UNDECANE

(CAS #1120-21-4)

GREENSCREEN® FOR SAFER CHEMICALS (GREENSCREEN®) ASSESSMENT

Prepared by:

ToxServices LLC

Assessment Date: February 24, 2025[1]

Expiration Date: February 24, 2030

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[1] The report was lasted updated on February 24, 2025. However, the last complete literature search was conducted on December 17, 2024.

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GreenScreen® Executive Summary for Undecane (CAS #1120-21-4)

Undecane is a linear C11 aliphatic hydrocarbon. It is used as feedstock for detergents, other industrial materials, reaction solvents, and solvents for industrial cleaning products. It is a component of consumer products such as car wax and lamp oil. It is used as a solvent in printing inks and degreasing products, and as a chemical intermediate for the production of chlorinated paraffins (C10-C30), n-paraffins (C10-C14), n-alcohol-paraffins (C11-C14), internal olefins and sulfonates, and citric acid. Additionally, it functions as a skin conditioning agent and emollient in cosmetic formulations. Undecane is a liquid under standard temperature and pressure. It has a high estimated vapor pressure, and low measured boiling point, indicating that it is volatile. It is slightly soluble in water.

Undecane was assigned a **GreenScreen Benchmark™ Score of 2** ("Use but Search for Safer Substitutes"). This score is based on the following hazard score combinations:

- Benchmark 2d
    - High Bioaccumulation-B + Moderate Group II Human Toxicity (eye irritation-IrE)
    - High B + High Group II Human Toxicity (single dose systemic toxicity-STs and skin irritation-IrS)
    - High B + Very High Ecotoxicity (chronic aquatic-CA)
- Benchmark 2f
    - Very High Ecotoxicity (CA)

A data gap (DG) exists for endocrine activity-E. As outlined in GreenScreen® Guidance Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), undecane meets requirements for a GreenScreen Benchmark™ Score of 2 despite the hazard data gap. In a worst-case scenario, if undecane were assigned a High score for the data gap E, it would be categorized as a Benchmark 1 Chemical.

New Approach Methodologies (NAMs) used in this GreenScreen® include *in silico* modeling for carcinogenicity, endocrine activity, respiratory sensitization, chronic aquatic toxicity, persistence, and bioaccumulation, and *in vitro* testing for genotoxicity, and endocrine activity. The quality, utility, and accuracy of NAM predictions are greatly influenced by two primary types of uncertainties:

- Type I: Uncertainties related to the input data used
- Type II: Uncertainties related to extrapolations made

Type I (input data) uncertainties in undecane's NAMs dataset includes lack of *in vivo* measured data for carcinogenicity, endocrine activity, respiratory sensitization, chronic aquatic toxicity for the fish trophic level, and bioaccumulation, and lack of validated test methods for respiratory sensitization. Undecane's Type II (extrapolation output) uncertainties include lack of defined applicability domains for Toxtree, ToxCast models, and OECD Toolbox structural alerts, limitations of *in vitro* genotoxicity assays in focusing on only a few events in the process of genotoxicity, and in mimicking *in vivo* conditions, Tox 21 EDSP high throughput screening assays' incomplete coverage of critical endocrine pathways and lack of consideration of toxicokinetics *in vivo,* and OECD Toolbox respiratory sensitization structural alerts' lack of consideration of non-immunological mechanisms.

GreenScreen® Hazard Summary for Undecane

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
						s	r*	s	r*	*	*								
L	**L**	*L*	*L*	DG	**L**	**H**	**L**	*L*	*L*	**L**	*L*	*H*	*M*	**L**	**vH**	*vL*	*H*	*L*	**M**

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. 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. Group II* Human Health endpoints are indicated by an * after the name of the hazard endpoint or after "repeat" for repeated exposure sub-endpoints. Please see Appendix A for a glossary of hazard acronyms.

GreenScreen® Chemical Assessment for Undecane (CAS #1120-21-4)

Method Version: GreenScreen® Version 1.4
Assessment Type[2]: Certified
Assessor Type: Licensed GreenScreen® Profiler

GreenScreen® Assessment (v.1.4) Prepared By:
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Date: December 3, 2024; February 19, 2025

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Date: December 17, 2024; February 24, 2025

Expiration Date: February 24, 2030[3]

Chemical Name: Undecane

CAS Number: 1120-21-4

Chemical Structure(s):

Also called:
Hendecane; n-Hendecane; Hendekan; Undekan; Decane, methyl- (PubChem 2024).

Suitable surrogates or moieties of chemicals used in this assessment (CAS #'s):
Limited data are available for undecane from the OECD SIDS initial assessment profiles on undecane (OECD 2010) and the C9-14 aliphatic (≤ 2% aromatic) hydrocarbon solvent category (OECD 2012), and the REACH registration dossier for undecane (ECHA, CAS #1120-21-4, 2024). Data on structurally similar hydrocarbons are therefore included where available.

Decane (CAS #124-18-5)

Structure not available
Hydrocarbons, C10-12, isoalkanes, <2% aromatics (CAS #N/A)

Structure not available
Hydrocarbons, C9-11, isoalkanes, cyclics, <2% aromatics (CAS #N/A)

Identify Applications/Functional Uses:
1. Solvent in printing inks and degreasing products
2. Chemical intermediate

[2] GreenScreen® reports are either "UNACCREDITED" (by unaccredited person), "AUTHORIZED" (by Authorized GreenScreen® Practitioner), or "CERTIFIED" (by Licensed GreenScreen® Profiler or equivalent).
[3] Assessments expire five years from the date of completion starting from January 1, 2019. An assessment expires three years from the date of completion if completed before January 1, 2019 (CPA 2018a).

3. Skin conditioning agent
4. Emollient
(HSDB 2017, EC 2024)

Known Impurities[4]:
No information is available. The screen is performed on the theoretical pure substance.

GreenScreen® Summary Rating for Undecane[5,6 7,8]: Undecane was assigned a **GreenScreen Benchmark™ Score of 2** ("Use but Search for Safer Substitutes") (CPA 2018b). This score is based on the following hazard score combinations:

- Benchmark 2d
  - High Bioaccumulation-B + Moderate Group II Human Toxicity (eye irritation-IrE)
  - High B + High Group II Human Toxicity (single dose systemic toxicity-STs and skin irritation-IrS)
  - High B + Very High Ecotoxicity (chronic aquatic-CA)
- Benchmark 2f
  - Very High Ecotoxicity (CA)

A data gap (DG) exists for endocrine activity-E. As outlined in GreenScreen® Guidance (CPA 2018b) Section 11.6.2.1 and Annex 5 (Conduct a Data Gap Analysis), undecane meets requirements for a GreenScreen Benchmark™ Score of 2 despite the hazard data gap. In a worst-case scenario, if undecane were assigned a High score for the data gap E, it would be categorized as a Benchmark 1 Chemical.

Figure 1: GreenScreen® Hazard Summary for Undecane

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
						s	r*	s	r*	*	*								
L	**L**	*L*	*L*	DG	**L**	**H**	**L**	*L*	*L*	**L**	*L*	*H*	*M*	**L**	**vH**	*vL*	*H*	*L*	**M**

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence in the hazard classification. 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. Group II* Human Health endpoints are indicated by an * after the name of the hazard endpoint or after "repeat" for repeated exposure sub-endpoints. Please see Appendix A for a glossary of hazard acronyms.

Environmental Transformation Products
Per GreenScreen® guidance (CPA 2018b), chemicals that degrade rapidly and completely (i.e., meet criteria for a Very Low for persistence) are not likely to form persistent biodegradation intermediates because the degradation intermediates will not persist long enough to be encountered after use or release

[4] Impurities of the chemical will be assessed at the product level instead of in this GreenScreen®.
[5] 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.
[6] See Appendix A for a glossary of hazard endpoint acronyms.
[7] For inorganic chemicals only, see GreenScreen® Guidance v1.4 Section 12 (Inorganic Chemical Assessment Procedure).
[8] For Systemic Toxicity and Neurotoxicity, repeated exposure data are preferred. Lack of single exposure data is not a Data Gap when repeated exposure data are available. In that case, lack of single exposure data may be represented as NA instead of DG. See GreenScreen® Guidance v1.4 Annex 2.

of the parent chemical (i.e., relevant). As undecane is readily biodegradable, it is not expected to have relevant transformation products.

Introduction

Undecane is a linear C11 aliphatic hydrocarbon. It is used as feedstock for detergents, other industrial materials, reaction solvents, and solvents for industrial cleaning products. It is a component of consumer products such as car wax and lamp oil (OECD 2010). It is used as a solvent in printing inks and degreasing products, and as a chemical intermediate for the production of chlorinated paraffins (C10-C30), n-paraffins (C10-C14), n-alcohol-paraffins (C11-C14), internal olefins and sulfonates, and citric acid (HSDB 2017). Additionally, it functions as a skin conditioning agent and emollient in cosmetic formulations (EC 2024). It is manufactured through the refinement of petroleum, in which n-paraffins are isolated from the kerosene fraction via adsorption to molecular sieves or adduction with urea and then distilled (PubChem 2024).

ToxServices assessed undecane against GreenScreen® Version 1.4 (CPA 2018b) following procedures outlined in ToxServices' SOPs (GreenScreen® Hazard Assessment) (ToxServices 2021).

U.S. EPA Safer Choice Program's Safer Chemical Ingredients List

The SCIL is a list of chemicals that meet the Safer Choice standard (U.S. EPA 2024a). It can be accessed at: http://www2.epa.gov/saferchoice/safer-ingredients. Chemicals on the SCIL have been assessed for compliance with the Safer Choice Standard and Criteria for Safer Chemical Ingredients (U.S. EPA 2024b).

Undecane is not listed on the U.S. EPA SCIL.

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 2018b). Pharos (Pharos 2024) is an online list-searching tool that is used to screen chemicals against all of the lists in the List Translator electronically. ToxServices also checks the U.S. Department of Transportation (U.S. DOT) lists (U.S. DOT 2008a,b),[9] which are not considered GreenScreen® Specified Lists but are additional information sources, in conjunction with the Pharos query. The output indicates benchmark or possible benchmark scores for each human health and environmental endpoint. The output for Undecane can be found in Appendix C.

- Undecane is an LT-P1 chemical when screened using Pharos, and therefore a full GreenScreen® is required.
- Undecane is not listed on the U.S. DOT list.
- Undecane is on the following lists for multiple endpoints:
    - EC CEPA DSL – Inherently Toxic in the Environment (iTE)
    - GHS Japan – H410 – Very toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment (chronic) – Category 1]
    - GHS New Zealand – Hazardous to the aquatic environment – chronic category 4
- Specified lists for single endpoints are reported in individual hazard endpoints in the hazard assessment section below.

[9] DOT lists are not required lists for GreenScreen® List Translator v1.4. They are reference lists only.

Hazard Statement and Occupational Control

One Globally Harmonized System of Classification and Labelling of Chemicals (GHS) hazard statement self-assigned by its ECHA dossier authors was identified for undecane, as indicated in Table 1. General personal protective equipment (PPE) recommendations are presented in Table 2, below. No occupational exposure limits (OELs) were identified.

Table 1: GHS H Statements for Undecane (CAS #1120-21-4) (ECHA, CAS #1120-21-4, 2024)

H Statement	H Statement Details
H304	May be fatal if swallowed and enters airways

Table 2: Occupational Exposure Limits and Recommended Personal Protective Equipment for Undecane (CAS #1120-21-4)

Personal Protective Equipment (PPE)	Reference	Occupational Exposure Limits (OEL)	Reference
PPE not required	ECHA, CAS #1120-21-4, 2024	None identified	

Physicochemical Properties of Undecane

Undecane is a liquid under standard temperature and pressure. It has a high estimated vapor pressure and relatively low boiling point, indicating that it is volatile. It is slightly soluble in water, and its higher estimated log K_{ow} of 5.25-6.23 indicates that it has the potential to bioaccumulate in aquatic biota.

Table 3: Physical and Chemical Properties of Undecane (CAS #1120-21-4)

Property	Value	Reference
Molecular formula	$C_{11}H_{24}$	PubChem 2024
SMILES Notation	CCCCCCCCCCC	PubChem 2024
Molecular weight	156.31 g/mol	PubChem 2024
Physical state	Liquid	PubChem 2024
Appearance	Clear, colorless	PubChem 2024
Melting point	-25.54°C	PubChem 2024
Boiling point	195-198°C	PubChem 2024
Vapor pressure	0.06 kPa at 25°C (est.)	ECHA, CAS #1120-21-4, 2024
Water solubility	0.014 mg/L at 25°C	PubChem 2024
Dissociation constant	Not applicable	ECHA, CAS #1120-21-4, 2024
Density/specific gravity	0.744 g/cm^3 at 15°C (ISO 12185)	ECHA, CAS #1120-21-4, 2024
Partition coefficient	Log K_{ow} = 5.25-6.23 at 20°C (est.)	ECHA, CAS #1120-21-4, 2024

Toxicokinetics

Undecane is readily absorbed via the inhalation route of exposure and distributed to various tissues, but especially fat tissue in rats. Undecane is predominantly distributed to the brain and a long-lasting redistribution from fat tissues to the brain can occur. Based on *in vitro* results, the amount of undecane that can be absorbed through the skin is expected to be very low (OECD 2010).

Hazard Classification Summary

Group I Human Health Effects (Group I Human)

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

Undecane was assigned a score of Low for carcinogenicity based on negative predictions from rule-based and statistical based models. GreenScreen® criteria classify chemicals as a Low hazard for carcinogenicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low due to the lack of experimental data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- Toxtree 2018
  - Based on its default structure, undecane does not have any structural alerts for genotoxic or nongenotoxic carcinogenicity (Appendix D).
- VEGA 2024
  - ToxServices predicted the carcinogenicity potential of undecane using the following six VEGA v.1.2.3 models: CAESAR v.2.1.10, ISS v.1.0.3, IRFMN/ISSCAN-CGX v.1.0.2, IRFMN/Antares v1.0.2, IRFMN oral classification v1.0.1, and IRFMN inhalation classification v1.0.1 models. If an external compound is beyond the defined scope of a given model, it is considered outside that model's applicability domain (AD) and cannot be associated with a reliable prediction (Sahigara 2007). Values for AD index (ADI) range from 0 (worst case) to 1 (best case). Generally, ADI values of > 0.70 indicate that the prediction has moderate or better predictivity (Gad 2016).
  - Undecane is outside the AD for three of the models: CAESAR v.2.1.10, ISS v.1.0.3, and IRFMN/Antares v.1.0.2. Therefore, ToxServices did not incorporate the results of these three models into the weight of evidence evaluation.
  - Undecane is inside the AD for the remaining three models (IRFMN-ISSCAN-CGX v.1.0.2, IRFMN oral classification v.1.0.1, and IRFMN inhalation classification v.1.0.1), and all three are predictions that undecane is negative for carcinogenicity (Appendix E).
- DTU 2024 (Appendix F)
  - Using the E Ultra FDA RCA Cancer model, undecane was predicted to be negative for carcinogenicity and was within the applicability domain for all datasets (i.e., Male Rat, Female Rat, Rat, Male Mouse, Female Mouse, Mouse, and Rodent).
  - Using the Leadscope FDA RCA Cancer model, the compound was outside the applicability domain for all datasets (i.e., Female Rat, Male Mouse, Female Mouse, Mouse, and Rodent), and the result is not included in the weight of evidence.
  - For the liver-specific cancer in rats or mouse model, the CASE Ultra, Leadscope, and SciQSAR models as well as the overall model battery predictions are negative and within the applicability domains.
- Based on the weight of evidence, a score of Low was assigned. Toxtree (a rule-based program) identified no structural alerts for genotoxic or nongenotoxic carcinogenicity for the target compound. Additionally, undecane was predicted to be a non-carcinogen by three rule-based models in VEGA, as well as all models of the statistical-based E Ultra and liver-specific cancer models that were within their respective applicability domains.

