Response to EPA's Hazard Characterization of the Gasoline Blending Streams Category
The American Petroleum Institute Petroleum HPV Testing Group
June 17, 2013

The following comments are in response to EPA's Hazard Characterization (HC) for the Gasoline Blending Streams Category (U.S. EPA, 2011). This Category was sponsored by the American Petroleum Institute (API) Petroleum HPV Testing Group (Testing Group) as part of EPA's HPV Chemical Challenge Program (www.petroleumhpv.org).

Below is EPA's generic table of content for all the HPV Hazard Characterizations (HCs) they have prepared, including Gasoline Blending Streams. The Testing Group's comments are found on the page numbers indicated below.

Summary

1. The EPA hazard characterization for several Petroleum HPV Categories including Gasoline Blending Streams, refers to the category members as complex mixtures when in fact they are Class 2 UVCB substances. (HC pages 5, 8, 10, 31 and Table 1)

Substances on the US TSCA Inventory are divided into two classes for ease of identification (EPA 1995). Class 1 substances are those single compounds composed of molecules with particular atoms arranged in a definite, known structure. However, many commercial substances that are subject to TSCA are not Class 1 substances, because they have unknown or variable compositions or are composed of a complex combination of different molecules. These are designated Class 2 substances. Class 2 includes substances that have no definite molecular formula representation and either partial structural diagrams or no structural diagrams. These are the "UVCB" substances (Unknown or Variable compositions, Complex reaction products and Biological materials). An example of this kind of substance is given below.

CAS Number: 64741-42-0
CAS Name: Naphtha (petroleum), full-range straight-run
CAS Definition: A complex combination of hydrocarbons produced by distillation of crude oil. It consists of hydrocarbons having carbon numbers predominantly in the range of C4 through C11 and boiling in the range of approximately minus 20°C to 220°C (-4°F to 428°F).

Petroleum substances are subject to nomenclature rules developed jointly by the U.S. EPA and the American Petroleum Institute (EPA, 1995b) In that guidance document, EPA adopts the definitions of petroleum process stream terms provided in API's published reference document Petroleum Stream Terms Included in the Chemical Substance Inventory under TSCA (1983, reprinted in 1985). The Stream Terms definitions include the CAS definition and registry number, the source of the substance and process (i.e., last refining step), short name, indication of carbon number, and indication of distillation range (or other appropriate characteristic). Therefore all members of the Gasoline Blending Streams Category are UVCB substances, not mixtures, under EPA's nomenclature guidance.

Skin Irritation

EPA comments that "aromatic naphthas are irritating to rabbit eyes." (Summary, p. 7) This statement is based upon data for Naphtha (petroleum), catalytic reformed (CAS 68955-35-1; paraffins 32.1%, olefins 0.5%, naphthenes 3.7%, aromatics 63.3%), which EPA has characterized (p. 73) as "moderately irritating to rabbit eyes" However, the test scores in this study for conjunctivitis and chemosis are insufficient to classify the results as irritating. No evidence of effects to the cornea or iris were observed at any time. Neither the conjunctivae score of 1.33 nor the chemosis score of 1.83 for the 24, 48, and 72 hours observations are sufficient for classification for eye irritation (i.e., GHS criteria of $\geq$ 2.0 for either score; OSHA minimum criteria of 2.5 and 2.0 for conjunctival redness and chemosis, respectively, or a 24-hour Draize score of > 25/110). Since the threshold for classification for eye irritation was not met, the appropriate interpretation would be that aromatic naphthas are not irritating to rabbit eyes.

Carcinogenicity

EPA cites the results of a chronic inhalation study with wholly-vaporized gasoline (PS-6) in rats as positive, causing increases incidence of renal carcinomas, sarcomas and adenomas in males. (HC page 76) But EPA does not point out that several years ago EPA found that these kidney lesions were species and sex specific and not relevant to humans (EPA, 1991). Furthermore, real-world inhalation exposure to gasoline is weighted towards the more volatile constituents making it markedly different from the wholly-vaporized material.

More recent studies on chronic exposure to gasoline vapor in rats have been reported (Benson et al., 2011). The abstract states, "The studies were conducted to compare the toxicity and potential carcinogenicity of evaporative emissions from unleaded gasoline (GVC) and gasoline containing the oxygenate methyl tertiary-butyl ether (MTBE; GMVC). The test materials were manufactured to mimic vapors people would be exposed to during refueling at gas stations. Fifty F344 rats per gender per exposure level per test article were exposed 6 h/d, 5 d/wk for 104 wk in whole body chambers. Target total vapor concentrations were 0, 2, 10, or 20 g/m3 for the control, low-, mid-, and high-level exposures, respectively. Endpoints included survival, body weights, clinical observations, organs weights, and histopathology. GVC and GMVC exerted no marked effects on survival or clinical observations and few effects on organ weights. Terminal body weights were reduced in all mid- and high-level GVC groups and high-level GMVC groups. The major proliferative lesions attributable to gasoline exposure with or without MTBE were renal tubule adenomas and carcinomas in male rats. GMV exposure led to elevated testicular mesothelioma incidence and an increased trend for thyroid carcinomas in males. GVMC inhalation caused an increased trend for testicular tumors with exposure concentration. Mid- and high-level exposures of GVC and GMVC led to elevated incidences of nasal respiratory epithelial degeneration. Overall, in these chronic studies conducted under identical conditions, the health effects in F344 rats following 2-yr of GVC or GMVC exposure were comparable in the production of renal adenomas and carcinomas in male rats and similar in other endpoints." The male rat kidney lesions in this study were identical to those previously discounted by EPA as not relevant to humans. (See above.)

Neurotoxicity

EPA points out the lack of neurological effects found in most animal studies done by inhalation exposure and the Testing Group agrees with that assessment. The one animal study EPA considered "positive" for neurotoxicity was a 13-week study on Naphtha (petroleum), light catalytic reformed (LCRN), conducted at doses up to 27.8 mg/l. (HC page 78) However, the increased motor activity was only observed at the high-dose and was not accompanied by changes in functional operational battery tests or neuropathology. For perspective, the Globally Harmonized System for Hazard Classification and Labelling of Chemicals (United Nations, 2011) requires target organ labeling for repeat-dose effects only when they occur at vapor concentrations below 1 mg/l. The high dose in the LCRN study (27.8 mg/l) represents 75% of the lower-explosive-limit, a concentration well above most human exposures, and far above accepted cut-offs for hazard classification.

EPA suggests that the neurotoxicity of gasoline is well-established in humans and that information on the human neurotoxicity of gasoline may be found in the ATSDR Toxicological Profile for Automotive Gasoline. (HC page 78) However, that ATSDR document says, "The majority of the data on the neurological effects of gasoline have come from case reports describing patients, usually adolescents, who were chronic gasoline sniffers (Owens et al.

1985). In most instances, the exposure concentrations could not be determined and the lead content in the gasoline was not specified." Case studies from the era of leaded gasoline cannot be considered relevant to current day exposures. The Testing Group agrees that chronic gasoline sniffing is harmful to several target organs including the nervous system, but EPA's HC significantly overstates the neurotoxic hazard of gasoline and gasoline blending streams. EPA should acknowledge that the evidence of neurological effects is based on observations of substance abuse (an intentional misuse), not with exposures associated with anticipated occupational and consumer uses.

4. Hazard to the Environment

The Testing Group disagrees with the approach that EPA used to evaluate the ecotoxicity hazards of the Gasoline Blending Streams Category. The endpoint values cited by EPA for read across to all category members were calculated based on measured concentrations of selected hydrocarbons used to verify the presence of hydrocarbons in the water accommodated fractions (WAFs). The Testing Group maintains that aquatic toxicity endpoints are more accurately expressed as 'loading rates'. Loading rates are a reflection of the composition and chemistry of the substance and implicitly accounts for dissolution and volatilization of individual hydrocarbon constituents. Loading rates are a more effective means of comparing two substances to each other because the composition of WAFs varies with composition of the test substance.

Below is a summary of the EPA findings (HC page 7).

EPA states, "Based on the category member CASRN 64741-66-8, the 96-h LC50 for fish is 0.31 mg/L (lowest value) and the 48-h EC50 value to aquatic invertebrates is 0.56 mg/L (lowest value). Based on the category member CASRN 64741-46-4, the 96-h EC50 for algae is 0.26 mg/L (lowest value) for biomass. Based on the category member CASRN 64741-66-8, the lowest values for the chronic 21-d EC50 are 1.9 mg/L (based on survival), and 0.14 mg/L (based on reproduction), and the lowest 21-d chronic NOEC values are 0.23 mg/L (based on survival), and 0.03 mg/L (based on reproduction)."

In Section 4, Hazard to the Environment, EPA cites the following tests and endpoints in their HC, all calculated based on measured concentrations of selected hydrocarbons (HC pages 127-134).

Acute Toxicity to Fish (fathead minnow: *Pimephales promelas*)	
Paraffinic Naphthas	
Naphtha (petroleum), light alkylate (CASRN 64741-66-8)	96-h LC50 = 0.305 mg/L
Naphtha (petroleum), light alkylate (CASRN 64741-66-8)	14-d LC50 = 0.15 mg/L
Olefinic Naphthas	
Naphtha (petroleum), light catalytic cracked (CASRN 64741-55-5)	96-h LC50 = 4.1 mg/L
Naphtha (petroleum), light catalytic cracked (CASRN 64741-55-5)	14-d LC50 = 1.5 mg/L
Naphthenic Naphthas	
Naphtha (petroleum), light straight-run (CASRN 64741-46-4)	96-h LC50 = 0.689 mg/L
Aromatic Naphthas	
Naphtha (petroleum), light catalytic reformed (CASRN 64741-63-5)	96-h LC50 = 11 mg/L
Naphtha (petroleum), light catalytic reformed (CASRN 64741-63-5)	14-d LC50 = 0.67 mg/L

Acute Toxicity to Aquatic Invertebrates (Cladoceran: *Daphnia magna*)
Paraffinic Naphthas Naphtha (petroleum), light alkylate (CASRN 64741-66-8) 48-h LC50 = 0.556 mg/L
Olefinic Naphthas Naphtha (petroleum), light catalytic cracked (CASRN 64741-55-5) 48-h LC50 = 1.4 mg/L
Naphthenic Naphthas Naphtha (petroleum), light straight-run (CASRN 64741-46-4) 48-h LC50 = 0.65 mg/L
Aromatic Naphthas Naphtha (petroleum), light catalytic reformed (CASRN 64741-63-5) 48-h LC50 = 2.6 mg/L
Toxicity to Aquatic Plants (Alga: *Pseudokirchneriella subcapitata*)
Paraffinic Naphthas Naphtha (petroleum), light alkylate (CASRN 64741-66-8) 96-h LC50 = 0.741 mg/L
Olefinic Naphthas Naphtha (petroleum), light catalytic cracked (CASRN 64741-55-5) 96-h LC50 = 4.6 mg/L
Naphthenic Naphthas Naphtha (petroleum), light straight-run (CASRN 64741-46-4) 96-h LC50 = 0.26 mg/L
Aromatic Naphthas Naphtha (petroleum), light catalytic reformed (CASRN 64741-63-5) 96-h LC50 =1.76 mg/L
Chronic Toxicity to Aquatic Invertebrates (Cladoceran: *Daphnia magna*)
Paraffinic Naphthas Naphtha (petroleum), light alkylate (CASRN 64741-66-8) 21-d EC50 (survival) = >0.46 mg/L 21-d NOEC (survival) = 0.23 mg/L 21-d EC50 (reproduction) = 0.14 mg/L 21-d NOEC (reproduction) = 0.032 mg/L
Olefinic Naphthas Naphtha (petroleum), light catalytic cracked (CASRN 64741-55-5) 21-d EC50 (survival) =1.9 mg/L 21-d NOEC (survival) = 0.68 mg/L 21-d EC50 (reproduction) = 0.55 mg/L 21-d NOEC (reproduction) = 0.11 mg/L
Aromatic Naphthas Naphtha (petroleum), light catalytic reformed (CASRN 64741-63-5) 21-d EC50 (survival) = 7.5 mg/L 21-d NOEC (survival) = 3.8 mg/L 21-d EC50 (reproduction) = 3.2 mg/L 21-d NOEC (reproduction) = <0.069 mg/L

As stated earlier, the endpoint values cited by EPA for read across to all category members were calculated based on measured concentrations of selected hydrocarbons used to verify the presence of hydrocarbons in the water accommodated fractions (WAFs). The Testing Group maintains that when toxicity endpoints are more accurately expressed as 'loading rates', the products in the Gasoline Blending Streams Category are expected to exhibit aquatic toxicity in the range from 1 to 200 mg/L for the three trophic levels. Loading is a reflection of the composition and chemistry of the substance and implicitly accounts for dissolution and volatilization of individual hydrocarbon constituents. Loading is a more effective means of

comparing two substances to each other because the composition of WAFs varies with composition of the test substance.

