Naphtha, Petroleum, Hydrotreated Heavy (CAS# 64742-48-9) GreenScreen® for Safer Chemicals (GreenScreen®) Assessment

Prepared for:

Washington State Department of Ecology

Prepared by:

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GreenScreen® Executive Summary for Naphtha, Petroleum, Hydrotreated Heavy (CAS #64742-48-9)

Naphtha, petroleum, hydrotreated heavy is a chemical that is primarily used as a solvent in a variety of applications including: extraction, cleaning, degreasing, aerosols, paints, wood preservatives, asphalt products, lacquers, and varnishes.

Naphtha, petroleum, hydrotreated heavy was assigned a GreenScreen® Benchmark Score of 1 ("Avoid – Chemical of high concern") as it has Very High bioaccumulation (B), Very High ecotoxicity (acute aquatic toxicity (AA) and chronic aquatic toxicity (CA)), High Group I Toxicity (carcinogenicity (C) and mutagenicity (M)), and High Group II* Toxicity (neurotoxicity (repeated dose) (Nr*)). This corresponds to GreenScreen® benchmark classification 1d and 1e in CPA 2011. Data gaps (DG) exist for endocrine activity (E), systemic toxicity (single dose), and respiratory sensitization (SnR*). As outlined in CPA (2013) Section 12.2 (Step 8 – Conduct a Data Gap Analysis to assign a final Benchmark score), naphtha, petroleum, hydrotreated heavy meets requirements for a GreenScreen® Benchmark Score of 1 despite the hazard data gaps. In a worst-case scenario, if naphtha, petroleum, hydrotreated heavy were assigned a High score for the data gap endocrine activity (E), it would be still be categorized as a Benchmark 1 Chemical.

GreenScreen® Benchmark Score for Relevant Route of Exposure:
As a standard approach for GreenScreen® evaluations, all exposure routes (oral, dermal, and inhalation) were evaluated together, so the GreenScreen® Benchmark Score of 1 ("Avoid – Chemicals of high concern") is applicable for all routes of exposure.

GreenScreen® Hazard Ratings for Naphtha, Petroleum, Hydrotreated Heavy

Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						single	repeated*	single	repeated*										
H	H	L	M	DG	L	DG	L	M	H	L	DG	H	L	vH	vH	L	vH	L	M

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated (modeled) values, authoritative B lists, screening lists, weak analogues, and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Please see Appendix A for a glossary of hazard acronyms.

GreenScreen® Assessment for Naphtha, Petroleum, Hydrotreated Heavy (CAS #64742-48-9)

Method Version: GreenScreen® Version 1.2[1]
Assessment Type[2]: Certified

Chemical Name: Naphtha, petroleum, hydrotreated heavy

CAS Number: 64742-48-9

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Organization: ToxServices LLC
Date: October 14, 2014

Confirm application of the *de minimus* rule[3]: N/A

Chemical Structure(s):
Naphtha, petroleum, hydrotreated heavy is identified as a complex combination of hydrocarbons ranging from C6 – C13. The aromatic or hexane concentration is not greater than 0.1% by volume. Depending on the material and the production processes, the composition and physical properties of naphtha, petroleum, hydrotreated heavy can greatly vary.

Also called: Hydrotreated heavy naphtha (petroleum); Hydrotreated light steam cracked naphtha residuum (petroleum) (ChemIDplus 2014)

Chemical Structure(s) of Chemical Surrogates Used in the GreenScreen®:
Few data were available for naphtha, petroleum, hydrotreated heavy (CAS# 64742-48-9). Naphtha, petroleum, hydrotreated heavy is a member of U.S. EPA's Gasoline Blending Streams category (U.S. EPA 2011). Members of the category are petroleum refinery streams used in the blending of gasoline. They are similar complex mixtures with carbon numbers ranging from C4-C12 and a boiling point range between -20 and 230 ºC. Members of this category are expected to have similar environmental fate and toxicity profiles. As supporting chemicals, U.S. EPA's assessment of this category included data on light naphtha, n-hexane rich (No CAS#) and various gasoline samples (CAS# 86290-81-5 or No CAS#). Since few data were available for naphtha, petroleum, hydrotreated heavy, data for the following members of and supporting chemicals for U.S. EPA's Gasoline Blending Streams category were also evaluated:

- Naphtha (petroleum), heavy thermal cracked (CAS# 64741-83-9)
- Naphtha (petroleum), light straight-run (CAS# 64741-46-4)

[1] Use GreenScreen® Assessment Procedure (Guidance) V1.2

[2] GreenScreen® reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen® Practitioner), "CERTIFIED" (by Licensed GreenScreen® Profiler or equivalent) or "CERTIFIED WITH VERIFICATION" (Certified or Authorized assessment that has passed GreenScreen® Verification Program)

[3] Every chemical in a material or formulation should be assessed if it is:
1. intentionally added and/or
2. present at greater than or equal to 100 ppm

- Naphtha (petroleum), light catalytic cracked (CAS# 64741-55-5)
- Naphtha (petroleum), sweetened (CAS# 64741-87-3)
- Naphtha (petroleum), catalytically reformed (CAS# 68955-35-1)
- Naphtha (petroleum), light alkylate (CAS# 64741-66-8)
- Naphtha (petroleum), heavy catalytic cracked (CAS# 64741-54-4)
- Naphtha (petroleum), full-range coker (CAS# 68513-02-0)
- Naphtha (petroleum), heavy catalytic reformed (CAS# 64741-68-0)
- Naphtha (petroleum), heavy straight run (CAS# 64741-41-9)
- Solvent naphtha (petroleum), light arom. (CAS# 64742-95-6)
- Various compositions of unleaded gasoline (No CAS#)
- Gasoline (CAS# 86290-81-5)

Naphtha, petroleum, hydrotreated heavy is a member of the Danish Environmental Protection Agency's White Spirit category (ECHA 2009). Members of this category are petroleum substances derived from crude oil. They are a complex mixture of saturated aliphatic and alicyclic C7-C12 hydrocarbons with a maximum content of 25% C7-C12 alkyl aromatic hydrocarbons. Members of this category are expected to have similar environmental fate and toxicity profiles. Since few data were available for naphtha, petroleum hydrotreated heavy, data for the following members of the Danish Environmental Protection Agency's White Spirit category were also evaluated:

- Solvent naphtha (petroleum), medium aliphatic (CAS# 64742-88-7)
- Naphtha (petroleum), hydrodesulphurized heavy (CAS# 64742-82-1)
- Naphtha (petroleum), solvent-refined heavy (CAS# 64741-92-0)

Due to the significant degree of structural similarity and physicochemical properties between these chemicals and naphtha, petroleum, hydrotreated heavy, the surrogates identified above are considered to be strong surrogates for naphtha, petroleum, hydrotreated heavy by ToxServices.

Identify Applications/Functional Uses: (Inglewood Oil Field 2012)
1. Extraction solvent.
2. Cleaning solvent.
3. Degreasing solvent.
4. Used as a solvent in aerosols, paints, wood preservatives, asphalt products, lacquers, and varnishes.
5. Component of the gelling agent used in hydraulic fracturing fluids.

GreenScreen® Summary Rating for Naphtha, Petroleum, Hydrotreated Heavy[4]:
Naphtha, petroleum, hydrotreated heavy was assigned a GreenScreen® Benchmark Score of 1 ("Avoid – Chemical of high concern") as it has Very High bioaccumulation (B), Very High Ecotoxicity (acute aquatic toxicity (AA) and chronic aquatic toxicity (CA)), high Group I Toxicity (carcinogenicity (C) and mutagenicity (M)), and high Group II* Toxicity (neurotoxicity (repeated dose) (Nr*)). This corresponds to GreenScreen® benchmark classification 1d and 1e in CPA 2011, 2012a. Data gaps (DG) exist for endocrine activity (E), systemic toxicity (single dose), and respiratory sensitization (SnR*). As outlined in CPA (2013) Section 12.2 (Step 8 – Conduct a Data

[4] For inorganic chemicals with low human and ecotoxicity across all hazard endpoints and low bioaccumulation potential, persistence alone will not be deemed problematic. Inorganic chemicals that are only persistent will be evaluated under the criteria for Benchmark 4.

Gap Analysis to assign a final Benchmark score), naphtha, petroleum, hydrotreated heavy meets requirements for a GreenScreen® Benchmark Score of 1 despite the hazard data gaps. In a worst-case scenario, if naphtha, petroleum, hydrotreated heavy were assigned a High score for the data gap endocrine activity (E), it would be still be categorized as a Benchmark 1 Chemical.