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

Undecane was assigned a score of Low for mutagenicity/genotoxicity based on a lack of genotoxicity effects seen in bacteria (mutagenicity) and mammalian cells (chromosomal aberration). GreenScreen® criteria classify chemicals as a Low hazard for mutagenicity/genotoxicity when negative data are available for both gene mutations and chromosome aberrations, and they are not GHS classified (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data on the target chemical.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- OECD 2010
  - *In vitro:* Undecane was not mutagenic in a GLP-compliant bacterial reverse mutation assay conducted in accordance with OECD Guidelines 471 and 472. *Salmonella typhimurium* test strains TA98, TA100, TA1535, and TA1537, as well as *Escherichia coli* strain WP_2 *uvr*A, were exposed to undecane (99% purity) at concentrations of 0, 313, 625, 1,250, 2,500 and 5,000 µg/plate in the presence or absence of exogenous metabolic activation (SD rat liver induced with phenobarbital and 5,6-benzoflavone). A vehicle of acetone was used. The positive controls were AF-2 (furylfuramide), sodium azide, 9-aminoacridine, and 2-aminoanthracene. No cytotoxicity was reported. There were no increases in mutation frequency detected in any test strains with treatment in the presence or absence of metabolic activation. The vehicle and positive controls were valid (Klimisch 1, Reliable without restrictions).
  - *In vitro:* Undecane was not clastogenic in a GLP-compliant chromosome aberration assay conducted in accordance with Japan Guidelines for Screening Mutagenicity Testing of Chemicals. Chinese hamster lung (CHL/IU) cells were exposed to undecane (99% purity) at concentrations of 0, 0.40, 0.80, 1.6 mg/mL in the presence or absence of exogenous metabolic activation (rat liver induced with phenobarbital and 5,6-benzoflavone). A vehicle of acetone was used. The positive controls were mitomycin C and cyclophosphamide. Cytotoxicity was reported at the highest concentration of 1.6 mg/mL both in the presence and absence of metabolic activation. Undecane did not induce structural chromosomal aberrations or polyploidy at any of the concentrations tested in the presence or absence of metabolic activation. The vehicle and positive controls were valid (Klimisch 1, reliable without restrictions).

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

Undecane was assigned a score of Low for reproductive toxicity based on no effects seen on reproductive parameters in an OECD Guideline 422 study in rats. GreenScreen® criteria classify chemicals as a Low hazard for reproductive toxicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low as it is based on a screening study.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- OECD 2012, ECHA, CAS #1120-21-4, 2024
  - *Oral:* Undecane was tested in a GLP-compliant combined reproduction and developmental toxicity screening test conducted in a manner similar to OECD Guideline 422. Sprague-Dawley rats (12/sex/dose) received undecane at doses of 0, 100, 300, or 1,000 mg/kg/day via gavage for 14 days prior to mating, through the mating period, and for a total of 46 days

(males) or through lactation day 3 (females). There were no effects on the sex cycle of females, copulation and conception, pathological changes to the testis, epididymis, ovary, or number of pups. Study authors identified a NOAEL of 1,000 mg/kg/day, the highest dose tested, for reproductive toxicity (Klimisch 1, Reliable without restrictions).

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M, or L): *L*
Undecane was assigned a score of Low for developmental toxicity based on no developmental toxicity effects seen in a combined reproduction and developmental toxicity screening test in rats. GreenScreen® criteria classify chemicals as a Low hazard for developmental toxicity when adequate negative data are available and they are not GHS classified (CPA 2018b). The confidence in the score is low as it is based on a screening study.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- OECD 2010, 2012, ECHA, CAS #1120-21-4, 2024
  - *Oral:* In the previously described GLP-unspecified combined reproduction and developmental toxicity screening test conducted in a manner similar to OECD Guideline 422 in 1996, Sprague-Dawley rats (12/sex/dose) were administered undecane (purity 99%) at doses of 0, 100, 300, or 1,000 mg/kg/day via gavage for 14 days prior to mating, through the mating period, and for a total of 46 days (males) or through lactation day 3 (females). No significant treatment related effects on systemic toxicity were observed; however, slight to moderate irritation to the non-glandular mucosa of the stomach was observed and considered related to the dosing method used. There were no treatment related effects on the offspring survival, mean litter size, sex ratio, body weight, and external and internal abnormalities. Study authors identified a NOAEL of 1,000 mg/kg/day, the highest dose tested, for maternal and developmental toxicity (Klimisch 1, Reliable without restriction).
    - The authors of the ECHA dossier did not identify treatment-related adverse effects on maternal toxicity. OECD (2010) identified a NOAEL of 300 mg/kg/day for maternal and developmental toxicity based on a reduction in body weight gain for offspring that may be due to general maternal toxicity; however, no treatment related effects on maternal toxicity were identified (OECD 2010). However, OECD (2012) considered reduction in body weight gain for the mid-dose group not treatment related as this effect was not observed in the high dose group; therefore OECD (2012) identified a NOAEL of 1,000 mg/kg/day, the highest dose tested, for developmental toxicity.

Endocrine Activity (E) Score (H, M, or L): DG
Undecane was assigned a score of Data Gap for endocrine activity based on insufficient data identified for this endpoint. The negative results from *in vitro* high throughput screening assays for interactions with estrogen, androgen, thyroid, and steroidogenesis pathways, and inactive prediction by ToxCast models for estrogen receptor activity are insufficient to determine the *in vivo* activity for endocrine pathways.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- U.S. EPA 2024c
  - Undecane was inactive in 18/18 estrogen receptor (ER) assays, 15/15 androgen receptor (AR) assays, 17/17 thyroid receptor assays, and 2/2 steroidogenesis assays performed as part

of the U.S. EPA's Endocrine Disruptor Screening Program (EDSP) in the 21st Century (Appendix D).
  - Undecane was predicted to be inactive for estrogen agonism, antagonism and binding by the CERAPP Potency Level (from literature) ToxCast model.

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

Note: Group II and Group II* endpoints are distinguished in the v 1.4 Benchmark system (the asterisk indicates repeated exposure). For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints. See GreenScreen® Guidance v1.4, Annex 2 for more details.

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

Undecane was assigned a score of Low for acute toxicity based on an oral LD_{50} > 2,000 mg/kg in rats. GreenScreen® criteria classify chemicals as a Low hazard for acute toxicity when oral LD_{50} values are < 2,000 mg/kg (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- OECD 2010
  - *Oral*: LD_{50} > 2,000 mg/kg in male and female Wistar rats (GLP-compliant, OECD Guideline 401) (Klimisch 1, reliable without restrictions)
  - *Inhalation*: 8-hour LC_{50} > 2.82 mg/L saturated vapor in male rats (strain not reported) (GLP compliance and test method not reported) (Klimisch 2, reliable without restrictions)
    - *ToxServices converted this value to a 4-hour vapor LC_{50} as follows: 4-hour LC_{50} = LC_{50} at 8 hours * $8^{1/2}/2$ = 2.82 mg/L * $8^{1/2}/2$ = 4.0 mg/L. Therefore, the 4-hour LC_{50} > 4.0 mg/L.*

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST-single) (Group II) Score (vH, H, M, or L): H

Undecane was assigned a score of High for systemic toxicity (single dose) based ToxServices classifying it as a GHS Category 1 aspiration hazard. GreenScreen® criteria classify chemicals as a High hazard for systemic toxicity (single dose) when they are GHS Category 1 aspiration hazards (CPA 2018b). Confidence is high based on the physicochemical properties and support from an authoritative body (i.e., OECD).

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* GHS Japan: H335 – May cause respiratory irritation [Specific target organ toxicity – single exposure – Category 3]
    - Based on descriptions of mucous membrane and upper respiratory tract irritation from Patty's Toxicology (2001) (NITE 2010)
- OECD 2010
  - *Oral*: In the previously described GLP-compliant oral acute toxicity study conducted according to OECD Guideline 401, Crj:CD(SD) rats (5/sex/dose) were given single gavage doses of 0, 500, 1,000 or 2,000 mg/kg undecane. Diarrhea was observed on the day of dosing both in treatment and control groups, which disappeared the next day. Therefore, study authors attributed this effect to the vehicle of olive oil. There were no other effects on clinical signs, body weight, or gross necropsy (Klimisch 1, reliable without restriction).

  - *Inhalation*: In an inhalation acute toxicity study in male rats, an 8-hour LC_{50} was calculated to be > 2.82 mg/L saturated undecane vapor. No treatment related effects on clinical signs, body weights, gross pathology and histopathology were observed (Klimisch 2, reliable with restrictions).
- HSDB 2017
  - Industrial exposure to undecane causes irritation to the upper respiratory tract.
  - *Inhalation:* Kristiansen and Nielsen (1988) studied the sensory irritation effects of n-alkane vapors from C7 to C11 in mice. The maximum irritation reaction within the first 10 minutes of exposure decreased as carbon chain lengths increased, reflecting a decrease in intrinsic activity. The RD_{50} (concentration at which respiratory rate depressed by 50%) was determined to be 17,400 ppm for heptane, and RD_{50} values could not be determined for other C8-C11 n-alkanes due to lower response levels. However, the threshold concentration (i.e., RD_0) decreased with increasing carbon chain length, reflecting an increase in potency. Additional analysis indicated the increase in potency by chain length was due to differences in distribution between the gas/air phase and the receptor phase. The study authors derived upper limits for sensory irritation, as references in the occupational setting, to be 1,205, 605, and 125 ppm for heptane, octane and nonane, respectively. The authors could not derive a limit for undecane due to "low intrinsic activity". Overall, the study authors concluded the pulmonary irritation potential for n-alkanes with 7-11 carbons to be weak, with the exception of heptane.
- ECHA, CAS #1120-21-4, 2024
  - Undecane has a kinematic viscosity of 1.597 mm^2/s at 20°C according to the ISO 3104 test (Klimisch 2, reliable with restrictions)
- Based on the weight of evidence, a score of High was assigned. Japan classified undecane to GHS Category 3 based on qualitative descriptions, and no additional information was available. No respiratory irritation was found in an acute inhalation study in rats and in another study designed to investigate respiratory irritation of n-alkane vapors in mice. Therefore, ToxServices discounted Japan's classification. On the other hand, GHS criteria classify chemicals as aspiration hazards Category 1 when they are hydrocarbons, alcohols, or ketones with a kinematic viscosity of ≤ 20 mm^2/s at 40°C along with consideration of surface tension, water solubility, boiling point, and volatility (UN 2023). There were no signs of aspiration identified in animal studies described previously. However, undecane is a hydrocarbon with a kinematic viscosity of 1.597 mm^2/s at 20°C. Though the viscosity at 40°C is unknown, it is expected to be lower than 1.597 mm^2/s, as kinematic viscosity decreases with temperature for liquids. Furthermore, OECD concluded that C9-C14 aliphatic hydrocarbon solvents such as undecane pose aspiration hazards if taken into the lung in a liquid state due to their physical and chemical properties (i.e., viscosity). Therefore, undecane meets the criteria for GHS Category 1 Aspiration hazard.

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST-repeat) (Group II*) Score (H, M, or L): L

Undecane was assigned a score of Low for systemic toxicity (repeated dose) based on a lack of systemic effects seen in a combined reproduction and developmental toxicity screening assay in rats. GreenScreen® criteria classify chemicals as a Low hazard for systemic toxicity (repeated dose) when adequate negative data are available and the chemical is GHS not classified (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.

- OECD 2012, ECHA, CAS #1120-21-4, 2024
    - *Oral:* In the previously described GLP-unspecified combined reproduction and developmental toxicity screening test conducted in a manner similar to OECD Guideline 422, Sprague-Dawley rats (12/sex/dose) were administered undecane (purity 99%) at doses of 0, 100, 300, or 1,000 mg/kg/day via gavage for 14 days prior to mating, through the mating period, and for a total of 46 days (males) or through lactation day 3 (females). No significant treatment related effects on systemic toxicity were observed, including clinical signs, body weight, food consumption, hematology, clinical biochemistry, organ weights, gross pathology, or histopathology. The following observations in the top dose groups were reported to not be toxicologically relevant due to a lack of related histopathology findings: clinical sign of salivation; reduced weight gain with reduced food consumption for males; increased body weights and increased food consumption for females; decreased hemoglobin concentration and albumin; increased white blood cell count, α2-globulin, glutamic-pyruvic transaminase (GPT), and cholinesterase; and increased absolute and relative liver weights for males and females. Slight to moderate irritation to the non-glandular mucosa of the stomach was observed and considered related to the dosing method used. No additional histopathological findings were reported. Study authors identified a NOAEL of 1,000 mg/kg/day, the highest dose tested, for systemic toxicity (Klimisch 1, reliable without restriction).

Neurotoxicity (single dose, N-single) (Group II) Score (vH, H, M, or L): *L*
Undecane was assigned a score of Low for neurotoxicity (single dose) based on lack of clinical signs and gross pathology findings indicative of neurotoxicity in acute oral and inhalation toxicity studies at oral doses up to 2,000 mg/kg in rats and with saturated undecane vapor. GreenScreen® criteria classify chemicals as a Low hazard for neurotoxicity (single dose) when adequate data are available and they are not classified under GHS (CPA 2018b). Confidence in the score is reduced due to lack of specific neurotoxicity examinations in standard acute toxicity studies.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- OECD 2010
    - *Oral*: In the previously described GLP-compliant oral acute toxicity study conducted according to OECD Guideline 401, Crj:CD(SD) rats (5/sex/dose) were given single gavage doses of 0, 500, 1,000 or 2,000 mg/kg undecane. There were no effects on clinical signs, or gross necropsy (Klimisch 1, reliable without restriction).
    - *Inhalation*: In an inhalation acute toxicity study in male rats, an 8-hour LC_{50} was calculated to be > 2.82 mg/L saturated undecane vapor. No treatment related effects on clinical signs, gross pathology and histopathology were observed (Klimisch 2, reliable with restrictions).

Neurotoxicity (repeated dose, N-repeated) (Group II*) Score (H, M, or L): *L*
Undecane was assigned a score of Low for neurotoxicity (repeated dose) based on no neurotoxic effects seen in rats in a combined reproduction and developmental toxicity screening assay in rats with the close surrogate decane. GreenScreen® criteria classify chemicals as a Low hazard for neurotoxicity (repeated dose) when adequate negative data are available and the chemical is not GHS classified (CPA 2018b). The confidence in the score is low as white mineral spirit which contains 10-25% aromatics, is associated with neurotoxicity in humans, which may or may not be relevant to undecane.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.