Gasoline Blending Streams show a relatively narrow range of aquatic toxicity because the constituent chemicals of those products are neutral organic hydrocarbons whose toxic mode of action is non-polar narcosis. Hydrocarbons are equitoxic in tissues where the toxic mechanism of short-term toxicity for these chemicals is disruption of biological membrane function (van Wezel and Opperhuizen, 1995). The differences between toxicities (i.e., LC/LL5O, EC/EL50) can be explained by the differences between the target tissue-partitioning behavior of the individual chemicals Verbruggen et al., 2000). The existing fish toxicity database for hydrophobic neutral chemicals supports a critical body residue (CBR, the internal concentration that causes mortality) of between approximately 2-8 mmol/kg fish (wet weight) (McGrath and Di Toro, 2009). When normalized to lipid content the CBR is approximately 50 µmol/g of lipid for most organisms (Di Toro et al., 2000).

Petroleum UVCB substances with a range of carbon numbers and water solubility as those in this category are expected to exhibit lower toxicity compared to the most toxic constituent alone. This occurs because the aqueous concentration of the constituent is a function of the partitioning of the constituents between the bulk hydrocarbon and water. Within the carbon number range of products in this category, a C9 hydrocarbon alone would be expected to exhibit the greatest toxicity based on the relationship of Kow with aquatic toxicity. However, products in this category are not composed of a single chemical and because two different products with a similar carbon number range can contain varying proportions of those carbon numbers, it is possible that different toxicities are expressed for the same organism. Thus, two products representing low or high carbon number ranges in this category can show different toxicities.

The Testing Group believes it is inappropriate for EPA to use these concentration values when they represent only an undetermined fraction of the dissolved hydrocarbons in the test solutions. Therefore, these 'toxic' concentrations represent lower acute toxicity values than what would have been calculated based on a complete analysis of the dissolved hydrocarbon composition. Additionally, the specific compounds of interest were different depending on the test substance, so the compounds measured in the light alkylate naphtha WAF differ from those measured in the light catalytic cracked naphtha WAF, as was true for each test substance. The following example In Table 1 shows the analyses of hydrocarbon constituents in the light straight-run naphtha (CASRN 64741-46-4) and the components selected for concentration determination of the WAFs. This illustrates how the endpoints of the toxicity tests based on measured data are artificially low.

Table 1. List of hydrocarbon constituents in CASRN 64741-46-4.

Compound	Weight % in Test Substance
butane	5.6
n-pentane	16.3
n-heptane	2.0
n-hexane	6.3
n-octane	0.8
n-nonane	0.1
isopentane	22.5
2,3 dimethyl butane	1.1
2 methyl pentane	7.0
3 methyl pentane	3.7
2,3 dimethyl pentane	0.8
2 methyl hexane	0.8
3 methyl hexane	1.4
2 methyl heptane	1.0
3 methyl heptane	0.5
4 methyl heptane	0.2
cyclopentane	1.7
methyl cyclopentane	4.6
dimethyl cyclopentane isomers	4.1
ethyl cyclopentane	0.5
trimethylcyclopentane isomers	2.4
methyl ethyl cyclopentane (3 isomers)	0.8
cyclohexane	1.7
methyl cyclohexane	2.5
dimethylcyclohexane isomers	1.6
trimethylcyclohexane isomers	0.9
benzene	0.8
toluene	1.1
m-xylene	0.3
p-xylene	0.1
o-xylene	0.2
ethylbenzene	0.3

The yellow highlighted compounds were those measured in the WAFs.

Sum of individual measurements (yellow highlight) **does not** reflect the concentration of all possible hydrocarbons dissolved in the WAFs.

Many of the most abundant constituents in the straight run naphtha shown in the example were not included in the analysis of the WAFs (e.g., n-pentane, iso-pentane, and others). These would be expected to contribute to the total dissolved hydrocarbons in the WAF because many have significant water solubilities and exist in significant proportions in the naphtha stream. Consequently the measured hydrocarbons cited in these studies do not represent the total hydrocarbon components to which the organisms were exposed, and the toxicological endpoints calculated on the basis of those measurements are artificially low.

The more appropriate and realistic evaluation of petroleum mixture aquatic toxicity is determined using composition of the petroleum product and QSAR based models, such as Petrotox (Redman et al. 2012). Toxicity QSARs may be used to provide LL50 estimates for

hydrocarbons or blocks where acute toxicity data are not available, since these are well established for hydrocarbons (details are included in the EU Technical Guidance Document (TGD) which recommends procedures for risk assessment). Furthermore, the use of QSAR allows for extrapolation of lethal loading (LL50) values to hydrocarbons or blocks that are beyond the solubility 'cut-off' and have no measured LC50 value. This provides a conservative approach for assessing the partial contribution of hydrocarbons or blocks that are individually not expected to exert toxicity.

The Petrotox spreadsheet model predicts the aquatic toxicity of complex petroleum substances from petroleum substance composition. Substance composition is characterized by specifying mass fractions in constituent hydrocarbon blocks (HBs), based on available analytical information. The HBs are defined by their mass fractions within a defined carbon number range or boiling point interval. Physicochemical properties of the HBs are approximated by assigning representative hydrocarbons from a database of individual hydrocarbons with associated physicochemical properties. A three-phase fate model is used to simulate the distribution of each structure among the water-, air-, and oil-phase liquid in the laboratory test system. Toxicity is then computed based on the predicted aqueous concentrations and aquatic toxicity of each structure and the target lipid model. The toxicity of the complex substance is computed assuming additivity of the contribution of the individual assigned hydrocarbons. This is valid since small non-polar hydrocarbons are equitoxic in tissues (van Wezel and Opperhuizen, 1995).

There are two situations when it may be necessary to estimate the toxicity of a petroleum-substance viz., to validate test results and to predict toxicity when data are lacking. This approach requires that the chemical composition of the petroleum substance should be known. In this procedure, the dissolved concentrations of individual hydrocarbons from a petroleum substance are estimated for a given loading rate and then normalized by their acute toxicity to yield Toxic Units (TU) which can be summed to predict the toxicity of the parent material (see below). As previously described, the quantity of any particular component of a petroleum substance detected in the water phase is related to the loading rate. Theoretically, using closed test systems brought to equilibrium, simple equilibrium partitioning and mass balance calculations may be used to estimate the concentration of each hydrocarbon constituent in water. The hydrocarbon/water partition coefficient (Kp) for each of the components is an essential part of the calculation. The details of this calculation approach have been published (Peterson 1994).

Further simplification is obtained by combining the concentration calculations for isomers of particular hydrocarbon species (e.g. iso-hexanes), since all of the isomers have essentially the same values of log Kow and Kp. This procedure is the equivalent of the "hydrocarbon block method" used in the risk assessment of petroleum substances (CONCAWE 1996; Hermens et al. 1985). Experimental Kp values simply related to Kow (Peterson 1994; Cline et al. 1991), for individual hydrocarbons are available in the published literature. In order to calculate the joint toxic action of a mixture of hydrocarbons dissolved in water, the concentrations cannot be added directly. Since each component will have a different toxicity, the concentration of each component must be scaled to its toxicity. This is done by division of the concentration by the toxicity (by the LL50 in the case of acute toxicity). The resulting values express the concentrations in equivalent "toxic units."

Thus, the sum of TUs for the components of a mixture will equal one at the LL50 of the mixture. Considerable experimental support for this conceptual framework has been developed, which

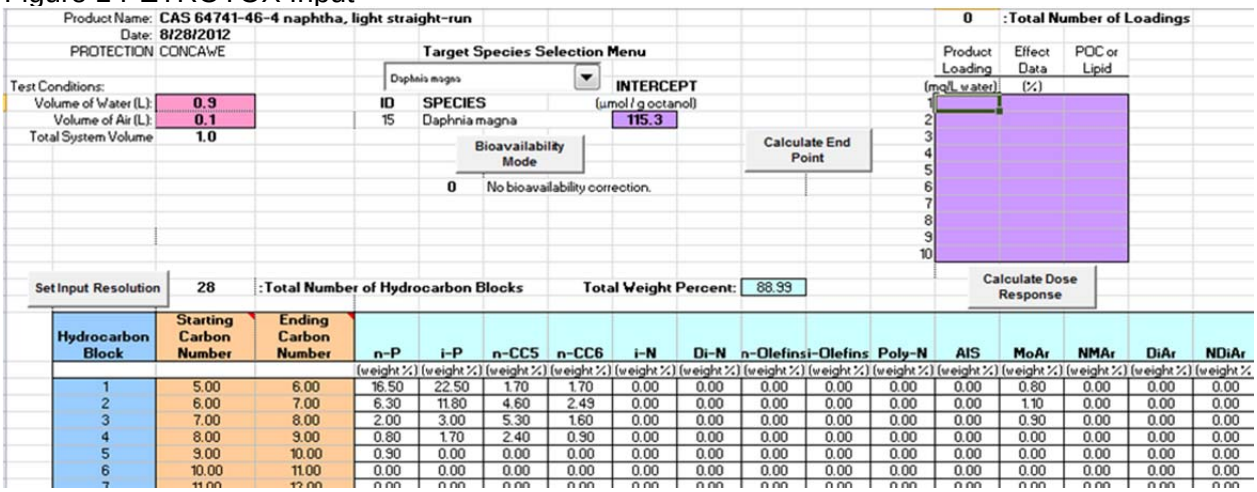
confirms that mixtures of substances exerting toxicity via a common mechanism, are additive and further, that hydrocarbons act through a common mechanism of non-polar narcosis (Hermens et al. 1985; Deneer et al. 1988).

Given the compositional analysis (together with consideration of the variability of composition of the particular petroleum substance), acute toxicity can be calculated. This toxicity calculation is conservative in that it assumes that each component is maximally dissolved (completely equilibrated with un-dissolved phase) and that there are no losses from solution (due to adsorption to surfaces, absorption to test organisms or volatilization, etc.). While the model is built on these assumptions, variability in test methods and laboratory procedures will result in discrepancies between empirical and modeled endpoints. For gasoline blending streams, tests were conducted in sealed test vessels with zero headspace. In practice, WAF preparations cannot totally meet the expectations of the model. Thus, headspace above the vortex in the WAF preparation vessel and the method of distribution of the WAFs to the test vessels would allow some volatile loss.

Using the composition for CAS 64741-46-4 reported above, daphnid toxicity was calculated and results are shown below. The calculated lethal loading of 15 mg/L is similar to the actual LL50 determined for this stream as reported in the Testing Group's robust summary. However, the total dissolved concentration of hydrocarbons in the water phase (Figure 2) is approximately 5.08 mg/L, based on partitioning behavior and test conditions, which is significantly higher concentration than the 0.65 mg/L reported by EPA. See Appendix A for additional Petrotox analyses which compares predicted dissolved hydrocarbon concentration corresponding to the empirical EL/LL 50 values. Finally, EC50/LC50 values will not remain constant for untested streams identified by the same CAS number unless the new stream compositions are identical to those already evaluated. Since the composition of these petroleum streams may vary due to crude oil source and specific site refinery processes even for the same CAS number, it is unlikely that the hydrocarbon constituent's concentration will remain constant for process streams.

