	0	0	0	5014	6813	5830	5575	0
373	0	0	0	0	0	5189	6813	4672	5573	0
374	0	0	0	0	0	5432	6893	3960	5144	0
375	0	0	0	0	0	5885	6973	2622	4716	0
376	0	0	0	0	0	6523	7053	2179	6416	0
377	0	0	0	0	0	7148	7301	1649	8967	0
378	0	0	0	0	0	7744	7386	1385	12369	0
379	0	0	0	0	0	8781	7645	1122	16622	0
380	0	0	0	0	0	10073	7733	1039	17470	0
381	0	0	0	0	0	10189	8097	955	17042	0
382	0	0	0	0	0	10789	8191	782	15338	0
383	0	0	0	0	0	11295	8381	430	13209	0
384	0	0	0	0	0	11690	8576	615	5971	0
385	0	0	0	0	0	12238	8877	623	5544	0
386	0	0	0	0	0	12240	9189	628	5116	0
387	0	0	0	0	0	11965	9403	547	4475	0
388	0	0	0	0	0	11696	9621	464	3834	0
389	0	0	0	0	0	11433	9845	468	3832	0

390	0	0	0	0	0	10924	9960	295	3830	0
391	0	0	0	0	0	10679	9960	33	4254	0
392	0	0	0	0	0	10680	9961	2	5528	0
393	0	0	0	0	0	10681	10077	0	6375	0
394	0	0	0	0	0	10930	10077	0	6373	0
395	0	0	0	0	0	11442	10194	0	5946	0
396	0	0	0	0	0	12396	9964	0	4667	0
397	0	0	0	0	0	14057	9851	0	3812	0
398	0	0	0	0	0	15761	9518	0	4236	0
399	0	0	0	0	0	15943	9410	0	5085	0
400	0	0	0	0	0	17075	8989	0	8913	0
401	0	0	0	0	0	17876	8587	0	14442	0
402	0	0	0	0	0	19366	8108	0	20397	0
403	0	0	0	0	0	21221	7570	0	23372	0
404	0	0	0	0	0	23791	7067	0	18689	0
405	0	0	0	0	0	24906	6374	0	12305	0
406	0	0	0	0	0	26074	6089	0	6770	0
407	0	0	0	0	0	26679	5684	0	1236	0
408	0	0	0	0	0	26989	5246	0	809	0
409	0	0	0	0	0	26083	4842	0	381	0
410	0	0	0	0	0	24083	4468	0	379	0
411	0	0	0	0	0	21734	4077	0	377	0
412	0	0	0	0	0	19170	3720	0	0	0
413	0	0	0	0	0	17103	3355	0	0	0
414	0	0	0	0	0	15612	2958	0	0	0
415	0	0	0	0	0	14580	2668	0	0	0
416	0	0	0	0	0	14091	2352	0	0	0
417	0	0	0	0	0	13933	2097	0	0	0
418	0	0	0	0	0	13934	1913	0	0	0
419	0	0	0	0	0	14096	1687	0	0	0
420	0	0	0	0	0	14423	1487	0	0	0
421	0	0	0	0	0	15273	1296	0	0	0
422	0	0	0	0	0	16358	1155	0	0	0
423	0	0	0	0	0	17925	1019	0	0	0
424	0	0	0	0	0	20327	878	0	0	0
425	0	0	0	0	0	22275	810	0	0	0
426	0	0	0	0	0	24409	674	0	0	0
427	0	0	0	0	0	26747	581	0	0	0
428	0	0	0	0	0	28001	500	0	0	0

429	0	0	0	0	0	28980	446	0	0	0
430	0	0	0	0	0	29654	0	0	0	0
431	0	0	0	0	0	31043	0	0	0	0
432	0	0	0	0	0	32129	0	0	0	0
433	0	0	0	0	0	33254	0	0	0	0
434	0	0	0	0	0	34026	0	0	0	0
435	0	0	0	0	0	33644	0	0	0	0
436	0	0	0	0	0	31063	0	0	0	0
437	0	0	0	0	0	26781	0	0	0	0
438	0	0	0	0	0	17756	0	0	0	0
439	0	0	0	0	0	14132	0	0	0	0
440	0	0	0	0	0	10503	0	0	0	0
441	0	0	0	0	0	8171	0	0	0	0
442	0	0	0	0	0	5735	0	0	0	0
443	0	0	0	0	0	4166	0	0	0	0
444	0	0	0	0	0	2731	0	0	0	0
445	0	0	0	0	0	2053	0	0	0	0
446	0	0	0	0	0	1579	0	0	0	0
447	0	0	0	0	0	1201	0	0	0	0
448	0	0	0	0	0	945	0	0	0	0
449	0	0	0	0	0	796	0	0	0	0
450	0	0	0	0	0	656	0	0	0	0

[a] $\varepsilon(\lambda)$ for phenanthrene measured in solvent cyclohexane [56].

[b] $\varepsilon(\lambda)$ for naphthalene measured in solvent cyclohexane [56].

[c] $\varepsilon(\lambda)$ for fluorene measured in solvent ethanol [74].

[d] $\varepsilon(\lambda)$ for acenaphthene measured in solvent ethanol [74].

[e] $\varepsilon(\lambda)$ for benzo[*b*]fluorene measured in solvent ethanol [74].

[f] $\varepsilon(\lambda)$ for perylene measured in solvent ethanol [74].

[g] $\varepsilon(\lambda)$ for bezanthrone measured in solvent ethanol [74].

[h] $\varepsilon(\lambda)$ for benzo[*b*]fluoranthene measured in solvent cyclohexane [56].

[i] $\varepsilon(\lambda)$ for benzo[*k*]fluoranthene measured in solvent benzene [74].

[j] $\varepsilon(\lambda)$ for benzo[*a*]fluorene measured in solvent ethanol [74].

Table A.6-a. Irradiance spectra ($I(\lambda)$) for the light sources used in the experimental data presented in Table A1 at 1 nm wavelength (λ) intervals.

λ (nm)	$I^a(\lambda)$ (μW/cm^2/nm)	$I^b(\lambda)$ (μW/cm^2/nm)	$I^c(\lambda)$ (μW/cm^2/nm)	$I^d(\lambda)$ (μW/cm^2/nm)	$I^e(\lambda)$ (μW/cm^2/nm)	$I^f(\lambda)$ (μW/cm^2/nm)	$I^g(\lambda)$ (μW/cm^2/nm)	$I^h(\lambda)$ (μW/cm^2/nm)	$I^i(\lambda)$ (μW/cm^2/nm)	$I^j(\lambda)$ (μW/cm^2/nm)
280	0	0	0.001	0	0	0	4.380	0	0	2.400
281	0	0	0.001	0	0	0	4.380	0	0	2.400
282	0	0	0.001	0	0	0	3.285	0	0	2.400
283	0	0	0.001	0	0	0	2.737	0	0	2.400
284	0	0	0.001	0	0	0	2.190	0	0	2.400
285	0	0	0.001	0	0	0	8.212	0	0	2.400
286	0	0	0.001	0	0	0	8.212	0	0	2.400
287	0	0	0.001	0	0	0	7.664	0	0	2.400
288	0	0	0.001	0	0	0	7.117	0	0	2.400
289	0	0	0.001	0	0	0	4.380	0	0	2.400
290	0	0.262	0.001	0	0	0	6.569	0.002	0	2.400
291	0	0.262	0.001	0	0	0	8.759	0.002	0	2.400
292	0	0.262	0.001	0	0	0	10.949	0.002	0	2.400
293	0	0.262	0.001	0	0	0	13.139	0.002	0	2.400
294	0	0.262	0.001	0	0	0	8.759	0.003	0	2.400
295	0	0.262	0.001	0.001	0	0	10.128	0.003	0	2.400
296	0	0.231	0.001	0.001	0	0	11.496	0.003	0	2.400
297	0	0.201	0.001	0.001	0	0	12.865	0.002	0	2.400
298	0	0.633	0.001	0.001	0	0	13.549	0.002	0	2.400
299	0	0.602	0.001	0.001	0	0	14.234	0.003	0	2.400
300	5.610	1.030	0.001	0.001	1.1	0	13.686	0.005	0	2.400
301	5.570	1.940	0.001	0.001	1.09	0	13.686	0.007	0	3.559
302	5.020	2.390	0.001	0.001	1.08	0	12.591	0.007	0	4.718

303	4.620	2.840	0.001	0.001	1.07	0	16.697	0.012	0	4.718
304	4.260	3.770	0.001	0.002	1.06	0	20.803	0.013	0	4.718
305	5.260	4.680	0.001	0.008	1.27	0	14.781	0.012	0	4.718
306	7.860	5.600	0.001	0.011	1.37	0	16.423	0.013	0	8.984
307	11.000	7.010	0.001	0.010	1.470	0	18.066	0.013	0	13.250
308	14.700	7.920	0.001	0.008	1.460	0	19.708	0.014	0	13.250
309	17.800	9.800	0.001	0.007	1.450	0	20.529	0.015	0	13.250
310	20.900	11.700	0.001	0.005	1.660	0	21.350	0.018	0	13.250
311	23.100	13.500	0.001	0.005	1.870	0	23.540	0.021	0	19.574
312	23.500	17.800	0.001	0.004	2.090	0	25.730	0.032	0	25.898
313	21.100	26.400	0.001	0.004	2.300	0	27.920	0.058	0	25.898
314	17.200	21.100	0.001	0.004	2.730	0	29.015	0.073	0	25.898
315	14.300	22.500	0.001	0.003	2.940	0	30.110	0.018	0	25.898
316	10.500	23.400	0.001	0.002	3.150	0	15.876	0.018	0	31.720
317	7.460	25.300	0.001	0.002	3.810	0	21.761	0.018	0	37.542
318	4.700	28.100	0.001	0.002	4.470	0	27.646	0.018	0	37.542
319	3.240	30.500	0.001	0.002	4.910	0	33.531	0.018	0	37.542
320	2.880	32.800	0.001	0.001	5.350	0	39.416	0.019	0	37.542
321	2.900	35.200	0.001	0.001	6.670	0	26.277	0.021	0.006	42.159
322	2.990	38.000	0.001	0.001	7.550	0	32.710	0.021	0.008	46.777
323	3.050	40.900	0.001	0.001	9.330	0	39.142	0.024	0.009	46.777
324	3.090	43.200	0.001	0.001	11.100	0	45.575	0.027	0.010	46.777
325	3.240	45.600	0.001	0.001	12.000	0	52.007	0.025	0.013	46.777
326	3.600	47.900	0.001	0.001	14.600	0	36.131	0.024	0.016	56.513
327	4.450	50.300	0.001	0.001	16.000	0	30.657	0.025	0.019	66.250
328	5.520	52.200	0.001	0.001	18.200	0	47.628	0.028	0.021	66.250
329	6.570	55.500	0.001	0.001	20.400	0	56.113	0.029	0.023	66.250
330	7.680	56.900	0.001	0.001	22.600	0	64.599	0.033	0.027	66.250
331	8.760	59.700	0.001	0.002	27.100	0	52.555	0.034	0.028	64.594

332	9.400	61.600	0.001	0.002	29.300	0	41.058	0.037	0.030	62.937
333	9.870	62.100	0.001	0.002	33.300	0	39.964	0.040	0.034	62.937
334	9.240	65.400	0.001	0.002	37.300	0	82.117	0.050	0.044	62.937
335	8.620	67.700	0.001	0.002	40.900	1.630	81.569	0.050	0.045	62.937
336	7.430	69.100	0.001	0.002	45.300	1.630	65.693	0.045	0.044	65.547
337	6.290	70.000	0.002	0.001	47.500	1.620	53.650	0.046	0.048	68.157
338	5.400	70.900	0.002	0.001	52.000	1.620	68.431	0.049	0.051	68.157
339	4.470	71.400	0.002	0.001	56.000	1.620	75.821	0.052	0.053	68.157
340	3.700	72.300	0.002	0.001	59.600	1.620	83.212	0.055	0.058	68.157
341	3.400	72.700	0.002	0.001	62.700	1.620	73.905	0.058	0.062	67.655
342	3.330	73.200	0.003	0.001	67.100	1.620	64.599	0.060	0.064	67.153
343	3.300	73.100	0.003	0.001	76.500	1.860	69.389	0.063	0.069	67.153
344	3.210	73.100	0.004	0.001	77.400	2.090	74.179	0.064	0.073	67.153
345	3.090	73.100	0.003	0.001	79.600	2.150	78.969	0.066	0.077	67.153
346	2.980	72.500	0.608	0.001	83.600	2.210	83.759	0.068	0.077	69.864
347	2.900	72.000	0.959	0.002	87.600	2.240	84.580	0.072	0.081	72.574
348	2.870	71.500	1.040	0.002	90.700	2.270	85.401	0.072	0.082	72.574
349	2.630	70.500	1.080	0.002	94.300	2.260	86.223	0.072	0.083	72.574
350	2.620	69.500	1.080	0.002	96.500	2.260	86.633	0.074	0.085	72.574
351	2.660	68.500	1.080	0.002	97.800	2.260	87.044	0.075	0.087	73.979
352	2.630	68.000	1.080	0.003	99.100	2.320	85.402	0.076	0.088	75.384
353	2.590	67.000	1.080	0.005	99.600	2.350	84.854	0.076	0.089	75.384
354	2.550	65.500	1.020	0.016	100.000	2.380	84.307	0.077	0.090	75.384
355	2.620	64.100	0.969	0.026	99.100	2.370	86.223	0.078	0.091	75.384
356	3.540	62.600	0.893	0.031	98.600	2.370	88.139	0.078	0.091	75.384
357	8.430	60.600	0.863	0.039	97.300	2.370	87.591	0.078	0.091	75.384
358	16.500	59.600	0.832	0.038	95.900	2.370	89.234	0.077	0.091	75.384
359	35.500	57.700	0.764	0.037	93.300	2.370	90.876	0.075	0.091	75.384
360	54.400	55.700	0.673	0.037	92.500	2.370	92.518	0.073	0.088	75.384

361	74.400	53.800	0.633	0.029	88.800	2.360	93.339	0.074	0.088	84.619
362	91.600	51.800	0.612	0.021	85.200	2.360	94.161	0.076	0.086	93.854
363	106.000	51.800	0.592	0.020	83.400	3.990	93.613	0.098	0.090	93.854
364	113.000	54.600	0.536	0.018	79.800	3.320	91.423	0.153	0.097	93.854
365	108.000	64.600	0.507	0.017	74.900	4.040	90.329	0.249	0.124	93.854
366	93.100	48.300	0.479	0.017	72.200	3.680	89.781	0.234	0.188	93.854
367	72.600	41.100	0.440	0.016	67.100	3.260	88.686	0.092	0.090	93.854
368	55.700	39.100	0.372	0.013	61.900	2.650	95.256	0.060	0.079	93.854
369	38.400	37.700	0.343	0.012	58.300	2.200	94.708	0.056	0.073	93.854
370	20.400	34.700	0.314	0.011	54.000	2.170	93.066	0.054	0.071	93.854
371	9.670	33.200	0.277	0.010	49.000	2.110	91.971	0.053	0.070	95.912
372	4.950	32.300	0.255	0.010	46.700	2.040	95.803	0.050	0.066	97.970
373	3.110	30.800	0.235	0.013	42.700	2.040	94.708	0.047	0.066	97.970
374	2.550	29.300	0.234	0.013	40.000	2.040	93.613	0.046	0.063	97.970
375	2.360	27.400	0.215	0.014	35.500	2.040	92.518	0.044	0.063	97.970
376	2.290	25.900	0.198	0.014	31.300	2.040	91.971	0.044	0.060	97.970
377	2.230	23.900	0.181	0.014	29.700	2.040	90.876	0.042	0.057	97.970
378	2.110	22.400	0.177	0.015	26.600	2.030	89.781	0.040	0.055	97.970
379	2.020	21.000	0.173	0.015	23.400	2.030	89.234	0.039	0.053	97.970
380	1.970	19.500	0.153	0.017	20.300	2.030	88.686	0.036	0.051	97.970
381	1.930	18.000	0.138	0.018	17.400	2.030	87.591	0.035	0.051	97.418
382	1.910	16.100	0.131	0.020	16.700	2.030	87.044	0.034	0.050	96.866
383	1.920	15.100	0.124	0.021	14.000	2.020	86.496	0.034	0.050	96.866
384	2.070	13.600	0.118	0.022	11.800	2.020	85.949	0.032	0.049	96.866
385	2.270	12.600	0.114	0.024	9.980	2.020	88.139	0.033	0.048	96.866
386	2.470	11.600	0.109	0.029	9.070	2.020	86.496	0.032	0.048	96.866
387	2.600	10.600	0.100	0.033	7.730	2.020	95.256	0.031	0.047	96.866
388	2.730	9.610	0.088	0.036	6.6	2.020	91.423	0.031	0.047	96.866
389	2.830	9.090	0.082	0.040	5.27	2.010	90.876	0.029	0.047	96.866

390	2.730	8.090	0.075	0.044	4.57	2.010	89.781	0.029	0.047	96.866
391	2.540	7.100	0.069	0.048	4.12	2.040	88.686	0.031	0.045	115.134
392	2.380	6.570	0.066	0.127	2.76	2.070	85.949	0.030	0.044	133.403
393	2.160	6.060	0.063	0.201	2.31	2.070	99.088	0.030	0.042	133.403
394	1.910	5.080	0.063	0.242	1.86	2.120	98.540	0.029	0.043	133.403
395	1.880	4.540	0.059	0.231	1.4	2.120	97.993	0.029	0.045	133.403
396	2.680	4.510	0.055	0.226	0.937	2.120	97.445	0.031	0.046	133.403
397	5.910	4.440	0.052	0.220	0.926	2.120	96.898	0.033	0.046	133.403
398	10.900	4.410	0.049	0.202	0.468	2.120	96.350	0.034	0.047	133.403
399	18.300	4.370	0.045	0.183	0.011	2.300	94.161	0.035	0.049	133.403
400	25.800	4.350	0.041	0.161	0	2.300	107.847	0.035	0.052	133.403
401	33.700	0.000	0.038	0.138	0	2.290	107.299	0	0	141.584
402	41.200	0.000	0.033	0.129	0	3.800	106.752	0	0	149.765
403	45.300	0	0.030	0.120	0	6.020	104.015	0	0	149.765
404	46.100	0	0.027	0.116	0	11.500	101.277	0	0	149.765
405	42.300	0	0.025	0.112	0	9.570	100.182	0	0	149.765
406	37.400	0	0.023	0.108	0	6.800	118.796	0	0	149.765
407	31.400	0	0.019	0.104	0	4.510	102.372	0	0	149.765
408	23.300	0	0.018	0.104	0	2.820	101.825	0	0	149.765
409	17.100	0	0.018	0.104	0	3.060	100.730	0	0	149.765
410	9.700	0	0.016	0.104	0	2.820	102.920	0	0	149.765
411	5.880	0	0.014	0.104	0	2.400	125.912	0	0	150.116
412	4.000	0	0.013	0.104	0	2.510	125.629	0	0	150.468
413	2.870	0	0.012	0.104	0	2.570	125.346	0	0	150.468
414	2.290	0	0.011	0.104	0	2.600	125.062	0	0	150.468
415	1.980	0	0.010	0.114	0	2.630	134.735	0	0	150.468
416	1.940	0	0.009	0.124	0	2.690	124.779	0	0	150.468
417	1.890	0	0.008	0.133	0	2.690	124.818	0	0	150.468
418	1.870	0	0.007	0.143	0	2.680	128.103	0	0	150.468

419	1.890	0	0.006	0.175	0	2.700	131.387	0	0	150.468
420	1.970	0	0.006	0.191	0	2.750	134.672	0	0	150.468
421	2.000	0	0.005	0.207	0	2.800	136.314	0	0	142.337
422	2.070	0	0.005	0.261	0	2.800	137.956	0	0	134.206
423	2.160	0	0.005	0.315	0	2.800	134.672	0	0	134.206
424	2.280	0	0.004	0.396	0	2.850	136.347	0	0	134.206
425	2.470	0	0.004	0.548	0	2.850	138.022	0	0	134.206
426	2.990	0	0.003	0.512	0	2.910	139.697	0	0	134.206
427	4.470	0	0.003	0.494	0	2.970	140.535	0	0	134.206
428	10.900	0	0.003	0.476	0	3.030	141.372	0	0	134.206
429	22.900	0	0.003	0.414	0	3.030	142.000	0	0	134.206
430	34.600	0	0.003	0.378	0	3.100	143.223	0	0	134.206
431	53.300	0	0.003	0.361	0	3.140	144.000	0	0	147.607
432	67.800	0	0.003	0.343	0	3.200	145.073	0	0	161.008
433	81.200	0	0.002	0.332	0	3.380	134.672	0	0	161.008
434	87.900	0	0.002	0.321	0	3.560	144.690	0	0	161.008
435	90.000	0	0.003	0.309	0	36.300	145.022	0	0	161.008
436	80.600	0	0.003	0.298	0	32.100	145.188	0	0	161.008
437	66.200	0	0.003	0.298	0	27.900	145.354	0	0	161.008
438	54.200	0	0.004	0.297	0	8.550	145.520	0	0	161.008
439	36.000	0	0.005	0.288	0	7.950	145.686	0	0	161.008
440	21.600	0	0.005	0.278	0	3.910	145.852	0	0	161.008
441	12.400	0	0.004	0.268	0	3.550	146.018	0	0	173.605
442	5.410	0	0.004	0.258	0	3.300	146.350	0	0	186.203
443	3.290	0	0.003	0.258	0	3.420	146.516	0	0	186.203
444	2.700	0	0.003	0.258	0	3.540	146.682	0	0	186.203
445	2.420	0	0.003	0.258	0	3.600	146.847	0	0	186.203
446	2.250	0	0.003	0.258	0	3.600	147.013	0	0	186.203
447	2.190	0	0.003	0.258	0	3.600	147.179	0	0	186.203

448	2.090	0	0.002	0.258	0	3.650	147.345	0	0	186.203
449	1.990	0	0.002	0.269	0	3.710	149.453	0	0	186.203
450	1.980	0	0.002	0.263	0	3.710	149.590	0	0	186.203
451	1.890	0	0.002	0.257	0	3.710	149.658	0	0	187.909
452	1.840	0	0.002	0.257	0	3.710	149.727	0	0	189.616
453	1.850	0	0.002	0.257	0	3.770	149.795	0	0	189.616
454	1.770	0	0.001	0.257	0	3.880	149.829	0	0	189.616
455	1.780	0	0.001	0.257	0	3.880	150.000	0	0	189.616
456	1.760	0	0.001	0.257	0	3.940	150.000	0	0	189.616
457	1.720	0	0.001	0.257	0	3.940	150.000	0	0	189.616
458	1.730	0	0.001	0.257	0	3.940	150.000	0	0	189.616
459	1.680	0	0.001	0.257	0	4.000	150.000	0	0	189.616
460	1.690	0	0.001	0.257	0	4.060	150.000	0	0	189.616
461	1.680	0	0.001	0.257	0	4.050	150.000	0	0	187.558
462	1.650	0	0.001	0.257	0	4.050	150.000	0	0	185.500
463	1.690	0	0.001	0.257	0	4.110	150.000	0	0	185.500
464	1.680	0	0.001	0.257	0	4.110	150.000	0	0	185.500
465	1.680	0	0.001	0.261	0	4.170	150.000	0	0	185.500
466	1.740	0	0.001	0.266	0	4.170	150.000	0	0	185.500
467	1.750	0	0.001	0.266	0	4.220	150.000	0	0	185.500
468	1.760	0	0.001	0.266	0	4.220	148.673	0	0	185.500
469	1.810	0	0.001	0.266	0	4.280	149.005	0	0	185.500
470	1.830	0	0.001	0.266	0	4.280	149.337	0	0	185.500
471	1.840	0	0.001	0.266	0	4.280	149.668	0	0	187.457
472	1.830	0	0.001	0.266	0	4.330	150.000	0	0	189.415
473	1.850	0	0.001	0.266	0	4.330	149.863	0	0	189.415
474	1.880	0	0.001	0.266	0	4.330	149.727	0	0	189.415
475	1.870	0	0.001	0.266	0	4.330	149.384	0	0	189.415
476	1.850	0	0.001	0.272	0	4.330	149.316	0	0	189.415

477	1.850	0	0.001	0.277	0	4.330	149.453	0	0	189.415
478	1.860	0	0.001	0.277	0	4.380	148.905	0	0	189.415
479	1.900	0	0.001	0.277	0	4.380	148.905	0	0	189.415
480	1.910	0	0.001	0.277	0	4.440	148.905	0	0	189.415
481	1.950	0	0.001	0.277	0	4.440	148.905	0	0	183.492
482	1.960	0	0.001	0.277	0	4.500	148.905	0	0	177.570
483	2.010	0	0.001	0.277	0	4.490	148.905	0	0	177.570
484	2.090	0	0.001	0.277	0	4.490	148.905	0	0	177.570
485	2.300	0	0.001	0.276	0	4.490	148.358	0	0	177.570
486	2.530	0	0.001	0.276	0	4.490	148.084	0	0	177.570
487	2.790	0	0.001	0.276	0	4.490	147.947	0	0	177.570
488	2.950	0	0.001	0.276	0	4.490	147.810	0	0	177.570
489	3.230	0	0.001	0.275	0	4.480	147.263	0	0	177.570
490	3.350	0	0.001	0.275	0	4.480	146.786	0	0	177.570
491	3.360	0	0.001	0.275	0	4.480	146.547	0	0	177.570
492	3.340	0	0.001	0.270	0	4.480	146.309	0	0	177.570
493	3.200	0	0.001	0.262	0	4.540	145.831	0	0	177.570
494	2.880	0	0.001	0.250	0	4.600	145.593	0	0	177.570
495	2.710	0	0.001	0.240	0	4.630	145.354	0	0	177.570
496	2.430	0	0.001	0.238	0	4.650	145.558	0	0	177.570
497	2.190	0	0.001	0.238	0	4.650	145.761	0	0	177.570
498	2.070	0	0.001	0.238	0	4.530	145.965	0	0	177.570
499	2.030	0	0.001	0.238	0	4.410	146.066	0	0	177.570
500	1.950	0	0.001	0.238	0	4.400	146.168	0	0	177.570
501	1.900	0	0.001	0.237	0	4.400	145.620	0	0	179.226
502	1.880	0	0.001	0.237	0	4.400	143.363	0	0	180.883
503	1.890	0	0.001	0.237	0	4.400	143.791	0	0	180.883
504	1.930	0	0.001	0.237	0	4.400	144.218	0	0	180.883
505	1.910	0	0.001	0.237	0	4.460	144.646	0	0	180.883

506	1.900	0	0.001	0.237	0	4.580	145.073	0	0	180.883
507	1.950	0	0.001	0.237	0	4.630	144.148	0	0	180.883
508	1.940	0	0.001	0.236	0	4.690	143.223	0	0	180.883
509	1.940	0	0.001	0.236	0	4.690	141.372	0	0	180.883
510	1.980	0	0.001	0.236	0	4.690	142.949	0	0	180.883
511	1.980	0	0.001	0.236	0	4.690	144.526	0	0	174.659
512	1.970	0	0.001	0.236	0	4.690	144.525	0	0	168.436
513	2.020	0	0.001	0.236	0	4.740	144.524	0	0	168.436
514	1.990	0	0.001	0.215	0	4.770	144.252	0	0	168.436
515	1.990	0	0.001	0.215	0	4.800	144.115	0	0	168.436
516	2.020	0	0.001	0.215	0	4.860	144.047	0	0	168.436
517	1.980	0	0.001	0.215	0	4.920	143.978	0	0	168.436
518	2.010	0	0.001	0.215	0	4.920	143.841	0	0	168.436
519	2.020	0	0.001	0.214	0	4.910	143.773	0	0	168.436
520	2.010	0	0.001	0.214	0	4.970	143.705	0	0	168.436
521	2.050	0	0.001	0.214	0	4.970	143.568	0	0	173.103
522	2.040	0	0.001	0.214	0	5.030	143.499	0	0	177.771
523	2.080	0	0.001	0.213	0	5.030	143.431	0	0	177.771
524	2.100	0	0.001	0.213	0	5.150	143.300	0	0	177.771
525	2.110	0	0.001	0.213	0	5.140	143.157	0	0	177.771
526	2.180	0	0.001	0.213	0	5.140	143.020	0	0	177.771
527	2.220	0	0.001	0.213	0	5.140	142.952	0	0	177.771
528	2.260	0	0.001	0.213	0	5.140	142.883	0	0	177.771
529	2.330	0	0.001	0.213	0	5.140	141.788	0	0	177.771
530	2.450	0	0.001	0.212	0	5.130	137.389	0	0	177.771
531	2.570	0	0.001	0.212	0	5.130	138.215	0	0	176.215
532	2.650	0	0.001	0.212	0	5.130	139.041	0	0	174.659
533	2.750	0	0.002	0.220	0	5.130	139.867	0	0	174.659
534	2.900	0	0.001	0.228	0	5.130	140.693	0	0	174.659

535	3.010	0	0.002	0.235	0	5.130	140.146	0	0	174.659
536	3.090	0	0.002	0.239	0	5.120	138.104	0	0	174.659
537	3.490	0	0.002	0.243	0	5.120	136.062	0	0	174.659
538	5.250	0	0.002	0.267	0	5.120	137.831	0	0	174.659
539	10.700	0	0.002	0.279	0	5.120	138.715	0	0	174.659
540	25.700	0	0.002	0.292	0	5.120	139.599	0	0	174.659
541	45.000	0	0.002	0.299	0	5.120	139.325	0	0	174.659
542	65.800	0	0.002	0.306	0	5.050	139.052	0	0	174.659
543	87.200	0	0.002	0.313	0	5.050	138.778	0	0	174.659
544	106.000	0	0.002	0.320	0	5.050	138.641	0	0	174.659
545	118.000	0	0.002	0.320	0	5.050	138.504	0	0	174.659
546	120.000	0	0.002	0.330	0	5.050	137.956	0	0	174.659
547	114.000	0	0.002	0.330	0	5.160	137.682	0	0	174.659
548	98.300	0	0.002	0.330	0	27.500	137.409	0	0	174.659
549	79.000	0	0.002	0.343	0	22.400	137.135	0	0	174.659
550	54.700	0	0.002	0.348	0	17.200	136.998	0	0	174.659
551	36.300	0	0.002	0.351	0	11.400	136.861	0	0	170.343
552	17.000	0	0.002	0.354	0	8.140	136.314	0	0	166.027
553	8.610	0	0.002	0.360	0	4.850	136.177	0	0	166.027
554	5.430	0	0.002	0.365	0	4.790	136.040	0	0	166.027
555	4.200	0	0.002	0.365	0	4.790	135.903	0	0	166.027
556	3.850	0	0.002	0.365	0	4.760	135.835	0	0	166.027
557	3.710	0	0.002	0.365	0	4.730	135.766	0	0	166.027
558	3.550	0	0.002	0.364	0	4.780	135.219	0	0	166.027
559	3.430	0	0.002	0.364	0	4.720	135.219	0	0	166.027
560	3.340	0	0.002	0.364	0	4.720	135.219	0	0	166.027
561	3.330	0	0.002	0.364	0	4.720	135.219	0	0	166.027
562	3.340	0	0.002	0.363	0	4.720	135.219	0	0	166.027
563	3.300	0	0.002	0.363	0	4.720	134.945	0	0	166.027

564	3.310	0	0.002	0.363	0	4.710	134.808	0	0	166.027
565	3.380	0	0.002	0.363	0	4.710	134.672	0	0	166.027
566	3.420	0	0.002	0.363	0	4.710	134.398	0	0	166.027
567	3.580	0	0.002	0.363	0	4.710	134.261	0	0	166.027
568	4.030	0	0.002	0.362	0	4.710	134.124	0	0	166.027
569	5.710	0	0.002	0.358	0	4.700	133.447	0	0	166.027
570	9.400	0	0.002	0.355	0	4.700	132.770	0	0	166.027
571	20.200	0	0.002	0.353	0	4.700	132.093	0	0	160.706
572	37.500	0	0.002	0.349	0	4.700	131.416	0	0	155.386
573	57.700	0	0.002	0.346	0	4.700	131.250	0	0	155.386
574	77.600	0	0.002	0.344	0	4.690	131.167	0	0	155.386
575	98.200	0	0.002	0.333	0	4.690	131.084	0	0	155.386
576	110.000	0	0.002	0.327	0	4.690	130.918	0	0	155.386
577	116.000	0	0.002	0.324	0	4.700	130.835	0	0	155.386
578	117.000	0	0.002	0.321	0	4.960	130.752	0	0	155.386
579	104.000	0	0.001	0.310	0	5.230	133.029	0	0	155.386
580	87.200	0	0.001	0.304	0	5.050	132.892	0	0	155.386
581	67.300	0	0.001	0.301	0	5.470	132.824	0	0	155.386
582	45.200	0	0.001	0.298	0	5.890	132.756	0	0	155.386
583	30.300	0	0.001	0.291	0	5.460	132.619	0	0	155.386
584	16.000	0	0.001	0.284	0	5.340	132.550	0	0	155.386
585	8.520	0	0.001	0.278	0	5.160	132.482	0	0	155.386
586	5.930	0	0.001	0.271	0	4.730	132.345	0	0	155.386
587	4.660	0	0.001	0.271	0	4.730	132.277	0	0	155.386
588	4.360	0	0.001	0.271	0	4.730	132.208	0	0	155.386
589	4.080	0	0.001	0.270	0	4.730	132.071	0	0	155.386
590	3.990	0	0.001	0.261	0	4.730	132.003	0	0	155.386
591	3.880	0	0.001	0.253	0	4.730	131.934	0	0	158.097
592	3.790	0	0.000	0.244	0	4.720	131.141	0	0	160.807

593	3.770	0	0.000	0.235	0	4.720	130.744	0	0	160.807
594	3.660	0	0.000	0.229	0	4.720	130.348	0	0	160.807
595	3.640	0	0	0.224	0	4.660	129.951	0	0	160.807
596	3.620	0	0	0.219	0	4.660	129.554	0	0	160.807
597	3.580	0	0	0.213	0	4.660	129.677	0	0	160.807
598	3.610	0	0	0.209	0	4.650	129.219	0	0	160.807
599	3.570	0	0	0.204	0	4.650	128.761	0	0	160.807
600	3.560	0	0	0.199	0	4.650	129.800	0	0	160.807
601	3.590	0	0	0.194	0	4.650	130.320	0	0	160.807
602	3.580	0	0	0.182	0	4.650	130.839	0	0	160.807
603	3.620	0	0	0.170	0	4.640	130.702	0	0	160.807
604	3.640	0	0	0.165	0	4.700	130.634	0	0	160.807
605	3.630	0	0	0.163	0	4.700	130.566	0	0	160.807
606	3.690	0	0	0.161	0	4.700	130.360	0	0	160.807
607	3.690	0	0	0.154	0	4.700	130.326	0	0	160.807
608	3.740	0	0	0.147	0	4.700	130.292	0	0	160.807
609	3.770	0	0	0.140	0	4.690	130.155	0	0	160.807
610	3.750	0	0	0.133	0	4.690	130.019	0	0	160.807
611	3.790	0	0	0.130	0	4.690	129.882	0	0	157.745
612	3.770	0	0	0.128	0	4.690	129.813	0	0	154.684
613	3.790	0	0	0.127	0	4.690	129.745	0	0	154.684
614	3.790	0	0	0.125	0	4.690	129.608	0	0	154.684
615	3.750	0	0	0.124	0	4.680	129.540	0	0	154.684
616	3.780	0	0	0.122	0	4.680	129.471	0	0	154.684
617	3.760	0	0	0.121	0	4.740	129.197	0	0	154.684
618	3.820	0	0	0.117	0	4.740	129.197	0	0	154.684
619	3.870	0	0	0.113	0	4.740	129.197	0	0	154.684
620	3.900	0	0	0.109	0	4.730	128.922	0	0	154.684
621	3.990	0	0	0.105	0	4.730	128.785	0	0	154.684

622	4.010	0	0	0.100	0	4.730	128.647	0	0	154.684
623	4.080	0	0	0.095	0	4.730	128.510	0	0	154.684
624	4.060	0	0	0.093	0	4.730	128.372	0	0	154.684
625	4.060	0	0	0.091	0	4.730	128.235	0	0	154.684
626	4.040	0	0	0.087	0	4.720	128.097	0	0	154.684
627	4.000	0	0	0.085	0	4.720	128.235	0	0	154.684
628	4.010	0	0	0.083	0	4.660	128.374	0	0	154.684
629	3.940	0	0	0.079	0	4.660	128.512	0	0	154.684
630	3.970	0	0	0.077	0	4.660	128.650	0	0	154.684
631	3.960	0	0	0.075	0	4.650	128.513	0	0	153.228
632	3.990	0	0	0.073	0	4.650	128.445	0	0	151.773
633	4.010	0	0	0.070	0	4.590	128.376	0	0	151.773
634	4.030	0	0	0.068	0	4.590	128.239	0	0	151.773
635	4.030	0	0	0.065	0	4.590	128.171	0	0	151.773
636	4.070	0	0	0.062	0	4.590	128.102	0	0	151.773
637	4.070	0	0	0.059	0	4.520	127.769	0	0	151.773
638	4.130	0	0	0.057	0	4.520	127.436	0	0	151.773
639	4.100	0	0	0.055	0	4.520	127.103	0	0	151.773
640	4.140	0	0	0.054	0	4.460	126.770	0	0	151.773
641	4.140	0	0	0.047	0	4.460	128.102	0	0	151.773
642	4.180	0	0	0.043	0	4.450	127.965	0	0	151.773
643	4.180	0	0	0.039	0	4.450	127.897	0	0	151.773
644	4.190	0	0	0.038	0	4.450	127.829	0	0	151.773
645	4.220	0	0	0.037	0	4.390	127.692	0	0	151.773
646	4.230	0	0	0.036	0	4.390	127.623	0	0	151.773
647	4.270	0	0	0.035	0	4.390	127.555	0	0	151.773
648	4.260	0	0	0.034	0	4.320	127.208	0	0	151.773
649	4.300	0	0	0.033	0	4.320	126.861	0	0	151.773
650	4.290	0	0	0.032	0	4.260	126.514	0	0	151.773

651	4.350	0	0	0.029	0	4.260	126.167	0	0	149.163
652	4.330	0	0	0.027	0	4.260	125.473	0	0	146.553
653	4.380	0	0	0.026	0	4.200	125.126	0	0	146.553
654	4.370	0	0	0.025	0	4.190	124.779	0	0	146.553
655	4.430	0	0	0.024	0	4.070	125.336	0	0	146.553
656	4.410	0	0	0.024	0	4.010	125.893	0	0	146.553
657	4.450	0	0	0.024	0	4.010	126.450	0	0	146.553
658	4.460	0	0	0.022	0	4.010	127.007	0	0	146.553
659	4.500	0	0	0.020	0	3.940	125.561	0	0	146.553
660	4.510	0	0	0.020	0	3.940	124.838	0	0	146.553
661	4.520	0	0	0.019	0	3.880	124.115	0	0	146.553
662	4.540	0	0	0.019	0	3.820	125.288	0	0	146.553
663	4.560	0	0	0.018	0	3.810	125.874	0	0	146.553
664	4.580	0	0	0.017	0	3.810	126.460	0	0	146.553
665	4.590	0	0	0.017	0	3.810	125.376	0	0	146.553
666	4.640	0	0	0.016	0	3.810	124.292	0	0	146.553
667	4.690	0	0	0.016	0	3.810	123.208	0	0	146.553
668	4.760	0	0	0.015	0	3.750	122.124	0	0	146.553
669	4.790	0	0	0.014	0	3.680	123.071	0	0	146.553
670	4.850	0	0	0.013	0	3.620	123.545	0	0	146.553
671	4.890	0	0	0.013	0	3.620	124.018	0	0	134.257
672	4.920	0	0	0.012	0	3.620	124.492	0	0	121.960
673	4.920	0	0	0.011	0	3.560	124.965	0	0	121.960
674	4.940	0	0	0.011	0	3.560	125.439	0	0	121.960
675	4.940	0	0	0.010	0	3.490	125.912	0	0	121.960
676	4.930	0	0	0.010	0	3.430	125.365	0	0	121.960
677	4.900	0	0	0.009	0	3.370	124.818	0	0	121.960
678	4.910	0	0	0.008	0	3.340	124.681	0	0	121.960
679	4.910	0	0	0.008	0	3.300	124.544	0	0	121.960

680	4.940	0	0	0.008	0	3.300	124.407	0	0	121.960
681	4.950	0	0	0.007	0	3.240	124.270	0	0	121.960
682	5.010	0	0	0.007	0	3.180	124.270	0	0	121.960
683	4.990	0	0	0.007	0	3.180	124.270	0	0	121.960
684	5.060	0	0	0.007	0	3.180	124.270	0	0	121.960
685	5.160	0	0	0.007	0	3.170	124.270	0	0	121.960
686	5.440	0	0	0.006	0	3.110	124.270	0	0	121.960
687	5.760	0	0	0.006	0	3.050	123.723	0	0	121.960
688	6.130	0	0	0.006	0	3.020	123.175	0	0	121.960
689	6.530	0	0	0.006	0	2.990	122.902	0	0	121.960
690	6.680	0	0	0.005	0	3.040	122.765	0	0	121.960
691	6.790	0	0	0.005	0	2.920	122.628	0	0	129.740
692	6.880	0	0	0.005	0	2.980	122.628	0	0	137.519
693	6.700	0	0	0.005	0	2.950	122.080	0	0	137.519
694	6.450	0	0	0.005	0	2.920	121.533	0	0	137.519
695	6.220	0	0	0.004	0	2.920	120.985	0	0	137.519
696	5.780	0	0	0.004	0	2.790	120.712	0	0	137.519
697	5.570	0	0	0.004	0	2.790	120.575	0	0	137.519
698	5.410	0	0	0.004	0	2.760	120.438	0	0	137.519
699	5.390	0	0	0.004	0	2.730	119.891	0	0	137.519
700	5.390	0	0	0.004	0	2.730	119.343	0	0	137.519
701	5.390	0	0	0.004	0	2.660	117.153	0	0	137.519
702	5.460	0	0	0.003	0	2.600	116.606	0	0	137.519
703	5.490	0	0	0.003	0	2.600	118.796	0	0	137.519
704	5.630	0	0	0.003	0	2.570	118.248	0	0	137.519
705	5.750	0	0	0.003	0	2.540	112.774	0	0	137.519
706	5.910	0	0	0.003	0	2.480	112.774	0	0	137.519
707	6.010	0	0	0.003	0	2.470	112.774	0	0	137.519
708	6.070	0	0	0.003	0	2.350	112.774	0	0	137.519

709	6.160	0	0	0.002	0	2.290	112.774	0	0	137.519
710	6.110	0	0	0.002	0	2.290	108.394	0	0	137.519
711	6.100	0	0	0.002	0	2.290	96.898	0	0	125.775
712	6.030	0	0	0.002	0	2.280	99.088	0	0	114.030
713	5.910	0	0	0.002	0	2.280	101.277	0	0	114.030
714	5.840	0	0	0.002	0	2.280	103.467	0	0	114.030
715	5.740	0	0	0.002	0	2.220	105.657	0	0	114.030
716	5.770	0	0	0.002	0	2.220	105.109	0	0	114.030
717	5.740	0	0	0.002	0	2.150	97.993	0	0	114.030
718	5.770	0	0	0.002	0	2.150	97.582	0	0	114.030
719	5.790	0	0	0.002	0	2.150	97.172	0	0	115.285
720	5.820	0	0	0.002	0	2.090	96.761	0	0	116.540
721	5.840	0	0	0.002	0	2.090	96.556	0	0	116.540
722	5.850	0	0	0.002	0	2.080	96.350	0	0	116.540
723	5.910	0	0	0.001	0	2.020	95.963	0	0	116.540
724	5.880	0	0	0.001	0	2.020	95.769	0	0	116.540
725	5.930	0	0	0.001	0	2.020	95.575	0	0	116.540
726	5.940	0	0	0.001	0	1.960	95.689	0	0	122.512
727	5.980	0	0	0.001	0	1.950	95.803	0	0	128.485
728	5.990	0	0	0.001	0	1.950	95.580	0	0	128.485
729	6.000	0	0	0.001	0	1.890	95.357	0	0	128.485
730	6.050	0	0	0.001	0	1.890	95.134	0	0	128.485
731	6.030	0	0	0.001	0	1.830	95.023	0	0	128.485
732	6.070	0	0	0.001	0	1.830	94.912	0	0	128.485
733	6.070	0	0	0.001	0	1.820	95.256	0	0	128.485
734	6.120	0	0	0.001	0	1.820	92.518	0	0	128.485
735	6.110	0	0	0.001	0	1.820	93.203	0	0	128.485
736	6.150	0	0	0.001	0	1.820	93.887	0	0	128.485
737	6.180	0	0	0.001	0	1.790	94.571	0	0	128.485

738	6.200	0	0	0.001	0	1.820	95.256	0	0	128.485
739	6.230	0	0	0.001	0	1.750	92.518	0	0	128.485
740	6.230	0	0	0.001	0	1.750	96.487	0	0	128.485
741	6.290	0	0	0.001	0	1.630	100.456	0	0	126.829
742	6.260	0	0	0.001	0	1.630	104.425	0	0	125.172
743	6.310	0	0	0.001	0	1.560	108.394	0	0	125.172
744	6.300	0	0	0.001	0	1.560	103.467	0	0	125.172
745	6.350	0	0	0.001	0	1.560	100.221	0	0	125.172
746	6.350	0	0	0.001	0	1.560	102.401	0	0	125.172
747	6.370	0	0	0.001	0	1.560	104.582	0	0	125.172
748	6.420	0	0	0.001	0	1.560	106.762	0	0	125.172
749	6.420	0	0	0.001	0	1.550	108.942	0	0	125.172
750	6.470	0	0	0.001	0	1.550	97.993	0	0	125.172
751	6.460	0	0	0.001	0	1.550	101.004	0	0	125.172
752	6.520	0	0	0.001	0	1.490	104.014	0	0	125.172
753	6.510	0	0	0.001	0	1.430	107.025	0	0	125.172
754	6.560	0	0	0.001	0	1.430	110.036	0	0	124.118
755	6.560	0	0	0	0	1.420	109.489	0	0	123.064
756	6.610	0	0	0	0	1.420	109.626	0	0	123.064
757	6.600	0	0	0	0	1.420	109.763	0	0	123.064
758	6.630	0	0	0	0	1.420	109.899	0	0	123.064
759	6.650	0	0	0	0	1.420	109.968	0	0	99.224
760	6.660	0	0	0	0	1.420	110.036	0	0	75.384
761	6.670	0	0	0	0	1.350	91.423	0	0	75.384
762	6.680	0	0	0	0	1.350	95.940	0	0	75.384
763	6.720	0	0	0	0	1.350	100.456	0	0	75.384
764	6.719	0	0	0	0	1.350	104.973	0	0	92.700
765	6.759	0	0	0	0	1.350	107.231	0	0	110.015
766	6.768	0	0	0	0	1.340	109.489	0	0	110.015

767	6.849	0	0	0	0	1.340	93.613	0	0	110.015
768	6.848	0	0	0	0	1.340	74.453	0	0	110.015
769	6.950	0	0	0	0	1.310	53.650	0	0	113.880
770	7.003	0	0	0	0	1.280	36.131	0	0	117.744
771	7.145	0	0	0	0	1.220	34.489	0	0	117.744
772	7.175	0	0	0	0	1.150	97.445	0	0	117.744
773	7.257	0	0	0	0	1.150	85.402	0	0	117.744
774	7.258	0	0	0	0	1.150	67.336	0	0	117.744
775	7.316	0	0	0	0	1.150	45.985	0	0	117.744
776	7.275	0	0	0	0	1.150	31.752	0	0	117.744
777	7.252	0	0	0	0	1.140	95.256	0	0	117.744
778	7.216	0	0	0	0	1.140	30.657	0	0	117.744
779	7.182	0	0	0	0	1.080	29.836	0	0	117.744
780	7.123	0	0	0	0	1.080	29.015	0	0	117.744
781	7.115	0	0	0	0	1.080	28.467	0	0	115.335
782	7.149	0	0	0	0	1.080	23.540	0	0	112.926
783	7.166	0	0	0	0	1.070	59.672	0	0	112.926
784	7.178	0	0	0	0	1.070	95.803	0	0	112.926
785	7.163	0	0	0	0	1.070	63.777	0	0	112.926
786	7.193	0	0	0	0	1.070	47.765	0	0	112.926
787	7.236	0	0	0	0	1.070	31.752	0	0	112.926
788	7.243	0	0	0	0	1.000	29.015	0	0	112.926
789	7.245	0	0	0	0	1.000	26.825	0	0	112.926
790	7.235	0	0	0	0	0.999	24.635	0	0	112.926
791	7.265	0	0	0	0	0.968	32.984	0	0	112.926
792	7.308	0	0	0	0	0.937	37.158	0	0	112.926
793	7.323	0	0	0	0	0.934	41.332	0	0	112.926
794	7.335	0	0	0	0	0.933	45.506	0	0	112.926
795	7.329	0	0	0	0	0.932	49.681	0	0	112.926

796	7.348	0	0	0	0	0.930	53.855	0	0	112.926
797	7.396	0	0	0	0	0.927	58.029	0	0	112.926
798	7.373	0	0	0	0	0.926	36.679	0	0	112.926
799	7.389	0	0	0	0	0.925	56.934	0	0	112.926
800	7.479	0	0	0	0	0.922	77.190	0	0	112.926

[a]Ultra-Vitalux lamp: irradiation spectrum provided by Michael Ahrens through personal communication.

[b]Qpanel lamp: irradiation spectrum provided in Diamond et al. [68].

[c,d]Black light and Cool-white light: irradiation spectrum provided in Cody et al. [37].

[e]GE F40 BLB blacklight: irradiation spectrum provided in Gala and Giesy [38].

[f]SSR II: solar simulated radiation irradiation spectrum provided in Lampi et al. [36].

[g]SSR II: UVB-filtered solar simulated radiation irradiation spectrum provided in Lampi et al. [36].

[h]SSR I: solar simulated radiation irradiation spectrum provided by James T. Oris through personal communication.

[i]SolarConstant 1200 lamp: irradiation spectrum provided in [86]

[j]Solar radiation spectral variation was used as the light source spectrum for Newsted and Giesy [11] since the irradiance spectrum was not provided. Standard CWF lamps were combined with RPR-3500 (UVA), and RPR-3000A (UVB) lamps (Southern New England Ultraviolet, Branford, CT, USA) to simulate solar radiation. A combination of Chroma F40C50 white (General Electric, Cleveland, OH) and FS40 ultraviolet (Westinghouse, Bloomfield, NJ) fluorescent bulbs was used to simulate solar radiation.

Table A.6-b. Irradiance spectra ($I(\lambda)$) used by Diamond et al. [68].

λ (nm)	$I^a(\lambda)$ (μW/cm^2/nm)	$I^b(\lambda)$ (μW/cm^2/nm)	$I^c(\lambda)$ (μW/cm^2/nm)	$I^d(\lambda)$ (μW/cm^2/nm)	$I^e(\lambda)$ (μW/cm^2/nm)	$I^f(\lambda)$ (μW/cm^2/nm)
280	0.832	2.057	0.426	0.626	0.000	2.921
281	0.841	2.054	0.434	0.626	0.000	2.919
282	0.851	2.051	0.441	0.626	0.000	2.916
283	0.863	1.760	0.451	0.626	0.000	2.626
284	0.869	1.760	0.454	0.626	0.000	2.622
285	0.583	1.756	0.753	0.626	0.000	2.618
286	0.893	1.753	0.468	0.626	0.000	2.903
287	0.903	1.750	0.473	0.626	0.000	2.900
288	0.912	1.748	0.477	0.626	0.000	2.898
289	0.924	1.745	0.482	0.626	0.000	2.894
290	0.933	2.029	0.490	0.626	0.000	2.893
291	0.942	2.026	0.497	0.626	0.000	2.890
292	0.952	2.024	0.503	0.626	0.000	2.887
293	0.964	2.309	0.510	0.626	0.000	2.885
294	0.973	2.307	0.518	0.626	0.000	3.455
295	0.982	2.303	0.524	0.626	0.000	3.165
296	0.994	2.301	0.525	0.626	0.000	3.163
297	1.299	2.587	0.533	0.626	0.000	3.449
298	1.305	2.584	0.834	0.626	0.000	3.447
299	1.606	2.581	1.133	0.626	0.000	3.731
300	2.210	2.870	1.140	0.626	0.000	3.730
301	2.210	2.860	1.150	1.050	0.000	4.300

302	2.230	3.150	1.450	1.610	0.000	4.590
303	2.530	3.430	1.750	1.620	0.000	4.870
304	2.540	3.720	2.040	1.630	0.000	5.440
305	3.130	4.000	2.050	2.190	0.000	6.300
306	3.720	4.290	2.050	2.190	0.000	6.870
307	4.320	5.150	2.640	2.750	0.000	7.730
308	5.210	5.720	2.930	2.920	0.000	8.880
309	6.680	6.870	3.230	3.090	0.000	10.000
310	7.270	8.010	3.820	3.680	0.000	11.500
311	9.030	9.740	4.990	4.590	0.000	14.900
312	10.200	11.200	5.870	5.300	0.000	17.200
313	10.800	12.300	6.750	5.460	0.000	18.600
314	12.300	14.300	7.050	5.810	0.000	19.600
315	13.200	14.600	7.350	5.910	0.000	20.400
316	14.000	15.200	7.940	6.190	0.000	21.200
317	15.500	16.000	8.230	7.070	0.000	23.000
318	17.600	18.600	9.700	7.370	0.000	27.300
319	18.500	20.600	10.600	8.250	0.000	28.400
320	20.200	22.100	11.500	9.130	0.383	32.700
321	22.300	24.400	12.900	10.000	0.389	34.200
322	24.000	26.700	14.100	10.000	0.394	36.500
323	25.200	28.400	14.700	10.900	0.693	41.100
324	27.000	31.000	16.100	12.100	0.697	43.100
325	28.500	32.700	17.900	12.400	1.290	45.400
326	29.600	34.400	18.800	13.000	1.880	46.800
327	31.400	36.400	19.700	13.800	2.170	50.800

328	33.200	38.200	21.100	14.700	3.060	54.600
329	34.600	40.700	22.600	15.600	3.940	56.300
330	35.800	42.800	24.600	16.200	5.110	58.600
331	36.400	44.500	25.800	17.100	5.990	60.600
332	37.300	47.100	26.700	17.700	6.870	63.700
333	37.600	48.200	27.300	18.200	8.330	65.500
334	37.900	49.100	28.700	18.800	8.920	67.200
335	38.500	51.400	29.600	19.300	10.700	68.300
336	38.500	52.200	30.800	19.700	13.600	70.400
337	38.800	53.400	32.000	20.600	14.200	72.100
338	38.500	54.500	32.800	20.900	15.900	72.600
339	38.200	56.000	33.400	20.900	18.900	73.800
340	37.700	56.800	33.700	21.200	20.900	74.400
341	37.100	57.100	34.300	21.200	22.400	75.200
342	35.900	57.700	34.900	21.700	24.400	75.500
343	35.100	57.700	35.200	21.800	26.200	75.500
344	34.500	58.000	35.500	21.800	27.900	75.500
345	33.600	58.200	35.800	22.100	29.700	75.800
346	32.800	58.200	36.100	22.100	30.600	75.800
347	31.600	58.200	36.100	22.100	31.700	75.800
348	31.000	58.200	36.100	22.100	32.600	75.500
349	29.900	58.200	36.100	22.100	35.000	75.500
350	28.700	57.900	36.100	21.800	35.800	74.900
351	27.300	57.400	36.100	21.900	37.300	74.300
352	26.100	57.100	35.600	21.400	37.900	73.200
353	25.500	55.900	35.300	21.000	38.200	72.000

354	24.400	54.800	35.000	20.400	38.500	70.600
355	23.200	54.500	34.400	20.100	39.400	69.200
356	22.100	53.900	34.100	19.800	39.400	68.600
357	20.900	52.200	33.500	19.600	39.400	67.400
358	19.400	51.900	33.300	19.300	39.100	66.800
359	18.900	50.700	32.400	18.800	38.500	64.800
360	18.300	49.600	31.500	18.100	37.900	62.500
361	17.100	47.600	30.700	17.800	37.400	61.400
362	16.600	47.000	30.700	17.500	37.700	60.200
363	16.600	49.300	32.100	18.100	38.800	61.000
364	16.900	50.400	33.000	18.900	40.600	62.800
365	16.000	50.400	32.700	19.200	41.800	62.800
366	14.800	48.400	31.900	18.200	40.000	58.800
367	13.700	43.800	27.500	17.000	36.800	56.800
368	12.200	39.500	24.900	15.100	33.500	49.300
369	10.800	36.900	23.700	13.200	30.100	46.400
370	10.200	34.000	22.500	12.600	28.700	44.700
371	9.640	33.200	22.000	12.100	27.800	42.900
372	9.650	32.000	20.200	11.500	26.500	41.800
373	9.370	31.100	19.100	11.300	25.200	39.500
374	8.500	28.800	18.500	10.800	23.700	37.700
375	8.220	27.400	18.200	10.300	22.600	35.400
376	7.940	26.200	17.100	9.760	21.100	33.700
377	7.650	24.800	16.500	9.190	20.600	31.700
378	7.090	23.600	15.300	8.900	18.500	30.000
379	7.090	22.200	14.700	8.320	17.700	28.200

380	7.100	20.800	13.900	7.460	16.800	27.100
381	6.530	19.300	13.300	7.170	16.200	25.400
382	6.250	18.500	13.000	6.590	15.300	24.200
383	5.970	18.200	12.400	6.310	14.500	23.100
384	5.980	16.700	11.900	6.320	13.300	21.600
385	5.700	15.900	11.600	5.740	13.000	20.500
386	5.700	15.000	10.100	5.890	12.400	19.600
387	5.710	14.400	9.540	5.750	11.600	18.700
388	5.430	13.600	9.250	5.170	11.000	17.300
389	5.440	12.100	8.390	4.890	10.400	16.100
390	5.160	11.500	8.100	4.460	9.850	13.800
391	5.170	11.000	7.240	4.030	9.560	13.000
392	4.890	10.100	6.950	3.740	8.700	12.400
393	4.890	9.800	6.370	3.460	8.120	12.100
394	4.610	8.930	6.090	3.170	7.540	11.500
395	4.330	8.350	5.800	2.880	6.680	10.700
396	4.350	7.780	5.510	2.890	6.100	9.500
397	4.070	7.490	5.230	2.900	6.100	8.350

398	3.780	7.200	4.940	2.610	5.820	7.770
399	3.790	6.330	4.660	2.330	5.240	7.770
400	3.800	6.040	4.080	2.330	5.240	7.480

[a] KCr-filtered Qpanel lamp: irradiation spectrum provided in Diamond et al. [68]

[b]ND1-filtered Qpanel lamp: irradiation spectrum provided in Diamond et al. [68]

[c]ND2-filtered Qpanel lamp: irradiation spectrum provided in Diamond et al. [68]

[d]ND3-filtered Qpanel lamp: irradiation spectrum provided in Diamond et al. [68]

[e]Silica galss-filtered Qpanel lamp: irradiation spectrum provided in Diamond et al. [68]

[f] ND-unfiltered Qpanel lamp: irradiation spectrum provided in Diamond et al. [68].

A.2 Comparison between PAHs Absorption in Solvent Octanol and other Solvents (Cyclohexane or Ethanol)

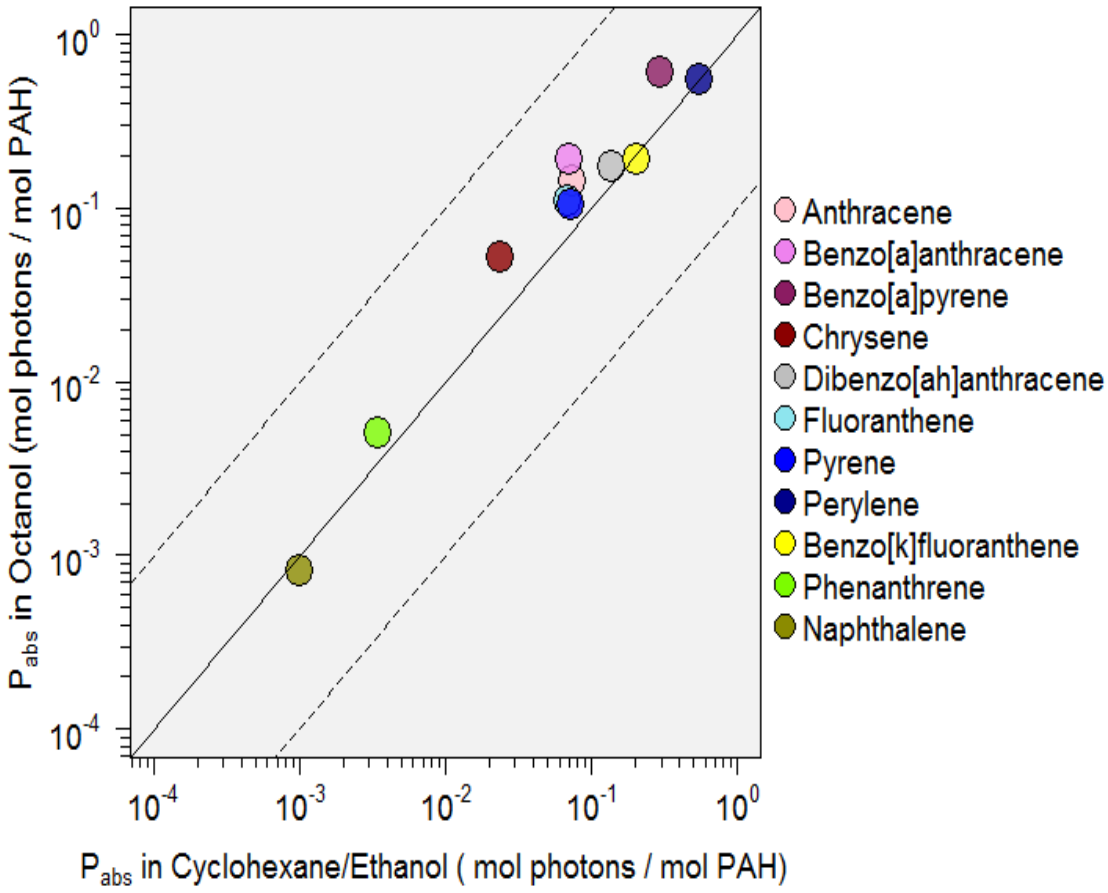

Figure A.1. P_{abs} (mol photon/mol PAH) calculated using Equation 3-5 based on PAHs $\varepsilon(\lambda)$ measured in octanol shown on y axis versus those calculated based on $\varepsilon(\lambda)$ measured in cyclohexane or ethanol (x axis). For $I(\lambda)$ and T_{exp} , solar radiation spectrum [87] and light exposure duration of 12 h are considered, respectively. P_{abs} are associated with the $\varepsilon(\lambda)$ measured in cyclohexane [56] except for perylene for which $\varepsilon(\lambda)$ is measured in ethanol [74].

A.3 Computational Example for PLC50 Prediction

Here a stepwise procedure to predict PLC50 of PAHs is provided. The example calculation is run for fluoranthene exposed to *Mysidopsis bahia* under SolarConstant 1200 radiation with UVB, UVA, and VIS intensities of I_{UVB} = 50 (μW/cm^2), I_{UVA} = 700 (μW/cm^2), and I_{VIS} = 4000 (μW/cm^2).

NLC50 Calculation

To calculate PLC50, the toxicity in the absence of light (NLC50) needs to be determined. Substituting $\log(K_{OW})$ = 5.19 for fluoranthene (Table S3) and $\log(C^*_{LN})$ = 1.535 (Table A4) in the NTLM (Equation 3) yields NLC50 = 42.763 (μg/L).

Light Absorption

Another key parameter to be determined is the dose of light energy (P_{abs}) which is expressed as moles of photons absorbed per mole of PAH in the PTLM framework. Due to the practical importance of the unit in which P_{abs} is expressed in this study, fist, the dimensional analysis used to obtain the dose of light in terms of moles of photon per mole of PAH is presented.

Dimensional Analysis

Energy Absorbed

The intensity of light delivered at wavelength λ is

$$I(\lambda)\ \left(\frac{\mu W}{cm^2\ nm}\right)=\left(\frac{10^{-2}J}{s\ m^2\ nm}\right) \tag{A-1}$$

Molar absorption coeffcient of the chemical at λ is

$$\varepsilon(\lambda)\ \left(\frac{1}{cm}\right)\left(\frac{L}{mol\ chem}\right) \tag{A-2}$$

The total energy absorbed for the light exposure duration T_{exp} (s) with the light spectrum spanning the range of wavelengths λ_1 to λ_1 is

$$E_{abs} = T_{exp}\int_{\lambda_1}^{\lambda_2} I_o(\lambda)\varepsilon(\lambda)d\lambda \quad \text{(A-3)}$$

$$\text{(s)}\left(\frac{10^{-2}\text{J}}{\text{s m}^2\text{nm}}\right)\left(\frac{\text{L}}{\text{cm mol chem}}\right)\text{(nm)}$$

After units conversion Equation A3 becomes

$$E_{abs} = \frac{T_{exp}}{10^3}\int_{\lambda_1}^{\lambda_2} I_o(\lambda)\varepsilon(\lambda)d\lambda \quad \left(\frac{\text{J}}{\text{mol chem}}\right) \quad \text{(A-4)}$$

Photon Absorbed

The energy of one of photons is

$$E_{photon} = \frac{h\,c}{\lambda} \quad \text{(A-5)}$$

where h is the Planck's constant (6.626×10^{-34} J.s), c is the speed of light (2.998×10^8 m/s), and λ is the wavelength of the photon. The energy of one mole of photons is

$$E_{mol\ photon} = \frac{N_A h\,c}{\lambda} \quad \text{(A-6)}$$

where N_A is the Avogadro number (6.022×10^{23}).

Substituting the numerical values of h, c, and N_A in Equation A6, energy of a mole of photons is quantified as

$$E_{mol\ photon} = \frac{0.11962}{\lambda(\text{m})}\left(\frac{\text{J m}}{\text{mol photon}}\right) \quad \text{(A-7)}$$

For λ in meters. Accrodingly, the conversion factor (CF) is

$$\mathrm{CF} = \frac{\lambda}{N_A h\, c}\left(\frac{\text{mol photon}}{\text{J}}\right) \tag{A-8}$$

Therefore, to convert E_{abs} (J/mol chem) to P_{abs} (mol photon/mol chem), the conversion factor is multiplied by E_{abs}

$$P_{\text{abs}}\left(\frac{\text{mol photon}}{\text{mol chem}}\right) = \mathrm{CF}\left(\frac{\text{mol photon}}{\text{J}}\right) \times E_{\text{abs}}\left(\frac{\text{J}}{\text{mol chem}}\right) \tag{A-9}$$

$$P_{\text{abs}} = \frac{T_{\text{exp}}}{10^3}\int_{\lambda_1}^{\lambda_2}\left(\frac{\lambda}{N_A h\, c}\right) I_o(\lambda)\varepsilon(\lambda)d\lambda \tag{A-10}$$

And Equation A10 is simplified to

$$P_{\text{abs}} = 0.00836 T_{\text{exp}}\int_{\lambda_1}^{\lambda_2} I_o(\lambda)\varepsilon(\lambda)\ \lambda\ d\lambda \tag{A-11}$$

Note that the respective units for T_{exp}, $I_o(\lambda)$, $\varepsilon(\lambda)$, and λ are (s),(μW/cm^2),(L/mol/cm), and (m).

P_{abs} Calculation Example

The total light emission dose from SolarConstant 1200 in UVB, UVA and VIS regions, E_{UVB} (μW/cm^2), E_{UVA} (μW/cm^2), and E_{VIS} (μW/cm^2) are calculated integrating the general incident light intensity ($I(\lambda)$) provided in Table A5 over UVB (λ_1 = 280, λ_2 = 320 nm), UVA (λ_1 = 320, λ_2 = 400 nm), and VIS (λ_1 = 400, λ_2 = 800 nm) regions, respectively (Equation A1).

$$E_{\text{X}} = \sum_{\lambda_1}^{\lambda_2} I(\lambda) \tag{A-12}$$

where E_{X} is quantified for UVB, UVA, and VIS regions as E_{UVB} = 439.865 (μW/cm^2), E_{UVA} = 6883.625 (μW/cm^2), and E_{VIS} = 60311.38 (μW/cm^2), respectively.

However, E_X is associated with the general irradiance and for a particular intensity that is exposed to the organisms (I_X), the factor by which the lamp irradiation intensity is reduced or amplified at each region (F_X) is determined dividing the incident light intenisites (I_X) by the respective emitted light (E_X):

$$F_X = \frac{I_X}{E_X} \tag{A-13}$$

F_X is used to determine the actual incident light irradiance spectrum, $I_{o\text{-}X}(\lambda)$, at each region as follow:

$$I_{o\text{-}X}(\lambda) = F_X I_X(\lambda) \tag{A-14}$$

As a case in point, for UVB region, F_{UVB} = (30/439.865) = 0.068 and $I_{o\text{-}UVB}(\lambda) = 0.068 I_{UVB}(\lambda)$, where λ ranges from 280 – 320 nm. Similarly, F_{UVA} = 0.102 and F_{VIS} = 0.066.

The light exposure duration, T_{exp}, is another important factor influencing amount of the absorbed light. The PTLM can accommodate both type of endpoints, phototoxic LC50s (PLC50s) and phototoxic LT50s (PLT50s). For PLC50s, T_{exp} is incorporated as total time of light exposure in Equation A5 to calculate P_{abs} . For example, T_{exp} = 32 h for a 48-h LC50 with a 16:8 h light:dark photoperiod. For LT50s, the light exposure regime is considered as continuous and therefore, T_{exp} = LT50. PLC50 is the concentration at which PLT50 was measured.

Utilizing Equation A-11, P_{abs} at each region is calculated substituting the corresponding wavelength range. For example for UVB, the absorbed dose is calculated as follow

$$P_{\text{abs-UVB}} = 0.00836 T_{\text{exp}} \int_{\lambda_1=2801}^{\lambda_2=320} I_{\text{o-UVB}}(\lambda)\varepsilon(\lambda)\ \lambda\ d\lambda$$
$$= 0.00836 \times 12 \times 3600 \times \int_{\lambda_1=2801}^{\lambda_2=320} 0.068 I_{\text{UVB}}(\lambda)\varepsilon(\lambda)\ \lambda\ d\lambda \quad \text{(A-15)}$$
$$= 13.875$$

Similarly, $P_{\text{abs-UVA}}$ =259.799 and $P_{\text{abs-VIS}}$ = 0. The total dose absorbed (mol photon/mol PAH) is

$$P_{\text{abs}} = P_{\text{abs-UVB}} + P_{\text{abs-UVA}} + P_{\text{abs-VIS}} = 311.828 \quad \text{(A-16)}$$

PLC50 Calculation

Finally, incorporating NLC50 = 42.763 (μg/L), P_{abs} = 311.828 (mol photon/mol PAH), a = 0.426, and R'^{*} = 0.511 in the PTLM (Equation A17) yields the predicted PLC50 =1.813 (μg/L)

$$\text{PLC50} = \frac{\text{NLC50}}{1 + \left(\frac{P_{\text{abs}}{}^{a}}{R'^{*}} \right)} \quad \text{(A-17)}$$

A.4 Diagnostic Plots

The diagnostic plots used to analyze how PTLM model (Equation 3-27) fit to the experimental data changes with the PAHs, organisms, the experimental data sources, and the light sources irradiance spectra are shown in Figure A2, Figure A3, Figure A4, and Figure A5, respectively. The PTLM model fits to the experimental data are shown as the curved lines and the dashed lines show one order of magnitude variations. Data with residuals greater than one order of magnitude are shown with plus symbols.

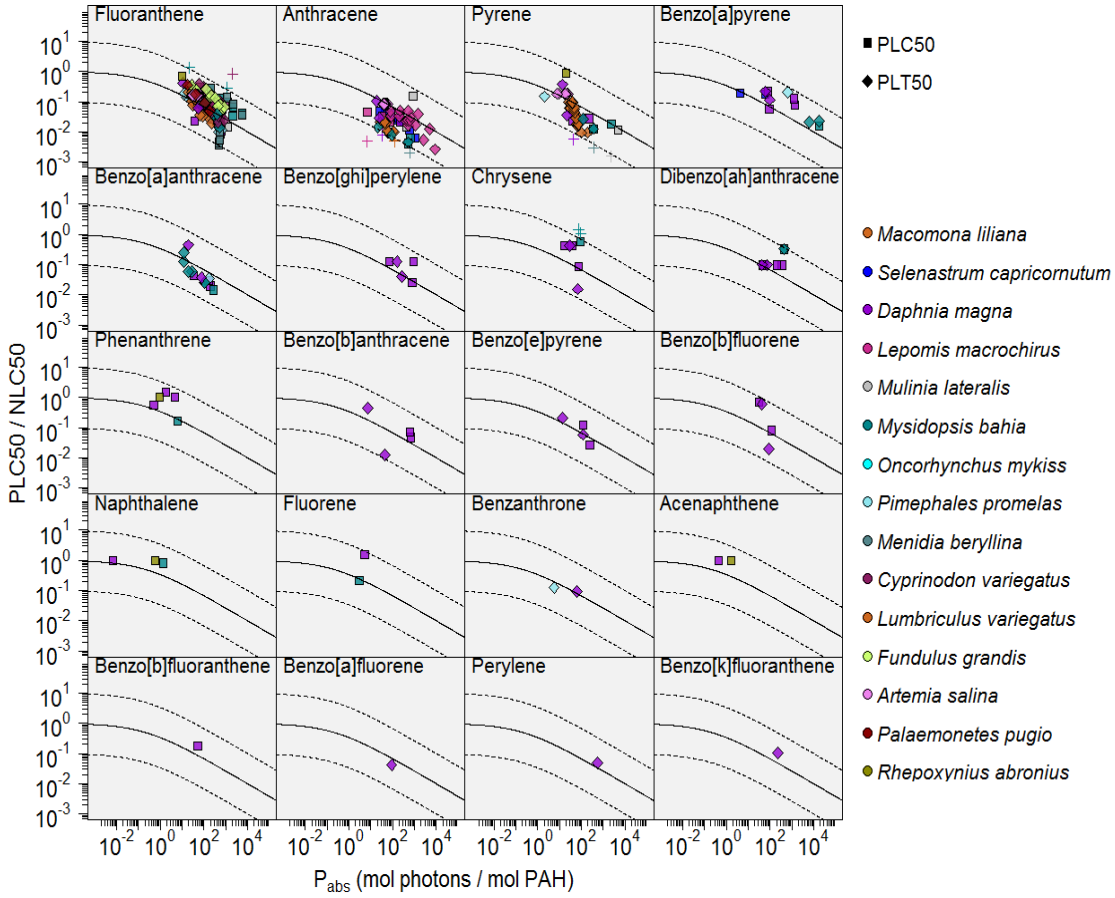

Figure A.2. The experimental PLC50s relative to NLC50s predicted by NTLM (Equation 3-4). Panels are separated by the chemicals. Organisms are color coded and described in the bottom legend. The top legend explains PLC50s obtained directly from the reported aqueous concentrations at 50% mortality (with PLC50 title), shown with the square symbols, while the experimental PLC50s corresponding to the reported phototoxic LT50 data (with PLT50 title) are shown with diamond symbols. Data with residuals greater than one order of magnitude are shown with plus symbols. The lines show the PTLM model fit (Equation 3-27). The dashed lines represent one order of magnitude uncertainties.

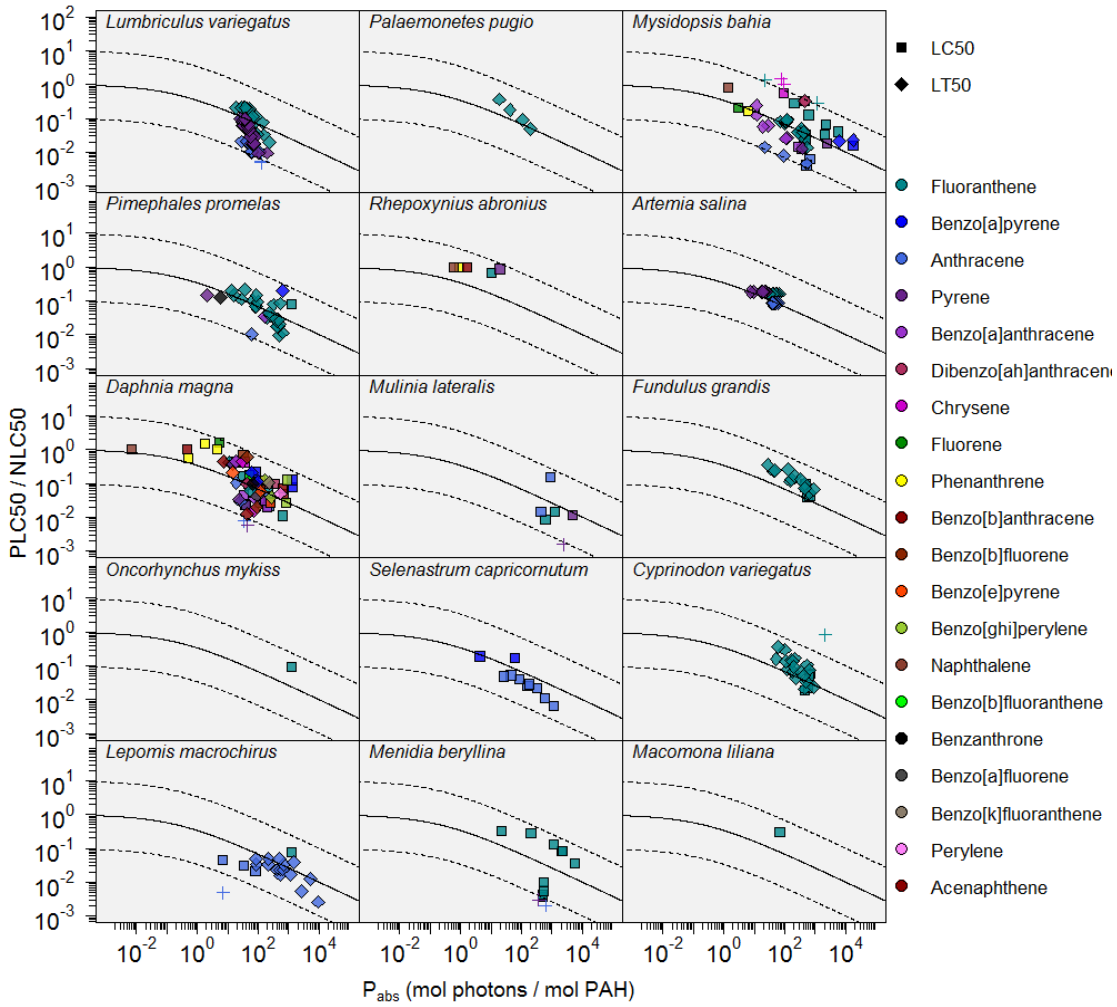

Figure A.3. The experimental PLC50s relative to NLC50s predicted by NTLM (Equation 3-4). Panels are separated by the organisms. Chemicals are color coded and described in the bottom legend. The top legend explains PLC50s obtained directly from the reported aqueous concentrations at 50% mortality (with PLC50 title), shown with the square symbols, while the experimental PLC50s corresponding to the reported phototoxic LT50 data (with PLT50 title) are shown with diamond symbols. Data with residuals greater than one order of magnitude are shown with plus symbols. The lines show the PTLM model fit (Equation 3-27). The dashed lines represent one order of magnitude uncertainties.

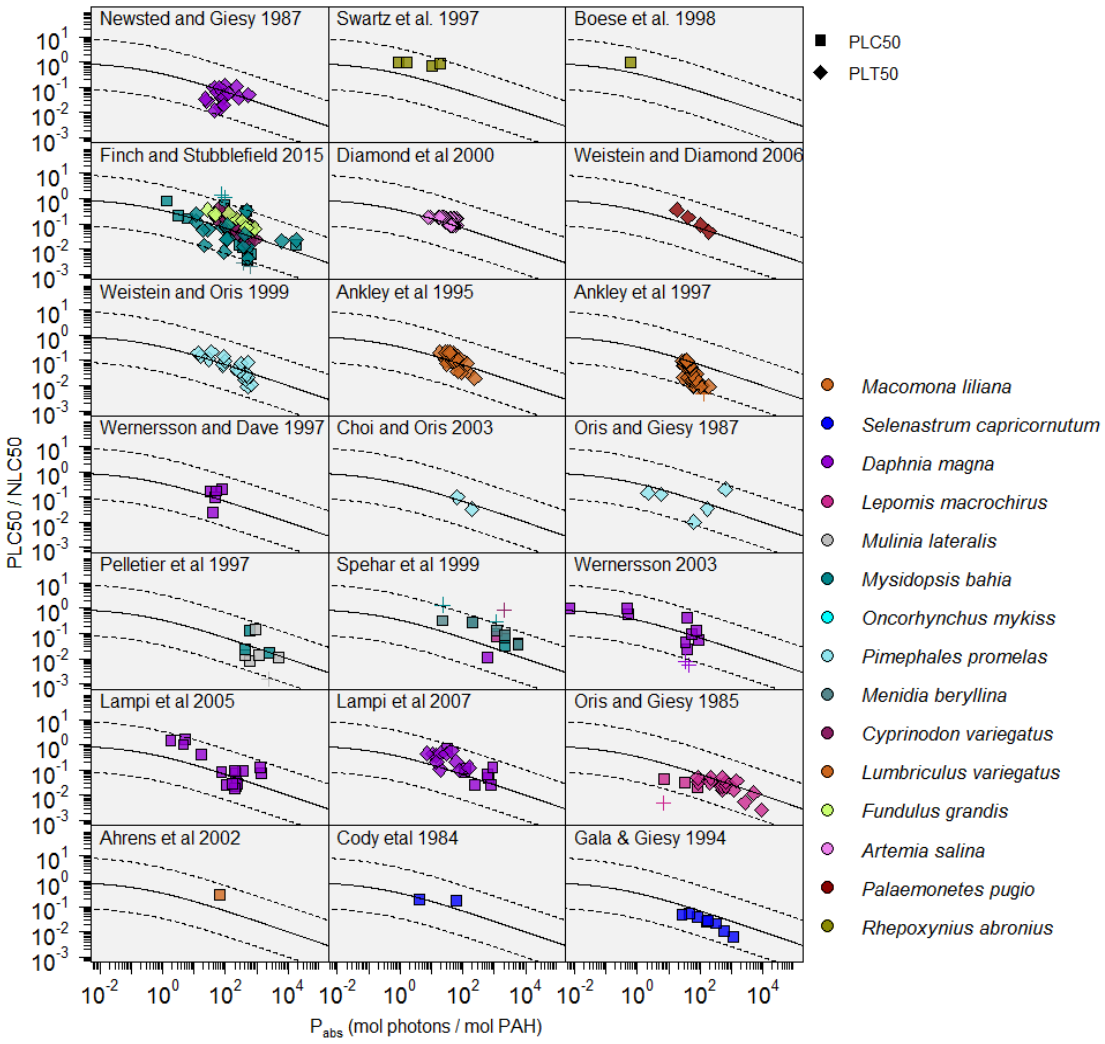

Figure A.4. The experimental PLC50s relative to NLC50s predicted by NTLM (Equation 3-4). Panels are separated by the data references. Organisms are color coded and described in the bottom legend. The top legend explains PLC50s obtained directly from the reported aqueous concentrations at 50% mortality (with PLC50 title), shown with the square symbols, while the experimental PLC50s corresponding to the reported phototoxic LT50 data (with PLT50 title) are shown with diamond symbols. Data with residuals greater than one order of magnitude are shown with plus symbols. The lines show the PTLM model fit (Equation 3-27). The dashed lines represent one order of magnitude uncertainties.