Figure 1: GreenScreen® Hazard Ratings for Naphtha, Petroleum, Hydrotreated Heavy

Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						single	repeated*	single	repeated*										
H	H	L	M	DG	L	DG	L	M	H	L	DG	H	L	vH	vH	L	vH	L	M

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated (modeled) values, authoritative B lists, screening lists, weak analogues, and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M, and L) instead of three (i.e., H, M, and L), and are based on single exposures instead of repeated exposures. Please see Appendix A for a glossary of hazard acronyms.

Transformation Products and Ratings:

Identify feasible and relevant fate and transformation products (i.e., dissociation products, transformation products, valence states) **and/or moieties of concern**[5]

No feasible and relevant transformation products were identified. CO, CO_2, and H_2O may be produced by combustion but are naturally occurring and are not assessed. Hydrolysis is a negligible transformation process as the hydrocarbons do not contain hydrolysable functional groups (U.S. EPA 2011).

Introduction

Naphtha, petroleum, hydrotreated heavy is identified as a complex combination of hydrocarbons ranging from C6-C13. The aromatic or hexane concentration is not greater than 0.1% by volume. Depending on the material and the production processes, the composition and physical properties of naphtha, petroleum, hydrotreated heavy can greatly vary. Naphtha, petroleum, hydrotreated heavy is primarily used as a solvent in a wide variety of applications.

ToxServices assessed naphtha, petroleum, hydrotreated heavy against GreenScreen® Version 1.2 (CPA 2013) following procedures outlined in ToxServices' SOP 1.37 (GreenScreen® Hazard Assessment) (ToxServices 2013).

GreenScreen® List Translator Screening Results

The GreenScreen® List Translator identifies specific authoritative or screening lists that should be searched to identify GreenScreen® benchmark 1 chemicals (CPA 2012b). Pharos (Pharos 2013) is an online list-searching tool that is used to screen chemicals against the List Translator electronically. The output indicates benchmark or possible benchmark scores for each human health and environmental endpoint. The output for naphtha, petroleum, hydrotreated heavy can be found in Appendix C, and classifications for specific endpoints can be found in the appropriate sections.

[5] A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

When a classification from GHS New Zealand was available for any endpoint, it was converted to the harmonized GHS classifications using the "Correlation between GHS and New Zealand HSNO Hazard Classes and Categories" document from the New Zealand Environmental Protection Authority (N.Z. EPA 2009).

Physicochemical Properties of Naphtha, Petroleum, Hydrotreated Heavy

Naphtha, petroleum, hydrotreated heavy is a liquid at room temperature. It is volatile with a high vapor pressure. It has low water solubility. The Log K_{ow} of 3.6-5.7 indicates some potential for bioaccumulation.

Table 1: Physical and Chemical Properties of Naphtha, Petroleum, Hydrotreated Heavy (CAS #64742-48-9)

Property	Value	Reference
Molecular formula	Unspecified (mixture)	
SMILES Notation	Unspecified (mixture)	
Molecular weight	Unspecified (mixture)	
Physical state	Liquid	U.S. EPA 2011
Appearance	Colorless liquid	U.S. EPA 2011
Melting point	< 25 ºC	U.S. EPA 2011
Vapor pressure	0.0602 – 184 mm Hg 25ºC	U.S. EPA 2011
Water solubility	0.33-161 mg/L	U.S. EPA 2011
Dissociation constant	N/A	
Density/specific gravity	0.75 – 0.8 g/cm^3 at 15ºC	ECHA 2014
Partition coefficient	Log K_{ow} = 3.6 – 5.7	U.S. EPA 2011

Hazard Classification Summary Section:

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M, or L): H

Naphtha, petroleum, hydrotreated heavy was assigned a score of High for carcinogenicity based on its presence on authoritative lists. Experimental data obtained with mice support naphtha, petroleum, hydrotreated heavy as having carcinogenic activity. GreenScreen® criteria classify chemicals as a high hazard for carcinogenicity when they are associated with EU Risk Phrase R45 or GHS Hazard Statement H350, or are classified as a Carcinogen Category 1B by EU CMR (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* EU CMR (1): Carcinogen Category 2 – Substances which should be regarded as if they are carcinogenic to man
  - *Authoritative:* EU R-Phrase: R45 May cause cancer
  - *Authoritative:* GHS H-Statement: H350 May cause cancer
  - *Authoritative:* EU CMR (2): Carcinogen Category 1B
  - *Screening:* not listed on any screening lists.
- No studies testing the carcinogenic potential of naphtha, petroleum, hydrotreated heavy have been performed. However, naphtha, petroleum, hydrotreated heavy may contain known carcinogens such as 4- to 6-membered fused-ring polycyclic aromatic hydrocarbons.
- ECHA 2014

  Unleaded gasoline (No CAS#)

- In a carcinogenicity study performed according to OECD Guideline 451, unleaded gasoline was administered to the skin of Swiss mice (n=50) three times per week for two years at a volume of 0.05 mL. One negative and two positive control groups were used; the negative control received no treatment and the positive control groups received benzo(a)pyrene (BaP) and BaP in acetone. The number of skin carcinomas, liver hemangiomas, lung adenomas, and malignant lymphomas in the group receiving the test substance was no greater than in the negative control group. Based on this study unleaded gasoline does not display carcinogenic potential in the absence of repeated dermal injury.

Naphtha (petroleum), heavy thermal cracked (CAS# 64741-83-9)

- In a GLP compliant combined chronic toxicity and carcinogenicity study performed according to OECD Guideline 453, thermal cracked naphtha was applied to the skin of male C3H mice (n=50) two times per week for two years at a volume of 0.05 mL. One negative and two positive control groups were used, the negative control received 0.05 mL toluene and the positive control groups received 0.01% or 0.04% benzo(a)pyrene (BaP) in toluene. Treatment produced an increased incidence of malignant dermal neoplasms.

Naphtha (petroleum), light straight-run (CAS# 64741-46-4)

- In a carcinogenicity study performed according to OECD Guideline 451 API Procedure, male C3H/HeJ mice were dermally exposed to light straight-run naphtha two times a week for up to one hundred and twenty-two weeks. This experiment tested the tumor initiating or promoting activity of light straight-run naphtha. Animals were exposed to 2.5 mg or 12.5 mg of the test substance for 2 weeks followed by treatment with 2.5 µg of the test substance for life. The test substance did not demonstrate tumor initiating or promoting activity. However, dermal application of the test substance caused the development of skin tumors. The authors noted that the development of skin tumors was secondary to repeated irritation and skin injury.

- Based on the weight of evidence, naphtha, petroleum, hydrotreated heavy is assigned a score of high. Carcinogenicity studies investigating the carcinogenic potential of thermal cracked naphtha and light straight-run naphtha found that dermal application of the test substance resulted in the development of skin tumors. Naphtha, petroleum, hydrotreated heavy is classified as a high carcinogenic hazard by the EU. Therefore, ToxServices classified naphtha, petroleum hydrotreated heavy as a High carcinogenic hazard.

Mutagenicity/Genotoxicity (M) Score (H, M, or L): H

Naphtha, petroleum, hydrotreated heavy was assigned a score of High for mutagenicity/genotoxicity based on positive results in *in vitro* and *in vivo* genotoxicity tests and on classification by the EU. GreenScreen® criteria classify chemicals as a high hazard for mutagenicity/genotoxicity when they are associated with EU Risk Phrase R46 or GHS H-Statement H340, or are classified as a Mutagen Category 1B by EU CMR (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* GHS H-Statement: H340 May cause genetic defects
  - *Authoritative:* EU CMR (2): Mutagen – Category 1B
  - *Authoritative:* EU R-Phrase: R46 May cause heritable genetic damage.
  - *Screening:* not listed on any screening lists.
- U.S. EPA 2011

  Naphtha (petroleum), light catalytic cracked (CAS# 64741-55-5)
  - Naphtha (petroleum), light catalytic cracked was equivocal for clastogenicity in a sister

chromatid exchange assay. Chinese hamster ovary cells were treated with 0.05-0.3 µL/mL without metabolic activation and 0.03-0.2 µL/mL with metabolic activation. Treatment in the presence of metabolic activation produced a significant increase in the frequency of sister chromatid exchange at two intermediate doses. Treatment in the absence of metabolic activation produced no changes.

Solvent naphtha (petroleum), light arom. (CAS# 64742-95-6)

- In a chromosomal aberration assay, solvent naphtha (petroleum), light arom. induced chromosomal aberrations in human lymphocytes. Human lymphocytes were treated with 2.5, 5, 10, or 25 µg/mL for 24 hours in the presence of metabolic activation and 2.5, 5, 10, or 20 µg/mL in the absence of metabolic activation. An increase in chromosomal aberrations was observed in all treatment groups with metabolic activation and at 20 µg/mL without metabolic activation.