In summary, the rationale presented in the above response supports the Testing Group's position that when toxicity endpoints are presented on the basis of loading rates, the products in the Gasoline Blending Streams Category are expected to exhibit acute aquatic toxicity in the range from 1 to 200 mg/L for the three trophic levels. Loading is a reflection of the composition and chemistry of the substance and is the more accurate manner in which to present the aquatic toxicity of petroleum substances.

Figure 1 PETROTOX Input



Product Name: CAS 64741-46-4 naphtha, light straight-run
Date: 8/28/2012
PROTECTION CONCAWE

Test Conditions:
Volume of Water (L): 0.9
Volume of Air (L): 0.1
Total System Volume 1.0

Target Species Selection Menu
Daphnia magna
ID 15 SPECIES Daphnia magna
INTERCEPT (umol / g octanol) 115.3

Bioavailability Mode
0 No bioavailability correction.

Calculate End Point

0 :Total Number of Loadings

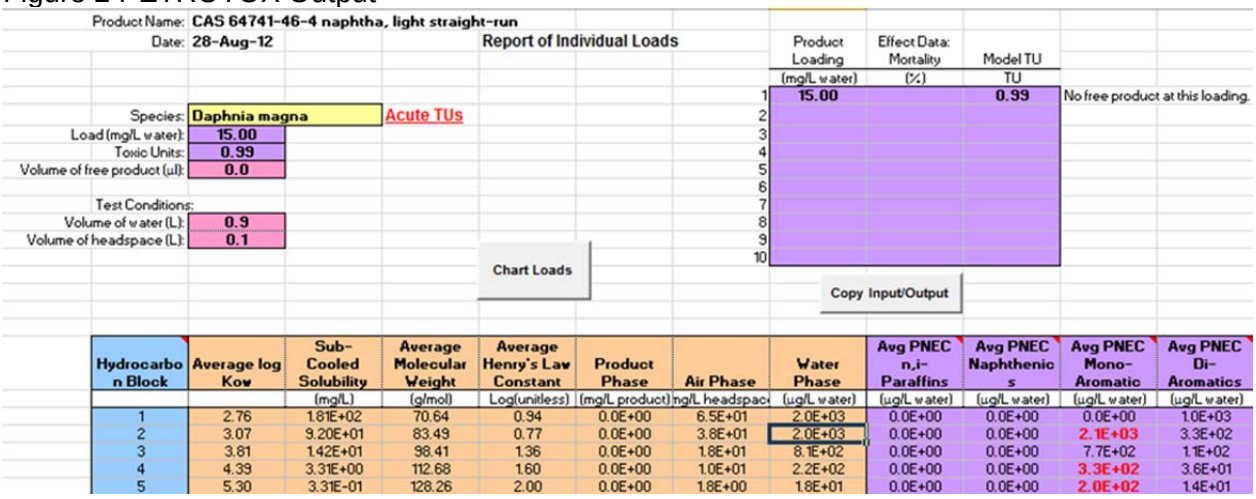
	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

Set Input Resolution 28 :Total Number of Hydrocarbon Blocks Total Weight Percent: 88.99

Calculate Dose Response

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P	i-P	n-CC5	n-CC6	i-N	Di-N	n-Olefins	i-Olefins	Poly-N	AIS	MoAr	NMAr	DiAr	NDiAr
			(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %
1	5.00	6.00	16.50	22.50	1.70	1.70	0.00	0.00	0.00	0.00	0.00	0.00	0.80	0.00	0.00	0.00
2	6.00	7.00	6.30	11.80	4.60	2.49	0.00	0.00	0.00	0.00	0.00	0.00	1.10	0.00	0.00	0.00
3	7.00	8.00	2.00	3.00	5.30	1.60	0.00	0.00	0.00	0.00	0.00	0.00	0.90	0.00	0.00	0.00
4	8.00	9.00	0.80	1.70	2.40	0.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure 2 PETROTOX Output



Product Name: CAS 64741-46-4 naphtha, light straight-run
Date: 28-Aug-12

Report of Individual Loads

Species: Daphnia magna Acute TUs
Load (mg/L water): 15.00
Toxic Units: 0.99
Volume of free product (ul): 0.0

Test Conditions:
Volume of water (L): 0.9
Volume of headspace (L): 0.1

Chart Loads

Copy Input/Output

	Product Loading (mg/L water)	Effect Data: Mortality (%)	Model TU TU	
1	15.00		0.99	No free product at this loading.
2				
3				
4				
5				
6				
7				
8				
9				
10				

Hydrocarbon Block	Average log Kow	Sub-Cooled Solubility	Average Molecular Weight	Average Henry's Law Constant	Product Phase	Air Phase	Water Phase	Avg PNEC n,i-Paraffins	Avg PNEC Naphthenics	Avg PNEC Mono-Aromatic	Avg PNEC Di-Aromatics
		(mg/L)	(g/mol)	Log(unitless)	(mg/L product)	ng/L headspac	(ug/L water)	(ug/L water)	(ug/L water)	(ug/L water)	(ug/L water)
1	2.76	1.81E+02	70.64	0.94	0.0E+00	6.5E+01	2.0E+03	0.0E+00	0.0E+00	0.0E+00	1.0E+03
2	3.07	9.20E+01	83.49	0.77	0.0E+00	3.8E+01	2.0E+03	0.0E+00	0.0E+00	2.1E+03	3.3E+02
3	3.81	1.42E+01	98.41	1.36	0.0E+00	1.8E+01	8.1E+02	0.0E+00	0.0E+00	7.7E+02	1.1E+02
4	4.39	3.31E+00	112.68	1.60	0.0E+00	1.0E+01	2.2E+02	0.0E+00	0.0E+00	3.3E+02	3.6E+01
5	5.30	3.31E-01	128.26	2.00	0.0E+00	1.8E+00	1.8E+01	0.0E+00	0.0E+00	2.0E+02	1.4E+01

Also in Section 4, Hazard to the Environment, EPA cites studies employing dilutions of water soluble fractions. (HC pages 128, 120). EPA cites the following two studies (one fish and one invertebrate) that used dilutions of a water soluble fraction as exposure solutions.
Solvent naphtha (petroleum), light arom. (CASRN 64742-95-6) 96-h LC50 = 1.03 mg/L
Solvent naphtha (petroleum), light arom. (CASRN 64742-95-6) 48-h EC50 = 1.2 mg/L

Results for petroleum UVCBs (multi-constituent, poorly soluble hydrocarbons) are expressed as lethal loadings (LL) rather than lethal concentrations (LC). Additionally, an inherent limitation of the dilution method is that the concentration of dissolved hydrocarbons in each successive dilution cannot be related back to a known amount of petroleum substance required to produce the observed effect. This is because the amount and composition of hydrocarbons in the dissolved phase is dependent upon the composition of the petroleum substance, temperature, and principally on the ratio of the volume of water to oil that comes in contact (Shiu et al. 1990). These factors led to the concept of 'loading rate' that is used to describe the total amount of petroleum product per unit volume of water used to prepare the WAFs. Loading rates provide a unifying concept for expressing the results of a toxicity test with poorly-soluble substances (European Eco-Labeling Criteria; ASTM 2009; GESAMP; OECD 2006; ECHA). Preparation of independent WAFs based on test substance loading rates is the appropriate procedure for substances in this category because they are petroleum UVCBs (multi-constituent hydrocarbons) whose constituent hydrocarbons vary in water solubility. The dissolution thermodynamics of a multi-constituent hydrocarbon in an aqueous medium limit the likelihood of consistent proportional concentrations of the constituent hydrocarbons at various test substance loading rates. For this reason,

- exposure solutions are not prepared from dilutions of a stock solution (the relative proportion of hydrocarbon constituents in the dilutions would not accurately reflect the relative concentration of those constituent chemicals in individually prepared, successively lower exposure solutions of the test material);
- separate exposure solutions are prepared at each exposure loading for products that are multi- constituent hydrocarbons; and

When compared on the basis of standard test methods and exposure solution preparation procedures, these gasoline blending streams are expected to produce a similar range of toxicity for the three trophic level species. Results expressed as measured concentrations of the fraction of the substance in solution are of little value since it will be virtually impossible to extrapolate to spill situations where the only relevant measures of concentration will be the amount of product spilled and the volume of the receiving environment (i.e., the loading rates).

References used in this response to EPA's HC of the Gasoline Blending Stream Category

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Appendix A
Estimation of Dissolved Hydrocarbon Concentration Corresponding to Petrotox EL/LL50 Output

The measured hydrocarbon concentrations used in the calculation of EC/LC50 endpoints cited in the EPA hazard characterization was shown to be an incomplete analysis of the potential dissolved hydrocarbon concentration. In spite of this, an estimate of those endpoints can be made using the available data for these streams. The table below provides the Petrotox modeled endpoints based on detailed hydrocarbon analyses of each CAS number, the water-phase hydrocarbon concentration corresponding to the effective or lethal loading rate (EL/LL50) from the Petrotox model, and the empirical data from the toxicity tests cited in the robust summaries.

Appendix Table A1. Petrotox Summary – Gasoline Naphthas Model Results and Empirical Data.

	Acute EL/LL50, mg/L		
	Algae	Daphnia	Fish
(P) Light Alkylate Naphtha (64741-66-8) Petrotox EL/LL50 Total HC	 2.13 0.34	 5.06 0.80	 5.36 0.85
Empirical, EL/LL50 EC/LC50	45 0.74	32 0.56	8.2 0.31
(O) Light Catalytic Cracked Naphtha (64741-55-5) Petrotox EL/LL50 Total HC	 3.44 1.63	 8.15 3.85	 8.71 4.08
Empirical, EL/LL50 EC/LC50	64 4.6	18 1.4	46 4.1
(N) Light Straight Run Naphtha (64741-46-6) Petrotox EL/LL50 Total HC	 6.36 2.14	 15 5.08	 16 5.40
Empirical, EL/LL50 EC/LC50	6.4 0.26	18 0.65	15 0.689
(A) Light Catalytic Reformed Naphtha (64741-63-5) Perotox EL/LL50 Total HC	 8.35 4.28	 19.79 10.14	 20.97 10.74
Empirical, EL/LL50 EC/LC50	8.5 1.7	10 2.6	34 11

Petrotox EL/LL50 = Petrotox output estimated toxicity endpoints for loading rates.
Total HC = Sum of Petrotox estimated water-phase hydrocarbon concentrations based on hydrocarbon block partitioning and solubility input.
Empirical EL/LL50 = endpoints provided by test data and summarized in the robust summary file of gasoline blending stream naphthas.
EC/LC50 = EPA-cited endpoints based on hydrocarbon analyses of WAF solutions used in testing.

One observation in the above table is that the modeled endpoints are more conservative than the empirical data (example: LAN (CAS 64741-66-8) modeled algal EL50 = 2.13 mg/L vs empirical EL50 = 45 mg/L). As discussed in the HC response, the Petrotox model may generate conservative endpoints since Petrotox assumes ideal behavior of the individual hydrocarbons in the WAFs with respect to partitioning and no losses of volatile components to the headspace during WAF preparation.

A second observation is that the dissolved hydrocarbon concentration corresponding to the Petrotox EL/LL50 values are generally higher than the empirical EC/LC50 endpoints. This is reasonable since it was shown that those values are based on analysis of several constituent compounds rather than all the dissolved components. By using the Petrotox EL/LL50 values:Total HC ratios, an estimate of the EC/LC50 values can be calculated. These ratios tend to be nearly constant across the different species, but unique for each naphtha stream. For the different PONA streams, the ratios of model EL/LL50:total HC are 6.3 (CAS# 64741-66-8), 2.1 (CAS# 64741-55-5), 3.0 (CAS# 64741-46-6), and 2.0 (CAS# 64741-63-5), respectively.

