Supporting Information for Low-Priority Substance 1-Docosanol (CASRN 661-19-8)

Final Designation

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Contents

Tables

1. Introduction

The Lautenberg amendments to the Toxic Substances Control Act (TSCA) require EPA to designate chemical substances as either High-Priority Substances for risk evaluation, or Low-Priority Substances for which risk evaluations are not warranted at this time (section 6(b)(1)(B) and implementing regulations (40 CFR 702.3)). A high-priority substance is defined as a chemical substance that the Administrator concludes, without consideration of costs or other non-risk factors, may present an unreasonable risk of injury to health or the environment because of a potential hazard and a potential route of exposure under the conditions of use, including an unreasonable risk to potentially exposed or susceptible subpopulations identified as relevant by the Administrator. If the Administrator concludes, based on information sufficient to establish, without consideration of costs or other non-risk factors, that the high-priority standard is not met, then the substance must be designated as a low-priority substance. 1-Docosanol is one of the 40 chemical substances initiated for prioritization as referenced in a March 21, 2019 notice (84 FR 10491)[1] and one of the 20 proposed as low-priority substances in an August 15, 2019 notice (84 FR 41712).[2]

As described under EPA's regulations at 40 CFR 702.9[3] and pursuant to section 6(b)(1)(A) of the statute, EPA generally used reasonably available information to screen the chemical substance under its conditions of use against the following criteria and considerations:

- the hazard and exposure potential of the chemical substance;
- persistence and bioaccumulation;
- potentially exposed or susceptible subpopulations;
- storage near significant sources of drinking water;
- conditions of use or significant changes in the conditions of use of the chemical substance;
- the chemical substance's production volume or significant changes in production volume; and
- other risk-based criteria that EPA determines to be relevant to the designation of the chemical substance's priority.

Designation of a low-priority substance is not a finding that the chemical substance does not present an unreasonable risk, but rather that the chemical does not meet the statutory criteria for a high-priority substance and that a risk evaluation is not warranted at the time. As explained in the preamble to the Prioritization Rule, "low-priority substance designations give the public notice of chemical substances for which the hazard and/or exposure potential is anticipated to be low or nonexistent and provides some insight into which chemical substances are likely not to need additional evaluation and risk management under TSCA." 82 FR 33753 at 33755. EPA is not precluded from later revising the designation based on reasonably available information, if warranted. 40 CFR 702.13; 702.15.

The screening review is not a risk evaluation, but rather a review of reasonably available information on the chemical substance that relates to the specific criteria and considerations in TSCA section

[1] https://www.federalregister.gov/documents/2019/03/21/2019-05404/initiation-of-prioritization-under-the-toxic-substances-control-act-tsca

[2] https://www.federalregister.gov/documents/2019/08/15/2019-17558/proposed-low-priority-substance-designation-under-the-toxic-substances-control-act-tsca-notice-of

[3] The prioritization process is explained in the *Procedures for Prioritization of Chemicals for Risk Evaluation Under the Toxic Substances Control Act* (82 FR 33753).

6(b)(1)(A) and 40 CFR 702.9. This paper documents the results of the screening review which supports the final designation of 1-docosanol as a low-priority substance. EPA has also prepared a general response to comments and, as applicable, chemical-specific responses to comments.

This risk-based, screening-level review is organized as follows:

- *Section 1 (Introduction):* This section explains the requirements of the Lautenberg amendments to the Toxic Substances Control Act (TSCA) and implementing regulations – including the criteria and considerations -- pertinent to prioritization and designation of low-priority substances.

- *Section 2 (Background on the Low-Priority Substance):* This section includes information on attributes of the chemical substance, including its structure, and relates them to its functionality.

- *Section 3 (Physical-Chemical Properties):* This section includes a description of the physical-chemical properties of the chemical substance and explains how these properties lead to the chemical's fate, transport, and exposure potential.

- *Section 4 (Relevant Assessment History):* This section includes an overview of the outcomes of other governing entities' assessments of the chemical substance.

- *Section 5 (Conditions of Use):* This section presents the chemical substance's known, intended, and reasonably foreseen conditions of use under TSCA.

- *Section 6 (Hazard Characterization):* This section summarizes the reasonably available hazard information and screens the information against low-concern benchmarks.

- *Section 7 (Exposure Characterization):* This section includes a qualitative summary of potential exposures to the chemical substance.

- *Section 8 (Summary of Findings):* In this section, EPA presents information pertinent to prioritization against each of the seven statutory and regulatory criteria and considerations, and makes a conclusion based on that evidence.

- *Section 9 (Final Designation):* In this section, EPA presents the final designation for this chemical substance.

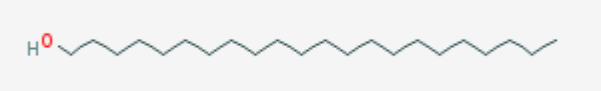
- *Appendix A (Conditions of Use Characterization):* This appendix contains a comprehensive list of TSCA and non-TSCA uses for the chemical substance from publicly available databases.

- *Appendix B (Hazard Characterization):* This appendix contains information on each of the studies used to support the hazard evaluation of the chemical substance.

- *Appendix C (Literature Search Outcomes):* This appendix includes literature search outcomes and rationales for studies that were identified in initial literature screening but were found to be off-topic or unacceptable for use in the screening-level review.

2. Background on 1-Docosanol

Table 1 below provides the CAS number, synonyms, and other information on 1-docosanol.

Table 1: 1-Docosanol at a Glance	
Chemical Name	1-Docosanol
CASRN	661-19-8
Synonyms	Docosan-1-ol; Behenyl alcohol; Docosanol; Behenic alcohol; Docosyl alcohol; n-Docosanol; Brassica alcohol
Trade Name(s)	Abreva; Tadenan; Lidavol; Lanette 22
Molecular Formula	$C_{22}H_{46}O$
Representative Structure	

1-Docosanol is a long-chain, saturated fatty alcohol that is a water-insoluble, waxy solid. Fatty alcohols are usually high-molecular-weight, straight-chain primary alcohols derived from natural fats and oils. Saturated fatty alcohols have no carbon-carbon double bonds, and have the formula – CH3(CH2)nOH – with variations in "n." Specifically, 1-docosanol is a saturated aliphatic alcohol with a 22-carbon chain, known as docosane, with a hydroxy group (-OH) at the terminal carbon and the formula CH3(CH2)21OH. This chemical has uses in consumer and industrial products, as well as in pharmaceutical products. 1-Docosanol functions as a thickener, emulsifier, emollient, and binder in a variety of applications and product sectors. Section 5 includes conditions of use for this chemical.

3. Physical-Chemical Properties

Table 2 lists physical-chemical properties for 1-docosanol. A chemical's physical-chemical properties provide a basis for understanding a chemical's behavior, including in the environment and in living organisms. These endpoints provide information generally needed to assess potential environmental release, exposure, and partitioning as well as insight into the potential for adverse toxicological effects.

Table 2: Physical-Chemical Properties for 1-Docosanol

Source/Model	Data Type	Endpoint	Endpoint Value	Notes
PubChem 2004	Experimental	State at room temperature	Solid	
Reported to the ECHA database 2019; HSDB 2006; ChemSpider 2019; EPISuitev.4.11[4]	Experimental	Molecular weight	327 g/mol	
EPISuitev.4.11	Experimental	Melting point	72.5°C	
EPISuitev.4.11	Calculated	Molecular weight	326.61 g/mol	
Lyman et al. 1990	Calculated	Molar volume	503 cm^3/mol	
ChemSpider 2019	Experimental	Water solubility	63600 at 30°C	This water solubility value seems unreasonably high considering the length of the carbon chain in 1-docosanol.
Reported to the ECHA database 2019	Experimental	Water solubility	<1 mg/L	Based on detection limit of method used.
EPISuitev.4.11	Estimated	Water solubility	$7.50x10^{-5}$ mg/L	
ChemSpider 2019	Experimental	Water solubility	$1.95x10^{-1}$ mol/L	This water solubility value seems unreasonably high considering the length of the carbon chain in 1-docosanol.
Reported to the ECHA database 2019	Experimental	Water solubility	$3.06x10^{-6}$ mol/L	
Reported to the ECHA database 2019	Experimental	Log K_{ow}	8.3	
EPISuitev.4.11	Estimated	Log K_{ow}	9.68	
EPISuitev.4.11	Estimated	Log K_{oa}	10.854	
EPISuitev.4.11	Estimated	Log K_{oc}	5.32 (MCI); 5.87 (K_{ow})	
HSDB 2006; EPISuitev.4.11	Experimental	Vapor pressure	0.22 mm Hg at 180°C	