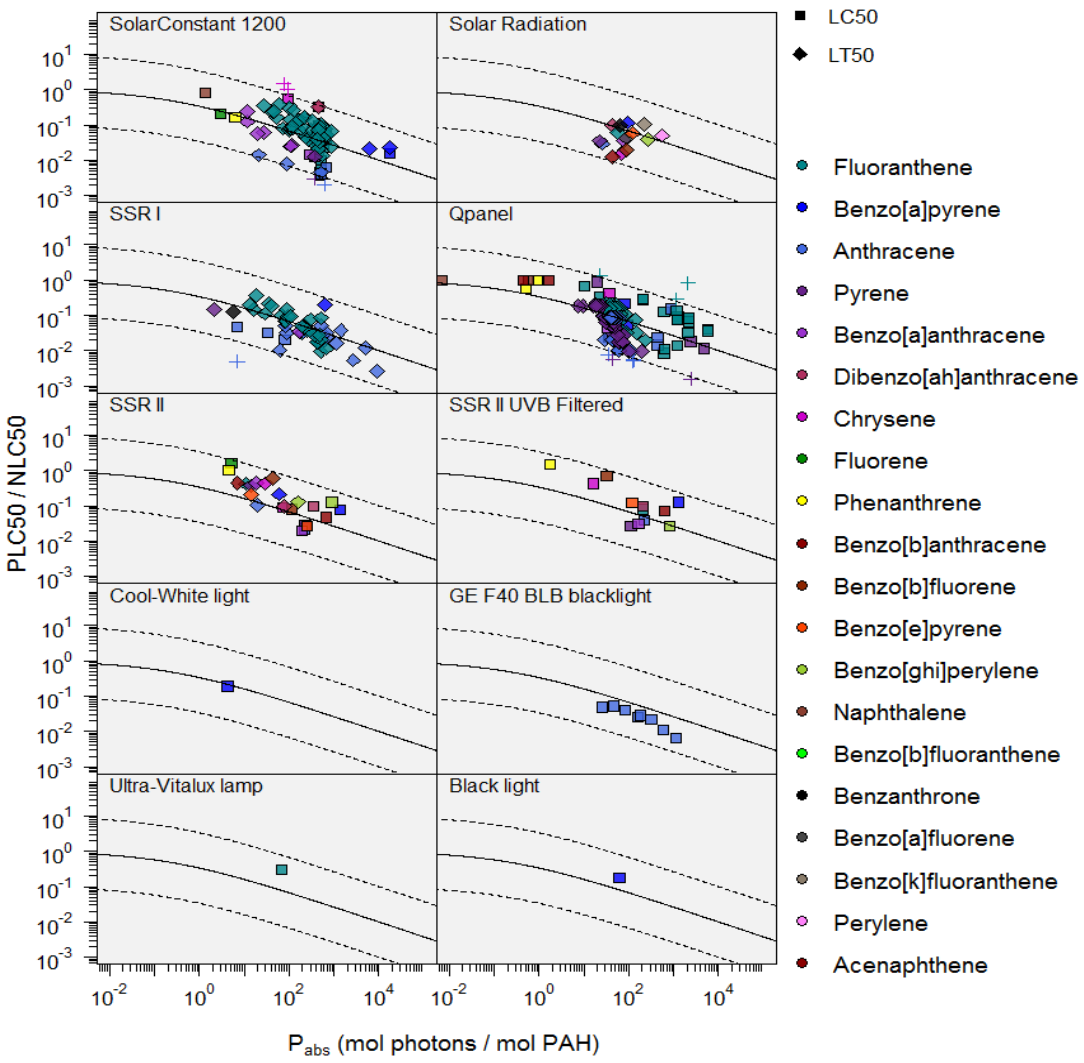

Figure A.5. The experimental PLC50s relative to NLC50s predicted by NTLM (Equation 3-4). Panels are separated by the light sources used to generate the phototoxic data.. Chemicals are color coded and described in the bottom legend. The top legend explains PLC50s obtained directly from the reported aqueous concentrations at 50% mortality (with PLC50 title), shown with the square symbols, while the experimental PLC50s corresponding to the reported phototoxic LT50 data (with PLT50 title) are shown with diamond symbols. Data with residuals greater than one order of magnitude are shown with plus symbols. The lines show the PTLM model fit (Equation 3-27). The dashed lines represent one order of magnitude uncertainties.

A.5 Residuals Analysis

For analysis of residuals, log of residuals are calculated as log(predicted PLC50) – log(observed PLC50). Figures A.6 and A.7 show the residuals with respect to the irradiance (P_{abs} / T_{exp}) and the total moles of photons absorbed per mole of PAH (P_{abs}), respectively. Figures A.6 and A.7 support the fact that the model prediction does not fall up at low or high light irradiance and total moles of photons absorbed per mole of PAH, respectively. Thus the residuals plots do not show any bias in the residuals against the irradiance and P_{abs}

The residuals against the light exposure time (T_{exp}) are presented in Figure S8 for continuous irradiation, as well as periodic irradiation associated with 48-h and 96-h PLC50s. For the periodic exposure, the light exposure time is up to about 80 h. The linear regression between the log of residuals and T_{exp} yielded slope = -0.071 (p-value = 0.244) for the 48-h periodic exposures and slope = -0.023 (p-value = 0.137) for the 96-h periodic exposures within 95% confidence interval. Both p-values suggest that the slopes are not significant so that there is no correlation between the residuals and the light exposure time. For the continuous light exposure, T_{exp} ranges from about 0.02 to up to 500 h. Comparion of the residuals to T_{exp} resulted in the slope of 0.002 (p-value = 0.003). Therefore, the slope and p-value suggest the PLC50 decreases slightly with the light exposure time in continuous light regime. The increase in phototoxicty at the longer exposure rejects the hypothesis of possibility of the repair mechanism. However, as expressed before, PTLM accommodates both types of endpoints, PLC50 and PLT50. The PLT50s fall into the category of the continuous light exposure regime for which it is assumed that T_{exp} = LT50. Yet, the slope of log of residuals against T_{exp} is very slight.

Therefore, the PTLM parameters (a and R^{r^*}) do not depend on the light intensity, total photons absorbed per mole PAH, and the ligth exposure duration.

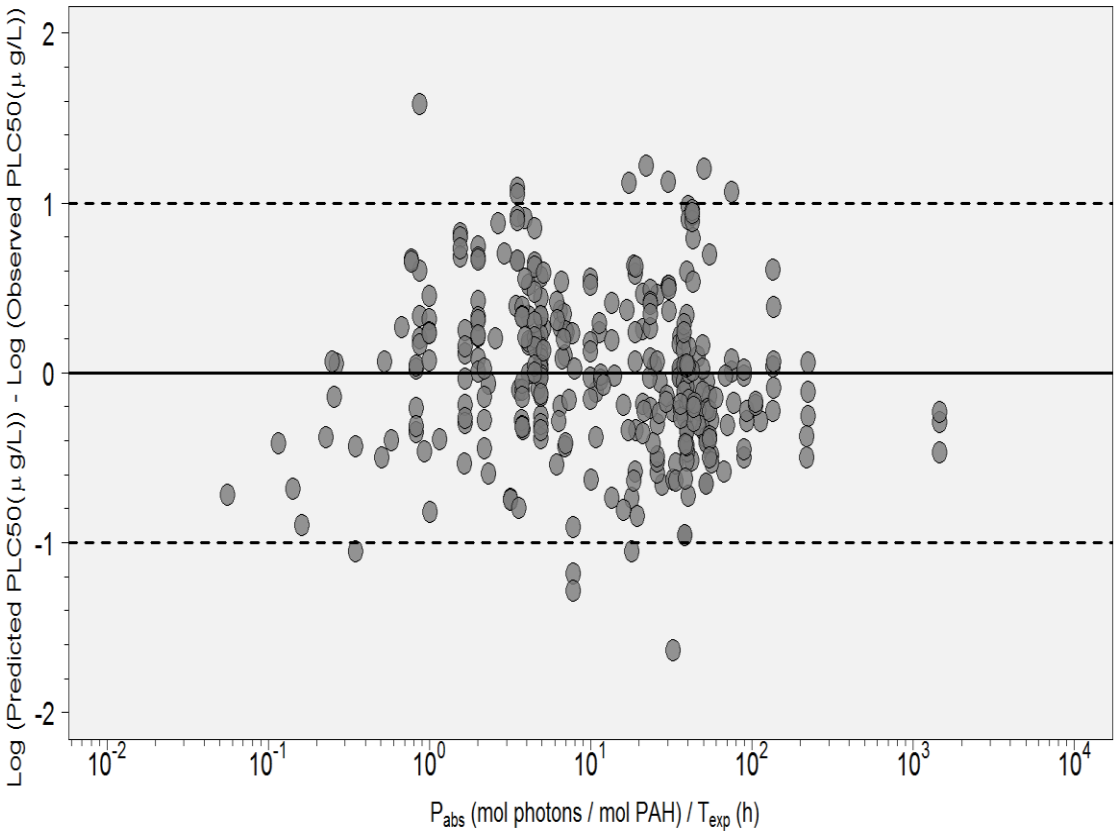

Figure A.6. Plot of log of residuals for PLC50 for 20 PAHs and 15 tested species used for the PTLM model versus the irradiance (P_{abs}/T_{exp}). Log of residuals (y-axis) are calculated as log(predicted PLC50 (µg/L)) – log (observed PLC50 (µg/L)).

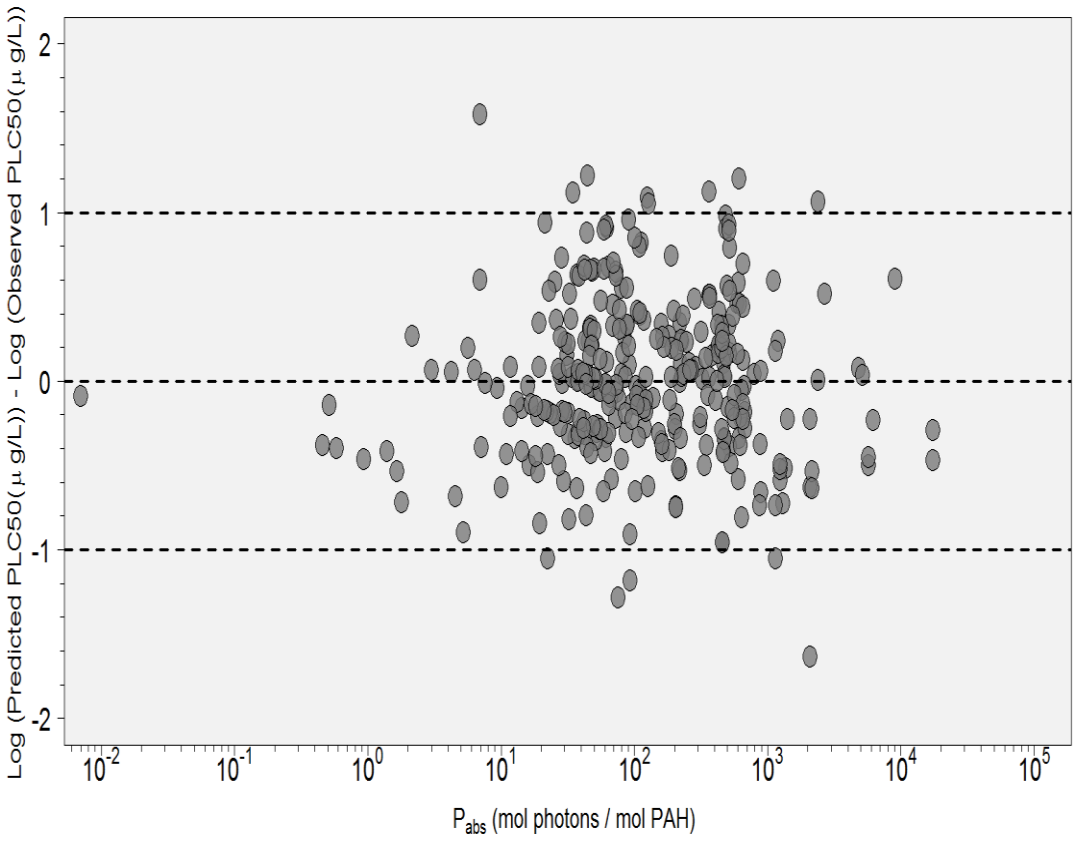

Figure A.7. Plot of log of residuals for PLC50 for 20 PAHs and 15 test species used for the PTLM model versus the absorbed light (P_{abs}). Log of residuals (y-axis) are calculated as log(predicted PLC50 (µg/L)) – log(observed PLC50 (µg/L)).

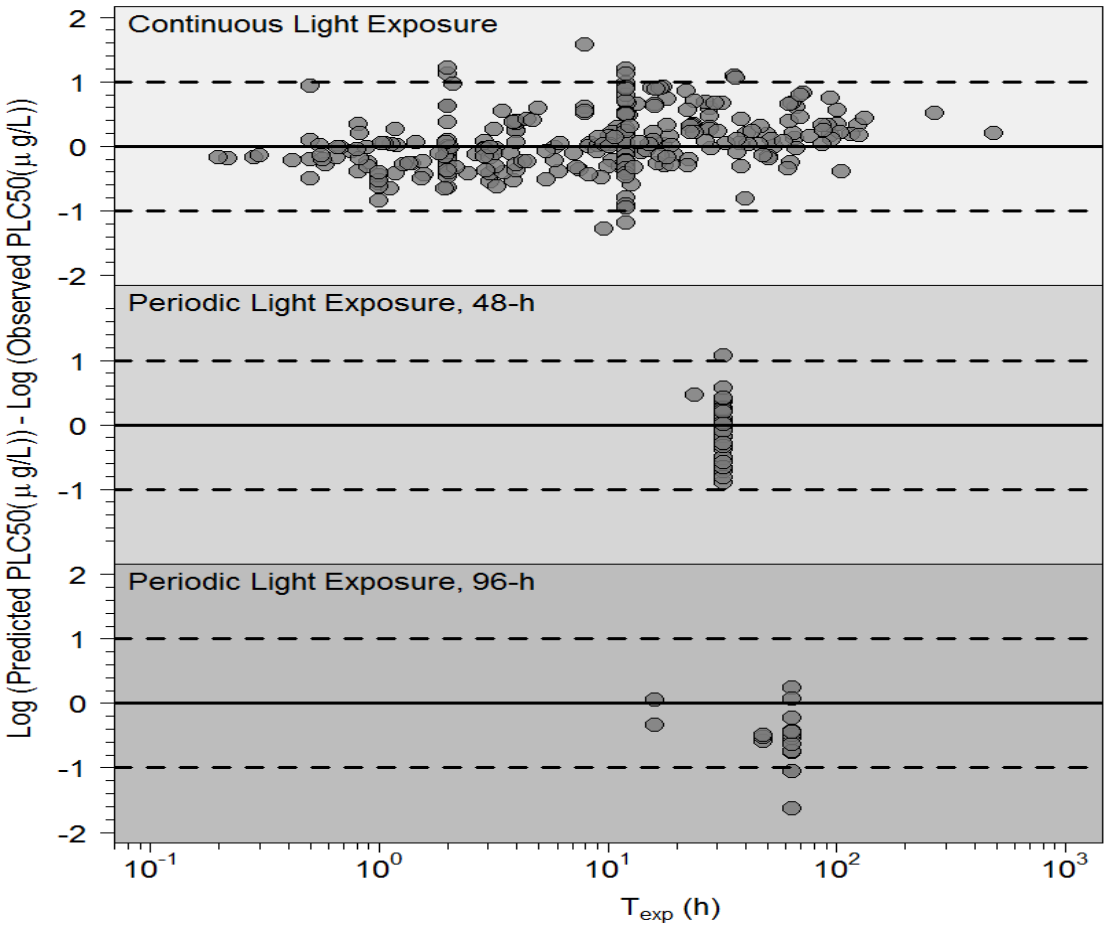

Figure A.8. Additional plot of log of residuals versus T_{exp} to analyze repair mechanism effect on the phototoxicity. Panels are separated based on light regime. From top to bottom, plots show the residuals for continuous light exposure and periodic exposures associated with 48-h and 96-h PLC50s, respectively. Log of residuals (y-axis) are calculated as log(predicted PLC50 (µg/L)) – log(observed PLC50 (µg/L)).

Appendix B

PHOTOTOXIC TARGET LIPID MODEL VALIDATION: PREDICTING PHOTOTOXICITY OF ALKYLATED PAHS, MIXTURES, AND NEAT AND WEATHERED PETROLEUM

B.1. Assumed Critical Target Lipid Body Burdens

a. **Table B.1.** CTLBBs backcalculated from the measured NLC50s associated with the species native to the Gulf of Mexico.

B.2. Molar Absorption Spectra of APAHs and other Phototoxic Chemicals in the WAF Solution of Macondo Crude Oil.

a. **Table B.2-a.** Molar absorption spectra of alkylated PAHs in the WAF solution at wavelength intervals of λ =1 (nm).
b. **Table B.2-b.** Molar absorption spectra of the phototoxic compounds in the WAF solution at wavelength intervals of λ =1 (nm).
c. **Table B.3.** Substituted molar absorption coefficients for the chemicals whole molar absoprtion coefficients are not available**.**

B.3. PTLM Validation for APAHs and other Phototoxic Compounds

a. **Figure B.1.** Predicted PLC50 (µg/L) vs. observed PLC50 (µg/L) for APAHs and other phototoxic chemicals. The organism are shown with different symbols. Chemical are color coded as described in the bottom legend. The solid diagonal lines indicate perfect agreement between predicted and observed PLC50s. The dashed lines represent one order of

magnitude uncertainties. The corresponding RMSE is equal to 0.483. The data are presented in Table B.3.

b. **Table B.4**. Observed PLC50s and experimental data used to predict PLC50s of APAHs and other phototoxic compounds shown in Figures 3-1 and B.1.

B.4. Narcotic Toxicity and Phototoxicity Data Associated with Binary and Ternary Mixtures of PAHs.

a. **Table B.5.** Data associate with the predicted and observed PTU values presented in Figures 4-2 and 4-3. The endpoints are 48h LC50.

B.5. Computational Example for Binary and Ternary Mixtures Phototoxicity Prediction.

B6. Observed and Predicted Macondo Crude Oil Narcotic Toxicity and Phototoxicity Data

a. **Table B.6**. Observed and predicted narcotic toxicity of neat and weathered Macondo crude oils exposed to the test organisms.

b. **Table B.7.** Observed and predicted phototoxicity of neat and weathered Macondo crude oils exposed to the test organisms.

B7. Chemical Compositions Data for the Components in Macondo Crude Oil WAF Solution.

a. **Table B.8.** Chemical compositions and concentrations of the components in the 100% WAF solution of MASS oil exposed to *Americamysis bahia* under natural solar radiation.

b. **Table B.9.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 100% WAF exposed to *Americamysis bahia* under natural solar radiation.

c. **Table B.10.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 25% WAF exposed to *Americamysis bahia* under natural solar radiation.

d. **Table B.11.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF exposed to *Americamysis bahia* under natural solar radiation.

e. **Table B.12.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF duplicate exposed to *Americamysis bahia* under natural solar radiation.

f. **Table B.13.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 100% WAF exposed to *Americamysis bahia* under natural solar radiation.

g. **Table B.14**. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 25% WAF exposed to *Americamysis bahia* under natural solar radiation.

h. **Table B.15.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF exposed to *Americamysis bahia* under natural solar radiation.

i. **Table B.16.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 100% WAF exposed to *Americamysis bahia* under artificial radiation.

j. **Table B.16.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 25% WAF exposed to *Americamysis bahia* under artificial radiation.

k. **Table B.17.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF exposed to *Americamysis bahia* under artificial radiation.

l. **Table B.18.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF duplicate exposed to *Americamysis bahia* under artificial radiation.

m. **Table B.19.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 100% WAF exposed to *Americamysis bahia* under natural solar radiation.

n. **Table B.20**. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in

Juniper oil at 25% WAF exposed to *Americamysis bahia* under natural solar radiation.

o. **Table B.21.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 6.25% WAF exposed to *Americamysis bahia* under natural solar radiation.

p. **Table B.22.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 6.25% WAF duplicate exposed to *Americamysis bahia* under natural solar radiation.

q. **Table B.23.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 100% WAF exposed to *Menidia beryllina* under natural solar radiation.

r. **Table B.24.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 25% WAF exposed to *Menidia beryllina* under natural solar radiation.

s. **Table B.25.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF exposed to *Menidia beryllina* under natural solar radiation.

t. **Table B.26.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in

MASS oil at 6.25% WAF duplicate exposed to *Menidia beryllina* under natural solar radiation.

u. **Table B.27.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 100% WAF exposed to *Menidia beryllina* under natural solar radiation.

v. **Table B.28.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 25% WAF exposed to *Menidia beryllina* under natural solar radiation.

w. **Table B.29.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF exposed to *Menidia beryllina* under natural solar radiation.

x. **Table B.30.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF duplicate exposed to *Menidia beryllina* under natural solar radiation.

y. **Table B.31.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 100% WAF exposed to *Menidia beryllina* under artificial radiation.

z. **Table B.32.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 25% WAF exposed to *Menidia beryllina* under artificial radiation

aa. **Table B.33.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF exposed to *Menidia beryllina* under artificial radiation.

bb. **Table B.34.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF duplicate exposed to *Menidia beryllina* under artificial radiation.

cc. **Table B.35.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 100% WAF exposed to *Menidia beryllina* natural solar radiation.

dd. **Table B.36.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 25% WAF exposed to *Menidia beryllina* natural solar radiation.

ee. **Table B.37.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 6.25% WAF exposed to *Menidia beryllina* natural solar radiation.

ff. **Table B.38**. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 6.25% WAF duplicate exposed to *Menidia beryllina* natural solar radiation.

gg. **Table B.39**. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 100% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

hh. **Table B.40.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 25% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

ii. **Table B.41.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

jj. **Table B.42** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF duplicate exposed to *Cyprinodon variegatus* under artificial radiation.

kk. **Table B.43.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 100% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

ll. **Table B.44.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 25% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

mm. Table B.45. Chemical compositions and concentrations of the components in the 6.25% WAF solution of Juniper oil exposed to *Cyprinodon variegatus* under artificial solar simulated radiation.

nn. Table B.46. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF duplicate exposed to *Cyprinodon variegatus* under artificial radiation.

oo. Table B.47. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 100% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

pp. Table B.48. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 25% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

qq. Table B.49. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 6.25% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

rr. Table B.50. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 6.25% WAF duplicate exposed to *Cyprinodon variegatus* under artificial radiation..

ss. **Table B.51.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 100% WAF exposed to *Fundulus grandis* under artificial radiation.

tt. **Table B.52.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 25% WAF exposed to *Fundulus grandis* under artificial radiation.

uu. **Table B.53.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF exposed to *Fundulus grandis* under artificial radiation.

vv. **Table B.54.** Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF duplicate exposed to *Fundulus grandis* under artificial radiation.

B.8. Hourly Natural Sunlight and Simulated Solar Radiation Intensities

a. **Table B.55**. Hourly natural radiation intensities exposed to *Americamysis bahia*.

b. **Table B.56**. Hourly artificial radiation intensities exposed to *Americamysis bahia*.

c. **Table B.57**. Hourly natural radiation intensities exposed to *Menidia beryllina*.

d. **Table B.58**. Hourly artificial radiation intensities exposed to *Menidia beryllina*.
e. **Table B.59.** Hourly artificial radiation intensities exposed to *Cyprinodon variegatus*.
f. **Table B.60.** Hourly artificial radiation intensities exposed to *Fundulus grandis*.

B.9. Computational Example for Oil Narcotic Toxicity and Phototoxicity

B.1 Assumed Critical Target Lipid Body Burdens

Table B.1. CTLBBs backcalculated from the measured NLC50s associated with the species native to the Gulf of Mexico.

Organism	Age	PAH	NLC50 (μg/L)	C^*_{LN} (μmol/g octanol)
Americamysis bahia	3 d	Fluoranthene	32.200	25.810
Menidia beryllina	7 d	Fluoranthene	37.160	29.786
Cyprinodon variegatus	7 d	Naphthalene	3889.000	113.501
Fundulus grandis	7 d	Naphthalene	5423.000	106.170

B.2 Molar Absorption Spectra of APAHs and other Phototoxic Chemicals in the WAF Solution of Macondo Crude Oil

Table B.2-a. Molar absorption spectra of alkylated PAHs in the WAF solution at wavelength intervals of λ =1 (nm).

λ (nm)	$\varepsilon^a(\lambda)$ (L/mol/cm)	$\varepsilon^b(\lambda)$ (L/mol/cm)	$\varepsilon^c(\lambda)$ (L/mol/cm)	$\varepsilon^d(\lambda)$ (L/mol/cm)	$\varepsilon^e(\lambda)$ (L/mol/cm)	$\varepsilon^f(\lambda)$ (L/mol/cm)	$\varepsilon^g(\lambda)$ (L/mol/cm)
280	3793	3586	6611	3793	384	5577	13208
281	3750	3537	6763	3750	359	4648	11786
282	3541	3441	7163	3541	328	3537	10759
283	3383	3442	7586	3383	310	3192	10164
284	3308	3396	7412	3308	297	2982	9941
285	3206	3350	6996	3206	275	2849	9830
286	3200	3213	6453	3200	262	2770	9834
287	2986	3126	5951	2986	254	2754	9506
288	2852	2876	5617	2852	248	2818	9226
289	2601	2468	5370	2601	240	2883	8983
290	2263	2270	5180	2263	235	3018	8885
291	1947	1791	5248	1947	238	3088	8688
292	1660	1474	5359	1660	238	3269	8791
293	1318	1100	5370	1318	241	3461	9102
294	1011	984	5610	1011	250	3631	9423
295	677	893	5740	677	268	4250	9981
296	537	799	5806	537	292	4500	10694

297	467	695	4997	467	331	4818	10577
298	421	613	4301	421	339	5339	10342
299	379	421	3377	379	371	5717	10345
300	338	398	2129	338	411	5850	10116
301	301	404	1711	301	433	5985	9550
302	297	433	1358	297	446	6337	9386
303	340	484	1018	340	452	6633	9456
304	423	440	837	423	468	6865	9789
305	449	410	741	449	496	7351	9991
306	419	388	712	419	520	7872	10492
307	356	394	745	356	604	9290	11371
308	292	428	754	292	653	9772	11908
309	276	679	661	276	700	10957	12589
310	283	792	592	283	761	11868	13059
311	293	625	515	293	844	12338	12915
312	293	521	509	293	902	13456	12342
313	268	435	492	268	981	13458	9936
314	236	403	419	236	1028	13458	8566
315	200	423	340	200	1053	12429	7943
316	168	487	336	168	1091	12430	8005
317	179	537	433	179	1109	12645	8576
318	368	501	491	368	1144	13012	9550
319	481	349	464	481	1172	13934	10715
320	409	316	306	409	1221	14585	11827
321	224	308	276	224	1272	15801	12817
322	121	436	299	121	1333	17706	13578
323	0	636	287	0	1429	19624	13895
324	0	1008	227	0	1497	23545	13804
325	0	995	134	0	1569	27307	12618

326	0	482	96	0	1701	30258	11324
327	0	359	73	0	1866	32035	9652
328	0	189	0	0	2023	28589	7594
329	0	0	0	0	2219	21753	5091
330	0	0	0	0	2433	15635	3532
331	0	0	0	0	2608	13795	2624
332	0	0	0	0	2672	12812	1995
333	0	0	0	0	2644	12887	1517
334	0	0	0	0	2558	13545	1369
335	0	0	0	0	2475	15119	1141
336	0	0	0	0	2450	17937	984
337	0	0	0	0	2453	19877	871
338	0	0	0	0	2455	24121	774
339	0	0	0	0	2458	27350	723
340	0	0	0	0	2576	38497	675
341	0	0	0	0	2761	45676	638
342	0	0	0	0	3098	50039	603
343	0	0	0	0	3398	50045	624
344	0	0	0	0	3945	47279	705
345	0	0	0	0	4376	30324	803
346	0	0	0	0	5012	14629	776
347	0	0	0	0	5559	4324	632
348	0	0	0	0	5772	2392	464
349	0	0	0	0	5650	1569	419
350	0	0	0	0	5342	1338	410
351	0	0	0	0	4772	1308	410
352	0	0	0	0	4312	1449	420
353	0	0	0	0	4078	1549	430
354	0	0	0	0	3813	1625	420

355	0	0	0	0	3524	996	346
356	0	0	0	0	3489	766	285
357	0	0	0	0	3532	603	288
358	0	0	0	0	3744	537	302
359	0	0	0	0	3968	475	346
360	0	0	0	0	4157	434	451
361	0	0	0	0	4665	378	721
362	0	0	0	0	5175	323	790
363	0	0	0	0	6077	282	809
364	0	0	0	0	7218	272	722
365	0	0	0	0	8285	263	427
366	0	0	0	0	8783	260	196
367	0	0	0	0	8595	251	0
368	0	0	0	0	8220	232	0
369	0	0	0	0	6780	63	0
370	0	0	0	0	5720	53	0
371	0	0	0	0	4664	72	0
372	0	0	0	0	3892	141	0
373	0	0	0	0	3246	214	0
374	0	0	0	0	2933	342	0
375	0	0	0	0	2786	533	0
376	0	0	0	0	2761	366	0
377	0	0	0	0	2844	169	0
378	0	0	0	0	3049	113	0
379	0	0	0	0	3232	0	0
380	0	0	0	0	3424	0	0
381	0	0	0	0	4508	0	0
382	0	0	0	0	4724	0	0
383	0	0	0	0	4783	0	0

384	0	0	0	0	5428	0	0
385	0	0	0	0	6826	0	0
386	0	0	0	0	7486	0	0
387	0	0	0	0	8496	0	0
388	0	0	0	0	8314	0	0
389	0	0	0	0	7096	0	0
390	0	0	0	0	5162	0	0
391	0	0	0	0	4307	0	0
392	0	0	0	0	2994	0	0
393	0	0	0	0	2280	0	0
394	0	0	0	0	1621	0	0
395	0	0	0	0	1193	0	0
396	0	0	0	0	784	0	0
397	0	0	0	0	692	0	0
398	0	0	0	0	392	0	0
399	0	0	0	0	312	0	0
400	0	0	0	0	222	0	0

[a] $\varepsilon(\lambda)$ for 1-methylnaphthalene measured in solvent ethanol [56].

[b] $\varepsilon(\lambda)$ for 2,6-dimethylnaphthalene measured in solvent isooctane [56].

[c] $\varepsilon(\lambda)$ for 1,6,7-trimethylnaphthalene measured in solvent hexane [56].

[d] $\varepsilon(\lambda)$ for 9-methylphenanthrene measured in solvent cyclohexane [56].

[e] $\varepsilon(\lambda)$ for 9-methylanthracene measured in solvent ethanol [56].

[f] $\varepsilon(\lambda)$ for 1-methylpyrene measured in solvent hexane [56].

[g] $\varepsilon(\lambda)$ for 1-methylchrysene measured in solvent ethanol [56].

Table B.2-b. Table B2-b. Molar absorption spectra of the phototoxic compounds in the WAF solution at wavelength intervals of λ =1 (nm).

λ (nm)	$\varepsilon^a(\lambda)$ (L/mol/cm)	$\varepsilon^b(\lambda)$ (L/mol/cm)	$\varepsilon^c(\lambda)$ (L/mol/cm)	$\varepsilon^d(\lambda)$ (L/mol/cm)	$\varepsilon^e(\lambda)$ (L/mol/cm)	$\varepsilon^f(\lambda)$ (L/mol/cm)	$\varepsilon^g(\lambda)$ (L/mol/cm)	$\varepsilon^h(\lambda)$ (L/mol/cm)
280	0	1109	15285	1201	5993	20922	14613	650
281	0	1200	15763	1188	6344	20169	13451	635
282	0	1333	15429	1188	6718	19417	12909	620
283	0	1369	14635	1244	6793	18476	12136	620
284	0	1540	14324	1288	7328	18268	11171	612
285	0	1667	14167	1380	7786	18924	11912	598
286	0	1875	14308	1530	8242	20454	12823	597
287	0	2628	14005	1777	8625	20961	13366	597
288	0	3409	12740	1993	9130	21477	13859	597
289	0	2635	11469	2210	9555	22688	11976	603
290	0	1214	10326	2522	10231	23720	10599	603
291	0	559	9199	2754	10585	28704	9521	613
292	0	301	8457	2951	11246	28974	8581	624
293	0	166	8022	3228	11727	29247	8161	631
294	0	58	7852	3357	12555	28356	7907	653
295	0	24	7847	3500	13291	28003	8799	683
296	0	19	8263	3665	13441	28186	9994	707
297	0	19	8173	3709	12986	28904	11121	732
298	0	19	7435	3928	11850	30515	11882	749
299	0	20	5319	4161	10449	32825	14057	793
300	0	21	0	4210	9645	34808	14996	840
301	0	22	0	4359	8902	35884	14981	879
302	0	25	0	4670	7850	37316	12176	910

303	0	28	0	5004	6922	39641	8000	964
304	0	31	0	5240	5635	39110	5506	1033
305	0	34	0	5878	4433	36792	3573	1094
306	0	37	0	6016	3409	31974	2468	1159
307	0	41	0	6228	2259	27335	1370	1228
308	0	43	0	6522	1737	21535	1056	1286
309	0	50	0	0	1291	19307	785	1346
310	0	60	0	0	1345	17169	715	1426
311	7	72	0	0	1382	17350	631	1528
312	6	78	0	0	1479	18783	606	1600
313	4	89	0	0	1621	20215	582	1714
314	3	98	0	0	1735	22718	583	1816
315	3	106	0	0	1816	26651	583	1946
316	3	116	0	0	1900	35048	609	2061
317	3	129	0	0	1966	33266	636	2183
318	2	133	0	0	2081	25456	637	2313
319	2	123	0	0	2129	17167	612	2450
320	2	117	0	0	2254	11671	564	2595
321	2	126	0	0	2305	9353	497	2797
322	2	123	0	0	2279	7928	477	2878
323	2	127	0	0	2304	6593	458	3048
324	2	141	0	0	2278	6150	449	3192
325	2	134	0	0	2102	5440	431	3342
326	2	141	0	0	1812	5978	387	3540
327	2	145	0	0	1598	5982	373	3793
328	2	134	0	0	1458	6165	315	3926
329	2	61	0	0	1425	5990	297	4159
330	2	25	0	0	1491	5994	310	4254
331	2	0	0	0	1543	6534	317	4558

332	2	0	0	0	1810	6449	352	4828
333	2	0	0	0	2128	6898	368	4997
334	1	0	0	0	2407	7080	376	5232
335	1	0	0	0	2434	7620	361	5542
336	1	0	0	0	2406	8071	305	5736
337	1	0	0	0	2074	8342	275	6076
338	1	0	0	0	1708	9061	243	6436
339	1	0	0	0	1439	9600	223	6897
340	1	0	0	0	0	9962	206	7391
341	1	0	0	0	0	10501	202	7560
342	1	0	0	0	0	10683	194	7468
343	1	0	0	0	0	11044	190	7293
344	1	0	0	0	0	11405	178	7162
345	1	0	0	0	0	11588	164	7158
346	1	0	0	0	0	11591	151	7112
347	1	0	0	0	0	11773	151	7275
348	1	0	0	0	0	11955	165	7356
349	1	0	0	0	0	12040	180	7438
350	1	0	0	0	0	12143	200	7743
351	1	0	0	0	0	12323	232	7966
352	1	0	0	0	0	12506	209	8537
353	1	0	0	0	0	13046	143	9256
354	1	0	0	0	0	13586	111	10152
355	1	0	0	0	0	14126	0	10265
356	1	0	0	0	0	14843	0	9679
357	1	0	0	0	0	15740	0	8814
358	1	0	0	0	0	16637	0	7842
359	1	0	0	0	0	17355	0	7309
360	1	0	0	0	0	17538	0	6813

361	1	0	0	0	0	17541	0	6499
362	1	0	0	0	0	17366	0	5953
363	1	0	0	0	0	16812	0	5613
364	1	0	0	0	0	16661	0	5324
365	1	0	0	0	0	16485	0	5079
366	1	0	0	0	0	15775	0	4845
367	1	0	0	0	0	15421	0	4569
368	1	0	0	0	0	15246	0	4384
369	1	0	0	0	0	14715	0	4207
370	1	0	0	0	0	14361	0	4060
371	1	0	0	0	0	14187	0	3785
372	1	0	0	0	0	13833	0	3695
373	1	0	0	0	0	13479	0	3525
374	1	0	0	0	0	13305	0	3402
375	1	0	0	0	0	13487	0	3323
376	1	0	0	0	0	14384	0	3151
377	1	0	0	0	0	15102	0	3131
378	1	0	0	0	0	15563	0	3056
379	1	0	0	0	0	15745	0	3020
380	1	0	0	0	0	14757	0	2983
381	1	0	0	0	0	14403	0	2880
382	1	0	0	0	0	13694	0	2747
383	1	0	0	0	0	13518	0	2591
384	1	0	0	0	0	13165	0	2305
385	1	0	0	0	0	13268	0	2075
386	1	0	0	0	0	13173	0	1762
387	1	0	0	0	0	13177	0	1363
388	1	0	0	0	0	13002	0	1199
389	1	0	0	0	0	12826	0	961

390	1	0	0	0	0	11545	0	761
391	1	0	0	0	0	10614	0	549
392	1	0	0	0	0	9623	0	361
393	1	0	0	0	0	8556	0	286
394	1	0	0	0	0	7845	0	199
395	1	0	0	0	0	6082	0	0
396	1	0	0	0	0	5953	0	0
397	1	0	0	0	0	5807	0	0
398	1	0	0	0	0	5783	0	0
399	1	0	0	0	0	5815	0	0
400	1	0	0	0	0	5863	0	0
401	0	0	0	0	0	5931	0	0
402	0	0	0	0	0	6014	0	0
403	0	0	0	0	0	6047	0	0
404	0	0	0	0	0	6132	0	0
405	0	0	0	0	0	6129	0	0
406	0	0	0	0	0	6172	0	0
407	0	0	0	0	0	6173	0	0
408	0	0	0	0	0	6194	0	0
409	0	0	0	0	0	6271	0	0
410	0	0	0	0	0	6197	0	0
411	0	0	0	0	0	6139	0	0
412	0	0	0	0	0	5987	0	0
413	0	0	0	0	0	5880	0	0
414	0	0	0	0	0	5751	0	0
415	0	0	0	0	0	5496	0	0
416	0	0	0	0	0	5295	0	0
417	0	0	0	0	0	5184	0	0
418	0	0	0	0	0	5055	0	0

419	0	0	0	0	0	4908	0	0
420	0	0	0	0	0	4868	0	0
421	0	0	0	0	0	4845	0	0
422	0	0	0	0	0	4842	0	0
423	0	0	0	0	0	4748	0	0
424	0	0	0	0	0	4655	0	0
425	0	0	0	0	0	4579	0	0
426	0	0	0	0	0	4538	0	0
427	0	0	0	0	0	4553	0	0
428	0	0	0	0	0	4600	0	0
429	0	0	0	0	0	4544	0	0
430	0	0	0	0	0	4361	0	0
431	0	0	0	0	0	4124	0	0
432	0	0	0	0	0	4086	0	0
433	0	0	0	0	0	4045	0	0
434	0	0	0	0	0	4040	0	0
435	0	0	0	0	0	3946	0	0
436	0	0	0	0	0	3710	0	0
437	0	0	0	0	0	3385	0	0
438	0	0	0	0	0	3006	0	0
439	0	0	0	0	0	2840	0	0
440	0	0	0	0	0	2534	0	0
441	0	0	0	0	0	2457	0	0
442	0	0	0	0	0	2149	0	0
443	0	0	0	0	0	1858	0	0
444	0	0	0	0	0	1772	0	0
445	0	0	0	0	0	1490	0	0
446	0	0	0	0	0	1452	0	0
447	0	0	0	0	0	1436	0	0

448	0	0	0	0	0	1409	0	0
449	0	0	0	0	0	1308	0	0
450	0	0	0	0	0	1154	0	0
451	0	0	0	0	0	1021	0	0
452	0	0	0	0	0	944	0	0
453	0	0	0	0	0	923	0	0
454	0	0	0	0	0	990	0	0
455	0	0	0	0	0	967	0	0
456	0	0	0	0	0	856	0	0
457	0	0	0	0	0	663	0	0
458	0	0	0	0	0	579	0	0
459	0	0	0	0	0	480	0	0
460	0	0	0	0	0	424	0	0
461	0	0	0	0	0	441	0	0
462	0	0	0	0	0	473	0	0
463	0	0	0	0	0	447	0	0
464	0	0	0	0	0	286	0	0
465	0	0	0	0	0	86	0	0
466	0	0	0	0	0	86	0	0
467	0	0	0	0	0	86	0	0
468	0	0	0	0	0	86	0	0
469	0	0	0	0	0	86	0	0
470	0	0	0	0	0	86	0	0
471	0	0	0	0	0	86	0	0
472	0	0	0	0	0	86	0	0
473	0	0	0	0	0	86	0	0
474	0	0	0	0	0	86	0	0
475	0	0	0	0	0	86	0	0
476	0	0	0	0	0	86	0	0

477	0	0	0	0	0	86	0	0
478	0	0	0	0	0	86	0	0
479	0	0	0	0	0	86	0	0
480	0	0	0	0	0	86	0	0
481	0	0	0	0	0	86	0	0
482	0	0	0	0	0	86	0	0
483	0	0	0	0	0	86	0	0
484	0	0	0	0	0	86	0	0
485	0	0	0	0	0	86	0	0
486	0	0	0	0	0	86	0	0
487	0	0	0	0	0	86	0	0
488	0	0	0	0	0	86	0	0
489	0	0	0	0	0	86	0	0
490	0	0	0	0	0	86	0	0
491	0	0	0	0	0	86	0	0
492	0	0	0	0	0	86	0	0
493	0	0	0	0	0	86	0	0
494	0	0	0	0	0	86	0	0
495	0	0	0	0	0	86	0	0
496	0	0	0	0	0	86	0	0
497	0	0	0	0	0	86	0	0
498	0	0	0	0	0	86	0	0
499	0	0	0	0	0	86	0	0
500	0	0	0	0	0	86	0	0

[a] $\varepsilon(\lambda)$ for benzothiophene measured in solvent ethanol [56].

[b] $\varepsilon(\lambda)$ for dibenzothiophene measured in solvent isooctane [56].

[c]$\varepsilon(\lambda)$ for dibenzofuran measured in solvent hexane [56].

[d]$\varepsilon(\lambda)$ for for acenaphthylene measured in solvent ethanol [56].

[e]$\varepsilon(\lambda)$ for carbazole measured in solvent ethanol [56].

[f]$\varepsilon(\lambda)$ for indeno[1,2,3-c,d]pyrene measured in solvent ethanol [56].

[g]$\varepsilon(\lambda)$ for retene measured in solvent ethanol [56].

[g]$\varepsilon(\lambda)$ for acridine measured in solvent ethanol [56].

Table B.3. Substituted molar absorption coefficients for the chemicals whole molar absorption coefficients are not available**.**

Chemical	Substitute chemical
2-methylphenanthrene	1-methylphenanthrene
3-methylphenanthrene	1-methylphenanthrene
3,6-dimethylphenanthrene	2,6-dimethylphenanthrene
2,3,6-trimethylphenanthrene	1,6,7-trimethylphenanthrene
2-methylanthracene	9-methylanthracene
2,3-dimethylanthracene	9-methylanthracene
1-methylpyrene	3-methylpyrene
1-methylfluorene	fluorene
alkylatednaphthalenes	1-methylnaphthalene
alkylatedphenanthrenes	9-methylphenanthrene
alkylatedanthracenes	9-methylanthracene
alkylatedpyrenes	3-methylpyrene
alkylatedchrysenes	1-methylchrysene
alkylatedfluorenes	fluorene
alkylatedbenzothiophenes	benzothiophene
alkylated dibenzothiophenes	dibenzothiophene

B.3 PTLM Validation for APAHs and other Phototoxic Compounds PTLM Validation for APAHs and other Phototoxic Compounds

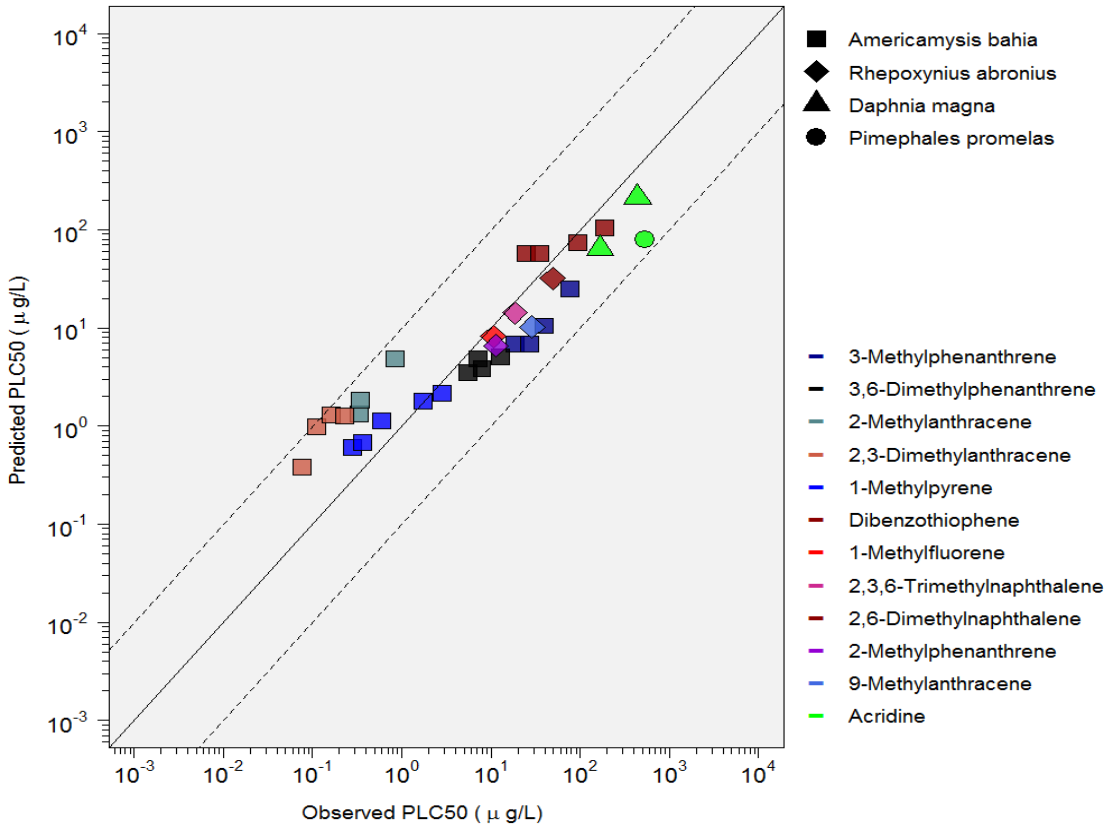

Figure B.1. Predicted PLC50 (µg/L) vs. observed PLC50 (µg/L) for APAHs and other phototoxic chemicals. The organism are shown with different symbols. Chemical are color coded as described in the bottom legend. The solid diagonal lines indicate perfect agreement between predicted and observed PLC50s. The dashed lines represent one order of magnitude uncertainties. The corresponding RMSE = 0.483. The data are presented in Table B.3.

Table B.4. Observed PLC50s and experimental data used to predict PLC50s of APAHs and other phototoxic compounds shown in Figures 4-1 and B.1.

Reference	PLC50 (µg/L)	Log(K_{ow})	Compound[a]	Organism[b]	NLC50 (µg/L)	End point	Light Source	T_{exp} (h)	I_{UVB} (µW/cm^2/nm)	I_{UVA} (µW/cm^2/nm)	I_{VIS} (µW/cm^2/nm)	P_{abs} (mol photn/mol chem)
[Finch]	18.60	5.036	3-MPHE	*A. bahia*	45.389	48 h EC50	SolarConstant	12	31.7	806	3940	11.851
[Finch]	5.48	5.34	3,6-DMPHE	*A. bahia*	25.291	48 h LC50	SolarConstant	12	30.5	803	4080	15.014
[Finch]	0.33	5.15	2-MANT	*A. bahia*	35.501	48 h LC50	SolarConstant	12	34.7	804	4690	415.474
[Finch]	0.08	5.69	2,3-DMANT	*A. bahia*	11.895	48 h LC50	SolarConstant	12	35.6	802	4510	606.808
[Finch]	0.28	5.48	1-MPYR	*A. bahia*	19.610	48 h LC50	SolarConstant	12	30	808	4460	672.146
[Finch]	24.80	4.341	DBTH	*A. bahia*	194.540	48 h LC50	SolarConstant	12	31.2	806	3740	1.586
[Finch]	26.90	5.036	3-MPHE	*A. bahia*	45.327	LT50	SolarConstant	12	31.7	806	3940	11.851
[Finch]	7.91	5.3	3,6-DMPHE	*A. bahia*	27.531	LT50	SolarConstant	12	30.5	803	4080	15.014
[Finch]	0.34	5.15	2-MANT	*A. bahia*	35.501	LT50	SolarConstant	5.43	34.7	804	4690	188.002
[Finch]	0.11	5.69	2,3-DMANT	*A. bahia*	11.895	LT50	SolarConstant	1.18	35.6	802	4510	59.669
[Finch]	0.36	5.48	1-MPYR	*A. bahia*	19.610	LT50	SolarConstant	9.23	30	808	4460	516.992
[Finch]	35.50	4.341	DBTH	*A. bahia*	194.540	LT50	SolarConstant	12	31.2	806	3740	1.586
[Finch]	38.90	5.036	3-MPHE	*A. bahia*	45.327	LT50	SolarConstant	3.51	31.7	806	3940	3.466
[Finch]	7.18	5.3	3,6-DMPHE	*A. bahia*	27.531	LT50	SolarConstant	6.31	30.5	803	4080	7.895
[Finch]	0.85	5.15	2-MANT	*A. bahia*	35.501	LT50	SolarConstant	0.46	34.7	804	4690	15.927

[Finch]	0.16	5.69	2,3-DMANT	*A. bahia*	11.895	LT50	SolarConstant	0.58	35.6	802	4510	29.329
[Finch]	0.59	5.48	1-MPYR	*A. bahia*	19.610	LT50	SolarConstant	2.57	30	808	4460	143.951
[Finch]	92.70	4.341	DBTH	*A. bahia*	194.540	LT50	SolarConstant	5.05	31.2	806	3740	0.667
[Finch]	76.20	5.036	3-MPHE	*A. bahia*	45.327	LT50	SolarConstant	0.13	31.7	806	3940	0.1284
[Finch]	12.60	5.3	3,6-DMPHE	*A. bahia*	27.531	LT50	SolarConstant	5.43	30.5	803	4080	6.794
[Finch]	0.23	5.69	2,3-DMANT	*A. bahia*	11.895	LT50	SolarConstant	0.61	35.6	802	4510	30.846
[Finch]	1.71	5.48	1-MPYR	*A. bahia*	19.610	LT50	SolarConstant	0.81	30	808	4460	45.370
[Finch]	190.00	4.341	DBTH	*A. bahia*	194.540	LT50	SolarConstant	1.11	31.2	806	3740	0.147
[Finch]	2.87	5.48	1-MPYR	*A. bahia*	19.610	LT50	SolarConstant	0.5	30	808	4460	8.006
[8]	10.60	4.37	1-MFLU	*R. abronius*	6.510	10 d LC50	Qpanel	1	128	279	0	0.012
[8]	18.50	4.57	2,3,6-TMPHE	*R. abronius*	3.994	10 d LC50	Qpanel	1	128	279	0	0.012
[8]	49.20	4.27	2,6-DMNAP	*R. abronius*	6.999	10 d LC50	Qpanel	1	128	279	0	0.057
[8]	11.40	5.04	2-MPHE	*R. abronius*	1.690	10 d LC50	Qpanel	1	128	279	0	0.0984
[8]	29.00	4.996	9-MANT	*R. abronius*	1.801	10 d LC50	Qpanel	1	128	279	0	1.757
[11]	440.10	4.48	ACR	*D. magna*	588.922	LT50	Solar Radiation[d]	0.897	25	120	680	0.800
[4]	525.00	4.48	ACR	*P. promelas*	623.82	LT50	SSR I[e]	4.3	20	95	0	19.689
[34]	168.00	4.48	ACR	*D. magna*	588.92	24 h LC50	Qpanel	2	0	320	0	27.894

[a]Abbreviations for compounds: 2-MPHE = 2-methylphenanthrene; 3-MPHE = 3-methylphenanthrene; 3,6-DMPHE = 3,6-dimethylphenanthrene; 2,3,6-TMPHE = 2,3,6-trimethylphenanthrene; 2,6-DMNAP = 2,6-dimethylnaphthalene; 2-MANT = 2-methylanthracene; 9-MANT = 9-methylanthracene; 2,3-DMANT = 2,3-dimethylanthracene; 1-MPYR = 1-methylpyrene; 1-MFLU = 1-methylfluorene; DBTH = dibenzothiophene; ACR = acridine.

[b]Abbreviations for organisms: *D. magna = Daphnia magna; A. bahia = Americamysis bahia; P. promelas = Pimephales promelas; R. abronius= Rhepoxynius abronius.*

B.4 Narcotic Toxicity and Phototoxicity Data Associated with Binary and Ternary Mixtures of PAHs.

Table B.5. Data associated with the predicted and observed PTU values presented in Figures 4-2 and 4-3. The endpoints are 48-h LC50.

Mixture	PAH[a]	$C_{W,i}$	Organism[b]	I_{UVB} (μW/cm²/nm)	I_{UVA} (μW/cm²/nm)	I_{VIS} (μW/cm²/nm)	P_{abs}[c] (mol photon/mol chem)	Predicted PLC50$_i$ (μg/L)	Predicted PTU$_i$[d]	Predicted PTU[e]	Observed PLC50$_i$	Observed PTU	%Mortality
PYR+ANT	PYR	0.19	*A. bahia*	30.8	809	6880	369.81	1.55	0.12	0.14	0.60	0.37	2.50
PYR+ANT	ANT	0.10	*A. bahia*	30.8	809	6880	363.28	4.82	0.02	0.14	0.62	0.37	2.50
PYR+ANT	PYR	0.19	*A. bahia*	30.8	809	6880	369.81	1.55	0.12	0.16	0.60	0.63	10.00
PYR+ANT	ANT	0.20	*A. bahia*	30.8	809	6880	363.28	4.82	0.04	0.16	0.62	0.63	10.00
PYR+ANT	PYR	0.39	*A. bahia*	30.8	809	6880	369.81	1.55	0.25	0.33	0.60	1.24	80.00
PYR+ANT	ANT	0.37	*A. bahia*	30.8	809	6880	363.28	4.82	0.08	0.33	0.62	1.24	80.00
PYR+ANT	PYR	0.62	*A. bahia*	30.8	809	6880	369.81	1.55	0.40	0.55	0.60	2.23	100.00
PYR+ANT	ANT	0.74	*A. bahia*	30.8	809	6880	363.28	4.82	0.15	0.55	0.62	2.23	100.00
PYR+ANT	PYR	1.29	*A. bahia*	30.8	809	6880	369.81	1.55	0.83	1.08	0.60	4.05	100.00
PYR+ANT	ANT	1.18	*A. bahia*	30.8	809	6880	363.28	4.82	0.24	1.08	0.62	4.05	100.00
PYR+FLA	PYR	0.12	*A. bahia*	31.1	804	6580	368.43	1.56	0.08	0.20	0.60	0.36	0.00
PYR+FLA	FLA	0.18	*A. bahia*	31.1	804	6580	312.69	1.45	0.12	0.72	1.07	0.36	0.00
PYR+FLA	PYR	0.19	*A. bahia*	31.1	804	6580	368.43	1.56	0.12	0.36	0.60	0.74	7.50
PYR+FLA	FLA	0.35	*A. bahia*	31.1	804	6580	312.69	1.45	0.24	1.48	1.07	0.74	7.50
PYR+FLA	PYR	0.32	*A. bahia*	31.1	804	6580	368.43	1.56	0.21	0.62	0.60	1.09	100.00

PYR+FLA	FLA	0.60	*A. bahia*	31.1	804	6580	312.69	1.45	0.41	2.18	1.07	1.09	100.00
PYR+FLA	PYR	0.74	*A. bahia*	31.1	804	6580	368.43	1.56	0.48	1.46	0.60	2.57	100.00
PYR+FLA	FLA	1.43	*A. bahia*	31.1	804	6580	312.69	1.45	0.98	5.14	1.07	2.57	100.00
PYR+FLA	PYR	1.31	*A. bahia*	31.1	804	6580	368.43	1.56	0.84	2.65	0.60	4.63	100.00
PYR+FLA	FLA	2.63	*A. bahia*	31.1	804	6580	312.69	1.45	1.81	9.26	1.07	4.63	100.00
PYR+ANT	ANT	0.10	*A. bahia*	30.2	807	6940	362.27	4.82	0.02	0.13	0.62	0.32	2.50
PYR+ANT	FLA	0.16	*A. bahia*	30.2	807	6940	313.39	1.45	0.11	0.13	1.07	0.32	2.50
PYR+ANT	ANT	0.17	*A. bahia*	30.2	807	6940	362.27	4.82	0.04	0.34	0.62	0.69	30.00
PYR+ANT	FLA	0.44	*A. bahia*	30.2	807	6940	313.39	1.45	0.30	0.34	1.07	0.69	30.00
PYR+ANT	ANT	0.33	*A. bahia*	30.2	807	6940	362.27	4.82	0.07	0.60	0.62	1.25	97.50
PYR+ANT	FLA	0.77	*A. bahia*	30.2	807	6940	313.39	1.45	0.53	0.60	1.07	1.25	97.50
PYR+ANT	ANT	0.61	*A. bahia*	30.2	807	6940	362.27	4.82	0.13	1.19	0.62	2.42	100.00
PYR+ANT	FLA	1.54	*A. bahia*	30.2	807	6940	313.39	1.45	1.06	1.19	1.07	2.42	100.00
PYR+ANT	ANT	1.17	*A. bahia*	30.2	807	6940	362.27	4.82	0.24	2.43	0.62	4.85	100.00
PYR+ANT	FLA	3.17	*A. bahia*	30.2	807	6940	313.39	1.45	2.19	2.43	1.07	4.85	100.00
PYR+ANT+FLA	PYR	0.10	*A. bahia*	30.2	799	6700	364.84	1.56	0.07	0.15	0.60	0.39	0.00
PYR+ANT+FLA	ANT	0.08	*A. bahia*	30.2	799	6700	358.74	4.84	0.02	0.15	0.62	0.39	0.00
PYR+ANT+FLA	FLA	0.10	*A. bahia*	30.2	799	6700	310.42	1.45	0.07	0.15	1.07	0.39	5.00
PYR+ANT+FLA	PYR	0.14	*A. bahia*	30.2	799	6700	364.84	1.56	0.09	0.24	0.60	0.59	5.00
PYR+ANT+FLA	ANT	0.12	*A. bahia*	30.2	799	6700	358.74	4.84	0.02	0.24	0.62	0.59	97.50
PYR+ANT+FLA	FLA	0.18	*A. bahia*	30.2	799	6700	310.42	1.45	0.13	0.24	1.07	0.59	97.50
PYR+ANT+FLA	PYR	0.21	*A. bahia*	30.2	799	6700	364.84	1.56	0.13	0.43	0.60	1.03	100.00
PYR+ANT+FLA	ANT	0.20	*A. bahia*	30.2	799	6700	358.74	4.84	0.04	0.43	0.62	1.03	100.00
PYR+ANT+FLA	FLA	0.37	*A. bahia*	30.2	799	6700	310.42	1.45	0.25	0.43	1.07	1.03	100.00
PYR+ANT+FLA	PYR	0.43	*A. bahia*	30.2	799	6700	364.84	1.56	0.28	0.90	0.60	2.06	100.00
PYR+ANT+FLA	ANT	0.38	*A. bahia*	30.2	799	6700	358.74	4.84	0.08	0.90	0.62	2.06	100.00

PYR+ANT+FLA	FLA	0.80	*A. bahia*	30.2	799	6700	310.42	1.45	0.55	0.90	1.07	2.06	100.00
PYR+ANT+FLA	PYR	0.75	*A. bahia*	30.2	799	6700	364.84	1.56	0.48	1.64	0.60	3.78	100.00
PYR+ANT+FLA	ANT	0.72	*A. bahia*	30.2	799	6700	358.74	4.84	0.15	1.64	0.62	3.78	100.00
PYR+ANT+FLA	FLA	1.48	*A. bahia*	30.2	799	6700	310.42	1.45	1.02	1.64	1.07	3.78	100.00
PYR+ANT	PYR	0.20	*M. beryllina*	28.9	803	5100	364.00	1.70	0.12	0.17	1.25	0.27	5.00
PYR+ANT	ANT	0.29	*M. beryllina*	28.9	803	5100	360.24	5.24	0.05	0.17	2.61	0.27	5.00
PYR+ANT	PYR	0.32	*M. beryllina*	28.9	803	5100	364.00	1.70	0.19	0.28	1.25	0.44	7.50
PYR+ANT	ANT	0.48	*M. beryllina*	28.9	803	5100	360.24	5.24	0.09	0.28	2.61	0.44	7.50
PYR+ANT	PYR	0.59	*M. beryllina*	28.9	803	5100	364.00	1.70	0.35	0.56	1.25	0.90	37.50
PYR+ANT	ANT	1.13	*M. beryllina*	28.9	803	5100	360.24	5.24	0.22	0.56	2.61	0.90	37.50
PYR+ANT	PYR	1.03	*M. beryllina*	28.9	803	5100	364.00	1.70	0.61	0.96	1.25	1.53	100.00
PYR+ANT	ANT	1.85	*M. beryllina*	28.9	803	5100	360.24	5.24	0.35	0.96	2.61	1.53	100.00
PYR+ANT	PYR	2.43	*M. beryllina*	28.9	803	5100	364.00	1.70	1.43	2.21	1.25	3.52	100.00
PYR+ANT	ANT	4.09	*M. beryllina*	28.9	803	5100	360.24	5.24	0.78	2.21	2.61	3.52	100.00
PYR+FLA	PYR	0.24	*M. beryllina*	28.7	802	5290	363.25	1.70	0.14	0.68	1.25	0.74	2.50
PYR+FLA	FLA	0.85	*M. beryllina*	28.7	802	5290	310.83	1.58	0.54	0.68	1.54	0.74	2.50
PYR+FLA	PYR	0.42	*M. beryllina*	28.7	802	5290	363.25	1.70	0.25	1.15	1.25	1.27	25.00
PYR+FLA	FLA	1.43	*M. beryllina*	28.7	802	5290	310.83	1.58	0.91	1.15	1.54	1.27	25.00
PYR+FLA	PYR	1.09	*M. beryllina*	28.7	802	5290	363.25	1.70	0.64	3.26	1.25	3.55	100.00
PYR+FLA	FLA	4.13	*M. beryllina*	28.7	802	5290	310.83	1.58	2.62	3.26	1.54	3.55	100.00
PYR+FLA	PYR	2.28	*M. beryllina*	28.7	802	5290	363.25	1.70	1.34	6.54	1.25	7.14	100.00
PYR+FLA	FLA	8.19	*M. beryllina*	28.7	802	5290	310.83	1.58	5.19	6.54	1.54	7.14	100.00
PYR+FLA	PYR	5.91	*M. beryllina*	28.7	802	5290	363.25	1.70	3.48	18.38	1.25	20.03	100.00

PYR+FLA	FLA	23.50	*M. beryllina*	28.7	802	5290	310.83	1.58	14.90	18.38	1.54	20.03	100.00
PYR+ANT	ANT	0.23	*M. beryllina*	29.2	807	5060	362.06	5.23	0.04	0.51	2.61	0.56	15.00
PYR+ANT	FLA	0.73	*M. beryllina*	29.2	807	5060	312.92	1.57	0.47	0.51	1.54	0.56	15.00
PYR+ANT	ANT	0.48	*M. beryllina*	29.2	807	5060	362.06	5.23	0.09	0.98	2.61	1.09	87.50
PYR+ANT	FLA	1.39	*M. beryllina*	29.2	807	5060	312.92	1.57	0.89	0.98	1.54	1.09	87.50
PYR+ANT	ANT	0.82	*M. beryllina*	29.2	807	5060	362.06	5.23	0.16	2.16	2.61	2.36	100.00
PYR+ANT	FLA	3.15	*M. beryllina*	29.2	807	5060	312.92	1.57	2.00	2.16	1.54	2.36	100.00
PYR+ANT	ANT	1.70	*M. beryllina*	29.2	807	5060	362.06	5.23	0.33	3.81	2.61	4.21	100.00
PYR+ANT	FLA	5.49	*M. beryllina*	29.2	807	5060	312.92	1.57	3.49	3.81	1.54	4.21	100.00
PYR+ANT	ANT	3.79	*M. beryllina*	29.2	807	5060	362.06	5.23	0.72	7.32	2.61	8.18	100.00
PYR+ANT	FLA	10.37	*M. beryllina*	29.2	807	5060	312.92	1.57	6.59	7.32	1.54	8.18	100.00
PYR+ANT+FLA	PYR	0.17	*M. beryllina*	29.4	797	4450	362.60	1.70	0.10	0.45	1.25	0.53	5.00
PYR+ANT+FLA	ANT	0.17	*M. beryllina*	29.4	797	4450	357.69	5.26	0.03	0.45	2.61	0.53	5.00
PYR+ANT+FLA	FLA	0.50	*M. beryllina*	29.4	797	4450	309.30	1.58	0.32	0.45	1.54	0.53	5.00
PYR+ANT+FLA	PYR	0.30	*M. beryllina*	29.4	797	4450	362.60	1.70	0.18	0.85	1.25	0.99	52.50
PYR+ANT+FLA	ANT	0.31	*M. beryllina*	29.4	797	4450	357.69	5.26	0.06	0.85	2.61	0.99	52.50
PYR+ANT+FLA	FLA	0.97	*M. beryllina*	29.4	797	4450	309.30	1.58	0.61	0.85	1.54	0.99	52.50
PYR+ANT+FLA	PYR	0.56	*M. beryllina*	29.4	797	4450	362.60	1.70	0.33	1.78	1.25	2.05	100.00
PYR+ANT+FLA	ANT	0.62	*M. beryllina*	29.4	797	4450	357.69	5.26	0.12	1.78	2.61	2.05	100.00
PYR+ANT+FLA	FLA	2.11	*M. beryllina*	29.4	797	4450	309.30	1.58	1.33	1.78	1.54	2.05	100.00
PYR+ANT+FLA	PYR	0.94	*M. beryllina*	29.4	797	4450	362.60	1.70	0.55	3.32	1.25	3.86	100.00
PYR+ANT+FLA	ANT	1.45	*M. beryllina*	29.4	797	4450	357.69	5.26	0.28	3.32	2.61	3.86	100.00

PYR+ANT+FLA	FLA	3.93	*M. beryllina*	29.4	797	4450	309.30	1.58	2.49	3.32	1.54	3.86	100.00
PYR+ANT+FLA	PYR	2.60	*M. beryllina*	29.4	797	4450	362.60	1.70	1.53	7.35	1.25	8.59	100.00
PYR+ANT+FLA	ANT	2.87	*M. beryllina*	29.4	797	4450	357.69	5.26	0.55	7.35	2.61	8.59	100.00
PYR+ANT+FLA	FLA	8.33	*M. beryllina*	29.4	797	4450	309.30	1.58	5.27	7.35	1.54	8.59	100.00

[a]Abbreviations for polycyclic aromatic hydrocarbons (PAHs): FLA = fluoranthene; ANT = anthracene; PYR = pyrene.

[b]Abbreviations for organisms: *A. bahia = Americamysis bahia; M. beryllina = Menidia beryllina.*

[c]The light source is SolarConstant 1200 and T_{exp}=12 (h).

[d]PTU_i denotes the phototoxic unit of the corresponding PAH.

[e]PTU is the total mixture PTU.

B.5 Computational Narcotic Toxicity and Phototoxicity Data Associated with Binary and Ternary Mixtures of PAHs.

Mixtures PTU_is can be readily predicted using Equations 4-6 and 4-8 which incorporate PTLM (Equation 4-2) and the additivity assumption. As a case in point, PLC50 predicted by the PTLM for pyrene and anthracene exposed to *Americamysis bahia* under SolarConstant 1200 lamp radiation for T_{exp}=12 (h) at the respective irradiance intensities for UVB, UVA, and VIS, I_{UVB} = 30.8 (μW/cm^2), I_{UVA} = 809 (μW/cm^2), and I_{VIS} = 6880 (μW/cm^2) are $PLC50_{pyrene}$ = 1.555 (μg/L) and $PLC50_{anthracene}$ = 4.816 (μg/L), respectively. Details of PLC50 calculations for single compounds are presented in Appendix A.3.

Exposing *Americamysis bahia* to a binary mixture composed the respective aqueous concentrations of pyrene and anthracene, $C_{w,pyrene}$ = 0.190 (μg/L) and $C_{w,anthracene}$ = 0.103 (μg/L), under the same light irradiance and duration results in the following PTU for the binary mixture:

$$\frac{C_{w,pyrene}}{PLC0_{pyrene}} + \frac{C_{w,anthracene}}{PLC0_{anthracene}} = \frac{0.190}{1.555} + \frac{0.103}{4.816} = 0.144 \quad \text{(B-1)}$$

Regarding ternary mixtures, for instance, for 12-h light exposure of *Americamysis bahia* (T_{exp}=12 (h)) to SolarConstant 1200 lamp at UVB, UVA, and VIS intensities of I_{UVB} = 30.200 (μW/cm^2), I_{UVA} = 799 (μW/cm^2), and I_{VIS} = 6700 (μW/cm^2), PTLM predicts the respective PLC50s of $PLC50_{pyrene}$=1.563 (μg/L), $PLC50_{anthracene}$=4.841 (μg/L), and $PLC50_{fluoranthene}$=1.455 (μg/L). Exposing the organisms to a ternary mixture of pyrene, anthracene, and fluoranthene with the aqueous concentrates of $C_{w,pyrene}$ = 0.749 (μg/L), $C_{w,anthracene}$ = 0.715 (μg/L), and $C_{w,fluoranthene}$ = 1.478 (μg/L) yields the following total PTU:

$$\frac{C_{\text{w,pyrene}}}{\text{PLC0}_{\text{pyrene}}} + \frac{C_{\text{w,anthracene}}}{\text{PLC0}_{\text{anthracene}}} + \frac{C_{\text{w,fluoranthene}}}{\text{PLC0}_{\text{fluoranthene}}} \quad \text{(B-2)}$$

$$= \frac{0.749}{1.563} + \frac{0.715}{4.841} + \frac{1.478}{1.455} = 1.643$$

PTU =1 at 50% mortality. Mortalities less and greater than 50% are expected below and above the PTU of unity, respectively. For the binary combination of pyrene and anthracene with the aqueous concentrations mentioned above, the mixture is not expected to be phototoxic to *Americamysis bahia* (Equation B-1), whereas Equation B-2 implies that the ternary mixture of pyrene, anthracene, and fluoranthene with the aforementioned aqueous concentrations has potential to be phototoxic to the organism.

B.6 Observed and Predicted Macondo Crude Oil Narcotic Toxicity and Phototoxicity Data

Table B.6. Observed and predicted narcotic toxicity of neat and weathered Macondo crude oils exposed to the test organisms.

	Observed NLC50 (%WAF)	**Predicted NLC50 (%WAF)**
Mass *Menidia beryllina*	>100	85.289
CTC *Menidia beryllina*	>100	646.554
Juniper *Menidia beryllina*	>100	2583.050
Mass *Americamysis bahia*	93.3	88.900
CTC *Americamysis bahia*	>100	964.803
Juniper *Americamysis bahia*	>100	1922.785
Mass *Cyprinodon variegatus*	>100	224.609
CTC *Cyprinodon variegatus*	>100	1914.777
Juniper *Cyprinodon variegatus*	>100	2007.176
Mass *Fundulus grandis*	>100	372.403
CTC *Fundulus grandis*	>100	1095.134
Juniper *Fundulus grandis*	>100	1353.034

Table B.7. Observed and predicted phototoxicity of neat and weathered Macondo crude oils exposed to the test organisms.

	Observed PLC50 (%WAF)	**Predicted PLC50 (%WAF)**
Mass Natural radiation *Menidia beryllina*	60.1	23.96
CTC Natural radiation *Menidia beryllina*	60.5	66.761
CTC Artificial radiation *Menidia beryllina*	70.8	33.897
Juniper Natural radiation *Menidia beryllina*	>100	231.329
Mass Natural radiation *Americamysis bahia*	20.3	23.686
CTC Natural radiation *Americamysis bahia*	32.3	101.929
CTC Artificial radiation *Americamysis bahia*	54.5	64.572
Juniper Natural radiation *Americamysis bahia*	51.2	153.58
Mass Artificial radiation *Cyprinodon variegatus*	>100	53.392
CTC Artificial radiation *Cyprinodon variegatus*	>100	141.231

Juniper Artificial radiation *Cyprinodon variegatus*	>100	403.882
Mass Artificial radiation *Fundulus grandis*	>100	75.347
CTC Artificial radiation *Fundulus grandis*	>100	157.466
Juniper Artificial radiation *Fundulus grandis*	>100	355.711

B.7 Chemical Compositions Data for the Components in Macondo Crude Oil WAF Solution

Table B.8. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 100% WAF exposed to *Americamysis bahia* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	22.739	23.100	46.329
2	C2-Naphthalenes	156.2	4.31	22.031	9.160	19.950
3	2-Methylnaphthalene	142.2	3.72	22.739	28.000	64.011
4	1-Methylnaphthalene	142.2	3.72	22.739	20.800	64.011
5	C3-Naphthalenes	170.26	4.77	22.031	2.040	8.069
6	Toluene	92.14	2.54	0.000	1640.000	7758.791
7	C1-Fluorenes	180.2	4.97	89.621	0.632	3.227
8	2,6-Dimethylnaphthalene	156.23	4.26	22.031	3.920	22.225
9	C1-Phenanthrenes/Anthracenes	192.3	4.26	976.945	0.959	6.018
10	m-XYLENE	106.2	3.09	0.000	419.000	2733.194
11	C2-Fluorenes	194.3	5.21	89.621	0.308	2.074
12	C4-Naphthalenes	184.3	5.18	22.031	0.463	3.610
13	Naphthalene	234.3	3.17	12.554	48.500	429.747
14	1,6,7-Trimethylnaphthalene	170.26	4.81	39.283	0.561	5.942
15	2-Methylanthracene	192.26	4.89	976.945	0.139	1.548
16	o-XYLENE	106.2	3.09	0.000	241.000	2733.194
17	4/9-Methylphenanthrene	192.26	4.89	78.492	0.376	4.311
18	1,2,4-Trimethylbenzene	120.2	3.63	0.000	75.200	966.074
19	Phenanthrene	178.2	4.35	46.039	1.010	15.764

20	Benzene	78.11	1.99	0.000	1200.000	21520.507
21	Fluorene	166.2	4.02	89.621	1.060	23.062
22	1-Methylphenanthrene	192.26	4.89	78.492	0.185	4.311
23	Methylcyclohexane	98.19	3.59	0.000	43.100	1105.638
24	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	41.800	1075.995
25	Ethylbenzene	106.2	3.03	0.000	117.000	3110.501
26	CYCLOHEXANE	84.16	3.18	0.000	85.500	2293.040
27	3-Methylphenanthrene	192.26	4.89	78.492	0.154	4.311
28	2-Methylphenanthrene	192.26	4.89	78.492	0.152	4.311
29	1,3,5-trimethylbenzene	120.2	3.63	0.000	27.000	966.074
30	p-XYLENE	106.2	3.09	0.000	66.500	2733.194
31	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	24.700	1075.995
32	C2-Dibenzothiophenes	214.3	5.13	6.751	0.160	7.172
33	Anthracene	178.2	4.35	613.291	0.116	5.569
34	Methylcyclopentane	84.16	3.1	0.000	55.600	2724.530
35	C1-Dibenzothiophenes	198.3	4.71	6.751	0.229	16.409
36	4-ETHYLTOLUENE	120.2	3.58	0.000	14.600	1075.995
37	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	4.070	367.163
38	C3-Benzothiophene	176.3	4.69	0.311	0.415	37.670
39	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	3.810	367.163
40	Propylbenzene	120.194	3.52	0.000	12.300	1224.471
41	CARBAZOLE	167.2	3.23	165.377	0.992	99.681
42	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	4.020	417.848
43	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	3.360	367.163
44	n-C5	72.15	2.8	0.000	39.800	4458.843
45	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	2.720	367.163
46	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	3.030	417.848
47	Isopropylbenzene	120.194	3.45	0.000	10.200	1423.864
48	Acenaphthene	154.2	4.15	64.349	0.126	18.424
49	Cyclopentane	70.13	2.68	0.000	37.100	5613.190

50	n-C6	86.18	3.29	0.000	12.000	1852.475
52	C4-Benzothiophene	190.3	5.18	0.311	0.090	14.143
53	m-cymene	134.2	4	0.000	3.030	485.890
54	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	2.270	367.217
55	Isopentane	72.15	2.72	0.000	32.200	5297.881
56	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	1.970	329.654
57	Pyrene	202.3	4.93	1126.734	0.008	1.408
59	Dibenzofuran	168.2	3.71	49.546	0.286	57.447
60	4-Methyldibenzothiophene	198.28	4.71	6.751	0.080	16.407
61	Dibenzothiophene	184.3	4.17	6.751	0.224	48.833
62	C2-Benzothiophene	162.25	4.13	0.311	0.513	115.901
67	Biphenyl	154.2	3.76	0.000	2.190	535.193
68	2/3-Methyldibenzothiophene	198.28	4.71	6.754	0.065	16.405
69	2-METHYLPENTANE	86.18	3.21	0.000	8.260	2201.062
71	3-Methylpentane	86.18	3.21	0.000	7.360	2201.062
76	Hydrindene	118.2	3.47	0.000	4.050	1341.169
77	4-isopropyltoluene	134.22	4	0.000	1.450	485.963
78	HEPTANE	100.2	3.78	0.000	2.110	749.158
79	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.948	367.217
80	Fluoranthene	202.3	4.93	835.591	0.004	1.594
81	3-methylhexane	100.2	3.71	0.000	2.060	871.151
82	1,2-Diethylbenzene	134.2	4.07	0.000	0.829	417.848
83	1-Methyldibenzothiophene	198.28	4.71	6.751	0.032	16.407
85	n-Butylbenzene	134.2	4.01	0.000	0.879	475.531
86	2-methylhexane	100.2	3.71	0.000	1.560	871.151
87	3-methylheptane	114.2	4.2	0.000	0.497	345.344
89	trans-Decalin	138.26	4.2	0.000	0.254	185.901
91	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.604	485.963
92	C1-Decalins	152.3	4.61	0.000	0.100	84.630
98	2,3-dimethylbutane	86.18	3.14	0.000	2.360	2559.484

103	C1-Benzothiophene	148.2	3.5365	0.311	0.225	380.424
104	Acenaphthylene	152.2	3.94	335.965	0.009	14.734
111	2,2-dimethylpentane	100.2	3.67	0.000	0.197	949.584
113	3-ethylhexane	114.2	4.2	0.000	0.055	345.344
115	cis-Decalin	138.26	4.2	0.000	0.017	185.901
118	Benzothiophene	134.2	2.99	0.311	0.037	1118.656
51	1-Decene	140.3	5.12	0.000	0.000	58.415
58	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	417.910
63	n-C10	142.29	5.25	0.000	0.000	44.767
64	n-C10	142.29	5.25	0.000	0.000	44.767
65	n-C10	142.3	5.25	0.000	0.000	44.770
66	n-C10	142.3	5.25	0.000	0.000	44.770
70	1-Nonene	126.2	4.62	0.000	0.000	154.357
72	n-C9	128.3	4.76	0.000	0.000	116.052
73	n-C9	128.3	4.76	0.000	0.000	116.052
74	n-C9	128.3	4.76	0.000	0.000	116.052
75	n-C9	128.3	4.76	0.000	0.000	116.052
84	n-C8	114.2	4.27	0.000	0.000	296.983
88	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	437.736
90	Octene-1	112.2	4.13	0.000	0.000	394.547
93	n-Pentylbenzene	148.2	4.5	0.000	0.000	234.765
94	n-C10	142.29	5.25	0.000	0.000	44.767
95	n-C10	142.29	5.25	0.000	0.000	44.767
96	n-C10	142.3	5.25	0.000	0.000	44.770
97	n-C10	142.3	5.25	0.000	0.000	44.770
99	2-methylheptane	114.2	4.2	0.000	0.000	345.344
100	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	477.147
101	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	410.437
102	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	437.851
105	n-C9	128.3	4.76	0.000	0.000	116.052

106	n-C9	128.3	4.76	0.000	0.000	116.052
107	n-C9	128.3	4.76	0.000	0.000	116.052
108	n-C9	128.3	4.76	0.000	0.000	116.052
109	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	410.437
110	2,3-dimethylhexane	114.2	4.12	0.000	0.000	410.329
112	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
114	tert-Butylbenzene	134.2	3.9	0.000	0.000	602.752
116	sec-Butylbenzene	134.2	3.94	0.000	0.000	552.966
117	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
119	n-C11	156.31	5.74	0.000	0.000	17.105
120	n-C11	156.31	5.74	0.000	0.000	17.105
121	n-C11	156.31	5.74	0.000	0.000	17.105
122	n-C11	156.31	5.74	0.000	0.000	17.105
123	n-C12	170.34	6.23	0.000	0.000	6.484
124	n-C12	170.34	6.23	0.000	0.000	6.484
125	n-C12	170.34	6.23	0.000	0.000	6.484
126	n-C12	170.34	6.23	0.000	0.000	6.484
127	n-C11	156.31	5.74	0.000	0.000	17.105
128	n-C11	156.31	5.74	0.000	0.000	17.105
129	n-C11	156.31	5.74	0.000	0.000	17.105
130	n-C11	156.31	5.74	0.000	0.000	17.105
131	n-C12	170.34	6.23	0.000	0.000	6.484
132	n-C12	170.34	6.23	0.000	0.000	6.484
133	n-C12	170.34	6.23	0.000	0.000	6.484
134	n-C12	170.34	6.23	0.000	0.000	6.484
135	n-C13	184.37	6.73	0.000	0.000	2.389
136	n-C14	198.4	7.22	0.000	0.000	0.894
137	n-C15	212.42	7.71	0.000	0.000	0.333
138	n-C16	226.45	8.2	0.000	0.000	0.123
139	n-C17	240.48	8.69	0.000	0.000	0.046

140	n-C18	254.5	9.18	0.000	0.000	0.017
141	n-C19	268.53	9.67	0.000	0.000	0.006
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.004
164	Pristane	268.525	9.38	0.000	0.000	0.012
165	Benzo(a)fluoranthene	252.3	6.11	4868.195	0.000	0.075
166	Benzo(b)fluorene	216.3	5.77	440.781	0.000	0.363
167	Benzo(k)fluoranthene	252.3	6.11	2735.614	0.000	0.095
168	Benzo[a]anthracene	228.3	5.52	743.532	0.000	0.529
169	Benzo[a]pyrene	252.3	6.11	3793.523	0.000	0.083

170	Benzo[b]fluoranthene	252.3	6.11	1622.042	0.000	0.119
171	Benzo[e]pyrene	252.3	6.11	906.904	0.000	0.151
172	Benzo[g,h,i]perylene	276.3	6.7	3006.420	0.000	0.028
173	C1-Chrysenes	242.3	6.0683	429.371	0.000	0.216
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1666.558	0.000	0.391
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.041
176	C2-Chrysenes	256.3	6.65	429.371	0.000	0.065
177	C2-Decalins	166.3	6.19	0.000	0.000	3.068
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1666.558	0.000	0.103
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.142
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	976.945	0.000	0.476
181	C3-Chrysenes	270.4	7.03	429.371	0.000	0.030
182	C3-Decalins	180.3	6.79	0.000	0.000	0.913
183	C3-Dibenzothiophenes	230.37	5.86	6.751	0.000	1.599
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1666.558	0.000	0.042
185	C3-Fluorenes	210.3	5.58	89.621	0.000	1.011
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.410
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	976.945	0.000	0.219
188	C4-Chrysenes	284.4	7.35	429.371	0.000	0.016
189	C4-Decalins	194.3	7.34	0.000	0.000	0.301
190	C4-Dibenzothiophenes	244.37	6.1	6.751	0.000	1.011
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1666.558	0.000	0.016
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.153
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	976.945	0.000	0.122
194	Chrysene	228.3	5.52	347.644	0.000	0.724
195	Dibenz(a,h)anthracene	278.4	6.7	1927.594	0.000	0.034
196	Indeno[1,2,3-cd]pyrene	276.3	6.7	5190.997	0.000	0.022
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	20.533
198	Perylene	252.3	6.11	8836.395	0.000	0.058
199	Retene	234.3	6.35	112.688	0.000	0.196

Table B.9. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 25% WAF exposed to *Americamysis bahia* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	22.739	6.380	46.329
2	C2-Naphthalenes	156.2	4.31	22.031	2.350	19.950
3	2-Methylnaphthalene	142.2	3.72	22.739	5.700	64.011
4	1-Methylnaphthalene	142.2	3.72	22.739	4.260	64.011
5	C3-Naphthalenes	170.26	4.77	22.031	0.481	8.069
6	C1-Fluorenes	180.2	4.97	89.621	0.164	3.227
7	Toluene	92.14	2.54	0.000	350.000	7758.791
8	2,6-Dimethylnaphthalene	156.23	4.26	22.031	1.000	22.225
9	C1-Phenanthrenes/Anthracenes	192.3	4.26	976.945	0.244	6.018
10	C2-Fluorenes	194.3	5.21	89.621	0.080	2.074
11	m-XYLENE	106.2	3.09	0.000	87.500	2733.194
12	C4-Naphthalenes	184.3	5.18	22.031	0.112	3.610
13	Naphthalene	234.3	3.17	12.554	10.700	429.747
14	1,6,7-Trimethylnaphthalene	170.26	4.81	39.283	0.135	5.942
15	4/9-Methylphenanthrene	192.26	4.89	78.492	0.094	4.311
16	o-XYLENE	106.2	3.09	0.000	58.000	2733.194
17	2-Methylanthracene	192.26	4.89	976.945	0.033	1.548
18	1,2,4-Trimethylbenzene	120.2	3.63	0.000	17.400	966.074
19	Phenanthrene	178.2	4.35	46.039	0.271	15.764
20	Fluorene	166.2	4.02	89.621	0.289	23.062
21	Benzene	78.11	1.99	0.000	254.000	21520.507
22	1-Methylphenanthrene	192.26	4.89	78.492	0.050	4.311
23	3-Methylphenanthrene	192.26	4.89	78.492	0.042	4.311

24	2-Methylphenanthrene	192.26	4.89	78.492	0.037	4.311
25	p-XYLENE	106.2	3.09	0.000	22.700	2733.194
26	Ethylbenzene	106.2	3.03	0.000	24.500	3110.501
27	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	8.350	1075.995
28	Methylcyclohexane	98.19	3.59	0.000	7.640	1105.638
30	CYCLOHEXANE	84.16	3.18	0.000	14.400	2293.040
31	C2-Dibenzothiophenes	214.3	5.13	6.751	0.042	7.172
32	1,3,5-trimethylbenzene	120.2	3.63	0.000	5.390	966.074
33	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	4.990	1075.995
38	Octene-1	112.2	4.13	0.000	1.540	394.547
39	Anthracene	178.2	4.35	613.291	0.020	5.569
41	Methylcyclopentane	84.16	3.1	0.000	9.410	2724.530
42	C3-Benzothiophene	176.3	4.69	0.311	0.119	37.670
43	C1-Dibenzothiophenes	198.3	4.71	6.751	0.052	16.409
48	4-ETHYLTOLUENE	120.2	3.58	0.000	2.980	1075.995
49	C4-Benzothiophene	190.3	5.18	0.311	0.038	14.143
50	CARBAZOLE	167.2	3.23	165.377	0.223	99.681
51	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.800	367.163
52	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.730	367.163
53	Propylbenzene	120.194	3.52	0.000	2.420	1224.471
55	Acenaphthene	154.2	4.15	64.349	0.032	18.424
56	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.632	367.163
57	Pyrene	202.3	4.93	1126.734	0.002	1.408
59	Isopropylbenzene	120.194	3.45	0.000	2.020	1423.864
60	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.513	367.217
61	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.582	417.848
62	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.510	367.163
63	n-C5	72.15	2.8	0.000	5.970	4458.843
64	Dibenzofuran	168.2	3.71	49.546	0.074	57.447