  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #124-18-5, 2024
  - *Surrogate: Decane (CAS #124-18-5):* In a GLP-compliant combined reproduction and developmental toxicity screening test conducted in a manner similar to OECD Guideline 422 in 1995, Sprague-Dawley rats (10/sex/dose) were administered surrogate decane (97% purity) at doses of 0, 25, 150, or 1,000 mg/kg/day via gavage for 14 days prior to mating, through the mating period, and for a total of 46 days (males) or through lactation day 4 (females). There were no test-related findings in neurobehavioral activity. Functional tests including startle reflex, open field test, and forelimb grip reflex performance were evaluated, and no treatment-related effects were observed. Additionally, histopathology and gross pathology findings did not report treatment related effects of the brain or spinal cord. Study authors identified a NOAEL of 1,000 mg/kg/day, the highest dose tested, for systemic toxicity, including neurotoxicity (Klimisch 1, reliable without restrictions).
- OECD 2012, McKee et al. 2018
  - OECD summarized a review of human literature demonstrating the potential for hydrocarbon solvents to cause chronic neurological effects in humans. The review focused on International Programme on Chemical Safety (IPCS), Scientific Committee on Occupational Exposure Limits (SCOEL), and European Chemicals Agency (ECHA) Committee for Risk Assessment (RAC) evaluations of epidemiological studies of white spirits, which is a C9-C11 aliphatic hydrocarbon solvent containing 15-20% aromatics. In epidemiological studies, this solvent has been associated with complaints of memory fatigue, impaired concentration, irritability, dizziness, headache, anxiety and apathy, and impairment in short-term visual memory tests and the symbol-digit test. Effects increased with duration of exposure. European Chemical Agency (ECHA)'s Risk Assessment Committee (RAC) concluded that chronic exposure to white spirits can cause effects in psychomotor, perception, and memory parameters, and disturbances in mood which can progress in severity. Studies are confounded by co-exposure to other solvents.
- Based on the weight of evidence, a score of Low was assigned. While human data on white spirits indicate neurotoxicity concerns, it is not clear if undecane or other hydrocarbon compounds (such as aromatics present at 15-20%) in the mixture contributed to the observed neurotoxicity. The aromatic fraction of white spirit (10-25%) is generally believed to be more toxic than the aliphatic fraction, and the epidemiological studies could not completely establish causal relationships between white spirit exposure and neurotoxicity observed in painters, due to co-exposure to other more volatile solvents. The combined reproduction and developmental toxicity screening test in rats on surrogate decane did not identify neurotoxicity in neurobehavioral assessments, functional tests, and organ weights, gross pathology, and histopathology of neuronal tissues. Therefore, undecane is GHS Not Classified based on the NOAEL of 1,000 mg/kg/day, which is above the duration-adjusted GHS cutoff of 200 mg/kg/day for Category 2.

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

Undecane was assigned a score of Low for skin sensitization based on no sensitization reactions seen in guinea pigs with the surrogate hydrocarbons, C10-12, isoalkanes, <2% aromatics. GreenScreen® criteria classify chemicals as a Low hazard for skin sensitization when adequate negative data are available and the chemical is not GHS classified (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data for a close structural surrogate.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.

- ECHA, CAS #1120-21-4, 2024
    - *Surrogate: Hydrocarbons, C10-12, isoalkanes, <2% aromatics (CAS #N/A)*: A non-GLP-compliant guinea pig maximization test conducted in 1977 in a manner similar to OECD Guideline 406 was performed with male and female guinea pigs (P strain, 10/sex/dose group, 5/sex in controls) for surrogate hydrocarbons, C10-C12, isoalkanes, < 2% aromatics (trade name: Shellsol TD, purity unspecified). The induction doses were applied as an intradermal injections of 0.1 mL 1.0% test substance in corn oil and topical application of 50% test substance under occlusion. The challenge dose was applied topically with 25% test substance under occlusive dressing. The dermal reactions were evaluated 24 and 48 hours after the removal of the dressing. No positive reactions were observed following the challenge dose and the study authors concluded that surrogate hydrocarbons, C10-C12, isoalkanes, < 2% aromatics (trade name: Shellsol TD) was not sensitizing to the skin in this study (Klimisch 2, reliable with restrictions).

Respiratory Sensitization (SnR) (Group II*) Score (H, M, or L): *L*
Undecane was assigned a score of Low for respiratory sensitization based on the lack of dermal sensitization potential according to the ECHA guidance (2017). GreenScreen® criteria classify chemicals as a Low hazard for respiratory sensitization when they are not GHS classified (CPA 2018b). The confidence in the score is low as this evaluation does not include non-immunologic mechanisms of respiratory sensitization, and no specific data are available for respiratory sensitization.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- OECD 2024
    - Undecane does not contain any structural alerts for respiratory sensitization (Appendix H).
- Based on the weight of evidence and guidance from ECHA regarding assessment of respiratory sensitization potential, a score of Low was assigned. The guidance from ECHA states that the mechanisms leading to respiratory sensitization are essentially similar to those leading to skin sensitization (ECHA 2017). ECHA recommended that if a chemical is not a dermal sensitizer based on high quality data, it is unlikely to be a respiratory sensitizer. ECHA also noted that this rationale does not cover respiratory hypersensitivity caused by non-immunological mechanisms, for which human experience is the main evidence of activity (ECHA 2017). As undecane was not sensitizing to the skin based on surrogate data (see skin sensitization section above), and a literature search did not find any human evidence of respiratory sensitization by undecane, and as undecane does not contain any structural alerts for respiratory sensitization (OECD 2024), undecane is not expected to be a respiratory sensitizer.

Skin Irritation/Corrosivity (IrS) (Group II) Score (vH, H, M, or L): *H*
Undecane was assigned a score of High for skin irritation/corrosivity based on some irritation effects seen in rabbits with several structural surrogates, leading to ToxServices' classification of GHS Category 2. GreenScreen® criteria classify chemicals as a High hazard for skin irritation/corrosivity when a chemical is considered a moderate irritant, which corresponds to the chemical being classified as GHS Category 2 (CPA 2018b). The confidence in the score is low as the levels of irritation vary among the surrogates.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #1120-21-4, 2024

- *Surrogate: Hydrocarbons, C9-11, isoalkanes, cyclics, <2% aromatics)*: In a GLP-compliant acute dermal toxicity study conducted in a manner similar to OECD Guideline 404, six male New Zealand White rabbits were exposed to 0.5 mL undiluted hydrocarbons, C9-11, isoalkanes, cyclics, <2% aromatics (tradename MRD-89-520, 100% purity) on the skin under semi-occlusion for 4 hours and observed for 7 days. The mean erythema score for all six animals across 24, 48 and 72 hours was 1.56, and the mean edema score was 0. Scores for individual animals were not reported. On day 7, three animals continued to exhibit signs of irritation with very slight erythema. Authors of the REACH dossier classified the test substance as not irritating (Klimisch 1, reliable without restriction).
  - *Insufficient data are reported for this study to perform GHS classification. According to the GHS criteria, mean scores of ≥ 1.5 and < 2.3 for erythema/eschar or for edema in at least 2 of 3 animals are classified to GHS Category 3 (UN 2023).*
- *Surrogate: Hydrocarbons, C10-12, isoalkanes, <2% aromatics (CAS #N/A)*: In a GLP-compliant acute dermal toxicity study conducted in a manner similar to OECD Guideline 404 in, three male New Zealand White rabbits were exposed to 0.5 mL undiluted hydrocarbons, C10-12, isoalkanes, <2% aromatics (tradename: MRD-00-710, purity unspecified) on the shaved skin under semi-occlusion for 4 hours and observed for 14 days. Dermal responses were observed in all animals including well-defined erythema and slight edema. The mean erythema score for all six animals across 24, 48 and 72 hours was 2.33, and the mean edema score was 1.1. All irritation was cleared by Day 14. Authors of the REACH dossier classified the test substance as a Category 2 dermal irritant (Klimisch 1, reliable without restriction).
  - *According to the GHS criteria, mean scores of ≥ 2.3 and ≤ 4.0 for erythema/eschar or for edema in at least 2 of 3 animals that are reversible within 14 days are classified to GHS Category 2 (UN 2023).*
- *Surrogate: Hydrocarbons, C10-12, isoalkanes, <2% aromatics (CAS #N/A)*: In a GLP-compliant acute dermal toxicity study conducted in a manner similar to OECD Guideline 404, three male New Zealand White rabbits were exposed to 0.5 mL undiluted hydrocarbons, C10-12, isoalkanes, < 2% aromatics (tradename Ecolane 90, purity unspecified) on the shaved skin under semi-occlusion for 4 hours and observed for 14 days. Dermal responses were observed in all animals including slight or well-defined erythema up to Day 10, and slight edema in two animals only on Day 1. The mean erythema score for each animal across 24, 48 and 72 hours were 1.3, 1.3, and 2.0, and the mean edema score for all animals was 0. All evidence of irritation was cleared by day 14. Study authors classified the test substance as not irritating (Klimisch 1, reliable without restriction).
  - *Based on the results of the above study, ToxServices did not classify hydrocarbons, C10-12, isoalkanes, < 2% aromatics under GHS criteria. According to the GHS criteria, mean scores of ≥ 1.5 and < 2.3 for erythema/eschar or for edema in at least 2 of 3 animals are classified to GHS Category 3 (UN 2023).*

- OECD 2012
  - OECD concluded that the C9-C14 aliphatic (≤ 2% aromatic) hydrocarbon solvents category of chemicals, including undecane, were minimally to slightly irritating to the skin of rabbits and not irritating to human skin under semi-occlusion, but produced irritation under occlusion, when evaporation was prevented. Furthermore, prolonged, or repeated exposure to this class of chemicals causes defatting of the skin leading to severe irritant dermatitis.
- Based on the weight of evidence, a score of High was conservatively assigned. Two surrogates, hydrocarbons, C10-12, isoalkanes, <2% aromatics and hydrocarbons, C9-11, isoalkanes, cyclics, < 2% aromatics, are not classified or classified to GHS Category 2, based on reliable animal data.

OECD concluded that this class of chemicals is at most slightly irritating to the skin of rabbits, non-irritating to the skin of humans except under occlusive conditions and/or with prolonged, repeated exposures (OECD 2012). ToxServices conservatively classified undecane as GHS Category 2.

Eye Irritation/Corrosivity (IrE) (Group II) Score (vH, H, M, or L): *M*
Undecane was assigned a score of Moderate for eye irritation/corrosivity based on the class of hydrocarbons, including undecane, are expected to be at most slightly irritating. GreenScreen® criteria classify chemicals as a Moderate hazard for eye irritation/corrosivity when found to be a mild irritant or GHS Category 3 (CPA 2018b). Confidence is low due to conflicting data from the surrogate hydrocatbons, C9-C11, isoalkanes, cyclics, <2% aromatics, indicating lack of ocular irritancy.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- ECHA, CAS #1120-21-4, 2024
  - *Surrogate: Hydrocarbons, C9-11, isoalkanes, cyclics, <2% aromatics)*: A GLP-compliant ocular irritation study conducted in a manner similar to OECD Guideline 405 was performed with six New Zealand White rabbits administered ocular instillations of 0.1 mL undiluted surrogate hydrocarbons, C9-C11, isoalkanes, cyclics, <2% aromatics (tradename: MRD-91-972, ~100% purity) without washing and with an observation period of 7 days following the instillation. At 24, 48, and 72 hours, the mean chemosis, conjunctivae, iris, and cornea opacity scores were 0. The study authors concluded that the test substance was not irritating to the eyes in this study (Klimisch 1, reliable without restriction)
  - *Surrogate*: *Decane (CAS #112-84-5):* A dose-response controlled, double blind study was performed with 63 human subjects randomly selected and exposed to concentrations of 0, 10, 35, or 100 µL/L surrogate n-decane. Dose-dependent irritation of the mucous membrane were observed as well as increased sensation of odor intensity and reduced air quality. Furthermore, reduced tear film stability of the eyes was evident at all concentrations and a dose-related increase in conjunctival polymorphonuclear leukocytes, a type of immune cell such as neutrophils, eosinophils, and basophils, was observed. Finally, adaptation was observed at the highest exposure level; however, these levels were not relevant to non-industrial environments (Klimisch 2, reliable with restrictions).
- OECD 2012
  - OECD concluded that the C9-C14 aliphatic (≤ 2% aromatic) hydrocarbon solvents category of chemicals, including undecane, were minimally to slightly irritating to the eyes of rabbits.
- Based on these results, a score of Moderate was assigned. Surrogate hydrocarbons, C9-C11, isoalkanes, cyclics, <2% aromatics was not irritating to the eyes of rabbits. A dose-response controlled study in humans exposed to surrogate n-decane identified a dose-dependent relationship for irritation of the eyes and mucous membranes at levels relevant to occupational settings; however, irritation concerns were low at levels below occupational levels. OECD concluded this category of chemicals is slightly to minimally irritating to the eyes in animal studies (OECD 2012). Therefore, based on human data and OECD's conclusion for this class of chemicals, ToxServices conservatively classified undecane to GHS Category 2B (mild) for eye irritation.

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M, or L): L
Undecane was assigned a score of Low for acute aquatic toxicity based on no effects seen up to the limits of water solubility. GreenScreen® criteria classify chemicals as a Low hazard for acute aquatic

toxicity when there are no effects seen at saturation (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data on the target chemical for all three trophic levels.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* GHS Japan: H400 – Very toxic to aquatic life [Hazardous to the aquatic environment (acute) – Category 1]
- PubChem 2024
  - Undecane has a measured water solubility of 0.014 mg/L at 25°C.
- OECD 2010
  - 96-hour LC_{50} in fish > 0.013 mg/L (*Oryzias latipes*, rice fish, measured) (GLP-compliant, OECD Guideline 203) (Klimisch 1, reliable without restrictions)
  - 48-hour mobility EC_{50} in daphnid = 0.011 mg/L (*Daphnia magna*, daphnid, measured) (GLP-compliant, OECD Guideline 202) (Klimisch 1, reliable without restrictions)
    - *Japan classified undecane to GHS Category 1 based on the results from this study (NITE 2010). While reduction in mobility was observed in this study within the measured soluble range, a solvent tetrahydrofuran was used to increase the solubility. The EC_0 of 0.0070 mg/L (measured concentration) is higher than the measured water solubility of 0.0044 mg/L without a solvent. Therefore, ToxServices did not heavily weigh this study in the overall weight of evidence.*
  - 72-hour growth rate and biomass EC_{50} in algae > 0.0059 mg/L (*Raphidocelis subcapitata*, microalga, measured) (GLP-compliant, OECD Guideline 201) (Klimisch 1, reliable without restrictions).
- ECHA, CAS#1120-21-4, 2024
  - 96-hour LL_{50} > 1,000 mg/L (nominal water accommodated fraction (WAF) loading rate) in saltwater amphipod (*Chaetogammarus marinus,* non-GLP, GESAMP No. 17(1982)) (Klimisch 2, reliable with restrictions)
  - 96-hour EL_{50} > 1,000 mg/L (nominal WAF loading rate) in *D. magna* (GESAMP No. 17(1982) (Klimisch 2, reliable with restrictions)
  - 96-hour LL_{50} > 1,000 mg/L (nominal WAF loading rate) in *Mysidopsis bahia* (shrimp-like crustacean in estuarine waters) (GESAMP No. 17(1982) (Klimisch 2, reliable with restrictions)
- As there were no effects seen up to the limit of water solubility, ToxServices assigned a score of Low.

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

Undecane was assigned a score of Very High for chronic aquatic toxicity based on a 21-day NOEC of 0.0057 mg/L. GreenScreen® criteria classify chemicals as a Very High hazard for chronic aquatic toxicity when chronic NOECs are < 0.1 mg/L (CPA 2018b). The confidence in the score is high as it is based on a reliable study on the target chemical.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- OECD 2010
  - 21-day reproduction NOEC in daphnid = 0.0057 mg/L (*D. magna*, daphnid, measured) (GLP-compliant, OECD Guideline 211). Reduced cumulative numbers of offspring produced were found at measured concentrations of 0.0083 mg/L and above (Klimisch 1, reliable without restrictions)

  - 72-hour growth rate and biomass NOEC in algae > 0.0059 mg/L (*P. subcapitata*, microalga, measured) (GLP-compliant, OECD Guideline 201) (Klimisch 1, reliable without restrictions)
- U.S. EPA 2022 (Appendix I)
  - Undecane is designated to the Neutral Organics ECOSAR chemical class. The most conservative predicted chronic values (ChVs) are 0.0082 mg/L in fish, 0.011 mg/L in daphnid, and 0.0079 mg/L in green algae. However, the predicted effect levels in fish and green algae exceed the chemical's measured water solubility of 0.0044 mg/L; therefore, these predicted results may not occur at saturation for these trophic levels.