[4] EPI Suite Physical Property Inputs – Melting Point = 72.5 deg C, SMILES: OCCCCCCCCCCCCCCCCCCCCCC

Table 2: Physical-Chemical Properties for 1-Docosanol				
Source/Model	**Data Type**	**Endpoint**	**Endpoint Value**	**Notes**
Reported to the ECHA database 2019	Experimental	Vapor pressure	$<7.5 \times 10^{-4}$ mm Hg (<0.001 mbar) at 38°C	
EPISuitev.4.11	Estimated	Vapor pressure	6.13×10^{-8} mm Hg	
EPISuitev.4.11	Estimated	Henry's Law	1.64×10^{-3} atm-m^3/mol (bond method) 4.88×10^{-3} (group method)	
EPISuitev.4.11	Estimated	Photolysis (volatilization)	2.49 hours (river) 7.45 days (lake)	
EPISuitev.4.11	Estimated	Photolysis (indirect)	3.97 hours ($T_{1/2}$)	OH rate constant 32.3 E-11 cm^3/molecules-second (12 hours day; 1.5E6 OH/cm^3)
EPISuitev.4.11	Estimated	Hydrolysis	Rate constants cannot be estimated	
EPISuitev.4.11	Estimated	Biodegradation potential	Ready prediction: Yes	
EPISuitev.4.11	Estimated	Wastewater treatment plant removal	99.8% Total Removal (56.6% biodegradation, 43.1% sludge, 0% air)	Input parameters: BioP = 40, BioA = 10 and BioS = 10 based on 37% in 28 days according to OECD 301B

EPA's Sustainable Futures/P2 Framework Manual[5] was used to interpret the physical-chemical properties provided in Table 2. Based on its reported physical form (PubChem, 2019) and measured melting point (EPISuite), 1-docosanol is a waxy solid under ambient conditions. In the solid form, 1-docosanol has the potential for exposure via direct dermal contact with the substance, through ingestion, and through inhalation of dust particles if they are generated. Based on its measured (Reported to the ECHA database, 2019) and estimated vapor pressures (EPISuite), 1-docosanol is not likely to be volatile at ambient temperatures. The estimated Henry's Law constant (EPISuite) for 1-docosanol reflects both the low volatility and low aqueous solubility of this compound; volatilization from water and aqueous solutions is expected to be minimal. Therefore, exposure via inhalation of vapors is expected to be minimal. Based on measured solubility data (Reported to the ECHA database, 2019), 1-docosanol is not considered water soluble, indicating that this substance is unlikely to dissolve in water and form an aqueous solution. Water insoluble substances have decreased potential for absorption through the gastrointestinal tract or lungs. Therefore, if exposed to the chemical in dust form, absorption through the lungs is unlikely. Based on its estimated log K_{ow} (EPISuite), 1-docosanol may cross lipid membranes; however, the structure of this substance indicates it has the potential to be metabolized, leading to a decreased likelihood of bioaccumulation. The estimated log K_{oc} (EPISuite) indicates this substance is immobile in soils and therefore unlikely to migrate into groundwater. 1-Docosanol is expected to have low persistence. Experimental biodegradation data for 1-docosanol indicate it is inherently biodegradable under aerobic conditions, and degradable under anaerobic conditions, indicating that this substance has the potential to break down into carbon dioxide and water. In addition, intermediate biodegradation products are expected to include fatty acids, which can be incorporated into biomass via normal metabolic processes.

3.1 References

ChemSpider. (2019). Docosanol. Retrieved from http://www.chemspider.com/Chemical-Structure.12100.html

European Chemicals Agency (ECHA). (2019). Docosan-1-ol. Retrieved from https://echa.europa.eu/substance-information/-/substanceinfo/100.010.498

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Lyman, Warren J., Reehl, W. F., Rosenblatt, D. H. (1990). Handbook of chemical property estimation methods: environmental behavior of organic compounds. American Chemical Society

PubChem (2004). Docosanol. Retrieved from https://pubchem.ncbi.nlm.nih.gov/compound/12620

U.S. EPA. (2019). Estimation Programs Interface Suite, v 4.11. United States Environmental Protection Agency, Washington, DC, USA

[5] https://www.epa.gov/sites/production/files/2015-05/documents/05.pdf

4. Relevant Assessment History

EPA assessed the toxicological profile of 1-docosanol and added the chemical to the Safer Choice Program's Safer Chemical Ingredients List (SCIL) in September 2017 under the functional class of emollients. The SCIL[6] is a continuously updated list of chemicals that meet low-concern Safer Choice criteria.[7]

EPA also reviewed international assessments of 1-docosanol. EPA identified assessments by the Organisation for Economic Co-operation and Development (OECD) and government agencies of Australia, Canada, Germany, and Japan.

The United Kingdom sponsored a long chain alcohol chemical category, which included 1-docosanol, as an OECD SIDS Initial Assessment Report (SIAR). The OECD SIAM 22[8] reviewed the SIAR in April 2006 and recommended 1-docosanol as low priority for further work based on the chemical's low hazard profile. EPA also reviewed 1-docosanol as part of a long chain alcohol hazard characterization in December 2009.[9]

The Australian Government's Department of Health National Industrial Chemicals Notification and Assessment Scheme (NICNAS) determined 1-docosanol to not pose an unreasonable risk to the health of workers and public health on the basis of the Tier I Inventory Multi-tiered Assessment and Prioritisation (IMAP) assessment.[10]

The Canadian Government, through an assessment of toxicity and exposure as part of its categorization of the Domestic Substance List, found that 1-docosanol did not meet its criteria for further attention.[11]

The German Environment Agency (UBA) designated 1-docosanol as "non-hazardous to water" in August 2018 based on an assessment of ecotoxicity and environmental fate.[12]

Japan's National Institute of Technology and Evaluation (NITE) categorized 1-docosanol as hazard class 4 for human health in 2017, the lowest-concern hazard ranking that NITE assigns.[13]

[6] https://www.epa.gov/saferchoice/safer-ingredients

[7] https://www.epa.gov/sites/production/files/2013-12/documents/dfe_master_criteria_safer_ingredients_v2_1.pdf

[8] https://hpvchemicals.oecd.org/UI/handler.axd?id=9802ef92-2c9d-4f21-877e-90b6133efd73

[9] https://chemview.epa.gov/chemview/proxy?filename=HC661198.pdf

[10] The IMAP framework is a science and risk-based framework for the assessment and prioritisation of chemicals on the Australian Inventory of Chemical Substances (AICS). It consists of 3 tiers of assessment, with the assessment effort increasing with each tier. https://www.nicnas.gov.au/chemical-information/imap-assessments/imap-assessments/human-health-assessments

[11] https://canadachemicals.oecd.org/ChemicalDetails.aspx?ChemicalID=A2958A06-5755-450B-9E53-81C208212012

[12] https://webrigoletto.uba.de/rigoletto/public/searchDetail.do?kennummer=656

[13] https://www.nite.go.jp/chem/jcheck/detail.action?cno=661-19-8&mno=2-3704&request_locale=en

5. Conditions of Use

Per TSCA section 3(4), the term "conditions of use" means the circumstances, as determined by the Administrator, under which a chemical substance is intended, known, or reasonably foreseen to be manufactured, processed, distributed in commerce, used, or disposed of. EPA assembled information on all uses of 1-docosanol (Appendix A) to inform which uses would be determined conditions of use.[14] One source of information that EPA used to help determine conditions of use is 2016 Chemical Data Reporting (CDR). The CDR rule (previously known as the Inventory Update Rule, or IUR), under TSCA section 8, requires manufacturers (including importers) to report information on the chemical substances they produce domestically or import into the U.S., generally above a reporting threshold of 25,000 lb. per site per year. CDR includes information on the manufacturing, processing, and use of chemical substances with information dating to the mid-1980s. CDR may not provide information on other life-cycle phases such as the chemical substance's end-of-life after use in products (i.e., disposal).