65	4-Methyldibenzothiophene	198.28	4.71	6.751	0.020	16.407
66	m-cymene	134.2	4	0.000	0.580	485.890
68	Isopentane	72.15	2.72	0.000	6.080	5297.881
69	Dibenzothiophene	184.3	4.17	6.751	0.056	48.833
70	Cyclopentane	70.13	2.68	0.000	6.380	5613.190
72	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.364	329.654
74	Biphenyl	154.2	3.76	0.000	0.587	535.193
75	C2-Benzothiophene	162.25	4.13	0.311	0.126	115.901
83	2/3-Methyldibenzothiophene	198.28	4.71	6.754	0.012	16.405
85	Hydrindene	118.2	3.47	0.000	0.880	1341.169
86	2-METHYLPENTANE	86.18	3.21	0.000	1.400	2201.062
88	Fluoranthene	202.3	4.93	835.591	0.001	1.594
89	4-isopropyltoluene	134.22	4	0.000	0.283	485.963
91	HEPTANE	100.2	3.78	0.000	0.386	749.158
92	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.185	367.217
93	1-Methyldibenzothiophene	198.28	4.71	6.751	0.007	16.407
94	3-methylhexane	100.2	3.71	0.000	0.379	871.151
95	1,2-Diethylbenzene	134.2	4.07	0.000	0.163	417.848
100	2-methylhexane	100.2	3.71	0.000	0.258	871.151
101	n-Butylbenzene	134.2	4.01	0.000	0.134	475.531
103	2,3-dimethylbutane	86.18	3.14	0.000	0.630	2559.484
104	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.114	485.963
107	C1-Benzothiophene	148.2	3.5365	0.311	0.062	380.424
109	Acenaphthylene	152.2	3.94	335.965	0.002	14.734
111	trans-Decalin	138.26	4.2	0.000	0.024	185.901
112	C1-Decalins	152.3	4.61	0.000	0.011	84.630
113	n-C8	114.2	4.27	0.000	0.035	296.983
116	2,2-dimethylpentane	100.2	3.67	0.000	0.033	949.584
117	cis-Decalin	138.26	4.2	0.000	0.002	185.901

118	Benzothiophene	134.2	2.99	0.311	0.009	1118.656
29	1-Decene	140.3	5.12	0.000	0.000	58.415
34	n-C10	142.29	5.25	0.000	0.000	44.767
35	n-C10	142.29	5.25	0.000	0.000	44.767
36	n-C10	142.3	5.25	0.000	0.000	44.770
37	n-C10	142.3	5.25	0.000	0.000	44.770
40	1-Nonene	126.2	4.62	0.000	0.000	154.357
44	n-C9	128.3	4.76	0.000	0.000	116.052
45	n-C9	128.3	4.76	0.000	0.000	116.052
46	n-C9	128.3	4.76	0.000	0.000	116.052
47	n-C9	128.3	4.76	0.000	0.000	116.052
54	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	417.848
58	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	437.736
67	n-C6	86.18	3.29	0.000	0.000	1852.475
71	n-Pentylbenzene	148.2	4.5	0.000	0.000	234.765
73	3-methylheptane	114.2	4.2	0.000	0.000	345.344
76	n-C10	142.29	5.25	0.000	0.000	44.767
77	n-C10	142.29	5.25	0.000	0.000	44.767
78	n-C10	142.3	5.25	0.000	0.000	44.770
79	n-C10	142.3	5.25	0.000	0.000	44.770
80	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	417.910
81	2-methylheptane	114.2	4.2	0.000	0.000	345.344
82	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	477.147
84	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	410.437
87	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	437.851
90	3-Methylpentane	86.18	3.21	0.000	0.000	2201.062
96	n-C9	128.3	4.76	0.000	0.000	116.052
97	n-C9	128.3	4.76	0.000	0.000	116.052
98	n-C9	128.3	4.76	0.000	0.000	116.052

99	n-C9	128.3	4.76	0.000	0.000	116.052
102	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	410.437
105	2,3-dimethylhexane	114.2	4.12	0.000	0.000	410.329
106	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
108	tert-Butylbenzene	134.2	3.9	0.000	0.000	602.752
110	3-ethylhexane	114.2	4.2	0.000	0.000	345.344
114	sec-Butylbenzene	134.2	3.94	0.000	0.000	552.966
115	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
119	n-C11	156.31	5.74	0.000	0.000	17.105
120	n-C11	156.31	5.74	0.000	0.000	17.105
121	n-C11	156.31	5.74	0.000	0.000	17.105
122	n-C11	156.31	5.74	0.000	0.000	17.105
123	n-C12	170.34	6.23	0.000	0.000	6.484
124	n-C12	170.34	6.23	0.000	0.000	6.484
125	n-C12	170.34	6.23	0.000	0.000	6.484
126	n-C12	170.34	6.23	0.000	0.000	6.484
127	n-C11	156.31	5.74	0.000	0.000	17.105
128	n-C11	156.31	5.74	0.000	0.000	17.105
129	n-C11	156.31	5.74	0.000	0.000	17.105
130	n-C11	156.31	5.74	0.000	0.000	17.105
131	n-C12	170.34	6.23	0.000	0.000	6.484
132	n-C12	170.34	6.23	0.000	0.000	6.484
133	n-C12	170.34	6.23	0.000	0.000	6.484
134	n-C12	170.34	6.23	0.000	0.000	6.484
135	n-C13	184.37	6.73	0.000	0.000	2.389
136	n-C14	198.4	7.22	0.000	0.000	0.894
137	n-C15	212.42	7.71	0.000	0.000	0.333
138	n-C16	226.45	8.2	0.000	0.000	0.123
139	n-C17	240.48	8.69	0.000	0.000	0.046

140	n-C18	254.5	9.18	0.000	0.000	0.017
141	n-C19	268.53	9.67	0.000	0.000	0.006
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.004
164	Pristane	268.525	9.38	0.000	0.000	0.012
165	Benzo(a)fluoranthene	252.3	6.11	4868.195	0.000	0.075
166	Benzo(b)fluorene	216.3	5.77	440.781	0.000	0.363
167	Benzo(k)fluoranthene	252.3	6.11	2735.614	0.000	0.095
168	Benzo[a]anthracene	228.3	5.52	743.532	0.000	0.529

169	Benzo[a]pyrene	252.3	6.11	3793.523	0.000	0.083
170	Benzo[b]fluoranthene	252.3	6.11	1622.042	0.000	0.119
171	Benzo[e]pyrene	252.3	6.11	906.904	0.000	0.151
172	Benzo[g,h,i]perylene	276.3	6.7	3006.420	0.000	0.028
173	C1-Chrysenes	242.3	6.0683	429.371	0.000	0.216
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1666.558	0.000	0.391
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.041
176	C2-Chrysenes	256.3	6.65	429.371	0.000	0.065
177	C2-Decalins	166.3	6.19	0.000	0.000	3.068
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1666.558	0.000	0.103
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.142
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	976.945	0.000	0.476
181	C3-Chrysenes	270.4	7.03	429.371	0.000	0.030
182	C3-Decalins	180.3	6.79	0.000	0.000	0.913
183	C3-Dibenzothiophenes	230.37	5.86	6.751	0.000	1.599
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1666.558	0.000	0.042
185	C3-Fluorenes	210.3	5.58	89.621	0.000	1.011
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.410
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	976.945	0.000	0.219
188	C4-Chrysenes	284.4	7.35	429.371	0.000	0.016
189	C4-Decalins	194.3	7.34	0.000	0.000	0.301
190	C4-Dibenzothiophenes	244.37	6.1	6.751	0.000	1.011
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1666.558	0.000	0.016
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.153
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	976.945	0.000	0.122
194	Chrysene	228.3	5.52	347.644	0.000	0.724
195	Dibenz(a,h)anthracene	278.4	6.7	1927.594	0.000	0.034
196	Indeno[1,2,3-cd]pyrene	276.3	6.7	5190.997	0.000	0.022
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	20.533

198	Perylene	252.3	6.11	8836.395	0.000	0.058
199	Retene	234.3	6.35	112.688	0.000	0.196

Table B.10. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF exposed to *Americamysis bahia* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	22.739	1.630	46.329
2	C2-Naphthalenes	156.2	4.31	22.031	0.540	19.950
3	2-Methylnaphthalene	142.2	3.72	22.739	1.480	64.011
4	1-Methylnaphthalene	142.2	3.72	22.739	1.130	64.011
5	C3-Naphthalenes	170.26	4.77	22.031	0.108	8.069
6	C1-Fluorenes	180.2	4.97	89.621	0.036	3.227
7	2,6-Dimethylnaphthalene	156.23	4.26	22.031	0.228	22.225
8	C2-Fluorenes	194.3	5.21	89.621	0.021	2.074
9	C1-Phenanthrenes/Anthracenes	192.3	4.26	976.945	0.059	6.018
10	Toluene	92.14	2.54	0.000	63.800	7758.791
11	C4-Naphthalenes	184.3	5.18	22.031	0.025	3.610
13	m-XYLENE	106.2	3.09	0.000	16.700	2733.194
14	Naphthalene	234.3	3.17	12.554	2.620	429.747
15	4/9-Methylphenanthrene	192.26	4.89	78.492	0.022	4.311
16	1,6,7-Trimethylnaphthalene	170.26	4.81	39.283	0.027	5.942
17	2-Methylanthracene	192.26	4.89	976.945	0.007	1.548
22	Phenanthrene	178.2	4.35	46.039	0.065	15.764
23	o-XYLENE	106.2	3.09	0.000	11.000	2733.194
25	1,2,4-Trimethylbenzene	120.2	3.63	0.000	3.410	966.074
30	3-Methylphenanthrene	192.26	4.89	78.492	0.013	4.311
31	Fluorene	166.2	4.02	89.621	0.066	23.062
32	1-Methylphenanthrene	192.26	4.89	78.492	0.011	4.311
33	Benzene	78.11	1.99	0.000	49.000	21520.507

35	2-Methylphenanthrene	192.26	4.89	78.492	0.008	4.311
37	p-XYLENE	106.2	3.09	0.000	4.930	2733.194
38	Ethylbenzene	106.2	3.03	0.000	4.760	3110.501
39	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	1.620	1075.995
41	C2-Dibenzothiophenes	214.3	5.13	6.751	0.010	7.172
43	Methylcyclohexane	98.19	3.59	0.000	1.380	1105.638
44	CYCLOHEXANE	84.16	3.18	0.000	2.680	2293.040
47	1,3,5-trimethylbenzene	120.2	3.63	0.000	1.030	966.074
53	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.960	1075.995
54	Anthracene	178.2	4.35	613.291	0.005	5.569
56	C4-Benzothiophene	190.3	5.18	0.311	0.011	14.143
58	C3-Benzothiophene	176.3	4.69	0.311	0.029	37.670
59	C1-Dibenzothiophenes	198.3	4.71	6.751	0.013	16.409
62	Methylcyclopentane	84.16	3.1	0.000	1.650	2724.530
64	4-ETHYLTOLUENE	120.2	3.58	0.000	0.568	1075.995
65	Pyrene	202.3	4.93	1126.734	0.001	1.408
66	Isopentane	72.15	2.72	0.000	2.660	5297.881
67	CARBAZOLE	167.2	3.23	165.377	0.049	99.681
68	Acenaphthene	154.2	4.15	64.349	0.008	18.424
69	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.150	367.163
70	Propylbenzene	120.194	3.52	0.000	0.454	1224.471
71	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.135	367.163
77	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.119	367.163
78	Dibenzofuran	168.2	3.71	49.546	0.017	57.447
79	4-Methyldibenzothiophene	198.28	4.71	6.751	0.005	16.407
81	Dibenzothiophene	184.3	4.17	6.751	0.013	48.833
82	Isopropylbenzene	120.194	3.45	0.000	0.378	1423.864
83	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.109	417.848
84	Biphenyl	154.2	3.76	0.000	0.139	535.193

85	n-C5	72.15	2.8	0.000	1.150	4458.843
86	C2-Benzothiophene	162.25	4.13	0.311	0.030	115.901
87	m-cymene	134.2	4	0.000	0.123	485.890
89	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.089	367.163
90	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.089	367.217
92	Cyclopentane	70.13	2.68	0.000	1.200	5613.190
93	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.069	329.654
99	Hydrindene	118.2	3.47	0.000	0.174	1341.169
100	2/3-Methyldibenzothiophene	198.28	4.71	6.754	0.002	16.405
101	4-isopropyltoluene	134.22	4	0.000	0.063	485.963
103	2-METHYLPENTANE	86.18	3.21	0.000	0.263	2201.062
104	1-Methyldibenzothiophene	198.28	4.71	6.751	0.002	16.407
106	1,2-Diethylbenzene	134.2	4.07	0.000	0.036	417.848
111	C1-Benzothiophene	148.2	3.5365	0.311	0.021	380.424
112	Acenaphthylene	152.2	3.94	335.965	0.001	14.734
113	2,3-dimethylbutane	86.18	3.14	0.000	0.120	2559.484
114	2,3-dimethylpentane	100.2	3.63	0.000	0.048	1035.079
115	C1-Decalins	152.3	4.61	0.000	0.003	84.630
116	trans-Decalin	138.26	4.2	0.000	0.005	185.901
118	Benzothiophene	134.2	2.99	0.311	0.002	1118.656
12	1-Decene	140.3	5.12	0.000	0.000	58.415
18	n-C10	142.29	5.25	0.000	0.000	44.767
19	n-C10	142.29	5.25	0.000	0.000	44.767
20	n-C10	142.3	5.25	0.000	0.000	44.770
21	n-C10	142.3	5.25	0.000	0.000	44.770
24	1-Nonene	126.2	4.62	0.000	0.000	154.357
26	n-C9	128.3	4.76	0.000	0.000	116.052
27	n-C9	128.3	4.76	0.000	0.000	116.052
28	n-C9	128.3	4.76	0.000	0.000	116.052

29	n-C9	128.3	4.76	0.000	0.000	116.052
34	Fluoranthene	202.3	4.93	835.591	0.000	1.594
36	n-C8	114.2	4.27	0.000	0.000	296.983
40	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	437.736
42	Octene-1	112.2	4.13	0.000	0.000	394.547
45	n-Pentylbenzene	148.2	4.5	0.000	0.000	234.765
46	3-methylheptane	114.2	4.2	0.000	0.000	345.344
48	n-C10	142.29	5.25	0.000	0.000	44.767
49	n-C10	142.29	5.25	0.000	0.000	44.767
50	n-C10	142.3	5.25	0.000	0.000	44.770
51	n-C10	142.3	5.25	0.000	0.000	44.770
52	2-methylheptane	114.2	4.2	0.000	0.000	345.344
55	HEPTANE	100.2	3.78	0.000	0.000	749.158
57	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	477.147
60	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	410.437
61	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	437.851
63	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	417.910
72	n-C9	128.3	4.76	0.000	0.000	116.052
73	n-C9	128.3	4.76	0.000	0.000	116.052
74	n-C9	128.3	4.76	0.000	0.000	116.052
75	n-C9	128.3	4.76	0.000	0.000	116.052
76	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	417.848
80	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	410.437
88	n-C6	86.18	3.29	0.000	0.000	1852.475
91	2,3-dimethylhexane	114.2	4.12	0.000	0.000	410.329
94	n-Butylbenzene	134.2	4.01	0.000	0.000	475.531
95	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
96	tert-Butylbenzene	134.2	3.9	0.000	0.000	602.752
97	2-methylhexane	100.2	3.71	0.000	0.000	871.151

98	3-ethylhexane	114.2	4.2	0.000	0.000	345.344
102	3-methylhexane	100.2	3.71	0.000	0.000	871.151
105	3-Methylpentane	86.18	3.21	0.000	0.000	2201.062
107	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	367.217
108	sec-Butylbenzene	134.2	3.94	0.000	0.000	552.966
109	2,2-dimethylpentane	100.2	3.67	0.000	0.000	949.584
110	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	485.963
117	cis-Decalin	138.26	4.2	0.000	0.000	185.901
119	n-C11	156.31	5.74	0.000	0.000	17.105
120	n-C11	156.31	5.74	0.000	0.000	17.105
121	n-C11	156.31	5.74	0.000	0.000	17.105
122	n-C11	156.31	5.74	0.000	0.000	17.105
123	n-C12	170.34	6.23	0.000	0.000	6.484
124	n-C12	170.34	6.23	0.000	0.000	6.484
125	n-C12	170.34	6.23	0.000	0.000	6.484
126	n-C12	170.34	6.23	0.000	0.000	6.484
127	n-C11	156.31	5.74	0.000	0.000	17.105
128	n-C11	156.31	5.74	0.000	0.000	17.105
129	n-C11	156.31	5.74	0.000	0.000	17.105
130	n-C11	156.31	5.74	0.000	0.000	17.105
131	n-C12	170.34	6.23	0.000	0.000	6.484
132	n-C12	170.34	6.23	0.000	0.000	6.484
133	n-C12	170.34	6.23	0.000	0.000	6.484
134	n-C12	170.34	6.23	0.000	0.000	6.484
135	n-C13	184.37	6.73	0.000	0.000	2.389
136	n-C14	198.4	7.22	0.000	0.000	0.894
137	n-C15	212.42	7.71	0.000	0.000	0.333
138	n-C16	226.45	8.2	0.000	0.000	0.123
139	n-C17	240.48	8.69	0.000	0.000	0.046

140	n-C18	254.5	9.18	0.000	0.000	0.017
141	n-C19	268.53	9.67	0.000	0.000	0.006
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.004
164	Pristane	268.525	9.38	0.000	0.000	0.012
165	Benzo(a)fluoranthene	252.3	6.11	4868.195	0.000	0.075
166	Benzo(b)fluorene	216.3	5.77	440.781	0.000	0.363
167	Benzo(k)fluoranthene	252.3	6.11	2735.614	0.000	0.095
168	Benzo[a]anthracene	228.3	5.52	743.532	0.000	0.529

169	Benzo[a]pyrene	252.3	6.11	3793.523	0.000	0.083
170	Benzo[b]fluoranthene	252.3	6.11	1622.042	0.000	0.119
171	Benzo[e]pyrene	252.3	6.11	906.904	0.000	0.151
172	Benzo[g,h,i]perylene	276.3	6.7	3006.420	0.000	0.028
173	C1-Chrysenes	242.3	6.0683	429.371	0.000	0.216
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1666.558	0.000	0.391
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.041
176	C2-Chrysenes	256.3	6.65	429.371	0.000	0.065
177	C2-Decalins	166.3	6.19	0.000	0.000	3.068
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1666.558	0.000	0.103
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.142
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	976.945	0.000	0.476
181	C3-Chrysenes	270.4	7.03	429.371	0.000	0.030
182	C3-Decalins	180.3	6.79	0.000	0.000	0.913
183	C3-Dibenzothiophenes	230.37	5.86	6.751	0.000	1.599
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1666.558	0.000	0.042
185	C3-Fluorenes	210.3	5.58	89.621	0.000	1.011
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.410
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	976.945	0.000	0.219
188	C4-Chrysenes	284.4	7.35	429.371	0.000	0.016
189	C4-Decalins	194.3	7.34	0.000	0.000	0.301
190	C4-Dibenzothiophenes	244.37	6.1	6.751	0.000	1.011
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1666.558	0.000	0.016
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.153
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	976.945	0.000	0.122
194	Chrysene	228.3	5.52	347.644	0.000	0.724
195	Dibenz(a,h)anthracene	278.4	6.7	1927.594	0.000	0.034
196	Indeno[1,2,3-cd]pyrene	276.3	6.7	5190.997	0.000	0.022
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	20.533

198	Perylene	252.3	6.11	8836.395	0.000	0.058
199	Retene	234.3	6.35	112.688	0.000	0.196

Table B.11. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF duplicate exposed to *Americamysis bahia* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	22.739	1.820	46.329
2	C2-Naphthalenes	156.2	4.31	22.031	0.565	19.950
3	2-Methylnaphthalene	142.2	3.72	22.739	1.660	64.011
4	1-Methylnaphthalene	142.2	3.72	22.739	1.250	64.011
5	C3-Naphthalenes	170.26	4.77	22.031	0.112	8.069
6	C1-Fluorenes	180.2	4.97	89.621	0.038	3.227
7	C2-Fluorenes	194.3	5.21	89.621	0.023	2.074
8	2,6-Dimethylnaphthalene	156.23	4.26	22.031	0.236	22.225
9	C1-Phenanthrenes/Anthracenes	192.3	4.26	976.945	0.061	6.018
10	Toluene	92.14	2.54	0.000	63.600	7758.791
11	C4-Naphthalenes	184.3	5.18	22.031	0.027	3.610
12	Naphthalene	234.3	3.17	12.554	3.020	429.747
13	m-XYLENE	106.2	3.09	0.000	16.000	2733.194
14	4/9-Methylphenanthrene	192.26	4.89	78.492	0.021	4.311
15	2-Methylanthracene	192.26	4.89	976.945	0.007	1.548
16	1,6,7-Trimethylnaphthalene	170.26	4.81	39.283	0.028	5.942
17	Phenanthrene	178.2	4.35	46.039	0.068	15.764
18	o-XYLENE	106.2	3.09	0.000	11.000	2733.194
19	1,2,4-Trimethylbenzene	120.2	3.63	0.000	3.360	966.074
20	3-Methylphenanthrene	192.26	4.89	78.492	0.014	4.311
21	Fluorene	166.2	4.02	89.621	0.072	23.062

22	1-Methylphenanthrene	192.26	4.89	78.492	0.012	4.311
23	Benzene	78.11	1.99	0.000	49.800	21520.507
24	p-XYLENE	106.2	3.09	0.000	5.580	2733.194
25	2-Methylphenanthrene	192.26	4.89	78.492	0.008	4.311
26	C2-Dibenzothiophenes	214.3	5.13	6.751	0.012	7.172
27	Ethylbenzene	106.2	3.03	0.000	4.680	3110.501
28	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	1.560	1075.995
29	Methylcyclohexane	98.19	3.59	0.000	1.340	1105.638
30	CYCLOHEXANE	84.16	3.18	0.000	2.620	2293.040
31	1,3,5-trimethylbenzene	120.2	3.63	0.000	1.010	966.074
32	Anthracene	178.2	4.35	613.291	0.005	5.569
33	C3-Benzothiophene	176.3	4.69	0.311	0.034	37.670
34	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.950	1075.995
35	C1-Dibenzothiophenes	198.3	4.71	6.751	0.012	16.409
36	C4-Benzothiophene	190.3	5.18	0.311	0.010	14.143
37	Methylcyclopentane	84.16	3.1	0.000	1.690	2724.530
38	Pyrene	202.3	4.93	1126.734	0.001	1.408
39	Isopentane	72.15	2.72	0.000	2.860	5297.881
40	CARBAZOLE	167.2	3.23	165.377	0.053	99.681
41	4-ETHYLTOLUENE	120.2	3.58	0.000	0.544	1075.995
42	Acenaphthene	154.2	4.15	64.349	0.008	18.424
43	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.147	367.163
44	Propylbenzene	120.194	3.52	0.000	0.434	1224.471
45	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.126	367.163
46	Dibenzofuran	168.2	3.71	49.546	0.018	57.447
47	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.115	367.163
48	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.103	367.163
49	C2-Benzothiophene	162.25	4.13	0.311	0.032	115.901
50	Biphenyl	154.2	3.76	0.000	0.146	535.193
51	Dibenzothiophene	184.3	4.17	6.751	0.013	48.833

52	Isopropylbenzene	120.194	3.45	0.000	0.373	1423.864
53	m-cymene	134.2	4	0.000	0.125	485.890
54	4-Methyldibenzothiophene	198.28	4.71	6.751	0.004	16.407
55	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.092	367.217
56	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.102	417.848
57	n-C5	72.15	2.8	0.000	1.070	4458.843
58	Cyclopentane	70.13	2.68	0.000	1.190	5613.190
59	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.065	329.654
60	Hydrindene	118.2	3.47	0.000	0.181	1341.169
61	4-isopropyltoluene	134.22	4	0.000	0.060	485.963
62	C1-Benzothiophene	148.2	3.5365	0.311	0.044	380.424
63	2-METHYLPENTANE	86.18	3.21	0.000	0.256	2201.062
64	2/3-Methyldibenzothiophene	198.28	4.71	6.754	0.002	16.405
65	1-Methyldibenzothiophene	198.28	4.71	6.751	0.002	16.407
66	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.031	367.217
67	Acenaphthylene	152.2	3.94	335.965	0.001	14.734
68	n-Butylbenzene	134.2	4.01	0.000	0.027	475.531
69	2,3-dimethylbutane	86.18	3.14	0.000	0.116	2559.484
70	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.019	485.963
71	trans-Decalin	138.26	4.2	0.000	0.005	185.901
72	Benzothiophene	134.2	2.99	0.311	0.003	1118.656
73	1-Decene	140.3	5.12	0.000	0.000	58.415
74	n-C10	142.29	5.25	0.000	0.000	44.767
75	n-C10	142.29	5.25	0.000	0.000	44.767
76	n-C10	142.3	5.25	0.000	0.000	44.770
77	n-C10	142.3	5.25	0.000	0.000	44.770
78	Fluoranthene	202.3	4.93	835.591	0.000	1.594
79	1-Nonene	126.2	4.62	0.000	0.000	154.357
80	n-C9	128.3	4.76	0.000	0.000	116.052
81	n-C9	128.3	4.76	0.000	0.000	116.052

82	n-C9	128.3	4.76	0.000	0.000	116.052
83	n-C9	128.3	4.76	0.000	0.000	116.052
84	n-C10	142.29	5.25	0.000	0.000	44.767
85	n-C10	142.29	5.25	0.000	0.000	44.767
86	n-C10	142.3	5.25	0.000	0.000	44.770
87	n-C10	142.3	5.25	0.000	0.000	44.770
88	n-C8	114.2	4.27	0.000	0.000	296.983
89	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	437.736
90	Octene-1	112.2	4.13	0.000	0.000	394.547
91	n-Pentylbenzene	148.2	4.5	0.000	0.000	234.765
92	3-methylheptane	114.2	4.2	0.000	0.000	345.344
93	2-methylheptane	114.2	4.2	0.000	0.000	345.344
94	HEPTANE	100.2	3.78	0.000	0.000	749.158
95	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	477.147
96	n-C9	128.3	4.76	0.000	0.000	116.052
97	n-C9	128.3	4.76	0.000	0.000	116.052
98	n-C9	128.3	4.76	0.000	0.000	116.052
99	n-C9	128.3	4.76	0.000	0.000	116.052
100	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	410.437
101	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	437.851
102	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	417.848
103	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	410.437
104	2,3-dimethylhexane	114.2	4.12	0.000	0.000	410.329
105	n-C6	86.18	3.29	0.000	0.000	1852.475
106	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	417.910
107	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
108	tert-Butylbenzene	134.2	3.9	0.000	0.000	602.752
109	2-methylhexane	100.2	3.71	0.000	0.000	871.151
110	3-ethylhexane	114.2	4.2	0.000	0.000	345.344
111	3-methylhexane	100.2	3.71	0.000	0.000	871.151

112	3-Methylpentane	86.18	3.21	0.000	0.000	2201.062
113	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	417.848
114	sec-Butylbenzene	134.2	3.94	0.000	0.000	552.966
115	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
116	2,2-dimethylpentane	100.2	3.67	0.000	0.000	949.584
117	C1-Decalins	152.3	4.61	0.000	0.000	84.630
118	cis-Decalin	138.26	4.2	0.000	0.000	185.901
119	n-C11	156.31	5.74	0.000	0.000	17.105
120	n-C11	156.31	5.74	0.000	0.000	17.105
121	n-C11	156.31	5.74	0.000	0.000	17.105
122	n-C11	156.31	5.74	0.000	0.000	17.105
123	n-C12	170.34	6.23	0.000	0.000	6.484
124	n-C12	170.34	6.23	0.000	0.000	6.484
125	n-C12	170.34	6.23	0.000	0.000	6.484
126	n-C12	170.34	6.23	0.000	0.000	6.484
127	n-C11	156.31	5.74	0.000	0.000	17.105
128	n-C11	156.31	5.74	0.000	0.000	17.105
129	n-C11	156.31	5.74	0.000	0.000	17.105
130	n-C11	156.31	5.74	0.000	0.000	17.105
131	n-C12	170.34	6.23	0.000	0.000	6.484
132	n-C12	170.34	6.23	0.000	0.000	6.484
133	n-C12	170.34	6.23	0.000	0.000	6.484
134	n-C12	170.34	6.23	0.000	0.000	6.484
135	n-C13	184.37	6.73	0.000	0.000	2.389
136	n-C14	198.4	7.22	0.000	0.000	0.894
137	n-C15	212.42	7.71	0.000	0.000	0.333
138	n-C16	226.45	8.2	0.000	0.000	0.123
139	n-C17	240.48	8.69	0.000	0.000	0.046
140	n-C18	254.5	9.18	0.000	0.000	0.017
141	n-C19	268.53	9.67	0.000	0.000	0.006

142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.004
164	Pristane	268.525	9.38	0.000	0.000	0.012
165	Benzo(a)fluoranthene	252.3	6.11	4868.195	0.000	0.075
166	Benzo(b)fluorene	216.3	5.77	440.781	0.000	0.363
167	Benzo(k)fluoranthene	252.3	6.11	2735.614	0.000	0.095
168	Benzo[a]anthracene	228.3	5.52	743.532	0.000	0.529
169	Benzo[a]pyrene	252.3	6.11	3793.523	0.000	0.083
170	Benzo[b]fluoranthene	252.3	6.11	1622.042	0.000	0.119
171	Benzo[e]pyrene	252.3	6.11	906.904	0.000	0.151

172	Benzo[g,h,i]perylene	276.3	6.7	3006.420	0.000	0.028
173	C1-Chrysenes	242.3	6.0683	429.371	0.000	0.216
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1666.558	0.000	0.391
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.041
176	C2-Chrysenes	256.3	6.65	429.371	0.000	0.065
177	C2-Decalins	166.3	6.19	0.000	0.000	3.068
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1666.558	0.000	0.103
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.142
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	976.945	0.000	0.476
181	C3-Chrysenes	270.4	7.03	429.371	0.000	0.030
182	C3-Decalins	180.3	6.79	0.000	0.000	0.913
183	C3-Dibenzothiophenes	230.37	5.86	6.751	0.000	1.599
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1666.558	0.000	0.042
185	C3-Fluorenes	210.3	5.58	89.621	0.000	1.011
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.410
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	976.945	0.000	0.219
188	C4-Chrysenes	284.4	7.35	429.371	0.000	0.016
189	C4-Decalins	194.3	7.34	0.000	0.000	0.301
190	C4-Dibenzothiophenes	244.37	6.1	6.751	0.000	1.011
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1666.558	0.000	0.016
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.153
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	976.945	0.000	0.122
194	Chrysene	228.3	5.52	347.644	0.000	0.724
195	Dibenz(a,h)anthracene	278.4	6.7	1927.594	0.000	0.034
196	Indeno[1,2,3-cd]pyrene	276.3	6.7	5190.997	0.000	0.022
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	20.533
198	Perylene	252.3	6.11	8836.395	0.000	0.058
199	Retene	234.3	6.35	112.688	0.000	0.196

Table B.12. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 100% WAF exposed to *Americamysis bahia* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	90.165	0.381	2.069
2	C1-Fluorenes	180.2	4.97	90.165	0.493	3.219
3	C3-Naphthalenes	170.26	4.77	22.395	0.953	8.020
4	C1-Phenanthrenes/Anthracenes	192.3	4.26	961.094	0.623	6.059
5	C4-Naphthalenes	184.3	5.18	22.395	0.232	3.588
6	C2-Naphthalenes	156.2	4.31	22.395	1.280	19.828
7	1-Methylphenanthrene	192.26	4.89	80.120	0.211	4.276
8	1,6,7-Trimethylnaphthalene	170.26	4.81	40.378	0.282	5.879
9	Phenanthrene	178.2	4.35	46.965	0.725	15.643
10	4/9-Methylphenanthrene	192.26	4.89	80.120	0.179	4.276
11	2-Methylphenanthrene	192.26	4.89	80.120	0.154	4.276
12	3-Methylphenanthrene	192.26	4.89	80.120	0.149	4.276
13	2,6-Dimethylnaphthalene	156.23	4.26	22.395	0.487	22.088
14	C2-Dibenzothiophenes	214.3	5.13	6.876	0.141	7.127
15	Fluorene	166.2	4.02	90.165	0.398	23.006
16	C1-Dibenzothiophenes	198.3	4.71	6.876	0.202	16.305
18	Pyrene	202.3	4.93	1120.979	0.009	1.411
19	4-Methyldibenzothiophene	198.28	4.71	6.876	0.079	16.303
21	C1-Naphthalenes	142.2	3.87	23.422	0.147	45.817
22	Dibenzothiophene	184.3	4.17	6.876	0.149	48.524

27	2-Methylanthracene	192.26	4.89	961.094	0.004	1.558
28	2/3-Methyldibenzothiophene	198.28	4.71	6.878	0.041	16.301
29	Fluoranthene	202.3	4.93	825.740	0.004	1.602
30	1-Methylnaphthalene	142.2	3.72	23.422	0.132	63.303
31	1-Methyldibenzothiophene	198.28	4.71	6.876	0.033	16.303
33	2-Methylnaphthalene	142.2	3.72	23.422	0.100	63.303
34	C4-Benzothiophene	190.3	5.18	0.307	0.022	14.179
37	Acenaphthene	154.2	4.15	65.963	0.020	18.245
39	Dibenzofuran	168.2	3.71	51.047	0.060	56.785
45	C3-Benzothiophene	176.3	4.69	0.307	0.033	37.766
60	Anthracene	178.2	4.35	603.704	0.002	5.605
65	C2-Benzothiophene	162.25	4.13	0.307	0.020	116.197
67	Biphenyl	154.2	3.76	0.000	0.086	535.193
74	Acenaphthylene	152.2	3.94	335.899	0.002	14.735
91	CARBAZOLE	167.2	3.23	167.183	0.005	99.246
104	Naphthalene	234.3	3.17	12.930	0.011	425.173
109	C1-Benzothiophene	148.2	3.5365	0.307	0.006	381.394
110	m-XYLENE	106.2	3.09	0.000	0.027	2733.194
111	p-XYLENE	106.2	3.09	0.000	0.015	2733.194
113	Ethylbenzene	106.2	3.03	0.000	0.016	3110.501
114	3-Methylpentane	86.18	3.21	0.000	0.010	2201.062
116	trans-Decalin	138.26	4.2	0.000	0.000	185.901
17	1-Decene	140.3	5.12	0.000	0.000	58.415
20	1-Nonene	126.2	4.62	0.000	0.000	154.357
23	n-C9	128.3	4.76	0.000	0.000	116.052
24	n-C9	128.3	4.76	0.000	0.000	116.052
25	n-C9	128.3	4.76	0.000	0.000	116.052
26	n-C9	128.3	4.76	0.000	0.000	116.052
32	n-C8	114.2	4.27	0.000	0.000	296.983

35	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	437.736
36	Octene-1	112.2	4.13	0.000	0.000	394.547
38	3-methylheptane	114.2	4.2	0.000	0.000	345.344
40	n-C10	142.29	5.25	0.000	0.000	44.767
41	n-C10	142.29	5.25	0.000	0.000	44.767
42	n-C10	142.3	5.25	0.000	0.000	44.770
43	n-C10	142.3	5.25	0.000	0.000	44.770
44	2-methylheptane	114.2	4.2	0.000	0.000	345.344
46	HEPTANE	100.2	3.78	0.000	0.000	749.158
47	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	477.147
48	n-C10	142.29	5.25	0.000	0.000	44.767
49	n-C10	142.29	5.25	0.000	0.000	44.767
50	n-C10	142.3	5.25	0.000	0.000	44.770
51	n-C10	142.3	5.25	0.000	0.000	44.770
52	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	410.437
53	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	437.851
54	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	417.910
55	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	367.163
56	n-C9	128.3	4.76	0.000	0.000	116.052
57	n-C9	128.3	4.76	0.000	0.000	116.052
58	n-C9	128.3	4.76	0.000	0.000	116.052
59	n-C9	128.3	4.76	0.000	0.000	116.052
61	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	410.437
62	2,3-dimethylhexane	114.2	4.12	0.000	0.000	410.329
63	Methylcyclohexane	98.19	3.59	0.000	0.000	1105.638
64	n-Butylbenzene	134.2	4.01	0.000	0.000	475.531
66	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
68	tert-Butylbenzene	134.2	3.9	0.000	0.000	602.752
69	2-methylhexane	100.2	3.71	0.000	0.000	871.151

70	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	367.217
71	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	417.848
72	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	367.163
73	3-ethylhexane	114.2	4.2	0.000	0.000	345.344
75	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	417.848
76	3-methylhexane	100.2	3.71	0.000	0.000	871.151
77	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
78	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
79	Hydrindene	118.2	3.47	0.000	0.000	1341.169
80	n-C5	72.15	2.8	0.000	0.000	4458.843
81	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2201.062
82	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	417.848
83	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	367.217
84	Propylbenzene	120.194	3.52	0.000	0.000	1224.471
85	4-isopropyltoluene	134.22	4	0.000	0.000	485.963
86	sec-Butylbenzene	134.2	3.94	0.000	0.000	552.966
87	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
88	2,2-dimethylpentane	100.2	3.67	0.000	0.000	949.584
89	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	966.074
90	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	485.963
92	m-cymene	134.2	4	0.000	0.000	485.890
93	CYCLOHEXANE	84.16	3.18	0.000	0.000	2293.040
94	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
95	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
96	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1075.995
97	Isopropylbenzene	120.194	3.45	0.000	0.000	1423.864
98	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	329.654
99	n-C6	86.18	3.29	0.000	0.000	1852.475
100	Isopentane	72.15	2.72	0.000	0.000	5297.881

101	Methylcyclopentane	84.16	3.1	0.000	0.000	2724.530
102	n-Pentylbenzene	148.2	4.5	0.000	0.000	234.765
103	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2559.484
105	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	966.074
106	o-XYLENE	106.2	3.09	0.000	0.000	2733.194
107	Cyclopentane	70.13	2.68	0.000	0.000	5613.190
108	C1-Decalins	152.3	4.61	0.000	0.000	84.630
112	cis-Decalin	138.26	4.2	0.000	0.000	185.901
115	Toluene	92.14	2.54	0.000	0.000	7758.791
117	Benzothiophene	134.2	2.99	0.307	0.000	1121.508
118	Benzene	78.11	1.99	0.000	0.000	21520.507
119	n-C11	156.31	5.74	0.000	0.000	17.105
120	n-C11	156.31	5.74	0.000	0.000	17.105
121	n-C11	156.31	5.74	0.000	0.000	17.105
122	n-C11	156.31	5.74	0.000	0.000	17.105
123	n-C12	170.34	6.23	0.000	0.000	6.484
124	n-C12	170.34	6.23	0.000	0.000	6.484
125	n-C12	170.34	6.23	0.000	0.000	6.484
126	n-C12	170.34	6.23	0.000	0.000	6.484
127	n-C11	156.31	5.74	0.000	0.000	17.105
128	n-C11	156.31	5.74	0.000	0.000	17.105
129	n-C11	156.31	5.74	0.000	0.000	17.105
130	n-C11	156.31	5.74	0.000	0.000	17.105
131	n-C12	170.34	6.23	0.000	0.000	6.484
132	n-C12	170.34	6.23	0.000	0.000	6.484
133	n-C12	170.34	6.23	0.000	0.000	6.484
134	n-C12	170.34	6.23	0.000	0.000	6.484
135	n-C13	184.37	6.73	0.000	0.000	2.389
136	n-C14	198.4	7.22	0.000	0.000	0.894

137	n-C15	212.42	7.71	0.000	0.000	0.333
138	n-C16	226.45	8.2	0.000	0.000	0.123
139	n-C17	240.48	8.69	0.000	0.000	0.046
140	n-C18	254.5	9.18	0.000	0.000	0.017
141	n-C19	268.53	9.67	0.000	0.000	0.006
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.004
164	Pristane	268.525	9.38	0.000	0.000	0.012
165	Benzo(a)fluoranthene	252.3	6.11	5005.988	0.000	0.074

166	Benzo(b)fluorene	216.3	5.77	445.576	0.000	0.361
167	Benzo(k)fluoranthene	252.3	6.11	2757.828	0.000	0.095
168	Benzo[a]anthracene	228.3	5.52	740.704	0.000	0.530
169	Benzo[a]pyrene	252.3	6.11	3756.755	0.000	0.083
170	Benzo[b]fluoranthene	252.3	6.11	1608.219	0.000	0.119
171	Benzo[e]pyrene	252.3	6.11	906.300	0.000	0.151
172	Benzo[g,h,i]perylene	276.3	6.7	2976.961	0.000	0.028
173	C1-Chrysenes	242.3	6.0683	431.978	0.000	0.216
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1647.337	0.000	0.393
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.041
176	C2-Chrysenes	256.3	6.65	431.978	0.000	0.065
177	C2-Decalins	166.3	6.19	0.000	0.000	3.068
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1647.337	0.000	0.103
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.142
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	961.094	0.000	0.479
181	C3-Chrysenes	270.4	7.03	431.978	0.000	0.030
182	C3-Decalins	180.3	6.79	0.000	0.000	0.913
183	C3-Dibenzothiophenes	230.37	5.86	6.876	0.000	1.589
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1647.337	0.000	0.042
185	C3-Fluorenes	210.3	5.58	90.165	0.000	1.009
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.410
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	961.094	0.000	0.221
188	C4-Chrysenes	284.4	7.35	431.978	0.000	0.016
189	C4-Decalins	194.3	7.34	0.000	0.000	0.301
190	C4-Dibenzothiophenes	244.37	6.1	6.876	0.000	1.005
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1647.337	0.000	0.016
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.153
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	961.094	0.000	0.123
194	Chrysene	228.3	5.52	351.996	0.000	0.720

195	Dibenz(a,h)anthracene	278.4	6.7	1935.638	0.000	0.034
196	Indeno[1,2,3-cd]pyrene	276.3	6.7	5232.487	0.000	0.022
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	20.533
198	Perylene	252.3	6.11	9113.504	0.000	0.057
199	Retene	234.3	6.35	115.167	0.000	0.194

Table B.13. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 25% WAF exposed to *Americamysis bahia* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	90.16475963	0.09	2.06943
2	C1-Fluorenes	180.2	4.97	90.16475963	0.113	3.21938
3	C3-Naphthalenes	170.26	4.77	22.39529722	0.205	8.01956
4	C1-Phenanthrenes/Anthracenes	192.3	4.26	961.0939304	0.146	6.05856
5	C2-Naphthalenes	156.2	4.31	22.39529722	0.275	19.828
6	C4-Naphthalenes	184.3	5.18	22.39529722	0.0493	3.58759
7	1-Methylphenanthrene	192.26	4.89	80.12049697	0.0485	4.2764
8	Phenanthrene	178.2	4.35	46.9645413	0.176	15.6433
9	1,6,7-Trimethylnaphthalene	170.26	4.81	40.3782977	0.0634	5.87944
10	4/9-Methylphenanthrene	192.26	4.89	80.12049697	0.0421	4.2764
11	2-Methylphenanthrene	192.26	4.89	80.12049697	0.0355	4.2764
12	3-Methylphenanthrene	192.26	4.89	80.12049697	0.0354	4.2764
14	2,6-Dimethylnaphthalene	156.23	4.26	22.39529722	0.101	22.0883
15	C2-Dibenzothiophenes	214.3	5.13	6.875629883	0.0322	7.12677
16	Fluorene	166.2	4.02	90.16475963	0.0937	23.0064
22	C1-Dibenzothiophenes	198.3	4.71	6.875629883	0.0403	16.3047
28	4-Methyldibenzothiophene	198.28	4.71	6.875629883	0.018	16.3031
37	Dibenzothiophene	184.3	4.17	6.875629883	0.0343	48.5239
38	Fluoranthene	202.3	4.93	825.7399979	0.00113	1.6017
39	C1-Naphthalenes	142.2	3.87	23.42213237	0.0316	45.8169
42	2-Methylanthracene	192.26	4.89	961.0939304	0.00096	1.55811
44	1-Methylnaphthalene	142.2	3.72	23.42213237	0.0282	63.3033
45	1-Methyldibenzothiophene	198.28	4.71	6.875629883	0.00697	16.3031
51	2-Methylnaphthalene	142.2	3.72	23.42213237	0.0223	63.3033

52	C4-Benzothiophene	190.3	5.18	0.307302064	0.00478	14.1791
57	2/3-Methyldibenzothiophene	198.28	4.71	6.87757334	0.00458	16.3015
59	Acenaphthene	154.2	4.15	65.96335464	0.00485	18.2455
60	C3-Benzothiophene	176.3	4.69	0.307302064	0.00979	37.7661
61	Dibenzofuran	168.2	3.71	51.04682344	0.0139	56.7848
76	Anthracene	178.2	4.35	603.70449	0.0006	5.60494
91	C2-Benzothiophene	162.25	4.13	0.307302064	0.00572	116.197
96	Acenaphthylene	152.2	3.94	335.8990774	0.00059	14.7353
100	Biphenyl	154.2	3.76	0	0.0193	535.193
108	Naphthalene	234.3	3.17	12.92968243	0.00676	425.173
109	CARBAZOLE	167.2	3.23	167.1829159	0.00146	99.2458
110	C1-Benzothiophene	148.2	3.5365	0.307302064	0.00506	381.394
112	m-XYLENE	106.2	3.09	0	0.0272	2733.19
114	o-XYLENE	106.2	3.09	0	0.0148	2733.19
115	p-XYLENE	106.2	3.09	0	0.0144	2733.19
116	trans-Decalin	138.26	4.2	0	0.00047	185.901
13	1-Decene	140.3	5.12	0	0	58.4149
17	1-Nonene	126.2	4.62	0	0	154.357
18	n-C9	128.3	4.76	0	0	116.052
19	n-C9	128.3	4.76	0	0	116.052
20	n-C9	128.3	4.76	0	0	116.052
21	n-C9	128.3	4.76	0	0	116.052
23	n-C8	114.2	4.27	0	0	296.983
24	Pyrene	202.3	4.93	1120.979231	0	1.411
25	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0	0	437.736
26	Octene-1	112.2	4.13	0	0	394.547
27	n-Pentylbenzene	148.2	4.5	0	0	234.765
29	3-methylheptane	114.2	4.2	0	0	345.344
30	n-C10	142.29	5.25	0	0	44.7672

31	n-C10	142.29	5.25	0	0	44.7672
32	n-C10	142.3	5.25	0	0	44.7704
33	n-C10	142.3	5.25	0	0	44.7704
34	2-methylheptane	114.2	4.2	0	0	345.344
35	HEPTANE	100.2	3.78	0	0	749.158
36	2,3,4-trimethylpentane	114.2	4.05	0	0	477.147
40	2,5-Dimethylhexane	114.23	4.12	0	0	410.437
41	Pentane, 2,3,3-trimethyl	114.23	4.09	0	0	437.851
43	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0	0	417.91
46	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0	0	367.163
47	n-C9	128.3	4.76	0	0	116.052
48	n-C9	128.3	4.76	0	0	116.052
49	n-C9	128.3	4.76	0	0	116.052
50	n-C9	128.3	4.76	0	0	116.052
53	n-C10	142.29	5.25	0	0	44.7672
54	n-C10	142.29	5.25	0	0	44.7672
55	n-C10	142.3	5.25	0	0	44.7704
56	n-C10	142.3	5.25	0	0	44.7704
58	1,1,3-trimethylpentane	114.23	4.12	0	0	410.437
62	2,3-dimethylhexane	114.2	4.12	0	0	410.329
63	Methylcyclohexane	98.19	3.59	0	0	1105.64
64	n-Butylbenzene	134.2	4.01	0	0	475.531
65	2,4-dimethylpentane	100.2	3.63	0	0	1035.08
66	tert-Butylbenzene	134.2	3.9	0	0	602.752
67	2-methylhexane	100.2	3.71	0	0	871.151
68	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0	0	367.217
69	1-Methyl-2-n-Propylbenzene	134.2	4.07	0	0	417.848
70	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0	0	367.163
71	3-ethylhexane	114.2	4.2	0	0	345.344

72	1-methyl-3-n-propylbenzene	134.2	4.07	0	0	417.848
73	3-methylhexane	100.2	3.71	0	0	871.151
74	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0	0	367.163
75	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0	0	367.163
77	Hydrindene	118.2	3.47	0	0	1341.17
78	n-C5	72.15	2.8	0	0	4458.84
79	2-METHYLPENTANE	86.18	3.21	0	0	2201.06
80	1,2-Diethylbenzene	134.2	4.07	0	0	417.848
81	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0	0	367.217
82	Propylbenzene	120.194	3.52	0	0	1224.47
83	4-isopropyltoluene	134.22	4	0	0	485.963
84	sec-Butylbenzene	134.2	3.94	0	0	552.966
85	2,3-dimethylpentane	100.2	3.63	0	0	1035.08
86	3-Methylpentane	86.18	3.21	0	0	2201.06
87	2,2-dimethylpentane	100.2	3.67	0	0	949.584
88	1,2,4-Trimethylbenzene	120.2	3.63	0	0	966.074
89	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0	0	485.963
90	m-cymene	134.2	4	0	0	485.89
92	Ethylbenzene	106.2	3.03	0	0	3110.5
93	CYCLOHEXANE	84.16	3.18	0	0	2293.04
94	1-Methyl-3-ethylbenzene	120.2	3.58	0	0	1076
95	1-Methyl-2-ethylbenzene	120.2	3.58	0	0	1076
97	4-ETHYLTOLUENE	120.2	3.58	0	0	1076
98	Isopropylbenzene	120.194	3.45	0	0	1423.86
99	1,2,4,5-Tetramethylbenzene	134.2	4.18	0	0	329.654
101	n-C6	86.18	3.29	0	0	1852.48
102	Isopentane	72.15	2.72	0	0	5297.88
103	Methylcyclopentane	84.16	3.1	0	0	2724.53
104	2,3-dimethylbutane	86.18	3.14	0	0	2559.48

105	1,3,5-trimethylbenzene	120.2	3.63	0	0	966.074
106	Cyclopentane	70.13	2.68	0	0	5613.19
107	C1-Decalins	152.3	4.61	0	0	84.6303
111	Toluene	92.14	2.54	0	0	7758.79
113	cis-Decalin	138.26	4.2	0	0	185.901
117	Benzothiophene	134.2	2.99	0.307302064	0	1121.51
118	Benzene	78.11	1.99	0	0	21520.5
120	n-C11	156.31	5.74	0	0	17.1054
121	n-C11	156.31	5.74	0	0	17.1054
122	n-C11	156.31	5.74	0	0	17.1054
123	n-C11	156.31	5.74	0	0	17.1054
124	n-C12	170.34	6.23	0	0	6.48369
125	n-C12	170.34	6.23	0	0	6.48369
126	n-C12	170.34	6.23	0	0	6.48369
127	n-C12	170.34	6.23	0	0	6.48369
128	n-C11	156.31	5.74	0	0	17.1054
129	n-C11	156.31	5.74	0	0	17.1054
130	n-C11	156.31	5.74	0	0	17.1054
131	n-C11	156.31	5.74	0	0	17.1054
132	n-C12	170.34	6.23	0	0	6.48369
133	n-C12	170.34	6.23	0	0	6.48369
134	n-C12	170.34	6.23	0	0	6.48369
135	n-C12	170.34	6.23	0	0	6.48369
136	n-C13	184.37	6.73	0	0	2.38889
137	n-C14	198.4	7.22	0	0	0.89414
138	n-C15	212.42	7.71	0	0	0.33298
139	n-C16	226.45	8.2	0	0	0.12347
140	n-C17	240.48	8.69	0	0	0.04561
141	n-C18	254.5	9.18	0	0	0.01679

142	n-C19	268.53	9.67	0	0	0.00616
143	n-C20	282.56	10.1	0	0	0.00257
144	n-C21	296.59	10.6	0	0	0.00092
145	n-C22	310.61	11.1	0	0	0.00033
146	n-C23	324.64	11.6	0	0	0.00012
147	n-C24	338.67	12.1	0	0	4.13E-05
148	n-C25	352.69	12.6	0	0	1.46E-05
149	n-C26	366.72	13.1	0	0	5.18E-06
150	n-C27	380.75	13.6	0	0	1.83E-06
151	n-C28	394.77	14	0	0	8.02E-07
152	n-C29	408.8	14.5	0	0	2.83E-07
153	n-C30	422.83	15	0	0	9.95E-08
154	n-C31	436.86	15.5	0	0	3.50E-08
155	n-C32	450.88	16	0	0	1.23E-08
156	n-C33	464.91	16.5	0	0	4.32E-09
157	n-C34	478.94	17	0	0	1.51E-09
158	n-C35	492.96	17.5	0	0	5.30E-10
159	n-C36	506.981	18	0	0	1.86E-10

160	n-C37	521	18.5	0	0	6.50E-11
161	n-C38	535	19	0	0	2.27E-11
162	n-C39	549.1	19.49	0	0	8.11E-12
163	n-C40	563.1	19.9	0	0	3.44E-12
164	Phytane	282.56	9.87	0	0	0.00421
165	Pristane	268.525	9.38	0	0	0.01151
166	Benzo(a)fluoranthene	252.3	6.11	5005.988094	0	0.074
167	Benzo(b)fluorene	216.3	5.77	445.5757446	0	0.3613
168	Benzo(k)fluoranthene	252.3	6.11	2757.828056	0	0.09503
169	Benzo[a]anthracene	228.3	5.52	740.7044592	0	0.53012
170	Benzo[a]pyrene	252.3	6.11	3756.755306	0	0.08348
171	Benzo[b]fluoranthene	252.3	6.11	1608.219145	0	0.11905
172	Benzo[e]pyrene	252.3	6.11	906.2998108	0	0.1511
173	Benzo[g,h,i]perylene	276.3	6.7	2976.960526	0	0.02826
174	C1-Chrysenes	242.3	6.0683	431.9778606	0	0.21552
175	C1-Fluoranthenes/Pyrene	216.3	5.4803	1647.33694	0	0.39257
176	C1-naphthobenzothiophenes	248.3	6.38	0	0	3.04146
177	C2-Chrysenes	256.3	6.65	431.9778606	0	0.06507
178	C2-Decalins	166.3	6.19	0	0	3.06788
179	C2-Fluoranthenes/Pyrene	230.3	6.13	1647.33694	0	0.10305
180	C2-naphthobenzothiophenes	262.4	6.86	0	0	1.14233
181	C2-Phenanthrenes/Anthracenes	206.3	5.47	961.0939304	0	0.47899
182	C3-Chrysenes	270.4	7.03	431.9778606	0	0.03027
183	C3-Decalins	180.3	6.79	0	0	0.91273
184	C3-Dibenzothiophenes	230.37	5.86	6.875629883	0	1.58861
185	C3-Fluoranthenes/Pyrene	244.34	6.57	1647.33694	0	0.04235

186	C3-Fluorenes	210.3	5.58	90.16475963	0	1.00901
187	C3-naphthobenzothiophenes	276.4	7.36	0	0	0.4096
188	C3-Phenanthrenes/Anthracenes	220.3	5.86	961.0939304	0	0.2207
189	C4-Chrysenes	284.4	7.35	431.9778606	0	0.01597
190	C4-Decalins	194.3	7.34	0	0	0.30062
191	C4-Dibenzothiophenes	244.37	6.1	6.875629883	0	1.00461
192	C4-Fluoranthenes/Pyrenes	258.34	7.05	1647.33694	0	0.01592
193	C4-naphthobenzothiophenes	290.4	7.84	0	0	0.15295
194	C4-Phenanthrenes/Anthracenes	234.3	6.16	961.0939304	0	0.12296
195	Chrysene	228.3	5.52	351.9959346	0	0.71988
196	Dibenz(a,h)anthracene	278.4	6.7	1935.637545	0	0.03409
197	Indeno[1,2,3-cd]pyrene	276.3	6.7	5232.486974	0	0.0223
198	Naphthobenzothiophenes	178.2	5.34	0	0	20.5331
199	Perylene	252.3	6.11	9113.504386	0	0.0575
200	Retene	234.3	6.35	115.1674186	0	0.19401

Table B.14. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF exposed to *Americamysis bahia* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	90.165	0.025	2.069
2	C1-Fluorenes	180.2	4.97	90.165	0.026	3.219
4	C3-Naphthalenes	170.26	4.77	22.395	0.050	8.020
5	C1-Phenanthrenes/Anthracenes	192.3	4.26	961.094	0.036	6.059
6	C4-Naphthalenes	184.3	5.18	22.395	0.013	3.588
8	C2-Naphthalenes	156.2	4.31	22.395	0.065	19.828
13	Phenanthrene	178.2	4.35	46.965	0.044	15.643
14	1-Methylphenanthrene	192.26	4.89	80.120	0.012	4.276
15	1,6,7-Trimethylnaphthalene	170.26	4.81	40.378	0.014	5.879
16	4/9-Methylphenanthrene	192.26	4.89	80.120	0.010	4.276
17	3-Methylphenanthrene	192.26	4.89	80.120	0.009	4.276
18	2-Methylphenanthrene	192.26	4.89	80.120	0.008	4.276
23	C2-Dibenzothiophenes	214.3	5.13	6.876	0.009	7.127
26	2,6-Dimethylnaphthalene	156.23	4.26	22.395	0.024	22.088
27	Fluorene	166.2	4.02	90.165	0.023	23.006
37	C1-Dibenzothiophenes	198.3	4.71	6.876	0.010	16.305
50	4-Methyldibenzothiophene	198.28	4.71	6.876	0.005	16.303
53	Fluoranthene	202.3	4.93	825.740	0.000	1.602
55	C1-Naphthalenes	142.2	3.87	23.422	0.008	45.817
57	2/3-Methyldibenzothiophene	198.28	4.71	6.878	0.003	16.301
60	Dibenzothiophene	184.3	4.17	6.876	0.008	48.524
71	1-Methylnaphthalene	142.2	3.72	23.422	0.007	63.303

72	1-Methyldibenzothiophene	198.28	4.71	6.876	0.002	16.303
74	Acenaphthene	154.2	4.15	65.963	0.002	18.245
76	2-Methylnaphthalene	142.2	3.72	23.422	0.006	63.303
108	Acenaphthylene	152.2	3.94	335.899	0.000	14.735
110	C2-Benzothiophene	162.25	4.13	0.307	0.002	116.197
111	Naphthalene	234.3	3.17	12.930	0.005	425.173
113	C1-Benzothiophene	148.2	3.5365	0.307	0.004	381.394
114	Biphenyl	154.2	3.76	0.000	0.005	535.193
3	1-Decene	140.3	5.12	0.000	0.000	58.415
7	1-Nonene	126.2	4.62	0.000	0.000	154.357
9	n-C9	128.3	4.76	0.000	0.000	116.052
10	n-C9	128.3	4.76	0.000	0.000	116.052
11	n-C9	128.3	4.76	0.000	0.000	116.052
12	n-C9	128.3	4.76	0.000	0.000	116.052
19	n-C8	114.2	4.27	0.000	0.000	296.983
20	2-Methylanthracene	192.26	4.89	961.094	0.000	1.558
21	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	437.736
22	Octene-1	112.2	4.13	0.000	0.000	394.547
24	n-Pentylbenzene	148.2	4.5	0.000	0.000	234.765
25	3-methylheptane	114.2	4.2	0.000	0.000	345.344
28	n-C10	142.29	5.25	0.000	0.000	44.767
29	n-C10	142.29	5.25	0.000	0.000	44.767
30	n-C10	142.3	5.25	0.000	0.000	44.770
31	n-C10	142.3	5.25	0.000	0.000	44.770
32	2-methylheptane	114.2	4.2	0.000	0.000	345.344
33	HEPTANE	100.2	3.78	0.000	0.000	749.158
34	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	477.147
35	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	410.437
36	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	437.851
38	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	417.910

39	Anthracene	178.2	4.35	603.704	0.000	5.605
40	Pyrene	202.3	4.93	1120.979	0.000	1.411
41	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	367.163
42	n-C9	128.3	4.76	0.000	0.000	116.052
43	n-C9	128.3	4.76	0.000	0.000	116.052
44	n-C9	128.3	4.76	0.000	0.000	116.052
45	n-C9	128.3	4.76	0.000	0.000	116.052
46	n-C10	142.29	5.25	0.000	0.000	44.767
47	n-C10	142.29	5.25	0.000	0.000	44.767
48	n-C10	142.3	5.25	0.000	0.000	44.770
49	n-C10	142.3	5.25	0.000	0.000	44.770
51	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	410.437
52	2,3-dimethylhexane	114.2	4.12	0.000	0.000	410.329
54	Methylcyclohexane	98.19	3.59	0.000	0.000	1105.638
56	n-Butylbenzene	134.2	4.01	0.000	0.000	475.531
58	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
59	C4-Benzothiophene	190.3	5.18	0.307	0.000	14.179
61	tert-Butylbenzene	134.2	3.9	0.000	0.000	602.752
62	2-methylhexane	100.2	3.71	0.000	0.000	871.151
63	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	367.217
64	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	417.848
65	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	367.163
66	3-ethylhexane	114.2	4.2	0.000	0.000	345.344
67	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	417.848
68	3-methylhexane	100.2	3.71	0.000	0.000	871.151
69	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
70	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
73	Hydrindene	118.2	3.47	0.000	0.000	1341.169
75	n-C5	72.15	2.8	0.000	0.000	4458.843
77	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2201.062

78	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	417.848
79	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	367.217
80	Propylbenzene	120.194	3.52	0.000	0.000	1224.471
81	p-XYLENE	106.2	3.09	0.000	0.000	2733.194
82	Dibenzofuran	168.2	3.71	51.047	0.000	56.785
83	4-isopropyltoluene	134.22	4	0.000	0.000	485.963
84	C3-Benzothiophene	176.3	4.69	0.307	0.000	37.766
85	sec-Butylbenzene	134.2	3.94	0.000	0.000	552.966
86	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
87	3-Methylpentane	86.18	3.21	0.000	0.000	2201.062
88	2,2-dimethylpentane	100.2	3.67	0.000	0.000	949.584
89	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	966.074
90	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	485.963
91	CARBAZOLE	167.2	3.23	167.183	0.000	99.246
92	m-cymene	134.2	4	0.000	0.000	485.890
93	Ethylbenzene	106.2	3.03	0.000	0.000	3110.501
94	CYCLOHEXANE	84.16	3.18	0.000	0.000	2293.040
95	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
96	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
97	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1075.995
98	m-XYLENE	106.2	3.09	0.000	0.000	2733.194
99	Isopropylbenzene	120.194	3.45	0.000	0.000	1423.864
100	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	329.654
101	n-C6	86.18	3.29	0.000	0.000	1852.475
102	Isopentane	72.15	2.72	0.000	0.000	5297.881
103	Methylcyclopentane	84.16	3.1	0.000	0.000	2724.530
104	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2559.484
105	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	966.074
106	o-XYLENE	106.2	3.09	0.000	0.000	2733.194
107	Cyclopentane	70.13	2.68	0.000	0.000	5613.190

109	C1-Decalins	152.3	4.61	0.000	0.000	84.630
112	trans-Decalin	138.26	4.2	0.000	0.000	185.901
115	cis-Decalin	138.26	4.2	0.000	0.000	185.901
116	Toluene	92.14	2.54	0.000	0.000	7758.791
117	Benzothiophene	134.2	2.99	0.307	0.000	1121.508
118	Benzene	78.11	1.99	0.000	0.000	21520.507
119	n-C11	156.31	5.74	0.000	0.000	17.105
120	n-C11	156.31	5.74	0.000	0.000	17.105
121	n-C11	156.31	5.74	0.000	0.000	17.105
122	n-C11	156.31	5.74	0.000	0.000	17.105
123	n-C12	170.34	6.23	0.000	0.000	6.484
124	n-C12	170.34	6.23	0.000	0.000	6.484
125	n-C12	170.34	6.23	0.000	0.000	6.484
126	n-C12	170.34	6.23	0.000	0.000	6.484
127	n-C11	156.31	5.74	0.000	0.000	17.105
128	n-C11	156.31	5.74	0.000	0.000	17.105
129	n-C11	156.31	5.74	0.000	0.000	17.105
130	n-C11	156.31	5.74	0.000	0.000	17.105
131	n-C12	170.34	6.23	0.000	0.000	6.484
132	n-C12	170.34	6.23	0.000	0.000	6.484
133	n-C12	170.34	6.23	0.000	0.000	6.484
134	n-C12	170.34	6.23	0.000	0.000	6.484
135	n-C13	184.37	6.73	0.000	0.000	2.389
136	n-C14	198.4	7.22	0.000	0.000	0.894
137	n-C15	212.42	7.71	0.000	0.000	0.333
138	n-C16	226.45	8.2	0.000	0.000	0.123
139	n-C17	240.48	8.69	0.000	0.000	0.046
140	n-C18	254.5	9.18	0.000	0.000	0.017
141	n-C19	268.53	9.67	0.000	0.000	0.006
142	n-C20	282.56	10.1	0.000	0.000	0.003

143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.004
164	Pristane	268.525	9.38	0.000	0.000	0.012
165	Benzo(a)fluoranthene	252.3	6.11	5005.988	0.000	0.074
166	Benzo(b)fluorene	216.3	5.77	445.576	0.000	0.361
167	Benzo(k)fluoranthene	252.3	6.11	2757.828	0.000	0.095
168	Benzo[a]anthracene	228.3	5.52	740.704	0.000	0.530
169	Benzo[a]pyrene	252.3	6.11	3756.755	0.000	0.083
170	Benzo[b]fluoranthene	252.3	6.11	1608.219	0.000	0.119
171	Benzo[e]pyrene	252.3	6.11	906.300	0.000	0.151
172	Benzo[g,h,i]perylene	276.3	6.7	2976.961	0.000	0.028

173	C1-Chrysenes	242.3	6.0683	431.978	0.000	0.216
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1647.337	0.000	0.393
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.041
176	C2-Chrysenes	256.3	6.65	431.978	0.000	0.065
177	C2-Decalins	166.3	6.19	0.000	0.000	3.068
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1647.337	0.000	0.103
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.142
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	961.094	0.000	0.479
181	C3-Chrysenes	270.4	7.03	431.978	0.000	0.030
182	C3-Decalins	180.3	6.79	0.000	0.000	0.913
183	C3-Dibenzothiophenes	230.37	5.86	6.876	0.000	1.589
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1647.337	0.000	0.042
185	C3-Fluorenes	210.3	5.58	90.165	0.000	1.009
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.410
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	961.094	0.000	0.221
188	C4-Chrysenes	284.4	7.35	431.978	0.000	0.016
189	C4-Decalins	194.3	7.34	0.000	0.000	0.301
190	C4-Dibenzothiophenes	244.37	6.1	6.876	0.000	1.005
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1647.337	0.000	0.016
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.153
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	961.094	0.000	0.123
194	Chrysene	228.3	5.52	351.996	0.000	0.720
195	Dibenz(a,h)anthracene	278.4	6.7	1935.638	0.000	0.034
196	Indeno[1,2,3-cd]pyrene	276.3	6.7	5232.487	0.000	0.022
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	20.533
198	Perylene	252.3	6.11	9113.504	0.000	0.057
199	Retene	234.3	6.35	115.167	0.000	0.194

Table B.15. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 100% WAF exposed to *Americamysis bahia* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	86.335	0.627	2.105
2	C1-Fluorenes	180.2	4.97	86.335	0.776	3.275
3	C3-Naphthalenes	170.26	4.77	25.890	1.440	7.593
4	C1-Phenanthrenes/Anthracenes	192.3	4.26	1094.052	1.060	5.741
5	C4-Naphthalenes	184.3	5.18	25.890	0.374	3.397
6	C2-Naphthalenes	156.2	4.31	25.890	1.900	18.775
7	1,6,7-Trimethylnaphthalene	170.26	4.81	31.742	0.499	6.448
8	1-Methylphenanthrene	192.26	4.89	57.155	0.348	4.883
9	Phenanthrene	178.2	4.35	36.024	1.210	17.328
10	4/9-Methylphenanthrene	192.26	4.89	57.155	0.309	4.883
11	2-Methylphenanthrene	192.26	4.89	57.155	0.260	4.883
16	3-Methylphenanthrene	192.26	4.89	57.155	0.254	4.883
17	2,6-Dimethylnaphthalene	156.23	4.26	25.890	0.776	20.915
19	C2-Dibenzothiophenes	214.3	5.13	7.682	0.251	6.856
20	Fluorene	166.2	4.02	86.335	0.653	23.405
25	C1-Dibenzothiophenes	198.3	4.71	7.682	0.337	15.685
31	Pyrene	202.3	4.93	1537.862	0.014	1.237
33	4-Methyldibenzothiophene	198.28	4.71	7.682	0.128	15.683
38	Dibenzothiophene	184.3	4.17	7.682	0.246	46.679
40	2-Methylanthracene	192.26	4.89	1094.052	0.008	1.477
41	C1-Naphthalenes	142.2	3.87	18.052	0.243	50.496
44	2/3-Methyldibenzothiophene	198.28	4.71	7.315	0.071	15.955

51	Fluoranthene	202.3	4.93	892.248	0.006	1.551
54	1-Methyldibenzothiophene	198.28	4.71	7.682	0.051	15.683
55	1-Methylnaphthalene	142.2	3.72	18.052	0.221	69.768
60	2-Methylnaphthalene	142.2	3.72	18.052	0.172	69.768
62	Anthracene	178.2	4.35	658.663	0.013	5.407
66	C4-Benzothiophene	190.3	5.18	0.384	0.025	13.452
67	Acenaphthene	154.2	4.15	63.035	0.032	18.573
72	Dibenzofuran	168.2	3.71	31.142	0.099	68.688
75	C3-Benzothiophene	176.3	4.69	0.384	0.043	35.831
104	Acenaphthylene	152.2	3.94	458.617	0.004	12.971
106	C2-Benzothiophene	162.25	4.13	0.384	0.030	110.242
107	Biphenyl	154.2	3.76	0.000	0.140	535.193
109	CARBAZOLE	167.2	3.23	164.530	0.010	99.887
111	C1-Benzothiophene	148.2	3.5365	0.384	0.025	361.847
114	Toluene	92.14	2.54	0.000	0.246	7758.791
115	Naphthalene	234.3	3.17	10.738	0.012	454.697
12	n-C10	142.29	5.25	0.000	0.000	44.767
13	n-C10	142.29	5.25	0.000	0.000	44.767
14	n-C10	142.3	5.25	0.000	0.000	44.770
15	n-C10	142.3	5.25	0.000	0.000	44.770
18	1-Decene	140.3	5.12	0.000	0.000	58.415
21	n-C9	128.3	4.76	0.000	0.000	116.052
22	n-C9	128.3	4.76	0.000	0.000	116.052
23	n-C9	128.3	4.76	0.000	0.000	116.052
24	n-C9	128.3	4.76	0.000	0.000	116.052
26	1-Nonene	126.2	4.62	0.000	0.000	154.357
27	n-C10	142.29	5.25	0.000	0.000	44.767
28	n-C10	142.29	5.25	0.000	0.000	44.767
29	n-C10	142.3	5.25	0.000	0.000	44.770

30	n-C10	142.3	5.25	0.000	0.000	44.770
32	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	437.736
34	n-C8	114.2	4.27	0.000	0.000	296.983
35	n-Pentylbenzene	148.2	4.5	0.000	0.000	234.765
36	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	417.910
37	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	367.163
39	Octene-1	112.2	4.13	0.000	0.000	394.547
42	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	437.851
43	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	410.437
45	3-methylheptane	114.2	4.2	0.000	0.000	345.344
46	n-C9	128.3	4.76	0.000	0.000	116.052
47	n-C9	128.3	4.76	0.000	0.000	116.052
48	n-C9	128.3	4.76	0.000	0.000	116.052
49	n-C9	128.3	4.76	0.000	0.000	116.052
50	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	477.147
52	2-methylheptane	114.2	4.2	0.000	0.000	345.344
53	HEPTANE	100.2	3.78	0.000	0.000	749.158
56	tert-Butylbenzene	134.2	3.9	0.000	0.000	602.752
57	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	367.163
58	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
59	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
61	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	367.217
63	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	417.848
64	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	417.848
65	n-Butylbenzene	134.2	4.01	0.000	0.000	475.531
68	Methylcyclohexane	98.19	3.59	0.000	0.000	1105.638
69	sec-Butylbenzene	134.2	3.94	0.000	0.000	552.966
70	Hydrindene	118.2	3.47	0.000	0.000	1341.169

71	Propylbenzene	120.194	3.52	0.000	0.000	1224.471
73	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	367.217
74	n-C6	86.18	3.29	0.000	0.000	1852.475
76	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	410.437
77	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	966.074
78	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	417.848
79	2,3-dimethylhexane	114.2	4.12	0.000	0.000	410.329
80	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	485.963
81	m-cymene	134.2	4	0.000	0.000	485.890
82	Ethylbenzene	106.2	3.03	0.000	0.000	3110.501
83	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
84	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
85	4-isopropyltoluene	134.22	4	0.000	0.000	485.963
86	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
87	CYCLOHEXANE	84.16	3.18	0.000	0.000	2293.040
88	n-C5	72.15	2.8	0.000	0.000	4458.843
89	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1075.995
90	p-XYLENE	106.2	3.09	0.000	0.000	2733.194
91	2-methylhexane	100.2	3.71	0.000	0.000	871.151
92	Isopropylbenzene	120.194	3.45	0.000	0.000	1423.864
93	3-Methylpentane	86.18	3.21	0.000	0.000	2201.062
94	3-ethylhexane	114.2	4.2	0.000	0.000	345.344
95	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	966.074
96	3-methylhexane	100.2	3.71	0.000	0.000	871.151
97	2,2-dimethylpentane	100.2	3.67	0.000	0.000	949.584
98	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
99	Methylcyclopentane	84.16	3.1	0.000	0.000	2724.530
100	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2201.062
101	o-XYLENE	106.2	3.09	0.000	0.000	2733.194

102	m-XYLENE	106.2	3.09	0.000	0.000	2733.194
103	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	329.654
105	Cyclopentane	70.13	2.68	0.000	0.000	5613.190
108	Benzene	78.11	1.99	0.000	0.000	21520.507
110	Isopentane	72.15	2.72	0.000	0.000	5297.881
112	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2559.484
113	C1-Decalins	152.3	4.61	0.000	0.000	84.630
116	trans-Decalin	138.26	4.2	0.000	0.000	185.901
117	cis-Decalin	138.26	4.2	0.000	0.000	185.901
118	Benzothiophene	134.2	2.99	0.384	0.000	1064.029
119	n-C11	156.31	5.74	0.000	0.000	17.105
120	n-C11	156.31	5.74	0.000	0.000	17.105
121	n-C11	156.31	5.74	0.000	0.000	17.105
122	n-C11	156.31	5.74	0.000	0.000	17.105
123	n-C12	170.34	6.23	0.000	0.000	6.484
124	n-C12	170.34	6.23	0.000	0.000	6.484
125	n-C12	170.34	6.23	0.000	0.000	6.484
126	n-C12	170.34	6.23	0.000	0.000	6.484
127	n-C11	156.31	5.74	0.000	0.000	17.105
128	n-C11	156.31	5.74	0.000	0.000	17.105
129	n-C11	156.31	5.74	0.000	0.000	17.105
130	n-C11	156.31	5.74	0.000	0.000	17.105
131	n-C12	170.34	6.23	0.000	0.000	6.484
132	n-C12	170.34	6.23	0.000	0.000	6.484
133	n-C12	170.34	6.23	0.000	0.000	6.484
134	n-C12	170.34	6.23	0.000	0.000	6.484
135	n-C13	184.37	6.73	0.000	0.000	2.389
136	n-C14	198.4	7.22	0.000	0.000	0.894
137	n-C15	212.42	7.71	0.000	0.000	0.333

138	n-C16	226.45	8.2	0.000	0.000	0.123
139	n-C17	240.48	8.69	0.000	0.000	0.046
140	n-C18	254.5	9.18	0.000	0.000	0.017
141	n-C19	268.53	9.67	0.000	0.000	0.006
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.004
164	Pristane	268.525	9.38	0.000	0.000	0.012
165	Benzo(a)fluoranthene	252.3	6.11	3030.873	0.000	0.091
166	Benzo(b)fluorene	216.3	5.77	593.982	0.000	0.321

167	Benzo(k)fluoranthene	252.3	6.11	2756.635	0.000	0.095
168	Benzo[a]anthracene	228.3	5.52	791.538	0.000	0.516
169	Benzo[a]pyrene	252.3	6.11	3969.164	0.000	0.082
170	Benzo[b]fluoranthene	252.3	6.11	1681.435	0.000	0.117
171	Benzo[e]pyrene	252.3	6.11	1161.480	0.000	0.136
172	Benzo[g,h,i]perylene	276.3	6.7	3235.538	0.000	0.027
173	C1-Chrysenes	242.3	6.0683	562.984	0.000	0.193
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1961.818	0.000	0.365
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.041
176	C2-Chrysenes	256.3	6.65	562.984	0.000	0.058
177	C2-Decalins	166.3	6.19	0.000	0.000	3.068
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1961.818	0.000	0.096
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.142
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1094.052	0.000	0.454
181	C3-Chrysenes	270.4	7.03	562.984	0.000	0.027
182	C3-Decalins	180.3	6.79	0.000	0.000	0.913
183	C3-Dibenzothiophenes	230.37	5.86	7.682	0.000	1.528
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1961.818	0.000	0.039
185	C3-Fluorenes	210.3	5.58	86.335	0.000	1.027
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.410
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1094.052	0.000	0.209
188	C4-Chrysenes	284.4	7.35	562.984	0.000	0.014
189	C4-Decalins	194.3	7.34	0.000	0.000	0.301
190	C4-Dibenzothiophenes	244.37	6.1	7.682	0.000	0.966
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1961.818	0.000	0.015
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.153
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1094.052	0.000	0.117
194	Chrysene	228.3	5.52	452.808	0.000	0.649
195	Dibenz(a,h)anthracene	278.4	6.7	1957.920	0.000	0.034

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	4665.545	0.000	0.023
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	20.533
198	Perylene	252.3	6.11	4968.758	0.000	0.074
199	Retene	234.3	6.35	84.725	0.000	0.219

Table B.16. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 25% WAF exposed to *Americamysis bahia* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	86.33531802	0.151	2.105306
2	C1-Fluorenes	180.2	4.97	86.33531802	0.183	3.275195
7	C3-Naphthalenes	170.26	4.77	25.89030265	0.333	7.593481
8	C1-Phenanthrenes/Anthracenes	192.3	4.26	1094.052007	0.25	5.741368
10	C4-Naphthalenes	184.3	5.18	25.89030265	0.0977	3.396985
11	C2-Naphthalenes	156.2	4.31	25.89030265	0.445	18.77454
16	Phenanthrene	178.2	4.35	36.02380848	0.299	17.32777
17	1,6,7-Trimethylnaphthalene	170.26	4.81	31.74227949	0.111	6.447692
18	1-Methylphenanthrene	192.26	4.89	57.15488994	0.082	4.883013
19	4/9-Methylphenanthrene	192.26	4.89	57.15488994	0.0727	4.883013
21	2-Methylphenanthrene	192.26	4.89	57.15488994	0.0609	4.883013
22	3-Methylphenanthrene	192.26	4.89	57.15488994	0.0599	4.883013
27	2,6-Dimethylnaphthalene	156.23	4.26	25.89030265	0.179	20.91475
29	C2-Dibenzothiophenes	214.3	5.13	7.682460823	0.0551	6.855788
33	Fluorene	166.2	4.02	86.33531802	0.158	23.40525
43	C1-Dibenzothiophenes	198.3	4.71	7.682460823	0.0658	15.68476
47	Pyrene	202.3	4.93	1537.861713	0.00404	1.237053
56	4-Methyldibenzothiophene	198.28	4.71	7.682460823	0.0293	15.68318
63	Dibenzothiophene	184.3	4.17	7.682460823	0.0583	46.6789
64	2-Methylanthracene	192.26	4.89	1094.052007	0.0018	1.476539
65	Fluoranthene	202.3	4.93	892.248225	0.00185	1.551127

66	C1-Naphthalenes	142.2	3.87	18.05244405	0.0562	50.49592
81	1-Methyldibenzothiophene	198.28	4.71	7.682460823	0.0117	15.68318
83	1-Methylnaphthalene	142.2	3.72	18.05244405	0.0506	69.768
87	2-Methylnaphthalene	142.2	3.72	18.05244405	0.0401	69.768
88	Anthracene	178.2	4.35	658.6633485	0.00292	5.407047
90	2/3-Methyldibenzothiophene	198.28	4.71	7.314847726	0.00818	15.95481
95	Acenaphthene	154.2	4.15	63.03500663	0.00797	18.57328
96	C4-Benzothiophene	190.3	5.18	0.384072873	0.00562	13.45239
99	C3-Benzothiophene	176.3	4.69	0.384072873	0.0128	35.83052
101	Dibenzofuran	168.2	3.71	31.14197165	0.0239	68.68768
108	Acenaphthylene	152.2	3.94	458.6172196	0.00114	12.9706
109	C2-Benzothiophene	162.25	4.13	0.384072873	0.00759	110.2416
110	Biphenyl	154.2	3.76	0	0.0339	535.1928
113	C1-Benzothiophene	148.2	3.5365	0.384072873	0.00866	361.847
114	CARBAZOLE	167.2	3.23	164.5299081	0.00212	99.8873
3	n-C10	142.29	5.25	0	0	44.76723
4	n-C10	142.29	5.25	0	0	44.76723
5	n-C10	142.3	5.25	0	0	44.77038
6	n-C10	142.3	5.25	0	0	44.77038
9	1-Decene	140.3	5.12	0	0	58.41489
12	n-C9	128.3	4.76	0	0	116.052
13	n-C9	128.3	4.76	0	0	116.052
14	n-C9	128.3	4.76	0	0	116.052
15	n-C9	128.3	4.76	0	0	116.052
20	1-Nonene	126.2	4.62	0	0	154.3566
23	n-C10	142.29	5.25	0	0	44.76723
24	n-C10	142.29	5.25	0	0	44.76723
25	n-C10	142.3	5.25	0	0	44.77038
26	n-C10	142.3	5.25	0	0	44.77038

28	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0	0	437.7357
30	n-C8	114.2	4.27	0	0	296.9833
31	n-Pentylbenzene	148.2	4.5	0	0	234.7654
32	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0	0	417.9103
34	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0	0	367.1626
35	Octene-1	112.2	4.13	0	0	394.547
36	Pentane, 2,3,3-trimethyl	114.23	4.09	0	0	437.8507
37	2,5-Dimethylhexane	114.23	4.12	0	0	410.4366
38	3-methylheptane	114.2	4.2	0	0	345.344
39	n-C9	128.3	4.76	0	0	116.052
40	n-C9	128.3	4.76	0	0	116.052
41	n-C9	128.3	4.76	0	0	116.052
42	n-C9	128.3	4.76	0	0	116.052
44	2,3,4-trimethylpentane	114.2	4.05	0	0	477.1468
45	2-methylheptane	114.2	4.2	0	0	345.344
46	HEPTANE	100.2	3.78	0	0	749.1583
48	tert-Butylbenzene	134.2	3.9	0	0	602.7516
49	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0	0	367.1626
50	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0	0	367.1626
51	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0	0	367.1626
52	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0	0	367.2173
53	1-Methyl-2-n-Propylbenzene	134.2	4.07	0	0	417.8481
54	1-methyl-3-n-propylbenzene	134.2	4.07	0	0	417.8481
55	n-Butylbenzene	134.2	4.01	0	0	475.5305
57	Methylcyclohexane	98.19	3.59	0	0	1105.638
58	sec-Butylbenzene	134.2	3.94	0	0	552.9659
59	Hydrindene	118.2	3.47	0	0	1341.169
60	Propylbenzene	120.194	3.52	0	0	1224.471
61	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0	0	367.2173

62	n-C6	86.18	3.29	0	0	1852.475
67	1,1,3-trimethylpentane	114.23	4.12	0	0	410.4366
68	1,2,4-Trimethylbenzene	120.2	3.63	0	0	966.0739
69	1,2-Diethylbenzene	134.2	4.07	0	0	417.8481
70	2,3-dimethylhexane	114.2	4.12	0	0	410.3288
71	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0	0	485.9629
72	m-cymene	134.2	4	0	0	485.8905
73	Ethylbenzene	106.2	3.03	0	0	3110.501
74	2,4-dimethylpentane	100.2	3.63	0	0	1035.079
75	1-Methyl-2-ethylbenzene	120.2	3.58	0	0	1075.995
76	4-isopropyltoluene	134.22	4	0	0	485.9629
77	1-Methyl-3-ethylbenzene	120.2	3.58	0	0	1075.995
78	CYCLOHEXANE	84.16	3.18	0	0	2293.04
79	n-C5	72.15	2.8	0	0	4458.843
80	4-ETHYLTOLUENE	120.2	3.58	0	0	1075.995
82	p-XYLENE	106.2	3.09	0	0	2733.194
84	2-methylhexane	100.2	3.71	0	0	871.1513
85	Isopropylbenzene	120.194	3.45	0	0	1423.864
86	3-Methylpentane	86.18	3.21	0	0	2201.062
89	3-ethylhexane	114.2	4.2	0	0	345.344
91	1,3,5-trimethylbenzene	120.2	3.63	0	0	966.0739
92	3-methylhexane	100.2	3.71	0	0	871.1513
93	2,2-dimethylpentane	100.2	3.67	0	0	949.5844
94	2,3-dimethylpentane	100.2	3.63	0	0	1035.079
97	Methylcyclopentane	84.16	3.1	0	0	2724.53
98	2-METHYLPENTANE	86.18	3.21	0	0	2201.062
100	o-XYLENE	106.2	3.09	0	0	2733.194
102	m-XYLENE	106.2	3.09	0	0	2733.194
103	1,2,4,5-Tetramethylbenzene	134.2	4.18	0	0	329.654