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): *vL*
Undecane was assigned a score of Very Low for persistence based on being found to be readily biodegradable with the major compartment being water. GreenScreen® criteria classify chemicals as a Very Low hazard for persistence when the major compartment is water and it meets the 10-day window in a ready biodegradation assay (CPA 2018b). The confidence in the score is low as the 10-day window is determined through modeled instead of experimental data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.
  - *Screening:* Not present on any screening lists for this endpoint.
- OECD 2010
  - In a ready biodegradability test conducted according to OECD Guideline 301C (Modified MITI Test (I)) (GLP compliance not specified), non-adapted activated sludge was exposed to undecane (99% purity) at a starting concentration of 100 mg/L for 28 days. A degradation rate of 100% was achieved after 28 days. No data were identified on the 10-day window; however, authors concluded that the test substance is readily biodegradable (Klimisch 1, reliable without restriction).
    - *ToxServices notes that the 10-day window does not apply to OECD 301C tests (OECD 2001).*
- U.S. EPA 2017
  - The BIOWIN modeling Ready Biodegradable Predictor indicates that undecane is expected to be readily biodegradable. Fugacity modeling (MCI method) predicts 68.1% will partition to water with a half-life of 8.67 days, 3.65% will partition to sediment with a half-life of 77.92 days, and 4.59% will partition to soil with a half-life of 17.33 days (Appendix J).
- Based on the weight of evidence, ToxServices assigned a score of Very Low. Although undecane was found to be readily biodegradable in an OECD Guideline 301C assay, the 10-day window does not apply to this type of assay. As a pragmatic approach, chemicals that pass this test are considered readily biodegradable (OECD 2001). Modeling output shows that the major compartment for undecane is water, and as it is predicted to have a half life of 8.67 days, it is expected to meet the 10-day biodegradation window.

Bioaccumulation (B) Score (vH, H, M, L, or vL): *H*
Undecane was assigned a score of High for bioaccumulation based on an estimated BAF value of 2,014. GreenScreen® criteria classify chemicals as a High hazard for bioaccumulation when the BCF or BAF is >1,000 to 5,000 (CPA 2018b). The confidence in the score is low as it is based on modeled data.

- Authoritative and Screening Lists
  - *Authoritative:* Not present on any authoritative lists for this endpoint.

    - *Screening:* Not present on any screening lists for this endpoint.
- OECD 2010, 2012
    - OECD concluded that undecane has moderate bioaccumulation potential based on an estimated BCF value of 1,420 and estimated log K_{ow} value of 5.74. Additionally, in its evaluation of the C9-C14 aliphatic hydrocarbons solvent chemical class, OECD concluded that these chemicals have a potential to bioaccumulate.
- U.S. EPA 2017
    - BCFBAF predicts a BCF of 120.9 using the regression based model based on an estimated log K_{ow} of 5.74, and a BAF of 2,014 using the Arnot-Gobas model for the upper trophic level, taking metabolism into consideration (Appendix J).

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M, or L): *L*
Undecane was assigned a score of Low for reactivity based on the lack of structural alerts for oxidizing and explosive properties. GreenScreen® criteria classify chemicals as a Low hazard for reactivity when it does not warrant GHS classification for any of the reactivity sub-endpoints and the chemical is not present on authoritative or screening lists (CPA 2018b). The confidence in the score is low based on the lack of measured data on explosivity.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:* Not present on any screening lists for this endpoint.
- No measured data were identified. Therefore, screening procedures for explosivity were used here to estimate the reactivity property of Undecane. These procedures are listed in the GHS (UN 2023).
    - Based on the structure of its components or moieties, undecane is not considered explosive or self-reactive due to lack of functional groups associated with explosive or self-reactive properties (See Appendix K).
    - Based on the structure of its components or moieties, undecane is not considered to have oxidizing properties as it does not contain any structural groups known to be correlated with a tendency to react exothermally with combustible materials.

Flammability (F) Score (vH, H, M, or L): M
Undecane was assigned a score of Moderate for flammability based on ToxServices classifying it to GHS classification of GHS Category 3, as well as being listed on two screening lists as GHS Category 3. GreenScreen® criteria classify chemicals as a Moderate hazard for flammability when classified as a GHS 3 or 4 flammable liquid (CPA 2018b). The confidence in the score is high as it is based on reliable experimental data.

- Authoritative and Screening Lists
    - *Authoritative:* Not present on any authoritative lists for this endpoint.
    - *Screening:*
        - GHS Japan: H226 – Flammable liquid and vapor (Flammable liquids – Category 3)
        - GHS New Zealand: Flammable liquids category 3
- ECHA, CAS #1120-21-4, 2024
    - A flash point of 65°C was established for undecane in a non-GLP compliant flammability test conducted using the Pensky-Martens closed cup method (Klimisch 2, reliable with restrictions).
        - The flash point is > 60°C and < 93°C corresponds to a GHS classification of Category 4 (UN 2023).

- ThermoFisher Scientific 2023
    - A material safety data sheet labeled undecane as Category 3 Flammable Liquid and identified the flashpoint for undecane as 60°C in a Pensky-Martens closed cup according to ASTM D93, BS EN 22719, BS 2000 Part 404, IP 404, ISO 2719, and AS/NZS 2106.
- Based on an experimental flash point of 60-65ºC, undecane is flammable, but not pyrophoric. Therefore, ToxServices conservatively classified undecane as a flammable liquid Category 3 under GHS criteria (UN 2023) based on measured flash points ≥ 23°C and ≤ 60°C.

Use of New Approach Methodologies (NAMs)[10] in the Assessment, Including Uncertainty Analyses of Input and Output

New Approach Methodologies (NAMs) used in this GreenScreen® include *in silico* modeling for carcinogenicity, endocrine activity, respiratory sensitization, chronic aquatic toxicity, persistence, and bioaccumulation, and *in vitro* testing for genotoxicity, and endocrine activity. NAMs are non-animal alternatives that can be used alone or in combination to provide information for safety assessment (Madden et al. 2020). At present, there is not a uniformly accepted framework on how to report and apply individual NAMs (U.S. EPA 2020, OECD 2020). The expanded application of NAMs greatly amplifies the need to communicate uncertainties associated with their use. As defined by EFSA (2018), uncertainty is "a general term referring to all types of limitations in available knowledge that affect the range and probability of possible answers to an assessment question." The quality, utility, and accuracy of NAM predictions are greatly influenced by two primary types of uncertainties (OECD 2020):

- Type I: Uncertainties related to the input data used
- Type II: Uncertainties related to extrapolations made

As shown in Table 4, Type I (input data) uncertainties in undecane's NAMs dataset includes lack of *in vivo* measured data for carcinogenicity, endocrine activity, respiratory sensitization, chronic aquatic toxicity for the fish trophic level, and bioaccumulation, and lack of validated test methods for respiratory sensitization. Undecane's Type II (extrapolation output) uncertainties include lack of defined applicability domains for Toxtree, ToxCast models, and OECD Toolbox structural alerts, limitations of *in vitro* genotoxicity assays in focusing on only a few events in the process of genotoxicity, and in mimicking *in vivo* conditions, Tox 21 EDSP high throughput screening assays' incomplete coverage of critical endocrine pathways and lack of consideration of toxicokinetics *in vivo,* and OECD Toolbox respiratory sensitization structural alerts' lack of consideration of non-immunological mechanisms. Some of undecane's type II uncertainties were alleviated by the use of *in vitro* test batteries and/or in combination of *in vivo* data.

Table 4: Summary of NAMs Used in the GreenScreen® Assessment, Including Uncertainty Analyses	
Uncertainty Analyses (OECD 2020)	
Type I Uncertainty: Data/Model Input	**Carcinogenicity:** No experimental data are identified. **Endocrine activity:** No *in vivo* experimental data are identified. **Respiratory sensitization**: No experimental data are available and there are no validated test methods. **Chronic aquatic toxicity:** No measured data are available for the fish trophic level. **Bioaccumulation:** No experimental BCF/BAF data are identified.
Type II Uncertainty: Extrapolation Output	**Carcinogenicity**: Toxtree only identifies structural alerts (SAs), and no applicability domain can be defined (Toxtree 2018). **Genotoxicity:** The bacterial reverse mutation assay (as defined in OECD Guideline 471) only tests point-mutation inducing activity in non-mammalian cells, and the exogenous metabolic activation

[10] NAMs refers to any non-animal technology, methodology, approach, or combination thereof that inform chemical hazard and risk assessments. NAMs include *in silico*/computational tools, *in vitro* biological profiling (e.g., cell cultures, 2,3-D organotypic culture systems, genomics/transcriptomics, organs on a chip), and frameworks (i.e., adverse outcome pathways (AOPs), defined approaches (DA), integrated approaches to testing and assessment (IATA).

	system does not entirely mimic *in vivo* conditions[11]. The *in vitro* chromosome aberration assay (OECD Guideline 473) does not measure aneuploidy and it only measures structural chromosomal aberrations. The exogenous metabolic activation system does not entirely mirror *in vivo* metabolism[12]. **Endocrine activity:** ToxCast models don't define applicability domain; the *in vivo* relevance of EDSP Tox 21 screening assays is unknown due to lack of consideration of metabolism and other toxicokinetic factors. EDSP Tox 21 assays do not cover all critical endocrine pathways. **Respiratory sensitization**: The OECD Toolbox only identifies structural alerts, and does not define applicability domains. Additionally, the ECHA guidance (2017), on which the use of OECD Toolbox structural alerts is based, does not evaluate non-immunologic mechanisms for respiratory sensitization.

Endpoint	NAMs Data Available and Evaluated? (Y/N)	Types of NAMs Data (*in silico* modeling/*in vitro* biological profiling/frameworks)
Carcinogenicity	Y	*In silico* modeling: VEGA/Toxtree/ /Danish QSAR
Mutagenicity	Y	*In vitro* data: Bacterial reverse mutation assay/*in vitro* chromosome aberration assay
Reproductive toxicity	N	
Developmental toxicity	N	
Endocrine activity	Y	*In vitro* high throughput data: EDSP Tox 21 screening assays *In silico* modeling: ToxCast models
Acute mammalian toxicity	N	
Single exposure systemic toxicity	N	
Repeated exposure systemic toxicity	N	
Single exposure neurotoxicity	N	
Repeated exposure neurotoxicity	N	
Skin sensitization	N	
Respiratory sensitization	Y	*In silico* modeling: OECD Toolbox structural alerts
Skin irritation	N	
Eye irritation	N	
Acute aquatic toxicity	N	

[11] https://www.oecd-ilibrary.org/docserver/9789264071247-en.pdf?expires=1614097593&id=id&accname=guest&checksum=89925F80B9F4BD2FFC6E90F94A0EE427
[12] https://www.oecd-ilibrary.org/docserver/9789264264649-en.pdf?expires=1614098015&id=id&accname=guest&checksum=6A4F9CE52EA974F5A74793DD54D54352

Chronic aquatic toxicity	Y	*In silico* modeling: ECOSAR modeling
Persistence	Y	*In silico* modeling: EPI Suite™ Non-animal testing: OECD Guideline 301C ready biodegradability test
Bioaccumulation	Y	*In silico* modeling: EPI Suite™

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APPENDIX A: Hazard Classification 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 Undecane (CAS #1120-21-4)

TOXSERVICES
TOXICOLOGY RISK ASSESSMENT CONSULTING

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	Undecane	1120-21-4	*L*	L	*L*	*L*	DG	L	H	L	*L*	*L*	L	*L*	*H*	*M*	L	vH	*vL*	*H*	*L*	M

Table 3: Hazard Summary Table

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

Table 4

Chemical Name	Preliminary GreenScreen® Benchmark Score
Undecane	2

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

Table 6

Chemical Name	Final GreenScreen® Benchmark Score
Undecane	2

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												
2	Yes	Yes	Yes	Yes	Yes							2
3												
4												

APPENDIX C: Pharos Output for Undecane (CAS #1120-21-4)

1120-21-4

n-Undecane

ALSO CALLED 1714962-75-0, 214-300-6, DTXSID9021689, Hendecane, n-C11H24, n-Hendecane, N-UNDECANE, UND, undecan,...

View all synonyms (14)

SHARE PROFILE

HAZARDS | PROPERTIES | FUNCTIONAL USES | RESOURCES

All Hazards View

Show PubMed Results | REQUEST ASSESSMENT | ADD TO COMPARISON

		Group I Human					Group II and II* Human								Ecotox			Fate		Physical		Mult	Non-GSLT			
	GREENSCREEN®	C	M	R	D	E	AT	ST	ST	N	N	SnS	SnR	IrS	IrE	AA	CA	ATB	P	B	Rx	F	Mult	PBT	GW	O	Other
List Hazard Summary	LT-P1	-	-	-	-	-	pC	H	-	-	-	-	-	pC	pC	vH	-	-	-	-	-	M	M	-	-	-	R