By dividing that ratio into the empirical EL/LL50 values, the revised EC/LC50 endpoints can be obtained. The resulting quotient reflects the adjusted dissolved hydrocarbon concentration corresponding to the EL/LL50 values. For the light alkylate naphtha stream (CAS# 64741-66-8) the revised endpoints for the three trophic level species are as follows:

Algae EC50: 45/6.3 = 7.1 mg/L
Daphnia EC50: 32/6.3 = 5.1 mg/L
Fish LC50: 8.2/6.3 = 1.3 mg/L

In each case, concentrations estimated in this manner are higher than the empirical data. This calculation represents the endpoint values if the full complement of dissolved hydrocarbons in the WAF had been quantified. For this exercise to be valid it is assumed that the empirical endpoints were derived using valid exposure solutions preparations and testing methods (i.e., WAFs prepared in a manner to prevent loss of hydrocarbons and testing in closed vessels with zero or minimal headspace). These conditions appeared to be met in the naphtha tests. Additionally, the Petrotox-derived ratio of modeled EL/LL50 to dissolved hydrocarbon should be a valid representation of dissolution dynamics since the model is based on known physico-chemical properties assigned to the respective blocks.

Figure A1. Light Alkylate Naphtha (64741-66-8) Input modeled for S. capricornutum.

Product Name: **CAS #64741-66-8, light alkylate naphtha**
Date: **8/30/2012**
PROTECTION CONCAWE

0 **:Total Number of Loadings**

Target Species Selection Menu

Test Conditions:
Volume of Water (L): **0.9**
Volume of Air (L): **0.1**
Total System Volume (L): **1.0**

ID	**SPECIES**	**INTERCEPT** (µmol / g octanol)
40	Selenastrum capricornutum	**48.6**

0 No bioavailability correction.

	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

27 **:Total Number of Hydrocarbon Blocks** **Total Weight Percent:** 98.60

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P	i-P	n-CC5	n-CC6	i-N	Di-N	n-Olefins	i-Olefins	Poly-N	AIS	MoAr	NMAr	DiAr	NDiAr	PolyAr	ArS
			(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)
1	5.00	6.00	0.23	12.62	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6.00	7.00	0.00	7.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	7.00	8.00	0.00	7.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	8.00	9.00	0.00	57.58	0.00	0.00	9.44	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.00	2.70	0.00	0.00	1.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.04	0.40	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	12.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	13.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	14.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	15.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	16.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	17.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	18.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure A2. Light Alkylate Naphtha (64741-66-8) Output modeled for S. capricornutum.

Product Name: **CAS #64741-66-8, light alkylate naphtha**
Date: **30-Aug-12**

LL50/NOEL and PNEC Report

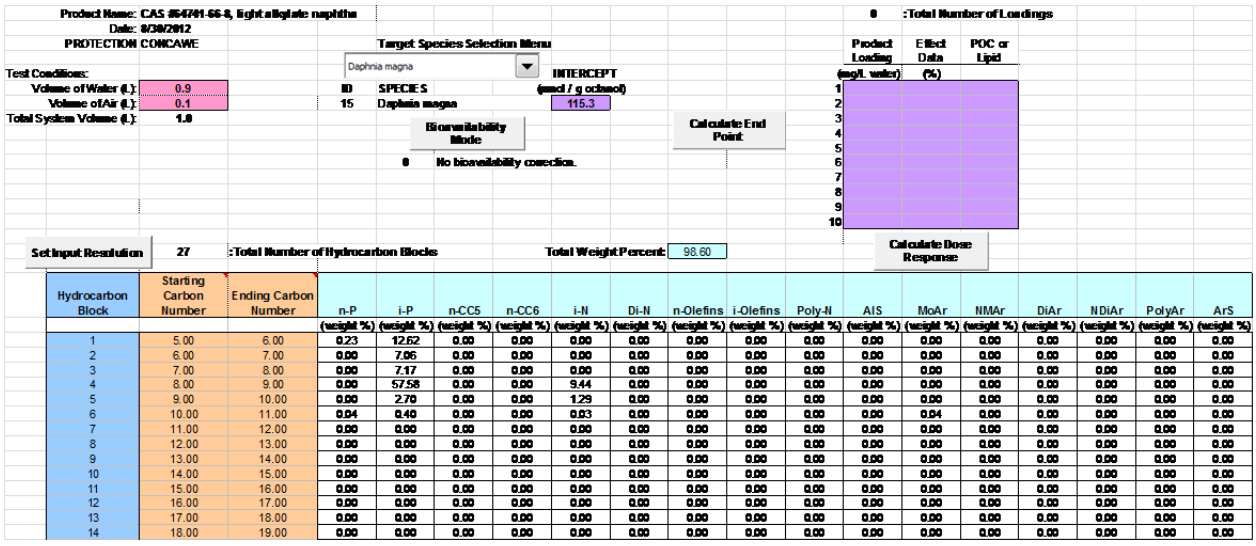
	Load (mg/L water)	**TU** Acute TUs
LL50:	2.13	1.00

Species: **Selenastrum capricornutum** **Acute TUs**
Model LL50 (mg/L water) **2.13** No free product at this loading.
Total Toxic Units: **1.00**

Test Conditions:
Volume of water (L): **0.9**
Volume of headspace (L): **0.1**
Volume of free product **0.0**

Hydrocarbon Block	Average log Kow	Average Sub-Cooled Solubility	Average Molecular Weight	Average Henry's Law Constant	Product Phase	Air Phase	Water Phase	Avg PNEC n,i-Paraffins	Avg PNEC Naphthenics	Avg PNEC Mono-Aromatic	Avg PNEC Di-Aromatics	Avg PNEC Poly-Aromatics
		(mg/L)	(g/mol)	Log(unitless)	(mg/L product)	mg/L headspace	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)
1	3.09	6.79E+01	72.15	1.56	0.0E+00	2.7E+00	7.1E+01	1.2E+02	1.0E+03	0.0E+00	0.0E+00	0.0E+00
2	3.66	1.69E+01	86.18	1.84	0.0E+00	1.7E+00	2.5E+01	4.2E+01	3.3E+02	2.1E+03	0.0E+00	0.0E+00
3	4.21	4.43E+00	100.20	2.09	0.0E+00	1.9E+00	1.5E+01	2.0E+01	1.1E+02	7.7E+02	0.0E+00	0.0E+00
4	4.59	1.94E+00	113.56	1.80	0.0E+00	1.6E+01	2.1E+02	4.0E+00	3.6E+01	3.3E+02	0.0E+00	0.0E+00
5	5.19	4.32E-01	127.85	2.09	0.0E+00	9.7E-01	1.3E+01	2.4E+00	1.4E+01	2.0E+02	0.0E+00	0.0E+00
6	4.97	1.05E+00	138.54	1.06	0.0E+00	1.3E-01	1.6E+00	7.2E-01	3.9E+00	6.9E+01	1.1E+02	0.0E+00
7	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	5.4E-01	1.3E+00	3.0E+01	4.6E+01	0.0E+00
8	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	5.7E-01	9.9E-01	1.4E+01	2.3E+01	6.3E+01
9	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	6.7E-01	1.0E+00	6.7E+00	1.0E+01	2.9E+01
10	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	7.2E-01	1.1E+00	2.6E+00	5.4E+00	1.1E+01

Figure A3. Light Alkylate Naphtha (64741-66-8) Input modeled for D. magna.



Product Name: CAS #64741-66-8, light alkylate naphtha
Date: 8/30/2012
PROTECTION CONCAWE

Test Conditions:
Volume of Water (L): 0.9
Volume of Air (L): 0.1
Total System Volume (L): 1.0

Target Species Selection Menu: Daphnia magna
ID 15 SPECIES Daphnia magna
INTERCEPT (umol / g octanol) 115.3

Bioavailability Mode
0 No bioavailability correction.

Calculate End Point

0 :Total Number of Loadings

	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

Set Input Resolution 27 :Total Number of Hydrocarbon Blocks Total Weight Percent: 98.60

Calculate Dose Response

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P	i-P	n-CC5	n-CC6	i-N	Di-N	n-Olefins	i-Olefins	Poly-N	AIS	MoAr	NMAr	DiAr	NDiAr	PolyAr	ArS
			(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)
1	5.00	6.00	0.23	12.62	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6.00	7.00	0.00	7.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	7.00	8.00	0.00	7.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	8.00	9.00	0.00	57.58	0.00	0.00	9.44	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.00	2.70	0.00	0.00	1.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.04	0.40	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	12.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	13.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	14.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	15.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	16.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	17.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	18.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure A4. Light Alkylate Naphtha (64741-66-8) Output modeled for D. magna.

Product Name: CAS #64741-66-8, light alkylate naphtha
Date: 30-Aug-12

LL50/NOEL and PNEC Report

	Load (mg/L water)	TU Acute TUs
LL50:	5.06	1.00

Species: Daphnia magna
Acute TUs
Model LL50 (mg/L water): 5.06
No free product at this loading.
Total Toxic Units: 1.00

Test Conditions:
Volume of water (L): 0.9
Volume of headspace (L): 0.1
Volume of free product: 0.0

Hydrocarbon Block	Average log Kow	Average Sub-Cooled Solubility	Average Molecular Weight	Average Henry's Law Constant	Product Phase	Air Phase	Water Phase	Avg PNEC n,i-Paraffins	Avg PNEC Naphthenics	Avg PNEC Mono-Aromatic	Avg PNEC Di-Aromatics	Avg PNEC Poly-Aromatics
		(mg/L)	(g/mol)	Log(unitless)	(mg/L product)	mg/L headspace	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)
1	3.09	6.79E+01	72.15	1.56	0.0E+00	6.5E+00	1.7E+02	1.2E+02	1.0E+03	0.0E+00	0.0E+00	0.0E+00
2	3.66	1.69E+01	86.18	1.84	0.0E+00	4.0E+00	5.9E+01	4.2E+01	3.3E+02	2.1E+03	0.0E+00	0.0E+00
3	4.21	4.43E+00	100.20	2.09	0.0E+00	4.4E+00	3.6E+01	2.0E+01	1.1E+02	7.7E+02	0.0E+00	0.0E+00
4	4.59	1.94E+00	113.56	1.80	0.0E+00	3.9E+01	5.0E+02	4.0E+00	3.6E+01	3.3E+02	0.0E+00	0.0E+00
5	5.19	4.32E-01	127.85	2.09	0.0E+00	2.3E+00	3.2E+01	2.4E+00	1.4E+01	2.0E+02	0.0E+00	0.0E+00
6	4.97	1.05E+00	138.54	1.06	0.0E+00	3.0E-01	3.7E+00	7.2E-01	3.9E+00	6.9E+01	1.1E+02	0.0E+00
7	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	5.4E-01	1.3E+00	3.0E+01	4.6E+01	0.0E+00
8	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	5.7E-01	9.9E-01	1.4E+01	2.3E+01	6.3E+01
9	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	6.7E-01	1.0E+00	6.7E+00	1.0E+01	2.9E+01
10	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	7.2E-01	1.1E+00	2.6E+00	5.4E+00	1.1E+01
11	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	6.9E-01	1.1E+00	1.2E+00	2.4E+00	5.0E+00
12	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.0E+00	1.2E+00	1.0E+00	1.0E+00	2.2E+00
13	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.1E+00	1.4E+00	1.0E+00	7.2E-01	1.0E+00
14	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.1E+00	1.7E+00	1.0E+00	6.5E-01	8.3E-01

Figure A5. Light Alkylate Naphtha (64741-66-8) Input modeled for P. promelas.

Product Name: **CAS 64741-66-8; light alkylate naphtha (LAN)**
Date: **9/14/2012**
PROTECTION CONCAWE

Target Species Selection Menu

ID	SPECIES	INTERCEPT (μmol / g octanol)
34	Pimephales promelas	122.2

0 No bioavailability correction.

Test Conditions:
Volume of Water (L): 0.9
Volume of Air (L): 0.1
Total System Volume (L): 1.0

0 :Total Number of Loadings

	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

27 :Total Number of Hydrocarbon Blocks

Total Weight Percent: 98.60

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P	i-P	n-CC5	n-CC6	i-N	Di-N	n-Olefins	i-Olefins	Poly-N	AIS	MoAr	NMAr	DiAr	NDiAr	PolyAr	ArS
			(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)
1	5.00	6.00	0.23	12.62	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6.00	7.00	0.00	7.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	7.00	8.00	0.00	7.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	8.00	9.00	0.00	57.58	0.00	0.00	9.44	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.00	2.70	0.00	0.00	1.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.04	0.40	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	12.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	13.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	14.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	15.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	16.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	17.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	18.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure A6. Light Alkylate Naphtha (64741-66-8) Output modeled for P. promelas.