Based on CDR, 1-docosanol is manufactured domestically and imported. It is an organic sodium salt used in processing (incorporation into formulation, mixture or reaction and processing as a reactant for plastic materials and resin manufacturing, soap, cleaning compound, and toilet preparation manufacturing, paper manufacturing, paint and coating additives, products and other applications). 1-Docosanol is used in a variety of industrial applications, including oil and gas drilling, extraction, and support activities, as well as commercial products, including plastics and rubbers. Consumer uses include paper products, paints and coatings, and laundry and dishwashing products, among others. Based on the known manufacturing, processing, and uses of this chemical substance, EPA assumes distribution in commerce. Based on CDR, five facilities reported that 1-docosanol was not recycled (e.g., not recycled, remanufactured, reprocessed, or reused), and one facility reported recycling information as confidential business information (CBI). No information on disposal is found in CDR or through EPA's Toxics Release Inventory (TRI) Program[15] because 1-docosanol is not a TRI-reportable chemical. Although reasonably available information did not specify additional types of disposal, for purposes of this prioritization designation, EPA assumed end-of-life pathways that include releases to air, wastewater, surface water, and land via solid and liquid waste based on the conditions of use (e.g., incineration, landfill).

To supplement CDR, EPA conducted research through the publicly available databases listed in Appendix A (Table A.2) and performed additional internet searches to clarify conditions of use or find additional occupational[16] and consumer uses. This research improved the Agency's understanding of the conditions of use for 1-docosanol. Although EPA identified uses of 1-docosanol in personal care products, the screening review covered TSCA conditions of use for the chemical substance and personal care products were not considered in EPA's assessment. Exclusions to TSCA's regulatory scope regarding "chemical substance" can be found at TSCA section 3(2). Table 3 lists the conditions of use 1-docosanol considered for chemical substance prioritization, per TSCA

[14] The prioritization process, including the definition of conditions of use, is explained in the *Procedures for Prioritization of Chemicals for Risk Evaluation Under the Toxic Substances Control Act* (82 FR 33753).

[15] https://www.epa.gov/toxics-release-inventory-tri-program

[16] Occupational uses include industrial and/or commercial uses

section 3(4). Table 3 reflects the TSCA uses determined as conditions of use listed in Table A.3 (Appendix A).

Table 3: Conditions of Use for 1-Docosanol			
Life Cycle Stage	**Category**	**Subcategory of Use**	**Source**
Manufacturing	Domestic manufacture	Domestic manufacture- information on whether domestically manufactured was not reported.	EPA (2017b)
	Import	Import- manufacture	EPA (2017b)
Processing	Processing-incorporation into formulation, mixture or reaction	Processing aids not otherwise listed- paper manufacturing; soap, cleaning compound, and toilet preparation manufacturing, plastic materials and resin manufacturing	EPA (2017b)
		Surface active agents- paper manufacturing	
		Surface active agents- soap, cleaning compound, and toilet preparation manufacturing	
		Paint additives and coating additives not described by other categories- paint and coating manufacture	
		Lubricant and lubricant additives- petroleum lubricating oil and grease manufacturing	
		Other- all other chemical product and preparation manufacturing, paper manufacturing	
	Processing as a reactant	Processing aids, not otherwise listed- paper manufacturing	
		Surface active agents- soap, cleaning compound, and toilet preparation manufacturing	
	Other	Agricultural additive manufacturing; textiles, apparel, and leather manufacturing	Synapse Information Resources (n.d.), CPCat (2019)
	Lubricants and lubricant additives	Food-contact metallic manufacturing	Synapse Information Resources (n.d.),CPCat (2019)
	Recycling	Recycling	EPA (2017b)[17]
Distribution	Distribution	Distribution	EPA (2017b)
Industrial uses	Other	Oil and gas drilling, extraction, and support activities	Synapse Information Resources (n.d.), CPCat (2019)
	Processing aids, not otherwise listed	Anti-foaming agent	CPCat (2019)
	Surface active agents	Surfactant	CPCat (2019)

[17] In the 2016 CDR, five facilities reported that 1-docosanol was not recycled (e.g., not recycled, remanufactured, reprocessed, or reused), and one facility reported recycling information as CBI (EPA 2017b).

Table 3: Conditions of Use for 1-Docosanol			
Life Cycle Stage	**Category**	**Subcategory of Use**	**Source**
Commercial	Plastic and rubber products not elsewhere classified		EPA (2017b)
Commercial/ consumer	Paper products		EPA (2017b)
	Paints and coatings		EPA (2017b)
Consumer	Laundry and dishwashing products		EPA (2017b)
	Window and door sealant		DeLima Associates (2016a)
Disposal	Releases to air, wastewater, solid and liquid wastes		Though not explicitly identified, releases from disposal were assumed to be reasonably foreseen[18]

[18] See Section 5 for a discussion on why releases were assumed to be reasonably foreseen for purposes of this prioritization designation.

6. Hazard Characterization

EPA reviewed primary literature and other data sources to identify reasonably available information. This literature review approach[19] is tailored to capture the reasonably available information associated with low-hazard chemicals. EPA also used this process to verify the reasonably available information for reliability, completeness, and consistency. EPA reviewed the reasonably available information to identify relevant, quality studies to evaluate the hazard potential for 1-docosanol against the endpoints listed below. EPA's New Chemicals Program has used these endpoints for decades to evaluate chemical substances under TSCA[20] and EPA toxicologists rely on these endpoints as key indicators of potential human health and environmental effects. These endpoints also align with internationally accepted hazard characterization criteria, such as the Globally Harmonized System of Classification and Labelling of Chemicals[21] as noted above in Section 4 and form the basis of the comparative hazard assessment of chemicals.

Human health endpoints evaluated: Acute mammalian toxicity, repeated dose toxicity, carcinogenicity, mutagenicity/genotoxicity, reproductive and developmental toxicity, neurotoxicity, skin sensitization, respiratory sensitization, immunotoxicity and eye and skin irritation.

Environmental fate and effects endpoints evaluated: Aquatic toxicity, environmental persistence, and bioaccumulation.

The low-concern criteria used to evaluate both human health and environmental fate and effects are included in Table 4 below.

Table 4: Low concern Criteria for Human Health and Environmental Fate and Effects

Human Health				
Acute Mammalian Toxicity[22]	**Very High**	**High**	**Moderate**	**Low**
Oral LD50 (mg/kg)	≤ 50	> 50 – 300	> 300 - 2000	> 2000
Dermal LD50 (mg/kg)	≤ 200	> 200 – 1000	> 1000 - 2000	> 2000
Inhalation LC50 (vapor/gas) (mg/L)	≤ 2	> 2 – 10	> 10 - 20	> 20
Inhalation LC50 (dust/mist/fume) (mg/L)	≤ 0.5	> 0.5 - 1.0	> 1.0 - 5	> 5

[19] Discussed in the document "Approach Document for Screening Hazard Information for Low-Priority Substances Under TSCA," which can be found at https://www.regulations.gov/document?D=EPA-HQ-OPPT-2019-0450-0002.

[20] https://www.epa.gov/sustainable-futures/sustainable-futures-p2-framework-manual

[21] https://www.unece.org/fileadmin/DAM/trans/danger/publi/ghs/ghs_rev07/English/ST_SG_AC10_30_Rev7e.pdf

[22] Values derived from GHS criteria (*Chapter 3.1: Acute Toxicity.* 2009, United Nations).