Hazard Lists

DOWNLOAD LISTS

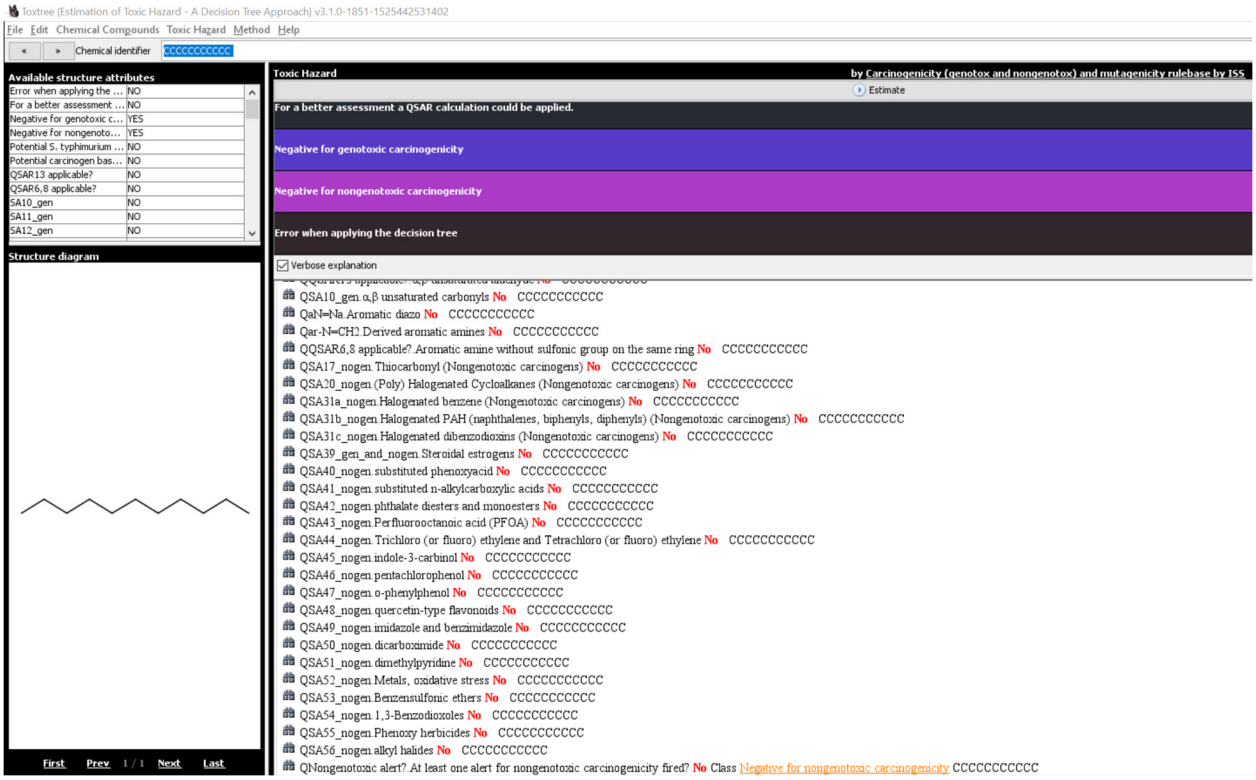
ENDPOINT	HAZARD LEVEL	GREENSCREEN®	LIST NAME	HAZARD DESCRIPTION	OTHER LISTS
Acute Mammalian Toxicity	pC	NoGS	DK-EPA - Danish Advisory List	Acute Tox. 4 - Harmful if swallowed (modeled)	
Systemic Toxicity/Organ Effects-Single Exposure	H	LT-UNK	GHS - Japan	H335 - May cause respiratory irritation [Specific target organ toxicity - Single exposure - Category 3]	+1
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H335 - May cause respiratory irritation (unverified) [Specific target organ toxicity - single exposure; Respiratory tract irritation - Category 3]	
Skin Irritation/Corrosivity	pC	NoGS	EU - Manufacturer REACH hazard submissions	H315 - Causes skin irritation (unverified) [Skin corrosion/irritation - Category 2]	
Eye Irritation/Corrosivity	pC	NoGS	EU - Manufacturer REACH hazard submissions	H319 - Causes serious eye irritation (unverified) [Serious eye damage/eye irritation - Category 2A]	

Acute Aquatic Toxicity	vH	LT-UNK	GHS - Japan	H400 - Very toxic to aquatic life [Hazardous to the aquatic environment (acute) - Category 1]	
Flammability	M	LT-UNK	GHS - Japan	H226 - Flammable liquid and vapour [Flammable liquids - Category 3]	+2
	M	LT-UNK	GHS - New Zealand	Flammable liquids category 3	
	M	LT-UNK	Québec CSST - WHMIS 1988	Class B3 - Combustible liquids	
Carcinogenicity,Mutagenicity/Genotoxicity Reproductive Toxicity, Developmental Toxicity, Acute Mammalian Toxicity, or System Toxicity/Organ Effects.	U	LT-UNK	Québec CSST - WHMIS 1988	Class D2B - Toxic material causing other toxic effects	
Systemic Toxicity/Organ Effects (Single Exposure - Aspiration Hazard)	pC	LT-UNK	GHS - Japan	H304 - May be fatal if swallowed and enters airways [Aspiration hazard - Category 1]	+1
	pC	NoGS	EU - Manufacturer REACH hazard submissions	H304 - May be fatal if swallowed and enters airways (unverified) [Aspiration hazard - Category 1]	
Acute aquatic toxicity; Chronic aquatic toxicity	U	LT-UNK	EC - CEPA DSL	Inherently Toxic in the Environment (iTE)	
T & P and/or B [(Chronic Aquatic Toxicity and sometimes Persistence) or (Acute Aquatic Toxicity and Persistence and/or Bioaccumulation)]	U	LT-P1	GHS - Japan	H410 - Very toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment (chronic) - Category 1]	
T & P and/or B [(Chronic Aquatic Toxicity and Persistence) or (Acute Aquatic Toxicity and Persistence and/or Bioaccumulation)]	M	LT-UNK	GHS - New Zealand	Hazardous to the aquatic environment - chronic category 4	

Restricted Substance Lists (8)

- Australia - National Industrial Chemicals Notification and Assessments (NICNAS): NICNAS
- EC - CEPA DSL: DSL-all
- EU - PACT-RMOA Substances: Substances selected for RMOA or hazard assessment
- Food Contact Chemicals Database (FCCdb): Food Contact Chemicals Database Version 5.0
- Food Contact Chemicals of Concern (FCCoCL): Food Contact Chemicals of Concern List (FCCoCL) - TIER 3
- FPF Priority Substance List from FCCdb: FPF Priority Substance List from FCCdb

APPENDIX D: Toxtree Carcinogenicity Results for Undecane (CAS #1120-21-4)



APPENDIX E: VEGA Carcinogenicity Results for Undecane (CAS #1120-21-4)

1. Prediction Summary

Prediction for compound Molecule 0 -

Prediction: Reliability:

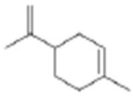
Prediction is Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- Accuracy of prediction for similar molecules found in the training set is not adequate
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: CCCCCCCCCCC
Experimental value: -
Predicted Carcinogen activity: Carcinogen
P(Carcinogen): 0.817
P(NON-Carcinogen): 0.183
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

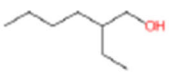
Compound #1

CAS: 111-68-2
Dataset id:357 (Test Set)
SMILES: NCCCCCCC
Similarity: 0.726
Experimental value : NON-Carcinogen
Predicted value : Carcinogen



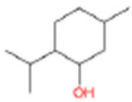
Compound #2

CAS: 5989-27-5
Dataset id:412 (Training Set)
SMILES: C=C(C)C1CC=C(C)CC1
Similarity: 0.723
Experimental value : Carcinogen
Predicted value : NON-Carcinogen



Compound #3

CAS: 104-76-7
Dataset id:314 (Training Set)
SMILES: OCC(CC)CCCC
Similarity: 0.717
Experimental value : NON-Carcinogen
Predicted value : Carcinogen

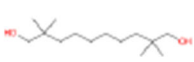


Compound #4

CAS: 89-78-1
Dataset id:427 (Training Set)
SMILES: OC1CC(C)CCC1(C(C)C)
Similarity: 0.692
Experimental value : NON-Carcinogen
Predicted value : Carcinogen

Compound #5

CAS: 1643-20-5
Dataset id:273 (Training Set)
SMILES: [O-][N+](C)(C)CCCCCCCCCCCC
Similarity: 0.683
Experimental value : NON-Carcinogen
Predicted value : Carcinogen



Compound #6

CAS: 35449-36-6
Dataset id:345 (Training Set)
SMILES: OCC(C)(C)CCCCCCC(C)(C)CO
Similarity: 0.678
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.724 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✖	Accuracy of prediction for similar molecules Accuracy index = 0 Explanation: Accuracy of prediction for similar molecules found in the training set is not adequate..
✖	Concordance for similar molecules Concordance index = 0.498 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✔	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✔	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..
✔	Model class assignment reliability Pos/Non-Pos difference = 0.633 Explanation: model class assignment is well defined..
✔	Neural map neurons concordance Neurons concordance = 1 Explanation: predicted value agrees with experimental values of training set compounds laying in the same neuron..

Symbols explanation:

✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

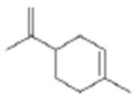
Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is NON-Carcinogen, but the result may be not reliable. A check of the information given in the following section should be done, paying particular attention to the following issues:
- Only moderately similar compounds with known experimental value in the training set have been found
- Accuracy of prediction for similar molecules found in the training set is not adequate
- similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: CCCCCCCCCCC
Experimental value: -
Predicted Carcinogen activity: NON-Carcinogen
Structural Alerts: -
Reliability: The predicted compound is outside the Applicability Domain of the model
Remarks:
- none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

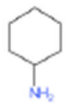


Compound #1

CAS: 5989-27-5
Dataset id:267 (Training Set)
SMILES: C=C(C)C1CC=C(C)CC1
Similarity: 0.723
Experimental value : Carcinogen
Predicted value : NON-Carcinogen

Compound #2

CAS: 1643-20-5
Dataset id:879 (Training Set)
SMILES: [O-][N+](C)(C)CCCCCCCCCCCC
Similarity: 0.683
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen



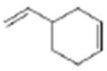
Compound #3

CAS: 108-91-8
Dataset id:834 (Training Set)
SMILES: NC1CCCCC1
Similarity: 0.657
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #4

CAS: 68107-26-6
Dataset id:527 (Training Set)
SMILES: O=NN(C)CCCCCCCCCCC
Similarity: 0.656
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): SA21 Alkyl and aryl N-nitroso groups



Compound #5

CAS: 100-40-3
Dataset id:238 (Training Set)
SMILES: C=CC1CC=CCC1
Similarity: 0.655
Experimental value : Carcinogen
Predicted value : NON-Carcinogen

Compound #6

CAS: 75881-22-0
Dataset id:762 (Training Set)
SMILES: O=NN(C)CCCCCCCCCC
Similarity: 0.655
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): SA21 Alkyl and aryl N-nitroso groups

3.2 Applicability Domain:
Measured Applicability Domain Scores

✖	Global AD Index AD index = 0.579 Explanation: The predicted compound is outside the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.702 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✖	Accuracy of prediction for similar molecules Accuracy index = 0.478 Explanation: Accuracy of prediction for similar molecules found in the training set is not adequate..
✖	Concordance for similar molecules Concordance index = 0.478 Explanation: similar molecules found in the training set have experimental values that disagree with the predicted value..
✔	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✔ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✖ The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

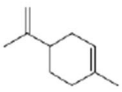
Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is Possible NON-Carcinogen, but the result shows some critical aspects, which require to be checked:
- Only moderately similar compounds with known experimental value in the training set have been found
- some similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: CCCCCCCCCCC
Experimental value: -
Predicted Carcinogenic activity: Possible NON-Carcinogen
No. alerts for carcinogenicity: 0
Structural Alerts: -
Reliability: The predicted compound could be out of the Applicability Domain of the model
Remarks:
none

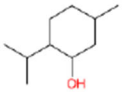
3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values



Compound #1

CAS: 5989-27-5
Dataset id:218 (Training Set)
SMILES: C=C(C)C1CC=C(C)CC1
Similarity: 0.723
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 39



Compound #2

CAS: 15356-70-4
Dataset id:654 (Training Set)
SMILES: OC1CC(C)CCC1(C(C)C)
Similarity: 0.692
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

Compound #3

CAS: 1643-20-5
Dataset id:777 (Training Set)
SMILES: [O-][N+](C)(C)CCCCCCCCCCCC
Similarity: 0.683
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

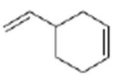
Compound #4

CAS: 108-91-8
Dataset id:748 (Training Set)
SMILES: NC1CCCCC1
Similarity: 0.657
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

Compound #5

CAS: 68107-26-6
Dataset id:439 (Training Set)
SMILES: O=NN(C)CCCCCCCCCCC
Similarity: 0.656
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 1; Carcinogenity alert no. 14; Carcinogenity alert no. 27



Compound #6

CAS: 100-40-3
Dataset id:196 (Training Set)
SMILES: C=CC1CC=CCC1
Similarity: 0.655
Experimental value : Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 39

3.2 Applicability Domain:
Measured Applicability Domain Scores

⚠	Global AD Index AD index = 0.75 Explanation: The predicted compound could be out of the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.698 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
✓	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
⚠	Concordance for similar molecules Concordance index = 0.649 Explanation: some similar molecules found in the training set have experimental values that disagree with the predicted value..
✓	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0 -

Prediction: Reliability:

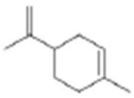
Prediction is Possible NON-Carcinogen, but the result shows some critical aspects, which require to be checked:
- Only moderately similar compounds with known experimental value in the training set have been found
- Accuracy of prediction for similar molecules found in the training set is not optimal
- some similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0
Compound SMILES: CCCCCCCCCCC
Experimental value: -
Predicted Carcinogenic activity: Possible NON-Carcinogen
No. alerts for carcinogenicity: 0
Structural Alerts: -
Reliability: The predicted compound could be out of the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

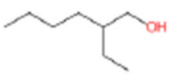
Compound #1

CAS: 111-68-2
Dataset id:357 (Test Set)
SMILES: NCCCCCCC
Similarity: 0.726
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen



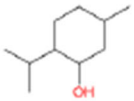
Compound #2

CAS: 5989-27-5
Dataset id:412 (Training Set)
SMILES: C=C(C)C1CC=C(C)CC1
Similarity: 0.723
Experimental value : Carcinogen
Predicted value : Possible NON-Carcinogen



Compound #3

CAS: 104-76-7
Dataset id:314 (Training Set)
SMILES: OCC(CC)CCCC
Similarity: 0.717
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen



Compound #4

CAS: 89-78-1
Dataset id:427 (Training Set)
SMILES: OC1CC(C)CCC1(C(C)C)
Similarity: 0.692
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

Compound #5

CAS: 1643-20-5
Dataset id:273 (Training Set)
SMILES: [O-][N+](C)(C)CCCCCCCCCCCC
Similarity: 0.683
Experimental value : NON-Carcinogen
Predicted value : Carcinogen

Alerts (not found also in the target): Carcinogenity alert no. 64

Compound #6

CAS: 35449-36-6
Dataset id:345 (Training Set)
SMILES: OCC(C)(C)CCCCCCC(C)(C)CO
Similarity: 0.678
Experimental value : NON-Carcinogen
Predicted value : Possible NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

⚠	Global AD Index AD index = 0.693 Explanation: The predicted compound could be out of the Applicability Domain of the model.
⚠	Similar molecules with known experimental value Similarity index = 0.722 Explanation: Only moderately similar compounds with known experimental value in the training set have been found..
⚠	Accuracy of prediction for similar molecules Accuracy index = 0.666 Explanation: Accuracy of prediction for similar molecules found in the training set is not optimal..
⚠	Concordance for similar molecules Concordance index = 0.666 Explanation: some similar molecules found in the training set have experimental values that disagree with the predicted value..
✓	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is NON-Carcinogen, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections.

Compound: Molecule 0
Compound SMILES: CCCCCCCCCCC
Experimental value: -
Predicted Oral Carcinogenic class: NON-Carcinogen
Reliability: The predicted compound is into the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: 124-18-5
Dataset id:425 (Training Set)
SMILES: CCCCCCCCCC
Similarity: 0.981
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #2

CAS: 111-84-2
Dataset id:610 (Training Set)
SMILES: CCCCCCCCC
Similarity: 0.961
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #3

CAS: 110-54-3
Dataset id:540 (Training Set)
SMILES: CCCCCC
Similarity: 0.847
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #4

CAS: 30501-43-0
Dataset id:692 (Training Set)
SMILES: CC1(C)(CCCCC1(C)(C))
Similarity: 0.841
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #5

CAS: 108-87-2
Dataset id:587 (Training Set)
SMILES: CC1CCCCC1
Similarity: 0.809
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #6

CAS: 109-66-0
Dataset id:626 (Training Set)
SMILES: CCCCC
Similarity: 0.8
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

✓	Global AD Index AD index = 0.985 Explanation: The predicted compound is into the Applicability Domain of the model.
✓	Similar molecules with known experimental value Similarity index = 0.971 Explanation: Strongly similar compounds with known experimental value in the training set have been ..
✓	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✓	Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✓	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✓	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

1. Prediction Summary

Prediction for compound Molecule 0 -

Prediction: Reliability:

Prediction is NON-Carcinogen, the result appears reliable. Anyhow, you should check it through the evaluation of the information given in the following sections.