Product Name: **CAS 64741-66-8; light alkylate naphtha (LAN)**
Date: **14-Sep-12**

LL50/NOEL and PNEC Report

Species: **Pimephales promelas** **Acute TUs**
Model LL50 (mg/L water): **5.36** No free product at this loading.
Total Toxic Units: **1.00**

	(mg/L water)	Acute TUs
LL50:	5.36	1.00

Test Conditions:
Volume of water (L): 0.9
Volume of headspace (L): 0.1
Volume of free product: 0.0

Hydrocarbon Block	Average log Kow	Average Sub-Cooled Solubility	Average Molecular Weight	Average Henry's Law Constant	Product Phase	Air Phase	Water Phase	Avg PNEC n,i-Paraffins	Avg PNEC Naphthenics	Avg PNEC Mono-Aromatic	Avg PNEC Di-Aromatics	Avg PNEC Poly-Aromatics
		(mg/L)	(g/mol)	Log(unitless)	(mg/L product)	mg/L headspace	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)
1	3.09	6.79E+01	72.15	1.56	0.0E+00	6.9E+00	1.8E+02	1.2E+02	1.0E+03	0.0E+00	0.0E+00	0.0E+00
2	3.66	1.69E+01	86.18	1.84	0.0E+00	4.3E+00	6.2E+01	4.2E+01	3.3E+02	2.1E+03	0.0E+00	0.0E+00
3	4.21	4.43E+00	100.20	2.09	0.0E+00	4.7E+00	3.9E+01	2.0E+01	1.1E+02	7.7E+02	0.0E+00	0.0E+00
4	4.59	1.94E+00	113.56	1.80	0.0E+00	4.1E+01	5.3E+02	4.0E+00	3.6E+01	3.3E+02	0.0E+00	0.0E+00
5	5.19	4.32E-01	127.85	2.09	0.0E+00	2.4E+00	3.4E+01	2.4E+00	1.4E+01	2.0E+02	0.0E+00	0.0E+00
6	4.97	1.05E+00	138.54	1.06	0.0E+00	3.2E-01	3.9E+00	7.2E-01	3.9E+00	6.9E+01	1.1E+02	0.0E+00
7	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	5.4E-01	1.3E+00	3.0E+01	4.6E+01	0.0E+00
8	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	5.7E-01	9.9E-01	1.4E+01	2.3E+01	6.3E+01
9	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	6.7E-01	1.0E+00	6.7E+00	1.0E+01	2.9E+01
10	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	7.2E-01	1.1E+00	2.6E+00	5.4E+00	1.1E+01
11	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	6.9E-01	1.1E+00	1.2E+00	2.4E+00	5.0E+00
12	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.0E+00	1.2E+00	1.0E+00	1.0E+00	2.2E+00
13	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.1E+00	1.4E+00	1.0E+00	7.2E-01	1.0E+00
14	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.1E+00	1.7E+00	1.0E+00	6.5E-01	8.3E-01

Figure A7. Light Catalytic Cracked Naphtha (64741-55-5) Input modeled for S. capricornutum.

Product Name: **CAS 64741-55-5; light catalytic cracked naphtha (LCCN)**
Date: **8/30/2012**
PROTECTION CONCAWE

Target Species Selection Menu

ID	SPECIES	INTERCEPT (μmol / g octanol)
40	Selenastrum capricornutum	48.6

0 No bioavailability correction.

Test Conditions:
Volume of Water (L): **0.9**
Volume of Air (L): **0.1**
Total System Volume (L): **1.0**

0 :Total Number of Loadings

	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

27 :Total Number of Hydrocarbon Blocks — Total Weight Percent: 96.73

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P	i-P	n-CC5	n-CC6	i-N	Di-N	n-Olefins	i-Olefins	Poly-N	AlS	MoAr	NMAr	DiAr	NDiAr	PolyAr	ArS
			(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)
1	5.00	6.00	1.69	4.70	0.50	0.00	0.00	0.00	15.65	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6.00	7.00	1.71	6.71	0.00	2.16	0.00	0.00	15.27	0.00	0.00	0.00	1.48	0.00	0.00	0.00	0.00	0.00
3	7.00	8.00	0.66	5.10	0.00	3.39	0.00	0.00	7.67	0.00	0.00	0.00	6.73	0.00	0.00	0.00	0.00	0.00
4	8.00	9.00	0.56	3.57	0.00	2.62	0.00	0.00	1.64	0.00	0.00	0.00	7.69	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.15	2.26	0.00	1.21	0.00	0.00	0.00	0.00	0.00	0.00	2.57	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.00	0.40	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.61	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	12.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	13.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	14.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	15.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	16.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	17.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	18.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure A8. Light Catalytic Cracked Naphtha (64741-55-5) Output modeled for S. capricornutum.

Product Name: **CAS 64741-55-5; light catalytic cracked naphtha (LCCN)**
Date: **30-Aug-12**

LL50/NOEL and PNEC Report

Species: **Selenastrum capricornutum** Acute TUs
Model LL50 (mg/L water): **3.44** No free product at this loading.
Total Toxic Units: **1.00**

Test Conditions:
Volume of water (L): **0.9**
Volume of headspace (L): **0.1**
Volume of free product: **0.0**

	Load (mg/L water)	TU Acute TUs
LL50:	3.44	1.00

Hydrocarbon Block	Average log Kow	Average Sub-Cooled Solubility (mg/L)	Average Molecular Weight (g/mol)	Average Henry's Law Constant Log(unitless)	Product Phase (mg/L product)	Air Phase mg/L headspace	Water Phase (μg/L water)	Avg PNEC n,i-Paraffins (μg/L water)	Avg PNEC Naphthenics (μg/L water)	Avg PNEC Mono-Aromatic (μg/L water)	Avg PNEC Di-Aromatics (μg/L water)	Avg PNEC Poly-Aromatics (μg/L water)
1	2.78	1.81E+02	70.54	0.96	0.0E+00	5.6E+00	3.8E+02	1.2E+02	1.0E+03	0.0E+00	0.0E+00	0.0E+00
2	3.17	6.98E+01	83.76	0.97	0.0E+00	8.0E+00	3.7E+02	4.2E+01	3.3E+02	2.1E+03	0.0E+00	0.0E+00
3	3.85	1.28E+01	98.52	1.42	0.0E+00	3.2E+00	3.3E+02	2.0E+01	1.1E+02	7.7E+02	0.0E+00	0.0E+00
4	4.03	1.02E+01	110.82	0.95	0.0E+00	5.7E+00	4.1E+02	4.0E+00	3.6E+01	3.3E+02	0.0E+00	0.0E+00
5	4.54	2.85E+00	124.98	1.14	0.0E+00	1.5E+00	1.1E+02	2.4E+00	1.4E+01	2.0E+02	0.0E+00	0.0E+00
6	5.04	8.36E-01	138.85	1.21	0.0E+00	2.0E-01	2.2E+01	7.2E-01	3.9E+00	6.9E+01	1.1E+02	0.0E+00
7	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	5.4E-01	1.3E+00	3.0E+01	4.6E+01	0.0E+00
8	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	5.7E-01	9.9E-01	1.4E+01	2.3E+01	6.3E+01
9	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	6.7E-01	1.0E+00	6.7E+00	1.0E+01	2.9E+01
10	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	7.2E-01	1.1E+00	2.6E+00	5.4E+00	1.1E+01
11	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	6.9E-01	1.1E+00	1.2E+00	2.4E+00	5.0E+00
12	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.0E+00	1.2E+00	1.0E+00	1.0E+00	2.2E+00
13	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.1E+00	1.4E+00	1.0E+00	7.2E-01	1.0E+00
14	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.1E+00	1.7E+00	1.0E+00	6.5E-01	8.3E-01

Figure A9. Light Catalytic Cracked Naphtha (64741-55-5) Input modeled for D. magna.

Product Name: **CAS 64741-55-5; light catalytic cracked naphtha (LCCN)**
Date: **8/30/2012**
PROTECTION CONCAWE

Target Species Selection Menu

ID	SPECIES	INTERCEPT (μmol / g octanol)
15	Daphnia magna	115.3

0 No bioavailability correction.

0 :Total Number of Loadings

	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

Test Conditions:
Volume of Water (L): **0.9**
Volume of Air (L): **0.1**
Total System Volume (L): **1.0**

27 :Total Number of Hydrocarbon Blocks — Total Weight Percent: 96.73

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P	i-P	n-CC5	n-CC6	i-N	Di-N	n-Olefins	i-Olefins	Poly-N	AlS	MoAr	NMAr	DiAr	NDiAr	PolyAr	ArS
			(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)
1	5.00	6.00	1.69	4.70	0.50	0.00	0.00	0.00	15.65	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6.00	7.00	1.71	6.71	0.00	2.16	0.00	0.00	15.27	0.00	0.00	0.00	1.48	0.00	0.00	0.00	0.00	0.00
3	7.00	8.00	0.66	5.10	0.00	3.39	0.00	0.00	7.67	0.00	0.00	0.00	6.73	0.00	0.00	0.00	0.00	0.00
4	8.00	9.00	0.56	3.57	0.00	2.62	0.00	0.00	1.64	0.00	0.00	0.00	7.69	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.15	2.26	0.00	1.21	0.00	0.00	0.00	0.00	0.00	0.00	2.57	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.00	0.40	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.61	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	12.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	13.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	14.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	15.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	16.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	17.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	18.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure A10. Light Catalytic Cracked Naphtha (64741-55-5) Output modeled for D. magna.

Product Name: **CAS 64741-55-5; light catalytic cracked naphtha (LCCN)**
Date: **30-Aug-12**

LL50/NOEL and PNEC Report

Species: **Daphnia magna** — **Acute TUs**
Model LL50 (mg/L water): **8.15** — No free product at this loading.
Total Toxic Units: **1.00**

	Load (mg/L water)	TU Acute TUs
LL50:	8.15	1.00

Test Conditions:
Volume of water (L): **0.9**
Volume of headspace (L): **0.1**
Volume of free product: **0.0**

Hydrocarbon Block	Average log Kow	Average Sub-Cooled Solubility	Average Molecular Weight	Average Henry's Law Constant	Product Phase	Air Phase	Water Phase	Avg PNEC n,i-Paraffins	Avg PNEC Naphthenics	Avg PNEC Mono-Aromatic	Avg PNEC Di-Aromatics	Avg PNEC Poly-Aromatics
		(mg/L)	(g/mol)	Log(unitless)	(mg/L product)	mg/L headspace	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)
1	2.78	1.81E+02	70.54	0.96	0.0E+00	1.3E+01	9.0E+02	1.2E+02	**1.0E+03**	0.0E+00	0.0E+00	0.0E+00
2	3.17	6.98E+01	83.76	0.97	0.0E+00	1.9E+01	8.8E+02	4.2E+01	3.3E+02	**2.1E+03**	0.0E+00	0.0E+00
3	3.85	1.28E+01	98.52	1.42	0.0E+00	7.5E+00	7.7E+02	2.0E+01	1.1E+02	**7.7E+02**	0.0E+00	0.0E+00
4	4.03	1.02E+01	110.82	0.95	0.0E+00	1.4E+01	9.8E+02	4.0E+00	3.6E+01	3.3E+02	0.0E+00	0.0E+00
5	4.54	2.85E+00	124.98	1.14	0.0E+00	3.6E+00	2.5E+02	2.4E+00	1.4E+01	2.0E+02	0.0E+00	0.0E+00
6	5.04	8.36E-01	138.85	1.21	0.0E+00	4.7E-01	5.2E+01	7.2E-01	3.9E+00	**6.9E+01**	**1.1E+02**	0.0E+00
7	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**5.4E-01**	**1.3E+00**	**3.0E+01**	**4.6E+01**	**0.0E+00**
8	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**5.7E-01**	**9.9E-01**	**1.4E+01**	**2.3E+01**	**6.3E+01**
9	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**6.7E-01**	**1.0E+00**	**6.7E+00**	**1.0E+01**	**2.9E+01**
10	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**7.2E-01**	**1.1E+00**	**2.6E+00**	**5.4E+00**	**1.1E+01**
11	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**6.9E-01**	**1.1E+00**	**1.2E+00**	**2.4E+00**	**5.0E+00**
12	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.0E+00**	**1.2E+00**	**1.0E+00**	**1.0E+00**	**2.2E+00**
13	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.1E+00**	**1.4E+00**	**1.0E+00**	**7.2E-01**	**1.0E+00**
14	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.1E+00**	**1.7E+00**	**1.0E+00**	**6.5E-01**	**8.3E-01**

Figure A11. Light Catalytic Cracked Naphtha (64741-55-5) Input modeled for P. promelas.