Table 4: Low concern Criteria for Human Health and Environmental Fate and Effects				
Repeated Dose Toxicity, Neurotoxicity, and Immunotoxicity (90-day study)[23]		**High**	**Moderate**	**Low**
Oral (mg/kg-bw/day)		< 10	10 - 100	> 100
Dermal (mg/kg-bw/day)		< 20	20 - 200	> 200
Inhalation (vapor/gas) (mg/L/6h/day)		< 0.2	0.2 - 1.0	> 1.0
Inhalation (dust/mist/fume) (mg/L/6h/day)		< 0.02	0.02 - 0.2	> 0.2
Reproductive and Developmental Toxicity[24]		**High**	**Moderate**	**Low**
Oral (mg/kg/day)		< 50	50 - 250	> 250
Dermal (mg/kg/day)		< 100	100 - 500	> 500
Inhalation (vapor, gas, mg/L/day)		< 1	1 - 2.5	> 2.5
Inhalation (dust/mist/fume, mg/L/day)		< 0.1	0.1 - 0.5	> 0.5
Mutagenicity/ Genotoxicity[25]	**Very High**	**High**	**Moderate**	**Low**
Germ cell mutagenicity	GHS Category 1A or 1B: Substances known to induce heritable mutations or to be regarded as if they induce heritable mutations in the germ cells of humans.	GHS Category 2: Substances which cause concern for humans owing to the possibility that they may induce heritable mutations in the germ cells of humans.	Evidence of mutagenicity support by positive results *in vitro* OR *in vivo* somatic cells of humans or animals	Negative for chromosomal aberrations and gene mutations, or no structural alerts.
Mutagenicity and Genotoxicity in Somatic Cells		OR Evidence of mutagenicity supported by positive results in *in vitro* AND *in vivo* somatic cells and/or germ cells of humans or animals.		

[23] Values from GHS criteria for Specific Target Organ Toxicity Repeated Exposure (*Chapter 3.9: Specific Target Organ Toxicity Repeated* Exposure. 2009, United Nations).

[24] Values derived from the US EPA's Office of Pollution Prevention & Toxics criteria for HPV chemical categorizations (*Methodology for Risk-Based Prioritization Under ChAMP*), and the EU REACH criteria for Annex IV (2007).

[25] From GHS criteria (*Chapter 3.5: Germ Cells Mutagenicity.* 2009, United Nations) and supplemented with considerations for mutagenicity and genotoxicity in cells other than germs cells.

Table 4: Low concern Criteria for Human Health and Environmental Fate and Effects				
Carcinogenicity[26]	**Very High**	**High**	**Moderate**	**Low**
	Known or presumed human carcinogen (GHS Category 1A and 1B)	Suspected human carcinogen (GHS Category 2)	Limited or marginal evidence of carcinogenicity in animals (and inadequate[27] evidence in humans)	Negative studies or robust mechanism-based SAR
Sensitization[28]		**High**	**Moderate**	**Low**
Skin sensitization		High frequency of sensitization in humans and/or high potency in animals (GHS Category 1A)	Low to moderate frequency of sensitization in human and/or low to moderate potency in animals (GHS Category 1B)	Adequate data available and not GHS Category 1A or 1B
Respiratory sensitization		Occurrence in humans or evidence of sensitization in humans based on animal or other tests (equivalent to GHS Category 1A or 1B)	Limited evidence including the presence of structural alerts	Adequate data available indicating lack of respiratory sensitization
Irritation/ Corrosivity[29]	**Very High**	**High**	**Moderate**	**Low**
Eye Irritation/ Corrosivity	Irritation persists for >21 days or corrosive	Clearing in 8-21 days, severely irritating	Clearing in 7 days or less, moderately irritating	Clearing in less than 24 hours, mildly irritating
Skin Irritation/ Corrosivity	Corrosive	Severe irritation at 72 hours	Moderate irritation at 72 hours	Mild or slight irritation at 72 hours

[26] Criteria mirror classification approach used by the IARC (*Preamble to the IARC Monographs: B. Scientific Review and Evaluation: 6. Evaluation and rationale.* 2006*)* and incorporate GHS classification scheme (*Chapter 3.6: Carcinogenicity.* 2009, United Nations).

[27] EPA's approach to determining the adequacy of information is discussed in the document "Approach Document for Screening Hazard Information for Low-Priority Substances Under TSCA", also released at proposal.

[28] Incorporates GHS criteria (*Chapter 3.4: Respiratory or Skin Sensitization.* 2009, United Nations).

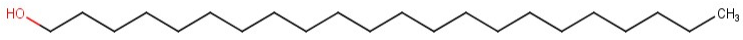
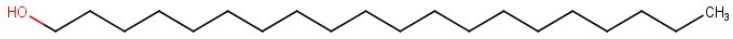
[29] Criteria derived from the Office of Pesticide Programs Acute Toxicity Categories (US EPA. *Label Review Manual.* 2010).

Table 4: Low concern Criteria for Human Health and Environmental Fate and Effects			
Environmental Fate and Effects			
Acute Aquatic Toxicity Value (L/E/IC50)[30]	**Chronic Aquatic Toxicity Value (L/E/IC50)[30]**	**Persistence (Measured in terms of level of biodegradation)[31]**	**Bioaccumulation Potential[32]**
May be low concern if ≤10 ppm…	…and ≤1 ppm…	…and the chemical meets the 10-day window as measured in a ready biodegradation test…	…and BCF/BAF < 1000.
Low concern if >10 ppm and <100 ppm…	…and >1 ppm and <10 ppm…	…and the chemical reaches the pass level within 28 days as measured in a ready biodegradation test	
Low concern if ≥100 ppm…	…and ≥ 10 ppm…	… and the chemical has a half-life < 60 days…	

6.1 Human Health Hazard

Below is a summary of the reasonably available information that EPA included in the hazard evaluation of 1-docosanol. In many cases, EPA used analogous chemicals to make findings for a given endpoint. Where this is the case, use of the analog is explained. If the chemical studied is not named, the study is for 1-docosanol. Appendix B contains more information on each study.

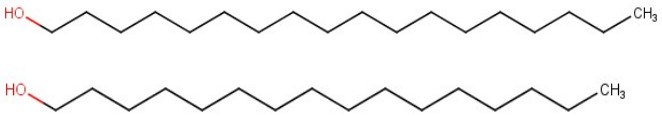
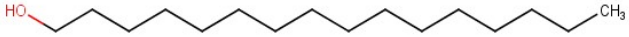
1-Docosanol is a linear C22 saturated aliphatic alcohol. EPA used best professional judgement to select analogs for 1-docosanol based on similarity in structure, physical-chemical properties, and functionality, with the assumption that these chemicals will have similar environmental transport and persistence characteristics, bioavailability and toxicity profiles. All analogs presented in Table 5 are long chain saturated aliphatic alcohols and have chain lengths from C16 to C20. Based on these factors, the environmental and toxicological effects of these analogs are expected to be very similar to each other and to 1-docosanol.

Table 5: 1-Docosanol and Analog Structures		
CASRN	**Name**	**Structure**
661-19-8	**1-Docosanol (C22)**	
629-96-9	**1-Eicosanol (C20)**	

[30] Derived from GHS criteria (*Chapter 4.1: Hazards to the Aquatic Environment.* 2009, United Nations), EPA OPPT New Chemicals Program (*Pollution Prevention (P2) Framework,* 2005*)* and OPPT's criteria for HPV chemical categorization (*Methodology for Risk Based Prioritization Under ChAMP. 2009).*

[31] Derived from OPPT's New Chemicals Program and DfE Master Criteria, and reflects OPPT policy on PBTs (*Design for the Environment Program Master Criteria for Safer Chemicals, 2010)*.

[32] Derived from OPPT's New Chemicals Program and Arnot & Gobas (2006) [Arnot, J.A. and F.A. Gobas, *A review of bioconcentration factor (BCF) and bioaccumulation factor (BAF) assessments for organic chemicals* in aquatic organisms. Environmental Reviews, 2006. 14: p. 257-297.]

Table 5: 1-Docosanol and Analog Structures		
112-92-5	1-Octadecanol (C18)	
67762-27-0	Alcohols, C16-18	 Representative structures
36653-82-4	Cetyl alcohol (C16)	

Alcohols, C16-18 and C18 unsaturated (CASRN 68002-94-8) was also included in analog data searches; relevant, quality studies[33] were only identified for the CASRNs listed in Table 5.

6.1.1 Absorption, Distribution, Metabolism, and Excretion

To review absorption, distribution, metabolism and excretion (ADME) endpoints without adequate quality[33] experimental data, EPA used widely accepted new approach methodologies (NAMs), such as modeling and estimation tools often based on physical-chemical properties, which provided information sufficient to fill these endpoints.