Compound: Molecule 0
Compound SMILES: CCCCCCCCCCC
Experimental value: -
Predicted Inhalation Carcinogenic class: NON-Carcinogen
Reliability: The predicted compound is into the Applicability Domain of the model
Remarks:
none

3.1 Applicability Domain:
Similar Compounds, with Predicted and Experimental Values

Compound #1

CAS: 124-18-5
Dataset id:389 (Training Set)
SMILES: CCCCCCCCCC
Similarity: 0.981
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #2

CAS: 111-84-2
Dataset id:593 (Training Set)
SMILES: CCCCCCCCC
Similarity: 0.961
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #3

CAS: 110-54-3
Dataset id:516 (Training Set)
SMILES: CCCCCC
Similarity: 0.847
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #4

CAS: 30501-43-0
Dataset id:687 (Training Set)
SMILES: CC1(C)(CCCCC1(C)(C))
Similarity: 0.841
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #5

CAS: 108-87-2
Dataset id:567 (Training Set)
SMILES: CC1CCCCC1
Similarity: 0.809
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

Compound #6

CAS: 109-66-0
Dataset id:612 (Training Set)
SMILES: CCCCC
Similarity: 0.8
Experimental value : NON-Carcinogen
Predicted value : NON-Carcinogen

3.2 Applicability Domain:
Measured Applicability Domain Scores

✓	Global AD Index AD index = 0.985 Explanation: The predicted compound is into the Applicability Domain of the model.
✓	Similar molecules with known experimental value Similarity index = 0.971 Explanation: Strongly similar compounds with known experimental value in the training set have been ..
✓	Accuracy of prediction for similar molecules Accuracy index = 1 Explanation: Accuracy of prediction for similar molecules found in the training set is good..
✓	Concordance for similar molecules Concordance index = 1 Explanation: Similar molecules found in the training set have experimental values that agree with the predicted value..
✓	Model's descriptors range check Descriptors range check = True Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set..
✓	Atom Centered Fragments similarity check ACF index = 1 Explanation: all atom centered fragment of the compound have been found in the compounds of the training set..

Symbols explanation:

✓ The feature has a good assessment, model is reliable regarding this aspect.

⚠ The feature has a non optimal assessment, this aspect should be reviewed by an expert.

✗ The feature has a bad assessment, model is not reliable regarding this aspect.

APPENDIX F: Danish QSAR Carcinogenicity Results for Undecane (CAS #1120-21-4)

Carcinogenicity

	E Ultra	Leadscope
FDA RCA Cancer Male Rat	NEG_IN	INC_OUT
FDA RCA Cancer Female Rat	NEG_IN	INC_OUT
FDA RCA Cancer Rat	NEG_IN	INC_OUT
FDA RCA Cancer Male Mouse	NEG_IN	INC_OUT
FDA RCA Cancer Female Mouse	NEG_IN	INC_OUT
FDA RCA Cancer Mouse	NEG_IN	NEG_OUT
FDA RCA Cancer Rodent	NEG_IN	INC_OUT

Commercial models from CASE Ultra and Leadscope

FDA RCA: Data from US Food and Drug Administration as part of Research Cooperation Agreement

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Carcinogenicity (genotox and nongenotox) alerts by ISS, alerts in:	
- parent only	No alert found
Oncologic Primary Classification, alerts in:	
- parent only	Not classified

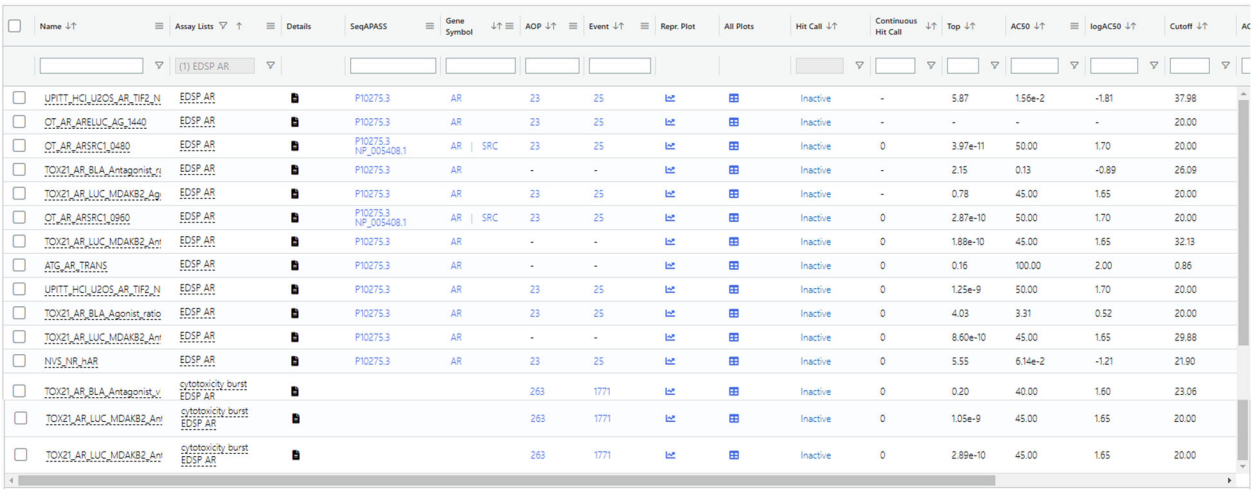
OECD QSAR Toolbox v.4.2 profilers

Profiler predictions are supporting information to be used together with the relevant QSAR predictions

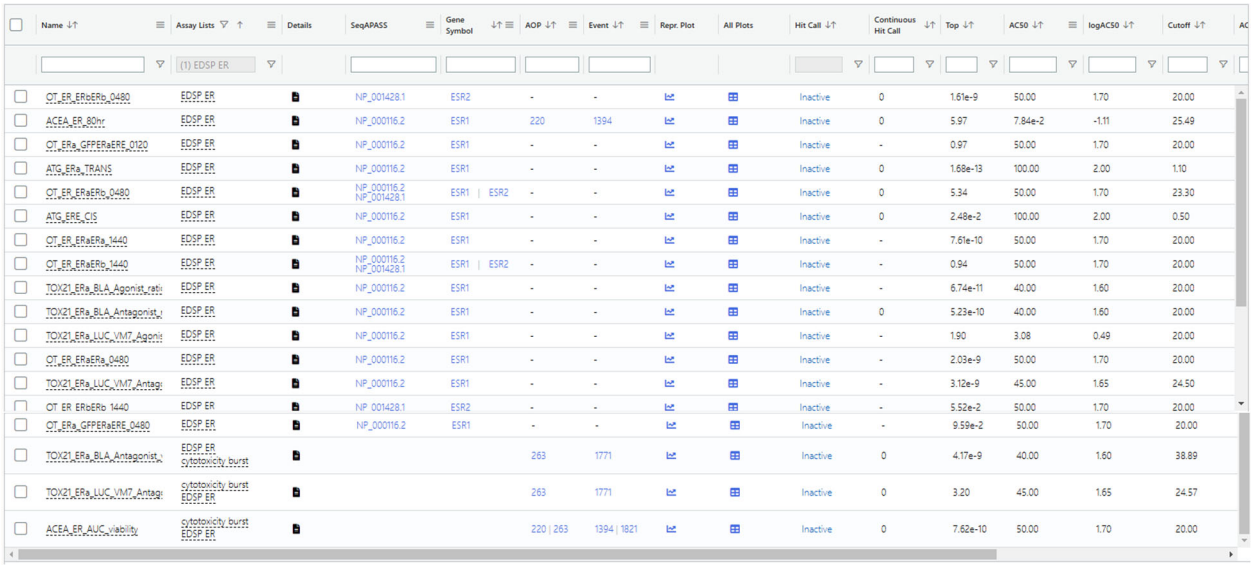
	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Liver Specific Cancer in Rat or Mouse		NEG_IN	NEG_IN	NEG_OUT	NEG_IN

DTU-developed models

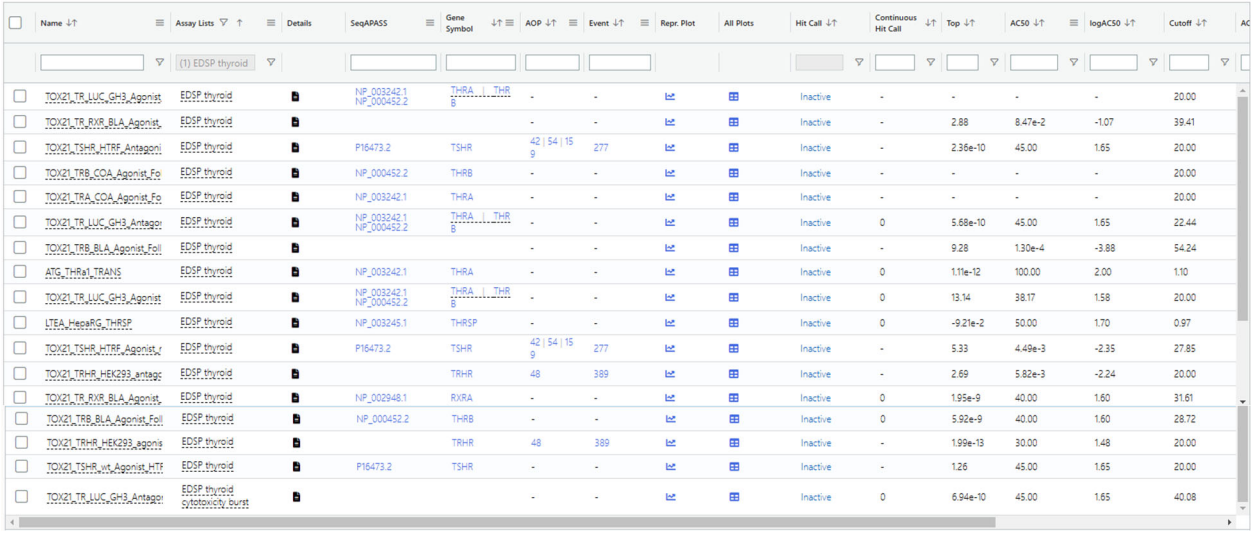
APPENDIX G: CompTox Endocrine Activity Results for Undecane (CAS #1120-21-4)



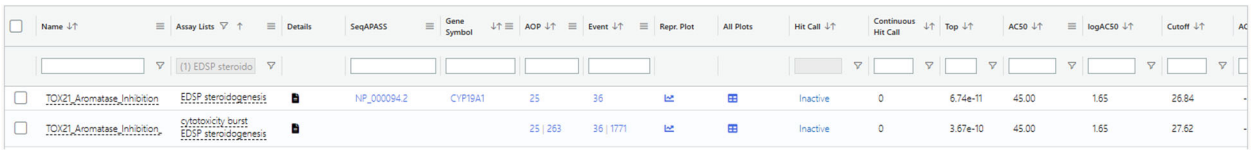
Name	Assay Lists	Details	SeqAPASS	Gene Symbol	AOP	Event	Repr. Plot	All Plots	Hit Call	Continuous Hit Call	Top	AC50	logAC50	Cutoff
	(1) EDSP AR													
UPITT_HCI_U2OS_AR_TIF2_N	EDSP AR		P10275.3	AR	23	25			Inactive	-	5.87	1.56e-2	-1.81	37.98
OT_AR_ARELUC_AG_1440	EDSP AR		P10275.3	AR	23	25			Inactive	-	-	-	-	20.00
OT_AR_ARSRC1_0480	EDSP AR		P10275.3 NP_005408.1	AR | SRC	23	25			Inactive	0	3.97e-11	50.00	1.70	20.00
TOX21_AR_BLA_Antagonist_r	EDSP AR		P10275.3	AR	-	-			Inactive	-	2.15	0.13	-0.89	26.09
TOX21_AR_LUC_MDAKB2_Ag	EDSP AR		P10275.3	AR	23	25			Inactive	-	0.78	45.00	1.65	20.00
OT_AR_ARSRC1_0960	EDSP AR		P10275.3 NP_005408.1	AR | SRC	23	25			Inactive	0	2.87e-10	50.00	1.70	20.00
TOX21_AR_LUC_MDAKB2_Ant	EDSP AR		P10275.3	AR	-	-			Inactive	0	1.88e-10	45.00	1.65	32.13
ATG_AR_TRANS	EDSP AR		P10275.3	AR	-	-			Inactive	0	0.16	100.00	2.00	0.86
UPITT_HCI_U2OS_AR_TIF2_N	EDSP AR		P10275.3	AR	23	25			Inactive	0	1.25e-9	50.00	1.70	20.00
TOX21_AR_BLA_Agonist_ratio	EDSP AR		P10275.3	AR	23	25			Inactive	0	4.03	3.31	0.52	20.00
TOX21_AR_LUC_MDAKB2_Ant	EDSP AR		P10275.3	AR	-	-			Inactive	0	8.60e-10	45.00	1.65	29.88
NVS_NR_hAR	EDSP AR		P10275.3	AR	23	25			Inactive	0	5.55	6.14e-2	-1.21	21.90
TOX21_AR_BLA_Antagonist_v	cytotoxicity burst EDSP AR				263	1771			Inactive	0	0.20	40.00	1.60	23.06
TOX21_AR_LUC_MDAKB2_Ant	cytotoxicity burst EDSP AR				263	1771			Inactive	0	1.05e-9	45.00	1.65	20.00
TOX21_AR_LUC_MDAKB2_Ant	cytotoxicity burst EDSP AR				263	1771			Inactive	0	2.89e-10	45.00	1.65	20.00