Product Name: **CAS 64741-55-5; light catalytic cracked naphtha (LSRN)**
Date: **9/14/2012**
PROTECTION CONCAWE

Target Species Selection Menu

	ID	SPECIES	INTERCEPT (μmol / g octanol)
	34	Pimephales promelas	122.2

Test Conditions:
Volume of Water (L): **0.9**
Volume of Air (L): **0.1**
Total System Volume (L): **1.0**

0 No bioavailability correction.

0 :Total Number of Loadings

	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

27 :Total Number of Hydrocarbon Blocks

Total Weight Percent: 97.82

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P	i-P	n-CC5	n-CC6	i-N	Di-N	n-Olefins	i-Olefins	Poly-N	AlS	MoAr	NMAr	DiAr	NDiAr	PolyAr	ArS
			(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)
1	5.00	6.00	1.77	5.42	0.50	0.00	0.00	0.00	15.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6.00	7.00	1.71	6.71	0.00	2.16	0.00	0.00	15.27	0.00	0.00	0.00	1.48	0.00	0.00	0.00	0.00	0.00
3	7.00	8.00	0.66	5.10	0.00	3.39	0.00	0.00	7.67	0.00	0.00	0.00	6.73	0.00	0.00	0.00	0.00	0.00
4	8.00	9.00	0.56	3.57	0.00	2.62	0.00	0.00	1.64	0.00	0.00	0.00	7.69	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.15	2.26	0.00	1.21	0.00	0.00	0.00	0.00	0.00	0.00	2.57	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.00	0.40	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.61	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	12.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	13.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	14.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	15.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	16.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	17.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	18.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure A12. Light Catalytic Cracked Naphtha (64741-55-5) Output modeled for P. promelas.

Date: **14-Sep-12**

LL50/NOEL and PNEC Report

Species: **Pimephales promelas** **Acute TUs**
Model LL50 (mg/L water): **8.71** No free product at this loading.
Total Toxic Units: **1.00**

	(mg/L water)	Acute TUs
LL50:	8.71	1.00

Test Conditions:
Volume of water (L): **0.9**
Volume of headspace (L): **0.1**
Volume of free product: **0.0**

Hydrocarbon Block	Average log Kow	Average Sub-Cooled Solubility	Average Molecular Weight	Average Henry's Law Constant	Product Phase	Air Phase	Water Phase	Avg PNEC n,i-Paraffins	Avg PNEC Naphthenics	Avg PNEC Mono-Aromatic	Avg PNEC Di-Aromatics	Avg PNEC Poly-Aromatics
		(mg/L)	(g/mol)	Log(unitless)	(mg/L product)	mg/L headspace	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)
1	2.78	1.81E+02	70.54	0.96	0.0E+00	1.5E+01	9.8E+02	1.2E+02	**1.0E+03**	0.0E+00	0.0E+00	0.0E+00
2	3.17	6.98E+01	83.76	0.97	0.0E+00	2.0E+01	9.3E+02	4.2E+01	3.3E+02	**2.1E+03**	0.0E+00	0.0E+00
3	3.85	1.28E+01	98.52	1.42	0.0E+00	7.9E+00	8.2E+02	2.0E+01	1.1E+02	7.7E+02	0.0E+00	0.0E+00
4	4.03	1.02E+01	110.82	0.95	0.0E+00	1.4E+01	1.0E+03	4.0E+00	3.6E+01	3.3E+02	0.0E+00	0.0E+00
5	4.54	2.85E+00	124.98	1.14	0.0E+00	3.8E+00	2.7E+02	2.4E+00	1.4E+01	2.0E+02	0.0E+00	0.0E+00
6	5.04	8.36E-01	138.85	1.21	0.0E+00	5.0E-01	5.5E+01	7.2E-01	3.9E+00	**6.9E+01**	**1.1E+02**	0.0E+00
7	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**5.4E-01**	**1.3E+00**	**3.0E+01**	**4.6E+01**	**0.0E+00**
8	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**5.7E-01**	**9.9E-01**	**1.4E+01**	**2.3E+01**	**6.3E+01**
9	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**6.7E-01**	**1.0E+00**	**6.7E+00**	**1.0E+01**	**2.9E+01**
10	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**7.2E-01**	**1.1E+00**	**2.6E+00**	**5.4E+00**	**1.1E+01**
11	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**6.9E-01**	**1.1E+00**	**1.2E+00**	**2.4E+00**	**5.0E+00**
12	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.0E+00**	**1.2E+00**	**1.0E+00**	**1.0E+00**	**2.2E+00**
13	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.1E+00**	**1.4E+00**	**1.0E+00**	**7.2E-01**	**1.0E+00**
14	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.1E+00**	**1.7E+00**	**1.0E+00**	**6.5E-01**	**8.3E-01**

Figure A13. Light Straight-Run Naphtha (64741-46-4) Input modeled for S. capricornutum.

Product Name: CAS 64741-46-4; light straight-run naphtha (LSRN)
Date: 10/2/2012
PROTECTION CONCAWE

Test Conditions:
Volume of Water (L): 0.9
Volume of Air (L): 0.1
Total System Volume (L): 1.0

Target Species Selection Menu: Selenastrum capricornutum
ID 40 SPECIES Selenastrum capricornutum INTERCEPT (umol / g octanol) 48.6

Bioavailability Mode: 0 No bioavailability correction.

Calculate End Point

0 :Total Number of Loadings

	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

Set Input Resolution: 27 :Total Number of Hydrocarbon Blocks

Total Weight Percent: 88.99

Calculate Dose Response

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P	i-P	n-CC5	n-CC6	i-N	Di-N	n-Olefins	i-Olefins	Poly-N	AIS	MoAr	NMAr	DiAr	NDiAr	PolyAr	ArS
			(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)
1	5.00	6.00	16.50	22.50	1.70	1.70	0.00	0.00	0.00	0.00	0.00	0.00	0.80	0.00	0.00	0.00	0.00	0.00
2	6.00	7.00	6.30	11.80	4.60	2.49	0.00	0.00	0.00	0.00	0.00	0.00	1.10	0.00	0.00	0.00	0.00	0.00
3	7.00	8.00	2.90	3.00	5.30	1.60	0.00	0.00	0.00	0.00	0.00	0.00	0.90	0.00	0.00	0.00	0.00	0.00
4	8.00	9.00	0.80	1.70	2.40	0.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	12.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	13.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	14.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	15.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	16.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	17.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	18.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure A14. Light Straight-Run Naphtha (64741-46-4) Output modeled for S. capricornutum.

Product Name: CAS 64741-46-4; light straight-run naphtha (LSRN)
Date: 02-Oct-12

LL50/NOEL and PNEC Report

Species: Selenastrum capricornutum
Acute TUs
Model LL50 (mg/L water): 6.36
No free product at this loading.
Total Toxic Units: 1.00

	(mg/L water)	Acute TUs
LL50:	6.36	1.00

Test Conditions:
Volume of water (L): 0.9
Volume of headspace (L): 0.1
Volume of free product: 0.0

Hydrocarbon Block	Average log Kow	Average Sub-Cooled Solubility	Average Molecular Weight	Average Henry's Law Constant	Product Phase	Air Phase	Water Phase	Avg PNEC n,i-Paraffins	Avg PNEC Naphthenics	Avg PNEC Mono-Aromatic	Avg PNEC Di-Aromatics	Avg PNEC Poly-Aromatics
		(mg/L)	(g/mol)	Log(unitless)	(mg/L product)	mg/L headspace	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)
1	2.76	1.81E+02	70.64	0.94	0.0E+00	2.7E+01	8.5E+02	1.2E+02	1.0E+03	0.0E+00	0.0E+00	0.0E+00
2	3.07	9.20E+01	83.49	0.77	0.0E+00	1.6E+01	8.6E+02	4.2E+01	3.3E+02	2.1E+03	0.0E+00	0.0E+00
3	3.81	1.42E+01	98.41	1.36	0.0E+00	7.6E+00	3.4E+02	2.0E+01	1.1E+02	7.7E+02	0.0E+00	0.0E+00
4	4.39	3.31E+00	112.68	1.60	0.0E+00	4.3E+00	9.2E+01	4.0E+00	3.6E+01	3.3E+02	0.0E+00	0.0E+00
5	5.30	3.31E-01	128.26	2.00	0.0E+00	7.5E-01	7.5E+00	2.4E+00	1.4E+01	2.0E+02	0.0E+00	0.0E+00
6	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	7.2E-01	3.9E+00	6.9E+01	1.1E+02	0.0E+00
7	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	5.4E-01	1.3E+00	3.0E+01	4.6E+01	0.0E+00
8	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	5.7E-01	9.9E-01	1.4E+01	2.3E+01	6.3E+01
9	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	6.7E-01	1.0E+00	6.7E+00	1.0E+01	2.9E+01
10	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	7.2E-01	1.1E+00	2.6E+00	5.4E+00	1.1E+01
11	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	6.9E-01	1.1E+00	1.2E+00	2.4E+00	5.0E+00
12	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.0E+00	1.2E+00	1.0E+00	1.0E+00	2.2E+00
13	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.1E+00	1.4E+00	1.0E+00	7.2E-01	1.0E+00
14	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.1E+00	1.7E+00	1.0E+00	6.5E-01	8.3E-01

Figure A15. Light Straight-Run Naphtha (64741-46-4) Input modeled for D. magna.

Product Name: **CAS 64741-46-4; light straight-run naphtha (LSRN)**
Date: **10/2/2012**
PROTECTION CONCAWE

0 **:Total Number of Loadings**

Target Species Selection Menu

Test Conditions:

Volume of Water (L):	**0.9**
Volume of Air (L):	**0.1**
Total System Volume (L):	**1.0**

ID	**SPECIES**	**INTERCEPT** (µmol / g octanol)
15	Daphnia magna	**115.3**

0 No bioavailability correction.

	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

27 **:Total Number of Hydrocarbon Blocks** **Total Weight Percent:** 88.99

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P	i-P	n-CC5	n-CC6	i-N	Di-N	n-Olefins	i-Olefins	Poly-N	AIS	MoAr	NMAr	DiAr	NDiAr	PolyAr	ArS
			(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)
1	5.00	6.00	16.50	22.50	1.70	1.70	0.00	0.00	0.00	0.00	0.00	0.00	0.80	0.00	0.00	0.00	0.00	0.00
2	6.00	7.00	6.30	11.80	4.60	2.49	0.00	0.00	0.00	0.00	0.00	0.00	1.10	0.00	0.00	0.00	0.00	0.00
3	7.00	8.00	2.00	3.00	5.30	1.60	0.00	0.00	0.00	0.00	0.00	0.00	0.90	0.00	0.00	0.00	0.00	0.00
4	8.00	9.00	0.80	1.70	2.40	0.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	12.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	13.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	14.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	15.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	16.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	17.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	18.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure A16. Light Straight-Run Naphtha (64741-46-4) Output modeled for D. magna.