104	Cyclopentane	70.13	2.68	0	0	5613.19
105	Toluene	92.14	2.54	0	0	7758.791
106	Benzene	78.11	1.99	0	0	21520.51
107	Isopentane	72.15	2.72	0	0	5297.881
111	2,3-dimethylbutane	86.18	3.14	0	0	2559.484
112	C1-Decalins	152.3	4.61	0	0	84.63028
115	trans-Decalin	138.26	4.2	0	0	185.9013
116	Naphthalene	234.3	3.17	10.73812435	0	454.6966
117	cis-Decalin	138.26	4.2	0	0	185.9013
118	Benzothiophene	134.2	2.99	0.384072873	0	1064.029
119	n-C11	156.31	5.74	0	0	17.10538
120	n-C11	156.31	5.74	0	0	17.10538
121	n-C11	156.31	5.74	0	0	17.10538
122	n-C11	156.31	5.74	0	0	17.10538
123	n-C12	170.34	6.23	0	0	6.483694
124	n-C12	170.34	6.23	0	0	6.483694
125	n-C12	170.34	6.23	0	0	6.483694
126	n-C12	170.34	6.23	0	0	6.483694
127	n-C11	156.31	5.74	0	0	17.10538
128	n-C11	156.31	5.74	0	0	17.10538
129	n-C11	156.31	5.74	0	0	17.10538
130	n-C11	156.31	5.74	0	0	17.10538
131	n-C12	170.34	6.23	0	0	6.483694
132	n-C12	170.34	6.23	0	0	6.483694
133	n-C12	170.34	6.23	0	0	6.483694
134	n-C12	170.34	6.23	0	0	6.483694
135	n-C13	184.37	6.73	0	0	2.38889
136	n-C14	198.4	7.22	0	0	0.894144
137	n-C15	212.42	7.71	0	0	0.332982

138	n-C16	226.45	8.2	0	0	0.123469
139	n-C17	240.48	8.69	0	0	0.045606
140	n-C18	254.5	9.18	0	0	0.016788
141	n-C19	268.53	9.67	0	0	0.006161
142	n-C20	282.56	10.1	0	0	0.002566
143	n-C21	296.59	10.6	0	0	0.000917
144	n-C22	310.61	11.1	0	0	0.000327
145	n-C23	324.64	11.6	0	0	0.000116
146	n-C24	338.67	12.1	0	0	4.13E-05
147	n-C25	352.69	12.6	0	0	1.46E-05
148	n-C26	366.72	13.1	0	0	5.18E-06
149	n-C27	380.75	13.6	0	0	1.83E-06
150	n-C28	394.77	14	0	0	8.02E-07
151	n-C29	408.8	14.5	0	0	2.83E-07
152	n-C30	422.83	15	0	0	9.95E-08
153	n-C31	436.86	15.5	0	0	3.50E-08
154	n-C32	450.88	16	0	0	1.23E-08
155	n-C33	464.91	16.5	0	0	4.32E-09
156	n-C34	478.94	17	0	0	1.51E-09
157	n-C35	492.96	17.5	0	0	5.30E-10
158	n-C36	506.981	18	0	0	1.86E-10
159	n-C37	521	18.5	0	0	6.50E-11
160	n-C38	535	19	0	0	2.27E-11
161	n-C39	549.1	19.49	0	0	8.11E-12
162	n-C40	563.1	19.9	0	0	3.44E-12
163	Phytane	282.56	9.87	0	0	0.004213
164	Pristane	268.525	9.38	0	0	0.01151
165	Benzo(a)fluoranthene	252.3	6.11	3030.873123	0	0.091345
166	Benzo(b)fluorene	216.3	5.77	593.981753	0	0.321001

167	Benzo(k)fluoranthene	252.3	6.11	2756.63538	0	0.095047
168	Benzo[a]anthracene	228.3	5.52	791.5377655	0	0.515768
169	Benzo[a]pyrene	252.3	6.11	3969.164117	0	0.081575
170	Benzo[b]fluoranthene	252.3	6.11	1681.435154	0	0.116861
171	Benzo[e]pyrene	252.3	6.11	1161.47982	0	0.136321
172	Benzo[g,h,i]perylene	276.3	6.7	3235.538164	0	0.027291
173	C1-Chrysenes	242.3	6.0683	562.9838065	0	0.19328
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1961.817865	0	0.364967
175	C1-naphthobenzothiophenes	248.3	6.38	0	0	3.041463
176	C2-Chrysenes	256.3	6.65	562.9838065	0	0.058359
177	C2-Decalins	166.3	6.19	0	0	3.067878
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1961.817865	0	0.095801
179	C2-naphthobenzothiophenes	262.4	6.86	0	0	1.142325
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1094.052007	0	0.453916
181	C3-Chrysenes	270.4	7.03	562.9838065	0	0.027145
182	C3-Decalins	180.3	6.79	0	0	0.912728
183	C3-Dibenzothiophenes	230.37	5.86	7.682460823	0	1.528203
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1961.817865	0	0.039376
185	C3-Fluorenes	210.3	5.58	86.33531802	0	1.026506
186	C3-naphthobenzothiophenes	276.4	7.36	0	0	0.409604
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1094.052007	0	0.209147
188	C4-Chrysenes	284.4	7.35	562.9838065	0	0.014325
189	C4-Decalins	194.3	7.34	0	0	0.300621
190	C4-Dibenzothiophenes	244.37	6.1	7.682460823	0	0.966414
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1961.817865	0	0.014796
192	C4-naphthobenzothiophenes	290.4	7.84	0	0	0.152948
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1094.052007	0	0.116522
194	Chrysene	228.3	5.52	452.8078727	0	0.649299
195	Dibenz(a,h)anthracene	278.4	6.7	1957.920341	0	0.03393

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	4665.544857	0	0.023404
197	Naphthobenzothiophenes	178.2	5.34	0	0	20.53305
198	Perylene	252.3	6.11	4968.758266	0	0.074229
199	Retene	234.3	6.35	84.72527191	0	0.219184

Table B.17. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF exposed to *Americamysis bahia* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	86.335	0.041	2.105
2	C1-Fluorenes	180.2	4.97	86.335	0.049	3.275
3	C4-Naphthalenes	184.3	5.18	25.890	0.043	3.397
4	C1-Phenanthrenes/Anthracenes	192.3	4.26	1094.052	0.066	5.741
5	C3-Naphthalenes	170.26	4.77	25.890	0.080	7.593
6	C2-Naphthalenes	156.2	4.31	25.890	0.103	18.775
7	Phenanthrene	178.2	4.35	36.024	0.082	17.328
8	1-Methylphenanthrene	192.26	4.89	57.155	0.021	4.883
9	1,6,7-Trimethylnaphthalene	170.26	4.81	31.742	0.027	6.448
10	4/9-Methylphenanthrene	192.26	4.89	57.155	0.019	4.883
11	3-Methylphenanthrene	192.26	4.89	57.155	0.016	4.883
12	2-Methylphenanthrene	192.26	4.89	57.155	0.016	4.883
13	2,6-Dimethylnaphthalene	156.23	4.26	25.890	0.040	20.915
14	Fluorene	166.2	4.02	86.335	0.042	23.405
15	C2-Dibenzothiophenes	214.3	5.13	7.682	0.012	6.856
16	Pyrene	202.3	4.93	1537.862	0.002	1.237
17	C1-Dibenzothiophenes	198.3	4.71	7.682	0.016	15.685
18	Fluoranthene	202.3	4.93	892.248	0.001	1.551
19	4-Methyldibenzothiophene	198.28	4.71	7.682	0.007	15.683
20	Dibenzothiophene	184.3	4.17	7.682	0.015	46.679
21	C1-Naphthalenes	142.2	3.87	18.052	0.016	50.496

22	1-Methyldibenzothiophene	198.28	4.71	7.682	0.003	15.683
23	1-Methylnaphthalene	142.2	3.72	18.052	0.014	69.768
24	2-Methylnaphthalene	142.2	3.72	18.052	0.011	69.768
25	Acenaphthene	154.2	4.15	63.035	0.002	18.573
26	Dibenzofuran	168.2	3.71	31.142	0.007	68.688
27	Acenaphthylene	152.2	3.94	458.617	0.001	12.971
28	C2-Benzothiophene	162.25	4.13	0.384	0.003	110.242
29	2/3-Methyldibenzothiophene	198.28	4.71	7.315	0.000	15.955
30	Biphenyl	154.2	3.76	0.000	0.009	535.193
31	C1-Benzothiophene	148.2	3.5365	0.384	0.004	361.847
32	CARBAZOLE	167.2	3.23	164.530	0.001	99.887
33	n-C10	142.29	5.25	0.000	2.360	44.767
34	n-C10	142.29	5.25	0.000	2.360	44.767
35	n-C10	142.3	5.25	0.000	2.360	44.770
36	n-C10	142.3	5.25	0.000	2.360	44.770
37	1-Decene	140.3	5.12	0.000	2.140	58.415
38	n-C9	128.3	4.76	0.000	2.520	116.052
39	n-C9	128.3	4.76	0.000	2.520	116.052
40	n-C9	128.3	4.76	0.000	2.520	116.052
41	n-C9	128.3	4.76	0.000	2.520	116.052
42	1-Nonene	126.2	4.62	0.000	2.060	154.357
43	n-C10	142.29	5.25	0.000	0.515	44.767
44	n-C10	142.29	5.25	0.000	0.515	44.767
45	n-C10	142.3	5.25	0.000	0.515	44.770
46	n-C10	142.3	5.25	0.000	0.515	44.770
47	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	3.630	437.736
48	n-C8	114.2	4.27	0.000	2.300	296.983
49	n-Pentylbenzene	148.2	4.5	0.000	1.780	234.765
50	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	2.890	417.910

51	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	2.000	367.163
52	Octene-1	112.2	4.13	0.000	2.060	394.547
53	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	2.000	437.851
54	2,5-Dimethylhexane	114.23	4.12	0.000	1.870	410.437
55	3-methylheptane	114.2	4.2	0.000	1.500	345.344
56	n-C9	128.3	4.76	0.000	0.501	116.052
57	n-C9	128.3	4.76	0.000	0.501	116.052
58	n-C9	128.3	4.76	0.000	0.501	116.052
59	n-C9	128.3	4.76	0.000	0.501	116.052
60	2,3,4-trimethylpentane	114.2	4.05	0.000	2.000	477.147
61	2-methylheptane	114.2	4.2	0.000	1.180	345.344
62	2-Methylanthracene	192.26	4.89	1094.052	0.005	1.477
63	HEPTANE	100.2	3.78	0.000	2.450	749.158
64	tert-Butylbenzene	134.2	3.9	0.000	1.900	602.752
65	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.928	367.163
66	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.910	367.163
67	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.909	367.163
68	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.862	367.217
69	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.910	417.848
70	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.864	417.848
71	n-Butylbenzene	134.2	4.01	0.000	0.903	475.531
72	Methylcyclohexane	98.19	3.59	0.000	1.890	1105.638
73	sec-Butylbenzene	134.2	3.94	0.000	0.913	552.966
74	Hydrindene	118.2	3.47	0.000	2.010	1341.169
75	Propylbenzene	120.194	3.52	0.000	1.820	1224.471
76	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.464	367.217
77	n-C6	86.18	3.29	0.000	2.340	1852.475
78	1,1,3-trimethylpentane	114.23	4.12	0.000	0.451	410.437
79	1,2,4-Trimethylbenzene	120.2	3.63	0.000	1.050	966.074

80	1,2-Diethylbenzene	134.2	4.07	0.000	0.435	417.848
81	2,3-dimethylhexane	114.2	4.12	0.000	0.416	410.329
82	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.464	485.963
83	m-cymene	134.2	4	0.000	0.454	485.890
84	Ethylbenzene	106.2	3.03	0.000	2.880	3110.501
85	Anthracene	178.2	4.35	658.663	0.005	5.407
86	2,4-dimethylpentane	100.2	3.63	0.000	0.928	1035.079
87	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.952	1075.995
88	4-isopropyltoluene	134.22	4	0.000	0.428	485.963
89	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.925	1075.995
90	CYCLOHEXANE	84.16	3.18	0.000	1.850	2293.040
91	n-C5	72.15	2.8	0.000	3.520	4458.843
92	4-ETHYLTOLUENE	120.2	3.58	0.000	0.821	1075.995
93	p-XYLENE	106.2	3.09	0.000	2.030	2733.194
94	2-methylhexane	100.2	3.71	0.000	0.596	871.151
95	Isopropylbenzene	120.194	3.45	0.000	0.926	1423.864
96	3-Methylpentane	86.18	3.21	0.000	1.340	2201.062
97	3-ethylhexane	114.2	4.2	0.000	0.178	345.344
98	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.463	966.074
99	3-methylhexane	100.2	3.71	0.000	0.416	871.151
100	2,2-dimethylpentane	100.2	3.67	0.000	0.453	949.584
101	2,3-dimethylpentane	100.2	3.63	0.000	0.462	1035.079
102	Methylcyclopentane	84.16	3.1	0.000	1.050	2724.530
103	C4-Benzothiophene	190.3	5.18	0.384	0.005	13.452
104	2-METHYLPENTANE	86.18	3.21	0.000	0.810	2201.062
105	o-XYLENE	106.2	3.09	0.000	0.964	2733.194
106	m-XYLENE	106.2	3.09	0.000	0.947	2733.194
107	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.110	329.654
108	Cyclopentane	70.13	2.68	0.000	1.620	5613.190

109	Toluene	92.14	2.54	0.000	1.960	7758.791
110	Benzene	78.11	1.99	0.000	3.130	21520.507
111	C3-Benzothiophene	176.3	4.69	0.384	0.005	35.831
112	Isopentane	72.15	2.72	0.000	0.497	5297.881
113	2,3-dimethylbutane	86.18	3.14	0.000	0.101	2559.484
114	C1-Decalins	152.3	4.61	0.000	0.003	84.630
115	trans-Decalin	138.26	4.2	0.000	0.003	185.901
116	Naphthalene	234.3	3.17	10.738	0.005	454.697
117	cis-Decalin	138.26	4.2	0.000	0.002	185.901
118	Benzothiophene	134.2	2.99	0.384	0.005	1064.029
119	n-C11	156.31	5.74	0.000	0.000	17.105
120	n-C11	156.31	5.74	0.000	0.000	17.105
121	n-C11	156.31	5.74	0.000	0.000	17.105
122	n-C11	156.31	5.74	0.000	0.000	17.105
123	n-C12	170.34	6.23	0.000	0.000	6.484
124	n-C12	170.34	6.23	0.000	0.000	6.484
125	n-C12	170.34	6.23	0.000	0.000	6.484
126	n-C12	170.34	6.23	0.000	0.000	6.484
127	n-C11	156.31	5.74	0.000	0.000	17.105
128	n-C11	156.31	5.74	0.000	0.000	17.105
129	n-C11	156.31	5.74	0.000	0.000	17.105
130	n-C11	156.31	5.74	0.000	0.000	17.105
131	n-C12	170.34	6.23	0.000	0.000	6.484
132	n-C12	170.34	6.23	0.000	0.000	6.484
133	n-C12	170.34	6.23	0.000	0.000	6.484
134	n-C12	170.34	6.23	0.000	0.000	6.484
135	n-C13	184.37	6.73	0.000	0.000	2.389
136	n-C14	198.4	7.22	0.000	0.000	0.894
137	n-C15	212.42	7.71	0.000	0.000	0.333

138	n-C16	226.45	8.2	0.000	0.000	0.123
139	n-C17	240.48	8.69	0.000	0.000	0.046
140	n-C18	254.5	9.18	0.000	0.000	0.017
141	n-C19	268.53	9.67	0.000	0.000	0.006
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.004
164	Pristane	268.525	9.38	0.000	0.000	0.012
165	Benzo(a)fluoranthene	252.3	6.11	3030.873	0.000	0.091
166	Benzo(b)fluorene	216.3	5.77	593.982	0.000	0.321

167	Benzo(k)fluoranthene	252.3	6.11	2756.635	0.000	0.095
168	Benzo[a]anthracene	228.3	5.52	791.538	0.000	0.516
169	Benzo[a]pyrene	252.3	6.11	3969.164	0.000	0.082
170	Benzo[b]fluoranthene	252.3	6.11	1681.435	0.000	0.117
171	Benzo[e]pyrene	252.3	6.11	1161.480	0.000	0.136
172	Benzo[g,h,i]perylene	276.3	6.7	3235.538	0.000	0.027
173	C1-Chrysenes	242.3	6.0683	562.984	0.000	0.193
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1961.818	0.000	0.365
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.041
176	C2-Chrysenes	256.3	6.65	562.984	0.000	0.058
177	C2-Decalins	166.3	6.19	0.000	0.000	3.068
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1961.818	0.000	0.096
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.142
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1094.052	0.000	0.454
181	C3-Chrysenes	270.4	7.03	562.984	0.000	0.027
182	C3-Decalins	180.3	6.79	0.000	0.000	0.913
183	C3-Dibenzothiophenes	230.37	5.86	7.682	0.000	1.528
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1961.818	0.000	0.039
185	C3-Fluorenes	210.3	5.58	86.335	0.000	1.027
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.410
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1094.052	0.000	0.209
188	C4-Chrysenes	284.4	7.35	562.984	0.000	0.014
189	C4-Decalins	194.3	7.34	0.000	0.000	0.301
190	C4-Dibenzothiophenes	244.37	6.1	7.682	0.000	0.966
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1961.818	0.000	0.015
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.153
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1094.052	0.000	0.117
194	Chrysene	228.3	5.52	452.808	0.000	0.649
195	Dibenz(a,h)anthracene	278.4	6.7	1957.920	0.000	0.034

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	4665.545	0.000	0.023
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	20.533
198	Perylene	252.3	6.11	4968.758	0.000	0.074
199	Retene	234.3	6.35	84.725	0.000	0.219

Table B.18. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF duplicate exposed to *Americamysis bahia* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	86.335	0.043	2.796
2	C1-Fluorenes	180.2	4.97	86.335	0.046	4.350
3	C4-Naphthalenes	184.3	5.18	25.890	0.0418	4.511
4	C1-Phenanthrenes/Anthracenes	192.3	4.26	1094.052	0.0622	7.625
5	C3-Naphthalenes	170.26	4.77	25.890	0.079	10.085
6	C2-Naphthalenes	156.2	4.31	25.890	0.102	24.934
7	Phenanthrene	178.2	4.35	36.024	0.0801	23.012
8	1-Methylphenanthrene	192.26	4.89	57.155	0.02	6.485
9	1,6,7-Trimethylnaphthalene	170.26	4.81	31.742	0.0258	8.563
10	4/9-Methylphenanthrene	192.26	4.89	57.155	0.0179	6.485
11	3-Methylphenanthrene	192.26	4.89	57.155	0.0152	6.485
12	2-Methylphenanthrene	192.26	4.89	57.155	0.0147	6.485
13	2,6-Dimethylnaphthalene	156.23	4.26	25.890	0.0392	27.776
14	Fluorene	166.2	4.02	86.335	0.0398	31.083
15	C2-Dibenzothiophenes	214.3	5.13	7.682	0.0105	9.105
16	C1-Dibenzothiophenes	198.3	4.71	7.682	0.0157	20.830
17	Fluoranthene	202.3	4.93	892.248	0.000936	2.060
18	4-Methyldibenzothiophene	198.28	4.71	7.682	0.0065	20.828
19	C1-Naphthalenes	142.2	3.87	18.052	0.0156	67.061
20	Dibenzothiophene	184.3	4.17	7.682	0.0142	61.992
21	1-Methylnaphthalene	142.2	3.72	18.052	0.0128	92.655
22	1-Methyldibenzothiophene	198.28	4.71	7.682	0.00281	20.828
23	2-Methylnaphthalene	142.2	3.72	18.052	0.0112	92.655

24	Acenaphthene	154.2	4.15	63.035	0.00278	24.666
25	Dibenzofuran	168.2	3.71	31.142	0.00657	91.221
26	Acenaphthylene	152.2	3.94	458.617	0.000624	17.226
27	C1-Benzothiophene	148.2	3.5365	0.384	0.0107	480.551
28	C2-Benzothiophene	162.25	4.13	0.384	0.00313	146.406
29	Biphenyl	154.2	3.76	0.000	0.00902	710.762
30	CARBAZOLE	167.2	3.23	164.530	0.000864	132.655
31	n-C10	142.29	5.25	0.000	2.36	59.453
32	n-C10	142.29	5.25	0.000	2.36	59.453
33	n-C10	142.3	5.25	0.000	2.36	59.457
34	n-C10	142.3	5.25	0.000	2.36	59.457
35	1-Decene	140.3	5.12	0.000	2.14	77.578
36	n-C10	142.29	5.25	0.000	1.03	59.453
37	n-C10	142.29	5.25	0.000	1.03	59.453
38	n-C10	142.3	5.25	0.000	1.03	59.457
39	n-C10	142.3	5.25	0.000	1.03	59.457
40	n-C9	128.3	4.76	0.000	2.52	154.123
41	n-C9	128.3	4.76	0.000	2.52	154.123
42	n-C9	128.3	4.76	0.000	2.52	154.123
43	n-C9	128.3	4.76	0.000	2.52	154.123
44	1-Nonene	126.2	4.62	0.000	2.06	204.993
45	n-C9	128.3	4.76	0.000	1	154.123
46	n-C9	128.3	4.76	0.000	1	154.123
47	n-C9	128.3	4.76	0.000	1	154.123
48	n-C9	128.3	4.76	0.000	1	154.123
49	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	3.63	581.335
50	Pyrene	202.3	4.93	1537.862	0.01	1.643
51	n-C8	114.2	4.27	0.000	2.3	394.408
52	n-Pentylbenzene	148.2	4.5	0.000	1.78	311.780

53	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	2.89	555.005
54	2-Methylanthracene	192.26	4.89	1094.052	0.00997	1.961
55	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	2	487.610
56	Octene-1	112.2	4.13	0.000	2.06	523.978
57	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	2	581.487
58	2,5-Dimethylhexane	114.23	4.12	0.000	1.87	545.080
59	3-methylheptane	114.2	4.2	0.000	1.5	458.634
60	2,3,4-trimethylpentane	114.2	4.05	0.000	2	633.674
61	2-methylheptane	114.2	4.2	0.000	1.18	458.634
62	HEPTANE	100.2	3.78	0.000	2.45	994.919
63	tert-Butylbenzene	134.2	3.9	0.000	1.9	800.484
64	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.928	487.610
65	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.91	487.610
66	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.909	487.610
67	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.862	487.683
68	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.91	554.923
69	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.864	554.923
70	n-Butylbenzene	134.2	4.01	0.000	0.903	631.528
71	Anthracene	178.2	4.35	658.663	0.00996	7.181
72	Methylcyclohexane	98.19	3.59	0.000	1.89	1468.342
73	sec-Butylbenzene	134.2	3.94	0.000	0.913	734.366
74	Hydrindene	118.2	3.47	0.000	2.01	1781.138
75	Propylbenzene	120.194	3.52	0.000	1.82	1626.158
76	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.464	487.683
77	n-C6	86.18	3.29	0.000	2.34	2460.178
78	1,1,3-trimethylpentane	114.23	4.12	0.000	0.451	545.080
79	1,2,4-Trimethylbenzene	120.2	3.63	0.000	1.05	1282.994
80	1,2-Diethylbenzene	134.2	4.07	0.000	0.435	554.923
81	2,3-dimethylhexane	114.2	4.12	0.000	0.416	544.937

82	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.464	645.383
83	m-cymene	134.2	4	0.000	0.454	645.286
84	Ethylbenzene	106.2	3.03	0.000	2.88	4130.898
85	2,4-dimethylpentane	100.2	3.63	0.000	0.928	1374.636
86	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.952	1428.974
87	4-isopropyltoluene	134.22	4	0.000	0.428	645.383
88	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.925	1428.974
89	CYCLOHEXANE	84.16	3.18	0.000	1.85	3045.269
90	n-C5	72.15	2.8	0.000	3.52	5921.563
91	4-ETHYLTOLUENE	120.2	3.58	0.000	0.821	1428.974
92	C4-Benzothiophene	190.3	5.18	0.384	0.01	17.865
93	p-XYLENE	106.2	3.09	0.000	2.03	3629.815
94	2-methylhexane	100.2	3.71	0.000	0.596	1156.932
95	Isopropylbenzene	120.194	3.45	0.000	0.926	1890.962
96	2/3-Methyldibenzothiophene	198.28	4.71	7.315	0.01	21.189
97	3-Methylpentane	86.18	3.21	0.000	1.34	2923.119
98	3-ethylhexane	114.2	4.2	0.000	0.178	458.634
99	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.463	1282.994
100	3-methylhexane	100.2	3.71	0.000	0.416	1156.932
101	2,2-dimethylpentane	100.2	3.67	0.000	0.453	1261.095
102	2,3-dimethylpentane	100.2	3.63	0.000	0.462	1374.636
103	Methylcyclopentane	84.16	3.1	0.000	1.05	3618.310
104	2-METHYLPENTANE	86.18	3.21	0.000	0.81	2923.119
105	o-XYLENE	106.2	3.09	0.000	0.964	3629.815
106	m-XYLENE	106.2	3.09	0.000	0.947	3629.815
107	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.11	437.797
108	Cyclopentane	70.13	2.68	0.000	1.62	7454.591
109	C3-Benzothiophene	176.3	4.69	0.384	0.01	47.585
110	Toluene	92.14	2.54	0.000	1.96	########

111	Benzene	78.11	1.99	0.000	3.13	########
112	Isopentane	72.15	2.72	0.000	0.497	7035.846
113	C1-Decalins	152.3	4.61	0.000	0.00647	112.393
114	2,3-dimethylbutane	86.18	3.14	0.000	0.101	3399.120
115	trans-Decalin	138.26	4.2	0.000	0.00647	246.886
116	Naphthalene	234.3	3.17	10.738	0.01	603.859
117	cis-Decalin	138.26	4.2	0.000	0.00356	246.886
118	Benzothiophene	134.2	2.99	0.384	0.01	1413.082
119	n-C11	156.31	5.74	0.000	0	22.717
120	n-C11	156.31	5.74	0.000	0	22.717
121	n-C11	156.31	5.74	0.000	0	22.717
122	n-C11	156.31	5.74	0.000	0	22.717
123	n-C12	170.34	6.23	0.000	0	8.611
124	n-C12	170.34	6.23	0.000	0	8.611
125	n-C12	170.34	6.23	0.000	0	8.611
126	n-C12	170.34	6.23	0.000	0	8.611
127	n-C11	156.31	5.74	0.000	0	22.717
128	n-C11	156.31	5.74	0.000	0	22.717
129	n-C11	156.31	5.74	0.000	0	22.717
130	n-C11	156.31	5.74	0.000	0	22.717
131	n-C12	170.34	6.23	0.000	0	8.611
132	n-C12	170.34	6.23	0.000	0	8.611
133	n-C12	170.34	6.23	0.000	0	8.611
134	n-C12	170.34	6.23	0.000	0	8.611
135	n-C13	184.37	6.73	0.000	0	3.173
136	n-C14	198.4	7.22	0.000	0	1.187
137	n-C15	212.42	7.71	0.000	0	0.442
138	n-C16	226.45	8.2	0.000	0	0.164
139	n-C17	240.48	8.69	0.000	0	0.061

140	n-C18	254.5	9.18	0.000	0	0.022
141	n-C19	268.53	9.67	0.000	0	0.008
142	n-C20	282.56	10.1	0.000	0	0.003
143	n-C21	296.59	10.6	0.000	0	0.001
144	n-C22	310.61	11.1	0.000	0	0.000
145	n-C23	324.64	11.6	0.000	0	0.000
146	n-C24	338.67	12.1	0.000	0	0.000
147	n-C25	352.69	12.6	0.000	0	0.000
148	n-C26	366.72	13.1	0.000	0	0.000
149	n-C27	380.75	13.6	0.000	0	0.000
150	n-C28	394.77	14	0.000	0	0.000
151	n-C29	408.8	14.5	0.000	0	0.000
152	n-C30	422.83	15	0.000	0	0.000
153	n-C31	436.86	15.5	0.000	0	0.000
154	n-C32	450.88	16	0.000	0	0.000
155	n-C33	464.91	16.5	0.000	0	0.000
156	n-C34	478.94	17	0.000	0	0.000
157	n-C35	492.96	17.5	0.000	0	0.000
158	n-C36	506.981	18	0.000	0	0.000
159	n-C37	521	18.5	0.000	0	0.000
160	n-C38	535	19	0.000	0	0.000
161	n-C39	549.1	19.49	0.000	0	0.000
162	n-C40	563.1	19.9	0.000	0	0.000
163	Phytane	282.56	9.87	0.000	0	0.006
164	Pristane	268.525	9.38	0.000	0	0.015
165	Benzo(a)fluoranthene	252.3	6.11	3030.873	0	0.121
166	Benzo(b)fluorene	216.3	5.77	593.982	0	0.426
167	Benzo(k)fluoranthene	252.3	6.11	2756.635	0	0.126
168	Benzo[a]anthracene	228.3	5.52	791.538	0	0.685

169	Benzo[a]pyrene	252.3	6.11	3969.164	0	0.108
170	Benzo[b]fluoranthene	252.3	6.11	1681.435	0	0.155
171	Benzo[e]pyrene	252.3	6.11	1161.480	0	0.181
172	Benzo[g,h,i]perylene	276.3	6.7	3235.538	0	0.036
173	C1-Chrysenes	242.3	6.0683	562.984	0	0.257
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1961.818	0	0.485
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0	4.039
176	C2-Chrysenes	256.3	6.65	562.984	0	0.078
177	C2-Decalins	166.3	6.19	0.000	0	4.074
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1961.818	0	0.127
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0	1.517
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1094.052	0	0.603
181	C3-Chrysenes	270.4	7.03	562.984	0	0.036
182	C3-Decalins	180.3	6.79	0.000	0	1.212
183	C3-Dibenzothiophenes	230.37	5.86	7.682	0	2.030
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1961.818	0	0.052
185	C3-Fluorenes	210.3	5.58	86.335	0	1.363
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0	0.544
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1094.052	0	0.278
188	C4-Chrysenes	284.4	7.35	562.984	0	0.019
189	C4-Decalins	194.3	7.34	0.000	0	0.399
190	C4-Dibenzothiophenes	244.37	6.1	7.682	0	1.283
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1961.818	0	0.020
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0	0.203
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1094.052	0	0.155
194	Chrysene	228.3	5.52	452.808	0	0.862
195	Dibenz(a,h)anthracene	278.4	6.7	1957.920	0	0.045
196	Indeno[1,2,3-cd]pyrene	276.3	6.7	4665.545	0	0.031
197	Naphthobenzothiophenes	178.2	5.34	0.000	0	27.269

198	Perylene	252.3	6.11	4968.758	0	0.099
199	Retene	234.3	6.35	84.725	0	0.291

Table B.19. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 100% WAF exposed to *Americamysis bahia* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	83.764	0.279	2.131
2	C1-Phenanthrenes/Anthracenes	192.3	4.26	921.897	0.621	6.164
3	C1-Fluorenes	180.2	4.97	83.764	0.192	3.315
4	1-Methylphenanthrene	192.26	4.89	71.473	0.214	4.473
5	4/9-Methylphenanthrene	192.26	4.89	71.473	0.180	4.473
6	2-Methylphenanthrene	192.26	4.89	71.473	0.148	4.473
7	3-Methylphenanthrene	192.26	4.89	71.473	0.142	4.473
8	C2-Dibenzothiophenes	214.3	5.13	6.161	0.152	7.403
9	C4-Naphthalenes	184.3	5.18	20.144	0.074	3.733
10	C3-Naphthalenes	170.26	4.77	20.144	0.165	8.344
11	Phenanthrene	178.2	4.35	41.949	0.304	16.342
12	C1-Dibenzothiophenes	198.3	4.71	6.161	0.180	16.936
13	1,6,7-Trimethylnaphthalene	170.26	4.81	35.520	0.054	6.176
14	Pyrene	202.3	4.93	1051.969	0.012	1.449
15	4-Methyldibenzothiophene	198.28	4.71	6.161	0.089	16.935
16	C2-Naphthalenes	156.2	4.31	20.144	0.095	20.630
17	2/3-Methyldibenzothiophene	198.28	4.71	6.161	0.054	16.934
18	Fluoranthene	202.3	4.93	785.130	0.005	1.635
19	Fluorene	166.2	4.02	83.764	0.063	23.687
20	1-Methyldibenzothiophene	198.28	4.71	6.161	0.028	16.935
21	2,6-Dimethylnaphthalene	156.23	4.26	20.144	0.032	22.981

22	Dibenzothiophene	184.3	4.17	6.161	0.068	50.404
23	C4-Benzothiophene	190.3	5.18	0.292	0.010	14.345
24	C3-Benzothiophene	176.3	4.69	0.292	0.013	38.209
25	2-Methylanthracene	192.26	4.89	921.897	0.000	1.585
26	C1-Naphthalenes	142.2	3.87	20.518	0.013	48.147
27	1-Methylnaphthalene	142.2	3.72	20.518	0.010	66.523
28	2-Methylnaphthalene	142.2	3.72	20.518	0.010	66.523
29	C2-Benzothiophene	162.25	4.13	0.292	0.014	117.558
30	Dibenzofuran	168.2	3.71	44.694	0.007	59.789
31	Acenaphthene	154.2	4.15	58.345	0.002	19.144
32	C1-Benzothiophene	148.2	3.5365	0.292	0.016	385.863
33	Naphthalene	234.3	3.17	11.329	0.009	446.010
34	CARBAZOLE	167.2	3.23	152.038	0.002	103.111
35	Biphenyl	154.2	3.76	0.000	0.007	535.193
36	Ethylbenzene	106.2	3.03	0.000	0.021	3110.501
37	trans-Decalin	138.26	4.2	0.000	0.000	185.901
38	1-Decene	140.3	5.12	0.000	0.000	58.415
39	n-C10	142.29	5.25	0.000	0.000	44.767
40	n-C10	142.29	5.25	0.000	0.000	44.767
41	n-C10	142.3	5.25	0.000	0.000	44.770
42	n-C10	142.3	5.25	0.000	0.000	44.770
43	1-Nonene	126.2	4.62	0.000	0.000	154.357
44	n-C9	128.3	4.76	0.000	0.000	116.052
45	n-C9	128.3	4.76	0.000	0.000	116.052
46	n-C9	128.3	4.76	0.000	0.000	116.052
47	n-C9	128.3	4.76	0.000	0.000	116.052
48	n-C8	114.2	4.27	0.000	0.000	296.983
49	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	437.736
50	Octene-1	112.2	4.13	0.000	0.000	394.547

51	n-Pentylbenzene	148.2	4.5	0.000	0.000	234.765
52	3-methylheptane	114.2	4.2	0.000	0.000	345.344
53	n-C10	142.29	5.25	0.000	0.000	44.767
54	n-C10	142.29	5.25	0.000	0.000	44.767
55	n-C10	142.3	5.25	0.000	0.000	44.770
56	n-C10	142.3	5.25	0.000	0.000	44.770
57	2-methylheptane	114.2	4.2	0.000	0.000	345.344
58	HEPTANE	100.2	3.78	0.000	0.000	749.158
59	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	477.147
60	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	410.437
61	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	437.851
62	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	417.910
63	Anthracene	178.2	4.35	578.353	0.000	5.705
64	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	367.163
65	n-C9	128.3	4.76	0.000	0.000	116.052
66	n-C9	128.3	4.76	0.000	0.000	116.052
67	n-C9	128.3	4.76	0.000	0.000	116.052
68	n-C9	128.3	4.76	0.000	0.000	116.052
69	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	410.437
70	2,3-dimethylhexane	114.2	4.12	0.000	0.000	410.329
71	Methylcyclohexane	98.19	3.59	0.000	0.000	1105.638
72	n-C6	86.18	3.29	0.000	0.000	1852.475
73	n-Butylbenzene	134.2	4.01	0.000	0.000	475.531
74	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
75	Toluene	92.14	2.54	0.000	0.000	7758.791
76	tert-Butylbenzene	134.2	3.9	0.000	0.000	602.752
77	2-methylhexane	100.2	3.71	0.000	0.000	871.151
78	Acenaphthylene	152.2	3.94	312.199	0.000	15.182
79	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	367.217

80	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	417.848
81	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	367.163
82	3-ethylhexane	114.2	4.2	0.000	0.000	345.344
83	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	417.848
84	3-methylhexane	100.2	3.71	0.000	0.000	871.151
85	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
86	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
87	Hydrindene	118.2	3.47	0.000	0.000	1341.169
88	n-C5	72.15	2.8	0.000	0.000	4458.843
89	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2201.062
90	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	417.848
91	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	367.217
92	Propylbenzene	120.194	3.52	0.000	0.000	1224.471
93	4-isopropyltoluene	134.22	4	0.000	0.000	485.963
94	sec-Butylbenzene	134.2	3.94	0.000	0.000	552.966
95	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
96	3-Methylpentane	86.18	3.21	0.000	0.000	2201.062
97	2,2-dimethylpentane	100.2	3.67	0.000	0.000	949.584
98	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	966.074
99	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	485.963
100	m-cymene	134.2	4	0.000	0.000	485.890
101	CYCLOHEXANE	84.16	3.18	0.000	0.000	2293.040
102	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
103	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
104	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1075.995
105	Isopropylbenzene	120.194	3.45	0.000	0.000	1423.864
106	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	329.654
107	Isopentane	72.15	2.72	0.000	0.000	5297.881
108	Methylcyclopentane	84.16	3.1	0.000	0.000	2724.530

109	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2559.484
110	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	966.074
111	Cyclopentane	70.13	2.68	0.000	0.000	5613.190
112	C1-Decalins	152.3	4.61	0.000	0.000	84.630
113	m-XYLENE	106.2	3.09	0.000	0.000	2733.194
114	cis-Decalin	138.26	4.2	0.000	0.000	185.901
115	o-XYLENE	106.2	3.09	0.000	0.000	2733.194
116	p-XYLENE	106.2	3.09	0.000	0.000	2733.194
117	Benzothiophene	134.2	2.99	0.292	0.000	1134.649
118	Benzene	78.11	1.99	0.000	0.000	21520.507
119	n-C11	156.31	5.74	0.000	0.000	17.105
120	n-C11	156.31	5.74	0.000	0.000	17.105
121	n-C11	156.31	5.74	0.000	0.000	17.105
122	n-C11	156.31	5.74	0.000	0.000	17.105
123	n-C12	170.34	6.23	0.000	0.000	6.484
124	n-C12	170.34	6.23	0.000	0.000	6.484
125	n-C12	170.34	6.23	0.000	0.000	6.484
126	n-C12	170.34	6.23	0.000	0.000	6.484
127	n-C11	156.31	5.74	0.000	0.000	17.105
128	n-C11	156.31	5.74	0.000	0.000	17.105
129	n-C11	156.31	5.74	0.000	0.000	17.105
130	n-C11	156.31	5.74	0.000	0.000	17.105
131	n-C12	170.34	6.23	0.000	0.000	6.484
132	n-C12	170.34	6.23	0.000	0.000	6.484
133	n-C12	170.34	6.23	0.000	0.000	6.484
134	n-C12	170.34	6.23	0.000	0.000	6.484
135	n-C13	184.37	6.73	0.000	0.000	2.389
136	n-C14	198.4	7.22	0.000	0.000	0.894
137	n-C15	212.42	7.71	0.000	0.000	0.333

138	n-C16	226.45	8.2	0.000	0.000	0.123
139	n-C17	240.48	8.69	0.000	0.000	0.046
140	n-C18	254.5	9.18	0.000	0.000	0.017
141	n-C19	268.53	9.67	0.000	0.000	0.006
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.004
164	Pristane	268.525	9.38	0.000	0.000	0.012
165	Benzo(a)fluoranthene	252.3	6.11	4637.391	0.000	0.076
166	Benzo(b)fluorene	216.3	5.77	405.248	0.000	0.376

167	Benzo(k)fluoranthene	252.3	6.11	2564.185	0.000	0.098
168	Benzo[a]anthracene	228.3	5.52	693.329	0.000	0.545
169	Benzo[a]pyrene	252.3	6.11	3571.194	0.000	0.085
170	Benzo[b]fluoranthene	252.3	6.11	1519.621	0.000	0.122
171	Benzo[e]pyrene	252.3	6.11	843.132	0.000	0.156
172	Benzo[g,h,i]perylene	276.3	6.7	2820.850	0.000	0.029
173	C1-Chrysenes	242.3	6.0683	396.598	0.000	0.223
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1565.526	0.000	0.401
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.041
176	C2-Chrysenes	256.3	6.65	396.598	0.000	0.067
177	C2-Decalins	166.3	6.19	0.000	0.000	3.068
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1565.526	0.000	0.105
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.142
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	921.897	0.000	0.487
181	C3-Chrysenes	270.4	7.03	396.598	0.000	0.031
182	C3-Decalins	180.3	6.79	0.000	0.000	0.913
183	C3-Dibenzothiophenes	230.37	5.86	6.161	0.000	1.650
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1565.526	0.000	0.043
185	C3-Fluorenes	210.3	5.58	83.764	0.000	1.039
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.410
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	921.897	0.000	0.225
188	C4-Chrysenes	284.4	7.35	396.598	0.000	0.017
189	C4-Decalins	194.3	7.34	0.000	0.000	0.301
190	C4-Dibenzothiophenes	244.37	6.1	6.161	0.000	1.044
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1565.526	0.000	0.016
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.153
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	921.897	0.000	0.125
194	Chrysene	228.3	5.52	319.110	0.000	0.749
195	Dibenz(a,h)anthracene	278.4	6.7	1783.769	0.000	0.035

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	4902.896	0.000	0.023
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	20.533
198	Perylene	252.3	6.11	8435.739	0.000	0.059
199	Retene	234.3	6.35	102.485	0.000	0.203

Table B.20. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 25% WAF exposed to *Americamysis bahia* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	83.764	0.076	2.131
2	C1-Phenanthrenes/Anthracenes	192.3	4.26	921.897	0.157	6.164
3	C1-Fluorenes	180.2	4.97	83.764	0.045	3.315
4	1-Methylphenanthrene	192.26	4.89	71.473	0.050	4.473
5	4/9-Methylphenanthrene	192.26	4.89	71.473	0.044	4.473
6	3-Methylphenanthrene	192.26	4.89	71.473	0.039	4.473
7	2-Methylphenanthrene	192.26	4.89	71.473	0.035	4.473
8	C3-Naphthalenes	170.26	4.77	20.144	0.046	8.344
9	C4-Naphthalenes	184.3	5.18	20.144	0.019	3.733
10	C2-Dibenzothiophenes	214.3	5.13	6.161	0.036	7.403
11	Phenanthrene	178.2	4.35	41.949	0.076	16.342
12	C1-Dibenzothiophenes	198.3	4.71	6.161	0.040	16.936
13	1,6,7-Trimethylnaphthalene	170.26	4.81	35.520	0.013	6.176
14	Pyrene	202.3	4.93	1051.969	0.003	1.449
15	C2-Naphthalenes	156.2	4.31	20.144	0.025	20.630
16	4-Methyldibenzothiophene	198.28	4.71	6.161	0.020	16.935
17	Fluoranthene	202.3	4.93	785.130	0.001	1.635
18	Fluorene	166.2	4.02	83.764	0.017	23.687
19	2/3-Methyldibenzothiophene	198.28	4.71	6.161	0.012	16.934
20	1-Methyldibenzothiophene	198.28	4.71	6.161	0.007	16.935
21	2,6-Dimethylnaphthalene	156.23	4.26	20.144	0.008	22.981

22	Dibenzothiophene	184.3	4.17	6.161	0.016	50.404
23	C3-Benzothiophene	176.3	4.69	0.292	0.011	38.209
24	C1-Naphthalenes	142.2	3.87	20.518	0.005	48.147
25	Acenaphthene	154.2	4.15	58.345	0.001	19.144
26	C2-Benzothiophene	162.25	4.13	0.292	0.005	117.558
27	Dibenzofuran	168.2	3.71	44.694	0.002	59.789
28	Naphthalene	234.3	3.17	11.329	0.008	446.010
29	C1-Benzothiophene	148.2	3.5365	0.292	0.007	385.863
30	CARBAZOLE	167.2	3.23	152.038	0.001	103.111
31	Ethylbenzene	106.2	3.03	0.000	0.018	3110.501
32	Benzothiophene	134.2	2.99	0.292	0.000	1134.649
33	1-Decene	140.3	5.12	0.000	0.000	58.415
34	n-C10	142.29	5.25	0.000	0.000	44.767
35	n-C10	142.29	5.25	0.000	0.000	44.767
36	n-C10	142.3	5.25	0.000	0.000	44.770
37	n-C10	142.3	5.25	0.000	0.000	44.770
38	1-Nonene	126.2	4.62	0.000	0.000	154.357
39	n-C9	128.3	4.76	0.000	0.000	116.052
40	n-C9	128.3	4.76	0.000	0.000	116.052
41	n-C9	128.3	4.76	0.000	0.000	116.052
42	n-C9	128.3	4.76	0.000	0.000	116.052
43	n-C8	114.2	4.27	0.000	0.000	296.983
44	2-Methylanthracene	192.26	4.89	921.897	0.000	1.585
45	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	437.736
46	Octene-1	112.2	4.13	0.000	0.000	394.547
47	n-Pentylbenzene	148.2	4.5	0.000	0.000	234.765
48	3-methylheptane	114.2	4.2	0.000	0.000	345.344
49	n-C10	142.29	5.25	0.000	0.000	44.767
50	n-C10	142.29	5.25	0.000	0.000	44.767

51	n-C10	142.3	5.25	0.000	0.000	44.770
52	n-C10	142.3	5.25	0.000	0.000	44.770
53	2-methylheptane	114.2	4.2	0.000	0.000	345.344
54	HEPTANE	100.2	3.78	0.000	0.000	749.158
55	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	477.147
56	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	410.437
57	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	437.851
58	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	417.910
59	Anthracene	178.2	4.35	578.353	0.000	5.705
60	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	367.163
61	n-C9	128.3	4.76	0.000	0.000	116.052
62	n-C9	128.3	4.76	0.000	0.000	116.052
63	n-C9	128.3	4.76	0.000	0.000	116.052
64	n-C9	128.3	4.76	0.000	0.000	116.052
65	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	410.437
66	2,3-dimethylhexane	114.2	4.12	0.000	0.000	410.329
67	Methylcyclohexane	98.19	3.59	0.000	0.000	1105.638
68	n-C6	86.18	3.29	0.000	0.000	1852.475
69	n-Butylbenzene	134.2	4.01	0.000	0.000	475.531
70	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
71	C4-Benzothiophene	190.3	5.18	0.292	0.000	14.345
72	tert-Butylbenzene	134.2	3.9	0.000	0.000	602.752
73	2-methylhexane	100.2	3.71	0.000	0.000	871.151
74	Acenaphthylene	152.2	3.94	312.199	0.000	15.182
75	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	367.217
76	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	417.848
77	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	367.163
78	3-ethylhexane	114.2	4.2	0.000	0.000	345.344
79	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	417.848

80	3-methylhexane	100.2	3.71	0.000	0.000	871.151
81	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
82	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
83	Hydrindene	118.2	3.47	0.000	0.000	1341.169
84	n-C5	72.15	2.8	0.000	0.000	4458.843
85	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2201.062
86	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	417.848
87	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	367.217
88	Propylbenzene	120.194	3.52	0.000	0.000	1224.471
89	1-Methylnaphthalene	142.2	3.72	20.518	0.000	66.523
90	4-isopropyltoluene	134.22	4	0.000	0.000	485.963
91	sec-Butylbenzene	134.2	3.94	0.000	0.000	552.966
92	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
93	3-Methylpentane	86.18	3.21	0.000	0.000	2201.062
94	2,2-dimethylpentane	100.2	3.67	0.000	0.000	949.584
95	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	966.074
96	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	485.963
97	2-Methylnaphthalene	142.2	3.72	20.518	0.000	66.523
98	m-cymene	134.2	4	0.000	0.000	485.890
99	CYCLOHEXANE	84.16	3.18	0.000	0.000	2293.040
100	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
101	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
102	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1075.995
103	Isopropylbenzene	120.194	3.45	0.000	0.000	1423.864
104	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	329.654
105	Toluene	92.14	2.54	0.000	0.000	7758.791
106	Isopentane	72.15	2.72	0.000	0.000	5297.881
107	Methylcyclopentane	84.16	3.1	0.000	0.000	2724.530
108	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2559.484

109	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	966.074
110	o-XYLENE	106.2	3.09	0.000	0.000	2733.194
111	Cyclopentane	70.13	2.68	0.000	0.000	5613.190
112	C1-Decalins	152.3	4.61	0.000	0.000	84.630
113	trans-Decalin	138.26	4.2	0.000	0.000	185.901
114	p-XYLENE	106.2	3.09	0.000	0.000	2733.194
115	cis-Decalin	138.26	4.2	0.000	0.000	185.901
116	m-XYLENE	106.2	3.09	0.000	0.000	2733.194
117	Biphenyl	154.2	3.76	0.000	0.000	535.193
118	Benzene	78.11	1.99	0.000	0.000	21520.507
119	n-C11	156.31	5.74	0.000	0.000	17.105
120	n-C11	156.31	5.74	0.000	0.000	17.105
121	n-C11	156.31	5.74	0.000	0.000	17.105
122	n-C11	156.31	5.74	0.000	0.000	17.105
123	n-C12	170.34	6.23	0.000	0.000	6.484
124	n-C12	170.34	6.23	0.000	0.000	6.484
125	n-C12	170.34	6.23	0.000	0.000	6.484
126	n-C12	170.34	6.23	0.000	0.000	6.484
127	n-C11	156.31	5.74	0.000	0.000	17.105
128	n-C11	156.31	5.74	0.000	0.000	17.105
129	n-C11	156.31	5.74	0.000	0.000	17.105
130	n-C11	156.31	5.74	0.000	0.000	17.105
131	n-C12	170.34	6.23	0.000	0.000	6.484
132	n-C12	170.34	6.23	0.000	0.000	6.484
133	n-C12	170.34	6.23	0.000	0.000	6.484
134	n-C12	170.34	6.23	0.000	0.000	6.484
135	n-C13	184.37	6.73	0.000	0.000	2.389
136	n-C14	198.4	7.22	0.000	0.000	0.894
137	n-C15	212.42	7.71	0.000	0.000	0.333

138	n-C16	226.45	8.2	0.000	0.000	0.123
139	n-C17	240.48	8.69	0.000	0.000	0.046
140	n-C18	254.5	9.18	0.000	0.000	0.017
141	n-C19	268.53	9.67	0.000	0.000	0.006
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.004
164	Pristane	268.525	9.38	0.000	0.000	0.012
165	Benzo(a)fluoranthene	252.3	6.11	4637.391	0.000	0.076
166	Benzo(b)fluorene	216.3	5.77	405.248	0.000	0.376

167	Benzo(k)fluoranthene	252.3	6.11	2564.185	0.000	0.098
168	Benzo[a]anthracene	228.3	5.52	693.329	0.000	0.545
169	Benzo[a]pyrene	252.3	6.11	3571.194	0.000	0.085
170	Benzo[b]fluoranthene	252.3	6.11	1519.621	0.000	0.122
171	Benzo[e]pyrene	252.3	6.11	843.132	0.000	0.156
172	Benzo[g,h,i]perylene	276.3	6.7	2820.850	0.000	0.029
173	C1-Chrysenes	242.3	6.0683	396.598	0.000	0.223
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1565.526	0.000	0.401
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.041
176	C2-Chrysenes	256.3	6.65	396.598	0.000	0.067
177	C2-Decalins	166.3	6.19	0.000	0.000	3.068
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1565.526	0.000	0.105
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.142
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	921.897	0.000	0.487
181	C3-Chrysenes	270.4	7.03	396.598	0.000	0.031
182	C3-Decalins	180.3	6.79	0.000	0.000	0.913
183	C3-Dibenzothiophenes	230.37	5.86	6.161	0.000	1.650
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1565.526	0.000	0.043
185	C3-Fluorenes	210.3	5.58	83.764	0.000	1.039
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.410
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	921.897	0.000	0.225
188	C4-Chrysenes	284.4	7.35	396.598	0.000	0.017
189	C4-Decalins	194.3	7.34	0.000	0.000	0.301
190	C4-Dibenzothiophenes	244.37	6.1	6.161	0.000	1.044
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1565.526	0.000	0.016
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.153
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	921.897	0.000	0.125
194	Chrysene	228.3	5.52	319.110	0.000	0.749
195	Dibenz(a,h)anthracene	278.4	6.7	1783.769	0.000	0.035

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	4902.896	0.000	0.023
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	20.533
198	Perylene	252.3	6.11	8435.739	0.000	0.059
199	Retene	234.3	6.35	102.485	0.000	0.203

Table B.21. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 6.25% WAF exposed to *Americamysis bahia* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	83.764	0.032	2.131
2	C1-Phenanthrenes/Anthracenes	192.3	4.26	921.897	0.047	6.164
3	C1-Fluorenes	180.2	4.97	83.764	0.012	3.315
4	3-Methylphenanthrene	192.26	4.89	71.473	0.015	4.473
5	C4-Naphthalenes	184.3	5.18	20.144	0.011	3.733
6	1-Methylphenanthrene	192.26	4.89	71.473	0.013	4.473
7	4/9-Methylphenanthrene	192.26	4.89	71.473	0.012	4.473
8	C3-Naphthalenes	170.26	4.77	20.144	0.021	8.344
9	2-Methylphenanthrene	192.26	4.89	71.473	0.010	4.473
10	C2-Dibenzothiophenes	214.3	5.13	6.161	0.010	7.403
11	Phenanthrene	178.2	4.35	41.949	0.021	16.342
12	Pyrene	202.3	4.93	1051.969	0.001	1.449
13	C1-Dibenzothiophenes	198.3	4.71	6.161	0.011	16.936
14	C2-Naphthalenes	156.2	4.31	20.144	0.012	20.630
15	1,6,7-Trimethylnaphthalene	170.26	4.81	35.520	0.003	6.176
16	Fluoranthene	202.3	4.93	785.130	0.001	1.635
17	4-Methyldibenzothiophene	198.28	4.71	6.161	0.005	16.935
18	Fluorene	166.2	4.02	83.764	0.006	23.687
19	C3-Benzothiophene	176.3	4.69	0.292	0.008	38.209
20	2/3-Methyldibenzothiophene	198.28	4.71	6.161	0.003	16.934
21	2,6-Dimethylnaphthalene	156.23	4.26	20.144	0.003	22.981

22	1-Methyldibenzothiophene	198.28	4.71	6.161	0.002	16.935
23	Dibenzothiophene	184.3	4.17	6.161	0.004	50.404
24	Acenaphthene	154.2	4.15	58.345	0.001	19.144
25	C2-Benzothiophene	162.25	4.13	0.292	0.004	117.558
26	Dibenzofuran	168.2	3.71	44.694	0.002	59.789
27	Naphthalene	234.3	3.17	11.329	0.008	446.010
28	C1-Benzothiophene	148.2	3.5365	0.292	0.006	385.863
29	Ethylbenzene	106.2	3.03	0.000	0.021	3110.501
30	CARBAZOLE	167.2	3.23	152.038	0.001	103.111
31	1-Decene	140.3	5.12	0.000	0.000	58.415
32	n-C10	142.29	5.25	0.000	0.000	44.767
33	n-C10	142.29	5.25	0.000	0.000	44.767
34	n-C10	142.3	5.25	0.000	0.000	44.770
35	n-C10	142.3	5.25	0.000	0.000	44.770
36	1-Nonene	126.2	4.62	0.000	0.000	154.357
37	n-C9	128.3	4.76	0.000	0.000	116.052
38	n-C9	128.3	4.76	0.000	0.000	116.052
39	n-C9	128.3	4.76	0.000	0.000	116.052
40	n-C9	128.3	4.76	0.000	0.000	116.052
41	n-C8	114.2	4.27	0.000	0.000	296.983
42	2-Methylanthracene	192.26	4.89	921.897	0.000	1.585
43	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	437.736
44	Octene-1	112.2	4.13	0.000	0.000	394.547
45	n-Pentylbenzene	148.2	4.5	0.000	0.000	234.765
46	3-methylheptane	114.2	4.2	0.000	0.000	345.344
47	n-C10	142.29	5.25	0.000	0.000	44.767
48	n-C10	142.29	5.25	0.000	0.000	44.767
49	n-C10	142.3	5.25	0.000	0.000	44.770
50	n-C10	142.3	5.25	0.000	0.000	44.770

51	2-methylheptane	114.2	4.2	0.000	0.000	345.344
52	HEPTANE	100.2	3.78	0.000	0.000	749.158
53	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	477.147
54	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	410.437
55	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	437.851
56	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	417.910
57	Anthracene	178.2	4.35	578.353	0.000	5.705
58	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	367.163
59	n-C9	128.3	4.76	0.000	0.000	116.052
60	n-C9	128.3	4.76	0.000	0.000	116.052
61	n-C9	128.3	4.76	0.000	0.000	116.052
62	n-C9	128.3	4.76	0.000	0.000	116.052
63	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	410.437
64	2,3-dimethylhexane	114.2	4.12	0.000	0.000	410.329
65	Methylcyclohexane	98.19	3.59	0.000	0.000	1105.638
66	n-C6	86.18	3.29	0.000	0.000	1852.475
67	n-Butylbenzene	134.2	4.01	0.000	0.000	475.531
68	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
69	C4-Benzothiophene	190.3	5.18	0.292	0.000	14.345
70	tert-Butylbenzene	134.2	3.9	0.000	0.000	602.752
71	2-methylhexane	100.2	3.71	0.000	0.000	871.151
72	Acenaphthylene	152.2	3.94	312.199	0.000	15.182
73	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	367.217
74	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	417.848
75	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	367.163
76	3-ethylhexane	114.2	4.2	0.000	0.000	345.344
77	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	417.848
78	3-methylhexane	100.2	3.71	0.000	0.000	871.151
79	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	367.163

80	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
81	Hydrindene	118.2	3.47	0.000	0.000	1341.169
82	n-C5	72.15	2.8	0.000	0.000	4458.843
83	C1-Naphthalenes	142.2	3.87	20.518	0.000	48.147
84	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2201.062
85	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	417.848
86	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	367.217
87	Propylbenzene	120.194	3.52	0.000	0.000	1224.471
88	4-isopropyltoluene	134.22	4	0.000	0.000	485.963
89	sec-Butylbenzene	134.2	3.94	0.000	0.000	552.966
90	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
91	3-Methylpentane	86.18	3.21	0.000	0.000	2201.062
92	2,2-dimethylpentane	100.2	3.67	0.000	0.000	949.584
93	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	966.074
94	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	485.963
95	1-Methylnaphthalene	142.2	3.72	20.518	0.000	66.523
96	m-cymene	134.2	4	0.000	0.000	485.890
97	CYCLOHEXANE	84.16	3.18	0.000	0.000	2293.040
98	2-Methylnaphthalene	142.2	3.72	20.518	0.000	66.523
99	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
100	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
101	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1075.995
102	Isopropylbenzene	120.194	3.45	0.000	0.000	1423.864
103	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	329.654
104	Isopentane	72.15	2.72	0.000	0.000	5297.881
105	Methylcyclopentane	84.16	3.1	0.000	0.000	2724.530
106	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2559.484
107	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	966.074
108	o-XYLENE	106.2	3.09	0.000	0.000	2733.194

109	Cyclopentane	70.13	2.68	0.000	0.000	5613.190
110	C1-Decalins	152.3	4.61	0.000	0.000	84.630
111	Toluene	92.14	2.54	0.000	0.000	7758.791
112	trans-Decalin	138.26	4.2	0.000	0.000	185.901
113	m-XYLENE	106.2	3.09	0.000	0.000	2733.194
114	cis-Decalin	138.26	4.2	0.000	0.000	185.901
115	Biphenyl	154.2	3.76	0.000	0.000	535.193
116	p-XYLENE	106.2	3.09	0.000	0.000	2733.194
117	Benzothiophene	134.2	2.99	0.292	0.000	1134.649
118	Benzene	78.11	1.99	0.000	0.000	21520.507
119	n-C11	156.31	5.74	0.000	0.000	17.105
120	n-C11	156.31	5.74	0.000	0.000	17.105
121	n-C11	156.31	5.74	0.000	0.000	17.105
122	n-C11	156.31	5.74	0.000	0.000	17.105
123	n-C12	170.34	6.23	0.000	0.000	6.484
124	n-C12	170.34	6.23	0.000	0.000	6.484
125	n-C12	170.34	6.23	0.000	0.000	6.484
126	n-C12	170.34	6.23	0.000	0.000	6.484
127	n-C11	156.31	5.74	0.000	0.000	17.105
128	n-C11	156.31	5.74	0.000	0.000	17.105
129	n-C11	156.31	5.74	0.000	0.000	17.105
130	n-C11	156.31	5.74	0.000	0.000	17.105
131	n-C12	170.34	6.23	0.000	0.000	6.484
132	n-C12	170.34	6.23	0.000	0.000	6.484
133	n-C12	170.34	6.23	0.000	0.000	6.484
134	n-C12	170.34	6.23	0.000	0.000	6.484
135	n-C13	184.37	6.73	0.000	0.000	2.389
136	n-C14	198.4	7.22	0.000	0.000	0.894
137	n-C15	212.42	7.71	0.000	0.000	0.333

138	n-C16	226.45	8.2	0.000	0.000	0.123
139	n-C17	240.48	8.69	0.000	0.000	0.046
140	n-C18	254.5	9.18	0.000	0.000	0.017
141	n-C19	268.53	9.67	0.000	0.000	0.006
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.004
164	Pristane	268.525	9.38	0.000	0.000	0.012
165	Benzo(a)fluoranthene	252.3	6.11	4637.391	0.000	0.076
166	Benzo(b)fluorene	216.3	5.77	405.248	0.000	0.376

167	Benzo(k)fluoranthene	252.3	6.11	2564.185	0.000	0.098
168	Benzo[a]anthracene	228.3	5.52	693.329	0.000	0.545
169	Benzo[a]pyrene	252.3	6.11	3571.194	0.000	0.085
170	Benzo[b]fluoranthene	252.3	6.11	1519.621	0.000	0.122
171	Benzo[e]pyrene	252.3	6.11	843.132	0.000	0.156
172	Benzo[g,h,i]perylene	276.3	6.7	2820.850	0.000	0.029
173	C1-Chrysenes	242.3	6.0683	396.598	0.000	0.223
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1565.526	0.000	0.401
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.041
176	C2-Chrysenes	256.3	6.65	396.598	0.000	0.067
177	C2-Decalins	166.3	6.19	0.000	0.000	3.068
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1565.526	0.000	0.105
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.142
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	921.897	0.000	0.487
181	C3-Chrysenes	270.4	7.03	396.598	0.000	0.031
182	C3-Decalins	180.3	6.79	0.000	0.000	0.913
183	C3-Dibenzothiophenes	230.37	5.86	6.161	0.000	1.650
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1565.526	0.000	0.043
185	C3-Fluorenes	210.3	5.58	83.764	0.000	1.039
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.410
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	921.897	0.000	0.225
188	C4-Chrysenes	284.4	7.35	396.598	0.000	0.017
189	C4-Decalins	194.3	7.34	0.000	0.000	0.301
190	C4-Dibenzothiophenes	244.37	6.1	6.161	0.000	1.044
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1565.526	0.000	0.016
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.153
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	921.897	0.000	0.125
194	Chrysene	228.3	5.52	319.110	0.000	0.749
195	Dibenz(a,h)anthracene	278.4	6.7	1783.769	0.000	0.035

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	4902.896	0.000	0.023
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	20.533
198	Perylene	252.3	6.11	8435.739	0.000	0.059
199	Retene	234.3	6.35	102.485	0.000	0.203

Table B.22. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 6.25% WAF duplicate exposed to *Americamysis bahia* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	83.764	0.025	2.131
2	C1-Phenanthrenes/Anthracenes	192.3	4.26	921.897	0.041	6.164
3	C1-Fluorenes	180.2	4.97	83.764	0.011	3.315
4	C4-Naphthalenes	184.3	5.18	20.144	0.012	3.733
5	3-Methylphenanthrene	192.26	4.89	71.473	0.013	4.473
6	1-Methylphenanthrene	192.26	4.89	71.473	0.012	4.473
7	C3-Naphthalenes	170.26	4.77	20.144	0.020	8.344
8	4/9-Methylphenanthrene	192.26	4.89	71.473	0.010	4.473
9	2-Methylphenanthrene	192.26	4.89	71.473	0.009	4.473
10	C2-Dibenzothiophenes	214.3	5.13	6.161	0.010	7.403
11	Phenanthrene	178.2	4.35	41.949	0.019	16.342
12	Pyrene	202.3	4.93	1051.969	0.001	1.449
13	C1-Dibenzothiophenes	198.3	4.71	6.161	0.011	16.936
14	1,6,7-Trimethylnaphthalene	170.26	4.81	35.520	0.004	6.176
15	C2-Naphthalenes	156.2	4.31	20.144	0.009	20.630
16	Fluoranthene	202.3	4.93	785.130	0.001	1.635
17	4-Methyldibenzothiophene	198.28	4.71	6.161	0.005	16.935
18	Fluorene	166.2	4.02	83.764	0.006	23.687
19	2/3-Methyldibenzothiophene	198.28	4.71	6.161	0.002	16.934
20	2,6-Dimethylnaphthalene	156.23	4.26	20.144	0.003	22.981
21	1-Methyldibenzothiophene	198.28	4.71	6.161	0.001	16.935

22	Dibenzothiophene	184.3	4.17	6.161	0.004	50.404
23	Dibenzofuran	168.2	3.71	44.694	0.002	59.789
24	Biphenyl	154.2	3.76	0.000	0.002	535.193
25	1-Decene	140.3	5.12	0.000	0.000	58.415
26	n-C10	142.29	5.25	0.000	0.000	44.767
27	n-C10	142.29	5.25	0.000	0.000	44.767
28	n-C10	142.3	5.25	0.000	0.000	44.770
29	n-C10	142.3	5.25	0.000	0.000	44.770
30	2-Methylanthracene	192.26	4.89	921.897	0.000	1.585
31	1-Nonene	126.2	4.62	0.000	0.000	154.357
32	n-C9	128.3	4.76	0.000	0.000	116.052
33	n-C9	128.3	4.76	0.000	0.000	116.052
34	n-C9	128.3	4.76	0.000	0.000	116.052
35	n-C9	128.3	4.76	0.000	0.000	116.052
36	n-C10	142.29	5.25	0.000	0.000	44.767
37	n-C10	142.29	5.25	0.000	0.000	44.767
38	n-C10	142.3	5.25	0.000	0.000	44.770
39	n-C10	142.3	5.25	0.000	0.000	44.770
40	n-C8	114.2	4.27	0.000	0.000	296.983
41	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	437.736
42	Octene-1	112.2	4.13	0.000	0.000	394.547
43	n-Pentylbenzene	148.2	4.5	0.000	0.000	234.765
44	3-methylheptane	114.2	4.2	0.000	0.000	345.344
45	Anthracene	178.2	4.35	578.353	0.000	5.705
46	2-methylheptane	114.2	4.2	0.000	0.000	345.344
47	HEPTANE	100.2	3.78	0.000	0.000	749.158
48	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	477.147
49	n-C9	128.3	4.76	0.000	0.000	116.052
50	n-C9	128.3	4.76	0.000	0.000	116.052

51	n-C9	128.3	4.76	0.000	0.000	116.052
52	n-C9	128.3	4.76	0.000	0.000	116.052
53	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	410.437
54	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	437.851
55	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	417.910
56	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	367.163
57	C4-Benzothiophene	190.3	5.18	0.292	0.000	14.345
58	Acenaphthylene	152.2	3.94	312.199	0.000	15.182
59	Acenaphthene	154.2	4.15	58.345	0.000	19.144
60	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	410.437
61	2,3-dimethylhexane	114.2	4.12	0.000	0.000	410.329
62	Methylcyclohexane	98.19	3.59	0.000	0.000	1105.638
63	n-C6	86.18	3.29	0.000	0.000	1852.475
64	n-Butylbenzene	134.2	4.01	0.000	0.000	475.531
65	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
66	tert-Butylbenzene	134.2	3.9	0.000	0.000	602.752
67	2-methylhexane	100.2	3.71	0.000	0.000	871.151
68	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	367.217
69	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	417.848
70	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	367.163
71	3-ethylhexane	114.2	4.2	0.000	0.000	345.344
72	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	417.848
73	3-methylhexane	100.2	3.71	0.000	0.000	871.151
74	C3-Benzothiophene	176.3	4.69	0.292	0.000	38.209
75	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
76	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	367.163
77	Hydrindene	118.2	3.47	0.000	0.000	1341.169
78	n-C5	72.15	2.8	0.000	0.000	4458.843
79	C1-Naphthalenes	142.2	3.87	20.518	0.000	48.147

80	CARBAZOLE	167.2	3.23	152.038	0.000	103.111
81	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2201.062
82	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	417.848
83	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	367.217
84	Propylbenzene	120.194	3.52	0.000	0.000	1224.471
85	p-XYLENE	106.2	3.09	0.000	0.000	2733.194
86	4-isopropyltoluene	134.22	4	0.000	0.000	485.963
87	sec-Butylbenzene	134.2	3.94	0.000	0.000	552.966
88	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1035.079
89	3-Methylpentane	86.18	3.21	0.000	0.000	2201.062
90	2,2-dimethylpentane	100.2	3.67	0.000	0.000	949.584
91	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	966.074
92	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	485.963
93	1-Methylnaphthalene	142.2	3.72	20.518	0.000	66.523
94	m-cymene	134.2	4	0.000	0.000	485.890
95	Ethylbenzene	106.2	3.03	0.000	0.000	3110.501
96	CYCLOHEXANE	84.16	3.18	0.000	0.000	2293.040
97	C1-Decalins	152.3	4.61	0.000	0.000	84.630
98	2-Methylnaphthalene	142.2	3.72	20.518	0.000	66.523
99	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
100	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1075.995
101	C2-Benzothiophene	162.25	4.13	0.292	0.000	117.558
102	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1075.995
103	m-XYLENE	106.2	3.09	0.000	0.000	2733.194
104	Isopropylbenzene	120.194	3.45	0.000	0.000	1423.864
105	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	329.654
106	Isopentane	72.15	2.72	0.000	0.000	5297.881
107	Methylcyclopentane	84.16	3.1	0.000	0.000	2724.530
108	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2559.484

109	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	966.074
110	o-XYLENE	106.2	3.09	0.000	0.000	2733.194
111	Cyclopentane	70.13	2.68	0.000	0.000	5613.190
112	Naphthalene	234.3	3.17	11.329	0.000	446.010
113	trans-Decalin	138.26	4.2	0.000	0.000	185.901
114	C1-Benzothiophene	148.2	3.5365	0.292	0.000	385.863
115	Toluene	92.14	2.54	0.000	0.000	7758.791
116	cis-Decalin	138.26	4.2	0.000	0.000	185.901
117	Benzothiophene	134.2	2.99	0.292	0.000	1134.649
118	Benzene	78.11	1.99	0.000	0.000	21520.507
119	n-C11	156.31	5.74	0.000	0.000	17.105
120	n-C11	156.31	5.74	0.000	0.000	17.105
121	n-C11	156.31	5.74	0.000	0.000	17.105
122	n-C11	156.31	5.74	0.000	0.000	17.105
123	n-C12	170.34	6.23	0.000	0.000	6.484
124	n-C12	170.34	6.23	0.000	0.000	6.484
125	n-C12	170.34	6.23	0.000	0.000	6.484
126	n-C12	170.34	6.23	0.000	0.000	6.484
127	n-C11	156.31	5.74	0.000	0.000	17.105
128	n-C11	156.31	5.74	0.000	0.000	17.105
129	n-C11	156.31	5.74	0.000	0.000	17.105
130	n-C11	156.31	5.74	0.000	0.000	17.105
131	n-C12	170.34	6.23	0.000	0.000	6.484
132	n-C12	170.34	6.23	0.000	0.000	6.484
133	n-C12	170.34	6.23	0.000	0.000	6.484
134	n-C12	170.34	6.23	0.000	0.000	6.484
135	n-C13	184.37	6.73	0.000	0.000	2.389
136	n-C14	198.4	7.22	0.000	0.000	0.894
137	n-C15	212.42	7.71	0.000	0.000	0.333

138	n-C16	226.45	8.2	0.000	0.000	0.123
139	n-C17	240.48	8.69	0.000	0.000	0.046
140	n-C18	254.5	9.18	0.000	0.000	0.017
141	n-C19	268.53	9.67	0.000	0.000	0.006
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.004
164	Pristane	268.525	9.38	0.000	0.000	0.012
165	Benzo(a)fluoranthene	252.3	6.11	4637.391	0.000	0.076
166	Benzo(b)fluorene	216.3	5.77	405.248	0.000	0.376

167	Benzo(k)fluoranthene	252.3	6.11	2564.185	0.000	0.098
168	Benzo[a]anthracene	228.3	5.52	693.329	0.000	0.545
169	Benzo[a]pyrene	252.3	6.11	3571.194	0.000	0.085
170	Benzo[b]fluoranthene	252.3	6.11	1519.621	0.000	0.122
171	Benzo[e]pyrene	252.3	6.11	843.132	0.000	0.156
172	Benzo[g,h,i]perylene	276.3	6.7	2820.850	0.000	0.029
173	C1-Chrysenes	242.3	6.0683	396.598	0.000	0.223
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1565.526	0.000	0.401
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.041
176	C2-Chrysenes	256.3	6.65	396.598	0.000	0.067
177	C2-Decalins	166.3	6.19	0.000	0.000	3.068
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1565.526	0.000	0.105
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.142
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	921.897	0.000	0.487
181	C3-Chrysenes	270.4	7.03	396.598	0.000	0.031
182	C3-Decalins	180.3	6.79	0.000	0.000	0.913
183	C3-Dibenzothiophenes	230.37	5.86	6.161	0.000	1.650
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1565.526	0.000	0.043
185	C3-Fluorenes	210.3	5.58	83.764	0.000	1.039
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.410
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	921.897	0.000	0.225
188	C4-Chrysenes	284.4	7.35	396.598	0.000	0.017
189	C4-Decalins	194.3	7.34	0.000	0.000	0.301
190	C4-Dibenzothiophenes	244.37	6.1	6.161	0.000	1.044
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1565.526	0.000	0.016
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.153
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	921.897	0.000	0.125
194	Chrysene	228.3	5.52	319.110	0.000	0.749
195	Dibenz(a,h)anthracene	278.4	6.7	1783.769	0.000	0.035

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	4902.896	0.000	0.023
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	20.533
198	Perylene	252.3	6.11	8435.739	0.000	0.059
199	Retene	234.3	6.35	102.485	0.000	0.203

Table B.23. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 100% WAF exposed to *Menidia beryllina* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	2-Methylnaphthalene	142.2	3.72	15.481	47.100	85.215
2	C1-Naphthalenes	142.2	3.87	15.481	31.200	61.676
3	C2-Naphthalenes	156.2	4.31	14.989	11.100	26.559
4	1-Methylnaphthalene	142.2	3.72	15.481	34.400	85.215
5	C3-Naphthalenes	170.26	4.77	14.989	2.520	10.742
6	2,6-Dimethylnaphthalene	156.23	4.26	14.989	6.130	29.586
7	C1-Fluorenes	180.2	4.97	60.440	0.856	4.349
8	Toluene	92.14	2.54	0.000	1500.000	8953.934
9	C1-Phenanthrenes/Anthracenes	192.3	4.26	663.598	1.220	8.150
10	Naphthalene	234.3	3.17	8.547	80.300	569.209
11	C2-Fluorenes	194.3	5.21	32.985	0.422	3.534
12	m-XYLENE	106.2	3.09	0.000	375.000	3154.207
13	C4-Naphthalenes	184.3	5.18	14.989	0.566	4.805
14	1,6,7-Trimethylnaphthalene	170.26	4.81	26.742	0.756	7.942
15	o-XYLENE	106.2	3.09	0.000	274.000	3154.207
16	4/9-Methylphenanthrene	192.26	4.89	53.414	0.464	5.786
17	1,2,4-Trimethylbenzene	120.2	3.63	0.000	85.200	1114.885
18	2-Methylanthracene	192.26	4.89	663.598	0.143	2.096
19	Phenanthrene	178.2	4.35	31.329	1.350	21.093
20	1-Methylphenanthrene	192.26	4.89	53.414	0.263	5.786
21	Fluorene	166.2	4.02	60.440	1.380	31.080

22	Benzene	78.11	1.99	0.000	1100.000	24835.468
23	2-Methylphenanthrene	192.26	4.89	53.414	0.212	5.786
24	3-Methylphenanthrene	192.26	4.89	53.414	0.211	5.786
25	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	43.000	1241.739
26	Ethylbenzene	106.2	3.03	0.000	105.000	3589.634
27	1,3,5-trimethylbenzene	120.2	3.63	0.000	27.800	1114.885
28	Methylcyclohexane	98.19	3.59	0.000	31.100	1275.948
29	CYCLOHEXANE	84.16	3.18	0.000	60.900	2646.253
30	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	26.100	1241.739
31	C2-Dibenzothiophenes	214.3	5.13	4.594	0.192	9.442
32	p-XYLENE	106.2	3.09	0.000	60.300	3154.207
33	Anthracene	178.2	4.35	416.623	0.124	7.534
34	C1-Dibenzothiophenes	198.3	4.71	4.594	0.308	21.601
35	4-ETHYLTOLUENE	120.2	3.58	0.000	15.200	1241.739
36	Methylcyclopentane	84.16	3.1	0.000	34.900	3144.209
37	C3-Benzothiophene	176.3	4.69	0.211	0.494	47.389
38	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	4.260	423.719
39	CARBAZOLE	167.2	3.23	112.488	1.170	134.251
40	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	3.670	423.719
41	Propylbenzene	120.194	3.52	0.000	12.000	1413.086
42	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	4.050	482.212
43	Isopentane	72.15	2.72	0.000	46.600	6113.952
44	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	3.100	423.719
45	Pyrene	202.3	4.93	765.804	0.013	1.907
46	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	2.780	423.719
47	n-C5	72.15	2.8	0.000	32.800	5145.671
48	C4-Benzothiophene	190.3	5.18	0.211	0.111	17.792
49	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	2.960	482.212
50	Acenaphthene	154.2	4.15	43.799	0.150	24.698

51	Isopropylbenzene	120.194	3.45	0.000	9.480	1643.193
52	m-cymene	134.2	4	0.000	2.990	560.736
53	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	1.950	380.433
54	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	2.170	423.782
55	4-Methyldibenzothiophene	198.28	4.71	4.594	0.110	21.599
56	Biphenyl	154.2	3.76	0.000	2.870	617.632
57	Dibenzofuran	168.2	3.71	33.732	0.352	76.887
58	2/3-Methyldibenzothiophene	198.28	4.71	4.594	0.096	21.599
59	Dibenzothiophene	184.3	4.17	4.594	0.279	64.285
60	n-C6	86.18	3.29	0.000	9.170	2137.825
61	Cyclopentane	70.13	2.68	0.000	25.500	6477.830
62	C2-Benzothiophene	162.25	4.13	0.211	0.542	145.804
63	HEPTANE	100.2	3.78	0.000	2.660	864.557
64	Hydrindene	118.2	3.47	0.000	4.430	1547.758
65	2-METHYLPENTANE	86.18	3.21	0.000	6.350	2540.108
66	4-isopropyltoluene	134.22	4	0.000	1.330	560.819
67	Fluoranthene	202.3	4.93	567.740	0.005	2.158
68	1-Methyldibenzothiophene	198.28	4.71	4.594	0.044	21.599
69	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.837	423.782
70	sec-Butylbenzene	134.2	3.94	0.000	1.230	638.143
71	3-Methylpentane	86.18	3.21	0.000	4.820	2540.108
72	n-Butylbenzene	134.2	4.01	0.000	0.974	548.780
73	1,2-Diethylbenzene	134.2	4.07	0.000	0.744	482.212
74	n-C8	114.2	4.27	0.000	0.511	342.730
75	3-methylhexane	100.2	3.71	0.000	1.490	1005.341
76	trans-Decalin	138.26	4.2	0.000	0.296	214.537
77	2-methylhexane	100.2	3.71	0.000	1.310	1005.341
78	C1-Decalins	152.3	4.61	0.000	0.123	97.666
79	2-methylheptane	114.2	4.2	0.000	0.431	398.540

80	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.487	560.819
81	Acenaphthylene	152.2	3.94	228.398	0.014	19.897
82	2,3-dimethylbutane	86.18	3.14	0.000	1.730	2953.740
83	C1-Benzothiophene	148.2	3.5365	0.211	0.232	478.575
84	1,1,3-trimethylpentane	114.23	4.12	0.000	0.088	473.659
85	cis-Decalin	138.26	4.2	0.000	0.024	214.537
86	2,2-dimethylpentane	100.2	3.67	0.000	0.098	1095.856
87	Benzothiophene	134.2	2.99	0.211	0.046	1407.273
88	1-Decene	140.3	5.12	0.000	0.000	67.413
89	n-C10	142.29	5.25	0.000	0.000	51.663
90	n-C10	142.29	5.25	0.000	0.000	51.663
91	n-C10	142.3	5.25	0.000	0.000	51.667
92	n-C10	142.3	5.25	0.000	0.000	51.667
93	1-Nonene	126.2	4.62	0.000	0.000	178.133
94	n-C9	128.3	4.76	0.000	0.000	133.928
95	n-C9	128.3	4.76	0.000	0.000	133.928
96	n-C9	128.3	4.76	0.000	0.000	133.928
97	n-C9	128.3	4.76	0.000	0.000	133.928
98	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
99	Octene-1	112.2	4.13	0.000	0.000	455.322
100	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
101	3-methylheptane	114.2	4.2	0.000	0.000	398.540
102	n-C10	142.29	5.25	0.000	0.000	51.663
103	n-C10	142.29	5.25	0.000	0.000	51.663
104	n-C10	142.3	5.25	0.000	0.000	51.667
105	n-C10	142.3	5.25	0.000	0.000	51.667
106	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
107	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
108	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296

109	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
110	n-C9	128.3	4.76	0.000	0.000	133.928
111	n-C9	128.3	4.76	0.000	0.000	133.928
112	n-C9	128.3	4.76	0.000	0.000	133.928
113	n-C9	128.3	4.76	0.000	0.000	133.928
114	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
115	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
116	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
117	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
118	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384

138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	3191.944	0.000	0.103
166	Benzo(b)fluorene	216.3	5.77	299.814	0.000	0.490

167	Benzo(k)fluoranthene	252.3	6.11	1838.684	0.000	0.130
168	Benzo[a]anthracene	228.3	5.52	505.386	0.000	0.716
169	Benzo[a]pyrene	252.3	6.11	2570.625	0.000	0.113
170	Benzo[b]fluoranthene	252.3	6.11	1102.129	0.000	0.161
171	Benzo[e]pyrene	252.3	6.11	616.524	0.000	0.204
172	Benzo[g,h,i]perylene	276.3	6.7	2042.215	0.000	0.038
173	C1-Chrysenes	242.3	6.0683	291.986	0.000	0.292
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1132.356	0.000	0.530
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	291.986	0.000	0.088
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1132.356	0.000	0.139
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	663.598	0.000	0.644
181	C3-Chrysenes	270.4	7.03	291.986	0.000	0.041
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	4.594	0.000	2.105
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1132.356	0.000	0.057
185	C3-Fluorenes	210.3	5.58	60.440	0.000	1.363
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	663.598	0.000	0.297
188	C4-Chrysenes	284.4	7.35	291.986	0.000	0.022
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	4.594	0.000	1.331
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1132.356	0.000	0.021
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	663.598	0.000	0.165
194	Chrysene	228.3	5.52	236.482	0.000	0.977
195	Dibenz(a,h)anthracene	278.4	6.7	1310.685	0.000	0.046

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	3470.160	0.000	0.031
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	5772.867	0.000	0.080
199	Retene	234.3	6.35	76.690	0.000	0.263

Table B.24. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 25% WAF exposed to *Menidia beryllina* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	15.481	8.410	61.676
2	2-Methylnaphthalene	142.2	3.72	15.481	10.200	85.215
3	C2-Naphthalenes	156.2	4.31	14.989	2.870	26.559
4	1-Methylnaphthalene	142.2	3.72	15.481	7.530	85.215
5	C3-Naphthalenes	170.26	4.77	14.989	0.612	10.742
6	Toluene	92.14	2.54	0.000	483.000	8953.934
7	C1-Fluorenes	180.2	4.97	60.440	0.212	4.349
8	2,6-Dimethylnaphthalene	156.23	4.26	14.989	1.360	29.586
9	m-XYLENE	106.2	3.09	0.000	121.000	3154.207
10	C1-Phenanthrenes/Anthracenes	192.3	4.26	663.598	0.306	8.150
11	Naphthalene	234.3	3.17	8.547	18.300	569.209
12	C2-Fluorenes	194.3	5.21	32.985	0.113	3.534
13	C4-Naphthalenes	184.3	5.18	14.989	0.134	4.805
14	o-XYLENE	106.2	3.09	0.000	75.100	3154.207
15	1,6,7-Trimethylnaphthalene	170.26	4.81	26.742	0.183	7.942
16	1,2,4-Trimethylbenzene	120.2	3.63	0.000	22.700	1114.885
17	4/9-Methylphenanthrene	192.26	4.89	53.414	0.115	5.786
18	2-Methylanthracene	192.26	4.89	663.598	0.035	2.096
19	Phenanthrene	178.2	4.35	31.329	0.346	21.093
20	Benzene	78.11	1.99	0.000	361.000	24835.468
21	1-Methylphenanthrene	192.26	4.89	53.414	0.070	5.786
22	Fluorene	166.2	4.02	60.440	0.356	31.080
23	p-XYLENE	106.2	3.09	0.000	32.600	3154.207
24	3-Methylphenanthrene	192.26	4.89	53.414	0.054	5.786