Naphtha (petroleum), light catalytic cracked (CAS# 64741-55-5)

- Naphtha (petroleum), light catalytic cracked induced sister chromatid exchange. B6C3F1 mice were treated with 0, 200, 1,200, or 2,400 mg/kg via i.p. injection. Treatment produced a significant increase in the frequency of sister chromatic exchange.
- Naphtha (petroleum), light catalytic cracked was not clastogenic in a bone marrow chromosomal aberration assay. Sprague-Dawley rats were treated with 0, 0.3, 1, or 3 g/kg via i.p. injection. Treatment did not produce chromosomal aberrations.

Naphtha (petroleum), sweetened (CAS# 64741-87-3)

- Naphtha (petroleum), sweetened was not clastogenic in a bone marrow chromosomal aberration assay. Sprague-Dawley rats were exposed to 0, 0.21, 0.99, or 6.7 mg/L via whole-body inhalation for 6 hours per day for 5 days. Treatment did not induce chromosomal aberrations.

Naphtha (petroleum), catalytic reformed (CAS# 68955-35-1)

- Naphtha (petroleum), catalytic reformed was not clastogenic in a bone marrow chromosomal aberration assay. Sprague-Dawley rats were treated with 0, 0.26, 0.82, or 2.42 g/kg via i.p. injection. Treatment did not produce chromosomal aberrations.

- Based on positive results in chromosomal aberration assays and sister chromatid exchange assays, naphtha, petroleum, hydrotreated heavy was assigned a High score for mutagenicity/genotoxicity.

Reproductive Toxicity (R) Score (H, M, or L): L

Naphtha, petroleum, hydrotreated heavy was assigned a score of Low for reproductive toxicity based on experimental data. GreenScreen® criteria classify chemicals as a low hazard for reproductive toxicity when there are adequate data available and negative, there are no structural alerts, and they are not classified under GHS (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* not listed on any screening lists.
- U.S. EPA 2011

  Naphtha (petroleum), light catalytic cracked (CAS# 64741-55-5)
  - *Inhalation:* A NOAEC of 23.9 mg/L/day was identified in a combined reproductive/developmental toxicity screening test in Sprague-Dawley rats. Animals were exposed to 0, 2.4, 7.9, or 23.8 mg/L naphtha (petroleum), light catalytic cracked for 6 hours per day, 7 days per week, for 30-47 days. Treatment commenced 14 days prior to mating and extended through gestation day 19. Treatment produced no adverse effects on parental body weight, food consumption, histology, fertility index, or number of

implantation sites.

- ECHA 2014

  Unleaded gasoline (No CAS#)

  - *Inhalation*: In a GLP-compliant 2-generation reproductive study performed according to OECD Guideline 416 using Sprague Dawley rats (n=30/sex/dose), animals received the test substance at doses of 0, 5,076 (±146), 10,247 (±249), and 20,241 (±373) mg/m^3 (analytical concentrations) via inhalation for 6 hours per day, 7 days per week. All animals were checked twice a day for viability and clinical signs were checked daily. Body weights were measured daily until mating, on GD 0, 7, 14, and 21, and on PPD 0, 4, 7, 14, and 21 for P1 and P2, and on PPD 28 for P1 only. Reproductive toxicity was assessed through evaluation of the following parameters: male and female fertility indices, male mating index, female fecundicity and gestational indices, mean litter size, mean days of gestation, female estrous cycle length, and number of females cycling normally. Ovarian and sperm evaluations were also performed. Offspring were counted and examined externally on a daily basis until PND 21. Pup body weight was assessed at PND 0, 4, 7, 14, and 21. From PND 21 to 28, pups were externally examined, and pups were weighed on PND 28 and 35. All surviving pups from both generations of offspring were evaluated for developmental landmarks, including pinna detachment, hair growth, incisor eruption, eye opening, and the development of the surface righting reflex. Postmortem analysis of the parental generation included measuring organ weights. Postmortem analysis of the offspring generation included necropsy of animals that died spontaneously or that were sacrificed in a moribund condition. No treatment-related effects were identified in any of the animals. The authors identified the parental and F1 NOAEC as at least 20,000 mg/m^3 (equivalent to the analytical dose of 20,241 mg/m^3 or 20.241 mg/L).

  Naphtha (petroleum), light alkylate (LAN-D) (CAS# 64741-66-8)

  - *Inhalation*: In a GLP-compliant reproduction and developmental toxicity screening test performed according to OECD Guideline 421, LAN-D was administered to groups of Sprague-Dawley rats (n=10/sex/group) at (analytical) doses of 0, 5,090, 12,490, and 24,960 mg/m^3 (0, 5.090, 12.490, and 24.960 mg/L). Animals were exposed 2 weeks prior to mating; dosing continued throughout gestation until PND 4 for females or for 8 consecutive weeks for males. Parental food consumption, body weights, organ weights, and reproductive indices were evaluated. No differences in effects were observed between the high doses and control groups. No information was provided as to why the lower dose groups were not evaluated. Pup birth weight, weight gain, and histopathogical analyses were all comparable to control. A viability index of greater than 97% was reported for all dose groups. The authors identified both the F1 and Parental Generation NOAECs as 24,700 mg/m^3 (24.700 mg/L).

- In summary, repeated exposure to surrogates of aliphatic petroleum distillates did not cause reproductive toxicity in male or female rats. These were high quality studies and performed according to OECD testing guidelines. Based on negative findings in experimental animals, ToxServices classified naphtha, petroleum, hydrotreated heavy as a Low hazard for this endpoint.

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): M

Naphtha, petroleum, hydrotreated heavy was assigned a score of Moderate for developmental toxicity based on experimental data. GreenScreen® criteria classify chemicals as a moderate hazard for developmental toxicity when there is marginal evidence of developmental toxicity in animals (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* not listed on any screening lists.
- ECHA 2009
  - In a neurobehavioral study, rats were prenatally exposed to 800 ppm (4,679 mg/m^3 = 4.679 mg/L) for 6 hours per day on gestation days 7-20. The offspring were monitored for 5 months. Exposure resulted in a 26% decrease in body weights of the exposed dams and a 7% decrease in body weight in the offspring. The offspring had significantly impaired learning and memory function.
- U.S. EPA 2011

  Naphtha (petroleum), light catalytic cracked (CAS# 64741-55-5)
  - A NOAEC of 23.9 mg/L/day (highest concentration tested) was identified in a combined reproductive/developmental inhalation toxicity test in Sprague-Dawley rats. Treatment produced no adverse effects on live birth index, number of litters, numbers of live and dead pups, pup survival, or pup body weight.

  Gasoline (CAS# 86290-81-5)
  - *Inhalation*: In a GLP-compliant prenatal development toxicity test performed according to OECD Guideline 414, pregnant rats were exposed to unleaded gasoline vapor condensate once daily on gestation days 6-19 via inhalation. Doses administered were 0, 2.7, 8, or 24 mg/L; 24 animals per dose were used. No treatment-related adverse effects on clinical chemistry and no grossly visible abnormalities were observed in the maternal generation. No developmental effects were observed during external, skeletal, or visceral examinations of fetuses. Based on the results of the study, the authors identified the developmental NOAEC as 24 mg/L/day.
  - *Inhalation*: A LOAEC of 6.2 mg/L/day was identified in a developmental toxicity study. Pregnant Sprague-Dawley rats were exposed to unleaded gasoline vapor for 6 hours per day on gestation days 6-15. Animals were exposed to 0, 1.6, or 6.3 mg/L unleaded gasoline vapor. Treatment produced an increase in the number of fetuses with skeletal variations which consisted primarily of changes related to retarded ossification.
- In summary prenatal exposure to aliphatic petroleum distillates impairs learning and memory of rat offspring. However, the authors of this study indicated that treatment resulted in a 26% decrease in body weight of exposed dams, indicating that maternal health may have been altered during the pregnancy. In a developmental study utilizing a supporting chemical, exposure to unleaded gasoline vapor during gestation resulted in skeletal variations in the offspring. Based on this study, ToxServices conservatively classified naphtha, petroleum, hydrotreated heavy as a Moderate hazard for this endpoint.

Endocrine Activity (E) Score (H, M, or L): DG

Naphtha, petroleum, hydrotreated heavy was assigned a Data Gap for endocrine disruption based on a lack of measured data.

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* not listed on any screening lists.
- Not listed as a potential endocrine disruptor on the EU Priority List of Suspected Endocrine Disruptors.
- Not listed as a potential endocrine disruptor on the OSPAR List of Chemicals of Possible Concern.
- No data were identified for this endpoint.