Product Name: **CAS 64741-46-4; light straight-run naphtha (LSRN)**
Date: **02-Oct-12**

LL50/NOEL and PNEC Report

Species: **Daphnia magna** **Acute TUs**

Model LL50 (mg/L water)	**15.08** No free product at this loading.
Total Toxic Units:	**1.00**

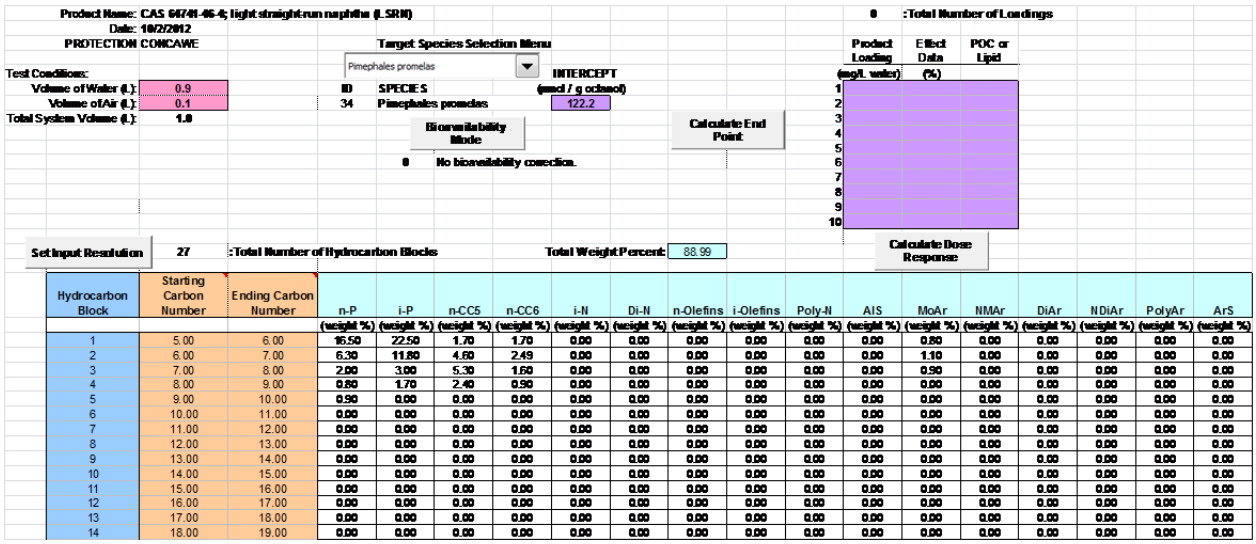
	(mg/L water)	Acute TUs
LL50:	15.08	1.00

Test Conditions:

Volume of water (L):	**0.9**
Volume of headspace (L):	**0.1**
Volume of free product	**0.0**

Hydrocarbon Block	Average log Kow	Average Sub-Cooled Solubility	Average Molecular Weight	Average Henry's Law Constant	Product Phase	Air Phase	Water Phase	Avg PNEC n,i-Paraffins	Avg PNEC Naphthenics	Avg PNEC Mono-Aromatic	Avg PNEC Di-Aromatics	Avg PNEC Poly-Aromatics
		(mg/L)	(g/mol)	Log(unitless)	(mg/L product)	mg/L headspace	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)
1	2.76	1.81E+02	70.64	0.94	0.0E+00	6.5E+01	2.0E+03	1.2E+02	1.0E+03	0.0E+00	0.0E+00	0.0E+00
2	3.07	9.20E+01	83.49	0.77	0.0E+00	3.8E+01	2.0E+03	4.2E+01	3.3E+02	**2.1E+03**	0.0E+00	0.0E+00
3	3.81	1.42E+01	98.41	1.36	0.0E+00	1.8E+01	8.1E+02	2.0E+01	1.1E+02	7.7E+02	0.0E+00	0.0E+00
4	4.39	3.31E+00	112.68	1.60	0.0E+00	1.0E+01	2.2E+02	4.0E+00	3.6E+01	**3.3E+02**	0.0E+00	0.0E+00
5	5.30	3.31E-01	128.26	2.00	0.0E+00	1.8E+00	1.8E+01	2.4E+00	1.4E+01	**2.0E+02**	0.0E+00	0.0E+00
6	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**7.2E-01**	**3.9E+00**	**6.9E+01**	**1.1E+02**	**0.0E+00**
7	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**5.4E-01**	**1.3E+00**	**3.0E+01**	**4.6E+01**	**0.0E+00**
8	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**5.7E-01**	**9.9E-01**	**1.4E+01**	**2.3E+01**	**6.3E+01**
9	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**6.7E-01**	**1.0E+00**	**6.7E+00**	**1.0E+01**	**2.9E+01**
10	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**7.2E-01**	**1.1E+00**	**2.6E+00**	**5.4E+00**	**1.1E+01**
11	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**6.9E-01**	**1.1E+00**	**1.2E+00**	**2.4E+00**	**5.0E+00**
12	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.0E+00**	**1.2E+00**	**1.0E+00**	**1.0E+00**	**2.2E+00**
13	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.1E+00**	**1.4E+00**	**1.0E+00**	**7.2E-01**	**1.0E+00**
14	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.1E+00**	**1.7E+00**	**1.0E+00**	**6.5E-01**	**8.3E-01**

Figure A17. Light Straight-Run Naphtha (64741-46-4) Input modeled for P. promelas.



Product Name: CAS 64741-46-4; light straight-run naphtha (LSRN)
Date: 10/2/2012
PROTECTION CONCAWE

Test Conditions:
Volume of Water (L): 0.9
Volume of Air (L): 0.1
Total System Volume (L): 1.0

Target Species Selection Menu: Pimephales promelas
ID 34 SPECIES Pimephales promelas
INTERCEPT (umol / g octanol) 122.2
Bioavailability Mode: 0 No bioavailability correction.
Calculate End Point

0 :Total Number of Loadings

	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

Set Input Resolution: 27 :Total Number of Hydrocarbon Blocks
Total Weight Percent: 88.99
Calculate Dose Response

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P	i-P	n-CC5	n-CC6	i-N	Di-N	n-Olefins	i-Olefins	Poly-N	AIS	MoAr	NMAr	DiAr	NDiAr	PolyAr	ArS
			(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)
1	5.00	6.00	16.50	22.50	1.70	1.70	0.00	0.00	0.00	0.00	0.00	0.00	0.80	0.00	0.00	0.00	0.00	0.00
2	6.00	7.00	6.30	11.80	4.60	2.49	0.00	0.00	0.00	0.00	0.00	0.00	1.10	0.00	0.00	0.00	0.00	0.00
3	7.00	8.00	2.90	3.00	5.30	1.60	0.00	0.00	0.00	0.00	0.00	0.00	0.90	0.00	0.00	0.00	0.00	0.00
4	8.00	9.00	0.80	1.70	2.40	0.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	12.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	13.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	14.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	15.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	16.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	17.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	18.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure A18. Light Straight-Run Naphtha (64741-46-4) Output modeled for P. promelas.

Product Name: CAS 64741-46-4; light straight-run naphtha (LSRN)
Date: 02-Oct-12

LL50/NOEL and PNEC Report

Species: Pimephales promelas
Acute TUs
Model LL50 (mg/L water): 15.98
No free product at this loading.
Total Toxic Units: 1.00

	(mg/L water)	Acute TUs
LL50:	15.98	1.00

Test Conditions:
Volume of water (L): 0.9
Volume of headspace (L): 0.1
Volume of free product: 0.0

Hydrocarbon Block	Average log Kow	Average Sub-Cooled Solubility	Average Molecular Weight	Average Henry's Law Constant	Product Phase	Air Phase	Water Phase	Avg PNEC n,i-Paraffins	Avg PNEC Naphthenics	Avg PNEC Mono-Aromatic	Avg PNEC Di-Aromatics	Avg PNEC Poly-Aromatics
		(mg/L)	(g/mol)	Log(unitless)	(mg/L product)	mg/L headspace	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)	(µg/L water)
1	2.76	1.81E+02	70.64	0.94	0.0E+00	6.9E+01	2.1E+03	1.2E+02	1.0E+03	0.0E+00	0.0E+00	0.0E+00
2	3.07	9.20E+01	83.49	0.77	0.0E+00	4.0E+01	2.2E+03	4.2E+01	3.3E+02	2.1E+03	0.0E+00	0.0E+00
3	3.81	1.42E+01	98.41	1.36	0.0E+00	1.9E+01	8.6E+02	2.0E+01	1.1E+02	7.7E+02	0.0E+00	0.0E+00
4	4.39	3.31E+00	112.68	1.60	0.0E+00	1.1E+01	2.3E+02	4.0E+00	3.6E+01	3.3E+02	0.0E+00	0.0E+00
5	5.30	3.31E-01	128.26	2.00	0.0E+00	1.9E+00	1.9E+01	2.4E+00	1.4E+01	2.0E+02	0.0E+00	0.0E+00
6	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	7.2E-01	3.9E+00	6.9E+01	1.1E+02	0.0E+00
7	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	5.4E-01	1.3E+00	3.0E+01	4.6E+01	0.0E+00
8	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	5.7E-01	9.9E-01	1.4E+01	2.3E+01	6.3E+01
9	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	6.7E-01	1.0E+00	6.7E+00	1.0E+01	2.9E+01
10	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	7.2E-01	1.1E+00	2.6E+00	5.4E+00	1.1E+01
11	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	6.9E-01	1.1E+00	1.2E+00	2.4E+00	5.0E+00
12	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.0E+00	1.2E+00	1.0E+00	1.0E+00	2.2E+00
13	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.1E+00	1.4E+00	1.0E+00	7.2E-01	1.0E+00
14	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	1.1E+00	1.7E+00	1.0E+00	6.5E-01	8.3E-01

Figure A19. Petrotox Input; Light Catalytic Reformed Naphtha (64741-63-5) model for S. capricornutum.

Product Name: **CAS 64741-63-5; light catalytic reformed naphtha (LCRN)**
Date: **8/30/2012**
PROTECTION CONCAWE

Target Species Selection Menu

	ID	SPECIES	INTERCEPT (μmol / g octanol)
	40	Selenastrum capricornutum	48.6

Test Conditions:
Volume of Water (L): **0.9**
Volume of Air (L): **0.1**
Total System Volume (L): **1.0**

0 No bioavailability correction.

0 :Total Number of Loadings

	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

27 :Total Number of Hydrocarbon Blocks — Total Weight Percent: 99.94

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P	i-P	n-CC5	n-CC6	i-N	Di-N	n-Olefins	i-Olefins	Poly-N	AlS	MoAr	NMAr	DiAr	NDiAr	PolyAr	ArS
			(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)
1	5.00	6.00	8.83	11.43	0.26	0.00	0.00	0.00	0.34	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6.00	7.00	4.69	11.54	0.00	0.62	0.00	0.00	0.27	0.00	0.00	0.00	8.37	0.00	0.00	0.00	0.00	0.00
3	7.00	8.00	3.59	14.11	0.00	1.18	0.00	0.00	0.28	0.00	0.00	0.00	29.77	0.00	0.00	0.00	0.00	0.00
4	8.00	9.00	0.40	2.72	0.00	0.27	0.00	0.00	0.01	0.00	0.00	0.00	1.26	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	12.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	13.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	14.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	15.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	16.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	17.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	18.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure A20. Petrotox Output; Light Catalytic Reformed Naphtha (64741-63-5) model for S. capricornutum.