Absorption

Because of its low water solubility, 1-docosanol is not expected to be absorbed from dermal, inhalation, or oral (from the gastrointestinal tract) exposures.

Distribution

Experimental data determined to be of adequate quality[34] on 1-docosanol or closely related analogs were not reasonably available for the assessment of distribution potential. Based on 1-docosanol's estimated log K_{ow}, 1-docosanol will likely be distributed to fatty tissues in the body. However, it is expected to be excreted through urine and feces (described below under Excretion).

Metabolism

Because quality experimental data[34] on 1-docosanol metabolite formation were not reasonably available, the Quantitative Structure-Activity Relationship (QSAR) toolbox[35] was used to run the rat liver S9 metabolism simulator, the skin metabolism simulator, and the *in vivo* rat metabolism simulator. The QSAR toolbox was used to identify putative 1-docosanol metabolites. All simulators reported docosanoic acid as a putative metabolite. The rat liver S9 and skin metabolism simulators

[33] This process is further discussed in the document "Approach Document for Screening Hazard Information for Low-Priority Substances Under TSCA."

[34] The literature search and review process to determine studies of adequate quality for inclusion in the screening review is further discussed in the document "Approach Document for Screening Hazard Information for Low-Priority Substances Under TSCA." https://www.regulations.gov/document?D=EPA-HQ-OPPT-2019-0450-0002.

35 https://www.oecd.org/chemicalsafety/risk-assessment/oecd-qsar-toolbox.htm

also predicted the C22 aldehyde docosanal. The *in vivo* rat metabolism simulator predicted various ketone metabolites and lower carbon (C10 – C18) containing fatty acids.

Excretion

To assess 1-docosanol's excretion pathways, EPA used read-across from 1-octadecanol and cetyl alcohol. Chinchilla rabbits were administered 1-octadecanol via oral gavage (OECD, 2006). Approximately 7.6% of the administered dose was measured as the glucuronide metabolite in urine 24 hours after dosing. Based on the data for 1-ocatdecanol, 1-docosanol is likely to be excreted as a glucuronide conjugate in small amounts in the urine. A study on Wistar rats exposed via oral gavage to analog cetyl alcohol measured 13.9% elimination in feces and 13.3% in urine (Freitag et al., 1982). One percent or less was retained in abdominal adipose tissue, liver, and lung, and 64.3% was retained in the carcass. Cetyl alcohol is an endogenous substance, is highly susceptible to oxidation via metabolic processes, and is involved in the metabolism of lipids and the biosynthesis of wax and plasmalogen in mammals.[36,37,38] The role of cetyl alcohol in these membrane-associated pathways likely accounts for the high measured retention in carcass. Due to 1-docosanol's low vapor pressure, gas exchange is unlikely to be a major pathway of excretion.

6.1.2 Acute Toxicity

EPA assessed the mammalian toxicity potential from acute oral exposures to 1-docosanol using experimental data. A study following OECD Guideline 423 exposed rats to 1-docosanol via oral gavage. The study authors reported no mortality in the single tested dose (2000 mg/kg), resulting in an LD_{50} greater than 2000 mg/kg (OECD, 2006; Reported to the ECHA database, 1997a). Another OECD 423 Guideline study in rats exposed to 1-docosanol via oral gavage reported no mortality at the highest tested dose of 10,000 mg/kg (OECD, 2006). A study on mice exposed to 1-docosanol via oral gavage also reported no mortality at the single tested dose of 1000 mg/kg, resulting in a LD_{50} greater than 1000 mg/kg (Elder, 1988). Given the limited dosing of the oral gavage study and that no mortality was observed in the other studies, these results provide sufficient information to indicate low concern for acute toxicity with LD_{50}s greater than the low-concern criteria benchmark of 2000 mg/kg.

EPA assessed mammalian toxicity from acute dermal exposures using read-across from C16-18 alcohols. Rabbits exposed to C16-18 alcohols dermally for 24 hours resulted in an LD_{50} greater than 8000 mg/kg (OECD, 2006). These results provide sufficient information to indicate low concern based on the dermal low-concern benchmark of 2000 mg/kg.

EPA assessed mammalian toxicity from acute inhalation exposures using read-across from C16-18 alcohols. Rats exposed to C16-18 alcohols via vapor inhalation for six hours and observed for 14 days resulted in no mortalities at the highest dose of 0.00014 mg/L (the saturated air concentration) (Reported to the ECHA database, 1979). Since no effects were observed at saturated air

[36] ChEBI 2019; Chemical Entities of Biological Interest - hexadecan-1-ol. Available from, as of November 26, 2019: https://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:16125

[37] HMDB 2019; Human Metabolome Database - 1-Hexadecanol. Available from, as of November 26, 2019: http://www.hmdb.ca/metabolites/HMDB0003424

[38] PubChem 2019; 1-Hexadecanol (Compound). U.S. National Library of Medicine. Available from, as of November 26, 2019: https://pubchem.ncbi.nlm.nih.gov/compound/1-Hexadecanol#section=Tissue-Locations

concentration, these results provide sufficient information to indicate low concern based on no effects at saturation.

6.1.3 Repeated Dose Toxicity

EPA assessed mammalian toxicity from repeated exposures to 1-docosanol using experimental data. A study on rats exposed via oral gavage to 1-docosanol for 26 weeks resulted in a no observed adverse effect level (NOAEL) of 1000 mg/kg-day (OECD, 2006; Iglesias et al., 2002a). Similarly, a 26-week study in dogs via oral gavage resulted in a NOAEL of 2000 mg/kg-day (Iglesias et al., 2002a). These results provide sufficient information to indicate low concern for toxicity from repeated exposures because the NOAELs meet the low-concern criteria benchmark of 100 mg/kg-day for a 90-day repeated dose study.

6.1.4 Reproductive and Developmental Toxicity

EPA assessed the potential for mammalian reproductive toxicity from 1-docosanol using experimental data. Rats were exposed to 1-docosanol by oral gavage for 71 days total, beginning during premating and extending through mating for males and beginning 15 days premating and extending through gestation day (GD) 20 for females (OECD, 2006; Iglesias et al., 2002c; U.S. EPA, 2002d). This study reported no adverse effects, resulting in a NOAEL of 1000 mg/kg-day. These results provide sufficient information to indicate low concern because the NOAEL meets the low-concern criteria benchmark of 250 mg/kg-day for reproductive toxicity.

EPA also assessed the potential for mammalian developmental toxicity from 1-docosanol using experimental data. A study on rabbits exposed to 1-docosanol by oral gavage during GD 6-19 reported a NOAEL of 2000 mg/kg-day (OECD, 2006; Iglesias et al., 2002c). In a second study, rats were exposed to 1-docosanol by oral gavage for 71 days total, beginning during premating and extending through mating for males and beginning 15 days during premating and extending through GD 20 for females (OECD, 2006; Iglesias et al., 2002c; U.S. EPA, 2002d). This study reported no adverse developmental effects, resulting in a NOAEL of 1000 mg/kg-day. These results provide sufficient information to indicate low concern for developmental toxicity by exceeding the low-concern criteria benchmark of 250 mg/kg-day.

6.1.5 Genotoxicity

EPA assessed experimental gene mutation and chromosomal aberration studies as an indicator of 1-docosanol's potential to cause genotoxicity. An *in vivo* gene mutation study in mice reported 1-docosanol as negative for inducing genotoxicity (OECD, 2006; Iglesias et al., 2002a; U.S. EPA, 2002c). This result is further supported by negative gene mutation findings in *in vitro* studies on bacteria species and Chinese hamster lung fibroblast cells exposed to 1-docosanol, with and without metabolic activation (OECD, 2006; Iglesias et al., 2002a, b; U.S. EPA, 2002b). Further, Chinese hamster lung fibroblast cells exposed to 1-docosanol were negative for chromosomal aberrations with and without metabolic activation (Iglesias et al., 2002a; U.S. EPA, 2002a). These results provide sufficient information to indicate a low concern for genotoxicity.