Group II and II* Human Health Effects (Group II and II* Human)

Note: Group II and Group II* endpoints are distinguished in the v 1.2 Benchmark system. For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints and test data for single or repeated exposures may be used. If data exist for single OR repeated exposures, then the endpoint is not considered a data gap. If data are available for both single and repeated exposures, then the more conservative value is used.

Acute Mammalian Toxicity (AT) Group II Score (vH, H, M, or L): L

Naphtha, petroleum, hydrotreated heavy was assigned a score of Low for acute toxicity based on measured data. GreenScreen® criteria classify chemicals as a low hazard for acute toxicity when values for inhalation LC_{50} are greater than 20 mg/L, oral LD_{50} values are greater than 2,000 mg/kg, or dermal LD_{50} values are greater than 2,000 mg/kg (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* not listed on any screening lists.
- U.S. EPA 2011

  Naphtha (petroleum), light alkylate (CAS# 64741-66-8)
  - *Oral:* LD_{50} greater than 7,000 mg/kg (Sprague-Dawley rats)
  - *Dermal:* LD_{50} greater than 2,000 mg/kg (New Zealand White Rabbits)
  - *Inhalation:* LC_{50} greater than 6.31 mg/L (Sprague-Dawley rats)

  Naphtha (petroleum), light catalytic cracked (CAS# 64741-55-5)
  - *Oral:* LD_{50} greater than 5,000 mg/kg
  - *Dermal:* LD_{50} greater than 3,000 mg/kg
  - *Inhalation:* LC_{50} greater than 5.3 mg/kg

  Naphtha (petroleum), catalytic reformed (CAS# 68955-35-1)
  - *Oral:* LD_{50} = 6,620 mg/kg (Sprague-Dawley rats, male)
  - *Oral:* LD_{50} = 5,390 mg/kg (Sprague-Dawley rats, female)
  - *Dermal:* LD_{50} greater than 2,000 mg/kg (New Zealand White rabbits)
  - *Inhalation:* LC_{50} greater than 5.22 mg/L

  Naphtha (petroleum), sweetened (CAS# 64741-87-3)
  - *Oral:* LD_{50} greater than 5,000 mg/kg (Sprague-Dawley rats)
  - *Dermal:* LD_{50} greater than 2,000 mg/kg (New Zealand White rabbits)
  - *Inhalation:* LC_{50} greater than 5.2 mg/L (Sprague-Dawley rats)

  Unleaded gasoline (No CAS#)
  - *Oral:* LD_{50} = 13,875 mg/kg
  - *Dermal:* LD_{50} greater than 3,700 mg/kg
- ESIS 2000
  - *Oral:* An LD_{50} of greater than 15,000 mg/kg was determined in rats.
  - *Oral:* An LD_{50} of greater than 5,000 mg/kg was determined in male albino rats. Animals were observed for 14 days. No animals died during the period of observation.
  - *Inhalation*: An LC_{50} of greater than12 mg/L was determined in the rat following a 6 hour exposure. Groups of male and female rats, mice, and guinea pigs (n=5/sex/species) were exposed to 12.19 mg/L of the test substance for 6 hours. Observations were made for 14 days following test substance administration; all animals survived to the end of the observation period and no significant clinical signs were observed. No gross lesions were observed at necropsy.

- *Dermal:* An LD_{50} of greater than 3,160 mg/kg was determined in male and female New Zealand White rabbits (n=3/sex) following a 24 hour exposure to 3,160 mg/kg. All animals survived treatment.

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)
***Group II Score (single dose)* (vH, H, M, or L):** DG
Naphtha, petroleum, hydrotreated heavy was assigned a Data Gap for systemic toxicity (single dose) based on a lack of identified data.

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* not listed on any screening lists.
- No data were identified.

***Group II* Score (repeated dose)* (H, M, or L): L**
Naphtha, petroleum, hydrotreated heavy was assigned a score of Low for systemic toxicity (repeated dose) based on subchronic toxicity studies of supporting chemicals. GreenScreen® criteria classify chemicals as a low hazard for systemic toxicity (repeated dose) when adequate data are available and adverse effects are not seen below the guidance values of 100 mg/kg/day for an oral study, 200 mg/kg/day for a dermal study, and 1.0 mg/L/6h/day for an inhalation (gas/vapor) study (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* not listed on any screening lists.
- U.S. EPA 2001
  - *Dermal:* In a repeated dose toxicity study, Fischer 344 rats were dermally exposed to 0, 500, 1,000, or 1,500 mg/kg in paraffin oil, once per day for 6 hours per day, 5 days per week, for 4 weeks. The test article was dermally applied over 10% of the body surface on the backs of rats clipped free of hair. Following application the animals were fitted with Elizabethan collars in order to reduce ingestions. After 6 hours the collars were removed and excess oil was wiped off. Food consumption was significantly decreased in male rats treated with 1,500 mg/kg/day during weeks 2 and 3 and in female rats treated with 1,000 mg/kg/day during week 2. Upon completion of the treatment period there was a dose-related increase in the white blood cells count of males and females which reached significance in the 1,500 mg/kg/day treatment group. The authors identified a LOAEL of 500 mg/kg/day in male Fischer 344 rats based on increased white blood cell count.
- ECHA 2014

  <u>Naphtha (petroleum), heavy catalytic cracked (CAS# 64741-54-4)</u>
  - *Oral*: Four naphtha streams, among fifteen hydrocarbon compounds, were administered to two groups of male F344 rats via gavage at doses of 500 mg/kg/day and 2,000 mg/kg/day. The test substance was administered 5 days per week for 4 weeks. The purpose of this study was to evaluate the nephrotoxicity of hydrocarbons. Lethargy was observed in both groups and significantly lower body weight gain was observed in the animals in the high dose group. The only histopathological difference found was in the kidneys of all male rats, which was α-2μ-globulin nephropathy. This effect is specific to male rats and is not considered to be biologically relevant in humans. A weak to moderate nephrotoxic dose-response was identified. The authors of the study identified the NOEL as less than 500 mg/kg.

  <u>Naphtha (petroleum), light catalytic cracked (CAS# 64741-55-5)</u>
  - *Dermal:* In a repeated dose dermal toxicity study performed according to OECD

Guideline 410, the test article was dermally administered to New Zealand White rabbits at doses of 200, 1,000, or 2,000 mg/kg/day for 6 hours per day under occlusive conditions three times per week for 4 weeks. Males treated with 2,000 mg/kg/day and females treated with 1,000 and 2,000 mg/kg/day had significantly lower body weights. Exposure to the test article caused moderate to severe dose-dependent dermal irritation, it did not cause systemic toxicity. The authors determined the systemic NOAEL was greater than 2,000 mg/kg/day.

Unleaded gasoline (No CAS#)

- *Dermal*: In a study previously described in the carcinogenicity section, unleaded gasoline was administered to the skin of Swiss mice (n=50) 3 times per week for 2 years at a volume of 0.05 mL. One negative and 2 positive control groups were used; the negative control received no treatment and the positive control groups received benzo(a)pyrene (BaP) and BaP in acetone. Hyperkeratosis, fibrosis of the dermis, extoabscess, and skin ulceration were observed at the treated areas. The authors concluded that the results of this study did not indicate that unleaded gasoline is a chronic dermal toxicant. As a result, the NOAEL was identified as 0.05 mL. This is approximately 532 mg/kg/day[6].
- *Inhalation*: F344 rats and B6C3F mice were exposed to unleaded gasoline vapor for 6 hours per day, 5 days per week for up to 113 weeks at concentrations of 322, 1,402, and 9,869 mg/m^3. These doses were identified as analytical concentrations[7]. After sacrifice, no consistent, compound-related changes were seen in mortality. Additionally, no consistent compound-related changes were seen in hematology or clinical chemistry parameters in either species. In both sexes of rats and in male mice exposed to the highest dose, a significant depression of body weight gain was observed. A compound-related increase in liver nodules and masses was seen at gross necropsy in female mice exposed to the highest dose level. Primary kidney neoplasms were observed in male rats exposed to the test article at all concentrations. This effect correlated histopathologically with an increased incidence and severity of regenerative epithelial changes and dilated tubules containing proteinaceous material. The effects observed in the kidney of male rats is suggestive of α-2μ-globulin nephropathy, which is not considered to be of biological significance in humans. The authors identified the NOAEC as 1,402 mg/m^3 based on decreased body weight gain in mice and rats at 9,869 mg/m^3. This is equivalent to 1,001 mg/m^3/day (1.001 mg/L/day) and 7,049 mg/m^3/day (7.049 mg/L/day), respectively, after converting to daily exposure. As a result, the LOAEC was identified as 9,869 mg/m^3 (9.869 mg/L/day).
- *Inhalation:* In a GLP compliant 90-day inhalation toxicity study performed according to EPA OPPTS 870.3465, Sprague-Dawley rats were exposed to 2,050, 10,148, or 20,324 mg/m^3 (equivalent to 2.050, 10.148, and 20.324 mg/L/day) for 6 hours per day, 5 days per week, for 13 weeks. Treatment had no effect on body weight gain, organ weights, hematology, gross pathology, or neurobehavior. Exposed males produced nephropathy, however the authors noted that this finding has been generally accepted as not relevant to human risk assessment. Animals exposed to 20.324 mg/L/day had a slight but reversible increase in red nasal discharge. The authors considered this effect to be due to irritation