Product Name: **CAS 64741-63-5; light catalytic reformed naphtha (LCRN)**
Date: **30-Aug-12**

LL50/NOEL and PNEC Report

Species: **Selenastrum capricornutum** **Acute TUs**
Model LL50 (mg/L water): **8.35** No free product at this loading.
Total Toxic Units: **1.00**

	(mg/L water)	Acute TUs
LL50:	8.35	1.00

Test Conditions:
Volume of water (L): **0.9**
Volume of headspace (L): **0.1**
Volume of free product **0.0**

Hydrocarbon Block	Average log Kow	Average Sub-Cooled Solubility	Average Molecular Weight	Average Henry's Law Constant	Product Phase	Air Phase	Water Phase	Avg PNEC n,i-Paraffins	Avg PNEC Naphthenics	Avg PNEC Mono-Aromatic	Avg PNEC Di-Aromatics	Avg PNEC Poly-Aromatics
		(mg/L)	(g/mol)	Log(unitless)	(mg/L product)	mg/L headspace	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)
1	2.78	1.81E+02	70.54	0.96	0.0E+00	1.7E+01	4.9E+02	1.2E+02	**1.0E+03**	0.0E+00	0.0E+00	0.0E+00
2	3.17	6.98E+01	83.76	0.97	0.0E+00	1.5E+01	9.8E+02	4.2E+01	3.3E+02	**2.1E+03**	0.0E+00	0.0E+00
3	3.85	1.28E+01	98.52	1.42	0.0E+00	1.9E+01	2.7E+03	2.0E+01	1.1E+02	7.7E+02	0.0E+00	0.0E+00
4	4.03	1.02E+01	110.82	0.95	0.0E+00	3.5E+00	1.5E+02	4.0E+00	3.6E+01	**3.3E+02**	0.0E+00	0.0E+00
5	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**2.4E+00**	**1.4E+01**	**2.0E+02**	**0.0E+00**	**0.0E+00**
6	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**7.2E-01**	**3.9E+00**	**6.9E+01**	**1.1E+02**	**0.0E+00**
7	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**5.4E-01**	**1.3E+00**	**3.0E+01**	**4.6E+01**	**0.0E+00**
8	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**5.7E-01**	**9.9E-01**	**1.4E+01**	**2.3E+01**	**6.3E+01**
9	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**6.7E-01**	**1.0E+00**	**6.7E+00**	**1.0E+01**	**2.9E+01**
10	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**7.2E-01**	**1.1E+00**	**2.6E+00**	**5.4E+00**	**1.1E+01**
11	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**6.9E-01**	**1.1E+00**	**1.2E+00**	**2.4E+00**	**5.0E+00**
12	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.0E+00**	**1.2E+00**	**1.0E+00**	**1.0E+00**	**2.2E+00**
13	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.1E+00**	**1.4E+00**	**1.0E+00**	**7.2E-01**	**1.0E+00**
14	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.1E+00**	**1.7E+00**	**1.0E+00**	**6.5E-01**	**8.3E-01**

Figure A21. Petrotox Input; Light Catalytic Reformed Naphtha (64741-63-5) model for D. magna.

Product Name: **CAS 64741-63-5; light catalytic reformed naphtha (LCRN)**
Date: **8/30/2012**
PROTECTION CONCAWE

Target Species Selection Menu

Test Conditions:
Volume of Water (L): **0.9**
Volume of Air (L): **0.1**
Total System Volume (L): **1.0**

ID	SPECIES	INTERCEPT (μmol / g octanol)
15	Daphnia magna	**115.3**

0 No bioavailability correction.

0 :Total Number of Loadings

	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

27 :Total Number of Hydrocarbon Blocks — Total Weight Percent: 99.94

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P	i-P	n-CC5	n-CC6	i-N	Di-N	n-Olefins	i-Olefins	Poly-N	AlS	MoAr	NMAr	DiAr	NDiAr	PolyAr	ArS
			(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)	(weight %)
1	5.00	6.00	8.83	11.43	0.26	0.00	0.00	0.00	0.34	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6.00	7.00	4.69	11.54	0.00	0.62	0.00	0.00	0.27	0.00	0.00	0.00	8.37	0.00	0.00	0.00	0.00	0.00
3	7.00	8.00	3.59	14.11	0.00	1.18	0.00	0.00	0.28	0.00	0.00	0.00	29.77	0.00	0.00	0.00	0.00	0.00
4	8.00	9.00	0.40	2.72	0.00	0.27	0.00	0.00	0.01	0.00	0.00	0.00	1.26	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	12.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	13.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	14.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	15.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	16.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	17.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	18.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure A22. Petrotox Output; Light Catalytic Reformed Naphtha (64741-63-5) model for D. magna.

Product Name: **CAS 64741-63-5; light catalytic reformed naphtha (LCRN)**
Date: **30-Aug-12**

LL50/NOEL and PNEC Report

Species: **Daphnia magna** — **Acute TUs**
Model LL50 (mg/L water): **19.79** — No free product at this loading.
Total Toxic Units: **1.00**

	(mg/L water)	Acute TUs
LL50:	19.79	1.00

Test Conditions:
Volume of water (L): **0.9**
Volume of headspace (L): **0.1**
Volume of free product **0.0**

Hydrocarbon Block	Average log Kow	Average Sub-Cooled Solubility	Average Molecular Weight	Average Henry's Law Constant	Product Phase	Air Phase	Water Phase	Avg PNEC n,i-Paraffins	Avg PNEC Naphthenics	Avg PNEC Mono-Aromatic	Avg PNEC Di-Aromatics	Avg PNEC Poly-Aromatics
		(mg/L)	(g/mol)	Log(unitless)	(mg/L product)	mg/L headspace	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)	(μg/L water)
1	2.78	1.81E+02	70.54	0.96	0.0E+00	4.0E+01	1.2E+03	1.2E+02	1.0E+03	0.0E+00	0.0E+00	0.0E+00
2	3.17	6.98E+01	83.76	0.97	0.0E+00	3.6E+01	2.3E+03	4.2E+01	3.3E+02	2.1E+03	0.0E+00	0.0E+00
3	3.85	1.28E+01	98.52	1.42	0.0E+00	4.4E+01	6.3E+03	2.0E+01	1.1E+02	7.7E+02	0.0E+00	0.0E+00
4	4.03	1.02E+01	110.82	0.95	0.0E+00	8.3E+00	3.5E+02	4.0E+00	3.6E+01	3.3E+02	0.0E+00	0.0E+00
5	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**2.4E+00**	**1.4E+01**	**2.0E+02**	**0.0E+00**	**0.0E+00**
6	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**7.2E-01**	**3.9E+00**	**6.9E+01**	**1.1E+02**	**0.0E+00**
7	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**5.4E-01**	**1.3E+00**	**3.0E+01**	**4.6E+01**	**0.0E+00**
8	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**5.7E-01**	**9.9E-01**	**1.4E+01**	**2.3E+01**	**6.3E+01**
9	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**6.7E-01**	**1.0E+00**	**6.7E+00**	**1.0E+01**	**2.9E+01**
10	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**7.2E-01**	**1.1E+00**	**2.6E+00**	**5.4E+00**	**1.1E+01**
11	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**6.9E-01**	**1.1E+00**	**1.2E+00**	**2.4E+00**	**5.0E+00**
12	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.0E+00**	**1.2E+00**	**1.0E+00**	**1.0E+00**	**2.2E+00**
13	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.1E+00**	**1.4E+00**	**1.0E+00**	**7.2E-01**	**1.0E+00**
14	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.1E+00**	**1.7E+00**	**1.0E+00**	**6.5E-01**	**8.3E-01**

Figure A23. Petrotox Input; Light Catalytic Reformed Naphtha (64741-63-5) model for P. promelas.

Product Name: **CAS 64741-63-5; light catalytic reformed naphtha (LCRN)**
Date: **9/14/2012**
PROTECTION CONCAWE

Target Species Selection Menu

ID	SPECIES	INTERCEPT (μmol / g octanol)
34	Pimephales promelas	122.2

0 No bioavailability correction.

Test Conditions:
Volume of Water (L): **0.9**
Volume of Air (L): **0.1**
Total System Volume (L): **1.0**

0 :Total Number of Loadings

	Product Loading (mg/L water)	Effect Data (%)	POC or Lipid
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			

27 :Total Number of Hydrocarbon Blocks — Total Weight Percent: 99.94

Hydrocarbon Block	Starting Carbon Number	Ending Carbon Number	n-P (weight %)	i-P (weight %)	n-CC5 (weight %)	n-CC6 (weight %)	i-N (weight %)	Di-N (weight %)	n-Olefins (weight %)	i-Olefins (weight %)	Poly-N (weight %)	AlS (weight %)	MoAr (weight %)	NMAr (weight %)	DiAr (weight %)	NDiAr (weight %)	PolyAr (weight %)	ArS (weight %)
1	5.00	6.00	8.83	11.43	0.26	0.00	0.00	0.00	0.34	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	6.00	7.00	4.69	11.54	0.00	0.62	0.00	0.00	0.27	0.00	0.00	0.00	8.37	0.00	0.00	0.00	0.00	0.00
3	7.00	8.00	3.59	14.11	0.00	1.18	0.00	0.00	0.28	0.00	0.00	0.00	29.77	0.00	0.00	0.00	0.00	0.00
4	8.00	9.00	0.40	2.72	0.00	0.27	0.00	0.00	0.01	0.00	0.00	0.00	1.26	0.00	0.00	0.00	0.00	0.00
5	9.00	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	10.00	11.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	11.00	12.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	12.00	13.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	13.00	14.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	14.00	15.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	15.00	16.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	16.00	17.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	17.00	18.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	18.00	19.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Figure A24. Petrotox Output; Light Catalytic Reformed Naphtha (64741-63-5) model for P. promelas.

Product Name: **CAS 64741-63-5; light catalytic reformed naphtha (LCRN)**
Date: **14-Sep-12**

LL50/NOEL and PNEC Report

Species: **Pimephales promelas** **Acute TUs**
Model LL50 (mg/L water): **20.97** No free product at this loading.
Total Toxic Units: **1.00**

	(mg/L water)	Acute TUs
LL50:	20.97	1.00

Test Conditions:
Volume of water (L): **0.9**
Volume of headspace (L): **0.1**
Volume of free product: **0.0**

Hydrocarbon Block	Average log Kow	Average Sub-Cooled Solubility (mg/L)	Average Molecular Weight (g/mol)	Average Henry's Law Constant Log(unitless)	Product Phase (mg/L product)	Air Phase mg/L headspace	Water Phase (μg/L water)	Avg PNEC n,i-Paraffins (μg/L water)	Avg PNEC Naphthenics (μg/L water)	Avg PNEC Mono-Aromatic (μg/L water)	Avg PNEC Di-Aromatics (μg/L water)	Avg PNEC Poly-Aromatics (μg/L water)
1	2.78	1.81E+02	70.54	0.96	0.0E+00	4.2E+01	1.2E+03	1.2E+02	1.0E+03	0.0E+00	0.0E+00	0.0E+00
2	3.17	6.98E+01	83.76	0.97	0.0E+00	3.8E+01	2.5E+03	4.2E+01	3.3E+02	2.1E+03	0.0E+00	0.0E+00
3	3.85	1.28E+01	98.52	1.42	0.0E+00	4.7E+01	6.7E+03	2.0E+01	1.1E+02	7.7E+02	0.0E+00	0.0E+00
4	4.03	1.02E+01	110.82	0.95	0.0E+00	8.8E+00	3.7E+02	4.0E+00	3.6E+01	3.3E+02	0.0E+00	0.0E+00
5	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**2.4E+00**	**1.4E+01**	**2.0E+02**	**0.0E+00**	**0.0E+00**
6	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**7.2E-01**	**3.9E+00**	**6.9E+01**	**1.1E+02**	**0.0E+00**
7	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**5.4E-01**	**1.3E+00**	**3.0E+01**	**4.6E+01**	**0.0E+00**
8	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**5.7E-01**	**9.9E-01**	**1.4E+01**	**2.3E+01**	**6.3E+01**
9	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**6.7E-01**	**1.0E+00**	**6.7E+00**	**1.0E+01**	**2.9E+01**
10	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**7.2E-01**	**1.1E+00**	**2.6E+00**	**5.4E+00**	**1.1E+01**
11	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**6.9E-01**	**1.1E+00**	**1.2E+00**	**2.4E+00**	**5.0E+00**
12	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.0E+00**	**1.2E+00**	**1.0E+00**	**1.0E+00**	**2.2E+00**
13	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.1E+00**	**1.4E+00**	**1.0E+00**	**7.2E-01**	**1.0E+00**
14	0.00	1.00E+00	0.00	0.00	0.0E+00	0.0E+00	0.0E+00	**1.1E+00**	**1.7E+00**	**1.0E+00**	**6.5E-01**	**8.3E-01**