25	2-Methylphenanthrene	192.26	4.89	53.414	0.053	5.786
26	Ethylbenzene	106.2	3.03	0.000	31.000	3589.634
27	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	10.600	1241.739
28	1,3,5-trimethylbenzene	120.2	3.63	0.000	6.740	1114.885
29	C2-Dibenzothiophenes	214.3	5.13	4.594	0.056	9.442
30	Methylcyclohexane	98.19	3.59	0.000	7.350	1275.948
31	CYCLOHEXANE	84.16	3.18	0.000	14.800	2646.253
33	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	6.250	1241.739
34	Anthracene	178.2	4.35	416.623	0.029	7.534
40	C1-Dibenzothiophenes	198.3	4.71	4.594	0.066	21.601
41	4-ETHYLTOLUENE	120.2	3.58	0.000	3.640	1241.739
42	Methylcyclopentane	84.16	3.1	0.000	8.740	3144.209
47	C3-Benzothiophene	176.3	4.69	0.211	0.124	47.389
48	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.918	423.719
49	Propylbenzene	120.194	3.52	0.000	2.780	1413.086
50	CARBAZOLE	167.2	3.23	112.488	0.261	134.251
51	C4-Benzothiophene	190.3	5.18	0.211	0.034	17.792
52	Pyrene	202.3	4.93	765.804	0.004	1.907
53	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.785	423.719
54	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.848	482.212
55	n-C5	72.15	2.8	0.000	8.400	5145.671
56	Acenaphthene	154.2	4.15	43.799	0.039	24.698
57	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.611	423.719
58	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.595	423.719
59	Isopropylbenzene	120.194	3.45	0.000	2.200	1643.193
60	Isopentane	72.15	2.72	0.000	8.110	6113.952
61	m-cymene	134.2	4	0.000	0.715	560.736
62	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.597	482.212
64	Biphenyl	154.2	3.76	0.000	0.750	617.632

65	4-Methyldibenzothiophene	198.28	4.71	4.594	0.026	21.599
66	n-C6	86.18	3.29	0.000	2.520	2137.825
67	Dibenzofuran	168.2	3.71	33.732	0.088	76.887
69	Dibenzothiophene	184.3	4.17	4.594	0.069	64.285
70	Cyclopentane	70.13	2.68	0.000	6.520	6477.830
71	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.426	423.782
74	C2-Benzothiophene	162.25	4.13	0.211	0.137	145.804
75	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.344	380.433
81	2/3-Methyldibenzothiophene	198.28	4.71	4.594	0.017	21.599
82	HEPTANE	100.2	3.78	0.000	0.587	864.557
83	Fluoranthene	202.3	4.93	567.740	0.001	2.158
85	2-METHYLPENTANE	86.18	3.21	0.000	1.630	2540.108
86	Hydrindene	118.2	3.47	0.000	0.993	1547.758
89	4-isopropyltoluene	134.22	4	0.000	0.296	560.819
90	1-Methyldibenzothiophene	198.28	4.71	4.594	0.011	21.599
91	3-Methylpentane	86.18	3.21	0.000	1.250	2540.108
93	sec-Butylbenzene	134.2	3.94	0.000	0.247	638.143
94	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.158	423.782
95	n-Butylbenzene	134.2	4.01	0.000	0.197	548.780
96	3-methylhexane	100.2	3.71	0.000	0.358	1005.341
97	1,2-Diethylbenzene	134.2	4.07	0.000	0.161	482.212
102	2-methylhexane	100.2	3.71	0.000	0.307	1005.341
103	n-C8	114.2	4.27	0.000	0.093	342.730
106	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.104	560.819
107	2,3-dimethylbutane	86.18	3.14	0.000	0.537	2953.740
108	Acenaphthylene	152.2	3.94	228.398	0.003	19.897
110	C1-Benzothiophene	148.2	3.5365	0.211	0.065	478.575
112	trans-Decalin	138.26	4.2	0.000	0.028	214.537
113	C1-Decalins	152.3	4.61	0.000	0.013	97.666

116	2,2-dimethylpentane	100.2	3.67	0.000	0.031	1095.856
117	cis-Decalin	138.26	4.2	0.000	0.002	214.537
118	Benzothiophene	134.2	2.99	0.211	0.012	1407.273
32	1-Decene	140.3	5.12	0.000	0.000	67.413
35	n-C10	142.29	5.25	0.000	0.000	51.663
36	n-C10	142.29	5.25	0.000	0.000	51.663
37	n-C10	142.3	5.25	0.000	0.000	51.667
38	n-C10	142.3	5.25	0.000	0.000	51.667
39	1-Nonene	126.2	4.62	0.000	0.000	178.133
43	n-C9	128.3	4.76	0.000	0.000	133.928
44	n-C9	128.3	4.76	0.000	0.000	133.928
45	n-C9	128.3	4.76	0.000	0.000	133.928
46	n-C9	128.3	4.76	0.000	0.000	133.928
63	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
68	Octene-1	112.2	4.13	0.000	0.000	455.322
72	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
73	3-methylheptane	114.2	4.2	0.000	0.000	398.540
76	n-C10	142.29	5.25	0.000	0.000	51.663
77	n-C10	142.29	5.25	0.000	0.000	51.663
78	n-C10	142.3	5.25	0.000	0.000	51.667
79	n-C10	142.3	5.25	0.000	0.000	51.667
80	2-methylheptane	114.2	4.2	0.000	0.000	398.540
84	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
87	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
88	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
92	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
98	n-C9	128.3	4.76	0.000	0.000	133.928
99	n-C9	128.3	4.76	0.000	0.000	133.928
100	n-C9	128.3	4.76	0.000	0.000	133.928

101	n-C9	128.3	4.76	0.000	0.000	133.928
104	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
105	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
109	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
111	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
114	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
115	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384
138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019

141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	3191.944	0.000	0.103
166	Benzo(b)fluorene	216.3	5.77	299.814	0.000	0.490
167	Benzo(k)fluoranthene	252.3	6.11	1838.684	0.000	0.130
168	Benzo[a]anthracene	228.3	5.52	505.386	0.000	0.716
169	Benzo[a]pyrene	252.3	6.11	2570.625	0.000	0.113

170	Benzo[b]fluoranthene	252.3	6.11	1102.129	0.000	0.161
171	Benzo[e]pyrene	252.3	6.11	616.524	0.000	0.204
172	Benzo[g,h,i]perylene	276.3	6.7	2042.215	0.000	0.038
173	C1-Chrysenes	242.3	6.0683	291.986	0.000	0.292
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1132.356	0.000	0.530
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	291.986	0.000	0.088
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1132.356	0.000	0.139
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	663.598	0.000	0.644
181	C3-Chrysenes	270.4	7.03	291.986	0.000	0.041
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	4.594	0.000	2.105
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1132.356	0.000	0.057
185	C3-Fluorenes	210.3	5.58	60.440	0.000	1.363
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	663.598	0.000	0.297
188	C4-Chrysenes	284.4	7.35	291.986	0.000	0.022
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	4.594	0.000	1.331
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1132.356	0.000	0.021
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	663.598	0.000	0.165
194	Chrysene	228.3	5.52	236.482	0.000	0.977
195	Dibenz(a,h)anthracene	278.4	6.7	1310.685	0.000	0.046
196	Indeno[1,2,3-cd]pyrene	276.3	6.7	3470.160	0.000	0.031
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	5772.867	0.000	0.080

199	Retene	234.3	6.35	76.690	0.000	0.263

Table B.25. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF exposed to *Menidia beryllina* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	15.481	2.070	61.676
2	C2-Naphthalenes	156.2	4.31	14.989	0.666	26.559
3	2-Methylnaphthalene	142.2	3.72	15.481	2.020	85.215
4	1-Methylnaphthalene	142.2	3.72	15.481	1.510	85.215
5	C3-Naphthalenes	170.26	4.77	14.989	0.140	10.742
6	C1-Fluorenes	180.2	4.97	60.440	0.051	4.349
7	2,6-Dimethylnaphthalene	156.23	4.26	14.989	0.310	29.586
8	Toluene	92.14	2.54	0.000	83.200	8953.934
9	C2-Fluorenes	194.3	5.21	32.985	0.032	3.534
10	C1-Phenanthrenes/Anthracenes	192.3	4.26	663.598	0.073	8.150
11	C4-Naphthalenes	184.3	5.18	14.989	0.034	4.805
12	m-XYLENE	106.2	3.09	0.000	21.700	3154.207
13	Naphthalene	234.3	3.17	8.547	3.500	569.209
15	1,6,7-Trimethylnaphthalene	170.26	4.81	26.742	0.042	7.942
16	4/9-Methylphenanthrene	192.26	4.89	53.414	0.027	5.786
17	o-XYLENE	106.2	3.09	0.000	14.300	3154.207
18	Phenanthrene	178.2	4.35	31.329	0.084	21.093
23	2-Methylanthracene	192.26	4.89	663.598	0.008	2.096
24	1,2,4-Trimethylbenzene	120.2	3.63	0.000	4.080	1114.885
26	1-Methylphenanthrene	192.26	4.89	53.414	0.017	5.786
27	Fluorene	166.2	4.02	60.440	0.086	31.080
32	Benzene	78.11	1.99	0.000	61.500	24835.468
33	3-Methylphenanthrene	192.26	4.89	53.414	0.014	5.786

34	p-XYLENE	106.2	3.09	0.000	6.900	3154.207
35	2-Methylphenanthrene	192.26	4.89	53.414	0.012	5.786
36	Ethylbenzene	106.2	3.03	0.000	6.030	3589.634
38	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	1.760	1241.739
39	C2-Dibenzothiophenes	214.3	5.13	4.594	0.013	9.442
42	1,3,5-trimethylbenzene	120.2	3.63	0.000	1.100	1114.885
44	CYCLOHEXANE	84.16	3.18	0.000	2.530	2646.253
46	Anthracene	178.2	4.35	416.623	0.007	7.534
47	Methylcyclohexane	98.19	3.59	0.000	1.130	1275.948
52	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	1.020	1241.739
54	Pyrene	202.3	4.93	765.804	0.001	1.907
55	C3-Benzothiophene	176.3	4.69	0.211	0.032	47.389
57	C4-Benzothiophene	190.3	5.18	0.211	0.012	17.792
58	C1-Dibenzothiophenes	198.3	4.71	4.594	0.014	21.601
61	Methylcyclopentane	84.16	3.1	0.000	1.560	3144.209
62	4-ETHYLTOLUENE	120.2	3.58	0.000	0.616	1241.739
64	Isopentane	72.15	2.72	0.000	2.780	6113.952
65	Acenaphthene	154.2	4.15	43.799	0.011	24.698
66	CARBAZOLE	167.2	3.23	112.488	0.052	134.251
67	n-C5	72.15	2.8	0.000	1.600	5145.671
72	Biphenyl	154.2	3.76	0.000	0.180	617.632
73	Dibenzofuran	168.2	3.71	33.732	0.022	76.887
74	4-Methyldibenzothiophene	198.28	4.71	4.594	0.006	21.599
75	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.119	423.719
76	Propylbenzene	120.194	3.52	0.000	0.395	1413.086
77	Fluoranthene	202.3	4.93	567.740	0.001	2.158
79	Dibenzothiophene	184.3	4.17	4.594	0.016	64.285
80	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.100	423.719
82	C2-Benzothiophene	162.25	4.13	0.211	0.034	145.804

83	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.110	482.212
84	Isopropylbenzene	120.194	3.45	0.000	0.327	1643.193
86	Cyclopentane	70.13	2.68	0.000	1.190	6477.830
87	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.076	423.719
88	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.071	423.719
89	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.075	482.212
91	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.057	423.782
94	Hydrindene	118.2	3.47	0.000	0.192	1547.758
95	1-Methyldibenzothiophene	198.28	4.71	4.594	0.003	21.599
97	2-METHYLPENTANE	86.18	3.21	0.000	0.280	2540.108
99	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.040	380.433
100	2/3-Methyldibenzothiophene	198.28	4.71	4.594	0.002	21.599
101	HEPTANE	100.2	3.78	0.000	0.089	864.557
102	3-Methylpentane	86.18	3.21	0.000	0.210	2540.108
109	Acenaphthylene	152.2	3.94	228.398	0.001	19.897
110	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.019	423.782
111	C1-Decalins	152.3	4.61	0.000	0.004	97.666
113	C1-Benzothiophene	148.2	3.5365	0.211	0.019	478.575
114	2,3-dimethylbutane	86.18	3.14	0.000	0.116	2953.740
115	n-Butylbenzene	134.2	4.01	0.000	0.021	548.780
116	trans-Decalin	138.26	4.2	0.000	0.006	214.537
117	cis-Decalin	138.26	4.2	0.000	0.000	214.537
118	Benzothiophene	134.2	2.99	0.211	0.003	1407.273
14	1-Decene	140.3	5.12	0.000	0.000	67.413
19	n-C10	142.29	5.25	0.000	0.000	51.663
20	n-C10	142.29	5.25	0.000	0.000	51.663
21	n-C10	142.3	5.25	0.000	0.000	51.667
22	n-C10	142.3	5.25	0.000	0.000	51.667

25	1-Nonene	126.2	4.62	0.000	0.000	178.133
28	n-C9	128.3	4.76	0.000	0.000	133.928
29	n-C9	128.3	4.76	0.000	0.000	133.928
30	n-C9	128.3	4.76	0.000	0.000	133.928
31	n-C9	128.3	4.76	0.000	0.000	133.928
37	n-C8	114.2	4.27	0.000	0.000	342.730
40	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
41	Octene-1	112.2	4.13	0.000	0.000	455.322
43	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
45	3-methylheptane	114.2	4.2	0.000	0.000	398.540
48	n-C10	142.29	5.25	0.000	0.000	51.663
49	n-C10	142.29	5.25	0.000	0.000	51.663
50	n-C10	142.3	5.25	0.000	0.000	51.667
51	n-C10	142.3	5.25	0.000	0.000	51.667
53	2-methylheptane	114.2	4.2	0.000	0.000	398.540
56	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
59	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
60	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
63	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
68	n-C9	128.3	4.76	0.000	0.000	133.928
69	n-C9	128.3	4.76	0.000	0.000	133.928
70	n-C9	128.3	4.76	0.000	0.000	133.928
71	n-C9	128.3	4.76	0.000	0.000	133.928
78	n-C6	86.18	3.29	0.000	0.000	2137.825
81	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
85	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
90	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
92	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598

93	2-methylhexane	100.2	3.71	0.000	0.000	1005.341
96	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
98	3-methylhexane	100.2	3.71	0.000	0.000	1005.341
103	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	482.212
104	4-isopropyltoluene	134.22	4	0.000	0.000	560.819
105	sec-Butylbenzene	134.2	3.94	0.000	0.000	638.143
106	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
107	2,2-dimethylpentane	100.2	3.67	0.000	0.000	1095.856
108	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	560.819
112	m-cymene	134.2	4	0.000	0.000	560.736
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032

137	n-C15	212.42	7.71	0.000	0.000	0.384
138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	3191.944	0.000	0.103

166	Benzo(b)fluorene	216.3	5.77	299.814	0.000	0.490
167	Benzo(k)fluoranthene	252.3	6.11	1838.684	0.000	0.130
168	Benzo[a]anthracene	228.3	5.52	505.386	0.000	0.716
169	Benzo[a]pyrene	252.3	6.11	2570.625	0.000	0.113
170	Benzo[b]fluoranthene	252.3	6.11	1102.129	0.000	0.161
171	Benzo[e]pyrene	252.3	6.11	616.524	0.000	0.204
172	Benzo[g,h,i]perylene	276.3	6.7	2042.215	0.000	0.038
173	C1-Chrysenes	242.3	6.0683	291.986	0.000	0.292
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1132.356	0.000	0.530
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	291.986	0.000	0.088
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1132.356	0.000	0.139
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	663.598	0.000	0.644
181	C3-Chrysenes	270.4	7.03	291.986	0.000	0.041
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	4.594	0.000	2.105
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1132.356	0.000	0.057
185	C3-Fluorenes	210.3	5.58	60.440	0.000	1.363
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	663.598	0.000	0.297
188	C4-Chrysenes	284.4	7.35	291.986	0.000	0.022
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	4.594	0.000	1.331
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1132.356	0.000	0.021
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	663.598	0.000	0.165
194	Chrysene	228.3	5.52	236.482	0.000	0.977

195	Dibenz(a,h)anthracene	278.4	6.7	1310.685	0.000	0.046
196	Indeno[1,2,3-cd]pyrene	276.3	6.7	3470.160	0.000	0.031
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	5772.867	0.000	0.080
199	Retene	234.3	6.35	76.690	0.000	0.263

Table B.26. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF duplicate exposed to *Menidia beryllina* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	15.481	2.230	61.676
2	C2-Naphthalenes	156.2	4.31	14.989	0.688	26.559
3	2-Methylnaphthalene	142.2	3.72	15.481	2.160	85.215
4	1-Methylnaphthalene	142.2	3.72	15.481	1.600	85.215
5	C3-Naphthalenes	170.26	4.77	14.989	0.141	10.742
6	C1-Fluorenes	180.2	4.97	60.440	0.051	4.349
7	2,6-Dimethylnaphthalene	156.23	4.26	14.989	0.319	29.586
8	Toluene	92.14	2.54	0.000	80.400	8953.934
9	C1-Phenanthrenes/Anthracenes	192.3	4.26	663.598	0.073	8.150
10	C2-Fluorenes	194.3	5.21	32.985	0.031	3.534
11	C4-Naphthalenes	184.3	5.18	14.989	0.034	4.805
12	Naphthalene	234.3	3.17	8.547	3.930	569.209
13	m-XYLENE	106.2	3.09	0.000	20.600	3154.207
14	1,6,7-Trimethylnaphthalene	170.26	4.81	26.742	0.040	7.942
15	o-XYLENE	106.2	3.09	0.000	13.800	3154.207
16	4/9-Methylphenanthrene	192.26	4.89	53.414	0.025	5.786
17	Phenanthrene	178.2	4.35	31.329	0.085	21.093
18	1,2,4-Trimethylbenzene	120.2	3.63	0.000	3.890	1114.885
19	2-Methylanthracene	192.26	4.89	663.598	0.007	2.096
20	1-Methylphenanthrene	192.26	4.89	53.414	0.018	5.786
21	Fluorene	166.2	4.02	60.440	0.091	31.080
22	Benzene	78.11	1.99	0.000	59.000	24835.468

23	3-Methylphenanthrene	192.26	4.89	53.414	0.014	5.786
24	p-XYLENE	106.2	3.09	0.000	6.640	3154.207
25	2-Methylphenanthrene	192.26	4.89	53.414	0.012	5.786
26	C2-Dibenzothiophenes	214.3	5.13	4.594	0.015	9.442
27	Ethylbenzene	106.2	3.03	0.000	5.740	3589.634
28	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	1.690	1241.739
29	1,3,5-trimethylbenzene	120.2	3.63	0.000	1.060	1114.885
30	Pyrene	202.3	4.93	765.804	0.002	1.907
31	CYCLOHEXANE	84.16	3.18	0.000	2.420	2646.253
32	Methylcyclohexane	98.19	3.59	0.000	1.140	1275.948
33	Anthracene	178.2	4.35	416.623	0.006	7.534
34	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.976	1241.739
35	C3-Benzothiophene	176.3	4.69	0.211	0.033	47.389
36	C1-Dibenzothiophenes	198.3	4.71	4.594	0.014	21.601
37	C4-Benzothiophene	190.3	5.18	0.211	0.011	17.792
38	4-ETHYLTOLUENE	120.2	3.58	0.000	0.594	1241.739
39	Methylcyclopentane	84.16	3.1	0.000	1.430	3144.209
40	Acenaphthene	154.2	4.15	43.799	0.011	24.698
41	CARBAZOLE	167.2	3.23	112.488	0.054	134.251
42	Biphenyl	154.2	3.76	0.000	0.190	617.632
43	Isopentane	72.15	2.72	0.000	1.860	6113.952
44	n-C5	72.15	2.8	0.000	1.520	5145.671
45	Dibenzofuran	168.2	3.71	33.732	0.022	76.887
46	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.118	423.719
47	4-Methyldibenzothiophene	198.28	4.71	4.594	0.006	21.599
48	Fluoranthene	202.3	4.93	567.740	0.001	2.158
49	Propylbenzene	120.194	3.52	0.000	0.370	1413.086
50	Dibenzothiophene	184.3	4.17	4.594	0.017	64.285
51	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.097	423.719
52	C2-Benzothiophene	162.25	4.13	0.211	0.033	145.804

53	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.105	482.212
54	Isopropylbenzene	120.194	3.45	0.000	0.298	1643.193
55	Cyclopentane	70.13	2.68	0.000	1.140	6477.830
56	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.074	423.719
57	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.076	482.212
58	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.066	423.719
59	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.054	423.782
60	1-Methyldibenzothiophene	198.28	4.71	4.594	0.003	21.599
61	Hydrindene	118.2	3.47	0.000	0.166	1547.758
62	2-METHYLPENTANE	86.18	3.21	0.000	0.264	2540.108
63	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.038	380.433
64	HEPTANE	100.2	3.78	0.000	0.079	864.557
65	3-Methylpentane	86.18	3.21	0.000	0.213	2540.108
66	2/3-Methyldibenzothiophene	198.28	4.71	4.594	0.002	21.599
67	C1-Decalins	152.3	4.61	0.000	0.007	97.666
68	C1-Benzothiophene	148.2	3.5365	0.211	0.028	478.575
69	n-Butylbenzene	134.2	4.01	0.000	0.029	548.780
70	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.022	423.782
71	2,3-dimethylbutane	86.18	3.14	0.000	0.133	2953.740
72	Acenaphthylene	152.2	3.94	228.398	0.001	19.897
73	trans-Decalin	138.26	4.2	0.000	0.007	214.537
74	cis-Decalin	138.26	4.2	0.000	0.001	214.537
75	Benzothiophene	134.2	2.99	0.211	0.003	1407.273
76	1-Decene	140.3	5.12	0.000	0.000	67.413
77	n-C10	142.29	5.25	0.000	0.000	51.663
78	n-C10	142.29	5.25	0.000	0.000	51.663
79	n-C10	142.3	5.25	0.000	0.000	51.667
80	n-C10	142.3	5.25	0.000	0.000	51.667
81	1-Nonene	126.2	4.62	0.000	0.000	178.133
82	n-C9	128.3	4.76	0.000	0.000	133.928

83	n-C9	128.3	4.76	0.000	0.000	133.928
84	n-C9	128.3	4.76	0.000	0.000	133.928
85	n-C9	128.3	4.76	0.000	0.000	133.928
86	n-C10	142.29	5.25	0.000	0.000	51.663
87	n-C10	142.29	5.25	0.000	0.000	51.663
88	n-C10	142.3	5.25	0.000	0.000	51.667
89	n-C10	142.3	5.25	0.000	0.000	51.667
90	n-C8	114.2	4.27	0.000	0.000	342.730
91	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
92	Octene-1	112.2	4.13	0.000	0.000	455.322
93	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
94	3-methylheptane	114.2	4.2	0.000	0.000	398.540
95	2-methylheptane	114.2	4.2	0.000	0.000	398.540
96	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
97	n-C9	128.3	4.76	0.000	0.000	133.928
98	n-C9	128.3	4.76	0.000	0.000	133.928
99	n-C9	128.3	4.76	0.000	0.000	133.928
100	n-C9	128.3	4.76	0.000	0.000	133.928
101	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
102	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
103	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
104	n-C6	86.18	3.29	0.000	0.000	2137.825
105	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
106	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
107	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
108	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
109	2-methylhexane	100.2	3.71	0.000	0.000	1005.341
110	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
111	3-methylhexane	100.2	3.71	0.000	0.000	1005.341
112	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	482.212

113	4-isopropyltoluene	134.22	4	0.000	0.000	560.819
114	sec-Butylbenzene	134.2	3.94	0.000	0.000	638.143
115	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
116	2,2-dimethylpentane	100.2	3.67	0.000	0.000	1095.856
117	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	560.819
118	m-cymene	134.2	4	0.000	0.000	560.736
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384
138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003

143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	3191.944	0.000	0.103
166	Benzo(b)fluorene	216.3	5.77	299.814	0.000	0.490
167	Benzo(k)fluoranthene	252.3	6.11	1838.684	0.000	0.130
168	Benzo[a]anthracene	228.3	5.52	505.386	0.000	0.716
169	Benzo[a]pyrene	252.3	6.11	2570.625	0.000	0.113
170	Benzo[b]fluoranthene	252.3	6.11	1102.129	0.000	0.161
171	Benzo[e]pyrene	252.3	6.11	616.524	0.000	0.204
172	Benzo[g,h,i]perylene	276.3	6.7	2042.215	0.000	0.038

173	C1-Chrysenes	242.3	6.0683	291.986	0.000	0.292
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1132.356	0.000	0.530
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	291.986	0.000	0.088
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1132.356	0.000	0.139
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	663.598	0.000	0.644
181	C3-Chrysenes	270.4	7.03	291.986	0.000	0.041
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	4.594	0.000	2.105
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1132.356	0.000	0.057
185	C3-Fluorenes	210.3	5.58	60.440	0.000	1.363
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	663.598	0.000	0.297
188	C4-Chrysenes	284.4	7.35	291.986	0.000	0.022
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	4.594	0.000	1.331
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1132.356	0.000	0.021
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	663.598	0.000	0.165
194	Chrysene	228.3	5.52	236.482	0.000	0.977
195	Dibenz(a,h)anthracene	278.4	6.7	1310.685	0.000	0.046
196	Indeno[1,2,3-cd]pyrene	276.3	6.7	3470.160	0.000	0.031
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	5772.867	0.000	0.080
199	Retene	234.3	6.35	76.690	0.000	0.263

Table B.27. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 100% WAF exposed to *Menidia beryllina* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	80.660	0.798	2.496
2	C1-Fluorenes	180.2	4.97	80.660	0.897	3.883
3	C3-Naphthalenes	170.26	4.77	19.514	1.580	9.744
4	C1-Phenanthrenes/Anthracenes	192.3	4.26	885.176	1.120	7.234
5	C4-Naphthalenes	184.3	5.18	19.514	0.405	4.359
6	C2-Naphthalenes	156.2	4.31	19.514	2.080	24.091
7	1,6,7-Trimethylnaphthalene	170.26	4.81	34.520	0.537	7.206
8	1-Methylphenanthrene	192.26	4.89	69.321	0.362	5.225
9	Phenanthrene	178.2	4.35	40.679	1.270	19.084
10	4/9-Methylphenanthrene	192.26	4.89	69.321	0.326	5.225
11	2-Methylphenanthrene	192.26	4.89	69.321	0.273	5.225
12	3-Methylphenanthrene	192.26	4.89	69.321	0.268	5.225
13	C2-Dibenzothiophenes	214.3	5.13	5.972	0.275	8.635
14	2,6-Dimethylnaphthalene	156.23	4.26	19.514	0.817	26.837
15	Fluorene	166.2	4.02	80.660	0.710	27.747
16	C1-Dibenzothiophenes	198.3	4.71	5.972	0.397	19.756
17	Pyrene	202.3	4.93	1013.086	0.015	1.698
18	4-Methyldibenzothiophene	198.28	4.71	5.972	0.140	19.754
19	C1-Naphthalenes	142.2	3.87	19.952	0.260	56.146
20	Dibenzothiophene	184.3	4.17	5.972	0.254	58.796
21	2/3-Methyldibenzothiophene	198.28	4.71	5.972	0.068	19.754
22	Fluoranthene	202.3	4.93	754.760	0.006	1.918

23	1-Methylnaphthalene	142.2	3.72	19.952	0.241	77.574
24	1-Methyldibenzothiophene	198.28	4.71	5.972	0.055	19.754
25	2-Methylnaphthalene	142.2	3.72	19.952	0.190	77.574
26	2-Methylanthracene	192.26	4.89	885.176	0.004	1.861
27	C4-Benzothiophene	190.3	5.18	0.281	0.037	16.705
28	Dibenzofuran	168.2	3.71	43.465	0.106	69.746
29	Acenaphthene	154.2	4.15	56.658	0.034	22.347
30	C3-Benzothiophene	176.3	4.69	0.281	0.049	44.493
31	Anthracene	178.2	4.35	555.417	0.007	6.694
32	Acenaphthylene	152.2	3.94	301.058	0.004	17.782
33	Biphenyl	154.2	3.76	0.000	0.146	617.632
34	C2-Benzothiophene	162.25	4.13	0.281	0.032	136.895
35	Naphthalene	234.3	3.17	11.017	0.016	519.927
36	C1-Benzothiophene	148.2	3.5365	0.281	0.010	449.333
37	1-Decene	140.3	5.12	0.000	0.000	67.413
38	n-C10	142.29	5.25	0.000	0.000	51.663
39	n-C10	142.29	5.25	0.000	0.000	51.663
40	n-C10	142.3	5.25	0.000	0.000	51.667
41	n-C10	142.3	5.25	0.000	0.000	51.667
42	1-Nonene	126.2	4.62	0.000	0.000	178.133
43	n-C9	128.3	4.76	0.000	0.000	133.928
44	n-C9	128.3	4.76	0.000	0.000	133.928
45	n-C9	128.3	4.76	0.000	0.000	133.928
46	n-C9	128.3	4.76	0.000	0.000	133.928
47	n-C8	114.2	4.27	0.000	0.000	342.730
48	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
49	Octene-1	112.2	4.13	0.000	0.000	455.322
50	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
51	3-methylheptane	114.2	4.2	0.000	0.000	398.540
52	n-C10	142.29	5.25	0.000	0.000	51.663

53	n-C10	142.29	5.25	0.000	0.000	51.663
54	n-C10	142.3	5.25	0.000	0.000	51.667
55	n-C10	142.3	5.25	0.000	0.000	51.667
56	2-methylheptane	114.2	4.2	0.000	0.000	398.540
57	HEPTANE	100.2	3.78	0.000	0.000	864.557
58	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
59	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
60	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
61	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
62	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	423.719
63	n-C9	128.3	4.76	0.000	0.000	133.928
64	n-C9	128.3	4.76	0.000	0.000	133.928
65	n-C9	128.3	4.76	0.000	0.000	133.928
66	n-C9	128.3	4.76	0.000	0.000	133.928
67	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
68	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
69	Methylcyclohexane	98.19	3.59	0.000	0.000	1275.948
70	n-Butylbenzene	134.2	4.01	0.000	0.000	548.780
71	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
72	Toluene	92.14	2.54	0.000	0.000	8953.934
73	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
74	2-methylhexane	100.2	3.71	0.000	0.000	1005.341
75	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	423.782
76	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	482.212
77	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	423.719
78	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
79	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	482.212
80	3-methylhexane	100.2	3.71	0.000	0.000	1005.341
81	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
82	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	423.719

83	Hydrindene	118.2	3.47	0.000	0.000	1547.758
84	n-C5	72.15	2.8	0.000	0.000	5145.671
85	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2540.108
86	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	482.212
87	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	423.782
88	Propylbenzene	120.194	3.52	0.000	0.000	1413.086
89	p-XYLENE	106.2	3.09	0.000	0.000	3154.207
90	4-isopropyltoluene	134.22	4	0.000	0.000	560.819
91	sec-Butylbenzene	134.2	3.94	0.000	0.000	638.143
92	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
93	3-Methylpentane	86.18	3.21	0.000	0.000	2540.108
94	2,2-dimethylpentane	100.2	3.67	0.000	0.000	1095.856
95	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
96	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	560.819
97	n-C6	86.18	3.29	0.000	0.000	2137.825
98	m-cymene	134.2	4	0.000	0.000	560.736
99	Ethylbenzene	106.2	3.03	0.000	0.000	3589.634
100	CYCLOHEXANE	84.16	3.18	0.000	0.000	2646.253
101	CARBAZOLE	167.2	3.23	147.059	0.000	120.597
102	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
103	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
104	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1241.739
105	m-XYLENE	106.2	3.09	0.000	0.000	3154.207
106	Isopropylbenzene	120.194	3.45	0.000	0.000	1643.193
107	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	380.433
108	Isopentane	72.15	2.72	0.000	0.000	6113.952
109	Methylcyclopentane	84.16	3.1	0.000	0.000	3144.209
110	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2953.740
111	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
112	o-XYLENE	106.2	3.09	0.000	0.000	3154.207

113	C1-Decalins	152.3	4.61	0.000	0.000	97.666
114	Cyclopentane	70.13	2.68	0.000	0.000	6477.830
115	Benzene	78.11	1.99	0.000	0.000	24835.468
116	trans-Decalin	138.26	4.2	0.000	0.000	214.537
117	cis-Decalin	138.26	4.2	0.000	0.000	214.537
118	Benzothiophene	134.2	2.99	0.281	0.000	1321.285
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384
138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003

143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	4444.987	0.000	0.090
166	Benzo(b)fluorene	216.3	5.77	391.970	0.000	0.439
167	Benzo(k)fluoranthene	252.3	6.11	2467.384	0.000	0.115
168	Benzo[a]anthracene	228.3	5.52	667.937	0.000	0.638
169	Benzo[a]pyrene	252.3	6.11	3431.470	0.000	0.100
170	Benzo[b]fluoranthene	252.3	6.11	1462.047	0.000	0.143
171	Benzo[e]pyrene	252.3	6.11	812.941	0.000	0.182
172	Benzo[g,h,i]perylene	276.3	6.7	2712.839	0.000	0.034

173	C1-Chrysenes	242.3	6.0683	383.098	0.000	0.261
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1505.075	0.000	0.470
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	383.098	0.000	0.079
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1505.075	0.000	0.123
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	885.176	0.000	0.572
181	C3-Chrysenes	270.4	7.03	383.098	0.000	0.037
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	5.972	0.000	1.925
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1505.075	0.000	0.051
185	C3-Fluorenes	210.3	5.58	80.660	0.000	1.217
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	885.176	0.000	0.264
188	C4-Chrysenes	284.4	7.35	383.098	0.000	0.019
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	5.972	0.000	1.217
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1505.075	0.000	0.019
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	885.176	0.000	0.147
194	Chrysene	228.3	5.52	308.794	0.000	0.876
195	Dibenz(a,h)anthracene	278.4	6.7	1722.147	0.000	0.041
196	Indeno[1,2,3-cd]pyrene	276.3	6.7	4708.378	0.000	0.027
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	8081.585	0.000	0.070
199	Retene	234.3	6.35	99.434	0.000	0.237

Table B.28. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 25% WAF exposed to *Menidia beryllina* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	80.660	0.184	2.496
2	C1-Fluorenes	180.2	4.97	80.660	0.196	3.883
3	C1-Phenanthrenes/Anthracenes	192.3	4.26	885.176	0.262	7.234
4	C3-Naphthalenes	170.26	4.77	19.514	0.340	9.744
5	C4-Naphthalenes	184.3	5.18	19.514	0.086	4.359
6	C2-Naphthalenes	156.2	4.31	19.514	0.454	24.091
7	1-Methylphenanthrene	192.26	4.89	69.321	0.084	5.225
8	Phenanthrene	178.2	4.35	40.679	0.303	19.084
9	1,6,7-Trimethylnaphthalene	170.26	4.81	34.520	0.113	7.206
10	4/9-Methylphenanthrene	192.26	4.89	69.321	0.075	5.225
11	2-Methylphenanthrene	192.26	4.89	69.321	0.062	5.225
12	3-Methylphenanthrene	192.26	4.89	69.321	0.062	5.225
13	2,6-Dimethylnaphthalene	156.23	4.26	19.514	0.173	26.837
14	Fluorene	166.2	4.02	80.660	0.164	27.747
15	C2-Dibenzothiophenes	214.3	5.13	5.972	0.050	8.635
16	C1-Dibenzothiophenes	198.3	4.71	5.972	0.072	19.756
17	Pyrene	202.3	4.93	1013.086	0.004	1.698
18	4-Methyldibenzothiophene	198.28	4.71	5.972	0.030	19.754
19	Dibenzothiophene	184.3	4.17	5.972	0.057	58.796
20	C1-Naphthalenes	142.2	3.87	19.952	0.053	56.146
21	2-Methylanthracene	192.26	4.89	885.176	0.002	1.861
22	Fluoranthene	202.3	4.93	754.760	0.002	1.918

23	1-Methylnaphthalene	142.2	3.72	19.952	0.051	77.574
24	1-Methyldibenzothiophene	198.28	4.71	5.972	0.012	19.754
25	C4-Benzothiophene	190.3	5.18	0.281	0.009	16.705
26	2-Methylnaphthalene	142.2	3.72	19.952	0.038	77.574
27	2/3-Methyldibenzothiophene	198.28	4.71	5.972	0.009	19.754
28	Acenaphthene	154.2	4.15	56.658	0.008	22.347
29	Dibenzofuran	168.2	3.71	43.465	0.024	69.746
30	C3-Benzothiophene	176.3	4.69	0.281	0.014	44.493
31	C2-Benzothiophene	162.25	4.13	0.281	0.008	136.895
32	Acenaphthylene	152.2	3.94	301.058	0.001	17.782
33	Biphenyl	154.2	3.76	0.000	0.032	617.632
34	Naphthalene	234.3	3.17	11.017	0.012	519.927
35	C1-Benzothiophene	148.2	3.5365	0.281	0.005	449.333
36	1-Decene	140.3	5.12	0.000	0.000	67.413
37	n-C10	142.29	5.25	0.000	0.000	51.663
38	n-C10	142.29	5.25	0.000	0.000	51.663
39	n-C10	142.3	5.25	0.000	0.000	51.667
40	n-C10	142.3	5.25	0.000	0.000	51.667
41	1-Nonene	126.2	4.62	0.000	0.000	178.133
42	n-C9	128.3	4.76	0.000	0.000	133.928
43	n-C9	128.3	4.76	0.000	0.000	133.928
44	n-C9	128.3	4.76	0.000	0.000	133.928
45	n-C9	128.3	4.76	0.000	0.000	133.928
46	n-C8	114.2	4.27	0.000	0.000	342.730
47	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
48	Octene-1	112.2	4.13	0.000	0.000	455.322
49	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
50	3-methylheptane	114.2	4.2	0.000	0.000	398.540
51	n-C10	142.29	5.25	0.000	0.000	51.663
52	n-C10	142.29	5.25	0.000	0.000	51.663

53	n-C10	142.3	5.25	0.000	0.000	51.667
54	n-C10	142.3	5.25	0.000	0.000	51.667
55	2-methylheptane	114.2	4.2	0.000	0.000	398.540
56	HEPTANE	100.2	3.78	0.000	0.000	864.557
57	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
58	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
59	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
60	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
61	Anthracene	178.2	4.35	555.417	0.000	6.694
62	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	423.719
63	n-C9	128.3	4.76	0.000	0.000	133.928
64	n-C9	128.3	4.76	0.000	0.000	133.928
65	n-C9	128.3	4.76	0.000	0.000	133.928
66	n-C9	128.3	4.76	0.000	0.000	133.928
67	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
68	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
69	Methylcyclohexane	98.19	3.59	0.000	0.000	1275.948
70	n-Butylbenzene	134.2	4.01	0.000	0.000	548.780
71	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
72	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
73	2-methylhexane	100.2	3.71	0.000	0.000	1005.341
74	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	423.782
75	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	482.212
76	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	423.719
77	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
78	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	482.212
79	3-methylhexane	100.2	3.71	0.000	0.000	1005.341
80	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
81	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
82	Hydrindene	118.2	3.47	0.000	0.000	1547.758

83	n-C5	72.15	2.8	0.000	0.000	5145.671
84	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2540.108
85	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	482.212
86	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	423.782
87	Propylbenzene	120.194	3.52	0.000	0.000	1413.086
88	p-XYLENE	106.2	3.09	0.000	0.000	3154.207
89	4-isopropyltoluene	134.22	4	0.000	0.000	560.819
90	n-C6	86.18	3.29	0.000	0.000	2137.825
91	sec-Butylbenzene	134.2	3.94	0.000	0.000	638.143
92	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
93	3-Methylpentane	86.18	3.21	0.000	0.000	2540.108
94	2,2-dimethylpentane	100.2	3.67	0.000	0.000	1095.856
95	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
96	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	560.819
97	m-cymene	134.2	4	0.000	0.000	560.736
98	Ethylbenzene	106.2	3.03	0.000	0.000	3589.634
99	CYCLOHEXANE	84.16	3.18	0.000	0.000	2646.253
100	CARBAZOLE	167.2	3.23	147.059	0.000	120.597
101	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
102	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
103	Toluene	92.14	2.54	0.000	0.000	8953.934
104	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1241.739
105	m-XYLENE	106.2	3.09	0.000	0.000	3154.207
106	Isopropylbenzene	120.194	3.45	0.000	0.000	1643.193
107	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	380.433
108	Isopentane	72.15	2.72	0.000	0.000	6113.952
109	Methylcyclopentane	84.16	3.1	0.000	0.000	3144.209
110	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2953.740
111	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
112	o-XYLENE	106.2	3.09	0.000	0.000	3154.207

113	C1-Decalins	152.3	4.61	0.000	0.000	97.666
114	Cyclopentane	70.13	2.68	0.000	0.000	6477.830
115	Benzene	78.11	1.99	0.000	0.000	24835.468
116	trans-Decalin	138.26	4.2	0.000	0.000	214.537
117	cis-Decalin	138.26	4.2	0.000	0.000	214.537
118	Benzothiophene	134.2	2.99	0.281	0.000	1321.285
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384
138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003

143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	4444.987	0.000	0.090
166	Benzo(b)fluorene	216.3	5.77	391.970	0.000	0.439
167	Benzo(k)fluoranthene	252.3	6.11	2467.384	0.000	0.115
168	Benzo[a]anthracene	228.3	5.52	667.937	0.000	0.638
169	Benzo[a]pyrene	252.3	6.11	3431.470	0.000	0.100
170	Benzo[b]fluoranthene	252.3	6.11	1462.047	0.000	0.143
171	Benzo[e]pyrene	252.3	6.11	812.941	0.000	0.182
172	Benzo[g,h,i]perylene	276.3	6.7	2712.839	0.000	0.034

173	C1-Chrysenes	242.3	6.0683	383.098	0.000	0.261
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1505.075	0.000	0.470
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	383.098	0.000	0.079
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1505.075	0.000	0.123
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	885.176	0.000	0.572
181	C3-Chrysenes	270.4	7.03	383.098	0.000	0.037
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	5.972	0.000	1.925
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1505.075	0.000	0.051
185	C3-Fluorenes	210.3	5.58	80.660	0.000	1.217
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	885.176	0.000	0.264
188	C4-Chrysenes	284.4	7.35	383.098	0.000	0.019
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	5.972	0.000	1.217
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1505.075	0.000	0.019
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	885.176	0.000	0.147
194	Chrysene	228.3	5.52	308.794	0.000	0.876
195	Dibenz(a,h)anthracene	278.4	6.7	1722.147	0.000	0.041
196	Indeno[1,2,3-cd]pyrene	276.3	6.7	4708.378	0.000	0.027
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	8081.585	0.000	0.070
199	Retene	234.3	6.35	99.434	0.000	0.237

Table B.29. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF exposed to *Menidia beryllina* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	80.660	0.049	2.496
2	C1-Fluorenes	180.2	4.97	80.660	0.051	3.883
3	C1-Phenanthrenes/Anthracenes	192.3	4.26	885.176	0.071	7.234
4	C3-Naphthalenes	170.26	4.77	19.514	0.086	9.744
5	C4-Naphthalenes	184.3	5.18	19.514	0.023	4.359
6	C2-Naphthalenes	156.2	4.31	19.514	0.122	24.091
7	1-Methylphenanthrene	192.26	4.89	69.321	0.024	5.225
8	Phenanthrene	178.2	4.35	40.679	0.082	19.084
9	1,6,7-Trimethylnaphthalene	170.26	4.81	34.520	0.028	7.206
10	4/9-Methylphenanthrene	192.26	4.89	69.321	0.019	5.225
11	3-Methylphenanthrene	192.26	4.89	69.321	0.017	5.225
12	2-Methylphenanthrene	192.26	4.89	69.321	0.017	5.225
13	2,6-Dimethylnaphthalene	156.23	4.26	19.514	0.045	26.837
14	Fluorene	166.2	4.02	80.660	0.044	27.747
15	C2-Dibenzothiophenes	214.3	5.13	5.972	0.012	8.635
16	Pyrene	202.3	4.93	1013.086	0.002	1.698
17	C1-Dibenzothiophenes	198.3	4.71	5.972	0.019	19.756
18	Fluoranthene	202.3	4.93	754.760	0.001	1.918
19	4-Methyldibenzothiophene	198.28	4.71	5.972	0.008	19.754
20	Dibenzothiophene	184.3	4.17	5.972	0.015	58.796
21	1-Methylnaphthalene	142.2	3.72	19.952	0.014	77.574

22	1-Methyldibenzothiophene	198.28	4.71	5.972	0.003	19.754
23	Dibenzofuran	168.2	3.71	43.465	0.007	69.746
24	2/3-Methyldibenzothiophene	198.28	4.71	5.972	0.002	19.754
25	Acenaphthylene	152.2	3.94	301.058	0.000	17.782
26	Naphthalene	234.3	3.17	11.017	0.009	519.927
27	Biphenyl	154.2	3.76	0.000	0.009	617.632
28	1-Decene	140.3	5.12	0.000	0.000	67.413
29	n-C10	142.29	5.25	0.000	0.000	51.663
30	n-C10	142.29	5.25	0.000	0.000	51.663
31	n-C10	142.3	5.25	0.000	0.000	51.667
32	n-C10	142.3	5.25	0.000	0.000	51.667
33	1-Nonene	126.2	4.62	0.000	0.000	178.133
34	n-C9	128.3	4.76	0.000	0.000	133.928
35	n-C9	128.3	4.76	0.000	0.000	133.928
36	n-C9	128.3	4.76	0.000	0.000	133.928
37	n-C9	128.3	4.76	0.000	0.000	133.928
38	n-C8	114.2	4.27	0.000	0.000	342.730
39	2-Methylanthracene	192.26	4.89	885.176	0.000	1.861
40	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
41	Octene-1	112.2	4.13	0.000	0.000	455.322
42	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
43	3-methylheptane	114.2	4.2	0.000	0.000	398.540
44	n-C10	142.29	5.25	0.000	0.000	51.663
45	n-C10	142.29	5.25	0.000	0.000	51.663
46	n-C10	142.3	5.25	0.000	0.000	51.667
47	n-C10	142.3	5.25	0.000	0.000	51.667
48	2-methylheptane	114.2	4.2	0.000	0.000	398.540
49	HEPTANE	100.2	3.78	0.000	0.000	864.557
50	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645

51	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
52	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
53	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
54	Anthracene	178.2	4.35	555.417	0.000	6.694
55	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	423.719
56	n-C9	128.3	4.76	0.000	0.000	133.928
57	n-C9	128.3	4.76	0.000	0.000	133.928
58	n-C9	128.3	4.76	0.000	0.000	133.928
59	n-C9	128.3	4.76	0.000	0.000	133.928
60	C1-Naphthalenes	142.2	3.87	19.952	0.000	56.146
61	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
62	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
63	Methylcyclohexane	98.19	3.59	0.000	0.000	1275.948
64	Acenaphthene	154.2	4.15	56.658	0.000	22.347
65	n-Butylbenzene	134.2	4.01	0.000	0.000	548.780
66	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
67	C4-Benzothiophene	190.3	5.18	0.281	0.000	16.705
68	2-Methylnaphthalene	142.2	3.72	19.952	0.000	77.574
69	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
70	2-methylhexane	100.2	3.71	0.000	0.000	1005.341
71	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	423.782
72	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	482.212
73	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	423.719
74	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
75	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	482.212
76	3-methylhexane	100.2	3.71	0.000	0.000	1005.341
77	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
78	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
79	Hydrindene	118.2	3.47	0.000	0.000	1547.758

80	n-C5	72.15	2.8	0.000	0.000	5145.671
81	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2540.108
82	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	482.212
83	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	423.782
84	Propylbenzene	120.194	3.52	0.000	0.000	1413.086
85	p-XYLENE	106.2	3.09	0.000	0.000	3154.207
86	4-isopropyltoluene	134.22	4	0.000	0.000	560.819
87	sec-Butylbenzene	134.2	3.94	0.000	0.000	638.143
88	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
89	3-Methylpentane	86.18	3.21	0.000	0.000	2540.108
90	2,2-dimethylpentane	100.2	3.67	0.000	0.000	1095.856
91	n-C6	86.18	3.29	0.000	0.000	2137.825
92	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
93	C3-Benzothiophene	176.3	4.69	0.281	0.000	44.493
94	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	560.819
95	m-cymene	134.2	4	0.000	0.000	560.736
96	Ethylbenzene	106.2	3.03	0.000	0.000	3589.634
97	CYCLOHEXANE	84.16	3.18	0.000	0.000	2646.253
98	CARBAZOLE	167.2	3.23	147.059	0.000	120.597
99	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
100	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
101	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1241.739
102	m-XYLENE	106.2	3.09	0.000	0.000	3154.207
103	Isopropylbenzene	120.194	3.45	0.000	0.000	1643.193
104	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	380.433
105	Isopentane	72.15	2.72	0.000	0.000	6113.952
106	Methylcyclopentane	84.16	3.1	0.000	0.000	3144.209
107	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2953.740
108	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	1114.885

109	o-XYLENE	106.2	3.09	0.000	0.000	3154.207
110	Cyclopentane	70.13	2.68	0.000	0.000	6477.830
111	C1-Decalins	152.3	4.61	0.000	0.000	97.666
112	C2-Benzothiophene	162.25	4.13	0.281	0.000	136.895
113	Benzene	78.11	1.99	0.000	0.000	24835.468
114	Toluene	92.14	2.54	0.000	0.000	8953.934
115	trans-Decalin	138.26	4.2	0.000	0.000	214.537
116	C1-Benzothiophene	148.2	3.5365	0.281	0.000	449.333
117	cis-Decalin	138.26	4.2	0.000	0.000	214.537
118	Benzothiophene	134.2	2.99	0.281	0.000	1321.285
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384

138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	4444.987	0.000	0.090
166	Benzo(b)fluorene	216.3	5.77	391.970	0.000	0.439

167	Benzo(k)fluoranthene	252.3	6.11	2467.384	0.000	0.115
168	Benzo[a]anthracene	228.3	5.52	667.937	0.000	0.638
169	Benzo[a]pyrene	252.3	6.11	3431.470	0.000	0.100
170	Benzo[b]fluoranthene	252.3	6.11	1462.047	0.000	0.143
171	Benzo[e]pyrene	252.3	6.11	812.941	0.000	0.182
172	Benzo[g,h,i]perylene	276.3	6.7	2712.839	0.000	0.034
173	C1-Chrysenes	242.3	6.0683	383.098	0.000	0.261
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1505.075	0.000	0.470
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	383.098	0.000	0.079
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1505.075	0.000	0.123
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	885.176	0.000	0.572
181	C3-Chrysenes	270.4	7.03	383.098	0.000	0.037
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	5.972	0.000	1.925
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1505.075	0.000	0.051
185	C3-Fluorenes	210.3	5.58	80.660	0.000	1.217
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	885.176	0.000	0.264
188	C4-Chrysenes	284.4	7.35	383.098	0.000	0.019
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	5.972	0.000	1.217
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1505.075	0.000	0.019
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	885.176	0.000	0.147
194	Chrysene	228.3	5.52	308.794	0.000	0.876
195	Dibenz(a,h)anthracene	278.4	6.7	1722.147	0.000	0.041

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	4708.378	0.000	0.027
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	8081.585	0.000	0.070
199	Retene	234.3	6.35	99.434	0.000	0.237

Table B.30. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF duplicate exposed to *Menidia beryllina* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	80.6598	0.0523	2.49581
2	C1-Fluorenes	180.2	4.97	80.6598	0.0514	3.8827
3	C1-Phenanthrenes/Anthracenes	192.3	4.26	885.176	0.0675	7.2344
4	C3-Naphthalenes	170.26	4.77	19.5142	0.0888	9.74368
5	C4-Naphthalenes	184.3	5.18	19.5142	0.0263	4.35889
6	C2-Naphthalenes	156.2	4.31	19.5142	0.123	24.0908
7	Phenanthrene	178.2	4.35	40.6789	0.0841	19.084
8	1-Methylphenanthrene	192.26	4.89	69.3211	0.0225	5.22482
9	1,6,7-Trimethylnaphthalene	170.26	4.81	34.5202	0.0272	7.20613
10	4/9-Methylphenanthrene	192.26	4.89	69.3211	0.0192	5.22482
11	2-Methylphenanthrene	192.26	4.89	69.3211	0.0178	5.22482
12	3-Methylphenanthrene	192.26	4.89	69.3211	0.0165	5.22482
13	2,6-Dimethylnaphthalene	156.23	4.26	19.5142	0.0462	26.8371
14	Fluorene	166.2	4.02	80.6598	0.0471	27.7466
15	C2-Dibenzothiophenes	214.3	5.13	5.97181	0.0126	8.63546
16	Pyrene	202.3	4.93	1013.09	0.00216	1.69822
17	C1-Dibenzothiophenes	198.3	4.71	5.97181	0.0181	19.7563
18	Fluoranthene	202.3	4.93	754.76	0.0011	1.91845
19	4-Methyldibenzothiophene	198.28	4.71	5.97181	0.00754	19.7543
20	Dibenzothiophene	184.3	4.17	5.97181	0.0156	58.7961
21	1-Methylnaphthalene	142.2	3.72	19.9522	0.0153	77.5743

22	1-Methyldibenzothiophene	198.28	4.71	5.97181	0.00336	19.7543
23	Dibenzofuran	168.2	3.71	43.4655	0.00715	69.7464
24	2/3-Methyldibenzothiophene	198.28	4.71	5.97181	0.00112	19.7543
25	Acenaphthylene	152.2	3.94	301.058	0.00062	17.7824
26	Naphthalene	234.3	3.17	11.0167	0.0128	519.927
27	Biphenyl	154.2	3.76	0	0.0109	617.632
28	Ethylbenzene	106.2	3.03	0	0.0181	3589.63
29	1-Decene	140.3	5.12	0	0	67.413
30	n-C10	142.29	5.25	0	0	51.6631
31	n-C10	142.29	5.25	0	0	51.6631
32	n-C10	142.3	5.25	0	0	51.6667
33	n-C10	142.3	5.25	0	0	51.6667
34	2-Methylanthracene	192.26	4.89	885.176	0	1.86051
35	1-Nonene	126.2	4.62	0	0	178.133
36	n-C9	128.3	4.76	0	0	133.928
37	n-C9	128.3	4.76	0	0	133.928
38	n-C9	128.3	4.76	0	0	133.928
39	n-C9	128.3	4.76	0	0	133.928
40	n-C10	142.29	5.25	0	0	51.6631
41	n-C10	142.29	5.25	0	0	51.6631
42	n-C10	142.3	5.25	0	0	51.6667
43	n-C10	142.3	5.25	0	0	51.6667
44	n-C8	114.2	4.27	0	0	342.73
45	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0	0	505.163
46	Octene-1	112.2	4.13	0	0	455.322
47	n-Pentylbenzene	148.2	4.5	0	0	270.928
48	3-methylheptane	114.2	4.2	0	0	398.54
49	Anthracene	178.2	4.35	555.417	0	6.69437
50	2-methylheptane	114.2	4.2	0	0	398.54

51	HEPTANE	100.2	3.78	0	0	864.557
52	2,3,4-trimethylpentane	114.2	4.05	0	0	550.645
53	n-C9	128.3	4.76	0	0	133.928
54	n-C9	128.3	4.76	0	0	133.928
55	n-C9	128.3	4.76	0	0	133.928
56	n-C9	128.3	4.76	0	0	133.928
57	2,5-Dimethylhexane	114.23	4.12	0	0	473.659
58	Pentane, 2,3,3-trimethyl	114.23	4.09	0	0	505.296
59	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0	0	482.284
60	C1-Naphthalenes	142.2	3.87	19.9522	0	56.1459
61	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0	0	423.719
62	C4-Benzothiophene	190.3	5.18	0.28077	0	16.7049
63	1,1,3-trimethylpentane	114.23	4.12	0	0	473.659
64	2,3-dimethylhexane	114.2	4.12	0	0	473.535
65	Acenaphthene	154.2	4.15	56.6577	0	22.3473
66	Methylcyclohexane	98.19	3.59	0	0	1275.95
67	2-Methylnaphthalene	142.2	3.72	19.9522	0	77.5743
68	n-Butylbenzene	134.2	4.01	0	0	548.78
69	2,4-dimethylpentane	100.2	3.63	0	0	1194.52
70	tert-Butylbenzene	134.2	3.9	0	0	695.598
71	2-methylhexane	100.2	3.71	0	0	1005.34
72	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0	0	423.782
73	1-Methyl-2-n-Propylbenzene	134.2	4.07	0	0	482.212
74	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0	0	423.719
75	3-ethylhexane	114.2	4.2	0	0	398.54
76	1-methyl-3-n-propylbenzene	134.2	4.07	0	0	482.212
77	3-methylhexane	100.2	3.71	0	0	1005.34
78	C3-Benzothiophene	176.3	4.69	0.28077	0	44.4935
79	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0	0	423.719

80	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0	0	423.719
81	Hydrindene	118.2	3.47	0	0	1547.76
82	n-C5	72.15	2.8	0	0	5145.67
83	CARBAZOLE	167.2	3.23	147.059	0	120.597
84	2-METHYLPENTANE	86.18	3.21	0	0	2540.11
85	1,2-Diethylbenzene	134.2	4.07	0	0	482.212
86	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0	0	423.782
87	Propylbenzene	120.194	3.52	0	0	1413.09
88	p-XYLENE	106.2	3.09	0	0	3154.21
89	4-isopropyltoluene	134.22	4	0	0	560.819
90	n-C6	86.18	3.29	0	0	2137.83
91	sec-Butylbenzene	134.2	3.94	0	0	638.143
92	2,3-dimethylpentane	100.2	3.63	0	0	1194.52
93	3-Methylpentane	86.18	3.21	0	0	2540.11
94	2,2-dimethylpentane	100.2	3.67	0	0	1095.86
95	1,2,4-Trimethylbenzene	120.2	3.63	0	0	1114.89
96	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0	0	560.819
97	m-cymene	134.2	4	0	0	560.736
98	CYCLOHEXANE	84.16	3.18	0	0	2646.25
99	C1-Decalins	152.3	4.61	0	0	97.6665
100	1-Methyl-3-ethylbenzene	120.2	3.58	0	0	1241.74
101	1-Methyl-2-ethylbenzene	120.2	3.58	0	0	1241.74
102	C2-Benzothiophene	162.25	4.13	0.28077	0	136.895
103	4-ETHYLTOLUENE	120.2	3.58	0	0	1241.74
104	m-XYLENE	106.2	3.09	0	0	3154.21
105	Isopropylbenzene	120.194	3.45	0	0	1643.19
106	1,2,4,5-Tetramethylbenzene	134.2	4.18	0	0	380.433
107	Isopentane	72.15	2.72	0	0	6113.95
108	Methylcyclopentane	84.16	3.1	0	0	3144.21

109	2,3-dimethylbutane	86.18	3.14	0	0	2953.74
110	1,3,5-trimethylbenzene	120.2	3.63	0	0	1114.89
111	o-XYLENE	106.2	3.09	0	0	3154.21
112	Cyclopentane	70.13	2.68	0	0	6477.83
113	trans-Decalin	138.26	4.2	0	0	214.537
114	C1-Benzothiophene	148.2	3.5365	0.28077	0	449.333
115	Toluene	92.14	2.54	0	0	8953.93
116	Benzene	78.11	1.99	0	0	24835.5
117	cis-Decalin	138.26	4.2	0	0	214.537
118	Benzothiophene	134.2	2.99	0.28077	0	1321.29
119	n-C11	156.31	5.74	0	0	19.7402
120	n-C11	156.31	5.74	0	0	19.7402
121	n-C11	156.31	5.74	0	0	19.7402
122	n-C11	156.31	5.74	0	0	19.7402
123	n-C12	170.34	6.23	0	0	7.48242
124	n-C12	170.34	6.23	0	0	7.48242
125	n-C12	170.34	6.23	0	0	7.48242
126	n-C12	170.34	6.23	0	0	7.48242
127	n-C11	156.31	5.74	0	0	19.7402
128	n-C11	156.31	5.74	0	0	19.7402
129	n-C11	156.31	5.74	0	0	19.7402
130	n-C11	156.31	5.74	0	0	19.7402
131	n-C12	170.34	6.23	0	0	7.48242
132	n-C12	170.34	6.23	0	0	7.48242
133	n-C12	170.34	6.23	0	0	7.48242
134	n-C12	170.34	6.23	0	0	7.48242
135	n-C13	184.37	6.73	0	0	2.75687
136	n-C14	198.4	7.22	0	0	1.03188
137	n-C15	212.42	7.71	0	0	0.38427

138	n-C16	226.45	8.2	0	0	0.14249
139	n-C17	240.48	8.69	0	0	0.05263
140	n-C18	254.5	9.18	0	0	0.01937
141	n-C19	268.53	9.67	0	0	0.00711
142	n-C20	282.56	10.1	0	0	0.00296
143	n-C21	296.59	10.6	0	0	0.00106
144	n-C22	310.61	11.1	0	0	0.00038
145	n-C23	324.64	11.6	0	0	0.00013
146	n-C24	338.67	12.1	0	0	4.77E-05
147	n-C25	352.69	12.6	0	0	1.69E-05
148	n-C26	366.72	13.1	0	0	5.98E-06
149	n-C27	380.75	13.6	0	0	2.11E-06
150	n-C28	394.77	14	0	0	9.25E-07
151	n-C29	408.8	14.5	0	0	3.26E-07
152	n-C30	422.83	15	0	0	1.15E-07
153	n-C31	436.86	15.5	0	0	4.04E-08
154	n-C32	450.88	16	0	0	1.42E-08
155	n-C33	464.91	16.5	0	0	4.98E-09
156	n-C34	478.94	17	0	0	1.75E-09
157	n-C35	492.96	17.5	0	0	6.12E-10
158	n-C36	506.981	18	0	0	2.14E-10
159	n-C37	521	18.5	0	0	7.50E-11
160	n-C38	535	19	0	0	2.62E-11
161	n-C39	549.1	19.49	0	0	9.35E-12
162	n-C40	563.1	19.9	0	0	3.96E-12
163	Phytane	282.56	9.87	0	0	0.00486
164	Pristane	268.525	9.38	0	0	0.01328
165	Benzo(a)fluoranthene	252.3	6.11	4444.99	0	0.08977
166	Benzo(b)fluorene	216.3	5.77	391.97	0	0.43945

167	Benzo(k)fluoranthene	252.3	6.11	2467.38	0	0.1149
168	Benzo[a]anthracene	228.3	5.52	667.937	0	0.63849
169	Benzo[a]pyrene	252.3	6.11	3431.47	0	0.10007
170	Benzo[b]fluoranthene	252.3	6.11	1462.05	0	0.14295
171	Benzo[e]pyrene	252.3	6.11	812.941	0	0.18241
172	Benzo[g,h,i]perylene	276.3	6.7	2712.84	0	0.03391
173	C1-Chrysenes	242.3	6.0683	383.098	0	0.26126
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1505.07	0	0.47042
175	C1-naphthobenzothiophenes	248.3	6.38	0	0	3.50996
176	C2-Chrysenes	256.3	6.65	383.098	0	0.07889
177	C2-Decalins	166.3	6.19	0	0	3.54045
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1505.07	0	0.12348
179	C2-naphthobenzothiophenes	262.4	6.86	0	0	1.31829
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	885.176	0	0.57196
181	C3-Chrysenes	270.4	7.03	383.098	0	0.03669
182	C3-Decalins	180.3	6.79	0	0	1.05332
183	C3-Dibenzothiophenes	230.37	5.86	5.97181	0	1.92491
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1505.07	0	0.05075
185	C3-Fluorenes	210.3	5.58	80.6598	0	1.21691
186	C3-naphthobenzothiophenes	276.4	7.36	0	0	0.4727
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	885.176	0	0.26353
188	C4-Chrysenes	284.4	7.35	383.098	0	0.01936
189	C4-Decalins	194.3	7.34	0	0	0.34693
190	C4-Dibenzothiophenes	244.37	6.1	5.97181	0	1.21728
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1505.07	0	0.01907
192	C4-naphthobenzothiophenes	290.4	7.84	0	0	0.17651
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	885.176	0	0.14682
194	Chrysene	228.3	5.52	308.794	0	0.87641
195	Dibenz(a,h)anthracene	278.4	6.7	1722.15	0	0.04131

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	4708.38	0	0.02691
197	Naphthobenzothiophenes	178.2	5.34	0	0	23.6959
198	Perylene	252.3	6.11	8081.58	0	0.0698
199	Retene	234.3	6.35	99.4344	0	0.23739

Table B.31. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 100% WAF exposed to *Menidia beryllina* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	130.346	0.930	2.062
2	C1-Fluorenes	180.2	4.97	130.346	1.010	3.208
3	C3-Naphthalenes	170.26	4.77	37.373	1.840	7.619
4	C1-Phenanthrenes/Anthracenes	192.3	4.26	1677.722	1.240	5.546
5	C2-Naphthalenes	156.2	4.31	37.373	2.430	18.839
6	C4-Naphthalenes	184.3	5.18	37.373	0.432	3.409
7	1,6,7-Trimethylnaphthalene	170.26	4.81	44.783	0.555	6.519
8	Phenanthrene	178.2	4.35	51.952	1.400	17.359
9	1-Methylphenanthrene	192.26	4.89	82.404	0.371	4.881
10	4/9-Methylphenanthrene	192.26	4.89	82.404	0.359	4.881
11	2-Methylphenanthrene	192.26	4.89	82.404	0.312	4.881
12	3-Methylphenanthrene	192.26	4.89	82.404	0.298	4.881
13	2,6-Dimethylnaphthalene	156.23	4.26	37.373	0.927	20.986
14	C2-Dibenzothiophenes	214.3	5.13	11.078	0.242	6.946
15	Fluorene	166.2	4.02	130.346	0.766	22.925
16	C1-Dibenzothiophenes	198.3	4.71	11.078	0.354	15.892
17	Pyrene	202.3	4.93	2291.602	0.016	1.209
18	4-Methyldibenzothiophene	198.28	4.71	11.078	0.141	15.891
19	C1-Naphthalenes	142.2	3.87	25.285	0.300	51.372
20	Dibenzothiophene	184.3	4.17	11.078	0.274	47.296
21	2/3-Methyldibenzothiophene	198.28	4.71	9.703	0.079	16.663

22	Fluoranthene	202.3	4.93	1355.371	0.006	1.505
23	1-Methyldibenzothiophene	198.28	4.71	11.078	0.058	15.891
24	1-Methylnaphthalene	142.2	3.72	25.285	0.254	70.978
25	2-Methylnaphthalene	142.2	3.72	25.285	0.210	70.978
26	C4-Benzothiophene	190.3	5.18	0.582	0.034	13.994
27	Acenaphthene	154.2	4.15	89.499	0.038	18.669
28	Dibenzofuran	168.2	3.71	43.589	0.115	69.670
29	Anthracene	178.2	4.35	1007.917	0.008	5.232
30	C3-Benzothiophene	176.3	4.69	0.582	0.051	37.274
31	Acenaphthylene	152.2	3.94	678.887	0.006	12.736
32	C2-Benzothiophene	162.25	4.13	0.582	0.037	114.684
33	Biphenyl	154.2	3.76	0.000	0.166	617.632
34	CARBAZOLE	167.2	3.23	241.556	0.010	98.693
35	C1-Benzothiophene	148.2	3.5365	0.582	0.027	376.428
36	Naphthalene	234.3	3.17	15.049	0.015	464.200
37	m-XYLENE	106.2	3.09	0.000	0.028	3154.207
38	trans-Decalin	138.26	4.2	0.000	0.002	214.537
39	Toluene	92.14	2.54	0.000	0.071	8953.934
40	o-XYLENE	106.2	3.09	0.000	0.018	3154.207
41	p-XYLENE	106.2	3.09	0.000	0.015	3154.207
42	Ethylbenzene	106.2	3.03	0.000	0.014	3589.634
43	n-C10	142.29	5.25	0.000	0.000	51.663
44	n-C10	142.29	5.25	0.000	0.000	51.663
45	n-C10	142.3	5.25	0.000	0.000	51.667
46	n-C10	142.3	5.25	0.000	0.000	51.667
47	1-Decene	140.3	5.12	0.000	0.000	67.413
48	n-C9	128.3	4.76	0.000	0.000	133.928
49	n-C9	128.3	4.76	0.000	0.000	133.928
50	n-C9	128.3	4.76	0.000	0.000	133.928

51	n-C9	128.3	4.76	0.000	0.000	133.928
52	1-Nonene	126.2	4.62	0.000	0.000	178.133
53	n-C10	142.29	5.25	0.000	0.000	51.663
54	n-C10	142.29	5.25	0.000	0.000	51.663
55	n-C10	142.3	5.25	0.000	0.000	51.667
56	n-C10	142.3	5.25	0.000	0.000	51.667
57	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
58	n-C8	114.2	4.27	0.000	0.000	342.730
59	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
60	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
61	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	423.719
62	Octene-1	112.2	4.13	0.000	0.000	455.322
63	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
64	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
65	3-methylheptane	114.2	4.2	0.000	0.000	398.540
66	n-C9	128.3	4.76	0.000	0.000	133.928
67	n-C9	128.3	4.76	0.000	0.000	133.928
68	n-C9	128.3	4.76	0.000	0.000	133.928
69	n-C9	128.3	4.76	0.000	0.000	133.928
70	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
71	2-Methylanthracene	192.26	4.89	1677.722	0.000	1.426
72	2-methylheptane	114.2	4.2	0.000	0.000	398.540
73	HEPTANE	100.2	3.78	0.000	0.000	864.557
74	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
75	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	423.719
76	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
77	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
78	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	423.782
79	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	482.212

80	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	482.212
81	n-Butylbenzene	134.2	4.01	0.000	0.000	548.780
82	Methylcyclohexane	98.19	3.59	0.000	0.000	1275.948
83	sec-Butylbenzene	134.2	3.94	0.000	0.000	638.143
84	Hydrindene	118.2	3.47	0.000	0.000	1547.758
85	Propylbenzene	120.194	3.52	0.000	0.000	1413.086
86	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	423.782
87	n-C6	86.18	3.29	0.000	0.000	2137.825
88	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
89	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
90	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	482.212
91	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
92	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	560.819
93	m-cymene	134.2	4	0.000	0.000	560.736
94	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
95	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
96	4-isopropyltoluene	134.22	4	0.000	0.000	560.819
97	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
98	CYCLOHEXANE	84.16	3.18	0.000	0.000	2646.253
99	n-C5	72.15	2.8	0.000	0.000	5145.671
100	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1241.739
101	2-methylhexane	100.2	3.71	0.000	0.000	1005.341
102	Isopropylbenzene	120.194	3.45	0.000	0.000	1643.193
103	3-Methylpentane	86.18	3.21	0.000	0.000	2540.108
104	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
105	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
106	3-methylhexane	100.2	3.71	0.000	0.000	1005.341
107	2,2-dimethylpentane	100.2	3.67	0.000	0.000	1095.856
108	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520

109	Methylcyclopentane	84.16	3.1	0.000	0.000	3144.209
110	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2540.108
111	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	380.433
112	Cyclopentane	70.13	2.68	0.000	0.000	6477.830
113	Benzene	78.11	1.99	0.000	0.000	24835.468
114	Isopentane	72.15	2.72	0.000	0.000	6113.952
115	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2953.740
116	C1-Decalins	152.3	4.61	0.000	0.000	97.666
117	cis-Decalin	138.26	4.2	0.000	0.000	214.537
118	Benzothiophene	134.2	2.99	0.582	0.000	1106.904
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384

138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	4780.805	0.000	0.087
166	Benzo(b)fluorene	216.3	5.77	860.457	0.000	0.318

167	Benzo(k)fluoranthene	252.3	6.11	4167.522	0.000	0.092
168	Benzo[a]anthracene	228.3	5.52	1186.537	0.000	0.503
169	Benzo[a]pyrene	252.3	6.11	6076.786	0.000	0.079
170	Benzo[b]fluoranthene	252.3	6.11	2548.196	0.000	0.113
171	Benzo[e]pyrene	252.3	6.11	1726.025	0.000	0.133
172	Benzo[g,h,i]perylene	276.3	6.7	4922.741	0.000	0.026
173	C1-Chrysenes	242.3	6.0683	826.307	0.000	0.190
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2971.001	0.000	0.354
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	826.307	0.000	0.057
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2971.001	0.000	0.093
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1677.722	0.000	0.438
181	C3-Chrysenes	270.4	7.03	826.307	0.000	0.027
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	11.078	0.000	1.548
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2971.001	0.000	0.038
185	C3-Fluorenes	210.3	5.58	130.346	0.000	1.005
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1677.722	0.000	0.202
188	C4-Chrysenes	284.4	7.35	826.307	0.000	0.014
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	11.078	0.000	0.979
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2971.001	0.000	0.014
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1677.722	0.000	0.113
194	Chrysene	228.3	5.52	655.692	0.000	0.643
195	Dibenz(a,h)anthracene	278.4	6.7	2902.389	0.000	0.033

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	7151.312	0.000	0.023
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	7919.021	0.000	0.070
199	Retene	234.3	6.35	121.648	0.000	0.219

Table B.32. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 25% WAF exposed to *Menidia beryllina* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	130.346	0.253	2.062
2	C1-Fluorenes	180.2	4.97	130.346	0.254	3.208
3	C1-Phenanthrenes/Anthracenes	192.3	4.26	1677.722	0.327	5.546
4	C3-Naphthalenes	170.26	4.77	37.373	0.439	7.619
5	C2-Naphthalenes	156.2	4.31	37.373	0.584	18.839
6	C4-Naphthalenes	184.3	5.18	37.373	0.104	3.409
7	Phenanthrene	178.2	4.35	51.952	0.363	17.359
8	1,6,7-Trimethylnaphthalene	170.26	4.81	44.783	0.130	6.519
9	1-Methylphenanthrene	192.26	4.89	82.404	0.097	4.881
10	4/9-Methylphenanthrene	192.26	4.89	82.404	0.092	4.881
11	2-Methylphenanthrene	192.26	4.89	82.404	0.079	4.881
12	3-Methylphenanthrene	192.26	4.89	82.404	0.077	4.881
13	2,6-Dimethylnaphthalene	156.23	4.26	37.373	0.218	20.986
14	Fluorene	166.2	4.02	130.346	0.188	22.925
15	C2-Dibenzothiophenes	214.3	5.13	11.078	0.053	6.946
16	C1-Dibenzothiophenes	198.3	4.71	11.078	0.074	15.892
17	Pyrene	202.3	4.93	2291.602	0.005	1.209
18	4-Methyldibenzothiophene	198.28	4.71	11.078	0.035	15.891
19	Dibenzothiophene	184.3	4.17	11.078	0.069	47.296
20	C1-Naphthalenes	142.2	3.87	25.285	0.073	51.372
21	Fluoranthene	202.3	4.93	1355.371	0.002	1.505

22	1-Methyldibenzothiophene	198.28	4.71	11.078	0.014	15.891
23	1-Methylnaphthalene	142.2	3.72	25.285	0.062	70.978
24	2-Methylnaphthalene	142.2	3.72	25.285	0.050	70.978
25	C4-Benzothiophene	190.3	5.18	0.582	0.008	13.994
26	Acenaphthene	154.2	4.15	89.499	0.010	18.669
27	2/3-Methyldibenzothiophene	198.28	4.71	9.703	0.008	16.663
28	Dibenzofuran	168.2	3.71	43.589	0.028	69.670
29	C3-Benzothiophene	176.3	4.69	0.582	0.015	37.274
30	C2-Benzothiophene	162.25	4.13	0.582	0.011	114.684
31	Biphenyl	154.2	3.76	0.000	0.040	617.632
32	C1-Benzothiophene	148.2	3.5365	0.582	0.009	376.428
33	trans-Decalin	138.26	4.2	0.000	0.001	214.537
34	Toluene	92.14	2.54	0.000	0.024	8953.934
35	n-C10	142.29	5.25	0.000	0.000	51.663
36	n-C10	142.29	5.25	0.000	0.000	51.663
37	n-C10	142.3	5.25	0.000	0.000	51.667
38	n-C10	142.3	5.25	0.000	0.000	51.667
39	1-Decene	140.3	5.12	0.000	0.000	67.413
40	n-C9	128.3	4.76	0.000	0.000	133.928
41	n-C9	128.3	4.76	0.000	0.000	133.928
42	n-C9	128.3	4.76	0.000	0.000	133.928
43	n-C9	128.3	4.76	0.000	0.000	133.928
44	1-Nonene	126.2	4.62	0.000	0.000	178.133
45	n-C10	142.29	5.25	0.000	0.000	51.663
46	n-C10	142.29	5.25	0.000	0.000	51.663
47	n-C10	142.3	5.25	0.000	0.000	51.667
48	n-C10	142.3	5.25	0.000	0.000	51.667
49	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
50	n-C8	114.2	4.27	0.000	0.000	342.730

51	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
52	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
53	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	423.719
54	Octene-1	112.2	4.13	0.000	0.000	455.322
55	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
56	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
57	3-methylheptane	114.2	4.2	0.000	0.000	398.540
58	n-C9	128.3	4.76	0.000	0.000	133.928
59	n-C9	128.3	4.76	0.000	0.000	133.928
60	n-C9	128.3	4.76	0.000	0.000	133.928
61	n-C9	128.3	4.76	0.000	0.000	133.928
62	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
63	2-Methylanthracene	192.26	4.89	1677.722	0.000	1.426
64	2-methylheptane	114.2	4.2	0.000	0.000	398.540
65	HEPTANE	100.2	3.78	0.000	0.000	864.557
66	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
67	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	423.719
68	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
69	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
70	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	423.782
71	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	482.212
72	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	482.212
73	n-Butylbenzene	134.2	4.01	0.000	0.000	548.780
74	Methylcyclohexane	98.19	3.59	0.000	0.000	1275.948
75	sec-Butylbenzene	134.2	3.94	0.000	0.000	638.143
76	Hydrindene	118.2	3.47	0.000	0.000	1547.758
77	Propylbenzene	120.194	3.52	0.000	0.000	1413.086
78	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	423.782
79	n-C6	86.18	3.29	0.000	0.000	2137.825

80	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
81	Anthracene	178.2	4.35	1007.917	0.000	5.232
82	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
83	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	482.212
84	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
85	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	560.819
86	m-cymene	134.2	4	0.000	0.000	560.736
87	Ethylbenzene	106.2	3.03	0.000	0.000	3589.634
88	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
89	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
90	4-isopropyltoluene	134.22	4	0.000	0.000	560.819
91	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
92	CYCLOHEXANE	84.16	3.18	0.000	0.000	2646.253
93	n-C5	72.15	2.8	0.000	0.000	5145.671
94	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1241.739
95	p-XYLENE	106.2	3.09	0.000	0.000	3154.207
96	2-methylhexane	100.2	3.71	0.000	0.000	1005.341
97	Isopropylbenzene	120.194	3.45	0.000	0.000	1643.193
98	3-Methylpentane	86.18	3.21	0.000	0.000	2540.108
99	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
100	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
101	3-methylhexane	100.2	3.71	0.000	0.000	1005.341
102	2,2-dimethylpentane	100.2	3.67	0.000	0.000	1095.856
103	Acenaphthylene	152.2	3.94	678.887	0.000	12.736
104	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
105	Methylcyclopentane	84.16	3.1	0.000	0.000	3144.209
106	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2540.108
107	o-XYLENE	106.2	3.09	0.000	0.000	3154.207
108	m-XYLENE	106.2	3.09	0.000	0.000	3154.207

109	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	380.433
110	Cyclopentane	70.13	2.68	0.000	0.000	6477.830
111	Benzene	78.11	1.99	0.000	0.000	24835.468
112	Isopentane	72.15	2.72	0.000	0.000	6113.952
113	CARBAZOLE	167.2	3.23	241.556	0.000	98.693
114	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2953.740
115	C1-Decalins	152.3	4.61	0.000	0.000	97.666
116	Naphthalene	234.3	3.17	15.049	0.000	464.200
117	cis-Decalin	138.26	4.2	0.000	0.000	214.537
118	Benzothiophene	134.2	2.99	0.582	0.000	1106.904
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384

138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	4780.805	0.000	0.087
166	Benzo(b)fluorene	216.3	5.77	860.457	0.000	0.318

167	Benzo(k)fluoranthene	252.3	6.11	4167.522	0.000	0.092
168	Benzo[a]anthracene	228.3	5.52	1186.537	0.000	0.503
169	Benzo[a]pyrene	252.3	6.11	6076.786	0.000	0.079
170	Benzo[b]fluoranthene	252.3	6.11	2548.196	0.000	0.113
171	Benzo[e]pyrene	252.3	6.11	1726.025	0.000	0.133
172	Benzo[g,h,i]perylene	276.3	6.7	4922.741	0.000	0.026
173	C1-Chrysenes	242.3	6.0683	826.307	0.000	0.190
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2971.001	0.000	0.354
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	826.307	0.000	0.057
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2971.001	0.000	0.093
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1677.722	0.000	0.438
181	C3-Chrysenes	270.4	7.03	826.307	0.000	0.027
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	11.078	0.000	1.548
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2971.001	0.000	0.038
185	C3-Fluorenes	210.3	5.58	130.346	0.000	1.005
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1677.722	0.000	0.202
188	C4-Chrysenes	284.4	7.35	826.307	0.000	0.014
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	11.078	0.000	0.979
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2971.001	0.000	0.014
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1677.722	0.000	0.113
194	Chrysene	228.3	5.52	655.692	0.000	0.643
195	Dibenz(a,h)anthracene	278.4	6.7	2902.389	0.000	0.033

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	7151.312	0.000	0.023
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	7919.021	0.000	0.070
199	Retene	234.3	6.35	121.648	0.000	0.219

Table B.33. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF exposed to *Menidia beryllina* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	Pyrene	202.3	4.93	2291.602	0.092	1.209
2	Fluoranthene	202.3	4.93	1355.371	0.057	1.505
3	C2-Fluorenes	194.3	5.21	130.346	0.063	2.062
4	C1-Phenanthrenes/Anthracenes	192.3	4.26	1677.722	0.158	5.546
5	C1-Fluorenes	180.2	4.97	130.346	0.065	3.208
6	C3-Naphthalenes	170.26	4.77	37.373	0.106	7.619
7	2-Methylanthracene	192.26	4.89	1677.722	0.013	1.426
8	4/9-Methylphenanthrene	192.26	4.89	82.404	0.043	4.881
9	1-Methylphenanthrene	192.26	4.89	82.404	0.043	4.881
10	C4-Naphthalenes	184.3	5.18	37.373	0.030	3.409
11	2-Methylphenanthrene	192.26	4.89	82.404	0.034	4.881
12	C2-Naphthalenes	156.2	4.31	37.373	0.125	18.839
13	Phenanthrene	178.2	4.35	51.952	0.114	17.359
14	3-Methylphenanthrene	192.26	4.89	82.404	0.032	4.881
15	Anthracene	178.2	4.35	1007.917	0.029	5.232
16	C2-Dibenzothiophenes	214.3	5.13	11.078	0.036	6.946
17	1,6,7-Trimethylnaphthalene	170.26	4.81	44.783	0.029	6.519
18	Acenaphthylene	152.2	3.94	678.887	0.055	12.736
19	2,6-Dimethylnaphthalene	156.23	4.26	37.373	0.043	20.986
20	Fluorene	166.2	4.02	130.346	0.045	22.925
21	C1-Dibenzothiophenes	198.3	4.71	11.078	0.027	15.892

22	2/3-Methyldibenzothiophene	198.28	4.71	9.703	0.012	16.663
23	4-Methyldibenzothiophene	198.28	4.71	11.078	0.011	15.891
24	C1-Naphthalenes	142.2	3.87	25.285	0.019	51.372
25	Dibenzothiophene	184.3	4.17	11.078	0.018	47.296
26	1-Methyldibenzothiophene	198.28	4.71	11.078	0.005	15.891
27	Acenaphthene	154.2	4.15	89.499	0.005	18.669
28	1-Methylnaphthalene	142.2	3.72	25.285	0.016	70.978
29	2-Methylnaphthalene	142.2	3.72	25.285	0.013	70.978
30	Dibenzofuran	168.2	3.71	43.589	0.006	69.670
31	Biphenyl	154.2	3.76	0.000	0.009	617.632
32	Toluene	92.14	2.54	0.000	0.016	8953.934
33	n-C10	142.29	5.25	0.000	0.000	51.663
34	n-C10	142.29	5.25	0.000	0.000	51.663
35	n-C10	142.3	5.25	0.000	0.000	51.667
36	n-C10	142.3	5.25	0.000	0.000	51.667
37	1-Decene	140.3	5.12	0.000	0.000	67.413
38	n-C10	142.29	5.25	0.000	0.000	51.663
39	n-C10	142.29	5.25	0.000	0.000	51.663
40	n-C10	142.3	5.25	0.000	0.000	51.667
41	n-C10	142.3	5.25	0.000	0.000	51.667
42	n-C9	128.3	4.76	0.000	0.000	133.928
43	n-C9	128.3	4.76	0.000	0.000	133.928
44	n-C9	128.3	4.76	0.000	0.000	133.928
45	n-C9	128.3	4.76	0.000	0.000	133.928
46	1-Nonene	126.2	4.62	0.000	0.000	178.133
47	n-C9	128.3	4.76	0.000	0.000	133.928
48	n-C9	128.3	4.76	0.000	0.000	133.928
49	n-C9	128.3	4.76	0.000	0.000	133.928
50	n-C9	128.3	4.76	0.000	0.000	133.928