6.1.6 Carcinogenicity

Experimental data determined to be of adequate quality[39] on 1-docosanol or closely-related analogs were not reasonably available for the assessment of carcinogenicity potential. EPA used widely accepted new approach methodologies (NAMs), such as publicly available quantitative structure activity relationship (QSAR) models and structural alerts (SA), to assess the carcinogenic potential for 1-docosanol. Based on OncoLogic[40] estimations, high molecular weight aliphatic alcohols like 1-docosanol (C > 20) are unlikely to be carcinogenic. In addition, processing 1-docosanol through a selection of other models did not identify any specific concern for carcinogenic potential. Structural alerts represent molecular functional groups or substructures that are known to be linked to the carcinogenic activity of chemicals. The most common structural alerts are those for electrophiles (either direct acting or following activation). Modulating factors that will impact the carcinogenic potential of a given electrophile will include its relative hardness or softness, its molecular flexibility or rigidity, and the balance between its reactivity and stability.[41] For this chemical, there is an absence of the types of reactive structural features that are present in genotoxic carcinogens. 1-Docosanol is not an electrophile. Further, the Virtual models for property Evaluation of chemicals within a Global Architecture (VEGA) models'[42] results indicate 1-docosanol has low potential to be carcinogenic or mutagenic with moderate and high reliability.

Applying expert scientific judgement based on the reasonably available information and weight of the scientific evidence, EPA finds that 1-docosanol's transformation profile, lack of structural alerts, non-carcinogenic predictions, and absence of genotoxicity in experimental studies provide sufficient information that this chemical has low concern for carcinogenicity.

6.1.7 Neurotoxicity

Though no guideline neurotoxicity studies were available for 1-docosanol or the identified analogs, repeated dose studies in rats and dogs for 1-docosanol reported no effects on the limited neurological endpoints that were evaluated (i.e., brain and spinal cord histopathology). 1-Docosanol did not produce histopathological lesions in the brain or spinal cord of dogs at oral gavage doses up to 2,000 mg/kg-day in a 26-week study (OECD, 2006). Similarly, in rats, no brain or spinal cord lesions were observed at oral gavage doses up to 1,000 mg/kg-day in a 26-week study (OECD, 2006; Iglesias et al., 2002a).

Assays related to neurological functions were identified in ToxCast;[43] however, data for 1-docosanol or analogs were not reasonably available for these assays.

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[39] The literature search and review process to determine studies of adequate quality for inclusion in the screening review is further discussed in the document "The Approach Document for Screening Hazard Information for Low-Priority Substances under TSCA." https://www.regulations.gov/document?D=EPA-HQ-OPPT-2019-0450-0002

[40] https://www.epa.gov/tsca-screening-tools/oncologictm-computer-system-evaluate-carcinogenic-potential-chemicals

[41] "Fundamental and Guiding Principles for (Q)SAR Analysis of Chemical Carcinogens with Mechanistic Considerations: Series on Testing and Assessment, No. 229." 2015. Environment Directorate, Joint Meeting of the Chemicals Committee and the Working Party on Chemicals, Pesticides and Biotechnology.

[42] There are four carcinogenicity models housed within the VEGA 1.1.4 software tool available from https://www.vegahub.eu. A summary of the results from these models is provided in Appendix B.

[43] https://comptox.epa.gov/dashboard Chemical specific assay list can be found at https://comptox.epa.gov/dashboard/dsstoxdb/results?search=661-19-8

Based on the neurological evidence from the repeated dose studies, and supporting evidence indicating low concern for other endpoints, such as acute, reproductive, and developmental toxicity, EPA has sufficient information to indicate low concern for neurotoxicity.

6.1.8 Skin Sensitization

Experimental data determined to be of adequate quality[44] on 1-docosanol or closely-related analogs were not reasonably available for the assessment of skin sensitization. EPA used widely accepted NAMs, such as the OECD QSAR Toolbox Version 4.2, which did not identify any structural alerts for protein binding potential by 1-docosanol in regard to skin sensitization. These results provide sufficient information to indicate low concern for skin sensitization by 1-docosanol.

6.1.9 Respiratory Sensitization

Experimental data determined to be of adequate quality[45] on 1-docosanol or closely related analogs were not reasonably available for the assessment of respiratory sensitization potential. To model respiratory sensitization potential for 1-docosanol, EPA used NAMs, such as the QSAR Toolbox, version 4.2 models[46] for keratinocyte gene expression; protein binding potency h-CLAT; protein binding potency cysteine; protein binding potency lysine; and respiratory sensitization. No structural alerts were identified for 1-docosanol. The results from these NAMs and weight of the scientific evidence provide sufficient information to indicate low concern for respiratory sensitization.

6.1.10 Immunotoxicity

EPA reviewed the literature for immunotoxicity endpoints such as lymphoid organ weight, histopathology, and immune function. Specific endpoints included immune system function (e.g., T-cell dependent antibody response), immunophenotyping (e.g., changes in cell types), natural killer cell activity, host resistance assays, macrophage neutrophil function, and cell-mediated immunity assays. Experimental data determined to be of adequate quality[47] on 1-docosanol or closely-related analogs were not reasonably available for the assessment of immunotoxicity potential.

Repeated dose testing is designed to be comprehensive in nature and is intended to address a wide range of possible impacts, including, but not limited to immunotoxicity. The testing required to address repeated dose toxicity typically includes routine clinical observations, hematology and clinical biochemistry, body weight/food and water consumption, as well as both gross necropsy and histopathology involving organs and organ systems. For example, repeated dose studies can evaluate

[44] The literature search and review process to determine studies of adequate quality for inclusion in the screening review is further discussed in the document "The Approach Document for Screening Hazard Information for Low-Priority Substances under TSCA." https://www.regulations.gov/document?D=EPA-HQ-OPPT-2019-0450-0002

[45] The literature search and review process to determine studies of adequate quality for inclusion in the screening review is further discussed in the document "Approach Document for Screening Hazard Information for Low-Priority Substances under TSCA." https://www.regulations.gov/document?D=EPA-HQ-OPPT-2019-0450-0002.

[46] The OECD QSAR Toolbox is one of EPA's listed new approach methodologies under TSCA 4(h)(2), available at https://www.epa.gov/sites/production/files/2019-12/documents/alternative_testing_nams_list_first_update_final.pdf

[47] The literature search and review process to determine studies of adequate quality for inclusion in the screening review is further discussed in the document "Approach Document for Screening Hazard Information for Low-Priority Substances under TSCA." https://www.regulations.gov/document?D=EPA-HQ-OPPT-2019-0450-0002.

changes to the spleen or thymus, which with accompanying histological changes or changes in hematological parameters can indicate potential for immunological toxicity. Where immune system-related endpoints were measured in repeated dose studies, any adverse effects would be incorporated into the lowest observed adverse effect level used against the low-concern benchmarks. Therefore, EPA relied on this information from repeated dose studies when it was reasonably available. For 1-docosanol, the included repeated dose studies did not report changes in lymphoid organ weights (thymus, spleen, lymph nodes), with accompanying histopathology, or hematological changes due to exposure to this chemical substance in mammals. These results provide sufficient information to indicate low concern for immunotoxicity potential from 1-docosanol.

6.1.11 Skin Irritation

EPA assessed the potential for skin irritation using a study following OECD Guideline 404 (OECD, 2006; Reported to the ECHA database, 1997c). Rabbits exposed dermally to 1-docosanol demonstrated negative results, providing sufficient information to indicate low concern for skin irritation from 1-docosanol.

6.1.12 Eye Irritation

EPA assessed 1-docosanol's potential to act as an eye irritant using experimental studies. A study following OECD Guideline 405 exposed rabbits to 1-docosanol via the eye (OECD, 2006; Reported to the ECHA database, 1997b, d). At one hour, all animals had slight conjunctival irritation. However, these results were completely reversible within 72 hours. Another study exposing rabbits to 1-docosanol reported that 2 hours and 6 hours post-exposure, all animals had conjunctival irritation (OECD, 2006; Elder, 1988). All effects were completely reversible within 24 hours. These results indicate 1-docosanol is moderately irritating to eyes. The weight of the scientific evidence for these results is discussed in Section 8.1.

6.1.13 Hazards to Potentially Exposed or Susceptible Subpopulations

The above information supports a low human health hazard finding for 1-docosanol based on low-concern criteria. This finding considers the endogenous nature of 1-docosanol and the potential for developmental toxicity, reproductive toxicity, and acute or repeated dose toxicity that may impact potentially exposed or susceptible subpopulations. Based on the hazard information discussed in Section 6, EPA did not identify populations with greater susceptibility to 1-docosanol.