[6] Using the density of 0.75 g/mL for naphtha, petroleum, hydrotreated heavy and the mean chronic time-weighted average body weight of male and female mice of 0.0302 kg listed by U.S. EPA (1988), 0.05 mL is approximately 1241 mg/kg. After adjustment of treatment frequency, the daily dose is 532 mg/kg/day

[7] Because the test substance was only administered for 5 days, it must be converted to a 7 day dosing regimen. Therefore, the doses to be assessed against guidance values should be calculated as follows: 322 * (5/7) = 230; 1,402 * (5/7) = 1,001; 9,869 * (5/7) = 7,049 mg/m^3/day
Converting these doses to mg/L/day was performed as follows: X mg/m^3/day ÷ 1,000 = X mg/L/day

at the site of contact. They determine the systemic NOAEC to be greater than 20.324 mg/L/day.

Naphtha (petroleum), full-range catalytically reformed (CAS# 68919-37-9)

- *Inhalation:* In a GLP-compliant 90-day inhalation toxicity study performed according to OECD Guideline 413, male and female Sprague-Dawley rats were exposed to 410, 1,970, or 8,050 mg/m^3 (equivalent to 4.1, 1.97, and 8.050 mg/L/day) for 6 hours per day, 5 days per week, for 13 weeks. Females rats exposed to 8.050 mg/L/day had significantly decreased white blood cell count. Also, treatment caused a significant increase in liver and kidney weight in males exposed to 8.050 mg/L/day. The authors identified a NOAEC of 1.97 mg/L/day and a LOAEC of 8.050 mg/L/day.

- In summary, the oral study identified a LOAEL of 500 mg/kg/day, the dermal studies identified LOAELs of 500 to greater than 2,000 mg/kg/day, and the inhalation studies identified LOAECs of 8.050 to greater than 20.324 mg/L. The values are greater than the guidance values of 100 mg/kg/day for an oral study, 200 mg/kg/day for a dermal study, and 1.0 mg/L/6h/day for an inhalation (gas/vapor) study for a Low score. Therefore, ToxServices assigned a score of Low for this endpoint.

Neurotoxicity (N)

***Group II Score (single dose)* (vH, H, M, or L): M**

Naphtha, petroleum, hydrotreated heavy was assigned a score of Moderate for neurotoxicity (single dose) based on classification of the chemical as GHS category 3. GreenScreen® criteria classify chemicals as a moderate hazard for neurotoxicity (single dose) when classified as GHS category 3 (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* not listed on any screening lists.
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006 and 2014).
- ECHA 2014

  Gasoline vapors
  - *Inhalation:* In an acute inhalation toxicity study, human volunteers were exposed to up to 1,296 mg/m^3 for 1 hour or up to 53,725 mg/m^3 for 10 min. Exposure to 4,320 mg/m^3 (equivalent to 4.320 mg/L) for 1 hour caused dizziness, nausea, and a headache. The authors identified the CNS LOAEL to be 4.320 mg/L.
- Based on the weight of evidence, a score of Moderate was assigned. Short term exposure to gasoline vapors caused dizziness, nausea, and a headache in human volunteers, warranting a classification of GHS Category 3 due to narcotic effects.

***Group II* Score (repeated dose)* (H, M, or L): H**

Naphtha, petroleum, hydrotreated heavy was assigned a score of High for neurotoxicity (repeated dose) based on data demonstrating that exposure to a chemical surrogate produced changes in the central and peripheral nervous system of humans, classifying it as GHS category 1. GreenScreen® criteria classify chemicals as a high hazard for neurotoxicity (repeated dose) when the chemical is classified as GHS Category 1 (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* not listed on any screening lists.
- Not classified as a developmental neurotoxicant (Grandjean and Landrigan 2006 and 2014).
- ECHA 2009

- *Inhalation:* Adult male rats were exposed to 2,330 or 4,670 mg/m^3 (equivalent to 2.33 and 4.67 mg/L) for 6 hours per day, 5 days per week for 6 months followed by an exposure free period of 70-80 days. Animals exposed to 4.67 mg/L had decreased motor activity during the dark cycle.
- *Inhalation:* Rats were exposed to 2,330 and 4,679 mg/m^3 (equivalent to 2.33 and 4.68 mg/L) for 6 hours per day, 5 days per week for 6 months. Treatment period was followed by an exposure free period of 70-80 days. The effect of treatment on the central nervous system was investigated by measuring sensory evoked potentials. Treatment induced concentration dependent changes in the flash evoked potential (FEP), somatosensory evoked potential (SEP), and auditory brain stem responses (ABR). The authors stated these results indicate that treatment affected the neurons of the retino-geniculate pathway, auditory pathway, and the cortical-subcortical network. They concluded that exposure to aliphatic petroleum distillates can induce long-lasting and potentially irreversible effects at 2.33 and 4.68 mg/L.

White spirit

- Numerous studies investigating the neurotoxic effects of exposure to white spirit in humans were summarized. Exposure to white spirit was generally due to occupational exposures in painters. Acute exposure resulted in reduced sense of taste, nausea, loss of appetite, headache, feeling of drunkenness, dizziness, and fatigue. These acute symptoms were reversible and disappeared during a period of exposure-free days (holidays or weekends). Chronic exposure resulted in memory impairment, forgetfulness, excessive fatigue, weariness, inability to concentrate, irritability, low frustration tolerance, headache, dizziness, apathy, lack of initiative, anxiety, nervousness, depression, low spirits, nausea, and blurred vision.

- ECHA 2014

  Unleaded Gasoline (No CAS#)

  - *Inhalation:* Fischer 344 rats were exposed to 5,056 ppm (equivalent to 21 mg/L[8]) for 6 hours per day, 5 days per week for 7, 12, or 18 months. Treatment did not produce any unique pathological changes.
- Based on the weight of evidence, naphtha, petroleum, hydrotreated heavy was assigned a High score. Experiments which exposed experimental animals to naphtha, petroleum, hydrotreated heavy via inhalation produced decreased motor activity and long-lasting effects to the rentino-geniculate pathway, auditory pathway, and cortical-subcortical pathway. The concentrations which produced these effects do not warrant GHS classification. However, data from human exposures to white spirit demonstrate that chronic exposure produces changes to the central and peripheral nervous system. Based on effects noted in humans, naphtha, petroleum, hydrotreated heavy was classified to GHS category 1 and hence a High hazard for this endpoint.

Skin Sensitization (SnS) Group II* Score (H, M, or L): L

Naphtha, petroleum, hydrotreated heavy was assigned a score of Low for skin sensitization based on negative experimental data. GreenScreen® criteria classify chemicals as a low hazard for skin sensitization when the chemical has adequate negative data available and it does not have structural alters and is not GHS classified (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* not listed on any screening lists.

[8] mg/L = (ppm)(MW)/(24,450) = (5,056)(100)/(24,450) = 21 mg/L using average molecular weight for unleaded gasoline (J.P. Morgan 2008).

- ECHA 2014
    - Naphtha, petroleum, hydrotreated heavy was applied to the skin of male Hartley Albino guinea pigs in 3 induction phases. The test substance was administered undiluted for the induction/challenge and challenge control group animals. The following criteria were evaluated: response grades, severity, and incidence at the time of challenge exposure. There was no difference in dermal responsiveness between the induction/challenge group and the naïve challenge control group. The positive control resulted in a significantly higher response in the induction challenge group than that observed in the naïve challenge control group. The authors of the study concluded that naphtha, petroleum, hydrotreated heavy was not dermally sensitizing.

Respiratory Sensitization (SnR) Group II* Score (H, M, or L): DG
Naphtha, petroleum, hydrotreated heavy was assigned a score of Data Gap for respiratory sensitization based on a lack of measured data.

- Authoritative and Screening Lists
    - *Authoritative:* not listed on any authoritative lists.
    - *Screening:* not listed on any screening lists.
- No data were identified for this endpoint.