51	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
52	n-C8	114.2	4.27	0.000	0.000	342.730
53	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
54	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
55	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	423.719
56	Octene-1	112.2	4.13	0.000	0.000	455.322
57	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
58	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
59	3-methylheptane	114.2	4.2	0.000	0.000	398.540
60	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
61	2-methylheptane	114.2	4.2	0.000	0.000	398.540
62	HEPTANE	100.2	3.78	0.000	0.000	864.557
63	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
64	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	423.719
65	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
66	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
67	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	423.782
68	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	482.212
69	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	482.212
70	n-Butylbenzene	134.2	4.01	0.000	0.000	548.780
71	Methylcyclohexane	98.19	3.59	0.000	0.000	1275.948
72	sec-Butylbenzene	134.2	3.94	0.000	0.000	638.143
73	Hydrindene	118.2	3.47	0.000	0.000	1547.758
74	Propylbenzene	120.194	3.52	0.000	0.000	1413.086
75	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	423.782
76	n-C6	86.18	3.29	0.000	0.000	2137.825
77	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
78	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
79	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	482.212

80	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
81	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	560.819
82	m-cymene	134.2	4	0.000	0.000	560.736
83	Ethylbenzene	106.2	3.03	0.000	0.000	3589.634
84	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
85	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
86	4-isopropyltoluene	134.22	4	0.000	0.000	560.819
87	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
88	C4-Benzothiophene	190.3	5.18	0.582	0.000	13.994
89	CYCLOHEXANE	84.16	3.18	0.000	0.000	2646.253
90	n-C5	72.15	2.8	0.000	0.000	5145.671
91	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1241.739
92	p-XYLENE	106.2	3.09	0.000	0.000	3154.207
93	2-methylhexane	100.2	3.71	0.000	0.000	1005.341
94	Isopropylbenzene	120.194	3.45	0.000	0.000	1643.193
95	3-Methylpentane	86.18	3.21	0.000	0.000	2540.108
96	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
97	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
98	3-methylhexane	100.2	3.71	0.000	0.000	1005.341
99	2,2-dimethylpentane	100.2	3.67	0.000	0.000	1095.856
100	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
101	Methylcyclopentane	84.16	3.1	0.000	0.000	3144.209
102	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2540.108
103	o-XYLENE	106.2	3.09	0.000	0.000	3154.207
104	m-XYLENE	106.2	3.09	0.000	0.000	3154.207
105	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	380.433
106	C3-Benzothiophene	176.3	4.69	0.582	0.000	37.274
107	Cyclopentane	70.13	2.68	0.000	0.000	6477.830
108	Benzene	78.11	1.99	0.000	0.000	24835.468

109	CARBAZOLE	167.2	3.23	241.556	0.000	98.693
110	C2-Benzothiophene	162.25	4.13	0.582	0.000	114.684
111	Isopentane	72.15	2.72	0.000	0.000	6113.952
112	C1-Decalins	152.3	4.61	0.000	0.000	97.666
113	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2953.740
114	trans-Decalin	138.26	4.2	0.000	0.000	214.537
115	C1-Benzothiophene	148.2	3.5365	0.582	0.000	376.428
116	Naphthalene	234.3	3.17	15.049	0.000	464.200
117	cis-Decalin	138.26	4.2	0.000	0.000	214.537
118	Benzothiophene	134.2	2.99	0.582	0.000	1106.904
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384

138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	4780.805	0.000	0.087
166	Benzo(b)fluorene	216.3	5.77	860.457	0.000	0.318

167	Benzo(k)fluoranthene	252.3	6.11	4167.522	0.000	0.092
168	Benzo[a]anthracene	228.3	5.52	1186.537	0.000	0.503
169	Benzo[a]pyrene	252.3	6.11	6076.786	0.000	0.079
170	Benzo[b]fluoranthene	252.3	6.11	2548.196	0.000	0.113
171	Benzo[e]pyrene	252.3	6.11	1726.025	0.000	0.133
172	Benzo[g,h,i]perylene	276.3	6.7	4922.741	0.000	0.026
173	C1-Chrysenes	242.3	6.0683	826.307	0.000	0.190
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2971.001	0.000	0.354
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	826.307	0.000	0.057
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2971.001	0.000	0.093
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1677.722	0.000	0.438
181	C3-Chrysenes	270.4	7.03	826.307	0.000	0.027
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	11.078	0.000	1.548
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2971.001	0.000	0.038
185	C3-Fluorenes	210.3	5.58	130.346	0.000	1.005
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1677.722	0.000	0.202
188	C4-Chrysenes	284.4	7.35	826.307	0.000	0.014
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	11.078	0.000	0.979
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2971.001	0.000	0.014
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1677.722	0.000	0.113
194	Chrysene	228.3	5.52	655.692	0.000	0.643
195	Dibenz(a,h)anthracene	278.4	6.7	2902.389	0.000	0.033

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	7151.312	0.000	0.023
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	7919.021	0.000	0.070
199	Retene	234.3	6.35	121.648	0.000	0.219

Table B.34. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF duplicate exposed to *Menidia beryllina* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	Pyrene	202.3	4.93	2291.602	0.092	1.209
2	Fluoranthene	202.3	4.93	1355.371	0.057	1.505
3	C2-Fluorenes	194.3	5.21	130.346	0.063	2.062
4	C1-Phenanthrenes/Anthracenes	192.3	4.26	1677.722	0.158	5.546
5	C1-Fluorenes	180.2	4.97	130.346	0.065	3.208
6	C3-Naphthalenes	170.26	4.77	37.373	0.106	7.619
7	2-Methylanthracene	192.26	4.89	1677.722	0.013	1.426
8	4/9-Methylphenanthrene	192.26	4.89	82.404	0.043	4.881
9	1-Methylphenanthrene	192.26	4.89	82.404	0.043	4.881
10	C4-Naphthalenes	184.3	5.18	37.373	0.030	3.409
11	2-Methylphenanthrene	192.26	4.89	82.404	0.034	4.881
12	C2-Naphthalenes	156.2	4.31	37.373	0.125	18.839
13	Phenanthrene	178.2	4.35	51.952	0.114	17.359
14	3-Methylphenanthrene	192.26	4.89	82.404	0.032	4.881
15	Anthracene	178.2	4.35	1007.917	0.029	5.232
16	C2-Dibenzothiophenes	214.3	5.13	11.078	0.036	6.946
17	1,6,7-Trimethylnaphthalene	170.26	4.81	44.783	0.029	6.519
18	Acenaphthylene	152.2	3.94	678.887	0.055	12.736
19	2,6-Dimethylnaphthalene	156.23	4.26	37.373	0.043	20.986
20	Fluorene	166.2	4.02	130.346	0.045	22.925
21	C1-Dibenzothiophenes	198.3	4.71	11.078	0.027	15.892

22	2/3-Methyldibenzothiophene	198.28	4.71	9.703	0.012	16.663
23	4-Methyldibenzothiophene	198.28	4.71	11.078	0.011	15.891
24	C1-Naphthalenes	142.2	3.87	25.285	0.019	51.372
25	Dibenzothiophene	184.3	4.17	11.078	0.018	47.296
26	1-Methyldibenzothiophene	198.28	4.71	11.078	0.005	15.891
27	Acenaphthene	154.2	4.15	89.499	0.005	18.669
28	1-Methylnaphthalene	142.2	3.72	25.285	0.016	70.978
29	2-Methylnaphthalene	142.2	3.72	25.285	0.013	70.978
30	Dibenzofuran	168.2	3.71	43.589	0.006	69.670
31	Biphenyl	154.2	3.76	0.000	0.009	617.632
32	Toluene	92.14	2.54	0.000	0.016	8953.934
33	n-C10	142.29	5.25	0.000	0.000	51.663
34	n-C10	142.29	5.25	0.000	0.000	51.663
35	n-C10	142.3	5.25	0.000	0.000	51.667
36	n-C10	142.3	5.25	0.000	0.000	51.667
37	1-Decene	140.3	5.12	0.000	0.000	67.413
38	n-C10	142.29	5.25	0.000	0.000	51.663
39	n-C10	142.29	5.25	0.000	0.000	51.663
40	n-C10	142.3	5.25	0.000	0.000	51.667
41	n-C10	142.3	5.25	0.000	0.000	51.667
42	n-C9	128.3	4.76	0.000	0.000	133.928
43	n-C9	128.3	4.76	0.000	0.000	133.928
44	n-C9	128.3	4.76	0.000	0.000	133.928
45	n-C9	128.3	4.76	0.000	0.000	133.928
46	1-Nonene	126.2	4.62	0.000	0.000	178.133
47	n-C9	128.3	4.76	0.000	0.000	133.928
48	n-C9	128.3	4.76	0.000	0.000	133.928
49	n-C9	128.3	4.76	0.000	0.000	133.928
50	n-C9	128.3	4.76	0.000	0.000	133.928

51	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
52	n-C8	114.2	4.27	0.000	0.000	342.730
53	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
54	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
55	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	423.719
56	Octene-1	112.2	4.13	0.000	0.000	455.322
57	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
58	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
59	3-methylheptane	114.2	4.2	0.000	0.000	398.540
60	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
61	2-methylheptane	114.2	4.2	0.000	0.000	398.540
62	HEPTANE	100.2	3.78	0.000	0.000	864.557
63	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
64	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	423.719
65	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
66	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
67	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	423.782
68	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	482.212
69	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	482.212
70	n-Butylbenzene	134.2	4.01	0.000	0.000	548.780
71	Methylcyclohexane	98.19	3.59	0.000	0.000	1275.948
72	sec-Butylbenzene	134.2	3.94	0.000	0.000	638.143
73	Hydrindene	118.2	3.47	0.000	0.000	1547.758
74	Propylbenzene	120.194	3.52	0.000	0.000	1413.086
75	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	423.782
76	n-C6	86.18	3.29	0.000	0.000	2137.825
77	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
78	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
79	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	482.212

80	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
81	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	560.819
82	m-cymene	134.2	4	0.000	0.000	560.736
83	Ethylbenzene	106.2	3.03	0.000	0.000	3589.634
84	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
85	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
86	4-isopropyltoluene	134.22	4	0.000	0.000	560.819
87	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
88	C4-Benzothiophene	190.3	5.18	0.582	0.000	13.994
89	CYCLOHEXANE	84.16	3.18	0.000	0.000	2646.253
90	n-C5	72.15	2.8	0.000	0.000	5145.671
91	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1241.739
92	p-XYLENE	106.2	3.09	0.000	0.000	3154.207
93	2-methylhexane	100.2	3.71	0.000	0.000	1005.341
94	Isopropylbenzene	120.194	3.45	0.000	0.000	1643.193
95	3-Methylpentane	86.18	3.21	0.000	0.000	2540.108
96	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
97	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
98	3-methylhexane	100.2	3.71	0.000	0.000	1005.341
99	2,2-dimethylpentane	100.2	3.67	0.000	0.000	1095.856
100	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
101	Methylcyclopentane	84.16	3.1	0.000	0.000	3144.209
102	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2540.108
103	o-XYLENE	106.2	3.09	0.000	0.000	3154.207
104	m-XYLENE	106.2	3.09	0.000	0.000	3154.207
105	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	380.433
106	C3-Benzothiophene	176.3	4.69	0.582	0.000	37.274
107	Cyclopentane	70.13	2.68	0.000	0.000	6477.830
108	Benzene	78.11	1.99	0.000	0.000	24835.468

109	CARBAZOLE	167.2	3.23	241.556	0.000	98.693
110	C2-Benzothiophene	162.25	4.13	0.582	0.000	114.684
111	Isopentane	72.15	2.72	0.000	0.000	6113.952
112	C1-Decalins	152.3	4.61	0.000	0.000	97.666
113	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2953.740
114	trans-Decalin	138.26	4.2	0.000	0.000	214.537
115	C1-Benzothiophene	148.2	3.5365	0.582	0.000	376.428
116	Naphthalene	234.3	3.17	15.049	0.000	464.200
117	cis-Decalin	138.26	4.2	0.000	0.000	214.537
118	Benzothiophene	134.2	2.99	0.582	0.000	1106.904
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384

138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	4780.805	0.000	0.087
166	Benzo(b)fluorene	216.3	5.77	860.457	0.000	0.318

167	Benzo(k)fluoranthene	252.3	6.11	4167.522	0.000	0.092
168	Benzo[a]anthracene	228.3	5.52	1186.537	0.000	0.503
169	Benzo[a]pyrene	252.3	6.11	6076.786	0.000	0.079
170	Benzo[b]fluoranthene	252.3	6.11	2548.196	0.000	0.113
171	Benzo[e]pyrene	252.3	6.11	1726.025	0.000	0.133
172	Benzo[g,h,i]perylene	276.3	6.7	4922.741	0.000	0.026
173	C1-Chrysenes	242.3	6.0683	826.307	0.000	0.190
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2971.001	0.000	0.354
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	826.307	0.000	0.057
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2971.001	0.000	0.093
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1677.722	0.000	0.438
181	C3-Chrysenes	270.4	7.03	826.307	0.000	0.027
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	11.078	0.000	1.548
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2971.001	0.000	0.038
185	C3-Fluorenes	210.3	5.58	130.346	0.000	1.005
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1677.722	0.000	0.202
188	C4-Chrysenes	284.4	7.35	826.307	0.000	0.014
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	11.078	0.000	0.979
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2971.001	0.000	0.014
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1677.722	0.000	0.113
194	Chrysene	228.3	5.52	655.692	0.000	0.643
195	Dibenz(a,h)anthracene	278.4	6.7	2902.389	0.000	0.033

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	7151.312	0.000	0.023
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	7919.021	0.000	0.070
199	Retene	234.3	6.35	121.648	0.000	0.219

Table B.35. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 100% WAF exposed to *Menidia beryllina* natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	60.950	0.262	2.786
2	C1-Phenanthrenes/Anthracenes	192.3	4.26	676.140	0.615	8.087
3	C1-Fluorenes	180.2	4.97	60.950	0.175	4.335
4	1-Methylphenanthrene	192.26	4.89	51.970	0.195	5.848
5	4/9-Methylphenanthrene	192.26	4.89	51.970	0.179	5.848
6	2-Methylphenanthrene	192.26	4.89	51.970	0.149	5.848
7	3-Methylphenanthrene	192.26	4.89	51.970	0.143	5.848
8	C2-Dibenzothiophenes	214.3	5.13	4.480	0.135	9.521
9	C3-Naphthalenes	170.26	4.77	14.660	0.153	10.830
10	C4-Naphthalenes	184.3	5.18	14.660	0.067	4.845
11	Phenanthrene	178.2	4.35	30.510	0.292	21.307
12	C1-Dibenzothiophenes	198.3	4.71	4.480	0.165	21.783
13	1,6,7-Trimethylnaphthalene	170.26	4.81	25.780	0.048	8.052
14	Pyrene	202.3	4.93	769.590	0.009	1.903
15	4-Methyldibenzothiophene	198.28	4.71	4.480	0.077	21.781
16	C2-Naphthalenes	156.2	4.31	14.660	0.073	26.776
17	2/3-Methyldibenzothiophene	198.28	4.71	4.480	0.049	21.781
18	Fluoranthene	202.3	4.93	575.260	0.004	2.146
19	Fluorene	166.2	4.02	60.950	0.057	30.978
20	1-Methyldibenzothiophene	198.28	4.71	4.480	0.027	21.781
21	2,6-Dimethylnaphthalene	156.23	4.26	14.660	0.028	29.828

22	Dibenzothiophene	184.3	4.17	4.480	0.056	64.828
23	2-Methylanthracene	192.26	4.89	676.140	0.002	2.080
24	C4-Benzothiophene	190.3	5.18	0.210	0.008	17.808
25	C3-Benzothiophene	176.3	4.69	0.210	0.012	47.433
26	C1-Naphthalenes	142.2	3.87	14.880	0.010	62.579
27	Toluene	92.14	2.54	0.000	1.180	8953.934
28	2-Methylnaphthalene	142.2	3.72	14.880	0.008	86.463
29	1-Methylnaphthalene	142.2	3.72	14.880	0.008	86.463
30	C2-Benzothiophene	162.25	4.13	0.210	0.012	145.939
31	Dibenzofuran	168.2	3.71	32.420	0.006	78.061
32	Acenaphthene	154.2	4.15	42.380	0.002	25.014
33	C1-Benzothiophene	148.2	3.5365	0.210	0.010	479.018
34	Acenaphthylene	152.2	3.94	228.140	0.000	19.906
35	Naphthalene	234.3	3.17	8.220	0.009	577.107
36	Biphenyl	154.2	3.76	0.000	0.006	617.632
37	1-Decene	140.3	5.12	0.000	0.000	67.413
38	n-C10	142.29	5.25	0.000	0.000	51.663
39	n-C10	142.29	5.25	0.000	0.000	51.663
40	n-C10	142.3	5.25	0.000	0.000	51.667
41	n-C10	142.3	5.25	0.000	0.000	51.667
42	1-Nonene	126.2	4.62	0.000	0.000	178.133
43	n-C9	128.3	4.76	0.000	0.000	133.928
44	n-C9	128.3	4.76	0.000	0.000	133.928
45	n-C9	128.3	4.76	0.000	0.000	133.928
46	n-C9	128.3	4.76	0.000	0.000	133.928
47	n-C8	114.2	4.27	0.000	0.000	342.730
48	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
49	Octene-1	112.2	4.13	0.000	0.000	455.322
50	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928

51	3-methylheptane	114.2	4.2	0.000	0.000	398.540
52	n-C10	142.29	5.25	0.000	0.000	51.663
53	n-C10	142.29	5.25	0.000	0.000	51.663
54	n-C10	142.3	5.25	0.000	0.000	51.667
55	n-C10	142.3	5.25	0.000	0.000	51.667
56	2-methylheptane	114.2	4.2	0.000	0.000	398.540
57	HEPTANE	100.2	3.78	0.000	0.000	864.557
58	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
59	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
60	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
61	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
62	Anthracene	178.2	4.35	424.130	0.000	7.479
63	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	423.719
64	n-C9	128.3	4.76	0.000	0.000	133.928
65	n-C9	128.3	4.76	0.000	0.000	133.928
66	n-C9	128.3	4.76	0.000	0.000	133.928
67	n-C9	128.3	4.76	0.000	0.000	133.928
68	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
69	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
70	Methylcyclohexane	98.19	3.59	0.000	0.000	1275.948
71	n-Butylbenzene	134.2	4.01	0.000	0.000	548.780
72	n-C6	86.18	3.29	0.000	0.000	2137.825
73	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
74	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
75	2-methylhexane	100.2	3.71	0.000	0.000	1005.341
76	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	423.782
77	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	482.212
78	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	423.719
79	3-ethylhexane	114.2	4.2	0.000	0.000	398.540

80	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	482.212
81	3-methylhexane	100.2	3.71	0.000	0.000	1005.341
82	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
83	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
84	Hydrindene	118.2	3.47	0.000	0.000	1547.758
85	n-C5	72.15	2.8	0.000	0.000	5145.671
86	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2540.108
87	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	482.212
88	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	423.782
89	Propylbenzene	120.194	3.52	0.000	0.000	1413.086
90	p-XYLENE	106.2	3.09	0.000	0.000	3154.207
91	4-isopropyltoluene	134.22	4	0.000	0.000	560.819
92	sec-Butylbenzene	134.2	3.94	0.000	0.000	638.143
93	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
94	3-Methylpentane	86.18	3.21	0.000	0.000	2540.108
95	2,2-dimethylpentane	100.2	3.67	0.000	0.000	1095.856
96	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
97	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	560.819
98	m-cymene	134.2	4	0.000	0.000	560.736
99	Ethylbenzene	106.2	3.03	0.000	0.000	3589.634
100	CYCLOHEXANE	84.16	3.18	0.000	0.000	2646.253
101	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
102	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
103	CARBAZOLE	167.2	3.23	110.810	0.000	135.058
104	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1241.739
105	m-XYLENE	106.2	3.09	0.000	0.000	3154.207
106	Isopropylbenzene	120.194	3.45	0.000	0.000	1643.193
107	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	380.433
108	Isopentane	72.15	2.72	0.000	0.000	6113.952

109	Methylcyclopentane	84.16	3.1	0.000	0.000	3144.209
110	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2953.740
111	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
112	o-XYLENE	106.2	3.09	0.000	0.000	3154.207
113	Cyclopentane	70.13	2.68	0.000	0.000	6477.830
114	C1-Decalins	152.3	4.61	0.000	0.000	97.666
115	Benzene	78.11	1.99	0.000	0.000	24835.468
116	trans-Decalin	138.26	4.2	0.000	0.000	214.537
117	cis-Decalin	138.26	4.2	0.000	0.000	214.537
118	Benzothiophene	134.2	2.99	0.210	0.000	1408.576
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384

138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	3326.260	0.000	0.101
166	Benzo(b)fluorene	216.3	5.77	295.350	0.000	0.493

167	Benzo(k)fluoranthene	252.3	6.11	1862.910	0.000	0.129
168	Benzo[a]anthracene	228.3	5.52	507.070	0.000	0.715
169	Benzo[a]pyrene	252.3	6.11	2612.960	0.000	0.112
170	Benzo[b]fluoranthene	252.3	6.11	1112.540	0.000	0.160
171	Benzo[e]pyrene	252.3	6.11	616.180	0.000	0.205
172	Benzo[g,h,i]perylene	276.3	6.7	2065.650	0.000	0.038
173	C1-Chrysenes	242.3	6.0683	289.380	0.000	0.293
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1146.990	0.000	0.527
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	289.380	0.000	0.088
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1146.990	0.000	0.138
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	676.140	0.000	0.639
181	C3-Chrysenes	270.4	7.03	289.380	0.000	0.041
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	4.480	0.000	2.122
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1146.990	0.000	0.057
185	C3-Fluorenes	210.3	5.58	60.950	0.000	1.359
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	676.140	0.000	0.295
188	C4-Chrysenes	284.4	7.35	289.380	0.000	0.022
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	4.480	0.000	1.342
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1146.990	0.000	0.021
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	676.140	0.000	0.164
194	Chrysene	228.3	5.52	232.480	0.000	0.984
195	Dibenz(a,h)anthracene	278.4	6.7	1302.120	0.000	0.046

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	3556.050	0.000	0.030
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	6039.440	0.000	0.079
199	Retene	234.3	6.35	74.490	0.000	0.266

Table B.36. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 25% WAF exposed to *Menidia beryllina* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	60.950	0.061	2.786
2	C1-Phenanthrenes/Anthracenes	192.3	4.26	676.140	0.147	8.087
3	C1-Fluorenes	180.2	4.97	60.950	0.042	4.335
4	1-Methylphenanthrene	192.26	4.89	51.970	0.048	5.848
5	4/9-Methylphenanthrene	192.26	4.89	51.970	0.043	5.848
6	2-Methylphenanthrene	192.26	4.89	51.970	0.035	5.848
7	3-Methylphenanthrene	192.26	4.89	51.970	0.034	5.848
8	C4-Naphthalenes	184.3	5.18	14.660	0.019	4.845
9	C3-Naphthalenes	170.26	4.77	14.660	0.038	10.830
10	Phenanthrene	178.2	4.35	30.510	0.071	21.307
11	C2-Dibenzothiophenes	214.3	5.13	4.480	0.029	9.521
12	C1-Dibenzothiophenes	198.3	4.71	4.480	0.038	21.783
13	Pyrene	202.3	4.93	769.590	0.003	1.903
14	1,6,7-Trimethylnaphthalene	170.26	4.81	25.780	0.011	8.052
15	4-Methyldibenzothiophene	198.28	4.71	4.480	0.017	21.781
16	C2-Naphthalenes	156.2	4.31	14.660	0.018	26.776
17	Fluoranthene	202.3	4.93	575.260	0.001	2.146
18	Fluorene	166.2	4.02	60.950	0.014	30.978
19	1-Methyldibenzothiophene	198.28	4.71	4.480	0.007	21.781
20	2/3-Methyldibenzothiophene	198.28	4.71	4.480	0.006	21.781
21	2,6-Dimethylnaphthalene	156.23	4.26	14.660	0.007	29.828

22	C4-Benzothiophene	190.3	5.18	0.210	0.004	17.808
23	Dibenzothiophene	184.3	4.17	4.480	0.013	64.828
24	C3-Benzothiophene	176.3	4.69	0.210	0.008	47.433
25	Toluene	92.14	2.54	0.000	0.273	8953.934
26	C2-Benzothiophene	162.25	4.13	0.210	0.004	145.939
27	Dibenzofuran	168.2	3.71	32.420	0.002	78.061
28	C1-Benzothiophene	148.2	3.5365	0.210	0.009	479.018
29	Naphthalene	234.3	3.17	8.220	0.011	577.107
30	Biphenyl	154.2	3.76	0.000	0.002	617.632
31	1-Decene	140.3	5.12	0.000	0.000	67.413
32	n-C10	142.29	5.25	0.000	0.000	51.663
33	n-C10	142.29	5.25	0.000	0.000	51.663
34	n-C10	142.3	5.25	0.000	0.000	51.667
35	n-C10	142.3	5.25	0.000	0.000	51.667
36	1-Nonene	126.2	4.62	0.000	0.000	178.133
37	n-C9	128.3	4.76	0.000	0.000	133.928
38	n-C9	128.3	4.76	0.000	0.000	133.928
39	n-C9	128.3	4.76	0.000	0.000	133.928
40	n-C9	128.3	4.76	0.000	0.000	133.928
41	n-C8	114.2	4.27	0.000	0.000	342.730
42	2-Methylanthracene	192.26	4.89	676.140	0.000	2.080
43	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
44	Octene-1	112.2	4.13	0.000	0.000	455.322
45	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
46	3-methylheptane	114.2	4.2	0.000	0.000	398.540
47	n-C10	142.29	5.25	0.000	0.000	51.663
48	n-C10	142.29	5.25	0.000	0.000	51.663
49	n-C10	142.3	5.25	0.000	0.000	51.667
50	n-C10	142.3	5.25	0.000	0.000	51.667

51	2-methylheptane	114.2	4.2	0.000	0.000	398.540
52	HEPTANE	100.2	3.78	0.000	0.000	864.557
53	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
54	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659
55	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
56	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
57	Anthracene	178.2	4.35	424.130	0.000	7.479
58	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	423.719
59	n-C9	128.3	4.76	0.000	0.000	133.928
60	n-C9	128.3	4.76	0.000	0.000	133.928
61	n-C9	128.3	4.76	0.000	0.000	133.928
62	n-C9	128.3	4.76	0.000	0.000	133.928
63	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
64	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
65	Methylcyclohexane	98.19	3.59	0.000	0.000	1275.948
66	n-C6	86.18	3.29	0.000	0.000	2137.825
67	n-Butylbenzene	134.2	4.01	0.000	0.000	548.780
68	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
69	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
70	2-methylhexane	100.2	3.71	0.000	0.000	1005.341
71	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	423.782
72	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	482.212
73	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	423.719
74	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
75	Acenaphthylene	152.2	3.94	228.140	0.000	19.906
76	Acenaphthene	154.2	4.15	42.380	0.000	25.014
77	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	482.212
78	3-methylhexane	100.2	3.71	0.000	0.000	1005.341
79	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	423.719

80	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
81	Hydrindene	118.2	3.47	0.000	0.000	1547.758
82	n-C5	72.15	2.8	0.000	0.000	5145.671
83	C1-Naphthalenes	142.2	3.87	14.880	0.000	62.579
84	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2540.108
85	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	482.212
86	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	423.782
87	Propylbenzene	120.194	3.52	0.000	0.000	1413.086
88	p-XYLENE	106.2	3.09	0.000	0.000	3154.207
89	4-isopropyltoluene	134.22	4	0.000	0.000	560.819
90	sec-Butylbenzene	134.2	3.94	0.000	0.000	638.143
91	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
92	3-Methylpentane	86.18	3.21	0.000	0.000	2540.108
93	2,2-dimethylpentane	100.2	3.67	0.000	0.000	1095.856
94	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
95	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	560.819
96	2-Methylnaphthalene	142.2	3.72	14.880	0.000	86.463
97	m-cymene	134.2	4	0.000	0.000	560.736
98	Ethylbenzene	106.2	3.03	0.000	0.000	3589.634
99	CYCLOHEXANE	84.16	3.18	0.000	0.000	2646.253
100	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
101	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
102	CARBAZOLE	167.2	3.23	110.810	0.000	135.058
103	1-Methylnaphthalene	142.2	3.72	14.880	0.000	86.463
104	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1241.739
105	m-XYLENE	106.2	3.09	0.000	0.000	3154.207
106	Isopropylbenzene	120.194	3.45	0.000	0.000	1643.193
107	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	380.433
108	Isopentane	72.15	2.72	0.000	0.000	6113.952

109	Methylcyclopentane	84.16	3.1	0.000	0.000	3144.209
110	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2953.740
111	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
112	o-XYLENE	106.2	3.09	0.000	0.000	3154.207
113	Cyclopentane	70.13	2.68	0.000	0.000	6477.830
114	C1-Decalins	152.3	4.61	0.000	0.000	97.666
115	Benzene	78.11	1.99	0.000	0.000	24835.468
116	trans-Decalin	138.26	4.2	0.000	0.000	214.537
117	cis-Decalin	138.26	4.2	0.000	0.000	214.537
118	Benzothiophene	134.2	2.99	0.210	0.000	1408.576
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384

138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	3326.260	0.000	0.101
166	Benzo(b)fluorene	216.3	5.77	295.350	0.000	0.493

167	Benzo(k)fluoranthene	252.3	6.11	1862.910	0.000	0.129
168	Benzo[a]anthracene	228.3	5.52	507.070	0.000	0.715
169	Benzo[a]pyrene	252.3	6.11	2612.960	0.000	0.112
170	Benzo[b]fluoranthene	252.3	6.11	1112.540	0.000	0.160
171	Benzo[e]pyrene	252.3	6.11	616.180	0.000	0.205
172	Benzo[g,h,i]perylene	276.3	6.7	2065.650	0.000	0.038
173	C1-Chrysenes	242.3	6.0683	289.380	0.000	0.293
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1146.990	0.000	0.527
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	289.380	0.000	0.088
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1146.990	0.000	0.138
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	676.140	0.000	0.639
181	C3-Chrysenes	270.4	7.03	289.380	0.000	0.041
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	4.480	0.000	2.122
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1146.990	0.000	0.057
185	C3-Fluorenes	210.3	5.58	60.950	0.000	1.359
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	676.140	0.000	0.295
188	C4-Chrysenes	284.4	7.35	289.380	0.000	0.022
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	4.480	0.000	1.342
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1146.990	0.000	0.021
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	676.140	0.000	0.164
194	Chrysene	228.3	5.52	232.480	0.000	0.984
195	Dibenz(a,h)anthracene	278.4	6.7	1302.120	0.000	0.046

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	3556.050	0.000	0.030
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	6039.440	0.000	0.079
199	Retene	234.3	6.35	74.490	0.000	0.266

Table B.37. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 6.25% WAF exposed to *Menidia beryllina* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	60.950	0.018	2.786
2	C1-Phenanthrenes/Anthracenes	192.3	4.26	676.140	0.039	8.087
3	C1-Fluorenes	180.2	4.97	60.950	0.011	4.335
4	1-Methylphenanthrene	192.26	4.89	51.970	0.013	5.848
5	4/9-Methylphenanthrene	192.26	4.89	51.970	0.011	5.848
6	3-Methylphenanthrene	192.26	4.89	51.970	0.010	5.848
7	C4-Naphthalenes	184.3	5.18	14.660	0.008	4.845
8	2-Methylphenanthrene	192.26	4.89	51.970	0.009	5.848
9	C3-Naphthalenes	170.26	4.77	14.660	0.013	10.830
10	C2-Dibenzothiophenes	214.3	5.13	4.480	0.008	9.521
11	Phenanthrene	178.2	4.35	30.510	0.019	21.307
12	Pyrene	202.3	4.93	769.590	0.001	1.903
13	1,6,7-Trimethylnaphthalene	170.26	4.81	25.780	0.003	8.052
14	C1-Dibenzothiophenes	198.3	4.71	4.480	0.008	21.783
15	Fluoranthene	202.3	4.93	575.260	0.001	2.146
16	C2-Naphthalenes	156.2	4.31	14.660	0.007	26.776
17	4-Methyldibenzothiophene	198.28	4.71	4.480	0.005	21.781
18	Fluorene	166.2	4.02	60.950	0.004	30.978
19	1-Methyldibenzothiophene	198.28	4.71	4.480	0.002	21.781
20	2/3-Methyldibenzothiophene	198.28	4.71	4.480	0.001	21.781
21	Dibenzothiophene	184.3	4.17	4.480	0.003	64.828

22	Naphthalene	234.3	3.17	8.220	0.008	577.107
23	Acenaphthylene	152.2	3.94	228.140	0.000	19.906
24	Dibenzofuran	168.2	3.71	32.420	0.001	78.061
25	Toluene	92.14	2.54	0.000	0.065	8953.934
26	Biphenyl	154.2	3.76	0.000	0.002	617.632
27	1-Decene	140.3	5.12	0.000	0.000	67.413
28	n-C10	142.29	5.25	0.000	0.000	51.663
29	n-C10	142.29	5.25	0.000	0.000	51.663
30	n-C10	142.3	5.25	0.000	0.000	51.667
31	n-C10	142.3	5.25	0.000	0.000	51.667
32	1-Nonene	126.2	4.62	0.000	0.000	178.133
33	n-C9	128.3	4.76	0.000	0.000	133.928
34	n-C9	128.3	4.76	0.000	0.000	133.928
35	n-C9	128.3	4.76	0.000	0.000	133.928
36	n-C9	128.3	4.76	0.000	0.000	133.928
37	n-C8	114.2	4.27	0.000	0.000	342.730
38	2-Methylanthracene	192.26	4.89	676.140	0.000	2.080
39	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	505.163
40	Octene-1	112.2	4.13	0.000	0.000	455.322
41	n-Pentylbenzene	148.2	4.5	0.000	0.000	270.928
42	3-methylheptane	114.2	4.2	0.000	0.000	398.540
43	n-C10	142.29	5.25	0.000	0.000	51.663
44	n-C10	142.29	5.25	0.000	0.000	51.663
45	n-C10	142.3	5.25	0.000	0.000	51.667
46	n-C10	142.3	5.25	0.000	0.000	51.667
47	2-methylheptane	114.2	4.2	0.000	0.000	398.540
48	HEPTANE	100.2	3.78	0.000	0.000	864.557
49	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	550.645
50	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	473.659

51	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	505.296
52	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	482.284
53	Anthracene	178.2	4.35	424.130	0.000	7.479
54	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	423.719
55	n-C9	128.3	4.76	0.000	0.000	133.928
56	n-C9	128.3	4.76	0.000	0.000	133.928
57	n-C9	128.3	4.76	0.000	0.000	133.928
58	n-C9	128.3	4.76	0.000	0.000	133.928
59	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	473.659
60	2,3-dimethylhexane	114.2	4.12	0.000	0.000	473.535
61	Methylcyclohexane	98.19	3.59	0.000	0.000	1275.948
62	n-Butylbenzene	134.2	4.01	0.000	0.000	548.780
63	2,4-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
64	C4-Benzothiophene	190.3	5.18	0.210	0.000	17.808
65	tert-Butylbenzene	134.2	3.9	0.000	0.000	695.598
66	n-C6	86.18	3.29	0.000	0.000	2137.825
67	2-methylhexane	100.2	3.71	0.000	0.000	1005.341
68	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	423.782
69	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	482.212
70	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	423.719
71	3-ethylhexane	114.2	4.2	0.000	0.000	398.540
72	Acenaphthene	154.2	4.15	42.380	0.000	25.014
73	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	482.212
74	3-methylhexane	100.2	3.71	0.000	0.000	1005.341
75	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
76	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	423.719
77	2,6-Dimethylnaphthalene	156.23	4.26	14.660	0.000	29.828
78	Hydrindene	118.2	3.47	0.000	0.000	1547.758
79	n-C5	72.15	2.8	0.000	0.000	5145.671

80	2-METHYLPENTANE	86.18	3.21	0.000	0.000	2540.108
81	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	482.212
82	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	423.782
83	Propylbenzene	120.194	3.52	0.000	0.000	1413.086
84	p-XYLENE	106.2	3.09	0.000	0.000	3154.207
85	4-isopropyltoluene	134.22	4	0.000	0.000	560.819
86	C1-Naphthalenes	142.2	3.87	14.880	0.000	62.579
87	sec-Butylbenzene	134.2	3.94	0.000	0.000	638.143
88	2,3-dimethylpentane	100.2	3.63	0.000	0.000	1194.520
89	3-Methylpentane	86.18	3.21	0.000	0.000	2540.108
90	2,2-dimethylpentane	100.2	3.67	0.000	0.000	1095.856
91	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
92	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	560.819
93	C3-Benzothiophene	176.3	4.69	0.210	0.000	47.433
94	m-cymene	134.2	4	0.000	0.000	560.736
95	Ethylbenzene	106.2	3.03	0.000	0.000	3589.634
96	CYCLOHEXANE	84.16	3.18	0.000	0.000	2646.253
97	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
98	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	1241.739
99	CARBAZOLE	167.2	3.23	110.810	0.000	135.058
100	2-Methylnaphthalene	142.2	3.72	14.880	0.000	86.463
101	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	1241.739
102	m-XYLENE	106.2	3.09	0.000	0.000	3154.207
103	Isopropylbenzene	120.194	3.45	0.000	0.000	1643.193
104	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	380.433
105	1-Methylnaphthalene	142.2	3.72	14.880	0.000	86.463
106	Isopentane	72.15	2.72	0.000	0.000	6113.952
107	Methylcyclopentane	84.16	3.1	0.000	0.000	3144.209
108	2,3-dimethylbutane	86.18	3.14	0.000	0.000	2953.740

109	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	1114.885
110	o-XYLENE	106.2	3.09	0.000	0.000	3154.207
111	Cyclopentane	70.13	2.68	0.000	0.000	6477.830
112	C1-Decalins	152.3	4.61	0.000	0.000	97.666
113	C2-Benzothiophene	162.25	4.13	0.210	0.000	145.939
114	Benzene	78.11	1.99	0.000	0.000	24835.468
115	trans-Decalin	138.26	4.2	0.000	0.000	214.537
116	C1-Benzothiophene	148.2	3.5365	0.210	0.000	479.018
117	cis-Decalin	138.26	4.2	0.000	0.000	214.537
118	Benzothiophene	134.2	2.99	0.210	0.000	1408.576
119	n-C11	156.31	5.74	0.000	0.000	19.740
120	n-C11	156.31	5.74	0.000	0.000	19.740
121	n-C11	156.31	5.74	0.000	0.000	19.740
122	n-C11	156.31	5.74	0.000	0.000	19.740
123	n-C12	170.34	6.23	0.000	0.000	7.482
124	n-C12	170.34	6.23	0.000	0.000	7.482
125	n-C12	170.34	6.23	0.000	0.000	7.482
126	n-C12	170.34	6.23	0.000	0.000	7.482
127	n-C11	156.31	5.74	0.000	0.000	19.740
128	n-C11	156.31	5.74	0.000	0.000	19.740
129	n-C11	156.31	5.74	0.000	0.000	19.740
130	n-C11	156.31	5.74	0.000	0.000	19.740
131	n-C12	170.34	6.23	0.000	0.000	7.482
132	n-C12	170.34	6.23	0.000	0.000	7.482
133	n-C12	170.34	6.23	0.000	0.000	7.482
134	n-C12	170.34	6.23	0.000	0.000	7.482
135	n-C13	184.37	6.73	0.000	0.000	2.757
136	n-C14	198.4	7.22	0.000	0.000	1.032
137	n-C15	212.42	7.71	0.000	0.000	0.384

138	n-C16	226.45	8.2	0.000	0.000	0.142
139	n-C17	240.48	8.69	0.000	0.000	0.053
140	n-C18	254.5	9.18	0.000	0.000	0.019
141	n-C19	268.53	9.67	0.000	0.000	0.007
142	n-C20	282.56	10.1	0.000	0.000	0.003
143	n-C21	296.59	10.6	0.000	0.000	0.001
144	n-C22	310.61	11.1	0.000	0.000	0.000
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.005
164	Pristane	268.525	9.38	0.000	0.000	0.013
165	Benzo(a)fluoranthene	252.3	6.11	3326.260	0.000	0.101
166	Benzo(b)fluorene	216.3	5.77	295.350	0.000	0.493

167	Benzo(k)fluoranthene	252.3	6.11	1862.910	0.000	0.129
168	Benzo[a]anthracene	228.3	5.52	507.070	0.000	0.715
169	Benzo[a]pyrene	252.3	6.11	2612.960	0.000	0.112
170	Benzo[b]fluoranthene	252.3	6.11	1112.540	0.000	0.160
171	Benzo[e]pyrene	252.3	6.11	616.180	0.000	0.205
172	Benzo[g,h,i]perylene	276.3	6.7	2065.650	0.000	0.038
173	C1-Chrysenes	242.3	6.0683	289.380	0.000	0.293
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	1146.990	0.000	0.527
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	3.510
176	C2-Chrysenes	256.3	6.65	289.380	0.000	0.088
177	C2-Decalins	166.3	6.19	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	230.3	6.13	1146.990	0.000	0.138
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	676.140	0.000	0.639
181	C3-Chrysenes	270.4	7.03	289.380	0.000	0.041
182	C3-Decalins	180.3	6.79	0.000	0.000	1.053
183	C3-Dibenzothiophenes	230.37	5.86	4.480	0.000	2.122
184	C3-Fluoranthenes/Pyrene	244.34	6.57	1146.990	0.000	0.057
185	C3-Fluorenes	210.3	5.58	60.950	0.000	1.359
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	676.140	0.000	0.295
188	C4-Chrysenes	284.4	7.35	289.380	0.000	0.022
189	C4-Decalins	194.3	7.34	0.000	0.000	0.347
190	C4-Dibenzothiophenes	244.37	6.1	4.480	0.000	1.342
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	1146.990	0.000	0.021
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	676.140	0.000	0.164
194	Chrysene	228.3	5.52	232.480	0.000	0.984
195	Dibenz(a,h)anthracene	278.4	6.7	1302.120	0.000	0.046

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	3556.050	0.000	0.030
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	23.696
198	Perylene	252.3	6.11	6039.440	0.000	0.079
199	Retene	234.3	6.35	74.490	0.000	0.266

Table B.38. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 6.25% WAF duplicate exposed to *Menidia beryllina* under natural solar radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	5.21	194.3	60.950	0.019	2.786
2	C1-Phenanthrenes/Anthracenes	4.26	192.3	676.140	0.038	8.087
3	C1-Fluorenes	4.97	180.2	60.950	0.011	4.335
4	C4-Naphthalenes	5.18	184.3	14.660	0.012	4.845
5	1-Methylphenanthrene	4.89	192.26	51.970	0.012	5.848
6	4/9-Methylphenanthrene	4.89	192.26	51.970	0.011	5.848
7	C3-Naphthalenes	4.77	170.26	14.660	0.018	10.830
8	3-Methylphenanthrene	4.89	192.26	51.970	0.009	5.848
9	2-Methylphenanthrene	4.89	192.26	51.970	0.009	5.848
10	C2-Dibenzothiophenes	5.13	214.3	4.480	0.010	9.521
11	Phenanthrene	4.35	178.2	30.510	0.020	21.307
12	Pyrene	4.93	202.3	769.590	0.002	1.903
13	1,6,7-Trimethylnaphthalene	4.81	170.26	25.780	0.004	8.052
14	C2-Naphthalenes	4.31	156.2	14.660	0.012	26.776
15	C1-Dibenzothiophenes	4.71	198.3	4.480	0.008	21.783
16	4-Methyldibenzothiophene	4.71	198.28	4.480	0.004	21.781
17	Fluorene	4.02	166.2	60.950	0.005	30.978
18	1-Methyldibenzothiophene	4.71	198.28	4.480	0.002	21.781
19	Dibenzothiophene	4.17	184.3	4.480	0.003	64.828
20	2/3-Methyldibenzothiophene	4.71	198.28	4.480	0.001	21.781
21	Naphthalene	3.17	234.3	8.220	0.014	577.107

22	Dibenzofuran	3.71	168.2	32.420	0.001	78.061
23	Toluene	2.54	92.14	0.000	0.054	8953.934
24	Biphenyl	3.76	154.2	0.000	0.003	617.632
25	1-Decene	5.12	140.3	0.000	0.000	67.413
26	n-C10	5.25	142.29	0.000	0.000	51.663
27	n-C10	5.25	142.29	0.000	0.000	51.663
28	n-C10	5.25	142.3	0.000	0.000	51.667
29	n-C10	5.25	142.3	0.000	0.000	51.667
30	1-Nonene	4.62	126.2	0.000	0.000	178.133
31	Fluoranthene	4.93	202.3	575.260	0.000	2.146
32	2-Methylanthracene	4.89	192.26	676.140	0.000	2.080
33	n-C9	4.76	128.3	0.000	0.000	133.928
34	n-C9	4.76	128.3	0.000	0.000	133.928
35	n-C9	4.76	128.3	0.000	0.000	133.928
36	n-C9	4.76	128.3	0.000	0.000	133.928
37	n-C10	5.25	142.29	0.000	0.000	51.663
38	n-C10	5.25	142.29	0.000	0.000	51.663
39	n-C10	5.25	142.3	0.000	0.000	51.667
40	n-C10	5.25	142.3	0.000	0.000	51.667
41	n-C8	4.27	114.2	0.000	0.000	342.730
42	2,2,4-TRIMETHYLPENTANE	4.09	114.2	0.000	0.000	505.163
43	Octene-1	4.13	112.2	0.000	0.000	455.322
44	n-Pentylbenzene	4.5	148.2	0.000	0.000	270.928
45	3-methylheptane	4.2	114.2	0.000	0.000	398.540
46	2-methylheptane	4.2	114.2	0.000	0.000	398.540
47	Anthracene	4.35	178.2	424.130	0.000	7.479
48	HEPTANE	3.78	100.2	0.000	0.000	864.557
49	2,3,4-trimethylpentane	4.05	114.2	0.000	0.000	550.645
50	n-C9	4.76	128.3	0.000	0.000	133.928

51	n-C9	4.76	128.3	0.000	0.000	133.928
52	n-C9	4.76	128.3	0.000	0.000	133.928
53	n-C9	4.76	128.3	0.000	0.000	133.928
54	2,5-Dimethylhexane	4.12	114.23	0.000	0.000	473.659
55	Pentane, 2,3,3-trimethyl	4.09	114.23	0.000	0.000	505.296
56	BENZENE, 1-METHYL-4-PROPYL-	4.07	134.22	0.000	0.000	482.284
57	1,3-dimethyl-4-ethylbenzene	4.13	134.2	0.000	0.000	423.719
58	C4-Benzothiophene	5.18	190.3	0.210	0.000	17.808
59	1,1,3-trimethylpentane	4.12	114.23	0.000	0.000	473.659
60	Acenaphthylene	3.94	152.2	228.140	0.000	19.906
61	Acenaphthene	4.15	154.2	42.380	0.000	25.014
62	2,3-dimethylhexane	4.12	114.2	0.000	0.000	473.535
63	Methylcyclohexane	3.59	98.19	0.000	0.000	1275.948
64	n-Butylbenzene	4.01	134.2	0.000	0.000	548.780
65	2,4-dimethylpentane	3.63	100.2	0.000	0.000	1194.520
66	2,6-Dimethylnaphthalene	4.26	156.23	14.660	0.000	29.828
67	tert-Butylbenzene	3.9	134.2	0.000	0.000	695.598
68	2-methylhexane	3.71	100.2	0.000	0.000	1005.341
69	n-C6	3.29	86.18	0.000	0.000	2137.825
70	1-ETHYL-2,3-DIMETHYLBENZENE	4.13	134.22	0.000	0.000	423.782
71	1-Methyl-2-n-Propylbenzene	4.07	134.2	0.000	0.000	482.212
72	1,4-dimethyl-2-ethylbenzene	4.13	134.2	0.000	0.000	423.719
73	3-ethylhexane	4.2	114.2	0.000	0.000	398.540
74	1-methyl-3-n-propylbenzene	4.07	134.2	0.000	0.000	482.212
75	3-methylhexane	3.71	100.2	0.000	0.000	1005.341
76	1,3-Dimethyl-5-Ethylbenzene	4.13	134.2	0.000	0.000	423.719
77	1,2-Dimethyl-4-Ethylbenzene	4.13	134.2	0.000	0.000	423.719
78	C3-Benzothiophene	4.69	176.3	0.210	0.000	47.433
79	C1-Naphthalenes	3.87	142.2	14.880	0.000	62.579

80	Hydrindene	3.47	118.2	0.000	0.000	1547.758
81	n-C5	2.8	72.15	0.000	0.000	5145.671
82	CARBAZOLE	3.23	167.2	110.810	0.000	135.058
83	2-METHYLPENTANE	3.21	86.18	0.000	0.000	2540.108
84	1,2-Diethylbenzene	4.07	134.2	0.000	0.000	482.212
85	1,3-Dimethyl-2-Ethylbenzene	4.13	134.22	0.000	0.000	423.782
86	Propylbenzene	3.52	120.194	0.000	0.000	1413.086
87	p-XYLENE	3.09	106.2	0.000	0.000	3154.207
88	2-Methylnaphthalene	3.72	142.2	14.880	0.000	86.463
89	4-isopropyltoluene	4	134.22	0.000	0.000	560.819
90	sec-Butylbenzene	3.94	134.2	0.000	0.000	638.143
91	2,3-dimethylpentane	3.63	100.2	0.000	0.000	1194.520
92	3-Methylpentane	3.21	86.18	0.000	0.000	2540.108
93	2,2-dimethylpentane	3.67	100.2	0.000	0.000	1095.856
94	1,2,4-Trimethylbenzene	3.63	120.2	0.000	0.000	1114.885
95	Benzene, 1-methyl-2-(1-methylethyl)-	4	134.22	0.000	0.000	560.819
96	1-Methylnaphthalene	3.72	142.2	14.880	0.000	86.463
97	m-cymene	4	134.2	0.000	0.000	560.736
98	Ethylbenzene	3.03	106.2	0.000	0.000	3589.634
99	CYCLOHEXANE	3.18	84.16	0.000	0.000	2646.253
100	C1-Decalins	4.61	152.3	0.000	0.000	97.666
101	1-Methyl-3-ethylbenzene	3.58	120.2	0.000	0.000	1241.739
102	1-Methyl-2-ethylbenzene	3.58	120.2	0.000	0.000	1241.739
103	4-ETHYLTOLUENE	3.58	120.2	0.000	0.000	1241.739
104	m-XYLENE	3.09	106.2	0.000	0.000	3154.207
105	Isopropylbenzene	3.45	120.194	0.000	0.000	1643.193
106	C2-Benzothiophene	4.13	162.25	0.210	0.000	145.939
107	1,2,4,5-Tetramethylbenzene	4.18	134.2	0.000	0.000	380.433
108	Isopentane	2.72	72.15	0.000	0.000	6113.952

109	Methylcyclopentane	3.1	84.16	0.000	0.000	3144.209
110	2,3-dimethylbutane	3.14	86.18	0.000	0.000	2953.740
111	1,3,5-trimethylbenzene	3.63	120.2	0.000	0.000	1114.885
112	o-XYLENE	3.09	106.2	0.000	0.000	3154.207
113	Cyclopentane	2.68	70.13	0.000	0.000	6477.830
114	trans-Decalin	4.2	138.26	0.000	0.000	214.537
115	C1-Benzothiophene	3.5365	148.2	0.210	0.000	479.018
116	Benzene	1.99	78.11	0.000	0.000	24835.468
117	cis-Decalin	4.2	138.26	0.000	0.000	214.537
118	Benzothiophene	2.99	134.2	0.210	0.000	1408.576
119	n-C11	5.74	156.31	0.000	0.000	19.740
120	n-C11	5.74	156.31	0.000	0.000	19.740
121	n-C11	5.74	156.31	0.000	0.000	19.740
122	n-C11	5.74	156.31	0.000	0.000	19.740
123	n-C12	6.23	170.34	0.000	0.000	7.482
124	n-C12	6.23	170.34	0.000	0.000	7.482
125	n-C12	6.23	170.34	0.000	0.000	7.482
126	n-C12	6.23	170.34	0.000	0.000	7.482
127	n-C11	5.74	156.31	0.000	0.000	19.740
128	n-C11	5.74	156.31	0.000	0.000	19.740
129	n-C11	5.74	156.31	0.000	0.000	19.740
130	n-C11	5.74	156.31	0.000	0.000	19.740
131	n-C12	6.23	170.34	0.000	0.000	7.482
132	n-C12	6.23	170.34	0.000	0.000	7.482
133	n-C12	6.23	170.34	0.000	0.000	7.482
134	n-C12	6.23	170.34	0.000	0.000	7.482
135	n-C13	6.73	184.37	0.000	0.000	2.757
136	n-C14	7.22	198.4	0.000	0.000	1.032
137	n-C15	7.71	212.42	0.000	0.000	0.384

138	n-C16	8.2	226.45	0.000	0.000	0.142
139	n-C17	8.69	240.48	0.000	0.000	0.053
140	n-C18	9.18	254.5	0.000	0.000	0.019
141	n-C19	9.67	268.53	0.000	0.000	0.007
142	n-C20	10.1	282.56	0.000	0.000	0.003
143	n-C21	10.6	296.59	0.000	0.000	0.001
144	n-C22	11.1	310.61	0.000	0.000	0.000
145	n-C23	11.6	324.64	0.000	0.000	0.000
146	n-C24	12.1	338.67	0.000	0.000	0.000
147	n-C25	12.6	352.69	0.000	0.000	0.000
148	n-C26	13.1	366.72	0.000	0.000	0.000
149	n-C27	13.6	380.75	0.000	0.000	0.000
150	n-C28	14	394.77	0.000	0.000	0.000
151	n-C29	14.5	408.8	0.000	0.000	0.000
152	n-C30	15	422.83	0.000	0.000	0.000
153	n-C31	15.5	436.86	0.000	0.000	0.000
154	n-C32	16	450.88	0.000	0.000	0.000
155	n-C33	16.5	464.91	0.000	0.000	0.000
156	n-C34	17	478.94	0.000	0.000	0.000
157	n-C35	17.5	492.96	0.000	0.000	0.000
158	n-C36	18	506.981	0.000	0.000	0.000
159	n-C37	18.5	521	0.000	0.000	0.000
160	n-C38	19	535	0.000	0.000	0.000
161	n-C39	19.49	549.1	0.000	0.000	0.000
162	n-C40	19.9	563.1	0.000	0.000	0.000
163	Phytane	9.87	282.56	0.000	0.000	0.005
164	Pristane	9.38	268.525	0.000	0.000	0.013
165	Benzo(a)fluoranthene	6.11	252.3	3326.260	0.000	0.101
166	Benzo(b)fluorene	5.77	216.3	295.350	0.000	0.493

167	Benzo(k)fluoranthene	6.11	252.3	1862.910	0.000	0.129
168	Benzo[a]anthracene	5.52	228.3	507.070	0.000	0.715
169	Benzo[a]pyrene	6.11	252.3	2612.960	0.000	0.112
170	Benzo[b]fluoranthene	6.11	252.3	1112.540	0.000	0.160
171	Benzo[e]pyrene	6.11	252.3	616.180	0.000	0.205
172	Benzo[g,h,i]perylene	6.7	276.3	2065.650	0.000	0.038
173	C1-Chrysenes	6.0683	242.3	289.380	0.000	0.293
174	C1-Fluoranthenes/Pyrene	5.4803	216.3	1146.990	0.000	0.527
175	C1-naphthobenzothiophenes	6.38	248.3	0.000	0.000	3.510
176	C2-Chrysenes	6.65	256.3	289.380	0.000	0.088
177	C2-Decalins	6.19	166.3	0.000	0.000	3.540
178	C2-Fluoranthenes/Pyrene	6.13	230.3	1146.990	0.000	0.138
179	C2-naphthobenzothiophenes	6.86	262.4	0.000	0.000	1.318
180	C2-Phenanthrenes/Anthracenes	5.47	206.3	676.140	0.000	0.639
181	C3-Chrysenes	7.03	270.4	289.380	0.000	0.041
182	C3-Decalins	6.79	180.3	0.000	0.000	1.053
183	C3-Dibenzothiophenes	5.86	230.37	4.480	0.000	2.122
184	C3-Fluoranthenes/Pyrene	6.57	244.34	1146.990	0.000	0.057
185	C3-Fluorenes	5.58	210.3	60.950	0.000	1.359
186	C3-naphthobenzothiophenes	7.36	276.4	0.000	0.000	0.473
187	C3-Phenanthrenes/Anthracenes	5.86	220.3	676.140	0.000	0.295
188	C4-Chrysenes	7.35	284.4	289.380	0.000	0.022
189	C4-Decalins	7.34	194.3	0.000	0.000	0.347
190	C4-Dibenzothiophenes	6.1	244.37	4.480	0.000	1.342
191	C4-Fluoranthenes/Pyrenes	7.05	258.34	1146.990	0.000	0.021
192	C4-naphthobenzothiophenes	7.84	290.4	0.000	0.000	0.177
193	C4-Phenanthrenes/Anthracenes	6.16	234.3	676.140	0.000	0.164
194	Chrysene	5.52	228.3	232.480	0.000	0.984
195	Dibenz(a,h)anthracene	6.7	278.4	1302.120	0.000	0.046

196	Indeno[1,2,3-cd]pyrene	6.7	276.3	3556.050	0.000	0.030
197	Naphthobenzothiophenes	5.34	178.2	0.000	0.000	23.696
198	Perylene	6.11	252.3	6039.440	0.000	0.079
199	Retene	6.35	234.3	74.490	0.000	0.266

Table B.39. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 100% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Naphthalenes	156.2	4.31	33.861	12.000	49.942
2	C1-Naphthalenes	142.2	3.87	22.060	31.300	138.041
3	2-Methylnaphthalene	142.2	3.72	22.060	29.800	190.725
4	C3-Naphthalenes	170.26	4.77	33.861	2.660	20.199
5	1-Methylnaphthalene	142.2	3.72	22.060	22.600	190.725
6	C1-Fluorenes	180.2	4.97	124.627	0.794	8.337
7	C1-Phenanthrenes/Anthracenes	192.3	4.26	1628.160	1.230	14.334
8	C2-Fluorenes	194.3	5.21	124.627	0.442	5.359
9	2,6-Dimethylnaphthalene	156.23	4.26	33.861	3.920	55.636
10	Toluene	92.14	2.54	0.000	1610.000	22856.420
11	C4-Naphthalenes	184.3	5.18	33.861	0.626	9.036
12	m-XYLENE	106.2	3.09	0.000	430.000	8051.643
13	2-Methylanthracene	192.26	4.89	1628.160	0.187	3.686
14	Naphthalene	234.3	3.17	13.139	56.300	1245.210
15	4/9-Methylphenanthrene	192.26	4.89	74.551	0.507	12.961
16	1,6,7-Trimethylnaphthalene	170.26	4.81	39.436	0.648	17.478
17	o-XYLENE	106.2	3.09	0.000	283.000	8051.643
18	1,2,4-Trimethylbenzene	120.2	3.63	0.000	90.800	2845.932
19	Phenanthrene	178.2	4.35	47.016	1.240	46.064
20	Fluorene	166.2	4.02	124.627	1.340	59.579
21	Benzene	78.11	1.99	0.000	1400.000	63396.698

22	CYCLOHEXANE	84.16	3.18	0.000	123.000	6755.006
23	1-Methylphenanthrene	192.26	4.89	74.551	0.232	12.961
24	Methylcyclohexane	98.19	3.59	0.000	55.800	3257.071
25	3-Methylphenanthrene	192.26	4.89	74.551	0.192	12.961
26	2-Methylphenanthrene	192.26	4.89	74.551	0.189	12.961
27	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	42.800	3169.746
28	Ethylbenzene	106.2	3.03	0.000	111.000	9163.144
29	Anthracene	178.2	4.35	975.919	0.161	13.537
30	C2-Dibenzothiophenes	214.3	5.13	10.025	0.199	18.379
31	Methylcyclopentane	84.16	3.1	0.000	83.100	8026.121
32	1,3,5-trimethylbenzene	120.2	3.63	0.000	27.600	2845.932
33	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	26.600	3169.746
34	Isopentane	72.15	2.72	0.000	112.000	15606.889
35	C1-Dibenzothiophenes	198.3	4.71	10.025	0.279	42.049
36	n-C5	72.15	2.8	0.000	83.500	13135.189
37	p-XYLENE	106.2	3.09	0.000	47.200	8051.643
38	C3-Benzothiophene	176.3	4.69	0.557	0.503	96.223
39	4-ETHYLTOLUENE	120.2	3.58	0.000	15.100	3169.746
40	Cyclopentane	70.13	2.68	0.000	72.000	16535.748
41	C4-Benzothiophene	190.3	5.18	0.557	0.156	36.127
42	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	4.330	1081.615
43	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	4.040	1081.615
44	Propylbenzene	120.194	3.52	0.000	13.300	3607.138
45	Pyrene	202.3	4.93	2154.955	0.011	3.166
46	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	4.230	1230.928
47	CARBAZOLE	167.2	3.23	223.309	0.863	260.088
48	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	3.460	1081.615
49	Acenaphthene	154.2	4.15	79.450	0.146	49.954
50	n-C6	86.18	3.29	0.000	15.200	5457.158

51	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	2.900	1081.615
52	Isopropylbenzene	120.194	3.45	0.000	11.000	4194.525
53	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	3.220	1230.928
54	m-cymene	134.2	4	0.000	3.240	1431.372
55	4-Methyldibenzothiophene	198.28	4.71	10.025	0.095	42.044
56	2-METHYLPENTANE	86.18	3.21	0.000	14.600	6484.052
57	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	2.420	1081.776
58	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	2.060	971.119
59	3-Methylpentane	86.18	3.21	0.000	13.400	6484.052
60	C2-Benzothiophene	162.25	4.13	0.557	0.599	296.055
61	Dibenzothiophene	184.3	4.17	10.025	0.250	125.139
62	2/3-Methyldibenzothiophene	198.28	4.71	8.675	0.087	44.264
63	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	2.340	1231.111
64	Dibenzofuran	168.2	3.71	37.994	0.324	187.515
65	Biphenyl	154.2	3.76	0.000	2.660	1576.610
66	Hydrindene	118.2	3.47	0.000	4.870	3950.913
67	4-isopropyltoluene	134.22	4	0.000	1.540	1431.585
68	1-Methyldibenzothiophene	198.28	4.71	10.025	0.042	42.044
69	Fluoranthene	202.3	4.93	1302.001	0.004	3.906
70	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	1.010	1081.776
71	sec-Butylbenzene	134.2	3.94	0.000	1.500	1628.968
72	3-methylhexane	100.2	3.71	0.000	2.140	2566.302
73	n-C10	142.29	5.25	0.000	0.095	131.879
74	n-C10	142.29	5.25	0.000	0.095	131.879
75	n-C10	142.3	5.25	0.000	0.095	131.888
76	n-C10	142.3	5.25	0.000	0.095	131.888
77	1,2-Diethylbenzene	134.2	4.07	0.000	0.880	1230.928
78	n-Butylbenzene	134.2	4.01	0.000	0.887	1400.853
79	2-methylhexane	100.2	3.71	0.000	1.420	2566.302

80	2,3-dimethylbutane	86.18	3.14	0.000	3.790	7539.916
81	2,3-dimethylpentane	100.2	3.63	0.000	1.530	3049.213
82	HEPTANE	100.2	3.78	0.000	1.060	2206.926
83	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.647	1431.585
84	trans-Decalin	138.26	4.2	0.000	0.202	547.642
85	C1-Decalins	152.3	4.61	0.000	0.086	249.310
86	Acenaphthylene	152.2	3.94	633.610	0.011	33.450
87	C1-Benzothiophene	148.2	3.5365	0.557	0.257	971.743
88	n-C8	114.2	4.27	0.000	0.157	874.875
89	2,2-dimethylpentane	100.2	3.67	0.000	0.298	2797.356
90	1,1,3-trimethylpentane	114.23	4.12	0.000	0.093	1209.094
91	cis-Decalin	138.26	4.2	0.000	0.013	547.642
92	Benzothiophene	134.2	2.99	0.557	0.047	2857.458
93	1-Decene	140.3	5.12	0.000	0.000	172.083
94	n-C9	128.3	4.76	0.000	0.000	341.874
95	n-C9	128.3	4.76	0.000	0.000	341.874
96	n-C9	128.3	4.76	0.000	0.000	341.874
97	n-C9	128.3	4.76	0.000	0.000	341.874
98	1-Nonene	126.2	4.62	0.000	0.000	454.715
99	n-C10	142.29	5.25	0.000	0.000	131.879
100	n-C10	142.29	5.25	0.000	0.000	131.879
101	n-C10	142.3	5.25	0.000	0.000	131.888
102	n-C10	142.3	5.25	0.000	0.000	131.888
103	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1289.514
104	n-Pentylbenzene	148.2	4.5	0.000	0.000	691.589
105	Octene-1	112.2	4.13	0.000	0.000	1162.286
106	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1289.853
107	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1209.094
108	3-methylheptane	114.2	4.2	0.000	0.000	1017.340

109	n-C9	128.3	4.76	0.000	0.000	341.874
110	n-C9	128.3	4.76	0.000	0.000	341.874
111	n-C9	128.3	4.76	0.000	0.000	341.874
112	n-C9	128.3	4.76	0.000	0.000	341.874
113	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1405.614
114	2-methylheptane	114.2	4.2	0.000	0.000	1017.340
115	tert-Butylbenzene	134.2	3.9	0.000	0.000	1775.630
116	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1208.777
117	2,4-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
118	3-ethylhexane	114.2	4.2	0.000	0.000	1017.340
119	n-C11	156.31	5.74	0.000	0.000	50.390
120	n-C11	156.31	5.74	0.000	0.000	50.390
121	n-C11	156.31	5.74	0.000	0.000	50.390
122	n-C11	156.31	5.74	0.000	0.000	50.390
123	n-C12	170.34	6.23	0.000	0.000	19.100
124	n-C12	170.34	6.23	0.000	0.000	19.100
125	n-C12	170.34	6.23	0.000	0.000	19.100
126	n-C12	170.34	6.23	0.000	0.000	19.100
127	n-C11	156.31	5.74	0.000	0.000	50.390
128	n-C11	156.31	5.74	0.000	0.000	50.390
129	n-C11	156.31	5.74	0.000	0.000	50.390
130	n-C11	156.31	5.74	0.000	0.000	50.390
131	n-C12	170.34	6.23	0.000	0.000	19.100
132	n-C12	170.34	6.23	0.000	0.000	19.100
133	n-C12	170.34	6.23	0.000	0.000	19.100
134	n-C12	170.34	6.23	0.000	0.000	19.100
135	n-C13	184.37	6.73	0.000	0.000	7.037
136	n-C14	198.4	7.22	0.000	0.000	2.634
137	n-C15	212.42	7.71	0.000	0.000	0.981

138	n-C16	226.45	8.2	0.000	0.000	0.364
139	n-C17	240.48	8.69	0.000	0.000	0.134
140	n-C18	254.5	9.18	0.000	0.000	0.049
141	n-C19	268.53	9.67	0.000	0.000	0.018
142	n-C20	282.56	10.1	0.000	0.000	0.008
143	n-C21	296.59	10.6	0.000	0.000	0.003
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.012
164	Pristane	268.525	9.38	0.000	0.000	0.034
165	Benzo(a)fluoranthene	252.3	6.11	4831.334	0.000	0.221
166	Benzo(b)fluorene	216.3	5.77	782.938	0.000	0.844

167	Benzo(k)fluoranthene	252.3	6.11	3994.076	0.000	0.240
168	Benzo[a]anthracene	228.3	5.52	1123.281	0.000	1.314
169	Benzo[a]pyrene	252.3	6.11	5890.368	0.000	0.204
170	Benzo[b]fluoranthene	252.3	6.11	2441.669	0.000	0.295
171	Benzo[e]pyrene	252.3	6.11	1618.083	0.000	0.350
172	Benzo[g,h,i]perylene	276.3	6.7	4737.382	0.000	0.069
173	C1-Chrysenes	242.3	6.0683	763.628	0.000	0.502
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2844.515	0.000	0.920
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	8.960
176	C2-Chrysenes	256.3	6.65	763.628	0.000	0.152
177	C2-Decalins	166.3	6.19	0.000	0.000	9.038
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2844.515	0.000	0.242
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	3.365
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1628.160	0.000	1.133
181	C3-Chrysenes	270.4	7.03	763.628	0.000	0.071
182	C3-Decalins	180.3	6.79	0.000	0.000	2.689
183	C3-Dibenzothiophenes	230.37	5.86	10.025	0.000	4.097
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2844.515	0.000	0.099
185	C3-Fluorenes	210.3	5.58	124.627	0.000	2.613
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.207
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1628.160	0.000	0.522
188	C4-Chrysenes	284.4	7.35	763.628	0.000	0.037
189	C4-Decalins	194.3	7.34	0.000	0.000	0.886
190	C4-Dibenzothiophenes	244.37	6.1	10.025	0.000	2.591
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2844.515	0.000	0.037
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.451
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1628.160	0.000	0.291
194	Chrysene	228.3	5.52	596.340	0.000	1.708
195	Dibenz(a,h)anthracene	278.4	6.7	2713.219	0.000	0.087

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	6963.391	0.000	0.058
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	60.488
198	Perylene	252.3	6.11	8099.812	0.000	0.178
199	Retene	234.3	6.35	109.500	0.000	0.583

Table B.40. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 25% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	22.060	8.280	138.041
2	C2-Naphthalenes	156.2	4.31	33.861	2.980	49.942
3	2-Methylnaphthalene	142.2	3.72	22.060	8.270	190.725
4	1-Methylnaphthalene	142.2	3.72	22.060	6.300	190.725
5	C3-Naphthalenes	170.26	4.77	33.861	0.664	20.199
6	C1-Fluorenes	180.2	4.97	124.627	0.208	8.337
7	2,6-Dimethylnaphthalene	156.23	4.26	33.861	1.210	55.636
8	C1-Phenanthrenes/Anthracenes	192.3	4.26	1628.160	0.305	14.334
9	C2-Fluorenes	194.3	5.21	124.627	0.112	5.359
10	Toluene	92.14	2.54	0.000	439.000	22856.420
11	C4-Naphthalenes	184.3	5.18	33.861	0.149	9.036
12	m-XYLENE	106.2	3.09	0.000	115.000	8051.643
13	Naphthalene	234.3	3.17	13.139	16.100	1245.210
14	2-Methylanthracene	192.26	4.89	1628.160	0.045	3.686
15	4/9-Methylphenanthrene	192.26	4.89	74.551	0.127	12.961
16	o-XYLENE	106.2	3.09	0.000	73.300	8051.643
17	1,6,7-Trimethylnaphthalene	170.26	4.81	39.436	0.157	17.478
18	1,2,4-Trimethylbenzene	120.2	3.63	0.000	22.400	2845.932
19	Phenanthrene	178.2	4.35	47.016	0.317	46.064
20	Benzene	78.11	1.99	0.000	375.000	63396.698
21	Fluorene	166.2	4.02	124.627	0.347	59.579

22	1-Methylphenanthrene	192.26	4.89	74.551	0.056	12.961
23	CYCLOHEXANE	84.16	3.18	0.000	26.500	6755.006
24	Methylcyclohexane	98.19	3.59	0.000	12.400	3257.071
25	3-Methylphenanthrene	192.26	4.89	74.551	0.047	12.961
26	2-Methylphenanthrene	192.26	4.89	74.551	0.046	12.961
27	Ethylbenzene	106.2	3.03	0.000	30.700	9163.144
28	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	10.600	3169.746
29	p-XYLENE	106.2	3.09	0.000	25.700	8051.643
30	C2-Dibenzothiophenes	214.3	5.13	10.025	0.058	18.379
31	Anthracene	178.2	4.35	975.919	0.036	13.537
32	1,3,5-trimethylbenzene	120.2	3.63	0.000	6.940	2845.932
33	Methylcyclopentane	84.16	3.1	0.000	18.300	8026.121
34	Isopentane	72.15	2.72	0.000	32.100	15606.889
35	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	6.460	3169.746
36	C1-Dibenzothiophenes	198.3	4.71	10.025	0.066	42.049
37	C3-Benzothiophene	176.3	4.69	0.557	0.129	96.223
38	Pyrene	202.3	4.93	2154.955	0.004	3.166
39	4-ETHYLTOLUENE	120.2	3.58	0.000	3.740	3169.746
40	n-C5	72.15	2.8	0.000	15.000	13135.189
41	C4-Benzothiophene	190.3	5.18	0.557	0.038	36.127
42	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	1.060	1081.615
43	Propylbenzene	120.194	3.52	0.000	3.090	3607.138
44	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.926	1081.615
45	Cyclopentane	70.13	2.68	0.000	14.100	16535.748
46	CARBAZOLE	167.2	3.23	223.309	0.211	260.088
47	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.981	1230.928
48	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.828	1081.615
49	Acenaphthene	154.2	4.15	79.450	0.037	49.954
50	n-C6	86.18	3.29	0.000	3.740	5457.158

51	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.720	1081.615
52	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.748	1230.928
53	Isopropylbenzene	120.194	3.45	0.000	2.510	4194.525
54	4-Methyldibenzothiophene	198.28	4.71	10.025	0.023	42.044
55	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.596	1081.776
56	m-cymene	134.2	4	0.000	0.777	1431.372
57	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.511	971.119
58	C2-Benzothiophene	162.25	4.13	0.557	0.151	296.055
59	Dibenzothiophene	184.3	4.17	10.025	0.063	125.139
60	2-METHYLPENTANE	86.18	3.21	0.000	3.030	6484.052
61	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.563	1231.111
62	Dibenzofuran	168.2	3.71	37.994	0.085	187.515
63	Biphenyl	154.2	3.76	0.000	0.697	1576.610
64	3-Methylpentane	86.18	3.21	0.000	2.700	6484.052
65	Fluoranthene	202.3	4.93	1302.001	0.002	3.906
66	n-C10	142.29	5.25	0.000	0.049	131.879
67	n-C10	142.29	5.25	0.000	0.049	131.879
68	n-C10	142.3	5.25	0.000	0.049	131.888
69	n-C10	142.3	5.25	0.000	0.049	131.888
70	2/3-Methyldibenzothiophene	198.28	4.71	8.675	0.013	44.264
71	Hydrindene	118.2	3.47	0.000	1.150	3950.913
72	4-isopropyltoluene	134.22	4	0.000	0.351	1431.585
73	1-Methyldibenzothiophene	198.28	4.71	10.025	0.010	42.044
74	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.253	1081.776
75	sec-Butylbenzene	134.2	3.94	0.000	0.335	1628.968
76	3-methylhexane	100.2	3.71	0.000	0.522	2566.302
77	1,2-Diethylbenzene	134.2	4.07	0.000	0.208	1230.928
78	n-Butylbenzene	134.2	4.01	0.000	0.194	1400.853
79	2-methylhexane	100.2	3.71	0.000	0.354	2566.302

80	HEPTANE	100.2	3.78	0.000	0.304	2206.926
81	2,3-dimethylbutane	86.18	3.14	0.000	1.020	7539.916
82	2,3-dimethylpentane	100.2	3.63	0.000	0.358	3049.213
83	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.148	1431.585
84	Acenaphthylene	152.2	3.94	633.610	0.003	33.450
85	C1-Decalins	152.3	4.61	0.000	0.019	249.310
86	trans-Decalin	138.26	4.2	0.000	0.037	547.642
87	C1-Benzothiophene	148.2	3.5365	0.557	0.064	971.743
88	2,2-dimethylpentane	100.2	3.67	0.000	0.064	2797.356
89	cis-Decalin	138.26	4.2	0.000	0.003	547.642
90	Benzothiophene	134.2	2.99	0.557	0.010	2857.458
91	1-Decene	140.3	5.12	0.000	0.000	172.083
92	n-C9	128.3	4.76	0.000	0.000	341.874
93	n-C9	128.3	4.76	0.000	0.000	341.874
94	n-C9	128.3	4.76	0.000	0.000	341.874
95	n-C9	128.3	4.76	0.000	0.000	341.874
96	1-Nonene	126.2	4.62	0.000	0.000	454.715
97	n-C10	142.29	5.25	0.000	0.000	131.879
98	n-C10	142.29	5.25	0.000	0.000	131.879
99	n-C10	142.3	5.25	0.000	0.000	131.888
100	n-C10	142.3	5.25	0.000	0.000	131.888
101	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1289.514
102	n-C8	114.2	4.27	0.000	0.000	874.875
103	n-Pentylbenzene	148.2	4.5	0.000	0.000	691.589
104	Octene-1	112.2	4.13	0.000	0.000	1162.286
105	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1289.853
106	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1209.094
107	3-methylheptane	114.2	4.2	0.000	0.000	1017.340
108	n-C9	128.3	4.76	0.000	0.000	341.874

109	n-C9	128.3	4.76	0.000	0.000	341.874
110	n-C9	128.3	4.76	0.000	0.000	341.874
111	n-C9	128.3	4.76	0.000	0.000	341.874
112	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1405.614
113	2-methylheptane	114.2	4.2	0.000	0.000	1017.340
114	tert-Butylbenzene	134.2	3.9	0.000	0.000	1775.630
115	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1209.094
116	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1208.777
117	2,4-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
118	3-ethylhexane	114.2	4.2	0.000	0.000	1017.340
119	n-C11	156.31	5.74	0.000	0.000	50.390
120	n-C11	156.31	5.74	0.000	0.000	50.390
121	n-C11	156.31	5.74	0.000	0.000	50.390
122	n-C11	156.31	5.74	0.000	0.000	50.390
123	n-C12	170.34	6.23	0.000	0.000	19.100
124	n-C12	170.34	6.23	0.000	0.000	19.100
125	n-C12	170.34	6.23	0.000	0.000	19.100
126	n-C12	170.34	6.23	0.000	0.000	19.100
127	n-C11	156.31	5.74	0.000	0.000	50.390
128	n-C11	156.31	5.74	0.000	0.000	50.390
129	n-C11	156.31	5.74	0.000	0.000	50.390
130	n-C11	156.31	5.74	0.000	0.000	50.390
131	n-C12	170.34	6.23	0.000	0.000	19.100
132	n-C12	170.34	6.23	0.000	0.000	19.100
133	n-C12	170.34	6.23	0.000	0.000	19.100
134	n-C12	170.34	6.23	0.000	0.000	19.100
135	n-C13	184.37	6.73	0.000	0.000	7.037
136	n-C14	198.4	7.22	0.000	0.000	2.634
137	n-C15	212.42	7.71	0.000	0.000	0.981

138	n-C16	226.45	8.2	0.000	0.000	0.364
139	n-C17	240.48	8.69	0.000	0.000	0.134
140	n-C18	254.5	9.18	0.000	0.000	0.049
141	n-C19	268.53	9.67	0.000	0.000	0.018
142	n-C20	282.56	10.1	0.000	0.000	0.008
143	n-C21	296.59	10.6	0.000	0.000	0.003
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.012
164	Pristane	268.525	9.38	0.000	0.000	0.034
165	Benzo(a)fluoranthene	252.3	6.11	4831.334	0.000	0.221
166	Benzo(b)fluorene	216.3	5.77	782.938	0.000	0.844

167	Benzo(k)fluoranthene	252.3	6.11	3994.076	0.000	0.240
168	Benzo[a]anthracene	228.3	5.52	1123.281	0.000	1.314
169	Benzo[a]pyrene	252.3	6.11	5890.368	0.000	0.204
170	Benzo[b]fluoranthene	252.3	6.11	2441.669	0.000	0.295
171	Benzo[e]pyrene	252.3	6.11	1618.083	0.000	0.350
172	Benzo[g,h,i]perylene	276.3	6.7	4737.382	0.000	0.069
173	C1-Chrysenes	242.3	6.0683	763.628	0.000	0.502
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2844.515	0.000	0.920
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	8.960
176	C2-Chrysenes	256.3	6.65	763.628	0.000	0.152
177	C2-Decalins	166.3	6.19	0.000	0.000	9.038
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2844.515	0.000	0.242
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	3.365
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1628.160	0.000	1.133
181	C3-Chrysenes	270.4	7.03	763.628	0.000	0.071
182	C3-Decalins	180.3	6.79	0.000	0.000	2.689
183	C3-Dibenzothiophenes	230.37	5.86	10.025	0.000	4.097
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2844.515	0.000	0.099
185	C3-Fluorenes	210.3	5.58	124.627	0.000	2.613
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.207
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1628.160	0.000	0.522
188	C4-Chrysenes	284.4	7.35	763.628	0.000	0.037
189	C4-Decalins	194.3	7.34	0.000	0.000	0.886
190	C4-Dibenzothiophenes	244.37	6.1	10.025	0.000	2.591
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2844.515	0.000	0.037
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.451
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1628.160	0.000	0.291
194	Chrysene	228.3	5.52	596.340	0.000	1.708
195	Dibenz(a,h)anthracene	278.4	6.7	2713.219	0.000	0.087

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	6963.391	0.000	0.058
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	60.488
198	Perylene	252.3	6.11	8099.812	0.000	0.178
199	Retene	234.3	6.35	109.500	0.000	0.583

Table B.41. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	22.060	1.900	138.041
2	C2-Naphthalenes	156.2	4.31	33.861	0.660	49.942
3	2-Methylnaphthalene	142.2	3.72	22.060	1.740	190.725
4	1-Methylnaphthalene	142.2	3.72	22.060	1.350	190.725
5	C3-Naphthalenes	170.26	4.77	33.861	0.133	20.199
6	C1-Fluorenes	180.2	4.97	124.627	0.051	8.337
7	C2-Fluorenes	194.3	5.21	124.627	0.029	5.359
8	C1-Phenanthrenes/Anthracenes	192.3	4.26	1628.160	0.073	14.334
9	2,6-Dimethylnaphthalene	156.23	4.26	33.861	0.267	55.636
10	C4-Naphthalenes	184.3	5.18	33.861	0.041	9.036
11	Toluene	92.14	2.54	0.000	64.000	22856.420
12	2-Methylanthracene	192.26	4.89	1628.160	0.010	3.686
13	Naphthalene	234.3	3.17	13.139	3.300	1245.210
14	4/9-Methylphenanthrene	192.26	4.89	74.551	0.030	12.961
15	1,6,7-Trimethylnaphthalene	170.26	4.81	39.436	0.038	17.478
16	m-XYLENE	106.2	3.09	0.000	17.300	8051.643
17	Phenanthrene	178.2	4.35	47.016	0.078	46.064
18	o-XYLENE	106.2	3.09	0.000	12.000	8051.643
19	Fluorene	166.2	4.02	124.627	0.083	59.579
20	1,2,4-Trimethylbenzene	120.2	3.63	0.000	3.940	2845.932
21	1-Methylphenanthrene	192.26	4.89	74.551	0.014	12.961

22	3-Methylphenanthrene	192.26	4.89	74.551	0.012	12.961
23	Benzene	78.11	1.99	0.000	56.600	63396.698
24	2-Methylphenanthrene	192.26	4.89	74.551	0.011	12.961
25	C2-Dibenzothiophenes	214.3	5.13	10.025	0.015	18.379
26	p-XYLENE	106.2	3.09	0.000	5.790	8051.643
27	Anthracene	178.2	4.35	975.919	0.008	13.537
28	Ethylbenzene	106.2	3.03	0.000	5.040	9163.144
29	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	1.700	3169.746
30	CYCLOHEXANE	84.16	3.18	0.000	3.570	6755.006
31	Pyrene	202.3	4.93	2154.955	0.002	3.166
32	Methylcyclohexane	98.19	3.59	0.000	1.570	3257.071
33	n-C6	86.18	3.29	0.000	2.340	5457.158
34	1,3,5-trimethylbenzene	120.2	3.63	0.000	1.150	2845.932
35	C1-Dibenzothiophenes	198.3	4.71	10.025	0.016	42.049
36	C3-Benzothiophene	176.3	4.69	0.557	0.032	96.223
37	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	1.060	3169.746
38	Methylcyclopentane	84.16	3.1	0.000	2.380	8026.121
39	4-ETHYLTOLUENE	120.2	3.58	0.000	0.606	3169.746
40	Acenaphthene	154.2	4.15	79.450	0.009	49.954
41	CARBAZOLE	167.2	3.23	223.309	0.045	260.088
42	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.177	1081.615
43	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.148	1081.615
44	Propylbenzene	120.194	3.52	0.000	0.481	3607.138
45	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.142	1081.615
46	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.161	1230.928
47	4-Methyldibenzothiophene	198.28	4.71	10.025	0.005	42.044
48	Dibenzothiophene	184.3	4.17	10.025	0.015	125.139
49	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.124	1081.615
50	Cyclopentane	70.13	2.68	0.000	1.840	16535.748

51	Dibenzofuran	168.2	3.71	37.994	0.021	187.515
52	C2-Benzothiophene	162.25	4.13	0.557	0.032	296.055
53	Biphenyl	154.2	3.76	0.000	0.163	1576.610
54	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.123	1230.928
55	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.104	1081.776
56	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.091	971.119
57	Isopropylbenzene	120.194	3.45	0.000	0.389	4194.525
58	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.100	1231.111
59	2-METHYLPENTANE	86.18	3.21	0.000	0.394	6484.052
60	1-Methyldibenzothiophene	198.28	4.71	10.025	0.002	42.044
61	Hydrindene	118.2	3.47	0.000	0.219	3950.913
62	3-Methylpentane	86.18	3.21	0.000	0.351	6484.052
63	2/3-Methyldibenzothiophene	198.28	4.71	8.675	0.002	44.264
64	4-isopropyltoluene	134.22	4	0.000	0.069	1431.585
65	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.040	1081.776
66	sec-Butylbenzene	134.2	3.94	0.000	0.056	1628.968
67	n-Butylbenzene	134.2	4.01	0.000	0.041	1400.853
68	1,2-Diethylbenzene	134.2	4.07	0.000	0.034	1230.928
69	Acenaphthylene	152.2	3.94	633.610	0.001	33.450
70	C1-Decalins	152.3	4.61	0.000	0.005	249.310
71	C1-Benzothiophene	148.2	3.5365	0.557	0.018	971.743
72	HEPTANE	100.2	3.78	0.000	0.040	2206.926
73	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.025	1431.585
74	trans-Decalin	138.26	4.2	0.000	0.006	547.642
75	Benzothiophene	134.2	2.99	0.557	0.002	2857.458
76	n-C10	142.29	5.25	0.000	0.000	131.879
77	n-C10	142.29	5.25	0.000	0.000	131.879
78	n-C10	142.3	5.25	0.000	0.000	131.888
79	n-C10	142.3	5.25	0.000	0.000	131.888