6.2 Environmental Hazard

To review environmental hazard endpoints without adequate quality[33] experimental data, EPA used widely accepted new approach methodologies (NAMs), such as modeling and estimation tools often based on physical-chemical properties, which provided information sufficient to fill these endpoints and form the basis for designation. EPA assessed environmental hazard for 1-docosanol based on available acute experimental data and estimated chronic toxicity values using the Ecological Structure Active Relationships (ECOSAR) Predictive Model.[48] Appendix B contains a summary of the reasonably available environmental hazard data.

[48] https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model

6.2.1 Acute Aquatic Toxicity

EPA assessed environmental hazard from acute exposures using experimental data on 1-docosanol and analogs. However, all of this data predicted effect levels at concentrations that exceed the water solubility of 1-docosanol (Table 3), indicating the physical-chemical properties of 1-docosanol limit the dissolved and bioavailable concentrations of the chemical in the water column such that acute toxicity is unlikely to be exhibited. Aquatic vertebrates exposed to 1-docosanol for 96 hours displayed no effects at the highest dose (1000 mg/L), resulting in an LC_{50} value greater than 1000 mg/L (OECD, 2006; Reported to the ECHA database, 2000). Aquatic invertebrates exposed to 1-octadecanol for 48 hours resulted in an EC_{50} of 1700 mg/L. Algae exposed to 1-octadecanol for 96 hours displayed no effects at the highest dose (250 mg/L unfiltered, 10 mg/L filtered), resulting in an EC_{50} greater than 10 mg/L. The effect concentrations for all three trophic levels exceed the water solubility of 1-docosanol, limiting the dissolved (and bioavailable) concentration of the chemical in the water column to the point that acute toxicity is unlikely to be exhibited. These results are also supported by ECOSAR estimations. The predicted and measured log K_{ow} values range from 8.3 to 9.68 (Table 3) for 1-docosanol and are greater than ECOSAR's acute benchmark[49] of log K_{ow} of 5. Chemicals with log K_{ow} values of 5 or greater are expected to result in no effects at saturation during a 48-hour to 96-hour test.[50] These results provide sufficient information to indicate that 1-docosanol is low concern for acute aquatic toxicity.

6.2.2 Chronic Aquatic Toxicity

EPA assessed environmental hazard from chronic exposures using experimental data on an analog and the ECOSAR Predictive Model. A study on aquatic invertebrates exposed to 1-octadecanol reported a no observed effect concentration (NOEC) of 0.98 mg/L at the highest dose tested in the study (OECD, 2006). Given the low water solubility of this chemical (Section 3), no effects are expected to aquatic invertebrates at dissolved aquatic concentrations. As further evidence, the range of log K_{ow} values for 1-docosanol (8.3 to 9.68, see Table 3) exceed the chronic benchmark for log K_{ow} of 8 for ECOSAR. Chemicals with log K_{ow} values of 8 or greater are expected to result in no effects at saturation even with long-term exposures.[50] Thus, ECOSAR predicts that the physical-chemical properties of 1-docosanol, specifically the high octanol water partition coefficient and low water solubility, limit the dissolved (and bioavailable) concentration of the chemical in the water column to the extent that chronic toxicity is unlikely to be exhibited. This conclusion is also supported by an OECD SIAR (OECD, 2006) and EPA's Hazard Characterization (U.S. EPA, 2009). Additionally, biodegradation (discussed below in Section 6.3.1) and sorption to sediments (described in Section 3) are expected to further reduce the dissolved concentration in the environment. Therefore, these results provide sufficient information to indicate 1-docosanol has low environmental hazard for aquatic vertebrates, aquatic invertebrates and algae.

[49] The limits of each QSAR must be understood if the results are to be interpreted properly. In general, when the log Kow is ≤ 5.0 for fish and daphnid, or ≤ 6.4 for green algae, ECOSAR provides reliable estimates for acute effects. If the log Kow exceeds those limits, empirical data indicate that the decreased solubility of these lipophilic chemicals results in "no effects at saturation." Source: https://www.epa.gov/sites/production/files/2015-05/documents/06.pdf

[50] https://www.epa.gov/sites/production/files/2015-05/documents/06.pdf

6.3 Persistence and Bioaccumulation Potential

6.3.1 Persistence

EPA assessed environmental persistence for 1-docosanol using experimental studies. An OECD 301B Guideline study reported that 1-docosanol degraded 37% in 28 days (OECD, 2006). While this result indicates 1-docosanol is not readily biodegradable under aerobic conditions, this substance is considered inherently biodegradable based on read-across from 1-octadecanol (OECD, 2006). Two studies following OECD Guideline 301D reported that 1-octadecanol degraded 69% (OECD, 2006) and 67% (OECD, 2006) in 28 days. An OECD Guideline 301B study reported that 1-docosanol degraded 37% in 28 days (OECD, 2006).

EPA assessed the potential for anaerobic biodegradation using read-across from cetyl alcohol. Cetyl alcohol reached 97% total degradation after 28 days using activated sludge from a municipal sewage treatment plant and an anaerobic sludge from a secondary digester of a municipal sewage treatment plant (Steber and Wierich, 1987). In another study under similar conditions, cetyl alcohol reached 90% degradation after 28 days (Nuck and Federle, 1996). These results indicate 1-docosanol is expected to biodegrade under anaerobic conditions based on read-across from cetyl alcohol.

No degradation products of concern were identified for this chemical substance. In addition, the analog 1-octadecanol had a half-life of 5.7 hours in brown water in an indirect photolysis study (Pittaway et al., 2015). These results provide sufficient information to indicate 1-docosanol will degrade under aerobic and anaerobic environments and has low persistence.

6.3.2 Bioaccumulation Potential

Fatty alcohols are known to be absorbed and metabolized by fish to form molecules for energy, growth and reproduction.[51] Because the chemicals have a role in endogenous physiological processes, they are not expected to bioconcentrate. Similar to its impact on aquatic toxicity, the low water solubility and high K_{ow} values of 1-docosonol will limit the dissolved and bioavailable concentration of the chemical in the water column. This conclusion is supported by experimental evidence from a study on aquatic vertebrates exposed to cetyl alcohol, which reported a BCF of 56 (Freitag et al., 1982). This result and the weight of the scientific evidence provide sufficient information to indicate 1-docosanol has low potential for bioaccumulation in the environment based on the low-concern benchmark of less than 1000.

[51] Douglas R. Tocher. {2003}. Metabolism and Functions of Lipids and Fatty Acids in Teleost Fish, Reviews in Fisheries Science, 11:2, 107-184

7. Exposure Characterization

EPA considered reasonably available information on exposure for 1-docosanol. In general, there is limited information on exposure for low hazard chemicals. EPA consulted sources of use information that include the CDR database and other databases and public sources. Of these sources, EPA determined that the CDR database contained the primary source of information on the conditions of use for this exposure characterization. EPA also consulted sources of use information from these other databases and public sources (listed in Table A.2). EPA used these sources only where they augmented information from the CDR database and to inform intended, known, or reasonably foreseeable uses (Section 5).

As shown in Tables 3 and A.3, 1-docosanol is used as a processing aid, additive and/or surfactant for soap, cleaning compounds, and toilet preparation manufacturing, paper manufacturing, paint and coating manufacturing and other applications, as well as in various industrial, consumer, and commercial uses as shown in Table 3. Non-TSCA uses, including those excluded under TSCA section 3(2), are beyond the scope of this assessment (See Table A.3).

Under the conditions of use identified in Table 3, EPA assessed the potential exposure to the following categories: the environment, the general population, and potentially exposed or susceptible subpopulations including workers and consumers.

7.1 Production Volume Information

Production volume information for 1-docosanol is based on an analysis of CDR data reported from 1986 to 2015.[52] The CDR database indicates that for reporting year 2015, six companies manufactured or imported 1-docosanol at six sites. From 1986 to 1998 reporting years, aggregate production volume for 1-docosanol was between 1,000,000 and 10,000,000 lbs., and in 2002 aggregate production volume was less at 10,000 to 500,000 lbs. From 2011 to 2015 reporting years, aggregate production volume for 1-docosanol then increased to 1,000,000 to 10,000,000 lbs. In general, since 1986, production volume has remained relatively stable, aside from a decrease in the 2002 reporting year.