Skin Irritation/Corrosivity (IrS) Group II Score (vH, H, M, or L): H
Naphtha, petroleum, hydrotreated heavy was assigned a score of High for skin irritation/corrosivity based on dermal irritation studies in rabbits. GreenScreen® criteria classify chemicals as a high hazard for skin irritation/corrosivity when data indicate that the chemical should be classified as GHS Category 2 (CPA 2012a).

- Authoritative and Screening Lists
    - *Authoritative:* not listed on any authoritative lists.
    - *Screening:* not listed on any screening lists.
- U.S. EPA 2011

  <u>Naphtha (petroleum), light alkylate (CAS# 64741-66-8)</u>
    - Application of 0.5 mL of naphtha (petroleum), light alkylate to intact or abraded skin under occluded conditions for 24 hours produced moderate irritation in rabbits. Treatment produced erythema and edema and the primary dermal irritation index was 3.9.

  <u>Naphtha (petroleum), full-range coker (CAS# 68513-02-0)</u>
    - Repeated exposure to 0.05 mL/kg naphtha (petroleum), full-range coker produced slight to moderate dermal irritation in rats.
- ECHA 2014

  <u>Unleaded gasoline (API 91-01 or API PS-6) (No CAS#)</u>
    - In a GLP-compliant dermal irritation study performed according to OECD Guideline 404, 0.5 mL of API 91-01 or API PS-6 was administered to the skin of New Zealand White rabbits. Animals were assigned one of four groups and were exposed to either test material under occlusive or semiocclusive conditions. Animals were treated for 4 hours and application sites were scored at 0.5, 1, 24, 48, and 72 hours and at 7 and 14 days after conclusion of the treatment. API 91-01 treatment caused moderate to severe erythema and slight edema. Mean erythema and edema scores for API 91-0 were 2.56 and 1.89, respectively. Erythema was fully reversible within 14 days. API PS-6 treatment caused moderate erythema, which was fully reversible within 14 days. Mean erythema and edema scores for API 91-0 were 2.39 and 1.39, respectively.

  <u>Naphtha (petroleum), heavy catalytic reformed (CAS# 64741-68-0)</u>

  - In a GLP-compliant acute dermal irritation test, 0.5 mL of heavy catalytically reformed naphtha was administered via occlusive patch onto the skin of New Zealand White rabbits for 24 hours. Treatment produced moderate to severe skin irritation. Erythema was not fully reversible within 14 days. Edema was fully reversible within 14 days. The authors noted that this test deviated from OECD Guidelines and should be used for supporting purposes only.

  Naphtha (petroleum), heavy catalytic cracked (CAS# 64741-54-4)
  - In a GLP compliant acute dermal irritation test, 0.5 mL of heavy catalytically cracked naphtha was administered onto the under occlusive conditions onto the skin of New Zealand White rabbits for 24 hours. Treatment produced erythema that persisted for 7 days and edema that persisted for 6 days. The mean erythema and edema scores were 1.3 and 0.7, respectively. The authors noted that this test deviated from OECD Guidelines and should be used for supporting purposes only.

- Based on the weight of evidence, a score of high was assigned. In a GLP-compliant skin irritation test API 91-01 caused erythema and edema with mean scores of 2.56 and 1.89, respectively. In the same study, API PS-6 caused erythema and edema with mean scores of 2.39 and 1.39, respectively. Based on GHS criteria, erythema scores of 2.3 to 4.0 warrant a classification as GHS Category 2, which corresponds to a score of High for this endpoint.

Eye Irritation/Corrosivity (IrE) Group II Score (vH, H, M, or L): L

Naphtha, petroleum, hydrotreated heavy was assigned a score of Low for eye irritation/corrosivity based on negative eye irritation tests in rabbits. GreenScreen® criteria classify chemicals as a low hazard for eye irritation/corrosivity when adequate data are available demonstrating that the chemical is not irritating, and the chemical is not present on authoritative or screening lists. (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* not listed on any screening lists.
- ECHA 2014

  Premium unleaded gasoline (No CAS#)
  - In a GLP-compliant eye irritation test, 0.1 mL of the test article was dripped onto the surface of the right eye of New Zealand White rabbits and rinsed 20-30 seconds later. Eye irritation was assessed 24, 48, 72 hours and 4 days following application of the test article. Application of the test article was not irritating to the eyes of New Zealand White rabbits. The mean conjunctivae redness, chemosis, corneal opacity, and iris lesion scores were each 0.

  100% Unleaded Cherry Point clear gasoline (F-62-01) (No CAS#)
  - In a GLP-compliant eye irritation test, 0.1 mL of the test article was dripped onto the surface of the right eye of New Zealand White rabbits and rinsed 20-30 seconds later, eye irritation was assessed at 24, 48, and 72 hours and 4 days following application of the test article. Application of the test article was not irritating to the eyes of New Zealand White rabbits. The mean corneal opacity, iris lesion, conjunctivae redness, and chemosis scores were 0, 0, 0.11, and 0, respectively.

  Naphtha (petroleum), light catalytic cracked (CAS# 64741-55-5)
  - In a GLP-compliant eye irritation test, 0.1 mL of the test article was instilled in the eyes of New Zealand White rabbits and eye irritation was assessed at 1, 24, 46, and 72 hours and 7 days following application of the test article. Ocular irritation was most prominent 28 hours after application. Irritation was reversible and subsided within 72 hours. The mean overall irritation scores at 24, 48, and 72 hours was 0.3, 0.7, and 0.0, respectively.

Supreme unleaded gasoline with ETBE (No CAS#)

- In a GLP-compliant eye irritation test performed according to OECD Guideline 405, 0.1 mL of the test article was instilled in the eyes of New Zealand White rabbits and ocular irritation was assessed at 1, 24, 48, and 72 hours and 4 days following application. Application of the test article did not cause ocular irritation. The mean corneal opacity, iris lesion, conjunctivae redness, and chemosis scores were 0, 0, 0.33, and 0.16, respectively.

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): vH

Naphtha, petroleum, hydrotreated heavy was assigned a score of Very High for acute aquatic toxicity based on measured data. GreenScreen® criteria classify chemicals as a very high hazard for acute aquatic toxicity when LC_{50} or EC_{50} values are less than or equal to 1 (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* DSL: DSL substances that are inherently toxic to aquatic organisms.
- ESIS 2000
  - 96 hour LC_{50} = 2,200 mg/L in *Pimephales promelas* (fish)
  - 96 hour LC_{50} = 4.3 mg/L in *Crangon crangon* (Crustacea)
- U.S. EPA 2011

  Naphtha (petroleum), light alkylate (CAS# 64741-66-8)
  - 96 hour LC_{50} = 0.31 mg/L in fish
  - 48 hour EC_{50} = 0.56 mg/L in aquatic invertebrates

  Naphtha (petroleum), light straight-run (CAS# 64741-46-4)
  - 96 hour EC_{50} = 0.26 mg/L in algae
- Based on the weight of evidence, naphtha, petroleum hydrotreated heavy is a Very High hazard for this endpoint.

Chronic Aquatic Toxicity (CA) Score (vH, H, M, or L): vH

Naphtha, petroleum, hydrotreated heavy was assigned a score of Very High for chronic aquatic toxicity based on measured data. GreenScreen® criteria classify chemicals as a very high hazard for chronic aquatic toxicity when NOEC values are less than 0.1 mg/L (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* DSL: DSL substances that are inherently toxic to aquatic organisms.
- U.S. EPA 2011

  Naphtha (petroleum), light alkylate (CAS# 64741-66-8)
  - 21-day EC_{50} = 1.9 mg/L (based on survival) in *Daphnia magna*
  - 21-day EC_{50} = 0.14 mg/L (based on reproduction) in *Daphnia magna*
  - 21 day NOEC = 0.23 mg/L (based on survival) in *Daphnia magna*
  - 21-day NOEC = 0.03 mg/L (based on reproduction) in *Daphnia magna*
- ECHA 2014
  - In a GLP-compliant Daphnia magna reproduction test performed according to OECD Guideline 211, the 21 day EL_{50} based on reproduction is 10 mg/L and based on mortality is greater than 40 mg/L.

- Based on the NOEC of 0.03 mg/L for the surrogate naphtha (petroleum), light alkylate in a 21-day study in daphnia, ToxServices classified naphtha, petroleum, hydrotreated heavy as a Very High hazard for this endpoint.

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): L
Naphtha, petroleum, hydrotreated heavy was assigned a score of Low for persistence based on experimental biodegradation tests for supporting chemicals. GreenScreen® criteria classify chemicals as a low hazard for persistence when the chemical is classified as GHS "Rapid degradability" (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative list.
  - *Screening:* DSL: DSL substances that are persistent.
- U.S. EPA 2011

  Naphtha (petroleum), heavy straight-run (CAS# 64741-41-9)
  - In a biodegradation test performed according to OECD Guideline 301F, naphtha, petroleum, heavy straight-run achieved greater than 77% biodegradation over 28 days, meeting the 10-day window. It was concluded that this substance is readily biodegradable.