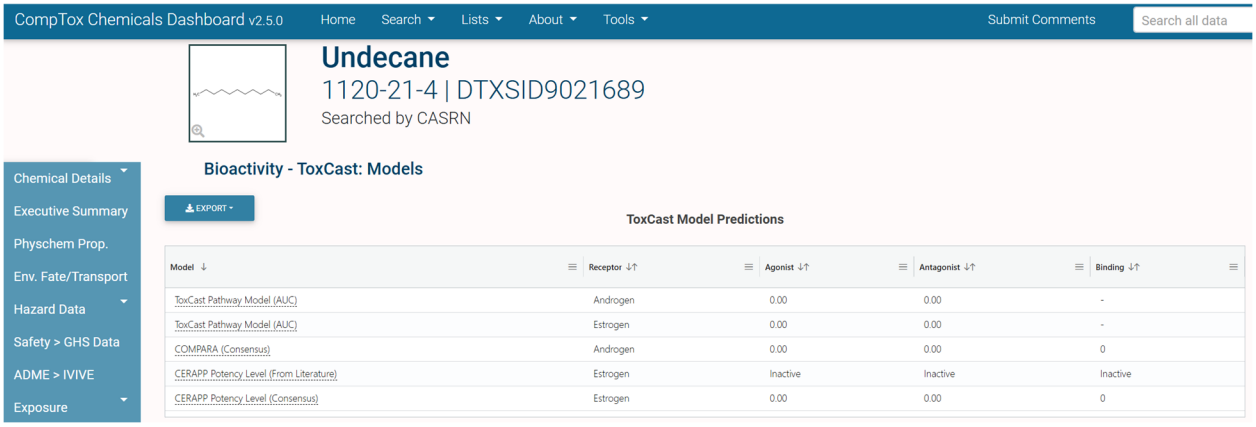
Name	Assay Lists	Details	SeqAPASS	Gene Symbol	AOP	Event	Repr. Plot	All Plots	Hit Call	Continuous Hit Call	Top	AC50	logAC50	Cutoff
	(1) EDSP ER													
OT_ER_ERbERb_0480	EDSP ER		NP_001428.1	ESR2	-	-			Inactive	0	1.61e-9	50.00	1.70	20.00
ACEA_ER_80hr	EDSP ER		NP_000116.2	ESR1	220	1394			Inactive	0	5.97	7.84e-2	-1.11	25.49
OT_ERa_GFPERaERE_0120	EDSP ER		NP_000116.2	ESR1	-	-			Inactive	-	0.97	50.00	1.70	20.00
ATG_ERa_TRANS	EDSP ER		NP_000116.2	ESR1	-	-			Inactive	0	1.68e-13	100.00	2.00	1.10
OT_ER_ERaERb_0480	EDSP ER		NP_000116.2 NP_001428.1	ESR1 | ESR2	-	-			Inactive	0	5.34	50.00	1.70	23.30
ATG_ERE_CIS	EDSP ER		NP_000116.2	ESR1	-	-			Inactive	0	2.48e-2	100.00	2.00	0.50
OT_ER_ERaERa_1440	EDSP ER		NP_000116.2	ESR1	-	-			Inactive	-	7.61e-10	50.00	1.70	20.00
OT_ER_ERaERb_1440	EDSP ER		NP_000116.2 NP_001428.1	ESR1 | ESR2	-	-			Inactive	-	0.94	50.00	1.70	20.00
TOX21_ERa_BLA_Agonist_rati	EDSP ER		NP_000116.2	ESR1	-	-			Inactive	-	6.74e-11	40.00	1.60	20.00
TOX21_ERa_BLA_Antagonist_r	EDSP ER		NP_000116.2	ESR1	-	-			Inactive	0	5.23e-10	40.00	1.60	20.00
TOX21_ERa_LUC_VM7_Agonis	EDSP ER		NP_000116.2	ESR1	-	-			Inactive	-	1.90	3.08	0.49	20.00
OT_ER_ERaERa_0480	EDSP ER		NP_000116.2	ESR1	-	-			Inactive	-	2.03e-9	50.00	1.70	20.00
TOX21_ERa_LUC_VM7_Antago	EDSP ER		NP_000116.2	ESR1	-	-			Inactive	-	3.12e-9	45.00	1.65	24.50
OT_ER_ERbERb_1440	EDSP ER		NP_001428.1	ESR2	-	-			Inactive	-	5.52e-2	50.00	1.70	20.00
OT_ERa_GFPERaERE_0480	EDSP ER		NP_000116.2	ESR1	-	-			Inactive	-	9.59e-2	50.00	1.70	20.00
TOX21_ERa_BLA_Antagonist_	EDSP ER cytotoxicity burst				263	1771			Inactive	0	4.17e-9	40.00	1.60	38.89
TOX21_ERa_LUC_VM7_Antago	cytotoxicity burst EDSP ER				263	1771			Inactive	0	3.20	45.00	1.65	24.57
ACEA_ER_AUC_viability	cytotoxicity burst EDSP ER				220 | 263	1394 | 1821			Inactive	0	7.62e-10	50.00	1.70	20.00



Name	Assay Lists	Details	SeqAPASS	Gene Symbol	AOP	Event	Repr. Plot	All Plots	Hit Call	Continuous Hit Call	Top	AC50	logAC50	Cutoff
	(1) EDSP thyroid													
TOX21_TR_LUC_GH3_Agonist	EDSP thyroid		NP_003242.1 NP_000452.2	THRA | THRB	-	-			Inactive	-	-	-	-	20.00
TOX21_TR_RXR_BLA_Agonist_	EDSP thyroid				-	-			Inactive	-	2.88	8.47e-2	-1.07	39.41
TOX21_TSHR_HTRF_Antagoni	EDSP thyroid		P16473.2	TSHR	42 | 54 | 159	277			Inactive	-	2.36e-10	45.00	1.65	20.00
TOX21_TRB_COA_Agonist_Fo	EDSP thyroid		NP_000452.2	THRB	-	-			Inactive	-	-	-	-	20.00
TOX21_TRA_COA_Agonist_Fo	EDSP thyroid		NP_003242.1	THRA	-	-			Inactive	-	-	-	-	20.00
TOX21_TR_LUC_GH3_Antago	EDSP thyroid		NP_003242.1 NP_000452.2	THRA | THRB	-	-			Inactive	0	5.68e-10	45.00	1.65	22.44
TOX21_TRB_BLA_Agonist_Foll	EDSP thyroid				-	-			Inactive	-	9.28	1.30e-4	-3.88	54.24
ATG_THRa1_TRANS	EDSP thyroid		NP_003242.1	THRA	-	-			Inactive	0	1.11e-12	100.00	2.00	1.10
TOX21_TR_LUC_GH3_Agonist	EDSP thyroid		NP_003242.1 NP_000452.2	THRA | THRB	-	-			Inactive	0	13.14	38.17	1.58	20.00
LTEA_HepaRG_THRSP	EDSP thyroid		NP_003245.1	THRSP	-	-			Inactive	0	-9.21e-2	50.00	1.70	0.97
TOX21_TSHR_HTRF_Agonist_r	EDSP thyroid		P16473.2	TSHR	42 | 54 | 159	277			Inactive	-	5.33	4.49e-3	-2.35	27.85
TOX21_TRHR_HEK293_antago	EDSP thyroid			TRHR	48	389			Inactive	-	2.69	5.82e-3	-2.24	20.00
TOX21_TR_RXR_BLA_Agonist_	EDSP thyroid		NP_002948.1	RXRA	-	-			Inactive	0	1.95e-9	40.00	1.60	31.61
TOX21_TRB_BLA_Agonist_Foll	EDSP thyroid		NP_000452.2	THRB	-	-			Inactive	0	5.92e-9	40.00	1.60	28.72
TOX21_TRHR_HEK293_agonis	EDSP thyroid			TRHR	48	389			Inactive	-	1.99e-13	30.00	1.48	20.00
TOX21_TSHR_wt_Agonist_HTF	EDSP thyroid		P16473.2	TSHR	-	-			Inactive	-	1.26	45.00	1.65	20.00
TOX21_TR_LUC_GH3_Antago	EDSP thyroid cytotoxicity burst				-	-			Inactive	0	6.94e-10	45.00	1.65	40.08

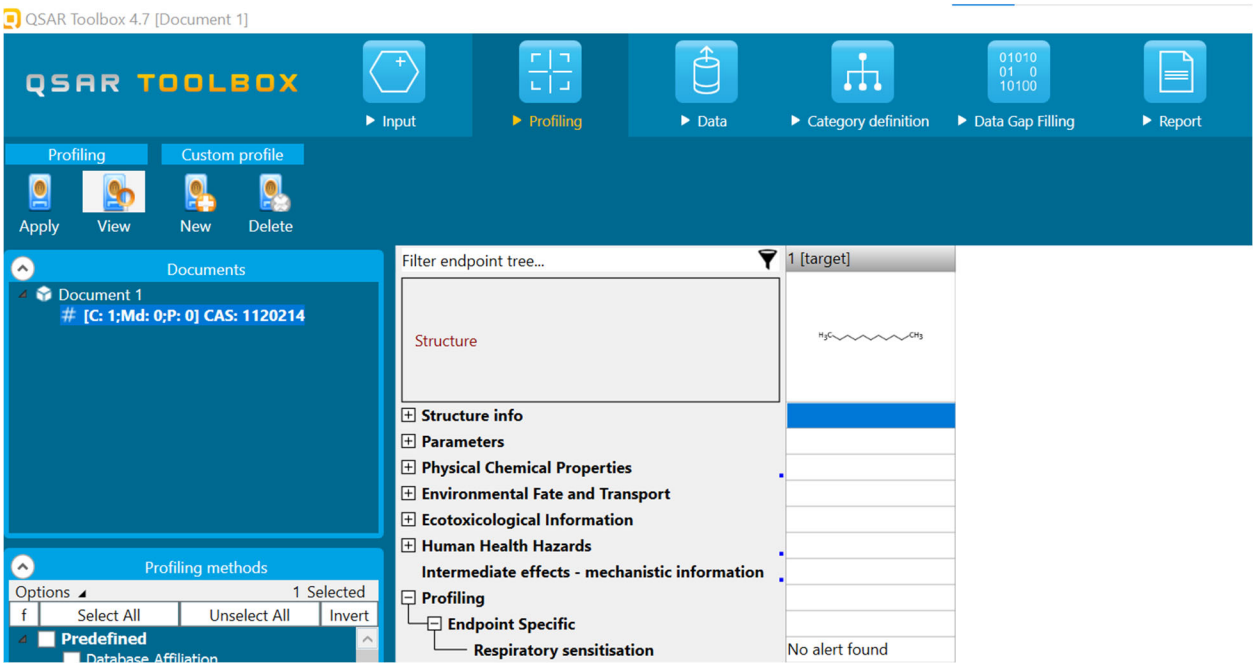


Name	Assay Lists	Details	SeqAPASS	Gene Symbol	AOP	Event	Repr. Plot	All Plots	Hit Call	Continuous Hit Call	Top	AC50	logAC50	Cutoff
	(1) EDSP steroido													
TOX21_Aromatase_Inhibition	EDSP steroidogenesis		NP_000094.2	CYP19A1	25	36			Inactive	0	6.74e-11	45.00	1.65	26.84
TOX21_Aromatase_Inhibition_	cytotoxicity burst EDSP steroidogenesis				25 | 263	36 | 1771			Inactive	0	3.67e-10	45.00	1.65	27.62

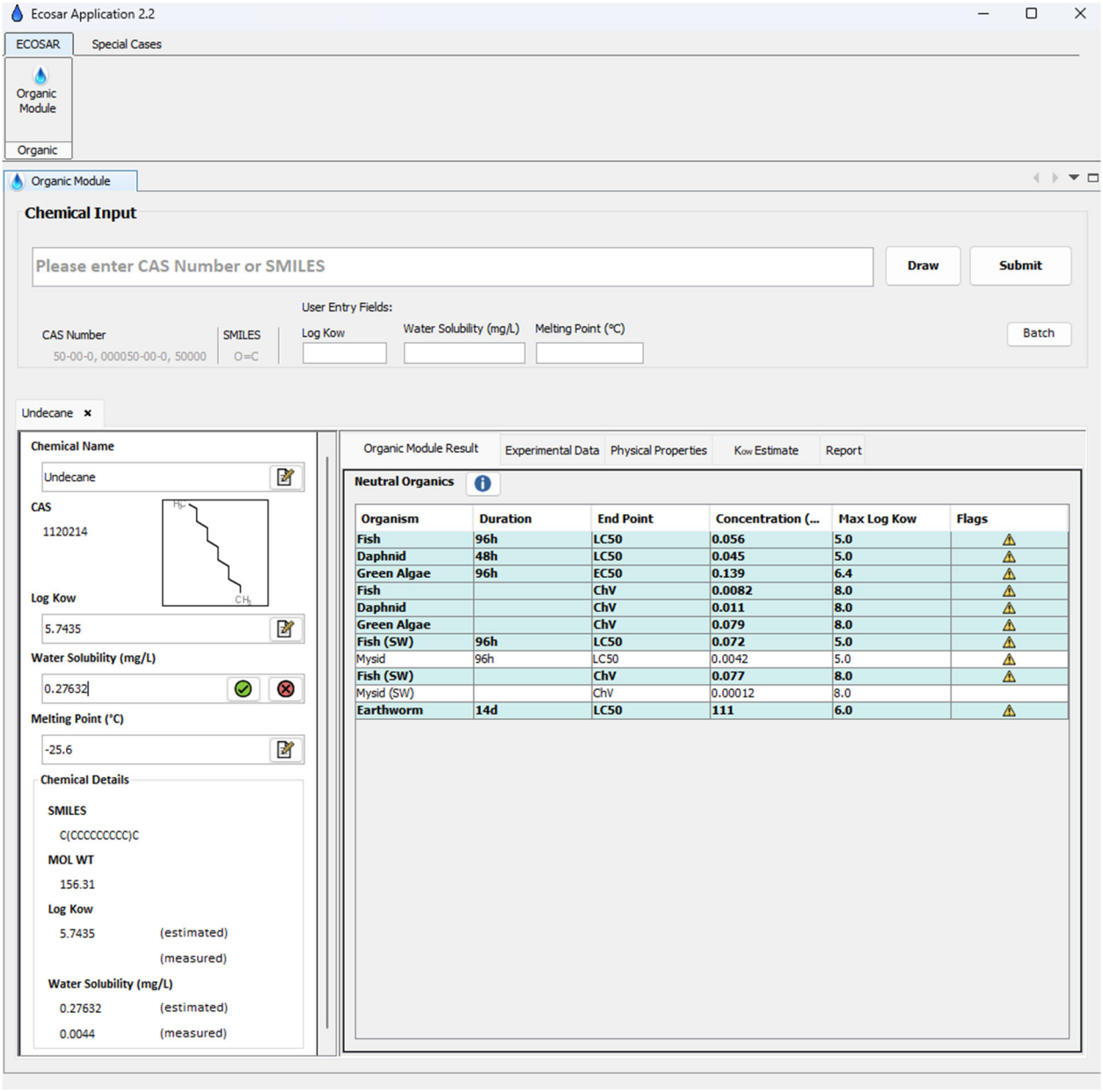


Model	Receptor	Agonist	Antagonist	Binding
ToxCast Pathway Model (AUC)	Androgen	0.00	0.00	-
ToxCast Pathway Model (AUC)	Estrogen	0.00	0.00	-
COMPARA (Consensus)	Androgen	0.00	0.00	0
CERAPP Potency Level (From Literature)	Estrogen	Inactive	Inactive	Inactive
CERAPP Potency Level (Consensus)	Estrogen	0.00	0.00	0

APPENDIX H: OECD Toolbox Respiratory Sensitization Results for Undecane (CAS #1120-21-4)



APPENDIX I: ECOSAR Modeling Results for Undecane (CAS #1120-21-4)



Organism	Duration	End Point	Concentration (...	Max Log Kow	Flags
Fish	**96h**	**LC50**	**0.056**	**5.0**	⚠
Daphnid	**48h**	**LC50**	**0.045**	**5.0**	⚠
Green Algae	**96h**	**EC50**	**0.139**	**6.4**	⚠
Fish		**ChV**	**0.0082**	**8.0**	⚠
Daphnid		**ChV**	**0.011**	**8.0**	⚠
Green Algae		**ChV**	**0.079**	**8.0**	⚠
Fish (SW)	**96h**	**LC50**	**0.072**	**5.0**	⚠
Mysid	96h	LC50	0.0042	5.0	⚠
Fish (SW)		**ChV**	**0.077**	**8.0**	⚠
Mysid (SW)		ChV	0.00012	8.0	
Earthworm	**14d**	**LC50**	**111**	**6.0**	⚠

APPENDIX J: EPI Suite™ Modeling Results for Undecane (CAS #1120-21-4)

(Estimated values included in the GreenScreen® are highlighted and bolded)

CAS Number: 001120-21-4
SMILES : C(CCCCCCCCC)C
CHEM : N-UNDECANE
MOL FOR: C11 H24
MOL WT : 156.31
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : 195.90
Melting Point (deg C) : -25.60
Vapor Pressure (mm Hg) : 0.412
Water Solubility (mg/L): 0.0044
Henry LC (atm-m3/mole) : ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.69 estimate) = 5.74

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 185.61 (Adapted Stein & Brown method)
Melting Pt (deg C): -32.36 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 0.629 (Mean VP of Antoine & Grain methods)
VP (Pa, 25 deg C) : 83.8 (Mean VP of Antoine & Grain methods)
MP (exp database): -25.6 deg C
BP (exp database): 195.9 deg C
VP (exp database): 4.12E-01 mm Hg (5.49E+001 Pa) at 25 deg C