80	1-Decene	140.3	5.12	0.000	0.000	172.083
81	n-C9	128.3	4.76	0.000	0.000	341.874
82	n-C9	128.3	4.76	0.000	0.000	341.874
83	n-C9	128.3	4.76	0.000	0.000	341.874
84	n-C9	128.3	4.76	0.000	0.000	341.874
85	1-Nonene	126.2	4.62	0.000	0.000	454.715
86	n-C10	142.29	5.25	0.000	0.000	131.879
87	n-C10	142.29	5.25	0.000	0.000	131.879
88	n-C10	142.3	5.25	0.000	0.000	131.888
89	n-C10	142.3	5.25	0.000	0.000	131.888
90	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1289.514
91	n-C8	114.2	4.27	0.000	0.000	874.875
92	n-Pentylbenzene	148.2	4.5	0.000	0.000	691.589
93	Octene-1	112.2	4.13	0.000	0.000	1162.286
94	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1289.853
95	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1209.094
96	3-methylheptane	114.2	4.2	0.000	0.000	1017.340
97	n-C9	128.3	4.76	0.000	0.000	341.874
98	n-C9	128.3	4.76	0.000	0.000	341.874
99	n-C9	128.3	4.76	0.000	0.000	341.874
100	n-C9	128.3	4.76	0.000	0.000	341.874
101	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1405.614
102	Fluoranthene	202.3	4.93	1302.001	0.000	3.906
103	2-methylheptane	114.2	4.2	0.000	0.000	1017.340
104	tert-Butylbenzene	134.2	3.9	0.000	0.000	1775.630
105	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1209.094
106	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1208.777
107	m-cymene	134.2	4	0.000	0.000	1431.372
108	2,4-dimethylpentane	100.2	3.63	0.000	0.000	3049.213

109	n-C5	72.15	2.8	0.000	0.000	13135.189
110	2-methylhexane	100.2	3.71	0.000	0.000	2566.302
111	3-ethylhexane	114.2	4.2	0.000	0.000	1017.340
112	3-methylhexane	100.2	3.71	0.000	0.000	2566.302
113	2,2-dimethylpentane	100.2	3.67	0.000	0.000	2797.356
114	2,3-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
115	C4-Benzothiophene	190.3	5.18	0.557	0.000	36.127
116	Isopentane	72.15	2.72	0.000	0.000	15606.889
117	2,3-dimethylbutane	86.18	3.14	0.000	0.000	7539.916
118	cis-Decalin	138.26	4.2	0.000	0.000	547.642
119	n-C11	156.31	5.74	0.000	0.000	50.390
120	n-C11	156.31	5.74	0.000	0.000	50.390
121	n-C11	156.31	5.74	0.000	0.000	50.390
122	n-C11	156.31	5.74	0.000	0.000	50.390
123	n-C12	170.34	6.23	0.000	0.000	19.100
124	n-C12	170.34	6.23	0.000	0.000	19.100
125	n-C12	170.34	6.23	0.000	0.000	19.100
126	n-C12	170.34	6.23	0.000	0.000	19.100
127	n-C11	156.31	5.74	0.000	0.000	50.390
128	n-C11	156.31	5.74	0.000	0.000	50.390
129	n-C11	156.31	5.74	0.000	0.000	50.390
130	n-C11	156.31	5.74	0.000	0.000	50.390
131	n-C12	170.34	6.23	0.000	0.000	19.100
132	n-C12	170.34	6.23	0.000	0.000	19.100
133	n-C12	170.34	6.23	0.000	0.000	19.100
134	n-C12	170.34	6.23	0.000	0.000	19.100
135	n-C13	184.37	6.73	0.000	0.000	7.037
136	n-C14	198.4	7.22	0.000	0.000	2.634
137	n-C15	212.42	7.71	0.000	0.000	0.981

138	n-C16	226.45	8.2	0.000	0.000	0.364
139	n-C17	240.48	8.69	0.000	0.000	0.134
140	n-C18	254.5	9.18	0.000	0.000	0.049
141	n-C19	268.53	9.67	0.000	0.000	0.018
142	n-C20	282.56	10.1	0.000	0.000	0.008
143	n-C21	296.59	10.6	0.000	0.000	0.003
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.012
164	Pristane	268.525	9.38	0.000	0.000	0.034
165	Benzo(a)fluoranthene	252.3	6.11	4831.334	0.000	0.221
166	Benzo(b)fluorene	216.3	5.77	782.938	0.000	0.844

167	Benzo(k)fluoranthene	252.3	6.11	3994.076	0.000	0.240
168	Benzo[a]anthracene	228.3	5.52	1123.281	0.000	1.314
169	Benzo[a]pyrene	252.3	6.11	5890.368	0.000	0.204
170	Benzo[b]fluoranthene	252.3	6.11	2441.669	0.000	0.295
171	Benzo[e]pyrene	252.3	6.11	1618.083	0.000	0.350
172	Benzo[g,h,i]perylene	276.3	6.7	4737.382	0.000	0.069
173	C1-Chrysenes	242.3	6.0683	763.628	0.000	0.502
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2844.515	0.000	0.920
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	8.960
176	C2-Chrysenes	256.3	6.65	763.628	0.000	0.152
177	C2-Decalins	166.3	6.19	0.000	0.000	9.038
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2844.515	0.000	0.242
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	3.365
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1628.160	0.000	1.133
181	C3-Chrysenes	270.4	7.03	763.628	0.000	0.071
182	C3-Decalins	180.3	6.79	0.000	0.000	2.689
183	C3-Dibenzothiophenes	230.37	5.86	10.025	0.000	4.097
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2844.515	0.000	0.099
185	C3-Fluorenes	210.3	5.58	124.627	0.000	2.613
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.207
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1628.160	0.000	0.522
188	C4-Chrysenes	284.4	7.35	763.628	0.000	0.037
189	C4-Decalins	194.3	7.34	0.000	0.000	0.886
190	C4-Dibenzothiophenes	244.37	6.1	10.025	0.000	2.591
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2844.515	0.000	0.037
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.451
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1628.160	0.000	0.291
194	Chrysene	228.3	5.52	596.340	0.000	1.708
195	Dibenz(a,h)anthracene	278.4	6.7	2713.219	0.000	0.087

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	6963.391	0.000	0.058
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	60.488
198	Perylene	252.3	6.11	8099.812	0.000	0.178
199	Retene	234.3	6.35	109.500	0.000	0.583

Table B.42. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF duplicate exposed to *Cyprinodon variegatus* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	22.060	1.970	138.041
2	C2-Naphthalenes	156.2	4.31	33.861	0.638	49.942
3	2-Methylnaphthalene	142.2	3.72	22.060	1.800	190.725
4	1-Methylnaphthalene	142.2	3.72	22.060	1.410	190.725
5	C3-Naphthalenes	170.26	4.77	33.861	0.129	20.199
6	C2-Fluorenes	194.3	5.21	124.627	0.030	5.359
7	C1-Fluorenes	180.2	4.97	124.627	0.045	8.337
8	C1-Phenanthrenes/Anthracenes	192.3	4.26	1628.160	0.067	14.334
9	2,6-Dimethylnaphthalene	156.23	4.26	33.861	0.255	55.636
10	C4-Naphthalenes	184.3	5.18	33.861	0.041	9.036
11	Naphthalene	234.3	3.17	13.139	3.490	1245.210
12	Toluene	92.14	2.54	0.000	57.900	22856.420
13	2-Methylanthracene	192.26	4.89	1628.160	0.009	3.686
14	4/9-Methylphenanthrene	192.26	4.89	74.551	0.028	12.961
15	m-XYLENE	106.2	3.09	0.000	15.500	8051.643
16	1,6,7-Trimethylnaphthalene	170.26	4.81	39.436	0.034	17.478
17	Phenanthrene	178.2	4.35	47.016	0.075	46.064
18	Fluorene	166.2	4.02	124.627	0.082	59.579
19	o-XYLENE	106.2	3.09	0.000	10.800	8051.643
20	1,2,4-Trimethylbenzene	120.2	3.63	0.000	3.320	2845.932
21	1-Methylphenanthrene	192.26	4.89	74.551	0.013	12.961

22	3-Methylphenanthrene	192.26	4.89	74.551	0.011	12.961
23	C2-Dibenzothiophenes	214.3	5.13	10.025	0.015	18.379
24	2-Methylphenanthrene	192.26	4.89	74.551	0.011	12.961
25	Benzene	78.11	1.99	0.000	50.600	63396.698
26	Anthracene	178.2	4.35	975.919	0.009	13.537
27	p-XYLENE	106.2	3.09	0.000	4.810	8051.643
28	Pyrene	202.3	4.93	2154.955	0.002	3.166
29	Ethylbenzene	106.2	3.03	0.000	4.480	9163.144
30	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	1.460	3169.746
31	CYCLOHEXANE	84.16	3.18	0.000	3.060	6755.006
32	n-C6	86.18	3.29	0.000	2.340	5457.158
33	Methylcyclohexane	98.19	3.59	0.000	1.240	3257.071
34	C3-Benzothiophene	176.3	4.69	0.557	0.034	96.223
35	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.968	2845.932
36	C1-Dibenzothiophenes	198.3	4.71	10.025	0.013	42.049
37	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.945	3169.746
38	Methylcyclopentane	84.16	3.1	0.000	1.860	8026.121
39	Acenaphthene	154.2	4.15	79.450	0.009	49.954
40	CARBAZOLE	167.2	3.23	223.309	0.042	260.088
41	4-ETHYLTOLUENE	120.2	3.58	0.000	0.490	3169.746
42	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.146	1081.615
43	4-Methyldibenzothiophene	198.28	4.71	10.025	0.005	42.044
44	C2-Benzothiophene	162.25	4.13	0.557	0.035	296.055
45	Dibenzothiophene	184.3	4.17	10.025	0.015	125.139
46	Propylbenzene	120.194	3.52	0.000	0.400	3607.138
47	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.119	1081.615
48	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.118	1081.615
49	Dibenzofuran	168.2	3.71	37.994	0.020	187.515
50	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.125	1230.928

51	Biphenyl	154.2	3.76	0.000	0.157	1576.610
52	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.105	1081.615
53	Cyclopentane	70.13	2.68	0.000	1.560	16535.748
54	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.102	1081.776
55	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.103	1230.928
56	Isopropylbenzene	120.194	3.45	0.000	0.340	4194.525
57	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.076	971.119
58	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.084	1231.111
59	1-Methyldibenzothiophene	198.28	4.71	10.025	0.002	42.044
60	Hydrindene	118.2	3.47	0.000	0.190	3950.913
61	2/3-Methyldibenzothiophene	198.28	4.71	8.675	0.002	44.264
62	2-METHYLPENTANE	86.18	3.21	0.000	0.279	6484.052
63	3-Methylpentane	86.18	3.21	0.000	0.268	6484.052
64	4-isopropyltoluene	134.22	4	0.000	0.057	1431.585
65	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.037	1081.776
66	n-Butylbenzene	134.2	4.01	0.000	0.040	1400.853
67	sec-Butylbenzene	134.2	3.94	0.000	0.043	1628.968
68	1,2-Diethylbenzene	134.2	4.07	0.000	0.030	1230.928
69	HEPTANE	100.2	3.78	0.000	0.048	2206.926
70	C1-Benzothiophene	148.2	3.5365	0.557	0.019	971.743
71	trans-Decalin	138.26	4.2	0.000	0.008	547.642
72	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.020	1431.585
73	Benzothiophene	134.2	2.99	0.557	0.003	2857.458
74	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1209.094
75	1-Decene	140.3	5.12	0.000	0.000	172.083
76	1-Nonene	126.2	4.62	0.000	0.000	454.715
77	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1289.514
78	2,2-dimethylpentane	100.2	3.67	0.000	0.000	2797.356
79	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1405.614

80	2,3-dimethylbutane	86.18	3.14	0.000	0.000	7539.916
81	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1208.777
82	2,3-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
83	2,4-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
84	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1209.094
85	2-methylheptane	114.2	4.2	0.000	0.000	1017.340
86	2-methylhexane	100.2	3.71	0.000	0.000	2566.302
87	3-ethylhexane	114.2	4.2	0.000	0.000	1017.340
88	3-methylheptane	114.2	4.2	0.000	0.000	1017.340
89	3-methylhexane	100.2	3.71	0.000	0.000	2566.302
90	Isopentane	72.15	2.72	0.000	0.000	15606.889
91	m-cymene	134.2	4	0.000	0.000	1431.372
92	n-C10	142.3	5.25	0.000	0.000	131.888
93	n-C10	142.3	5.25	0.000	0.000	131.888
94	n-C10	142.3	5.25	0.000	0.000	131.888
95	n-C10	142.3	5.25	0.000	0.000	131.888
96	n-C11	156.31	5.74	0.000	0.000	50.390
97	n-C11	156.31	5.74	0.000	0.000	50.390
98	n-C11	156.31	5.74	0.000	0.000	50.390
99	n-C11	156.31	5.74	0.000	0.000	50.390
100	n-C12	170.34	6.23	0.000	0.000	19.100
101	n-C12	170.34	6.23	0.000	0.000	19.100
102	n-C12	170.34	6.23	0.000	0.000	19.100
103	n-C12	170.34	6.23	0.000	0.000	19.100
104	n-C5	72.15	2.8	0.000	0.000	13135.189
105	n-C8	114.2	4.27	0.000	0.000	874.875
106	n-C9	128.3	4.76	0.000	0.000	341.874
107	n-C9	128.3	4.76	0.000	0.000	341.874
108	n-C9	128.3	4.76	0.000	0.000	341.874

109	n-C9	128.3	4.76	0.000	0.000	341.874
110	n-Pentylbenzene	148.2	4.5	0.000	0.000	691.589
111	Octene-1	112.2	4.13	0.000	0.000	1162.286
112	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1289.853
113	tert-Butylbenzene	134.2	3.9	0.000	0.000	1775.630
114	n-C10	142.29	5.25	0.000	0.000	131.879
115	n-C10	142.29	5.25	0.000	0.000	131.879
116	n-C10	142.29	5.25	0.000	0.000	131.879
117	n-C10	142.29	5.25	0.000	0.000	131.879
118	n-C11	156.31	5.74	0.000	0.000	50.390
119	n-C11	156.31	5.74	0.000	0.000	50.390
120	n-C11	156.31	5.74	0.000	0.000	50.390
121	n-C11	156.31	5.74	0.000	0.000	50.390
122	n-C12	170.34	6.23	0.000	0.000	19.100
123	n-C12	170.34	6.23	0.000	0.000	19.100
124	n-C12	170.34	6.23	0.000	0.000	19.100
125	n-C12	170.34	6.23	0.000	0.000	19.100
126	n-C13	184.37	6.73	0.000	0.000	7.037
127	n-C14	198.4	7.22	0.000	0.000	2.634
128	n-C15	212.42	7.71	0.000	0.000	0.981
129	n-C16	226.45	8.2	0.000	0.000	0.364
130	n-C17	240.48	8.69	0.000	0.000	0.134
131	n-C18	254.5	9.18	0.000	0.000	0.049
132	n-C19	268.53	9.67	0.000	0.000	0.018
133	n-C20	282.56	10.1	0.000	0.000	0.008
134	n-C21	296.59	10.6	0.000	0.000	0.003
135	n-C22	310.61	11.1	0.000	0.000	0.001
136	n-C23	324.64	11.6	0.000	0.000	0.000
137	n-C24	338.67	12.1	0.000	0.000	0.000

138	n-C25	352.69	12.6	0.000	0.000	0.000
139	n-C26	366.72	13.1	0.000	0.000	0.000
140	n-C27	380.75	13.6	0.000	0.000	0.000
141	n-C28	394.77	14	0.000	0.000	0.000
142	n-C29	408.8	14.5	0.000	0.000	0.000
143	n-C30	422.83	15	0.000	0.000	0.000
144	n-C31	436.86	15.5	0.000	0.000	0.000
145	n-C32	450.88	16	0.000	0.000	0.000
146	n-C33	464.91	16.5	0.000	0.000	0.000
147	n-C34	478.94	17	0.000	0.000	0.000
148	n-C35	492.96	17.5	0.000	0.000	0.000
149	n-C36	506.981	18	0.000	0.000	0.000
150	n-C37	521	18.5	0.000	0.000	0.000
151	n-C38	535	19	0.000	0.000	0.000
152	n-C39	549.1	19.49	0.000	0.000	0.000
153	n-C40	563.1	19.9	0.000	0.000	0.000
154	n-C9	128.3	4.76	0.000	0.000	341.874
155	n-C9	128.3	4.76	0.000	0.000	341.874
156	n-C9	128.3	4.76	0.000	0.000	341.874
157	n-C9	128.3	4.76	0.000	0.000	341.874
158	Phytane	282.56	9.87	0.000	0.000	0.012
159	Pristane	268.525	9.38	0.000	0.000	0.034
160	Acenaphthylene	152.2	3.94	633.610	0.000	33.450
161	Benzo(a)fluoranthene	252.3	6.11	4831.334	0.000	0.221
162	Benzo(b)fluorene	216.3	5.77	782.938	0.000	0.844
163	Benzo(k)fluoranthene	252.3	6.11	3994.076	0.000	0.240
164	Benzo[a]anthracene	228.3	5.52	1123.281	0.000	1.314
165	Benzo[a]pyrene	252.3	6.11	5890.368	0.000	0.204
166	Benzo[b]fluoranthene	252.3	6.11	2441.669	0.000	0.295

167	Benzo[e]pyrene	252.3	6.11	1618.083	0.000	0.350
168	Benzo[g,h,i]perylene	276.3	6.7	4737.382	0.000	0.069
169	C1-Chrysenes	242.3	6.0683	763.628	0.000	0.502
170	C1-Decalins	152.3	4.61	0.000	0.000	249.310
171	C1-Fluoranthenes/Pyrene	216.3	5.4803	2844.515	0.000	0.920
172	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	8.960
173	C2-Chrysenes	256.3	6.65	763.628	0.000	0.152
174	C2-Decalins	166.3	6.19	0.000	0.000	9.038
175	C2-Fluoranthenes/Pyrene	230.3	6.13	2844.515	0.000	0.242
176	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	3.365
177	C2-Phenanthrenes/Anthracenes	206.3	5.47	1628.160	0.000	1.133
178	C3-Chrysenes	270.4	7.03	763.628	0.000	0.071
179	C3-Decalins	180.3	6.79	0.000	0.000	2.689
180	C3-Dibenzothiophenes	230.37	5.86	10.025	0.000	4.097
181	C3-Fluoranthenes/Pyrene	244.34	6.57	2844.515	0.000	0.099
182	C3-Fluorenes	210.3	5.58	124.627	0.000	2.613
183	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.207
184	C3-Phenanthrenes/Anthracenes	220.3	5.86	1628.160	0.000	0.522
185	C4-Benzothiophene	190.3	5.18	0.557	0.000	36.127
186	C4-Chrysenes	284.4	7.35	763.628	0.000	0.037
187	C4-Decalins	194.3	7.34	0.000	0.000	0.886
188	C4-Dibenzothiophenes	244.37	6.1	10.025	0.000	2.591
189	C4-Fluoranthenes/Pyrenes	258.34	7.05	2844.515	0.000	0.037
190	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.451
191	C4-Phenanthrenes/Anthracenes	234.3	6.16	1628.160	0.000	0.291
192	Chrysene	228.3	5.52	596.340	0.000	1.708
193	cis-Decalin	138.26	4.2	0.000	0.000	547.642
194	Dibenz(a,h)anthracene	278.4	6.7	2713.219	0.000	0.087
195	Fluoranthene	202.3	4.93	1302.001	0.000	3.906

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	6963.391	0.000	0.058
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	60.488
198	Perylene	252.3	6.11	8099.812	0.000	0.178
199	Retene	234.3	6.35	109.500	0.000	0.583

Table B.43. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 100% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	131.253	0.678	5.249
2	C1-Fluorenes	180.2	4.97	131.253	0.835	8.166
3	C3-Naphthalenes	170.26	4.77	39.124	1.560	19.110
4	C1-Phenanthrenes/Anthracenes	192.3	4.26	1672.207	1.110	14.176
5	C4-Naphthalenes	184.3	5.18	39.124	0.380	8.549
6	C2-Naphthalenes	156.2	4.31	39.124	2.050	47.249
7	1,6,7-Trimethylnaphthalene	170.26	4.81	47.767	0.519	16.231
8	1-Methylphenanthrene	192.26	4.89	86.350	0.361	12.230
9	Phenanthrene	178.2	4.35	54.428	1.260	43.516
10	4/9-Methylphenanthrene	192.26	4.89	86.350	0.323	12.230
11	2-Methylphenanthrene	192.26	4.89	86.350	0.272	12.230
12	3-Methylphenanthrene	192.26	4.89	86.350	0.267	12.230
13	C2-Dibenzothiophenes	214.3	5.13	11.607	0.284	17.436
14	2,6-Dimethylnaphthalene	156.23	4.26	39.124	0.834	52.636
15	Fluorene	166.2	4.02	131.253	0.705	58.356
16	C1-Dibenzothiophenes	198.3	4.71	11.607	0.368	39.891
17	Pyrene	202.3	4.93	2337.740	0.014	3.060
18	4-Methyldibenzothiophene	198.28	4.71	11.607	0.134	39.887
19	C1-Naphthalenes	142.2	3.87	27.131	0.281	127.689
20	Dibenzothiophene	184.3	4.17	11.607	0.260	118.718
21	2-Methylanthracene	192.26	4.89	1672.207	0.008	3.646

22	2/3-Methyldibenzothiophene	198.28	4.71	10.239	0.075	41.726
23	Fluoranthene	202.3	4.93	1361.298	0.007	3.834
24	1-Methylnaphthalene	142.2	3.72	27.131	0.250	176.422
25	1-Methyldibenzothiophene	198.28	4.71	11.607	0.052	39.887
26	2-Methylnaphthalene	142.2	3.72	27.131	0.204	176.422
27	Anthracene	178.2	4.35	1006.340	0.012	13.365
28	C4-Benzothiophene	190.3	5.18	0.586	0.029	35.661
29	Acenaphthene	154.2	4.15	94.968	0.034	46.548
30	Dibenzofuran	168.2	3.71	46.797	0.107	173.022
31	C3-Benzothiophene	176.3	4.69	0.586	0.045	94.983
32	Acenaphthylene	152.2	3.94	696.287	0.004	32.172
33	C2-Benzothiophene	162.25	4.13	0.586	0.032	292.239
34	Biphenyl	154.2	3.76	0.000	0.151	1576.610
35	C1-Benzothiophene	148.2	3.5365	0.586	0.070	959.217
36	CARBAZOLE	167.2	3.23	249.410	0.012	248.678
37	Naphthalene	234.3	3.17	16.140	0.021	1154.840
38	Toluene	92.14	2.54	0.000	0.144	22856.420
39	cis-Decalin	138.26	4.2	0.000	0.001	547.642
40	Benzothiophene	134.2	2.99	0.586	0.000	2820.625
41	n-C10	142.29	5.25	0.000	0.000	131.879
42	n-C10	142.29	5.25	0.000	0.000	131.879
43	n-C10	142.3	5.25	0.000	0.000	131.888
44	n-C10	142.3	5.25	0.000	0.000	131.888
45	1-Decene	140.3	5.12	0.000	0.000	172.083
46	n-C9	128.3	4.76	0.000	0.000	341.874
47	n-C9	128.3	4.76	0.000	0.000	341.874
48	n-C9	128.3	4.76	0.000	0.000	341.874
49	n-C9	128.3	4.76	0.000	0.000	341.874
50	1-Nonene	126.2	4.62	0.000	0.000	454.715

51	n-C10	142.29	5.25	0.000	0.000	131.879
52	n-C10	142.29	5.25	0.000	0.000	131.879
53	n-C10	142.3	5.25	0.000	0.000	131.888
54	n-C10	142.3	5.25	0.000	0.000	131.888
55	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1289.514
56	n-C8	114.2	4.27	0.000	0.000	874.875
57	n-Pentylbenzene	148.2	4.5	0.000	0.000	691.589
58	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	1231.111
59	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
60	Octene-1	112.2	4.13	0.000	0.000	1162.286
61	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1289.853
62	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1209.094
63	3-methylheptane	114.2	4.2	0.000	0.000	1017.340
64	n-C9	128.3	4.76	0.000	0.000	341.874
65	n-C9	128.3	4.76	0.000	0.000	341.874
66	n-C9	128.3	4.76	0.000	0.000	341.874
67	n-C9	128.3	4.76	0.000	0.000	341.874
68	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1405.614
69	2-methylheptane	114.2	4.2	0.000	0.000	1017.340
70	HEPTANE	100.2	3.78	0.000	0.000	2206.926
71	tert-Butylbenzene	134.2	3.9	0.000	0.000	1775.630
72	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
73	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
74	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
75	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	1081.776
76	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	1230.928
77	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	1230.928
78	n-Butylbenzene	134.2	4.01	0.000	0.000	1400.853
79	Methylcyclohexane	98.19	3.59	0.000	0.000	3257.071

80	sec-Butylbenzene	134.2	3.94	0.000	0.000	1628.968
81	Hydrindene	118.2	3.47	0.000	0.000	3950.913
82	Propylbenzene	120.194	3.52	0.000	0.000	3607.138
83	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	1081.776
84	n-C6	86.18	3.29	0.000	0.000	5457.158
85	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1209.094
86	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
87	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	1230.928
88	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1208.777
89	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	1431.585
90	m-cymene	134.2	4	0.000	0.000	1431.372
91	Ethylbenzene	106.2	3.03	0.000	0.000	9163.144
92	2,4-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
93	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
94	4-isopropyltoluene	134.22	4	0.000	0.000	1431.585
95	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
96	CYCLOHEXANE	84.16	3.18	0.000	0.000	6755.006
97	n-C5	72.15	2.8	0.000	0.000	13135.189
98	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	3169.746
99	p-XYLENE	106.2	3.09	0.000	0.000	8051.643
100	2-methylhexane	100.2	3.71	0.000	0.000	2566.302
101	Isopropylbenzene	120.194	3.45	0.000	0.000	4194.525
102	3-Methylpentane	86.18	3.21	0.000	0.000	6484.052
103	3-ethylhexane	114.2	4.2	0.000	0.000	1017.340
104	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
105	3-methylhexane	100.2	3.71	0.000	0.000	2566.302
106	2,2-dimethylpentane	100.2	3.67	0.000	0.000	2797.356
107	2,3-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
108	Methylcyclopentane	84.16	3.1	0.000	0.000	8026.121

109	2-METHYLPENTANE	86.18	3.21	0.000	0.000	6484.052
110	o-XYLENE	106.2	3.09	0.000	0.000	8051.643
111	m-XYLENE	106.2	3.09	0.000	0.000	8051.643
112	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	971.119
113	Cyclopentane	70.13	2.68	0.000	0.000	16535.748
114	Benzene	78.11	1.99	0.000	0.000	63396.698
115	Isopentane	72.15	2.72	0.000	0.000	15606.889
116	2,3-dimethylbutane	86.18	3.14	0.000	0.000	7539.916
117	C1-Decalins	152.3	4.61	0.000	0.000	249.310
118	trans-Decalin	138.26	4.2	0.000	0.000	547.642
119	n-C11	156.31	5.74	0.000	0.000	50.390
120	n-C11	156.31	5.74	0.000	0.000	50.390
121	n-C11	156.31	5.74	0.000	0.000	50.390
122	n-C11	156.31	5.74	0.000	0.000	50.390
123	n-C12	170.34	6.23	0.000	0.000	19.100
124	n-C12	170.34	6.23	0.000	0.000	19.100
125	n-C12	170.34	6.23	0.000	0.000	19.100
126	n-C12	170.34	6.23	0.000	0.000	19.100
127	n-C11	156.31	5.74	0.000	0.000	50.390
128	n-C11	156.31	5.74	0.000	0.000	50.390
129	n-C11	156.31	5.74	0.000	0.000	50.390
130	n-C11	156.31	5.74	0.000	0.000	50.390
131	n-C12	170.34	6.23	0.000	0.000	19.100
132	n-C12	170.34	6.23	0.000	0.000	19.100
133	n-C12	170.34	6.23	0.000	0.000	19.100
134	n-C12	170.34	6.23	0.000	0.000	19.100
135	n-C13	184.37	6.73	0.000	0.000	7.037
136	n-C14	198.4	7.22	0.000	0.000	2.634
137	n-C15	212.42	7.71	0.000	0.000	0.981

138	n-C16	226.45	8.2	0.000	0.000	0.364
139	n-C17	240.48	8.69	0.000	0.000	0.134
140	n-C18	254.5	9.18	0.000	0.000	0.049
141	n-C19	268.53	9.67	0.000	0.000	0.018
142	n-C20	282.56	10.1	0.000	0.000	0.008
143	n-C21	296.59	10.6	0.000	0.000	0.003
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.012
164	Pristane	268.525	9.38	0.000	0.000	0.034
165	Benzo(a)fluoranthene	252.3	6.11	4589.933	0.000	0.226
166	Benzo(b)fluorene	216.3	5.77	898.179	0.000	0.797

167	Benzo(k)fluoranthene	252.3	6.11	4187.545	0.000	0.235
168	Benzo[a]anthracene	228.3	5.52	1204.593	0.000	1.277
169	Benzo[a]pyrene	252.3	6.11	6060.592	0.000	0.201
170	Benzo[b]fluoranthene	252.3	6.11	2564.123	0.000	0.289
171	Benzo[e]pyrene	252.3	6.11	1764.684	0.000	0.337
172	Benzo[g,h,i]perylene	276.3	6.7	4937.495	0.000	0.067
173	C1-Chrysenes	242.3	6.0683	853.377	0.000	0.479
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2991.384	0.000	0.901
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	8.960
176	C2-Chrysenes	256.3	6.65	853.377	0.000	0.145
177	C2-Decalins	166.3	6.19	0.000	0.000	9.038
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2991.384	0.000	0.237
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	3.365
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1672.207	0.000	1.121
181	C3-Chrysenes	270.4	7.03	853.377	0.000	0.067
182	C3-Decalins	180.3	6.79	0.000	0.000	2.689
183	C3-Dibenzothiophenes	230.37	5.86	11.607	0.000	3.887
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2991.384	0.000	0.097
185	C3-Fluorenes	210.3	5.58	131.253	0.000	2.559
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.207
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1672.207	0.000	0.516
188	C4-Chrysenes	284.4	7.35	853.377	0.000	0.036
189	C4-Decalins	194.3	7.34	0.000	0.000	0.886
190	C4-Dibenzothiophenes	244.37	6.1	11.607	0.000	2.458
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2991.384	0.000	0.037
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.451
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1672.207	0.000	0.288
194	Chrysene	228.3	5.52	684.656	0.000	1.613
195	Dibenz(a,h)anthracene	278.4	6.7	2973.351	0.000	0.084

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	7096.895	0.000	0.058
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	60.488
198	Perylene	252.3	6.11	7520.015	0.000	0.184
199	Retene	234.3	6.35	127.907	0.000	0.548

Table B.44. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 25% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	131.253	0.177	5.249
2	C1-Fluorenes	180.2	4.97	131.253	0.206	8.166
3	C1-Phenanthrenes/Anthracenes	192.3	4.26	1672.207	0.276	14.176
4	C3-Naphthalenes	170.26	4.77	39.124	0.359	19.110
5	C4-Naphthalenes	184.3	5.18	39.124	0.087	8.549
6	C2-Naphthalenes	156.2	4.31	39.124	0.475	47.249
7	Phenanthrene	178.2	4.35	54.428	0.326	43.516
8	1,6,7-Trimethylnaphthalene	170.26	4.81	47.767	0.121	16.231
9	1-Methylphenanthrene	192.26	4.89	86.350	0.090	12.230
10	4/9-Methylphenanthrene	192.26	4.89	86.350	0.080	12.230
11	2-Methylphenanthrene	192.26	4.89	86.350	0.067	12.230
12	3-Methylphenanthrene	192.26	4.89	86.350	0.067	12.230
13	C2-Dibenzothiophenes	214.3	5.13	11.607	0.068	17.436
14	2,6-Dimethylnaphthalene	156.23	4.26	39.124	0.192	52.636
15	Fluorene	166.2	4.02	131.253	0.175	58.356
16	C1-Dibenzothiophenes	198.3	4.71	11.607	0.077	39.891
17	Pyrene	202.3	4.93	2337.740	0.005	3.060
18	4-Methyldibenzothiophene	198.28	4.71	11.607	0.032	39.887
19	Fluoranthene	202.3	4.93	1361.298	0.003	3.834
20	Dibenzothiophene	184.3	4.17	11.607	0.064	118.718
21	C1-Naphthalenes	142.2	3.87	27.131	0.068	127.689

22	2-Methylanthracene	192.26	4.89	1672.207	0.002	3.646
23	1-Methylnaphthalene	142.2	3.72	27.131	0.060	176.422
24	1-Methyldibenzothiophene	198.28	4.71	11.607	0.013	39.887
25	2-Methylnaphthalene	142.2	3.72	27.131	0.050	176.422
26	2/3-Methyldibenzothiophene	198.28	4.71	10.239	0.010	41.726
27	C4-Benzothiophene	190.3	5.18	0.586	0.008	35.661
28	Acenaphthene	154.2	4.15	94.968	0.009	46.548
29	Anthracene	178.2	4.35	1006.340	0.002	13.365
30	Dibenzofuran	168.2	3.71	46.797	0.027	173.022
31	C3-Benzothiophene	176.3	4.69	0.586	0.013	94.983
32	Acenaphthylene	152.2	3.94	696.287	0.001	32.172
33	C2-Benzothiophene	162.25	4.13	0.586	0.010	292.239
34	Biphenyl	154.2	3.76	0.000	0.038	1576.610
35	CARBAZOLE	167.2	3.23	249.410	0.002	248.678
36	C1-Benzothiophene	148.2	3.5365	0.586	0.008	959.217
37	Toluene	92.14	2.54	0.000	0.047	22856.420
38	Benzothiophene	134.2	2.99	0.586	0.000	2820.625
39	n-C10	142.29	5.25	0.000	0.000	131.879
40	n-C10	142.29	5.25	0.000	0.000	131.879
41	n-C10	142.3	5.25	0.000	0.000	131.888
42	n-C10	142.3	5.25	0.000	0.000	131.888
43	1-Decene	140.3	5.12	0.000	0.000	172.083
44	n-C9	128.3	4.76	0.000	0.000	341.874
45	n-C9	128.3	4.76	0.000	0.000	341.874
46	n-C9	128.3	4.76	0.000	0.000	341.874
47	n-C9	128.3	4.76	0.000	0.000	341.874
48	1-Nonene	126.2	4.62	0.000	0.000	454.715
49	n-C10	142.29	5.25	0.000	0.000	131.879
50	n-C10	142.29	5.25	0.000	0.000	131.879

51	n-C10	142.3	5.25	0.000	0.000	131.888
52	n-C10	142.3	5.25	0.000	0.000	131.888
53	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1289.514
54	n-C8	114.2	4.27	0.000	0.000	874.875
55	n-Pentylbenzene	148.2	4.5	0.000	0.000	691.589
56	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	1231.111
57	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
58	Octene-1	112.2	4.13	0.000	0.000	1162.286
59	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1289.853
60	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1209.094
61	3-methylheptane	114.2	4.2	0.000	0.000	1017.340
62	n-C9	128.3	4.76	0.000	0.000	341.874
63	n-C9	128.3	4.76	0.000	0.000	341.874
64	n-C9	128.3	4.76	0.000	0.000	341.874
65	n-C9	128.3	4.76	0.000	0.000	341.874
66	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1405.614
67	2-methylheptane	114.2	4.2	0.000	0.000	1017.340
68	HEPTANE	100.2	3.78	0.000	0.000	2206.926
69	tert-Butylbenzene	134.2	3.9	0.000	0.000	1775.630
70	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
71	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
72	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
73	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	1081.776
74	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	1230.928
75	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	1230.928
76	n-Butylbenzene	134.2	4.01	0.000	0.000	1400.853
77	Methylcyclohexane	98.19	3.59	0.000	0.000	3257.071
78	sec-Butylbenzene	134.2	3.94	0.000	0.000	1628.968
79	Hydrindene	118.2	3.47	0.000	0.000	3950.913

80	Propylbenzene	120.194	3.52	0.000	0.000	3607.138
81	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	1081.776
82	n-C6	86.18	3.29	0.000	0.000	5457.158
83	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1209.094
84	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
85	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	1230.928
86	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1208.777
87	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	1431.585
88	m-cymene	134.2	4	0.000	0.000	1431.372
89	Ethylbenzene	106.2	3.03	0.000	0.000	9163.144
90	2,4-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
91	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
92	4-isopropyltoluene	134.22	4	0.000	0.000	1431.585
93	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
94	CYCLOHEXANE	84.16	3.18	0.000	0.000	6755.006
95	n-C5	72.15	2.8	0.000	0.000	13135.189
96	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	3169.746
97	p-XYLENE	106.2	3.09	0.000	0.000	8051.643
98	2-methylhexane	100.2	3.71	0.000	0.000	2566.302
99	Isopropylbenzene	120.194	3.45	0.000	0.000	4194.525
100	3-Methylpentane	86.18	3.21	0.000	0.000	6484.052
101	3-ethylhexane	114.2	4.2	0.000	0.000	1017.340
102	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
103	3-methylhexane	100.2	3.71	0.000	0.000	2566.302
104	2,2-dimethylpentane	100.2	3.67	0.000	0.000	2797.356
105	2,3-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
106	Methylcyclopentane	84.16	3.1	0.000	0.000	8026.121
107	2-METHYLPENTANE	86.18	3.21	0.000	0.000	6484.052
108	o-XYLENE	106.2	3.09	0.000	0.000	8051.643

109	m-XYLENE	106.2	3.09	0.000	0.000	8051.643
110	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	971.119
111	Cyclopentane	70.13	2.68	0.000	0.000	16535.748
112	Benzene	78.11	1.99	0.000	0.000	63396.698
113	Isopentane	72.15	2.72	0.000	0.000	15606.889
114	2,3-dimethylbutane	86.18	3.14	0.000	0.000	7539.916
115	C1-Decalins	152.3	4.61	0.000	0.000	249.310
116	trans-Decalin	138.26	4.2	0.000	0.000	547.642
117	Naphthalene	234.3	3.17	16.140	0.000	1154.840
118	cis-Decalin	138.26	4.2	0.000	0.000	547.642
119	n-C11	156.31	5.74	0.000	0.000	50.390
120	n-C11	156.31	5.74	0.000	0.000	50.390
121	n-C11	156.31	5.74	0.000	0.000	50.390
122	n-C11	156.31	5.74	0.000	0.000	50.390
123	n-C12	170.34	6.23	0.000	0.000	19.100
124	n-C12	170.34	6.23	0.000	0.000	19.100
125	n-C12	170.34	6.23	0.000	0.000	19.100
126	n-C12	170.34	6.23	0.000	0.000	19.100
127	n-C11	156.31	5.74	0.000	0.000	50.390
128	n-C11	156.31	5.74	0.000	0.000	50.390
129	n-C11	156.31	5.74	0.000	0.000	50.390
130	n-C11	156.31	5.74	0.000	0.000	50.390
131	n-C12	170.34	6.23	0.000	0.000	19.100
132	n-C12	170.34	6.23	0.000	0.000	19.100
133	n-C12	170.34	6.23	0.000	0.000	19.100
134	n-C12	170.34	6.23	0.000	0.000	19.100
135	n-C13	184.37	6.73	0.000	0.000	7.037
136	n-C14	198.4	7.22	0.000	0.000	2.634
137	n-C15	212.42	7.71	0.000	0.000	0.981

138	n-C16	226.45	8.2	0.000	0.000	0.364
139	n-C17	240.48	8.69	0.000	0.000	0.134
140	n-C18	254.5	9.18	0.000	0.000	0.049
141	n-C19	268.53	9.67	0.000	0.000	0.018
142	n-C20	282.56	10.1	0.000	0.000	0.008
143	n-C21	296.59	10.6	0.000	0.000	0.003
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.012
164	Pristane	268.525	9.38	0.000	0.000	0.034
165	Benzo(a)fluoranthene	252.3	6.11	4589.933	0.000	0.226
166	Benzo(b)fluorene	216.3	5.77	898.179	0.000	0.797

167	Benzo(k)fluoranthene	252.3	6.11	4187.545	0.000	0.235
168	Benzo[a]anthracene	228.3	5.52	1204.593	0.000	1.277
169	Benzo[a]pyrene	252.3	6.11	6060.592	0.000	0.201
170	Benzo[b]fluoranthene	252.3	6.11	2564.123	0.000	0.289
171	Benzo[e]pyrene	252.3	6.11	1764.684	0.000	0.337
172	Benzo[g,h,i]perylene	276.3	6.7	4937.495	0.000	0.067
173	C1-Chrysenes	242.3	6.0683	853.377	0.000	0.479
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2991.384	0.000	0.901
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	8.960
176	C2-Chrysenes	256.3	6.65	853.377	0.000	0.145
177	C2-Decalins	166.3	6.19	0.000	0.000	9.038
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2991.384	0.000	0.237
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	3.365
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1672.207	0.000	1.121
181	C3-Chrysenes	270.4	7.03	853.377	0.000	0.067
182	C3-Decalins	180.3	6.79	0.000	0.000	2.689
183	C3-Dibenzothiophenes	230.37	5.86	11.607	0.000	3.887
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2991.384	0.000	0.097
185	C3-Fluorenes	210.3	5.58	131.253	0.000	2.559
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.207
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1672.207	0.000	0.516
188	C4-Chrysenes	284.4	7.35	853.377	0.000	0.036
189	C4-Decalins	194.3	7.34	0.000	0.000	0.886
190	C4-Dibenzothiophenes	244.37	6.1	11.607	0.000	2.458
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2991.384	0.000	0.037
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.451
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1672.207	0.000	0.288
194	Chrysene	228.3	5.52	684.656	0.000	1.613
195	Dibenz(a,h)anthracene	278.4	6.7	2973.351	0.000	0.084

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	7096.895	0.000	0.058
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	60.488
198	Perylene	252.3	6.11	7520.015	0.000	0.184
199	Retene	234.3	6.35	127.907	0.000	0.548

Table B.45. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	131.253	0.048	5.249
2	C1-Fluorenes	180.2	4.97	131.253	0.052	8.166
3	C1-Phenanthrenes/Anthracenes	192.3	4.26	1672.207	0.071	14.176
4	C3-Naphthalenes	170.26	4.77	39.124	0.085	19.110
5	C4-Naphthalenes	184.3	5.18	39.124	0.024	8.549
6	C2-Naphthalenes	156.2	4.31	39.124	0.110	47.249
7	Phenanthrene	178.2	4.35	54.428	0.085	43.516
8	1-Methylphenanthrene	192.26	4.89	86.350	0.023	12.230
9	1,6,7-Trimethylnaphthalene	170.26	4.81	47.767	0.028	16.231
10	4/9-Methylphenanthrene	192.26	4.89	86.350	0.020	12.230
11	3-Methylphenanthrene	192.26	4.89	86.350	0.017	12.230
12	2-Methylphenanthrene	192.26	4.89	86.350	0.017	12.230
13	C2-Dibenzothiophenes	214.3	5.13	11.607	0.016	17.436
14	2,6-Dimethylnaphthalene	156.23	4.26	39.124	0.043	52.636
15	Pyrene	202.3	4.93	2337.740	0.002	3.060
16	Fluorene	166.2	4.02	131.253	0.044	58.356
17	C1-Dibenzothiophenes	198.3	4.71	11.607	0.018	39.891
18	Fluoranthene	202.3	4.93	1361.298	0.001	3.834
19	4-Methyldibenzothiophene	198.28	4.71	11.607	0.008	39.887
20	C1-Naphthalenes	142.2	3.87	27.131	0.021	127.689
21	Dibenzothiophene	184.3	4.17	11.607	0.016	118.718

22	2/3-Methyldibenzothiophene	198.28	4.71	10.239	0.005	41.726
23	1-Methylnaphthalene	142.2	3.72	27.131	0.017	176.422
24	2-Methylnaphthalene	142.2	3.72	27.131	0.015	176.422
25	1-Methyldibenzothiophene	198.28	4.71	11.607	0.003	39.887
26	C4-Benzothiophene	190.3	5.18	0.586	0.003	35.661
27	C3-Benzothiophene	176.3	4.69	0.586	0.006	94.983
28	Acenaphthene	154.2	4.15	94.968	0.003	46.548
29	Dibenzofuran	168.2	3.71	46.797	0.007	173.022
30	C1-Benzothiophene	148.2	3.5365	0.586	0.027	959.217
31	Acenaphthylene	152.2	3.94	696.287	0.001	32.172
32	C2-Benzothiophene	162.25	4.13	0.586	0.004	292.239
33	Biphenyl	154.2	3.76	0.000	0.010	1576.610
34	CARBAZOLE	167.2	3.23	249.410	0.001	248.678
35	Benzothiophene	134.2	2.99	0.586	0.001	2820.625
36	n-C10	142.29	5.25	0.000	0.000	131.879
37	n-C10	142.29	5.25	0.000	0.000	131.879
38	n-C10	142.3	5.25	0.000	0.000	131.888
39	n-C10	142.3	5.25	0.000	0.000	131.888
40	1-Decene	140.3	5.12	0.000	0.000	172.083
41	n-C9	128.3	4.76	0.000	0.000	341.874
42	n-C9	128.3	4.76	0.000	0.000	341.874
43	n-C9	128.3	4.76	0.000	0.000	341.874
44	n-C9	128.3	4.76	0.000	0.000	341.874
45	1-Nonene	126.2	4.62	0.000	0.000	454.715
46	n-C10	142.29	5.25	0.000	0.000	131.879
47	n-C10	142.29	5.25	0.000	0.000	131.879
48	n-C10	142.3	5.25	0.000	0.000	131.888
49	n-C10	142.3	5.25	0.000	0.000	131.888
50	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1289.514

51	n-C8	114.2	4.27	0.000	0.000	874.875
52	n-Pentylbenzene	148.2	4.5	0.000	0.000	691.589
53	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	1231.111
54	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
55	Octene-1	112.2	4.13	0.000	0.000	1162.286
56	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1289.853
57	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1209.094
58	3-methylheptane	114.2	4.2	0.000	0.000	1017.340
59	n-C9	128.3	4.76	0.000	0.000	341.874
60	n-C9	128.3	4.76	0.000	0.000	341.874
61	n-C9	128.3	4.76	0.000	0.000	341.874
62	n-C9	128.3	4.76	0.000	0.000	341.874
63	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1405.614
64	2-Methylanthracene	192.26	4.89	1672.207	0.000	3.646
65	2-methylheptane	114.2	4.2	0.000	0.000	1017.340
66	HEPTANE	100.2	3.78	0.000	0.000	2206.926
67	tert-Butylbenzene	134.2	3.9	0.000	0.000	1775.630
68	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
69	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
70	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
71	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	1081.776
72	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	1230.928
73	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	1230.928
74	n-Butylbenzene	134.2	4.01	0.000	0.000	1400.853
75	Methylcyclohexane	98.19	3.59	0.000	0.000	3257.071
76	sec-Butylbenzene	134.2	3.94	0.000	0.000	1628.968
77	Hydrindene	118.2	3.47	0.000	0.000	3950.913
78	Propylbenzene	120.194	3.52	0.000	0.000	3607.138
79	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	1081.776

80	n-C6	86.18	3.29	0.000	0.000	5457.158
81	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1209.094
82	Anthracene	178.2	4.35	1006.340	0.000	13.365
83	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
84	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	1230.928
85	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1208.777
86	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	1431.585
87	m-cymene	134.2	4	0.000	0.000	1431.372
88	Ethylbenzene	106.2	3.03	0.000	0.000	9163.144
89	2,4-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
90	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
91	4-isopropyltoluene	134.22	4	0.000	0.000	1431.585
92	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
93	CYCLOHEXANE	84.16	3.18	0.000	0.000	6755.006
94	n-C5	72.15	2.8	0.000	0.000	13135.189
95	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	3169.746
96	p-XYLENE	106.2	3.09	0.000	0.000	8051.643
97	2-methylhexane	100.2	3.71	0.000	0.000	2566.302
98	Isopropylbenzene	120.194	3.45	0.000	0.000	4194.525
99	3-Methylpentane	86.18	3.21	0.000	0.000	6484.052
100	3-ethylhexane	114.2	4.2	0.000	0.000	1017.340
101	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
102	3-methylhexane	100.2	3.71	0.000	0.000	2566.302
103	2,2-dimethylpentane	100.2	3.67	0.000	0.000	2797.356
104	2,3-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
105	Methylcyclopentane	84.16	3.1	0.000	0.000	8026.121
106	2-METHYLPENTANE	86.18	3.21	0.000	0.000	6484.052
107	o-XYLENE	106.2	3.09	0.000	0.000	8051.643
108	m-XYLENE	106.2	3.09	0.000	0.000	8051.643

109	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	971.119
110	Cyclopentane	70.13	2.68	0.000	0.000	16535.748
111	Toluene	92.14	2.54	0.000	0.000	22856.420
112	Benzene	78.11	1.99	0.000	0.000	63396.698
113	Isopentane	72.15	2.72	0.000	0.000	15606.889
114	2,3-dimethylbutane	86.18	3.14	0.000	0.000	7539.916
115	C1-Decalins	152.3	4.61	0.000	0.000	249.310
116	trans-Decalin	138.26	4.2	0.000	0.000	547.642
117	Naphthalene	234.3	3.17	16.140	0.000	1154.840
118	cis-Decalin	138.26	4.2	0.000	0.000	547.642
119	n-C11	156.31	5.74	0.000	0.000	50.390
120	n-C11	156.31	5.74	0.000	0.000	50.390
121	n-C11	156.31	5.74	0.000	0.000	50.390
122	n-C11	156.31	5.74	0.000	0.000	50.390
123	n-C12	170.34	6.23	0.000	0.000	19.100
124	n-C12	170.34	6.23	0.000	0.000	19.100
125	n-C12	170.34	6.23	0.000	0.000	19.100
126	n-C12	170.34	6.23	0.000	0.000	19.100
127	n-C11	156.31	5.74	0.000	0.000	50.390
128	n-C11	156.31	5.74	0.000	0.000	50.390
129	n-C11	156.31	5.74	0.000	0.000	50.390
130	n-C11	156.31	5.74	0.000	0.000	50.390
131	n-C12	170.34	6.23	0.000	0.000	19.100
132	n-C12	170.34	6.23	0.000	0.000	19.100
133	n-C12	170.34	6.23	0.000	0.000	19.100
134	n-C12	170.34	6.23	0.000	0.000	19.100
135	n-C13	184.37	6.73	0.000	0.000	7.037
136	n-C14	198.4	7.22	0.000	0.000	2.634
137	n-C15	212.42	7.71	0.000	0.000	0.981

138	n-C16	226.45	8.2	0.000	0.000	0.364
139	n-C17	240.48	8.69	0.000	0.000	0.134
140	n-C18	254.5	9.18	0.000	0.000	0.049
141	n-C19	268.53	9.67	0.000	0.000	0.018
142	n-C20	282.56	10.1	0.000	0.000	0.008
143	n-C21	296.59	10.6	0.000	0.000	0.003
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.012
164	Pristane	268.525	9.38	0.000	0.000	0.034
165	Benzo(a)fluoranthene	252.3	6.11	4589.933	0.000	0.226
166	Benzo(b)fluorene	216.3	5.77	898.179	0.000	0.797

167	Benzo(k)fluoranthene	252.3	6.11	4187.545	0.000	0.235
168	Benzo[a]anthracene	228.3	5.52	1204.593	0.000	1.277
169	Benzo[a]pyrene	252.3	6.11	6060.592	0.000	0.201
170	Benzo[b]fluoranthene	252.3	6.11	2564.123	0.000	0.289
171	Benzo[e]pyrene	252.3	6.11	1764.684	0.000	0.337
172	Benzo[g,h,i]perylene	276.3	6.7	4937.495	0.000	0.067
173	C1-Chrysenes	242.3	6.0683	853.377	0.000	0.479
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2991.384	0.000	0.901
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	8.960
176	C2-Chrysenes	256.3	6.65	853.377	0.000	0.145
177	C2-Decalins	166.3	6.19	0.000	0.000	9.038
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2991.384	0.000	0.237
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	3.365
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1672.207	0.000	1.121
181	C3-Chrysenes	270.4	7.03	853.377	0.000	0.067
182	C3-Decalins	180.3	6.79	0.000	0.000	2.689
183	C3-Dibenzothiophenes	230.37	5.86	11.607	0.000	3.887
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2991.384	0.000	0.097
185	C3-Fluorenes	210.3	5.58	131.253	0.000	2.559
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.207
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1672.207	0.000	0.516
188	C4-Chrysenes	284.4	7.35	853.377	0.000	0.036
189	C4-Decalins	194.3	7.34	0.000	0.000	0.886
190	C4-Dibenzothiophenes	244.37	6.1	11.607	0.000	2.458
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2991.384	0.000	0.037
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.451
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1672.207	0.000	0.288
194	Chrysene	228.3	5.52	684.656	0.000	1.613
195	Dibenz(a,h)anthracene	278.4	6.7	2973.351	0.000	0.084

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	7096.895	0.000	0.058
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	60.488
198	Perylene	252.3	6.11	7520.015	0.000	0.184
199	Retene	234.3	6.35	127.907	0.000	0.548

Table B.46. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in CTC oil at 6.25% WAF duplicate exposed to *Cyprinodon variegatus* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	131.253	0.044	5.249
2	C1-Fluorenes	180.2	4.97	131.253	0.050	8.166
3	C1-Phenanthrenes/Anthracenes	192.3	4.26	1672.207	0.067	14.176
4	C3-Naphthalenes	170.26	4.77	39.124	0.083	19.110
5	C4-Naphthalenes	184.3	5.18	39.124	0.025	8.549
6	C2-Naphthalenes	156.2	4.31	39.124	0.107	47.249
7	1-Methylphenanthrene	192.26	4.89	86.350	0.024	12.230
8	Phenanthrene	178.2	4.35	54.428	0.084	43.516
9	1,6,7-Trimethylnaphthalene	170.26	4.81	47.767	0.027	16.231
10	4/9-Methylphenanthrene	192.26	4.89	86.350	0.019	12.230
11	3-Methylphenanthrene	192.26	4.89	86.350	0.016	12.230
12	2-Methylphenanthrene	192.26	4.89	86.350	0.016	12.230
13	2,6-Dimethylnaphthalene	156.23	4.26	39.124	0.042	52.636
14	Fluorene	166.2	4.02	131.253	0.043	58.356
15	C2-Dibenzothiophenes	214.3	5.13	11.607	0.012	17.436
16	C1-Dibenzothiophenes	198.3	4.71	11.607	0.017	39.891
17	Fluoranthene	202.3	4.93	1361.298	0.001	3.834
18	C1-Naphthalenes	142.2	3.87	27.131	0.024	127.689
19	4-Methyldibenzothiophene	198.28	4.71	11.607	0.007	39.887
20	Dibenzothiophene	184.3	4.17	11.607	0.016	118.718
21	C1-Benzothiophene	148.2	3.5365	0.586	0.125	959.217

22	C4-Benzothiophene	190.3	5.18	0.586	0.004	35.661
23	1-Methylnaphthalene	142.2	3.72	27.131	0.018	176.422
24	2/3-Methyldibenzothiophene	198.28	4.71	10.239	0.004	41.726
25	2-Methylnaphthalene	142.2	3.72	27.131	0.015	176.422
26	1-Methyldibenzothiophene	198.28	4.71	11.607	0.003	39.887
27	C3-Benzothiophene	176.3	4.69	0.586	0.007	94.983
28	Acenaphthene	154.2	4.15	94.968	0.003	46.548
29	Dibenzofuran	168.2	3.71	46.797	0.007	173.022
30	Acenaphthylene	152.2	3.94	696.287	0.001	32.172
31	C2-Benzothiophene	162.25	4.13	0.586	0.004	292.239
32	Biphenyl	154.2	3.76	0.000	0.010	1576.610
33	CARBAZOLE	167.2	3.23	249.410	0.001	248.678
34	Benzothiophene	134.2	2.99	0.586	0.001	2820.625
35	n-C10	142.29	5.25	0.000	0.000	131.879
36	n-C10	142.29	5.25	0.000	0.000	131.879
37	n-C10	142.3	5.25	0.000	0.000	131.888
38	n-C10	142.3	5.25	0.000	0.000	131.888
39	1-Decene	140.3	5.12	0.000	0.000	172.083
40	n-C10	142.29	5.25	0.000	0.000	131.879
41	n-C10	142.29	5.25	0.000	0.000	131.879
42	n-C10	142.3	5.25	0.000	0.000	131.888
43	n-C10	142.3	5.25	0.000	0.000	131.888
44	n-C9	128.3	4.76	0.000	0.000	341.874
45	n-C9	128.3	4.76	0.000	0.000	341.874
46	n-C9	128.3	4.76	0.000	0.000	341.874
47	n-C9	128.3	4.76	0.000	0.000	341.874
48	1-Nonene	126.2	4.62	0.000	0.000	454.715
49	Pyrene	202.3	4.93	2337.740	0.000	3.060
50	n-C9	128.3	4.76	0.000	0.000	341.874

51	n-C9	128.3	4.76	0.000	0.000	341.874
52	n-C9	128.3	4.76	0.000	0.000	341.874
53	n-C9	128.3	4.76	0.000	0.000	341.874
54	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1289.514
55	2-Methylanthracene	192.26	4.89	1672.207	0.000	3.646
56	n-C8	114.2	4.27	0.000	0.000	874.875
57	n-Pentylbenzene	148.2	4.5	0.000	0.000	691.589
58	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	1231.111
59	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
60	Octene-1	112.2	4.13	0.000	0.000	1162.286
61	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1289.853
62	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1209.094
63	3-methylheptane	114.2	4.2	0.000	0.000	1017.340
64	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1405.614
65	2-methylheptane	114.2	4.2	0.000	0.000	1017.340
66	HEPTANE	100.2	3.78	0.000	0.000	2206.926
67	tert-Butylbenzene	134.2	3.9	0.000	0.000	1775.630
68	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
69	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
70	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
71	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	1081.776
72	Anthracene	178.2	4.35	1006.340	0.000	13.365
73	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	1230.928
74	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	1230.928
75	n-Butylbenzene	134.2	4.01	0.000	0.000	1400.853
76	Methylcyclohexane	98.19	3.59	0.000	0.000	3257.071
77	sec-Butylbenzene	134.2	3.94	0.000	0.000	1628.968
78	Hydrindene	118.2	3.47	0.000	0.000	3950.913
79	Propylbenzene	120.194	3.52	0.000	0.000	3607.138

80	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	1081.776
81	n-C6	86.18	3.29	0.000	0.000	5457.158
82	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1209.094
83	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
84	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	1230.928
85	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1208.777
86	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	1431.585
87	m-cymene	134.2	4	0.000	0.000	1431.372
88	Ethylbenzene	106.2	3.03	0.000	0.000	9163.144
89	2,4-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
90	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
91	4-isopropyltoluene	134.22	4	0.000	0.000	1431.585
92	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
93	CYCLOHEXANE	84.16	3.18	0.000	0.000	6755.006
94	n-C5	72.15	2.8	0.000	0.000	13135.189
95	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	3169.746
96	p-XYLENE	106.2	3.09	0.000	0.000	8051.643
97	2-methylhexane	100.2	3.71	0.000	0.000	2566.302
98	Isopropylbenzene	120.194	3.45	0.000	0.000	4194.525
99	3-Methylpentane	86.18	3.21	0.000	0.000	6484.052
100	3-ethylhexane	114.2	4.2	0.000	0.000	1017.340
101	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
102	3-methylhexane	100.2	3.71	0.000	0.000	2566.302
103	2,2-dimethylpentane	100.2	3.67	0.000	0.000	2797.356
104	2,3-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
105	Methylcyclopentane	84.16	3.1	0.000	0.000	8026.121
106	2-METHYLPENTANE	86.18	3.21	0.000	0.000	6484.052
107	o-XYLENE	106.2	3.09	0.000	0.000	8051.643
108	m-XYLENE	106.2	3.09	0.000	0.000	8051.643

109	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	971.119
110	Cyclopentane	70.13	2.68	0.000	0.000	16535.748
111	Toluene	92.14	2.54	0.000	0.000	22856.420
112	Benzene	78.11	1.99	0.000	0.000	63396.698
113	Isopentane	72.15	2.72	0.000	0.000	15606.889
114	C1-Decalins	152.3	4.61	0.000	0.000	249.310
115	2,3-dimethylbutane	86.18	3.14	0.000	0.000	7539.916
116	trans-Decalin	138.26	4.2	0.000	0.000	547.642
117	Naphthalene	234.3	3.17	16.140	0.000	1154.840
118	cis-Decalin	138.26	4.2	0.000	0.000	547.642
119	n-C11	156.31	5.74	0.000	0.000	50.390
120	n-C11	156.31	5.74	0.000	0.000	50.390
121	n-C11	156.31	5.74	0.000	0.000	50.390
122	n-C11	156.31	5.74	0.000	0.000	50.390
123	n-C12	170.34	6.23	0.000	0.000	19.100
124	n-C12	170.34	6.23	0.000	0.000	19.100
125	n-C12	170.34	6.23	0.000	0.000	19.100
126	n-C12	170.34	6.23	0.000	0.000	19.100
127	n-C11	156.31	5.74	0.000	0.000	50.390
128	n-C11	156.31	5.74	0.000	0.000	50.390
129	n-C11	156.31	5.74	0.000	0.000	50.390
130	n-C11	156.31	5.74	0.000	0.000	50.390
131	n-C12	170.34	6.23	0.000	0.000	19.100
132	n-C12	170.34	6.23	0.000	0.000	19.100
133	n-C12	170.34	6.23	0.000	0.000	19.100
134	n-C12	170.34	6.23	0.000	0.000	19.100
135	n-C13	184.37	6.73	0.000	0.000	7.037
136	n-C14	198.4	7.22	0.000	0.000	2.634
137	n-C15	212.42	7.71	0.000	0.000	0.981

138	n-C16	226.45	8.2	0.000	0.000	0.364
139	n-C17	240.48	8.69	0.000	0.000	0.134
140	n-C18	254.5	9.18	0.000	0.000	0.049
141	n-C19	268.53	9.67	0.000	0.000	0.018
142	n-C20	282.56	10.1	0.000	0.000	0.008
143	n-C21	296.59	10.6	0.000	0.000	0.003
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.012
164	Pristane	268.525	9.38	0.000	0.000	0.034
165	Benzo(a)fluoranthene	252.3	6.11	4589.933	0.000	0.226
166	Benzo(b)fluorene	216.3	5.77	898.179	0.000	0.797

167	Benzo(k)fluoranthene	252.3	6.11	4187.545	0.000	0.235
168	Benzo[a]anthracene	228.3	5.52	1204.593	0.000	1.277
169	Benzo[a]pyrene	252.3	6.11	6060.592	0.000	0.201
170	Benzo[b]fluoranthene	252.3	6.11	2564.123	0.000	0.289
171	Benzo[e]pyrene	252.3	6.11	1764.684	0.000	0.337
172	Benzo[g,h,i]perylene	276.3	6.7	4937.495	0.000	0.067
173	C1-Chrysenes	242.3	6.0683	853.377	0.000	0.479
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2991.384	0.000	0.901
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	8.960
176	C2-Chrysenes	256.3	6.65	853.377	0.000	0.145
177	C2-Decalins	166.3	6.19	0.000	0.000	9.038
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2991.384	0.000	0.237
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	3.365
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1672.207	0.000	1.121
181	C3-Chrysenes	270.4	7.03	853.377	0.000	0.067
182	C3-Decalins	180.3	6.79	0.000	0.000	2.689
183	C3-Dibenzothiophenes	230.37	5.86	11.607	0.000	3.887
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2991.384	0.000	0.097
185	C3-Fluorenes	210.3	5.58	131.253	0.000	2.559
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.207
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1672.207	0.000	0.516
188	C4-Chrysenes	284.4	7.35	853.377	0.000	0.036
189	C4-Decalins	194.3	7.34	0.000	0.000	0.886
190	C4-Dibenzothiophenes	244.37	6.1	11.607	0.000	2.458
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2991.384	0.000	0.037
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.451
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1672.207	0.000	0.288
194	Chrysene	228.3	5.52	684.656	0.000	1.613
195	Dibenz(a,h)anthracene	278.4	6.7	2973.351	0.000	0.084

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	7096.895	0.000	0.058
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	60.488
198	Perylene	252.3	6.11	7520.015	0.000	0.184
199	Retene	234.3	6.35	127.907	0.000	0.548

Table B.47. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 100% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	122.328	0.243	5.399
2	C1-Phenanthrenes/Anthracenes	192.3	4.26	1594.680	0.545	14.459
3	C1-Fluorenes	180.2	4.97	122.328	0.149	8.399
4	1-Methylphenanthrene	192.26	4.89	70.978	0.171	13.214
5	4/9-Methylphenanthrene	192.26	4.89	70.978	0.157	13.214
6	2-Methylphenanthrene	192.26	4.89	70.978	0.135	13.214
7	3-Methylphenanthrene	192.26	4.89	70.978	0.124	13.214
8	C2-Dibenzothiophenes	214.3	5.13	9.545	0.162	18.704
9	C4-Naphthalenes	184.3	5.18	32.258	0.058	9.205
10	C3-Naphthalenes	170.26	4.77	32.258	0.124	20.577
11	Phenanthrene	178.2	4.35	44.769	0.244	46.946
12	C1-Dibenzothiophenes	198.3	4.71	9.545	0.192	42.791
13	Pyrene	202.3	4.93	2084.628	0.010	3.210
14	n-Pentylbenzene	148.2	4.5	0.000	1.780	691.589
15	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	2.890	1231.111
16	4-Methyldibenzothiophene	198.28	4.71	9.545	0.098	42.787
17	1,6,7-Trimethylnaphthalene	170.26	4.81	37.111	0.040	17.892
18	2/3-Methyldibenzothiophene	198.28	4.71	8.229	0.063	45.097
19	C2-Naphthalenes	156.2	4.31	32.258	0.066	50.876
20	Fluoranthene	202.3	4.93	1270.157	0.004	3.946
21	Fluorene	166.2	4.02	122.328	0.044	60.024

22	n-C10	142.29	5.25	0.000	0.089	131.879
23	n-C10	142.29	5.25	0.000	0.089	131.879
24	n-C10	142.3	5.25	0.000	0.089	131.888
25	n-C10	142.3	5.25	0.000	0.089	131.888
26	1-Methyldibenzothiophene	198.28	4.71	9.545	0.025	42.787
27	2-Methylanthracene	192.26	4.89	1594.680	0.002	3.719
28	Dibenzothiophene	184.3	4.17	9.545	0.058	127.348
29	n-C6	86.18	3.29	0.000	2.340	5457.158
30	2,6-Dimethylnaphthalene	156.23	4.26	32.258	0.022	56.676
31	Ethylbenzene	106.2	3.03	0.000	2.880	9163.144
32	Anthracene	178.2	4.35	954.966	0.004	13.659
33	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.925	3169.746
34	p-XYLENE	106.2	3.09	0.000	2.030	8051.643
35	C4-Benzothiophene	190.3	5.18	0.543	0.007	36.363
36	o-XYLENE	106.2	3.09	0.000	0.964	8051.643
37	m-XYLENE	106.2	3.09	0.000	0.947	8051.643
38	C3-Benzothiophene	176.3	4.69	0.543	0.011	96.852
39	n-C9	128.3	4.76	0.000	0.031	341.874
40	n-C9	128.3	4.76	0.000	0.031	341.874
41	n-C9	128.3	4.76	0.000	0.031	341.874
42	n-C9	128.3	4.76	0.000	0.031	341.874
43	Toluene	92.14	2.54	0.000	1.960	22856.420
44	C1-Naphthalenes	142.2	3.87	20.674	0.011	141.434
45	1-Methylnaphthalene	142.2	3.72	20.674	0.008	195.413
46	2-Methylnaphthalene	142.2	3.72	20.674	0.008	195.413
47	C2-Benzothiophene	162.25	4.13	0.543	0.010	297.989
48	n-C8	114.2	4.27	0.000	0.027	874.875
49	Dibenzofuran	168.2	3.71	35.593	0.005	192.274
50	C1-Benzothiophene	148.2	3.5365	0.543	0.009	978.092

51	trans-Decalin	138.26	4.2	0.000	0.003	547.642
52	Naphthalene	234.3	3.17	12.318	0.007	1274.755
53	Biphenyl	154.2	3.76	0.000	0.004	1576.610
54	1-Decene	140.3	5.12	0.000	0.000	172.083
55	n-C9	128.3	4.76	0.000	0.000	341.874
56	n-C9	128.3	4.76	0.000	0.000	341.874
57	n-C9	128.3	4.76	0.000	0.000	341.874
58	n-C9	128.3	4.76	0.000	0.000	341.874
59	1-Nonene	126.2	4.62	0.000	0.000	454.715
60	n-C10	142.29	5.25	0.000	0.000	131.879
61	n-C10	142.29	5.25	0.000	0.000	131.879
62	n-C10	142.3	5.25	0.000	0.000	131.888
63	n-C10	142.3	5.25	0.000	0.000	131.888
64	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1289.514
65	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
66	Octene-1	112.2	4.13	0.000	0.000	1162.286
67	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1289.853
68	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1209.094
69	3-methylheptane	114.2	4.2	0.000	0.000	1017.340
70	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1405.614
71	2-methylheptane	114.2	4.2	0.000	0.000	1017.340
72	HEPTANE	100.2	3.78	0.000	0.000	2206.926
73	tert-Butylbenzene	134.2	3.9	0.000	0.000	1775.630
74	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
75	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
76	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
77	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	1081.776
78	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	1230.928
79	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	1230.928

80	n-Butylbenzene	134.2	4.01	0.000	0.000	1400.853
81	Methylcyclohexane	98.19	3.59	0.000	0.000	3257.071
82	sec-Butylbenzene	134.2	3.94	0.000	0.000	1628.968
83	Hydrindene	118.2	3.47	0.000	0.000	3950.913
84	Propylbenzene	120.194	3.52	0.000	0.000	3607.138
85	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	1081.776
86	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1209.094
87	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
88	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	1230.928
89	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1208.777
90	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	1431.585
91	m-cymene	134.2	4	0.000	0.000	1431.372
92	2,4-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
93	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
94	4-isopropyltoluene	134.22	4	0.000	0.000	1431.585
95	CYCLOHEXANE	84.16	3.18	0.000	0.000	6755.006
96	n-C5	72.15	2.8	0.000	0.000	13135.189
97	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	3169.746
98	2-methylhexane	100.2	3.71	0.000	0.000	2566.302
99	Isopropylbenzene	120.194	3.45	0.000	0.000	4194.525
100	3-Methylpentane	86.18	3.21	0.000	0.000	6484.052
101	3-ethylhexane	114.2	4.2	0.000	0.000	1017.340
102	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
103	3-methylhexane	100.2	3.71	0.000	0.000	2566.302
104	2,2-dimethylpentane	100.2	3.67	0.000	0.000	2797.356
105	2,3-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
106	Acenaphthylene	152.2	3.94	611.073	0.000	33.953
107	Methylcyclopentane	84.16	3.1	0.000	0.000	8026.121
108	2-METHYLPENTANE	86.18	3.21	0.000	0.000	6484.052

109	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	971.119
110	Cyclopentane	70.13	2.68	0.000	0.000	16535.748
111	Acenaphthene	154.2	4.15	75.030	0.000	51.095
112	Benzene	78.11	1.99	0.000	0.000	63396.698
113	Isopentane	72.15	2.72	0.000	0.000	15606.889
114	CARBAZOLE	167.2	3.23	214.531	0.000	264.349
115	2,3-dimethylbutane	86.18	3.14	0.000	0.000	7539.916
116	C1-Decalins	152.3	4.61	0.000	0.000	249.310
117	cis-Decalin	138.26	4.2	0.000	0.000	547.642
118	Benzothiophene	134.2	2.99	0.543	0.000	2876.127
119	n-C11	156.31	5.74	0.000	0.000	50.390
120	n-C11	156.31	5.74	0.000	0.000	50.390
121	n-C11	156.31	5.74	0.000	0.000	50.390
122	n-C11	156.31	5.74	0.000	0.000	50.390
123	n-C12	170.34	6.23	0.000	0.000	19.100
124	n-C12	170.34	6.23	0.000	0.000	19.100
125	n-C12	170.34	6.23	0.000	0.000	19.100
126	n-C12	170.34	6.23	0.000	0.000	19.100
127	n-C11	156.31	5.74	0.000	0.000	50.390
128	n-C11	156.31	5.74	0.000	0.000	50.390
129	n-C11	156.31	5.74	0.000	0.000	50.390
130	n-C11	156.31	5.74	0.000	0.000	50.390
131	n-C12	170.34	6.23	0.000	0.000	19.100
132	n-C12	170.34	6.23	0.000	0.000	19.100
133	n-C12	170.34	6.23	0.000	0.000	19.100
134	n-C12	170.34	6.23	0.000	0.000	19.100
135	n-C13	184.37	6.73	0.000	0.000	7.037
136	n-C14	198.4	7.22	0.000	0.000	2.634
137	n-C15	212.42	7.71	0.000	0.000	0.981

138	n-C16	226.45	8.2	0.000	0.000	0.364
139	n-C17	240.48	8.69	0.000	0.000	0.134
140	n-C18	254.5	9.18	0.000	0.000	0.049
141	n-C19	268.53	9.67	0.000	0.000	0.018
142	n-C20	282.56	10.1	0.000	0.000	0.008
143	n-C21	296.59	10.6	0.000	0.000	0.003
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.012
164	Pristane	268.525	9.38	0.000	0.000	0.034
165	Benzo(a)fluoranthene	252.3	6.11	5015.528	0.000	0.218
166	Benzo(b)fluorene	216.3	5.77	747.224	0.000	0.860

167	Benzo(k)fluoranthene	252.3	6.11	3937.473	0.000	0.241
168	Benzo[a]anthracene	228.3	5.52	1089.529	0.000	1.331
169	Benzo[a]pyrene	252.3	6.11	5779.613	0.000	0.205
170	Benzo[b]fluoranthene	252.3	6.11	2379.848	0.000	0.298
171	Benzo[e]pyrene	252.3	6.11	1563.329	0.000	0.355
172	Benzo[g,h,i]perylene	276.3	6.7	4626.123	0.000	0.069
173	C1-Chrysenes	242.3	6.0683	733.508	0.000	0.510
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2771.332	0.000	0.931
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	8.960
176	C2-Chrysenes	256.3	6.65	733.508	0.000	0.154
177	C2-Decalins	166.3	6.19	0.000	0.000	9.038
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2771.332	0.000	0.244
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	3.365
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1594.680	0.000	1.143
181	C3-Chrysenes	270.4	7.03	733.508	0.000	0.072
182	C3-Decalins	180.3	6.79	0.000	0.000	2.689
183	C3-Dibenzothiophenes	230.37	5.86	9.545	0.000	4.169
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2771.332	0.000	0.100
185	C3-Fluorenes	210.3	5.58	122.328	0.000	2.633
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.207
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1594.680	0.000	0.527
188	C4-Chrysenes	284.4	7.35	733.508	0.000	0.038
189	C4-Decalins	194.3	7.34	0.000	0.000	0.886
190	C4-Dibenzothiophenes	244.37	6.1	9.545	0.000	2.637
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2771.332	0.000	0.038
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.451
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1594.680	0.000	0.293
194	Chrysene	228.3	5.52	569.025	0.000	1.741
195	Dibenz(a,h)anthracene	278.4	6.7	2618.466	0.000	0.089

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	6932.949	0.000	0.058
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	60.488
198	Perylene	252.3	6.11	8498.796	0.000	0.174
199	Retene	234.3	6.35	104.029	0.000	0.595

Table B.48. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 25% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	122.328	0.054	5.399
2	C1-Phenanthrenes/Anthracenes	192.3	4.26	1594.680	0.131	14.459
3	C1-Fluorenes	180.2	4.97	122.328	0.036	8.399
4	1-Methylphenanthrene	192.26	4.89	70.978	0.041	13.214
5	4/9-Methylphenanthrene	192.26	4.89	70.978	0.037	13.214
6	n-Pentylbenzene	148.2	4.5	0.000	1.780	691.589
7	2-Methylphenanthrene	192.26	4.89	70.978	0.032	13.214
8	3-Methylphenanthrene	192.26	4.89	70.978	0.031	13.214
9	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	2.890	1231.111
10	C2-Dibenzothiophenes	214.3	5.13	9.545	0.037	18.704
11	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	2.000	1081.615
12	C4-Naphthalenes	184.3	5.18	32.258	0.016	9.205
13	C3-Naphthalenes	170.26	4.77	32.258	0.032	20.577
14	Phenanthrene	178.2	4.35	44.769	0.062	46.946
15	C1-Dibenzothiophenes	198.3	4.71	9.545	0.047	42.791
16	Pyrene	202.3	4.93	2084.628	0.003	3.210
17	4-Methyldibenzothiophene	198.28	4.71	9.545	0.023	42.787
18	1,6,7-Trimethylnaphthalene	170.26	4.81	37.111	0.009	17.892
19	n-C6	86.18	3.29	0.000	2.340	5457.158
20	n-C10	142.29	5.25	0.000	0.051	131.879
21	n-C10	142.29	5.25	0.000	0.051	131.879

22	n-C10	142.3	5.25	0.000	0.051	131.888
23	n-C10	142.3	5.25	0.000	0.051	131.888
24	C2-Naphthalenes	156.2	4.31	32.258	0.019	50.876
25	2/3-Methyldibenzothiophene	198.28	4.71	8.229	0.016	45.097
26	Fluoranthene	202.3	4.93	1270.157	0.001	3.946
27	Ethylbenzene	106.2	3.03	0.000	2.880	9163.144
28	p-XYLENE	106.2	3.09	0.000	2.030	8051.643
29	Fluorene	166.2	4.02	122.328	0.011	60.024
30	1-Methyldibenzothiophene	198.28	4.71	9.545	0.006	42.787
31	o-XYLENE	106.2	3.09	0.000	0.964	8051.643
32	m-XYLENE	106.2	3.09	0.000	0.947	8051.643
33	Dibenzothiophene	184.3	4.17	9.545	0.015	127.348
34	2,6-Dimethylnaphthalene	156.23	4.26	32.258	0.006	56.676
35	Toluene	92.14	2.54	0.000	1.960	22856.420
36	Anthracene	178.2	4.35	954.966	0.001	13.659
37	n-C9	128.3	4.76	0.000	0.015	341.874
38	n-C9	128.3	4.76	0.000	0.015	341.874
39	n-C9	128.3	4.76	0.000	0.015	341.874
40	n-C9	128.3	4.76	0.000	0.015	341.874
41	C1-Naphthalenes	142.2	3.87	20.674	0.006	141.434
42	1-Methylnaphthalene	142.2	3.72	20.674	0.004	195.413
43	2-Methylnaphthalene	142.2	3.72	20.674	0.004	195.413
44	Acenaphthene	154.2	4.15	75.030	0.001	51.095
45	C2-Benzothiophene	162.25	4.13	0.543	0.003	297.989
46	Dibenzofuran	168.2	3.71	35.593	0.002	192.274
47	trans-Decalin	138.26	4.2	0.000	0.003	547.642
48	C1-Benzothiophene	148.2	3.5365	0.543	0.004	978.092
49	Naphthalene	234.3	3.17	12.318	0.005	1274.755
50	Biphenyl	154.2	3.76	0.000	0.001	1576.610

51	1-Decene	140.3	5.12	0.000	0.000	172.083
52	n-C9	128.3	4.76	0.000	0.000	341.874
53	n-C9	128.3	4.76	0.000	0.000	341.874
54	n-C9	128.3	4.76	0.000	0.000	341.874
55	n-C9	128.3	4.76	0.000	0.000	341.874
56	1-Nonene	126.2	4.62	0.000	0.000	454.715
57	n-C10	142.29	5.25	0.000	0.000	131.879
58	n-C10	142.29	5.25	0.000	0.000	131.879
59	n-C10	142.3	5.25	0.000	0.000	131.888
60	n-C10	142.3	5.25	0.000	0.000	131.888
61	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1289.514
62	n-C8	114.2	4.27	0.000	0.000	874.875
63	Octene-1	112.2	4.13	0.000	0.000	1162.286
64	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1289.853
65	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1209.094
66	3-methylheptane	114.2	4.2	0.000	0.000	1017.340
67	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1405.614
68	2-Methylanthracene	192.26	4.89	1594.680	0.000	3.719
69	2-methylheptane	114.2	4.2	0.000	0.000	1017.340
70	HEPTANE	100.2	3.78	0.000	0.000	2206.926
71	tert-Butylbenzene	134.2	3.9	0.000	0.000	1775.630
72	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
73	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
74	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
75	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	1081.776
76	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	1230.928
77	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	1230.928
78	n-Butylbenzene	134.2	4.01	0.000	0.000	1400.853
79	Methylcyclohexane	98.19	3.59	0.000	0.000	3257.071

80	sec-Butylbenzene	134.2	3.94	0.000	0.000	1628.968
81	Hydrindene	118.2	3.47	0.000	0.000	3950.913
82	Propylbenzene	120.194	3.52	0.000	0.000	3607.138
83	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	1081.776
84	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1209.094
85	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
86	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	1230.928
87	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1208.777
88	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	1431.585
89	m-cymene	134.2	4	0.000	0.000	1431.372
90	2,4-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
91	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
92	4-isopropyltoluene	134.22	4	0.000	0.000	1431.585
93	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
94	CYCLOHEXANE	84.16	3.18	0.000	0.000	6755.006
95	n-C5	72.15	2.8	0.000	0.000	13135.189
96	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	3169.746
97	2-methylhexane	100.2	3.71	0.000	0.000	2566.302
98	Isopropylbenzene	120.194	3.45	0.000	0.000	4194.525
99	3-Methylpentane	86.18	3.21	0.000	0.000	6484.052
100	3-ethylhexane	114.2	4.2	0.000	0.000	1017.340
101	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
102	3-methylhexane	100.2	3.71	0.000	0.000	2566.302
103	2,2-dimethylpentane	100.2	3.67	0.000	0.000	2797.356
104	2,3-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
105	Acenaphthylene	152.2	3.94	611.073	0.000	33.953
106	Methylcyclopentane	84.16	3.1	0.000	0.000	8026.121
107	C4-Benzothiophene	190.3	5.18	0.543	0.000	36.363
108	2-METHYLPENTANE	86.18	3.21	0.000	0.000	6484.052

109	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	971.119
110	Cyclopentane	70.13	2.68	0.000	0.000	16535.748
111	Benzene	78.11	1.99	0.000	0.000	63396.698
112	C3-Benzothiophene	176.3	4.69	0.543	0.000	96.852
113	Isopentane	72.15	2.72	0.000	0.000	15606.889
114	CARBAZOLE	167.2	3.23	214.531	0.000	264.349
115	2,3-dimethylbutane	86.18	3.14	0.000	0.000	7539.916
116	C1-Decalins	152.3	4.61	0.000	0.000	249.310
117	cis-Decalin	138.26	4.2	0.000	0.000	547.642
118	Benzothiophene	134.2	2.99	0.543	0.000	2876.127
119	n-C11	156.31	5.74	0.000	0.000	50.390
120	n-C11	156.31	5.74	0.000	0.000	50.390
121	n-C11	156.31	5.74	0.000	0.000	50.390
122	n-C11	156.31	5.74	0.000	0.000	50.390
123	n-C12	170.34	6.23	0.000	0.000	19.100
124	n-C12	170.34	6.23	0.000	0.000	19.100
125	n-C12	170.34	6.23	0.000	0.000	19.100
126	n-C12	170.34	6.23	0.000	0.000	19.100
127	n-C11	156.31	5.74	0.000	0.000	50.390
128	n-C11	156.31	5.74	0.000	0.000	50.390
129	n-C11	156.31	5.74	0.000	0.000	50.390
130	n-C11	156.31	5.74	0.000	0.000	50.390
131	n-C12	170.34	6.23	0.000	0.000	19.100
132	n-C12	170.34	6.23	0.000	0.000	19.100
133	n-C12	170.34	6.23	0.000	0.000	19.100
134	n-C12	170.34	6.23	0.000	0.000	19.100
135	n-C13	184.37	6.73	0.000	0.000	7.037
136	n-C14	198.4	7.22	0.000	0.000	2.634
137	n-C15	212.42	7.71	0.000	0.000	0.981

138	n-C16	226.45	8.2	0.000	0.000	0.364
139	n-C17	240.48	8.69	0.000	0.000	0.134
140	n-C18	254.5	9.18	0.000	0.000	0.049
141	n-C19	268.53	9.67	0.000	0.000	0.018
142	n-C20	282.56	10.1	0.000	0.000	0.008
143	n-C21	296.59	10.6	0.000	0.000	0.003
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.012
164	Pristane	268.525	9.38	0.000	0.000	0.034
165	Benzo(a)fluoranthene	252.3	6.11	5015.528	0.000	0.218
166	Benzo(b)fluorene	216.3	5.77	747.224	0.000	0.860