  Naphtha (petroleum), light catalytic cracked (CAS# 64741-55-5)
  - In an inherent biodegradation test performed according to CONCAWE 1996/1997 aerobic test guideline, naphtha (petroleum), light catalytic cracked achieved 74% degradation over 28 days. Therefore, it is considered inherently biodegradable, with a biodegradation half-life of approximately 14 days.

  Naphtha (petroleum), light catalytic reformed (CAS# 64741-63-5)
  - In an inherent biodegradation test performed according to CONCAWE 1996/1997 aerobic test guideline, naphtha (petroleum), light catalytic cracked achieved 96% degradation over 28 days. Therefore, it is considered inherently biodegradable.

  Naphtha (petroleum), light alkylate (CAS# 64741-66-8)
  - In an inherent biodegradation test, naphtha (petroleum), light alkylate achieved 41% degradation in the CONCAWE test.
- U.S. EPA 2012
  - The BIOWIN modeling Ready Biodegradable Predictor indicates that Naphtha, petroleum, hydrotreated heavy is expected to be readily biodegradable (see Appendix D). Fugacity modeling predicts 68.1% will partition to water with a half-life of 9 days, 29% will partition to air with a half-life of 25.2 hours, and 1.57% will partition to soil with a half-life of 17 days.
- Based on the weight of evidence, naphtha, petroleum, hydrotreated heavy was assigned a score of low. In an OECD Guideline 301F test, naphtha (petroleum), heavy straight-run achieved 77% biodegradation after 28 days, but failed the 10-day biodegradation window. Also, in CONCAWE 1996/1997 aerobic tests, naphtha (petroleum), light catalytic cracked and naphtha (petroleum), light catalytic reformed achieved 74% and 96% degradation over 28 days, respectively. Fugacity modeling predicts that naphtha, petroleum, hydrotreated heavy will partition primarily to water. When the major compartment is water, GreenScreen® criteria specify a hazard score of Low if the chemical meets the 28-day window in a ready biodegradation test. Therefore, naphtha, petroleum, hydrotreated heavy is classified as GHS - "Rapid degradability" and assigned a score of Low for this endpoint.

Bioaccumulation (B) Score (vH, H, M, L, or vL): vH
Naphtha, petroleum, hydrotreated heavy was assigned a score of Very High for bioaccumulation based on measured data. GreenScreen® criteria classify chemicals as a very high hazard for bioaccumulation when log K_{ow} values are greater than 5.0 (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative list.
  - *Screening:* DSL: DSL substances that are bioaccumulative.
- U.S. EPA 2011
  - The log K_{ow} values range from 3.6 – 5.7.
  - The estimated bioaccumulation factor (BAF) ranges between 44-939.
- ECHA 2014
  - Based on modeling performed using EPI SuiteTM (2000), estimated BCF values range between 10 and 2,500.
- Based on the weight of the evidence, a score of Very High was assigned. Measured log K_{ow} values of 3.6-5.7 suggest potential for bioaccumulation. In addition, modeled BCF values of 10-2,500 indicate naphtha, petroleum, hydrotreated heavy may bioaccumulate. Naphtha, petroleum, hydrotreated heavy is a complex mixture of hydrocarbons, a score of very high was assigned to account for the possibility of a high proportion of bioaccumulative hydrocarbons in a given mixture.

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): L
Naphtha, petroleum, hydrotreated heavy was assigned a score of Low for reactivity based on its HMIS rating for reactivity. GreenScreen® criteria classify chemicals as a low hazard for reactivity when the chemical is not explosive, reactive with water, or self-reactive (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* not listed on any authoritative lists.
  - *Screening:* not listed on any screening lists.
- Exxon Mobil 2007
  - Naphtha, petroleum, hydrotreated heavy received an HMIS rating of 0 for reactivity ("Minimal Hazard: Materials which are normally stable even under fire conditions, and which will not react with water." (Paint.org 2014)).

Flammability (F) Score (vH, H, M, or L): M
Naphtha, petroleum, hydrotreated heavy was assigned a score of Moderate for flammability based on the WHMIS classification as Class B3 and measured data classifying the chemical as a GHS Category 3 flammable liquid. GreenScreen® criteria classify chemicals as a moderate hazard for flammability when the chemical is classified as GHS Category 3 (CPA 2012a).

- Authoritative and Screening Lists
  - *Authoritative:* U.S. DOT 49 CFR§172.101 Hazard/Division 3, Packing Group I, II, III (petroleum distillates)
  - *Screening:* WHMIS: Class B3 – Combustible liquids.
- IPCS 2001
  - Flammable
  - Flash point: 40-62ºC
- Exxon Mobil 2007
  - Naphtha, petroleum, hydrotreated heavy received an HMIS rating of 2 for flammability

("Moderate Hazard: Materials which must be moderately heated or exposed to high ambient temperatures before ignition will occur. Includes liquids having a flash point at or above 100 F but below 200 F." (Classes II and IIIA)).

- Based on the weight of evidence, a score of Moderate was assigned. IPCS (2001) classified naphtha, petroleum, hydrotreated heavy as flammable and stated the flash point is between 40-62ºC which classifies it as GHS Category 3. Naphtha, petroleum, hydrotreated heavy also received an HMIS rating of 2 for flammability, classifying it as a moderate hazard. This is consistent with classification by WHMIS as a Class B3 – combustible liquid.

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APPENDIX A: Hazard Benchmark Acronyms
(in alphabetical order)

(AA) Acute Aquatic Toxicity

(AT) Acute Mammalian Toxicity

(B) Bioaccumulation

(C) Carcinogenicity

(CA) Chronic Aquatic Toxicity

(D) Developmental Toxicity

(E) Endocrine Activity

(F) Flammability

(IrE) Eye Irritation/Corrosivity

(IrS) Skin Irritation/Corrosivity

(M) Mutagenicity and Genotoxicity

(N) Neurotoxicity

(P) Persistence

(R) Reproductive Toxicity

(Rx) Reactivity

(SnS) Sensitization- Skin

(SnR) Sensitization- Respiratory

(ST) Systemic/Organ Toxicity

APPENDIX B: Results of Automated GreenScreen® Score Calculation for Naphtha, Petroleum, Hydrotreated Heavy (CAS #64742-48-9)

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

GREEN SCREEN FOR SAFER CHEMICALS

GreenScreen® Score Inspector

Table 1: Hazard Table

			Group I Human					Group II and II* Human								Ecotox		Fate		Physical	
			Carcinogenicity	Mutagenicity/Genotoxicity	Reproductive Toxicity	Developmental Toxicity	Endocrine Activity	Acute Toxicity	Systemic Toxicity		Neurotoxicity		Skin Sensitization*	Respiratory Sensitization*	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Reactivity	Flammability
Table 2: Chemical Details									S	R *	S	R *	*	*								
Inorganic Chemical?	Chemical Name	CAS#	C	M	R	D	E	AT	STs	STr	Ns	Nr	SNS*	SNR*	IrS	IrE	AA	CA	P	B	Rx	F
No	Naphtha, petroleum, hydrotreated heavy	64742-48-9	H	H	L	M	DG	L	DG	L	M	H	L	DG	H	L	vH	vH	L	vH	L	M

Table 3: Hazard Summary Table

Benchmark	a	b	c	d	e	f	g
1	No	No	No	Yes	Yes		
2	STOP						
3	STOP						
4	STOP						

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Naphtha, petroleum, hydrotreated heavy	1

Note: Chemical has not undergone a data gap assessment. Not a Final GreenScreen™ Score

Table 6

Chemical Name	Final GreenScreen® Benchmark Score
Naphtha, petroleum, hydrotreated heavy	1

After Data gap Assessment
Note: No Data gap Assessment Done if Preliminary GS Benchmark Score is 1.