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 0.2763
log Kow used: 5.74 (estimated)
melt pt used: -25.60 deg C
Water Sol (Exper. database match) = 0.0044 mg/L (25 deg C)
Exper. Ref: YALKOWSKY,SH & DANNENFELSER,RM (1992)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 0.029256 mg/L

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

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 7.04E+000 atm-m3/mole (7.13E+005 Pa-m3/mole)
Group Method: 9.52E+000 atm-m3/mole (9.64E+005 Pa-m3/mole)
Exper Database: 1.93E+00 atm-m3/mole (1.96E+005 Pa-m3/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: 1.926E+001 atm-m3/mole (1.951E+006 Pa-m3/mole)
VP: 0.412 mm Hg (source: User-Entered)
WS: 0.0044 mg/L (source: User-Entered)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: 5.74 (KowWin est)
Log Kaw used: 1.897 (exp database)
Log Koa (KOAWIN v1.10 estimate): 3.843
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.8900
Biowin2 (Non-Linear Model) : 0.9888
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 3.4504 (days-weeks)
Biowin4 (Primary Survey Model) : 4.1604 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.6175
Biowin6 (MITI Non-Linear Model): 0.8233
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.2754
Ready Biodegradability Prediction: YES

Hydrocarbon Biodegradation (BioHCwin v1.01):
LOG BioHC Half-Life (days) : 1.0041
BioHC Half-Life (days) : 10.0938

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 54.9 Pa (0.412 mm Hg)
Log Koa (Koawin est): 3.843
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 5.46E-008
Octanol/air (Koa) model: 1.71E-009
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 1.97E-006
Mackay model : 4.37E-006
Octanol/air (Koa) model: 1.37E-007

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 12.5235 E-12 cm3/molecule-sec
Half-Life = 0.854 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 10.249 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
3.17E-006 (Junge-Pankow, Mackay avg)

1.37E-007 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc : 2644 L/kg (MCI method)
Log Koc: 3.422 (MCI method)
Koc : 9.58E+004 L/kg (Kow method)
Log Koc: 4.981 (Kow 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 = 2.082 (BCF = 120.9 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 0.6035 days (HL = 4.013 days)
Log BCF Arnot-Gobas method (upper trophic) = 3.152 (BCF = 1420)
Log BAF Arnot-Gobas method (upper trophic) = 3.304 (BAF = 2014)
log Kow used: 5.74 (estimated)

Volatilization from Water:
Henry LC: 1.93 atm-m3/mole (Henry experimental database)
Half-Life from Model River: 1.276 hours
Half-Life from Model Lake : 118.8 hours (4.948 days)

Removal In Wastewater Treatment (recommended maximum 95%):
Total removal: 99.85 percent
Total biodegradation: 0.18 percent
Total sludge adsorption: 57.81 percent
Total to Air: 41.86 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model: (MCI Method)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	**23.7**	**19.4**	**1000**
Water	**68.1**	**208**	**1000**
Soil	**4.59**	**416**	**1000**
Sediment	**3.65**	**1.87e+003**	**0**

Persistence Time: 72.3 hr

Level III Fugacity Model: (MCI Method with Water percents)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	23.7	19.4	1000
Water	68.1	208	1000
water	(66)		
biota	(1.81)		
suspended sediment	(0.262)		
Soil	4.59	416	1000

Sediment 3.65 1.87e+003 0
Persistence Time: 72.3 hr

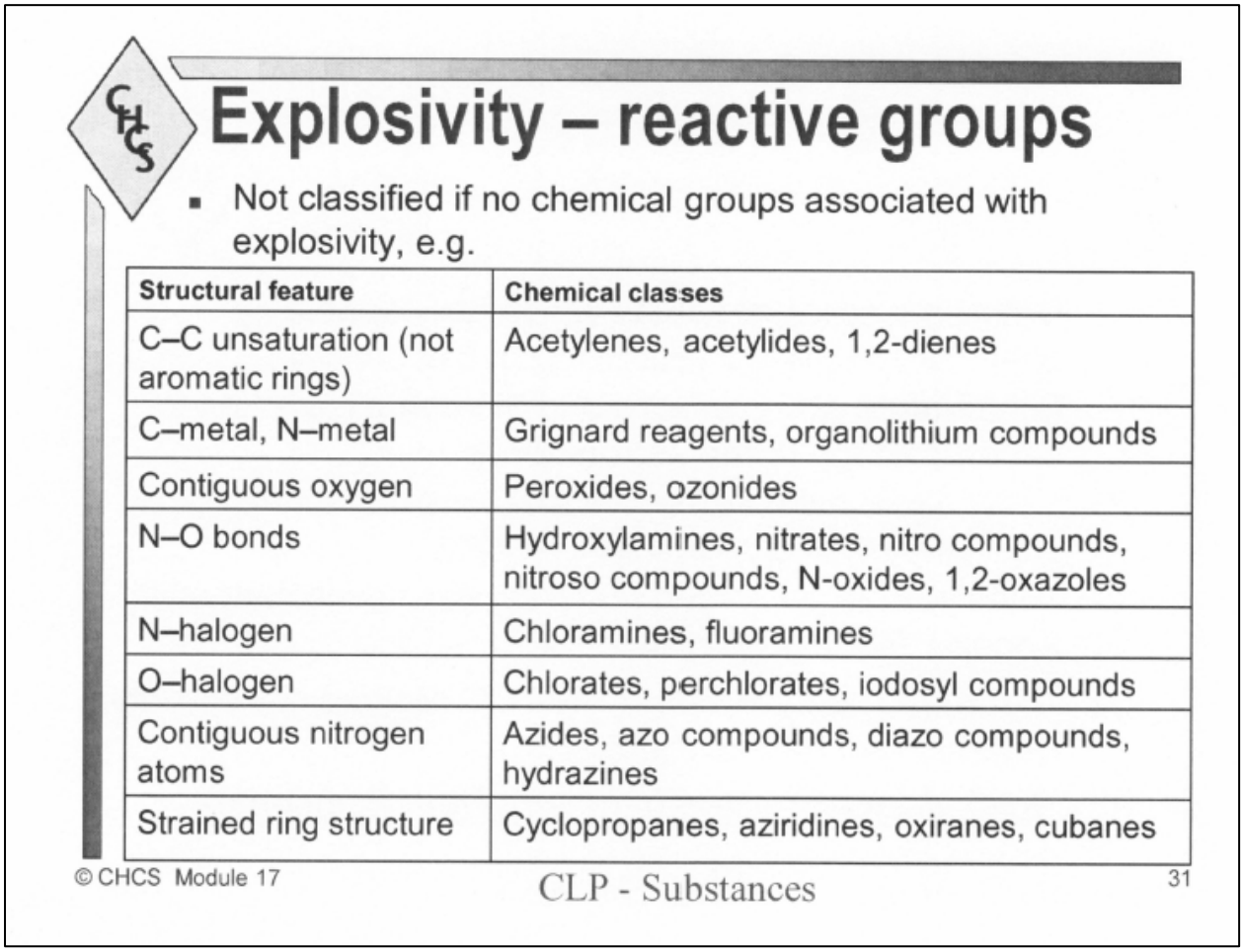
Level III Fugacity Model: (EQC Default)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	4.14	19.4	1000
Water	15	208	1000
water	(11)		
biota	(0.302)		
suspended sediment	(3.72)		
Soil	35.4	416	1000
Sediment	45.4	1.87e+003	0

Persistence Time: 302 hr

APPENDIX K: Known Structural Alerts for Reactivity

Explosivity – Abbreviated List



Explosivity – reactive groups

- Not classified if no chemical groups associated with explosivity, e.g.

Structural feature	Chemical classes
C–C unsaturation (not aromatic rings)	Acetylenes, acetylides, 1,2-dienes
C–metal, N–metal	Grignard reagents, organolithium compounds
Contiguous oxygen	Peroxides, ozonides
N–O bonds	Hydroxylamines, nitrates, nitro compounds, nitroso compounds, N-oxides, 1,2-oxazoles
N–halogen	Chloramines, fluoramines
O–halogen	Chlorates, perchlorates, iodosyl compounds
Contiguous nitrogen atoms	Azides, azo compounds, diazo compounds, hydrazines
Strained ring structure	Cyclopropanes, aziridines, oxiranes, cubanes

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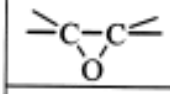
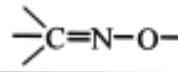
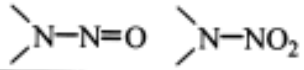
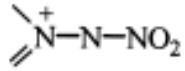
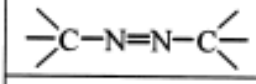
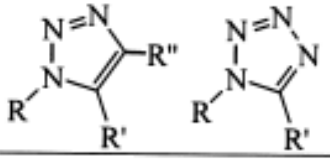
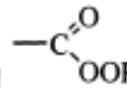
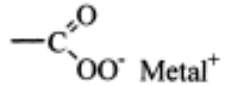
Explosivity – Full List

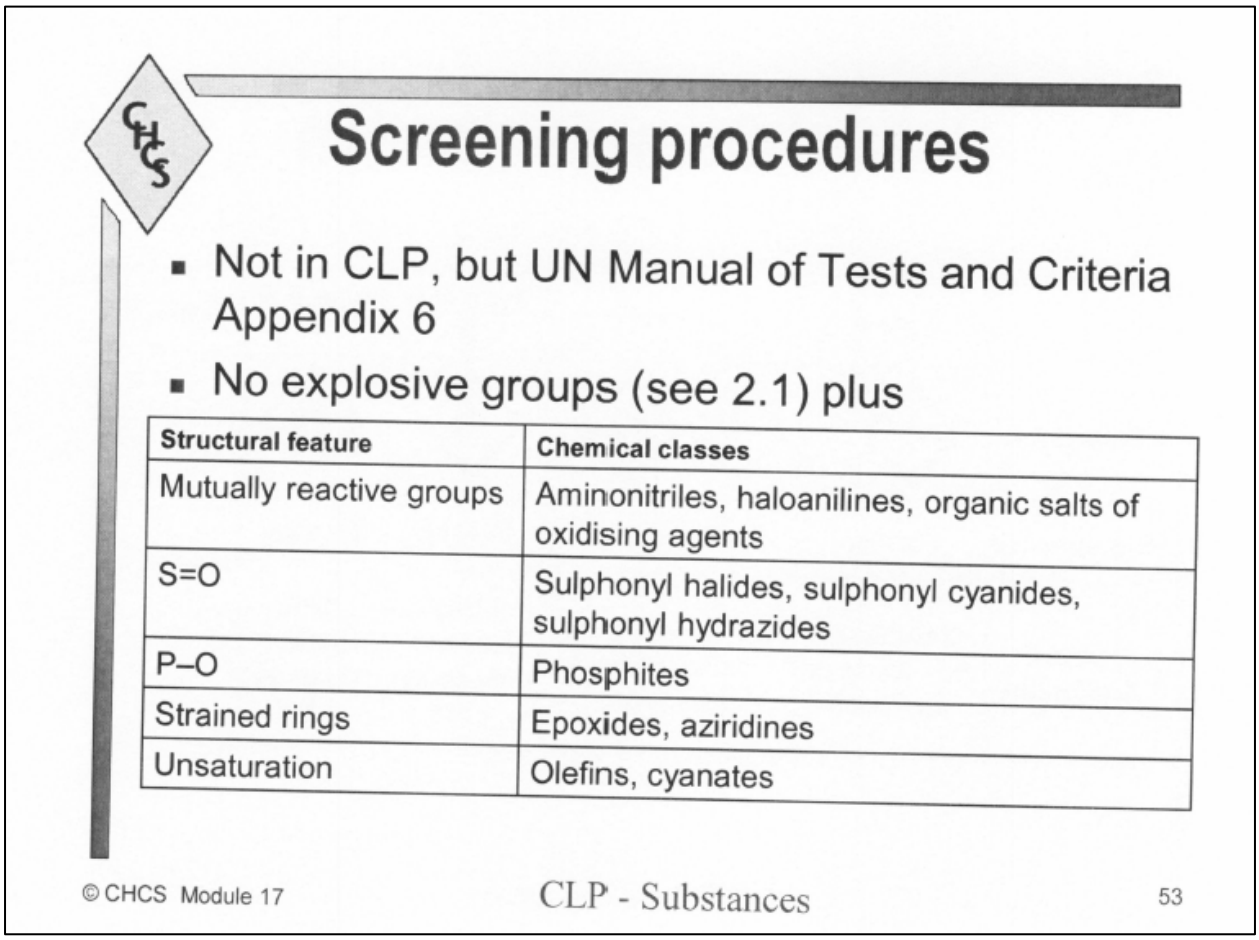
Table R.7.1-28 Chemical groups associated with explosive properties

Chemical group	Chemical Class
-C≡C- -C≡C-Metal -C≡C-Halogen	Acetylenic Compounds Metal Acetylides Haloacetylene Derivatives
	Diazo Compounds
-N=O -NO_2	Nitroso and Nitro Compounds,
R-O-N=O R-O-NO_2	Acyl or Alkyl Nitrites and Nitrates
	1,2-Epoxides
	Metal Fulminates or *aci*-Nitro Salts
	N-Metal Derivatives (especially heavy metals)
	N-Nitroso and N-Nitro Compounds
	N-Azolium Nitroimidates
	Azo Compounds
Ar-N=N-O-Ar	Arene Diazoates
$(ArN=N)_2O$, $(ArN=N)_2S$	Bis-Arenediazo Oxides and Sulfides
RN=N-NR'R''	Triazines
	High-nitrogen Compounds: e.g. Triazoles, Tetrazoles

Chemical group	Chemical Class
[1] ROOR', [2] 	Peroxy Compounds: [1] Alkyl hydroperoxides (R'=H), Peroxides (R'=organic); [2] Peroxo acids (R'=H), Peroxyesters (R'=organic)
[1] ROOMetal, [2] 	Metal peroxides, Peroxoacids salts
$-N_3$	Azides e.g. PbN_6, CH_3N_3
$^{-}O-C-N_2^{+}$	Arenediazonium oxides i.e. inner diazonium salts in which the counter ion is an oxide
Ar-N=N-S- Ar-N=N-S-Ar	Diazonium sulfides and derivatives, Arenediazo Aryl Sulfides
XO_n	Halogen Oxide: e.g. percholrates, bromates, etc
NX_3 e.g. $NC1_3$, $RNC1_2$	N-Halogen Compounds

Adapted from Bretherick (Bretherick's Handbook of Reactive Chemical Hazards 6th Ed., 1999, Butterworths, London)

Self-Reactive Substances



APPENDIX L: Change in Benchmark Score

Table 5 provides a summary of changes to the GreenScreen® Benchmark™ for Undecane. The original GreenScreen® assessment was performed in 2024 with slight update in 2025, under version 1.4 criteria and ToxServices assigned a Benchmark 2 (BM-2) score.

Table 5: Change in GreenScreen® Benchmark™ for Undecane

Date	GreenScreen® Benchmark™	GreenScreen® Version	Comment
December 17, 2024	BM-2	v. 1.4	Original GreenScreen® assessment.
February 24, 2025	BM-2	v. 1.4	No change in benchmark score. The confidence for the Low score for repeated exposure neurotoxicity is changed from high to low based on comments from Washington Department of Ecology

Licensed GreenScreen® Profilers

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