167	Benzo(k)fluoranthene	252.3	6.11	3937.473	0.000	0.241
168	Benzo[a]anthracene	228.3	5.52	1089.529	0.000	1.331
169	Benzo[a]pyrene	252.3	6.11	5779.613	0.000	0.205
170	Benzo[b]fluoranthene	252.3	6.11	2379.848	0.000	0.298
171	Benzo[e]pyrene	252.3	6.11	1563.329	0.000	0.355
172	Benzo[g,h,i]perylene	276.3	6.7	4626.123	0.000	0.069
173	C1-Chrysenes	242.3	6.0683	733.508	0.000	0.510
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2771.332	0.000	0.931
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	8.960
176	C2-Chrysenes	256.3	6.65	733.508	0.000	0.154
177	C2-Decalins	166.3	6.19	0.000	0.000	9.038
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2771.332	0.000	0.244
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	3.365
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1594.680	0.000	1.143
181	C3-Chrysenes	270.4	7.03	733.508	0.000	0.072
182	C3-Decalins	180.3	6.79	0.000	0.000	2.689
183	C3-Dibenzothiophenes	230.37	5.86	9.545	0.000	4.169
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2771.332	0.000	0.100
185	C3-Fluorenes	210.3	5.58	122.328	0.000	2.633
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.207
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1594.680	0.000	0.527
188	C4-Chrysenes	284.4	7.35	733.508	0.000	0.038
189	C4-Decalins	194.3	7.34	0.000	0.000	0.886
190	C4-Dibenzothiophenes	244.37	6.1	9.545	0.000	2.637
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2771.332	0.000	0.038
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.451
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1594.680	0.000	0.293
194	Chrysene	228.3	5.52	569.025	0.000	1.741
195	Dibenz(a,h)anthracene	278.4	6.7	2618.466	0.000	0.089

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	6932.949	0.000	0.058
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	60.488
198	Perylene	252.3	6.11	8498.796	0.000	0.174
199	Retene	234.3	6.35	104.029	0.000	0.595

Table B.49. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 6.25% WAF exposed to *Cyprinodon variegatus* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	122.328	0.016	5.399
2	n-Pentylbenzene	148.2	4.5	0.000	1.780	691.589
3	C1-Phenanthrenes/Anthracenes	192.3	4.26	1594.680	0.034	14.459
4	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	2.890	1231.111
5	C1-Fluorenes	180.2	4.97	122.328	0.010	8.399
6	1-Methylphenanthrene	192.26	4.89	70.978	0.010	13.214
7	3-Methylphenanthrene	192.26	4.89	70.978	0.010	13.214
8	4/9-Methylphenanthrene	192.26	4.89	70.978	0.009	13.214
9	C4-Naphthalenes	184.3	5.18	32.258	0.006	9.205
10	C3-Naphthalenes	170.26	4.77	32.258	0.013	20.577
11	2-Methylphenanthrene	192.26	4.89	70.978	0.008	13.214
12	C2-Dibenzothiophenes	214.3	5.13	9.545	0.009	18.704
13	n-C6	86.18	3.29	0.000	2.340	5457.158
14	Phenanthrene	178.2	4.35	44.769	0.018	46.946
15	Pyrene	202.3	4.93	2084.628	0.001	3.210
16	Ethylbenzene	106.2	3.03	0.000	2.880	9163.144
17	p-XYLENE	106.2	3.09	0.000	2.030	8051.643
18	C1-Dibenzothiophenes	198.3	4.71	9.545	0.009	42.791
19	1,6,7-Trimethylnaphthalene	170.26	4.81	37.111	0.003	17.892
20	C2-Naphthalenes	156.2	4.31	32.258	0.008	50.876
21	Fluoranthene	202.3	4.93	1270.157	0.001	3.946

22	4-Methyldibenzothiophene	198.28	4.71	9.545	0.005	42.787
23	o-XYLENE	106.2	3.09	0.000	0.964	8051.643
24	m-XYLENE	106.2	3.09	0.000	0.947	8051.643
25	Toluene	92.14	2.54	0.000	1.960	22856.420
26	Fluorene	166.2	4.02	122.328	0.004	60.024
27	2,6-Dimethylnaphthalene	156.23	4.26	32.258	0.003	56.676
28	1-Methyldibenzothiophene	198.28	4.71	9.545	0.001	42.787
29	C1-Naphthalenes	142.2	3.87	20.674	0.005	141.434
30	Dibenzothiophene	184.3	4.17	9.545	0.004	127.348
31	2/3-Methyldibenzothiophene	198.28	4.71	8.229	0.001	45.097
32	2-Methylnaphthalene	142.2	3.72	20.674	0.003	195.413
33	1-Methylnaphthalene	142.2	3.72	20.674	0.003	195.413
34	Naphthalene	234.3	3.17	12.318	0.009	1274.755
35	Dibenzofuran	168.2	3.71	35.593	0.001	192.274
36	trans-Decalin	138.26	4.2	0.000	0.003	547.642
37	Biphenyl	154.2	3.76	0.000	0.005	1576.610
38	C1-Benzothiophene	148.2	3.5365	0.543	0.002	978.092
39	n-C10	142.29	5.25	0.000	0.000	131.879
40	n-C10	142.29	5.25	0.000	0.000	131.879
41	n-C10	142.3	5.25	0.000	0.000	131.888
42	n-C10	142.3	5.25	0.000	0.000	131.888
43	1-Decene	140.3	5.12	0.000	0.000	172.083
44	n-C9	128.3	4.76	0.000	0.000	341.874
45	n-C9	128.3	4.76	0.000	0.000	341.874
46	n-C9	128.3	4.76	0.000	0.000	341.874
47	n-C9	128.3	4.76	0.000	0.000	341.874
48	1-Nonene	126.2	4.62	0.000	0.000	454.715
49	n-C10	142.29	5.25	0.000	0.000	131.879
50	n-C10	142.29	5.25	0.000	0.000	131.879

51	n-C10	142.3	5.25	0.000	0.000	131.888
52	n-C10	142.3	5.25	0.000	0.000	131.888
53	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1289.514
54	n-C8	114.2	4.27	0.000	0.000	874.875
55	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
56	Octene-1	112.2	4.13	0.000	0.000	1162.286
57	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1289.853
58	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1209.094
59	3-methylheptane	114.2	4.2	0.000	0.000	1017.340
60	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1405.614
61	n-C9	128.3	4.76	0.000	0.000	341.874
62	n-C9	128.3	4.76	0.000	0.000	341.874
63	n-C9	128.3	4.76	0.000	0.000	341.874
64	n-C9	128.3	4.76	0.000	0.000	341.874
65	2-Methylanthracene	192.26	4.89	1594.680	0.000	3.719
66	2-methylheptane	114.2	4.2	0.000	0.000	1017.340
67	HEPTANE	100.2	3.78	0.000	0.000	2206.926
68	tert-Butylbenzene	134.2	3.9	0.000	0.000	1775.630
69	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
70	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
71	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
72	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	1081.776
73	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	1230.928
74	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	1230.928
75	n-Butylbenzene	134.2	4.01	0.000	0.000	1400.853
76	Methylcyclohexane	98.19	3.59	0.000	0.000	3257.071
77	sec-Butylbenzene	134.2	3.94	0.000	0.000	1628.968
78	Hydrindene	118.2	3.47	0.000	0.000	3950.913
79	Propylbenzene	120.194	3.52	0.000	0.000	3607.138

80	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	1081.776
81	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1209.094
82	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
83	Anthracene	178.2	4.35	954.966	0.000	13.659
84	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	1230.928
85	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1208.777
86	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	1431.585
87	m-cymene	134.2	4	0.000	0.000	1431.372
88	2,4-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
89	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
90	4-isopropyltoluene	134.22	4	0.000	0.000	1431.585
91	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
92	CYCLOHEXANE	84.16	3.18	0.000	0.000	6755.006
93	n-C5	72.15	2.8	0.000	0.000	13135.189
94	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	3169.746
95	2-methylhexane	100.2	3.71	0.000	0.000	2566.302
96	Isopropylbenzene	120.194	3.45	0.000	0.000	4194.525
97	3-Methylpentane	86.18	3.21	0.000	0.000	6484.052
98	3-ethylhexane	114.2	4.2	0.000	0.000	1017.340
99	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
100	3-methylhexane	100.2	3.71	0.000	0.000	2566.302
101	2,2-dimethylpentane	100.2	3.67	0.000	0.000	2797.356
102	2,3-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
103	Acenaphthylene	152.2	3.94	611.073	0.000	33.953
104	Methylcyclopentane	84.16	3.1	0.000	0.000	8026.121
105	C4-Benzothiophene	190.3	5.18	0.543	0.000	36.363
106	2-METHYLPENTANE	86.18	3.21	0.000	0.000	6484.052
107	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	971.119
108	Cyclopentane	70.13	2.68	0.000	0.000	16535.748

109	Acenaphthene	154.2	4.15	75.030	0.000	51.095
110	Benzene	78.11	1.99	0.000	0.000	63396.698
111	C3-Benzothiophene	176.3	4.69	0.543	0.000	96.852
112	Isopentane	72.15	2.72	0.000	0.000	15606.889
113	CARBAZOLE	167.2	3.23	214.531	0.000	264.349
114	2,3-dimethylbutane	86.18	3.14	0.000	0.000	7539.916
115	C2-Benzothiophene	162.25	4.13	0.543	0.000	297.989
116	C1-Decalins	152.3	4.61	0.000	0.000	249.310
117	cis-Decalin	138.26	4.2	0.000	0.000	547.642
118	Benzothiophene	134.2	2.99	0.543	0.000	2876.127
119	n-C11	156.31	5.74	0.000	0.000	50.390
120	n-C11	156.31	5.74	0.000	0.000	50.390
121	n-C11	156.31	5.74	0.000	0.000	50.390
122	n-C11	156.31	5.74	0.000	0.000	50.390
123	n-C12	170.34	6.23	0.000	0.000	19.100
124	n-C12	170.34	6.23	0.000	0.000	19.100
125	n-C12	170.34	6.23	0.000	0.000	19.100
126	n-C12	170.34	6.23	0.000	0.000	19.100
127	n-C11	156.31	5.74	0.000	0.000	50.390
128	n-C11	156.31	5.74	0.000	0.000	50.390
129	n-C11	156.31	5.74	0.000	0.000	50.390
130	n-C11	156.31	5.74	0.000	0.000	50.390
131	n-C12	170.34	6.23	0.000	0.000	19.100
132	n-C12	170.34	6.23	0.000	0.000	19.100
133	n-C12	170.34	6.23	0.000	0.000	19.100
134	n-C12	170.34	6.23	0.000	0.000	19.100
135	n-C13	184.37	6.73	0.000	0.000	7.037
136	n-C14	198.4	7.22	0.000	0.000	2.634
137	n-C15	212.42	7.71	0.000	0.000	0.981

138	n-C16	226.45	8.2	0.000	0.000	0.364
139	n-C17	240.48	8.69	0.000	0.000	0.134
140	n-C18	254.5	9.18	0.000	0.000	0.049
141	n-C19	268.53	9.67	0.000	0.000	0.018
142	n-C20	282.56	10.1	0.000	0.000	0.008
143	n-C21	296.59	10.6	0.000	0.000	0.003
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.012
164	Pristane	268.525	9.38	0.000	0.000	0.034
165	Benzo(a)fluoranthene	252.3	6.11	5015.528	0.000	0.218
166	Benzo(b)fluorene	216.3	5.77	747.224	0.000	0.860

167	Benzo(k)fluoranthene	252.3	6.11	3937.473	0.000	0.241
168	Benzo[a]anthracene	228.3	5.52	1089.529	0.000	1.331
169	Benzo[a]pyrene	252.3	6.11	5779.613	0.000	0.205
170	Benzo[b]fluoranthene	252.3	6.11	2379.848	0.000	0.298
171	Benzo[e]pyrene	252.3	6.11	1563.329	0.000	0.355
172	Benzo[g,h,i]perylene	276.3	6.7	4626.123	0.000	0.069
173	C1-Chrysenes	242.3	6.0683	733.508	0.000	0.510
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2771.332	0.000	0.931
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	8.960
176	C2-Chrysenes	256.3	6.65	733.508	0.000	0.154
177	C2-Decalins	166.3	6.19	0.000	0.000	9.038
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2771.332	0.000	0.244
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	3.365
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1594.680	0.000	1.143
181	C3-Chrysenes	270.4	7.03	733.508	0.000	0.072
182	C3-Decalins	180.3	6.79	0.000	0.000	2.689
183	C3-Dibenzothiophenes	230.37	5.86	9.545	0.000	4.169
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2771.332	0.000	0.100
185	C3-Fluorenes	210.3	5.58	122.328	0.000	2.633
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.207
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1594.680	0.000	0.527
188	C4-Chrysenes	284.4	7.35	733.508	0.000	0.038
189	C4-Decalins	194.3	7.34	0.000	0.000	0.886
190	C4-Dibenzothiophenes	244.37	6.1	9.545	0.000	2.637
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2771.332	0.000	0.038
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.451
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1594.680	0.000	0.293
194	Chrysene	228.3	5.52	569.025	0.000	1.741
195	Dibenz(a,h)anthracene	278.4	6.7	2618.466	0.000	0.089

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	6932.949	0.000	0.058
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	60.488
198	Perylene	252.3	6.11	8498.796	0.000	0.174
199	Retene	234.3	6.35	104.029	0.000	0.595

Table B.50. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in Juniper oil at 6.25% WAF duplicate exposed to *Cyprinodon variegatus* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C2-Fluorenes	194.3	5.21	122.328	0.016	5.399
2	n-Pentylbenzene	148.2	4.5	0.000	1.780	691.589
3	C1-Phenanthrenes/Anthracenes	192.3	4.26	1594.680	0.034	14.459
4	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	2.890	1231.111
5	C1-Fluorenes	180.2	4.97	122.328	0.010	8.399
6	1-Methylphenanthrene	192.26	4.89	70.978	0.010	13.214
7	3-Methylphenanthrene	192.26	4.89	70.978	0.010	13.214
8	4/9-Methylphenanthrene	192.26	4.89	70.978	0.009	13.214
9	C4-Naphthalenes	184.3	5.18	32.258	0.006	9.205
10	C3-Naphthalenes	170.26	4.77	32.258	0.013	20.577
11	2-Methylphenanthrene	192.26	4.89	70.978	0.008	13.214
12	C2-Dibenzothiophenes	214.3	5.13	9.545	0.009	18.704
13	n-C6	86.18	3.29	0.000	2.340	5457.158
14	Phenanthrene	178.2	4.35	44.769	0.018	46.946
15	Pyrene	202.3	4.93	2084.628	0.001	3.210
16	p-XYLENE	106.2	3.09	0.000	2.030	8051.643
17	C1-Dibenzothiophenes	198.3	4.71	9.545	0.009	42.791
18	1,6,7-Trimethylnaphthalene	170.26	4.81	37.111	0.003	17.892
19	C2-Naphthalenes	156.2	4.31	32.258	0.008	50.876
20	Fluoranthene	202.3	4.93	1270.157	0.001	3.946
21	4-Methyldibenzothiophene	198.28	4.71	9.545	0.005	42.787

22	o-XYLENE	106.2	3.09	0.000	0.964	8051.643
23	m-XYLENE	106.2	3.09	0.000	0.947	8051.643
24	Toluene	92.14	2.54	0.000	1.960	22856.420
25	Fluorene	166.2	4.02	122.328	0.004	60.024
26	2,6-Dimethylnaphthalene	156.23	4.26	32.258	0.003	56.676
27	1-Methyldibenzothiophene	198.28	4.71	9.545	0.001	42.787
28	C1-Naphthalenes	142.2	3.87	20.674	0.005	141.434
29	Dibenzothiophene	184.3	4.17	9.545	0.004	127.348
30	2/3-Methyldibenzothiophene	198.28	4.71	8.229	0.001	45.097
31	2-Methylnaphthalene	142.2	3.72	20.674	0.003	195.413
32	1-Methylnaphthalene	142.2	3.72	20.674	0.003	195.413
33	Naphthalene	234.3	3.17	12.318	0.009	1274.755
34	Dibenzofuran	168.2	3.71	35.593	0.001	192.274
35	trans-Decalin	138.26	4.2	0.000	0.003	547.642
36	Biphenyl	154.2	3.76	0.000	0.005	1576.610
37	C1-Benzothiophene	148.2	3.5365	0.543	0.002	978.092
38	n-C10	142.29	5.25	0.000	0.000	131.879
39	n-C10	142.29	5.25	0.000	0.000	131.879
40	n-C10	142.3	5.25	0.000	0.000	131.888
41	n-C10	142.3	5.25	0.000	0.000	131.888
42	1-Decene	140.3	5.12	0.000	0.000	172.083
43	n-C9	128.3	4.76	0.000	0.000	341.874
44	n-C9	128.3	4.76	0.000	0.000	341.874
45	n-C9	128.3	4.76	0.000	0.000	341.874
46	n-C9	128.3	4.76	0.000	0.000	341.874
47	1-Nonene	126.2	4.62	0.000	0.000	454.715
48	n-C10	142.29	5.25	0.000	0.000	131.879
49	n-C10	142.29	5.25	0.000	0.000	131.879
50	n-C10	142.3	5.25	0.000	0.000	131.888

51	n-C10	142.3	5.25	0.000	0.000	131.888
52	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1289.514
53	n-C8	114.2	4.27	0.000	0.000	874.875
54	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
55	Octene-1	112.2	4.13	0.000	0.000	1162.286
56	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1289.853
57	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1209.094
58	3-methylheptane	114.2	4.2	0.000	0.000	1017.340
59	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1405.614
60	n-C9	128.3	4.76	0.000	0.000	341.874
61	n-C9	128.3	4.76	0.000	0.000	341.874
62	n-C9	128.3	4.76	0.000	0.000	341.874
63	n-C9	128.3	4.76	0.000	0.000	341.874
64	2-Methylanthracene	192.26	4.89	1594.680	0.000	3.719
65	2-methylheptane	114.2	4.2	0.000	0.000	1017.340
66	HEPTANE	100.2	3.78	0.000	0.000	2206.926
67	tert-Butylbenzene	134.2	3.9	0.000	0.000	1775.630
68	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.000	1081.615
69	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
70	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.000	1081.615
71	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.000	1081.776
72	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.000	1230.928
73	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.000	1230.928
74	n-Butylbenzene	134.2	4.01	0.000	0.000	1400.853
75	Methylcyclohexane	98.19	3.59	0.000	0.000	3257.071
76	sec-Butylbenzene	134.2	3.94	0.000	0.000	1628.968
77	Hydrindene	118.2	3.47	0.000	0.000	3950.913
78	Propylbenzene	120.194	3.52	0.000	0.000	3607.138
79	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	1081.776

80	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1209.094
81	1,2,4-Trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
82	Anthracene	178.2	4.35	954.966	0.000	13.659
83	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	1230.928
84	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1208.777
85	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	1431.585
86	m-cymene	134.2	4	0.000	0.000	1431.372
87	Ethylbenzene	106.2	3.03	0.000	0.000	9163.144
88	2,4-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
89	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
90	4-isopropyltoluene	134.22	4	0.000	0.000	1431.585
91	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	0.000	3169.746
92	CYCLOHEXANE	84.16	3.18	0.000	0.000	6755.006
93	n-C5	72.15	2.8	0.000	0.000	13135.189
94	4-ETHYLTOLUENE	120.2	3.58	0.000	0.000	3169.746
95	2-methylhexane	100.2	3.71	0.000	0.000	2566.302
96	Isopropylbenzene	120.194	3.45	0.000	0.000	4194.525
97	3-Methylpentane	86.18	3.21	0.000	0.000	6484.052
98	3-ethylhexane	114.2	4.2	0.000	0.000	1017.340
99	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.000	2845.932
100	3-methylhexane	100.2	3.71	0.000	0.000	2566.302
101	2,2-dimethylpentane	100.2	3.67	0.000	0.000	2797.356
102	2,3-dimethylpentane	100.2	3.63	0.000	0.000	3049.213
103	Acenaphthylene	152.2	3.94	611.073	0.000	33.953
104	Methylcyclopentane	84.16	3.1	0.000	0.000	8026.121
105	C4-Benzothiophene	190.3	5.18	0.543	0.000	36.363
106	2-METHYLPENTANE	86.18	3.21	0.000	0.000	6484.052
107	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.000	971.119
108	Cyclopentane	70.13	2.68	0.000	0.000	16535.748

109	Acenaphthene	154.2	4.15	75.030	0.000	51.095
110	Benzene	78.11	1.99	0.000	0.000	63396.698
111	C3-Benzothiophene	176.3	4.69	0.543	0.000	96.852
112	Isopentane	72.15	2.72	0.000	0.000	15606.889
113	CARBAZOLE	167.2	3.23	214.531	0.000	264.349
114	2,3-dimethylbutane	86.18	3.14	0.000	0.000	7539.916
115	C2-Benzothiophene	162.25	4.13	0.543	0.000	297.989
116	C1-Decalins	152.3	4.61	0.000	0.000	249.310
117	cis-Decalin	138.26	4.2	0.000	0.000	547.642
118	Benzothiophene	134.2	2.99	0.543	0.000	2876.127
119	n-C11	156.31	5.74	0.000	0.000	50.390
120	n-C11	156.31	5.74	0.000	0.000	50.390
121	n-C11	156.31	5.74	0.000	0.000	50.390
122	n-C11	156.31	5.74	0.000	0.000	50.390
123	n-C12	170.34	6.23	0.000	0.000	19.100
124	n-C12	170.34	6.23	0.000	0.000	19.100
125	n-C12	170.34	6.23	0.000	0.000	19.100
126	n-C12	170.34	6.23	0.000	0.000	19.100
127	n-C11	156.31	5.74	0.000	0.000	50.390
128	n-C11	156.31	5.74	0.000	0.000	50.390
129	n-C11	156.31	5.74	0.000	0.000	50.390
130	n-C11	156.31	5.74	0.000	0.000	50.390
131	n-C12	170.34	6.23	0.000	0.000	19.100
132	n-C12	170.34	6.23	0.000	0.000	19.100
133	n-C12	170.34	6.23	0.000	0.000	19.100
134	n-C12	170.34	6.23	0.000	0.000	19.100
135	n-C13	184.37	6.73	0.000	0.000	7.037
136	n-C14	198.4	7.22	0.000	0.000	2.634
137	n-C15	212.42	7.71	0.000	0.000	0.981

138	n-C16	226.45	8.2	0.000	0.000	0.364
139	n-C17	240.48	8.69	0.000	0.000	0.134
140	n-C18	254.5	9.18	0.000	0.000	0.049
141	n-C19	268.53	9.67	0.000	0.000	0.018
142	n-C20	282.56	10.1	0.000	0.000	0.008
143	n-C21	296.59	10.6	0.000	0.000	0.003
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.012
164	Pristane	268.525	9.38	0.000	0.000	0.034
165	Benzo(a)fluoranthene	252.3	6.11	5015.528	0.000	0.218
166	Benzo(b)fluorene	216.3	5.77	747.224	0.000	0.860

167	Benzo(k)fluoranthene	252.3	6.11	3937.473	0.000	0.241
168	Benzo[a]anthracene	228.3	5.52	1089.529	0.000	1.331
169	Benzo[a]pyrene	252.3	6.11	5779.613	0.000	0.205
170	Benzo[b]fluoranthene	252.3	6.11	2379.848	0.000	0.298
171	Benzo[e]pyrene	252.3	6.11	1563.329	0.000	0.355
172	Benzo[g,h,i]perylene	276.3	6.7	4626.123	0.000	0.069
173	C1-Chrysenes	242.3	6.0683	733.508	0.000	0.510
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2771.332	0.000	0.931
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	8.960
176	C2-Chrysenes	256.3	6.65	733.508	0.000	0.154
177	C2-Decalins	166.3	6.19	0.000	0.000	9.038
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2771.332	0.000	0.244
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	3.365
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1594.680	0.000	1.143
181	C3-Chrysenes	270.4	7.03	733.508	0.000	0.072
182	C3-Decalins	180.3	6.79	0.000	0.000	2.689
183	C3-Dibenzothiophenes	230.37	5.86	9.545	0.000	4.169
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2771.332	0.000	0.100
185	C3-Fluorenes	210.3	5.58	122.328	0.000	2.633
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.207
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1594.680	0.000	0.527
188	C4-Chrysenes	284.4	7.35	733.508	0.000	0.038
189	C4-Decalins	194.3	7.34	0.000	0.000	0.886
190	C4-Dibenzothiophenes	244.37	6.1	9.545	0.000	2.637
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2771.332	0.000	0.038
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.451
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1594.680	0.000	0.293
194	Chrysene	228.3	5.52	569.025	0.000	1.741
195	Dibenz(a,h)anthracene	278.4	6.7	2618.466	0.000	0.089

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	6932.949	0.000	0.058
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	60.488
198	Perylene	252.3	6.11	8498.796	0.000	0.174
199	Retene	234.3	6.35	104.029	0.000	0.595

Table B.51. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 100% WAF exposed to *Fundulus grandis* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	2-Methylnaphthalene	142.2	3.72	22.713	83.400	263.425
2	C1-Naphthalenes	142.2	3.87	22.713	48.600	190.659
3	1-Methylnaphthalene	142.2	3.72	22.713	61.400	263.425
4	C2-Naphthalenes	156.2	4.31	34.260	10.900	69.426
5	Naphthalene	234.3	3.17	13.523	162.000	1720.608
6	C3-Naphthalenes	170.26	4.77	34.260	2.490	28.080
7	2,6-Dimethylnaphthalene	156.23	4.26	34.260	6.060	77.340
8	C1-Fluorenes	180.2	4.97	123.371	0.786	11.689
9	C2-Fluorenes	194.3	5.21	123.371	0.446	7.514
10	C1-Phenanthrenes/Anthracenes	192.3	4.26	1597.323	1.170	20.176
11	C4-Naphthalenes	184.3	5.18	34.260	0.609	12.562
12	Toluene	92.14	2.54	0.000	1350.000	31915.982
13	m-XYLENE	106.2	3.09	0.000	412.000	11243.060
14	2-Methylanthracene	192.26	4.89	1597.323	0.171	5.189
15	1,6,7-Trimethylnaphthalene	170.26	4.81	40.427	0.651	24.174
16	4/9-Methylphenanthrene	192.26	4.89	75.479	0.470	18.010
17	o-XYLENE	106.2	3.09	0.000	250.000	11243.060
18	1,2,4-Trimethylbenzene	120.2	3.63	0.000	84.300	3973.969
19	Phenanthrene	178.2	4.35	47.595	1.230	64.017
20	Fluorene	166.2	4.02	123.371	1.340	83.532
21	1-Methylphenanthrene	192.26	4.89	75.479	0.244	18.010

22	Benzene	78.11	1.99	0.000	1160.000	88525.143
23	3-Methylphenanthrene	192.26	4.89	75.479	0.184	18.010
24	2-Methylphenanthrene	192.26	4.89	75.479	0.183	18.010
25	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	40.800	4426.133
26	Methylcyclohexane	98.19	3.59	0.000	39.000	4548.071
27	Ethylbenzene	106.2	3.03	0.000	107.000	12795.125
28	C2-Dibenzothiophenes	214.3	5.13	10.148	0.213	25.552
29	CYCLOHEXANE	84.16	3.18	0.000	78.600	9432.476
30	Anthracene	178.2	4.35	958.381	0.148	19.045
31	1,3,5-trimethylbenzene	120.2	3.63	0.000	27.000	3973.969
32	C1-Dibenzothiophenes	198.3	4.71	10.148	0.365	58.458
33	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	25.200	4426.133
34	p-XYLENE	106.2	3.09	0.000	63.500	11243.060
35	CARBAZOLE	167.2	3.23	223.878	1.780	362.804
36	Methylcyclopentane	84.16	3.1	0.000	50.100	11207.422
37	C3-Benzothiophene	176.3	4.69	0.550	0.497	134.811
38	4-ETHYLTOLUENE	120.2	3.58	0.000	15.100	4426.133
39	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	4.580	1510.332
40	C4-Benzothiophene	190.3	5.18	0.550	0.142	50.614
41	Pyrene	202.3	4.93	2143.908	0.012	4.430
42	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	3.900	1510.332
43	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	4.280	1718.828
44	Propylbenzene	120.194	3.52	0.000	12.500	5036.894
45	n-C5	72.15	2.8	0.000	42.200	18341.563
46	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	3.440	1510.332
47	Acenaphthene	154.2	4.15	81.144	0.150	69.175
48	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	2.960	1510.332
49	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	3.130	1718.828
50	n-C6	86.18	3.29	0.000	13.700	7620.202

51	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	2.350	1356.040
52	Isopropylbenzene	120.194	3.45	0.000	10.000	5857.102
53	Isopentane	72.15	2.72	0.000	36.500	21792.966
54	4-Methyldibenzothiophene	198.28	4.71	10.148	0.096	58.452
55	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	2.430	1510.557
56	m-cymene	134.2	4	0.000	2.990	1998.723
57	Dibenzothiophene	184.3	4.17	10.148	0.256	173.974
58	Cyclopentane	70.13	2.68	0.000	33.100	23089.995
59	Dibenzofuran	168.2	3.71	39.135	0.344	258.877
60	C2-Benzothiophene	162.25	4.13	0.550	0.530	414.781
61	Biphenyl	154.2	3.76	0.000	2.680	2201.529
62	2-METHYLPENTANE	86.18	3.21	0.000	9.230	9054.125
63	3-Methylpentane	86.18	3.21	0.000	7.620	9054.125
64	Fluoranthene	202.3	4.93	1283.084	0.005	5.487
65	1-Methyldibenzothiophene	198.28	4.71	10.148	0.047	58.452
66	HEPTANE	100.2	3.78	0.000	2.470	3081.681
67	Hydrindene	118.2	3.47	0.000	4.360	5516.930
68	2/3-Methyldibenzothiophene	198.28	4.71	8.823	0.045	61.438
69	4-isopropyltoluene	134.22	4	0.000	1.420	1999.020
70	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	1.000	1510.557
71	3-methylhexane	100.2	3.71	0.000	2.300	3583.503
72	n-Butylbenzene	134.2	4.01	0.000	1.210	1956.107
73	sec-Butylbenzene	134.2	3.94	0.000	1.340	2274.639
74	1,2-Diethylbenzene	134.2	4.07	0.000	0.800	1718.828
75	trans-Decalin	138.26	4.2	0.000	0.237	764.710
76	C1-Decalins	152.3	4.61	0.000	0.104	348.129
77	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.579	1999.020
78	Acenaphthylene	152.2	3.94	632.500	0.011	46.742
79	C1-Benzothiophene	148.2	3.5365	0.550	0.223	1361.440

80	2,3-dimethylbutane	86.18	3.14	0.000	1.670	10528.500
81	1,1,3-trimethylpentane	114.23	4.12	0.000	0.101	1688.341
82	cis-Decalin	138.26	4.2	0.000	0.032	764.710
83	Benzothiophene	134.2	2.99	0.550	0.042	4003.379
84	n-C10	142.29	5.25	0.000	0.000	184.151
85	n-C10	142.29	5.25	0.000	0.000	184.151
86	n-C10	142.3	5.25	0.000	0.000	184.164
87	n-C10	142.3	5.25	0.000	0.000	184.164
88	1-Decene	140.3	5.12	0.000	0.000	240.291
89	n-C9	128.3	4.76	0.000	0.000	477.383
90	n-C9	128.3	4.76	0.000	0.000	477.383
91	n-C9	128.3	4.76	0.000	0.000	477.383
92	n-C9	128.3	4.76	0.000	0.000	477.383
93	1-Nonene	126.2	4.62	0.000	0.000	634.950
94	n-C10	142.29	5.25	0.000	0.000	184.151
95	n-C10	142.29	5.25	0.000	0.000	184.151
96	n-C10	142.3	5.25	0.000	0.000	184.164
97	n-C10	142.3	5.25	0.000	0.000	184.164
98	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1800.637
99	n-C8	114.2	4.27	0.000	0.000	1221.648
100	n-Pentylbenzene	148.2	4.5	0.000	0.000	965.713
101	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	1719.085
102	Octene-1	112.2	4.13	0.000	0.000	1622.979
103	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1801.110
104	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1688.341
105	3-methylheptane	114.2	4.2	0.000	0.000	1420.581
106	n-C9	128.3	4.76	0.000	0.000	477.383
107	n-C9	128.3	4.76	0.000	0.000	477.383
108	n-C9	128.3	4.76	0.000	0.000	477.383

109	n-C9	128.3	4.76	0.000	0.000	477.383
110	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1962.755
111	2-methylheptane	114.2	4.2	0.000	0.000	1420.581
112	tert-Butylbenzene	134.2	3.9	0.000	0.000	2479.434
113	2-methylhexane	100.2	3.71	0.000	0.000	3583.503
114	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1687.898
115	2,4-dimethylpentane	100.2	3.63	0.000	0.000	4257.824
116	3-ethylhexane	114.2	4.2	0.000	0.000	1420.581
117	2,2-dimethylpentane	100.2	3.67	0.000	0.000	3906.139
118	2,3-dimethylpentane	100.2	3.63	0.000	0.000	4257.824
119	n-C11	156.31	5.74	0.000	0.000	70.363
120	n-C11	156.31	5.74	0.000	0.000	70.363
121	n-C11	156.31	5.74	0.000	0.000	70.363
122	n-C11	156.31	5.74	0.000	0.000	70.363
123	n-C12	170.34	6.23	0.000	0.000	26.671
124	n-C12	170.34	6.23	0.000	0.000	26.671
125	n-C12	170.34	6.23	0.000	0.000	26.671
126	n-C12	170.34	6.23	0.000	0.000	26.671
127	n-C11	156.31	5.74	0.000	0.000	70.363
128	n-C11	156.31	5.74	0.000	0.000	70.363
129	n-C11	156.31	5.74	0.000	0.000	70.363
130	n-C11	156.31	5.74	0.000	0.000	70.363
131	n-C12	170.34	6.23	0.000	0.000	26.671
132	n-C12	170.34	6.23	0.000	0.000	26.671
133	n-C12	170.34	6.23	0.000	0.000	26.671
134	n-C12	170.34	6.23	0.000	0.000	26.671
135	n-C13	184.37	6.73	0.000	0.000	9.827
136	n-C14	198.4	7.22	0.000	0.000	3.678
137	n-C15	212.42	7.71	0.000	0.000	1.370

138	n-C16	226.45	8.2	0.000	0.000	0.508
139	n-C17	240.48	8.69	0.000	0.000	0.188
140	n-C18	254.5	9.18	0.000	0.000	0.069
141	n-C19	268.53	9.67	0.000	0.000	0.025
142	n-C20	282.56	10.1	0.000	0.000	0.011
143	n-C21	296.59	10.6	0.000	0.000	0.004
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.017
164	Pristane	268.525	9.38	0.000	0.000	0.047
165	Benzo(a)fluoranthene	252.3	6.11	4721.971	0.000	0.312
166	Benzo(b)fluorene	216.3	5.77	790.615	0.000	1.173

167	Benzo(k)fluoranthene	252.3	6.11	3953.845	0.000	0.336
168	Benzo[a]anthracene	228.3	5.52	1114.179	0.000	1.841
169	Benzo[a]pyrene	252.3	6.11	5785.774	0.000	0.286
170	Benzo[b]fluoranthene	252.3	6.11	2408.970	0.000	0.414
171	Benzo[e]pyrene	252.3	6.11	1612.027	0.000	0.489
172	Benzo[g,h,i]perylene	276.3	6.7	4665.274	0.000	0.096
173	C1-Chrysenes	242.3	6.0683	765.693	0.000	0.700
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2807.331	0.000	1.292
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	12.511
176	C2-Chrysenes	256.3	6.65	765.693	0.000	0.211
177	C2-Decalins	166.3	6.19	0.000	0.000	12.620
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2807.331	0.000	0.339
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	4.699
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1597.323	0.000	1.595
181	C3-Chrysenes	270.4	7.03	765.693	0.000	0.098
182	C3-Decalins	180.3	6.79	0.000	0.000	3.755
183	C3-Dibenzothiophenes	230.37	5.86	10.148	0.000	5.696
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2807.331	0.000	0.139
185	C3-Fluorenes	210.3	5.58	123.371	0.000	3.664
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.685
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1597.323	0.000	0.735
188	C4-Chrysenes	284.4	7.35	765.693	0.000	0.052
189	C4-Decalins	194.3	7.34	0.000	0.000	1.237
190	C4-Dibenzothiophenes	244.37	6.1	10.148	0.000	3.602
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2807.331	0.000	0.052
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.629
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1597.323	0.000	0.409
194	Chrysene	228.3	5.52	602.317	0.000	2.375
195	Dibenz(a,h)anthracene	278.4	6.7	2706.502	0.000	0.122

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	6853.386	0.000	0.082
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	84.463
198	Perylene	252.3	6.11	7893.119	0.000	0.251
199	Retene	234.3	6.35	111.122	0.000	0.810

Table B.52. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 25% WAF exposed to *Fundulus grandis* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	22.713	8.720	190.659
2	C2-Naphthalenes	156.2	4.31	34.260	2.620	69.426
3	2-Methylnaphthalene	142.2	3.72	22.713	8.510	263.425
4	1-Methylnaphthalene	142.2	3.72	22.713	6.450	263.425
5	C3-Naphthalenes	170.26	4.77	34.260	0.527	28.080
6	C1-Fluorenes	180.2	4.97	123.371	0.180	11.689
7	2,6-Dimethylnaphthalene	156.23	4.26	34.260	1.170	77.340
8	C1-Phenanthrenes/Anthracenes	192.3	4.26	1597.323	0.263	20.176
9	C2-Fluorenes	194.3	5.21	123.371	0.095	7.514
10	Naphthalene	234.3	3.17	13.523	17.400	1720.608
11	C4-Naphthalenes	184.3	5.18	34.260	0.123	12.562
12	Toluene	92.14	2.54	0.000	269.000	31915.982
13	2-Methylanthracene	192.26	4.89	1597.323	0.037	5.189
14	m-XYLENE	106.2	3.09	0.000	75.800	11243.060
15	4/9-Methylphenanthrene	192.26	4.89	75.479	0.106	18.010
16	1,6,7-Trimethylnaphthalene	170.26	4.81	40.427	0.137	24.174
17	Phenanthrene	178.2	4.35	47.595	0.297	64.017
18	o-XYLENE	106.2	3.09	0.000	47.700	11243.060
19	1,2,4-Trimethylbenzene	120.2	3.63	0.000	16.400	3973.969
20	Fluorene	166.2	4.02	123.371	0.322	83.532
21	1-Methylphenanthrene	192.26	4.89	75.479	0.057	18.010

22	Benzene	78.11	1.99	0.000	225.000	88525.143
23	3-Methylphenanthrene	192.26	4.89	75.479	0.042	18.010
24	2-Methylphenanthrene	192.26	4.89	75.479	0.042	18.010
25	p-XYLENE	106.2	3.09	0.000	21.400	11243.060
26	Ethylbenzene	106.2	3.03	0.000	21.400	12795.125
27	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	7.360	4426.133
28	C2-Dibenzothiophenes	214.3	5.13	10.148	0.042	25.552
29	Anthracene	178.2	4.35	958.381	0.029	19.045
30	1,3,5-trimethylbenzene	120.2	3.63	0.000	4.760	3973.969
31	Methylcyclohexane	98.19	3.59	0.000	5.130	4548.071
32	CYCLOHEXANE	84.16	3.18	0.000	10.300	9432.476
33	C1-Dibenzothiophenes	198.3	4.71	10.148	0.062	58.458
34	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	4.620	4426.133
35	C3-Benzothiophene	176.3	4.69	0.550	0.126	134.811
36	Pyrene	202.3	4.93	2143.908	0.004	4.430
37	C4-Benzothiophene	190.3	5.18	0.550	0.039	50.614
38	CARBAZOLE	167.2	3.23	223.878	0.228	362.804
39	4-ETHYLTOLUENE	120.2	3.58	0.000	2.590	4426.133
40	Methylcyclopentane	84.16	3.1	0.000	6.340	11207.422
41	Acenaphthene	154.2	4.15	81.144	0.036	69.175
42	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.777	1510.332
43	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.652	1510.332
44	Propylbenzene	120.194	3.52	0.000	2.070	5036.894
45	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.670	1718.828
46	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.580	1510.332
47	4-Methyldibenzothiophene	198.28	4.71	10.148	0.021	58.452
48	Dibenzothiophene	184.3	4.17	10.148	0.059	173.974
49	C2-Benzothiophene	162.25	4.13	0.550	0.140	414.781
50	Isopentane	72.15	2.72	0.000	7.350	21792.966

51	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.500	1510.332
52	Fluoranthene	202.3	4.93	1283.084	0.002	5.487
53	Dibenzofuran	168.2	3.71	39.135	0.081	258.877
54	Biphenyl	154.2	3.76	0.000	0.673	2201.529
55	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.502	1718.828
56	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.386	1356.040
57	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.428	1510.557
58	2/3-Methyldibenzothiophene	198.28	4.71	8.823	0.017	61.438
59	Isopropylbenzene	120.194	3.45	0.000	1.620	5857.102
60	m-cymene	134.2	4	0.000	0.508	1998.723
61	n-C5	72.15	2.8	0.000	4.590	18341.563
62	n-C6	86.18	3.29	0.000	1.700	7620.202
63	Cyclopentane	70.13	2.68	0.000	4.380	23089.995
64	Hydrindene	118.2	3.47	0.000	0.858	5516.930
65	1-Methyldibenzothiophene	198.28	4.71	10.148	0.009	58.452
66	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.172	1510.557
67	4-isopropyltoluene	134.22	4	0.000	0.220	1999.020
68	2-METHYLPENTANE	86.18	3.21	0.000	0.982	9054.125
69	3-Methylpentane	86.18	3.21	0.000	0.891	9054.125
70	sec-Butylbenzene	134.2	3.94	0.000	0.197	2274.639
71	HEPTANE	100.2	3.78	0.000	0.247	3081.681
72	1,2-Diethylbenzene	134.2	4.07	0.000	0.133	1718.828
73	n-Butylbenzene	134.2	4.01	0.000	0.145	1956.107
74	3-methylhexane	100.2	3.71	0.000	0.245	3583.503
75	Acenaphthylene	152.2	3.94	632.500	0.003	46.742
76	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.094	1999.020
77	C1-Benzothiophene	148.2	3.5365	0.550	0.058	1361.440
78	C1-Decalins	152.3	4.61	0.000	0.011	348.129
79	2,3-dimethylbutane	86.18	3.14	0.000	0.303	10528.500

80	trans-Decalin	138.26	4.2	0.000	0.022	764.710
81	cis-Decalin	138.26	4.2	0.000	0.003	764.710
82	Benzothiophene	134.2	2.99	0.550	0.010	4003.379
83	n-C10	142.29	5.25	0.000	0.000	184.151
84	n-C10	142.29	5.25	0.000	0.000	184.151
85	n-C10	142.3	5.25	0.000	0.000	184.164
86	n-C10	142.3	5.25	0.000	0.000	184.164
87	1-Decene	140.3	5.12	0.000	0.000	240.291
88	n-C10	142.29	5.25	0.000	0.000	184.151
89	n-C10	142.29	5.25	0.000	0.000	184.151
90	n-C10	142.3	5.25	0.000	0.000	184.164
91	n-C10	142.3	5.25	0.000	0.000	184.164
92	n-C9	128.3	4.76	0.000	0.000	477.383
93	n-C9	128.3	4.76	0.000	0.000	477.383
94	n-C9	128.3	4.76	0.000	0.000	477.383
95	n-C9	128.3	4.76	0.000	0.000	477.383
96	1-Nonene	126.2	4.62	0.000	0.000	634.950
97	n-C9	128.3	4.76	0.000	0.000	477.383
98	n-C9	128.3	4.76	0.000	0.000	477.383
99	n-C9	128.3	4.76	0.000	0.000	477.383
100	n-C9	128.3	4.76	0.000	0.000	477.383
101	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1800.637
102	n-C8	114.2	4.27	0.000	0.000	1221.648
103	n-Pentylbenzene	148.2	4.5	0.000	0.000	965.713
104	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	1719.085
105	Octene-1	112.2	4.13	0.000	0.000	1622.979
106	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1801.110
107	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1688.341
108	3-methylheptane	114.2	4.2	0.000	0.000	1420.581

109	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1962.755
110	2-methylheptane	114.2	4.2	0.000	0.000	1420.581
111	tert-Butylbenzene	134.2	3.9	0.000	0.000	2479.434
112	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1688.341
113	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1687.898
114	2,4-dimethylpentane	100.2	3.63	0.000	0.000	4257.824
115	2-methylhexane	100.2	3.71	0.000	0.000	3583.503
116	3-ethylhexane	114.2	4.2	0.000	0.000	1420.581
117	2,2-dimethylpentane	100.2	3.67	0.000	0.000	3906.139
118	2,3-dimethylpentane	100.2	3.63	0.000	0.000	4257.824
119	n-C11	156.31	5.74	0.000	0.000	70.363
120	n-C11	156.31	5.74	0.000	0.000	70.363
121	n-C11	156.31	5.74	0.000	0.000	70.363
122	n-C11	156.31	5.74	0.000	0.000	70.363
123	n-C12	170.34	6.23	0.000	0.000	26.671
124	n-C12	170.34	6.23	0.000	0.000	26.671
125	n-C12	170.34	6.23	0.000	0.000	26.671
126	n-C12	170.34	6.23	0.000	0.000	26.671
127	n-C11	156.31	5.74	0.000	0.000	70.363
128	n-C11	156.31	5.74	0.000	0.000	70.363
129	n-C11	156.31	5.74	0.000	0.000	70.363
130	n-C11	156.31	5.74	0.000	0.000	70.363
131	n-C12	170.34	6.23	0.000	0.000	26.671
132	n-C12	170.34	6.23	0.000	0.000	26.671
133	n-C12	170.34	6.23	0.000	0.000	26.671
134	n-C12	170.34	6.23	0.000	0.000	26.671
135	n-C13	184.37	6.73	0.000	0.000	9.827
136	n-C14	198.4	7.22	0.000	0.000	3.678
137	n-C15	212.42	7.71	0.000	0.000	1.370

138	n-C16	226.45	8.2	0.000	0.000	0.508
139	n-C17	240.48	8.69	0.000	0.000	0.188
140	n-C18	254.5	9.18	0.000	0.000	0.069
141	n-C19	268.53	9.67	0.000	0.000	0.025
142	n-C20	282.56	10.1	0.000	0.000	0.011
143	n-C21	296.59	10.6	0.000	0.000	0.004
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.017
164	Pristane	268.525	9.38	0.000	0.000	0.047
165	Benzo(a)fluoranthene	252.3	6.11	4721.971	0.000	0.312
166	Benzo(b)fluorene	216.3	5.77	790.615	0.000	1.173

167	Benzo(k)fluoranthene	252.3	6.11	3953.845	0.000	0.336
168	Benzo[a]anthracene	228.3	5.52	1114.179	0.000	1.841
169	Benzo[a]pyrene	252.3	6.11	5785.774	0.000	0.286
170	Benzo[b]fluoranthene	252.3	6.11	2408.970	0.000	0.414
171	Benzo[e]pyrene	252.3	6.11	1612.027	0.000	0.489
172	Benzo[g,h,i]perylene	276.3	6.7	4665.274	0.000	0.096
173	C1-Chrysenes	242.3	6.0683	765.693	0.000	0.700
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2807.331	0.000	1.292
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	12.511
176	C2-Chrysenes	256.3	6.65	765.693	0.000	0.211
177	C2-Decalins	166.3	6.19	0.000	0.000	12.620
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2807.331	0.000	0.339
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	4.699
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1597.323	0.000	1.595
181	C3-Chrysenes	270.4	7.03	765.693	0.000	0.098
182	C3-Decalins	180.3	6.79	0.000	0.000	3.755
183	C3-Dibenzothiophenes	230.37	5.86	10.148	0.000	5.696
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2807.331	0.000	0.139
185	C3-Fluorenes	210.3	5.58	123.371	0.000	3.664
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.685
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1597.323	0.000	0.735
188	C4-Chrysenes	284.4	7.35	765.693	0.000	0.052
189	C4-Decalins	194.3	7.34	0.000	0.000	1.237
190	C4-Dibenzothiophenes	244.37	6.1	10.148	0.000	3.602
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2807.331	0.000	0.052
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.629
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1597.323	0.000	0.409
194	Chrysene	228.3	5.52	602.317	0.000	2.375
195	Dibenz(a,h)anthracene	278.4	6.7	2706.502	0.000	0.122

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	6853.386	0.000	0.082
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	84.463
198	Perylene	252.3	6.11	7893.119	0.000	0.251
199	Retene	234.3	6.35	111.122	0.000	0.810

Table B.53. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF exposed to *Fundulus grandis* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	22.713	1.980	190.659
2	C2-Naphthalenes	156.2	4.31	34.260	0.575	69.426
3	2-Methylnaphthalene	142.2	3.72	22.713	1.810	263.425
4	1-Methylnaphthalene	142.2	3.72	22.713	1.390	263.425
5	C3-Naphthalenes	170.26	4.77	34.260	0.122	28.080
6	C2-Fluorenes	194.3	5.21	123.371	0.029	7.514
7	C1-Fluorenes	180.2	4.97	123.371	0.043	11.689
8	C1-Phenanthrenes/Anthracenes	192.3	4.26	1597.323	0.068	20.176
9	2,6-Dimethylnaphthalene	156.23	4.26	34.260	0.251	77.340
10	C4-Naphthalenes	184.3	5.18	34.260	0.032	12.562
11	Naphthalene	234.3	3.17	13.523	3.500	1720.608
12	2-Methylanthracene	192.26	4.89	1597.323	0.009	5.189
13	Toluene	92.14	2.54	0.000	51.100	31915.982
14	4/9-Methylphenanthrene	192.26	4.89	75.479	0.026	18.010
15	m-XYLENE	106.2	3.09	0.000	15.200	11243.060
16	1,6,7-Trimethylnaphthalene	170.26	4.81	40.427	0.032	24.174
17	Phenanthrene	178.2	4.35	47.595	0.075	64.017
18	Fluorene	166.2	4.02	123.371	0.078	83.532
19	o-XYLENE	106.2	3.09	0.000	9.820	11243.060
20	1,2,4-Trimethylbenzene	120.2	3.63	0.000	3.140	3973.969
21	1-Methylphenanthrene	192.26	4.89	75.479	0.014	18.010

22	3-Methylphenanthrene	192.26	4.89	75.479	0.012	18.010
23	2-Methylphenanthrene	192.26	4.89	75.479	0.011	18.010
24	C2-Dibenzothiophenes	214.3	5.13	10.148	0.013	25.552
25	Pyrene	202.3	4.93	2143.908	0.002	4.430
26	Benzene	78.11	1.99	0.000	42.500	88525.143
27	Anthracene	178.2	4.35	958.381	0.007	19.045
28	p-XYLENE	106.2	3.09	0.000	3.990	11243.060
29	Ethylbenzene	106.2	3.03	0.000	3.980	12795.125
30	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	1.270	4426.133
31	C1-Dibenzothiophenes	198.3	4.71	10.148	0.015	58.458
32	C3-Benzothiophene	176.3	4.69	0.550	0.031	134.811
33	Fluoranthene	202.3	4.93	1283.084	0.001	5.487
34	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.837	3973.969
35	C4-Benzothiophene	190.3	5.18	0.550	0.011	50.614
36	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.823	4426.133
37	CYCLOHEXANE	84.16	3.18	0.000	1.460	9432.476
38	CARBAZOLE	167.2	3.23	223.878	0.054	362.804
39	Methylcyclohexane	98.19	3.59	0.000	0.676	4548.071
40	Acenaphthene	154.2	4.15	81.144	0.008	69.175
41	4-ETHYLTOLUENE	120.2	3.58	0.000	0.435	4426.133
42	4-Methyldibenzothiophene	198.28	4.71	10.148	0.005	58.452
43	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.134	1510.332
44	Dibenzothiophene	184.3	4.17	10.148	0.014	173.974
45	Methylcyclopentane	84.16	3.1	0.000	0.908	11207.422
46	Dibenzofuran	168.2	3.71	39.135	0.020	258.877
47	C2-Benzothiophene	162.25	4.13	0.550	0.031	414.781
48	Biphenyl	154.2	3.76	0.000	0.152	2201.529
49	Propylbenzene	120.194	3.52	0.000	0.344	5036.894
50	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.103	1510.332

51	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.098	1510.332
52	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.111	1718.828
53	2/3-Methyldibenzothiophene	198.28	4.71	8.823	0.004	61.438
54	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.091	1510.332
55	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.068	1356.040
56	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.074	1510.557
57	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.081	1718.828
58	Isopropylbenzene	120.194	3.45	0.000	0.260	5857.102
59	1-Methyldibenzothiophene	198.28	4.71	10.148	0.002	58.452
60	Hydrindene	118.2	3.47	0.000	0.184	5516.930
61	n-C5	72.15	2.8	0.000	0.584	18341.563
62	4-isopropyltoluene	134.22	4	0.000	0.055	1999.020
63	Cyclopentane	70.13	2.68	0.000	0.579	23089.995
64	sec-Butylbenzene	134.2	3.94	0.000	0.037	2274.639
65	2-METHYLPENTANE	86.18	3.21	0.000	0.139	9054.125
66	Acenaphthylene	152.2	3.94	632.500	0.001	46.742
67	HEPTANE	100.2	3.78	0.000	0.040	3081.681
68	3-Methylpentane	86.18	3.21	0.000	0.116	9054.125
69	C1-Benzothiophene	148.2	3.5365	0.550	0.014	1361.440
70	C1-Decalins	152.3	4.61	0.000	0.002	348.129
71	trans-Decalin	138.26	4.2	0.000	0.004	764.710
72	Benzothiophene	134.2	2.99	0.550	0.002	4003.379
73	n-C10	142.29	5.25	0.000	0.000	184.151
74	n-C10	142.29	5.25	0.000	0.000	184.151
75	n-C10	142.3	5.25	0.000	0.000	184.164
76	n-C10	142.3	5.25	0.000	0.000	184.164
77	1-Decene	140.3	5.12	0.000	0.000	240.291
78	n-C9	128.3	4.76	0.000	0.000	477.383
79	n-C9	128.3	4.76	0.000	0.000	477.383

80	n-C9	128.3	4.76	0.000	0.000	477.383
81	n-C9	128.3	4.76	0.000	0.000	477.383
82	1-Nonene	126.2	4.62	0.000	0.000	634.950
83	n-C10	142.29	5.25	0.000	0.000	184.151
84	n-C10	142.29	5.25	0.000	0.000	184.151
85	n-C10	142.3	5.25	0.000	0.000	184.164
86	n-C10	142.3	5.25	0.000	0.000	184.164
87	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1800.637
88	n-C8	114.2	4.27	0.000	0.000	1221.648
89	n-Pentylbenzene	148.2	4.5	0.000	0.000	965.713
90	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	1719.085
91	Octene-1	112.2	4.13	0.000	0.000	1622.979
92	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1801.110
93	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1688.341
94	3-methylheptane	114.2	4.2	0.000	0.000	1420.581
95	n-C9	128.3	4.76	0.000	0.000	477.383
96	n-C9	128.3	4.76	0.000	0.000	477.383
97	n-C9	128.3	4.76	0.000	0.000	477.383
98	n-C9	128.3	4.76	0.000	0.000	477.383
99	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1962.755
100	2-methylheptane	114.2	4.2	0.000	0.000	1420.581
101	tert-Butylbenzene	134.2	3.9	0.000	0.000	2479.434
102	n-Butylbenzene	134.2	4.01	0.000	0.000	1956.107
103	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	1510.557
104	n-C6	86.18	3.29	0.000	0.000	7620.202
105	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1688.341
106	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	1718.828
107	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1687.898
108	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	1999.020

109	m-cymene	134.2	4	0.000	0.000	1998.723
110	2,4-dimethylpentane	100.2	3.63	0.000	0.000	4257.824
111	2-methylhexane	100.2	3.71	0.000	0.000	3583.503
112	3-ethylhexane	114.2	4.2	0.000	0.000	1420.581
113	3-methylhexane	100.2	3.71	0.000	0.000	3583.503
114	2,2-dimethylpentane	100.2	3.67	0.000	0.000	3906.139
115	2,3-dimethylpentane	100.2	3.63	0.000	0.000	4257.824
116	Isopentane	72.15	2.72	0.000	0.000	21792.966
117	2,3-dimethylbutane	86.18	3.14	0.000	0.000	10528.500
118	cis-Decalin	138.26	4.2	0.000	0.000	764.710
119	n-C11	156.31	5.74	0.000	0.000	70.363
120	n-C11	156.31	5.74	0.000	0.000	70.363
121	n-C11	156.31	5.74	0.000	0.000	70.363
122	n-C11	156.31	5.74	0.000	0.000	70.363
123	n-C12	170.34	6.23	0.000	0.000	26.671
124	n-C12	170.34	6.23	0.000	0.000	26.671
125	n-C12	170.34	6.23	0.000	0.000	26.671
126	n-C12	170.34	6.23	0.000	0.000	26.671
127	n-C11	156.31	5.74	0.000	0.000	70.363
128	n-C11	156.31	5.74	0.000	0.000	70.363
129	n-C11	156.31	5.74	0.000	0.000	70.363
130	n-C11	156.31	5.74	0.000	0.000	70.363
131	n-C12	170.34	6.23	0.000	0.000	26.671
132	n-C12	170.34	6.23	0.000	0.000	26.671
133	n-C12	170.34	6.23	0.000	0.000	26.671
134	n-C12	170.34	6.23	0.000	0.000	26.671
135	n-C13	184.37	6.73	0.000	0.000	9.827
136	n-C14	198.4	7.22	0.000	0.000	3.678
137	n-C15	212.42	7.71	0.000	0.000	1.370

138	n-C16	226.45	8.2	0.000	0.000	0.508
139	n-C17	240.48	8.69	0.000	0.000	0.188
140	n-C18	254.5	9.18	0.000	0.000	0.069
141	n-C19	268.53	9.67	0.000	0.000	0.025
142	n-C20	282.56	10.1	0.000	0.000	0.011
143	n-C21	296.59	10.6	0.000	0.000	0.004
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.017
164	Pristane	268.525	9.38	0.000	0.000	0.047
165	Benzo(a)fluoranthene	252.3	6.11	4721.971	0.000	0.312
166	Benzo(b)fluorene	216.3	5.77	790.615	0.000	1.173

167	Benzo(k)fluoranthene	252.3	6.11	3953.845	0.000	0.336
168	Benzo[a]anthracene	228.3	5.52	1114.179	0.000	1.841
169	Benzo[a]pyrene	252.3	6.11	5785.774	0.000	0.286
170	Benzo[b]fluoranthene	252.3	6.11	2408.970	0.000	0.414
171	Benzo[e]pyrene	252.3	6.11	1612.027	0.000	0.489
172	Benzo[g,h,i]perylene	276.3	6.7	4665.274	0.000	0.096
173	C1-Chrysenes	242.3	6.0683	765.693	0.000	0.700
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2807.331	0.000	1.292
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	12.511
176	C2-Chrysenes	256.3	6.65	765.693	0.000	0.211
177	C2-Decalins	166.3	6.19	0.000	0.000	12.620
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2807.331	0.000	0.339
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	4.699
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1597.323	0.000	1.595
181	C3-Chrysenes	270.4	7.03	765.693	0.000	0.098
182	C3-Decalins	180.3	6.79	0.000	0.000	3.755
183	C3-Dibenzothiophenes	230.37	5.86	10.148	0.000	5.696
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2807.331	0.000	0.139
185	C3-Fluorenes	210.3	5.58	123.371	0.000	3.664
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.685
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1597.323	0.000	0.735
188	C4-Chrysenes	284.4	7.35	765.693	0.000	0.052
189	C4-Decalins	194.3	7.34	0.000	0.000	1.237
190	C4-Dibenzothiophenes	244.37	6.1	10.148	0.000	3.602
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2807.331	0.000	0.052
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.629
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1597.323	0.000	0.409
194	Chrysene	228.3	5.52	602.317	0.000	2.375
195	Dibenz(a,h)anthracene	278.4	6.7	2706.502	0.000	0.122

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	6853.386	0.000	0.082
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	84.463
198	Perylene	252.3	6.11	7893.119	0.000	0.251
199	Retene	234.3	6.35	111.122	0.000	0.810

Table B.54. Chemical compositions and chemical properties, photons absorbed, concentrations, and predicted PLC50 of the components in MASS oil at 6.25% WAF duplicate exposed to *Fundulus grandis* under artificial radiation.

	Compound	Molecular weight (g/mol)	log(K_{OW})	P_{abs} (mol photon/mol chem)	$C_{W,i}$ (µg/L)	PLC50 (µg/L)
1	C1-Naphthalenes	142.2	3.87	22.713	2.010	190.659
2	C2-Naphthalenes	156.2	4.31	34.260	0.570	69.426
3	2-Methylnaphthalene	142.2	3.72	22.713	1.840	263.425
4	1-Methylnaphthalene	142.2	3.72	22.713	1.410	263.425
5	C3-Naphthalenes	170.26	4.77	34.260	0.116	28.080
6	C2-Fluorenes	194.3	5.21	123.371	0.028	7.514
7	C1-Fluorenes	180.2	4.97	123.371	0.043	11.689
8	C1-Phenanthrenes/Anthracenes	192.3	4.26	1597.323	0.067	20.176
9	2,6-Dimethylnaphthalene	156.23	4.26	34.260	0.247	77.340
10	C4-Naphthalenes	184.3	5.18	34.260	0.030	12.562
11	Naphthalene	234.3	3.17	13.523	3.650	1720.608
12	2-Methylanthracene	192.26	4.89	1597.323	0.009	5.189
13	Toluene	92.14	2.54	0.000	48.900	31915.982
14	4/9-Methylphenanthrene	192.26	4.89	75.479	0.026	18.010
15	1,6,7-Trimethylnaphthalene	170.26	4.81	40.427	0.031	24.174
16	m-XYLENE	106.2	3.09	0.000	14.100	11243.060
17	Phenanthrene	178.2	4.35	47.595	0.075	64.017
18	Fluorene	166.2	4.02	123.371	0.078	83.532
19	o-XYLENE	106.2	3.09	0.000	9.450	11243.060
20	1-Methylphenanthrene	192.26	4.89	75.479	0.015	18.010
21	1,2,4-Trimethylbenzene	120.2	3.63	0.000	2.950	3973.969

22	3-Methylphenanthrene	192.26	4.89	75.479	0.012	18.010
23	2-Methylphenanthrene	192.26	4.89	75.479	0.011	18.010
24	Pyrene	202.3	4.93	2143.908	0.002	4.430
25	C2-Dibenzothiophenes	214.3	5.13	10.148	0.012	25.552
26	Benzene	78.11	1.99	0.000	40.900	88525.143
27	Anthracene	178.2	4.35	958.381	0.008	19.045
28	p-XYLENE	106.2	3.09	0.000	4.220	11243.060
29	Ethylbenzene	106.2	3.03	0.000	3.780	12795.125
30	1-Methyl-3-ethylbenzene	120.2	3.58	0.000	1.200	4426.133
31	C1-Dibenzothiophenes	198.3	4.71	10.148	0.014	58.458
32	Fluoranthene	202.3	4.93	1283.084	0.001	5.487
33	C3-Benzothiophene	176.3	4.69	0.550	0.030	134.811
34	C4-Benzothiophene	190.3	5.18	0.550	0.010	50.614
35	1,3,5-trimethylbenzene	120.2	3.63	0.000	0.774	3973.969
36	1-Methyl-2-ethylbenzene	120.2	3.58	0.000	0.762	4426.133
37	CYCLOHEXANE	84.16	3.18	0.000	1.370	9432.476
38	Methylcyclohexane	98.19	3.59	0.000	0.653	4548.071
39	CARBAZOLE	167.2	3.23	223.878	0.052	362.804
40	Acenaphthene	154.2	4.15	81.144	0.009	69.175
41	4-ETHYLTOLUENE	120.2	3.58	0.000	0.412	4426.133
42	4-Methyldibenzothiophene	198.28	4.71	10.148	0.005	58.452
43	Dibenzothiophene	184.3	4.17	10.148	0.015	173.974
44	1,2-Dimethyl-4-Ethylbenzene	134.2	4.13	0.000	0.121	1510.332
45	Dibenzofuran	168.2	3.71	39.135	0.020	258.877
46	C2-Benzothiophene	162.25	4.13	0.550	0.031	414.781
47	Methylcyclopentane	84.16	3.1	0.000	0.808	11207.422
48	Biphenyl	154.2	3.76	0.000	0.152	2201.529
49	1,4-dimethyl-2-ethylbenzene	134.2	4.13	0.000	0.098	1510.332
50	Propylbenzene	120.194	3.52	0.000	0.313	5036.894

51	1,3-Dimethyl-5-Ethylbenzene	134.2	4.13	0.000	0.092	1510.332
52	1-methyl-3-n-propylbenzene	134.2	4.07	0.000	0.096	1718.828
53	1,3-dimethyl-4-ethylbenzene	134.2	4.13	0.000	0.077	1510.332
54	1-ETHYL-2,3-DIMETHYLBENZENE	134.22	4.13	0.000	0.073	1510.557
55	1,2,4,5-Tetramethylbenzene	134.2	4.18	0.000	0.059	1356.040
56	1-Methyl-2-n-Propylbenzene	134.2	4.07	0.000	0.075	1718.828
57	Isopropylbenzene	120.194	3.45	0.000	0.240	5857.102
58	1-Methyldibenzothiophene	198.28	4.71	10.148	0.002	58.452
59	n-C5	72.15	2.8	0.000	0.580	18341.563
60	Hydrindene	118.2	3.47	0.000	0.167	5516.930
61	2/3-Methyldibenzothiophene	198.28	4.71	8.823	0.002	61.438
62	4-isopropyltoluene	134.22	4	0.000	0.049	1999.020
63	Cyclopentane	70.13	2.68	0.000	0.566	23089.995
64	2-METHYLPENTANE	86.18	3.21	0.000	0.146	9054.125
65	Acenaphthylene	152.2	3.94	632.500	0.001	46.742
66	sec-Butylbenzene	134.2	3.94	0.000	0.032	2274.639
67	3-Methylpentane	86.18	3.21	0.000	0.121	9054.125
68	HEPTANE	100.2	3.78	0.000	0.036	3081.681
69	C1-Benzothiophene	148.2	3.5365	0.550	0.014	1361.440
70	C1-Decalins	152.3	4.61	0.000	0.003	348.129
71	trans-Decalin	138.26	4.2	0.000	0.005	764.710
72	Benzothiophene	134.2	2.99	0.550	0.003	4003.379
73	n-C10	142.29	5.25	0.000	0.000	184.151
74	n-C10	142.29	5.25	0.000	0.000	184.151
75	n-C10	142.3	5.25	0.000	0.000	184.164
76	n-C10	142.3	5.25	0.000	0.000	184.164
77	1-Decene	140.3	5.12	0.000	0.000	240.291
78	n-C10	142.29	5.25	0.000	0.000	184.151
79	n-C10	142.29	5.25	0.000	0.000	184.151

80	n-C10	142.3	5.25	0.000	0.000	184.164
81	n-C10	142.3	5.25	0.000	0.000	184.164
82	n-C9	128.3	4.76	0.000	0.000	477.383
83	n-C9	128.3	4.76	0.000	0.000	477.383
84	n-C9	128.3	4.76	0.000	0.000	477.383
85	n-C9	128.3	4.76	0.000	0.000	477.383
86	1-Nonene	126.2	4.62	0.000	0.000	634.950
87	n-C9	128.3	4.76	0.000	0.000	477.383
88	n-C9	128.3	4.76	0.000	0.000	477.383
89	n-C9	128.3	4.76	0.000	0.000	477.383
90	n-C9	128.3	4.76	0.000	0.000	477.383
91	2,2,4-TRIMETHYLPENTANE	114.2	4.09	0.000	0.000	1800.637
92	n-C8	114.2	4.27	0.000	0.000	1221.648
93	n-Pentylbenzene	148.2	4.5	0.000	0.000	965.713
94	BENZENE, 1-METHYL-4-PROPYL-	134.22	4.07	0.000	0.000	1719.085
95	Octene-1	112.2	4.13	0.000	0.000	1622.979
96	Pentane, 2,3,3-trimethyl	114.23	4.09	0.000	0.000	1801.110
97	2,5-Dimethylhexane	114.23	4.12	0.000	0.000	1688.341
98	3-methylheptane	114.2	4.2	0.000	0.000	1420.581
99	2,3,4-trimethylpentane	114.2	4.05	0.000	0.000	1962.755
100	2-methylheptane	114.2	4.2	0.000	0.000	1420.581
101	tert-Butylbenzene	134.2	3.9	0.000	0.000	2479.434
102	n-Butylbenzene	134.2	4.01	0.000	0.000	1956.107
103	1,3-Dimethyl-2-Ethylbenzene	134.22	4.13	0.000	0.000	1510.557
104	n-C6	86.18	3.29	0.000	0.000	7620.202
105	1,1,3-trimethylpentane	114.23	4.12	0.000	0.000	1688.341
106	1,2-Diethylbenzene	134.2	4.07	0.000	0.000	1718.828
107	2,3-dimethylhexane	114.2	4.12	0.000	0.000	1687.898
108	Benzene, 1-methyl-2-(1-methylethyl)-	134.22	4	0.000	0.000	1999.020

109	m-cymene	134.2	4	0.000	0.000	1998.723
110	2,4-dimethylpentane	100.2	3.63	0.000	0.000	4257.824
111	2-methylhexane	100.2	3.71	0.000	0.000	3583.503
112	3-ethylhexane	114.2	4.2	0.000	0.000	1420.581
113	3-methylhexane	100.2	3.71	0.000	0.000	3583.503
114	2,2-dimethylpentane	100.2	3.67	0.000	0.000	3906.139
115	2,3-dimethylpentane	100.2	3.63	0.000	0.000	4257.824
116	Isopentane	72.15	2.72	0.000	0.000	21792.966
117	2,3-dimethylbutane	86.18	3.14	0.000	0.000	10528.500
118	cis-Decalin	138.26	4.2	0.000	0.000	764.710
119	n-C11	156.31	5.74	0.000	0.000	70.363
120	n-C11	156.31	5.74	0.000	0.000	70.363
121	n-C11	156.31	5.74	0.000	0.000	70.363
122	n-C11	156.31	5.74	0.000	0.000	70.363
123	n-C12	170.34	6.23	0.000	0.000	26.671
124	n-C12	170.34	6.23	0.000	0.000	26.671
125	n-C12	170.34	6.23	0.000	0.000	26.671
126	n-C12	170.34	6.23	0.000	0.000	26.671
127	n-C11	156.31	5.74	0.000	0.000	70.363
128	n-C11	156.31	5.74	0.000	0.000	70.363
129	n-C11	156.31	5.74	0.000	0.000	70.363
130	n-C11	156.31	5.74	0.000	0.000	70.363
131	n-C12	170.34	6.23	0.000	0.000	26.671
132	n-C12	170.34	6.23	0.000	0.000	26.671
133	n-C12	170.34	6.23	0.000	0.000	26.671
134	n-C12	170.34	6.23	0.000	0.000	26.671
135	n-C13	184.37	6.73	0.000	0.000	9.827
136	n-C14	198.4	7.22	0.000	0.000	3.678
137	n-C15	212.42	7.71	0.000	0.000	1.370

138	n-C16	226.45	8.2	0.000	0.000	0.508
139	n-C17	240.48	8.69	0.000	0.000	0.188
140	n-C18	254.5	9.18	0.000	0.000	0.069
141	n-C19	268.53	9.67	0.000	0.000	0.025
142	n-C20	282.56	10.1	0.000	0.000	0.011
143	n-C21	296.59	10.6	0.000	0.000	0.004
144	n-C22	310.61	11.1	0.000	0.000	0.001
145	n-C23	324.64	11.6	0.000	0.000	0.000
146	n-C24	338.67	12.1	0.000	0.000	0.000
147	n-C25	352.69	12.6	0.000	0.000	0.000
148	n-C26	366.72	13.1	0.000	0.000	0.000
149	n-C27	380.75	13.6	0.000	0.000	0.000
150	n-C28	394.77	14	0.000	0.000	0.000
151	n-C29	408.8	14.5	0.000	0.000	0.000
152	n-C30	422.83	15	0.000	0.000	0.000
153	n-C31	436.86	15.5	0.000	0.000	0.000
154	n-C32	450.88	16	0.000	0.000	0.000
155	n-C33	464.91	16.5	0.000	0.000	0.000
156	n-C34	478.94	17	0.000	0.000	0.000
157	n-C35	492.96	17.5	0.000	0.000	0.000
158	n-C36	506.981	18	0.000	0.000	0.000
159	n-C37	521	18.5	0.000	0.000	0.000
160	n-C38	535	19	0.000	0.000	0.000
161	n-C39	549.1	19.49	0.000	0.000	0.000
162	n-C40	563.1	19.9	0.000	0.000	0.000
163	Phytane	282.56	9.87	0.000	0.000	0.017
164	Pristane	268.525	9.38	0.000	0.000	0.047
165	Benzo(a)fluoranthene	252.3	6.11	4721.971	0.000	0.312
166	Benzo(b)fluorene	216.3	5.77	790.615	0.000	1.173

167	Benzo(k)fluoranthene	252.3	6.11	3953.845	0.000	0.336
168	Benzo[a]anthracene	228.3	5.52	1114.179	0.000	1.841
169	Benzo[a]pyrene	252.3	6.11	5785.774	0.000	0.286
170	Benzo[b]fluoranthene	252.3	6.11	2408.970	0.000	0.414
171	Benzo[e]pyrene	252.3	6.11	1612.027	0.000	0.489
172	Benzo[g,h,i]perylene	276.3	6.7	4665.274	0.000	0.096
173	C1-Chrysenes	242.3	6.0683	765.693	0.000	0.700
174	C1-Fluoranthenes/Pyrene	216.3	5.4803	2807.331	0.000	1.292
175	C1-naphthobenzothiophenes	248.3	6.38	0.000	0.000	12.511
176	C2-Chrysenes	256.3	6.65	765.693	0.000	0.211
177	C2-Decalins	166.3	6.19	0.000	0.000	12.620
178	C2-Fluoranthenes/Pyrene	230.3	6.13	2807.331	0.000	0.339
179	C2-naphthobenzothiophenes	262.4	6.86	0.000	0.000	4.699
180	C2-Phenanthrenes/Anthracenes	206.3	5.47	1597.323	0.000	1.595
181	C3-Chrysenes	270.4	7.03	765.693	0.000	0.098
182	C3-Decalins	180.3	6.79	0.000	0.000	3.755
183	C3-Dibenzothiophenes	230.37	5.86	10.148	0.000	5.696
184	C3-Fluoranthenes/Pyrene	244.34	6.57	2807.331	0.000	0.139
185	C3-Fluorenes	210.3	5.58	123.371	0.000	3.664
186	C3-naphthobenzothiophenes	276.4	7.36	0.000	0.000	1.685
187	C3-Phenanthrenes/Anthracenes	220.3	5.86	1597.323	0.000	0.735
188	C4-Chrysenes	284.4	7.35	765.693	0.000	0.052
189	C4-Decalins	194.3	7.34	0.000	0.000	1.237
190	C4-Dibenzothiophenes	244.37	6.1	10.148	0.000	3.602
191	C4-Fluoranthenes/Pyrenes	258.34	7.05	2807.331	0.000	0.052
192	C4-naphthobenzothiophenes	290.4	7.84	0.000	0.000	0.629
193	C4-Phenanthrenes/Anthracenes	234.3	6.16	1597.323	0.000	0.409
194	Chrysene	228.3	5.52	602.317	0.000	2.375
195	Dibenz(a,h)anthracene	278.4	6.7	2706.502	0.000	0.122

196	Indeno[1,2,3-cd]pyrene	276.3	6.7	6853.386	0.000	0.082
197	Naphthobenzothiophenes	178.2	5.34	0.000	0.000	84.463
198	Perylene	252.3	6.11	7893.119	0.000	0.251
199	Retene	234.3	6.35	111.122	0.000	0.810

Table 4-2. Hourly irradiance intensity of solar radiation exposed to *Americamysis bahia* in the computational example.

B.8 Hourly Natural Sunlight and Simulated Solar Radiation Intensities

Table B.55. Hourly natural radiation intensities exposed to *Americamysis bahia*.

Time (h)	I_{UVB} (μW/cm^2)	I_{UVA} (μW/cm^2)	I_{VIS} (μW/cm^2)
1	0.45	11.32	90.7
2	7.27	169.5	996
3	43.52	679	8480
4	82.16	1028	11930
5	160	1776	20680
6	217.4	2129	21330
7	286.6	2564	25390
8	310.2	2649	26920
9	313.4	2684	27290
10	278.7	2462	25560
11	211.9	2022	22090
12	156	1715	19950
13	88.5	1142	14690
14	37.97	573.2	7474
15	8.96	198.6	1251
16	0.54	17.53	144.2

Table B.56. Hourly artificial radiation intensities exposed to *Americamysis bahia*.

Time (h)	I_{UVB} (μW/cm^2)	I_{UVA} (μW/cm^2)	I_{VIS} (μW/cm^2)
1	6.620	18.060	8.697
2	6.620	18.060	8.697
3	11.524	30.876	15.147
4	11.524	30.876	15.147
5	23.377	62.885	30.858
6	23.377	62.885	30.858
7	23.377	62.885	30.858
8	23.377	62.885	30.858
9	12.397	33.766	16.545
10	12.397	33.766	16.545
11	6.515	18.533	8.980
12	6.515	18.533	8.980

Table B.57. Hourly natural radiation intensities exposed to *Menidia beryllina.*

Time (h)	I_{UVB} (μW/cm^2)	I_{UVA} (μW/cm^2)	I_{VIS} (μW/cm^2)
1	0.37	6.313	40.1
2	6.06	144.9	1186
3	41.07	642	8262
4	88	863	10320
5	194	2005	20620
6	208.3	2021	21630
7	258	2358	23920
8	271.1	2494	25820
9	153	1400	11720
10	106.4	949	8570
11	99	957	8600
12	50.22	564.8	5620
13	19.59	283.4	2253
14	4.54	121.32	1541
15	0.22	0.323	1634.8

Table B.58. Hourly artificial radiation intensities exposed to *Menidia beryllina*.

Time (h)	I_{UVB} (μW/cm^2)	I_{UVA} (μW/cm^2)	I_{VIS} (μW/cm^2)
1	94.49	817	3610
2	88.25	858	3700
3	196	1538	6990
4	177.5	1520	7340
5	266.2	2421	11220
6	266.2	2421	11220
7	261.7	2483	11440
8	261.7	2483	11440
9	164.3	1552	6760
10	159.1	1530	6740
11	86.74	840	3680
12	81.54	845	3600
13	91.8	860.5	3620
14	89.08	869.01	3600
15	168.3	1528	6760
16	161.3	1544	6840
17	260.7	2467	10930
18	260.7	2467	10930
19	260.3	2464	11030
20	260.3	2464	11030
21	153.2	1529	6560
22	154.2	1503	6550
23	89.38	831	3760
24	80.85	839	3680

Table B.59. Hourly artificial radiation intensities exposed to *Cyprinodon variegatus*.

Time (h)	I_{UVB} (μW/cm^2)	I_{UVA} (μW/cm^2)	I_{VIS} (μW/cm^2)
1	68.44	828.2	4160
2	79.01	808.4	3960
3	147.5	1479	7680
4	140.8	1476	8170
5	220.1	2371	11400
6	220.1	2371	11400
7	218.3	2360	11050
8	218.3	2360	11050
9	143.2	1491	6380
10	141.9	1492	6820
11	81.23	801.9	3670
12	76.01	812	3960
13	77.41	833	4740
14	84.66	834.1	4350
15	154.6	1469	7330
16	148.8	1531	7890
17	225	2411	11510
18	225	2411	11510
19	231.7	2386	11180
20	231.7	2386	11180
21	150.3	1525.4	6980
22	148.3	1539.3	7080
23	92.2	812	4360
24	78.7	822.3	4120

Table B.60. Hourly artificial radiation intensities exposed to *Fundulus grandis.*

Time (h)	I_{UVB} (μW/cm^2)	I_{UVA} (μW/cm^2)	I_{VIS} (μW/cm^2)
1	81.35	819	3710
2	85.15	751	3840
3	150.2	1501	7220
4	142.4	1449	6950
5	233.2	2319	10930
6	233.2	2319	10930
7	228.5	2316	11940
8	228.5	2316	11940
9	135.7	1423.6	7070
10	136.3	1433	7480
11	72.13	824.8	3750
12	73.06	811.9	3910
13	82.74	833.5	3780
14	75.5	648	3470
15	172.6	1504.6	6750
16	157.2	1558	6590
17	243.3	2362	10520
18	243.3	2362	10520
19	235.3	2305	11440
20	235.3	2305	11440
21	151.2	1496	7020
22	150.9	1524.3	7480
23	80.56	843.5	3790
24	83.9	838.1	4240

B.9 Computational Examples for Predicating Narcotic Toxicity and Phototoxicity of Petroleum

Americamysis bahia exposure to undiluted WAF solution of MASS oil is considered as a case in point for oil phototoxicity prediction. For 100% WAF solution of the MASS oil, the observed narcotic toxicity, NLC50 = 93.3 (%WAF) and PLC50 = 20.60 (%WAF) under natural solar radiation at the reported hourly UVB, UVA, and VIS intensities for 16 (h) light exposure (Table B.55). For the given concentration of the MASS oil WAF solution (Table B.7), NTU_i and PTU_i are calculated for all constituents identified in the WAF solution. For example, concentration of methylnaphthalene in the MASS oil at 100% WAF is reportedly $C_{w,i}$ = 47.1 (µg/L). Using Equation 4-1 and CTLBB provided in Table B.1, $NLC50_i$ = 620.85 (µg/L) for *Americamysis bahia.* Considering the sunlight exposure conditions provided in Table B.55 Equation 4-3 yields P_{abs} = 22.74 (mol photon/mol PAH) resulting in $PLC50_i$ = 85.21 (µg/L) (Equation 4-2). For step by step procedures for $NLC50_i$ and $PLC50_i$ calculations see Appendix A.3. Utilizing Equations 4-5 and 4-6, the respective NTU_i and PTU_i are calculated as 0.08 and 0.55. Likewise, NTU_is and PTU_is are calculated for all 199 compounds detected in the WAF solution for the subsequent computation of total narcotic and phototoxic TUs of the MASS oil using Equations 4-7 and 4-8 which are respectively quantified as NTU_{WAF} = 1.33 and PTU_{WAF} = 4.51.

Note that NTU_{NLC50}= 1 and PTU_{PLC50}= 1. The following proportion exists between concentration of WAF solution and the corresponding TU:

Toxic unit	**Concentration (%WAF)**
TU_{LC50} =1	LC50
TU_{WAF}	C_{exp} (%WAF)

Note that TU = 1 at LC50 (%WAF) and C_{exp} (%WAF) is the concentration of the WAF solution that produces TU_{WAF}. To proceed with predicting toxicity of undiluted MASS oil WAF solution (C_{exp} = 100 %WAF) to *Americamysis bahia* , in the absence of light in terms of %WAF, NLC50 (%WAF), NTU_{WAF} is substituted in Equation 4-12 as follow

$$\text{NLC50 (\%WAF)} = \frac{100}{NTU_{WAF}} = \frac{100}{1.33} = 75.19 \qquad \text{(B-3)}$$

Similarly, PTU_{WAF} is substituted in Equation 4-13 to predict PLC50 (%WAF)

$$\text{PLC50 (\%WAF)} = \frac{100}{PTU_{WAF}} \frac{100}{4.51} = 21.98 \qquad \text{(B-4)}$$

The compositions for the MASS oil are provided at the dilution factors of DF = 1/4 (C_{exp} = 25 %WAF) and DF= 1/16 (C_{exp} = 6.25 %WAF) as well (Tables B.9 through B.11). NTU_{WAF} and PTU_{WAF} for diluted solutions are plugged in Equations 4-12 and 4-13 to calculate the corresponding NLC50 and PLC50s. The predicted narcotic toxicity and phototoxicity of MASS oil is average of the calculated NLC50s and PLC50s for the three dilutions of 1, 1/4, and 1/16.

Appendix C

GLOSSARY

ANI	average number of *A. salina* nauplii immobilized per sample
$\bar{A}$	average number of quanta absorbed
c	speed of light
C	concentration of the sensitizer placed in solution with organism (the nauplii)
C_{L}	concentration of the chemical in the lipid fraction of the organism
C_{W}	aqueous concentration of the chemical
C_{LP}	concentration of photons absorbed in organism target lipid
C_{LRTS}	concentration of RTS in the lipid fraction
C^*_{LRTS}	narcotic critical target lipid body burden
C^*_{LN}	RTS critical target lipid body burden
$C^*_{\mathrm{PAH,W}}$	PAH aqueous concentration that causes 50% mortality
D_{L}	lethal damage
ED50	tissue concentration at which 50% mortality occurs
h	Planck's constant
I	incident light intensity
I_o	incident light intensity
J	absorption of light
k	a rate constant for accrual of damage
K_{LW}	lipid- water partition coefficient
K_{OW}	octanol-water partition coefficient
l	path length of organism (the nauplii)
LC50	median lethal concentration

LT50	median lethal time
M	percent mortality
N_A	Avogadro number
N_c	number of leaves in the control at time
NLC50	narcotic median lethal concentration
NLT50	narcotic median time
N_t	number of leaves in the sample treated with a given PAH
NTU	narcotic toxic unit
P_{abs}	number of photons absorbed by the PAH
PLC50	phototoxic median lethal concentration
PLT50	phototoxic median lethal time
PMF	photomodification factor
PSF	photosensitization factor
PTU	phototoxic unit
[PAH]i	the whole-body concentration of PAHi
R^*	ratio of critical body burdens
RLC50	phototoxic reactive species LC50
RMSE	root mean square error
R_o	concentration of chemical in tissue
RPA	relative potency activity
t	time
T_{exp}	time of exposure to the light
tp PAH_{eq}	total phototoxic PAH equivalents
TU	toxic unit
TUN	toxic unit for the narcotic-related toxicity
TUP	total phototoxic toxic unit
TUR	toxic unit for the RTS-related toxicity

T_λ	optical transmittance of the organism
A	the fraction of available sensitizer absorbed by organism (the nauplii)
Δc	chemical class correction
ε	molar absorption coefficient
λ	wavelength
ϕ	potency
Φ_{RTS}	quantum yield of RTS formation