Table 5: Data Gap Assessment Table

Datagap Criteria	a	b	c	d	e	f	g	h	i	j	bm4	End Result
1												1
2												
3												
4												

APPENDIX C: Pharos Output for Naphtha, Petroleum, Hydrotreated Heavy (CAS #64742-48-9)

HYDROTREATED HEAVY NAPHTHA (PETROLEUM)

CAS RN: 64742-48-9

Detailed Direct Hazard Listings — Quickscreen

PBT	Environment Canada - Domestic Substances List (DSL) Persistent, Bioaccumulative and inherently Toxic (PBiT) to aquatic organisms - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
PBT	Environment Canada - Domestic Substances List (DSL) Persistent, Bioaccumulative and inherently Toxic (PBiT) to humans - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
CANCER	EC - REACH Annex XVII (EU CMR (1)) Carcinogen Category 2 - Substances which should be regarded as if they are carcinogenic to man - GreenScreen Benchmark 1 (LT-1) - HPD
CANCER	EC - Risk Phrases (EU R-Phrases) R45: May cause cancer. - GreenScreen Benchmark 1 (LT-1) - HPD
CANCER	EC - CLP/GHS Hazard Statements (EU H-Statements) H350 May cause cancer - GreenScreen Benchmark 1 (LT-1) - HPD
CANCER	EC - CLP Inventory (EU CMR (2)) Carcinogen - Category 1B - GreenScreen Benchmark 1 (LT-1) - HPD
GENE MUTATION	EC - CLP/GHS Hazard Statements (EU H-Statements) H340 May cause genetic defects - GreenScreen Benchmark 1 (LT-1) - HPD
GENE MUTATION	EC - CLP Inventory (EU CMR (2)) Mutagen - Category 1B - GreenScreen Benchmark 1 (LT-1) - HPD
MAMMALIAN	EC - CLP/GHS Hazard Statements (EU H-Statements) H304: May be fatal if swallowed and enters airways - Not included in GreenScreen - HPD
FLAMMABLE	Québec CSST - WHMIS Classifications (WHMIS) Class B3 - Combustible liquids - GreenScreen Benchmark Unspecified (LT-U)
PBT	Environment Canada - Domestic Substances List (DSL) DSL substances that are Persistent - GreenScreen Benchmark Unspecified (LT-U)
PBT	Environment Canada - Domestic Substances List (DSL) DSL substances that are Bioaccumulative - GreenScreen Benchmark Unspecified (LT-U)
RESTRICTED LIST	ChemSec - Substitute List (SIN) Classified CMR (Carcinogen, Mutagen &/or Reproductive Toxicant) - GreenScreen Benchmark Possible 1 (LT-P1) - HPD
RESTRICTED LIST	Environment Canada - Domestic Substances List (DSL) Inherently Toxic in the Environment - GreenScreen Benchmark Unspecified (LT-U)

Compound Group Hazard Listings

RESTRICTED LIST	CA SCP Candidate Chemicals Full Candidate Chemical List - Not included in GreenScreen

APPENDIX D: EPISuite Modeling Results for Naphtha, Petroleum, Hydrotreated Heavy (CAS #64742-48-9)

CAS Number: 64742-48-9
SMILES: CCCCCCCCC
CHEM: Naphtha (petroleum), hydrotreated heavy
MOL FOR: C9 H20
MOL WT : 128.26
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log K_{ow} (octanol-water): ------
Boiling Point (deg C): ------
Melting Point (deg C): 25.00
Vapor Pressure (mm Hg): ------
Water Solubility (mg/L): ------
Henry LC (atm-m^3/mole): ------

Log Octanol-Water Partition Coef (SRC):
Log K_{ow} (K_{ow}WIN v1.68 estimate) = 4.76
Log K_{ow} (Exper. database match) = 5.65
Exper. Ref: DAYLIGHT (2003)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 142.69 (Adapted Stein & Brown method)
Melting Pt (deg C): -56.16 (Mean or Weighted MP)
VP (mm Hg,25 deg C): 4.96 (Mean VP of Antoine & Grain methods)
VP (Pa, 25 deg C): 661 (Mean VP of Antoine & Grain methods)
MP (exp database): -53.5 deg C
BP (exp database): 150.8 deg C
VP (exp database): 4.45E+00 mm Hg (5.93E+002 Pa) at 25 deg C

Water Solubility Estimate from Log K_{ow} (WSK_{ow} v1.42):
Water Solubility at 25 deg C (mg/L): 0.3415
log K_{ow} used: 5.65 (expK_{ow} database)
melt pt used: 25.00 deg C
Water Sol (Exper. database match) = 0.22 mg/L (25 deg C)
Exper. Ref: RIDDICK, J.A. ET AL. (1986)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 0.28467 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method: 4.00E+000 atm-m^3/mole (4.05E+005 Pa-m^3/mole)
Group Method: 4.77E+000 atm-m^3/mole (4.83E+005 Pa-m^3/mole)
Exper Database: 3.40E+00 atm-m^3/mole (3.45E+005 Pa-m^3/mole)

For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 2.451E+000 atm-m3/mole (2.484E+005 Pa-m^3/mole)
VP: 4.96 mm Hg (source: MPBPVP)
WS: 0.342 mg/L (source: $WSK_{ow}WIN$)

Log Octanol-Air Partition Coefficient (25 deg C) [K_{oa}WIN v1.10]:
Log K_{ow} used: 5.65 (exp database)
Log K_{aw} used: 2.143 (exp database)
Log K_{oa} (K_{oa}WIN v1.10 estimate): 3.507
Log K_{oa} (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model): 0.9033
Biowin2 (Non-Linear Model): 0.9924
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.5124 (days-weeks)
Biowin4 (Primary Survey Model): 4.2008 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model): 0.6773
Biowin6 (MITI Non-Linear Model): 0.8663
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.2234
Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
LOG BioHC Half-Life (days): 0.8713
BioHC Half-Life (days): 7.4345

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 593 Pa (4.45 mm Hg)
Log K_{oa} (K_{oa}WIN est): 3.507
Kp (particle/gas partition coef. (m^3/µg)):
Mackay model: 5.06E-009
Octanol/air (K_{oa}) model: 7.89E-010
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model: 1.83E-007
Mackay model: 4.04E-007
Octanol/air (K_{oa}) model: 6.31E-008

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 9.6974 E-12 cm^3/molecule-sec
Half-Life = 1.103 Days (12-hr. day; 1.5E6 OH/cm^3)
Half-Life = 13.236 Hrs.
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):

2.94E-007 (Junge-Pankow, Mackay avg)
6.31E-008 (K_{oa} method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (K_{oc}WIN v2.00):
K_{oc}: 796 L/kg (MCI method)
Log K_{oc}: 2.901 (MCI method)
K_{oc}: 8.003E+004 L/kg (K_{ow} method)
Log K_{oc}: 4.903 (K_{ow} method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 2.021 (BCF = 104.9 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 0.5983 days (HL = 3.965 days)
Log BCF Arnot-Gobas method (upper trophic) = 3.481 (BCF = 3029)
Log BAF Arnot-Gobas method (upper trophic) = 3.881 (BAF = 7601)
log K_{ow} used: 5.65 (expK_{ow} database)

Volatilization from Water:
Henry LC: 3.4 atm-m^3/mole (Henry experimental database)
Half-Life from Model River: 1.156 hours
Half-Life from Model Lake: 107.6 hours (4.482 days)

Removal in Wastewater Treatment (recommended maximum 95%):
Total removal: 99.92 percent
Total biodegradation: 0.17 percent
Total sludge adsorption: 56.95 percent
Total to Air: 42.80 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr.)	Emissions (kg/hr.)
Air	29	25.2	1000
Water	68.1	208	1000
Soil	1.57	416	1000
Sediment	1.37	1.87e+003	0

Persistence Time: 72.2 hr.

Sources to Check for GreenScreen® Hazard Assessment

Note: For a GreenScreen® Hazard Assessment, data queries should be initially limited to the following references. If data gaps exist after these references have been checked, additional references may be utilized.

U.S. EPA High Production Volume Information System (HPVIS):
http://www.epa.gov/hpvis/index.html

UNEP OECD Screening Information Datasets (SIDS):
http://www.chem.unep.ch/irptc/sids/OECDSIDS/sidspub.html

OECD Existing Chemicals Database: http://webnet.oecd.org/hpv/ui/SponsoredChemicals.aspx

European Chemical Substances Information System IUCLID Chemical Data Sheets:
http://esis.jrc.ec.europa.eu/index.php?PGM=dat

National Toxicology Program: http://ntp.niehs.nih.gov/

International Agency for the Research on Cancer:
http://monographs.iarc.fr/ENG/Classification/index.php

Human and Environmental Risk Assessment (HERA) on ingredients of household cleaning products:
http://www.heraproject.com/RiskAssessment.cfm

European Chemicals Agency (ECHA) REACH Dossiers: http://echa.europa.eu/

Licensed GreenScreen® Profilers

Naphtha, petroleum, hydrotreated heavy GreenScreen® Evaluation Prepared by:

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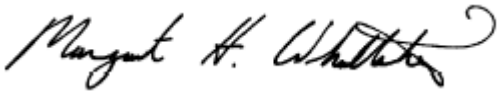
ToxServices LLC

Naphtha, petroleum, hydrotreated heavy GreenScreen® Evaluation QC'd by:



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