7.2 Exposures to the Environment

EPA expects most exposures to the environment to occur during the manufacture, import, processing, and industrial, commercial and consumer uses of 1-docosanol. Exposure is also possible from other uses, distribution and disposal. These activities could result in releases of 1-docosanol to media including surface water, landfills, and air.

EPA expects high levels of removal of 1-docosanol during wastewater treatment (either directly from the facility or indirectly via discharge to a municipal treatment facility or Publicly Owned Treatment Works (POTW), see Table 2). Further, 1-docosanol is expected to have low persistence (aerobic and

[52] The CDR requires manufacturers (including importers) to report information on the chemicals they produce domestically or import into the U.S above 25,000 lb. per site per year.

anaerobic biodegradation are discussed in Section 6.3.1) and has the potential to break down in the environment into carbon dioxide and water. Therefore, any release of the chemical to surface water is expected to be limited by its water solubility and break down, reducing exposure to aquatic organisms in the water column, benthic organisms, and groundwater sources of drinking water, including well water.

If disposed of in a landfill, this chemical is expected to degrade under aerobic and anaerobic conditions (aerobic and anaerobic biodegradation are discussed in Section 6.3.1).

If incineration releases during manufacturing and processing occur, EPA expects significant degradation of 1-docosanol to the point that it will not be present in air.

7.3 Exposures to the General Population

EPA expects the general population is unlikely to be exposed to 1-docosanol from the environmental releases described above. The general population is unlikely to be exposed to 1-docosanol via inhalation of ambient air because 1-docosanol is a solid, has a low vapor pressure, and will break down if incinerated. 1-Docosanol is also unlikely to be present in surface water because of low water solubility and its ability to degrade (aerobic and anaerobic biodegradation are discussed in Section 6.3.1), reducing the potential for the general population to be exposed by oral ingestion or dermal exposure. Given the low bioconcentration and bioaccumulation potential of 1-docosanol, oral exposure to 1-docosanol via fish ingestion is unlikely.

7.4 Exposures to Potentially Exposed or Susceptible Subpopulations

EPA identified workers as potentially exposed or susceptible subpopulations based on greater exposure to 1-docosanol than the general population during manufacturing, processing, distribution, use and disposal. EPA also identified consumers as a population that may experience greater exposure to 1-docosanol than the general population through use of paper products, paints and coatings, and laundry and dishwashing products, for example. EPA did not identify populations with greater susceptibility to 1-docosanol.

7.4.1 Exposures to Workers

Based on its reported physical form and measured melting point (Table 2), 1-docosanol is a solid under ambient conditions. Based on 1-docosanol's conditions of use (Table 3), workers may be exposed to solids through direct dermal contact with the substance and inhalation of dust if it is generated. 1-Docosanol is not expected to be a volatile substance, meaning workers are unlikely to be exposed through inhalation of vapors. Workers may be exposed to 1-docosanol in manufacturing, processing, distribution, use, and disposal.

7.4.2 Exposures to Consumers

Consumers could be exposed to 1-docosanol through the use of paper products, paints and coatings, laundry and dishwashing products, or others as specified in Table 3. For all these uses, if dermal contact does occur, 1-docosanol is expected to be minimally absorbed through the skin. If the chemical is in an aerosol product and inhalation exposure occurs, 1-docosanol's absorption from the lungs is unlikely. Consumer exposure through inhalation or incidental ingestion of dust if using

consumer products in a powdered form, such as powdered laundry and dishwashing products, is expected to be limited by minimal absorption. EPA does not include intentional misuse, such as people drinking products containing this chemical, as part of the known, intended, or reasonably foreseen conditions of use that could lead to an exposure (82 FR 33726). Thus, oral exposures will be incidental (meaning inadvertent and low in volume). 1-Docosanol is expected to be metabolized and excreted, further reducing the duration of exposure.

8. Summary of Findings

EPA has used reasonably available information on the following statutory and regulatory criteria and considerations to screen 1-docosanol against each of the priority designation considerations in 40 CFR 702.9(a), and discussed individually in this section, under its conditions of use:

- the hazard and exposure potential of the chemical substance (See Sections 6 and 7);
- persistence and bioaccumulation (See Section 6.3);
- potentially exposed or susceptible subpopulations (See Section 7.4);
- storage near significant sources of drinking water (See Section 8.4);
- conditions of use or significant changes in the conditions of use of the chemical substance (See Section 5);
- the chemical substance's production volume or significant changes in production volume (See Section 7.1); and
- other risk-based criteria that EPA determines to be relevant to the designation of the chemical substance's priority.

EPA conducted a risk-based, screening-level review based on the criteria and other considerations above and other relevant information described in 40 CFR 702.9(c) to inform the determination of whether the substance meets the standard of a high-priority substance. High-priority substance means a chemical substance that EPA determines, without consideration of costs or other non-risk factors, may present an unreasonable risk of injury to health or the environment because of a potential hazard and a potential route of exposure under the conditions of use, including an unreasonable risk to potentially exposed or susceptible subpopulations identified as relevant by EPA (40 CFR 702.3). Designation of a low-priority substance is not a finding that the chemical substance does not present an unreasonable risk, but rather that the chemical does not meet the statutory criteria for a high-priority substance and that a risk evaluation is not warranted at the time. This section explains the basis for the final designation and how EPA applied statutory and regulatory requirements, addressed rationales, and reached conclusions.

8.1 Hazard and Exposure Potential of the Chemical Substance

Approach: EPA evaluated the hazard and exposure potential of 1-docosanol. EPA used this information to inform its determination of whether 1-docosanol meets the statutory criteria and considerations for final designation as a low-priority substance.

- **Hazard potential:**

For 1-docosanol's hazard potential, EPA gathered information for a broad set of human health and environmental endpoints described in detail in Section 6 of this document. EPA screened this information against low-concern benchmarks. EPA found that 1-docosanol is of low concern for human health and environmental hazard across the range of endpoints in these low-concern criteria.

- **Exposure potential:**

To understand exposure potential, EPA gathered information on physical-chemical properties, production volumes, and the types of exposures likely to be faced by workers, the general population,

children, and consumers (discussed in Sections 3 and 7). EPA also gathered information on environmental releases. EPA identified workers, the general population, consumers, and the environment as most likely to experience exposures. EPA determined that while the general population, consumers, and workers may be exposed to 1-docosanol, exposure by dermal, ingestion and inhalation pathways is limited by 1-docosanol's physical-chemical properties. If 1-docosanol is released into the environment, its exposure potential will be minimal because of low water solubility, and further reduced through biodegradation under aerobic and anaerobic conditions.

Rationale: Although 1-docosanol may have potential to cause moderate eye irritation, the effects are reversible, thereby reducing concern for longer-term effects. TSCA conditions of use would be unlikely to result in frequent eye exposure because the use patterns do not involve intentional eye exposure. Workers could be exposed during processing, manufacturing, distribution, use, and disposal, through splashing of solutions or hand-to-face and eye contact. Other uses covered under TSCA, especially consumer uses in laundry and dishwashing products would be unlikely to result in more than incidental eye exposure. Eye irritation resulting from exposure in an occupational and consumer setting is mitigated primarily by the reversible nature of the effect and furthermore by the strong likelihood that any exposures would be self-limiting, especially by those who experience eye irritation from eye exposure.

Conclusion: Based on an initial analysis of reasonably available hazard and exposure information, EPA concludes that the risk-based, screening-level review under 40 CFR 702.9(a)(1) does not support a finding that 1-docosanol meets the standard for a high-priority substance. The reasonably available hazard and exposure information described above provides sufficient information to support this finding. EPA does not find that unlikely, infrequent, and temporary occurrence of potential moderate eye irritation meets the standard for a high-priority substance (i.e., that the substance "may present an unreasonable risk of injury to health").

8.2 Persistence and Bioaccumulation

Approach: EPA has evaluated both the persistence and bioaccumulation potential of 1-docosanol based on a set of EPA and internationally accepted measurement tools and benchmarks that are sound indicators of persistence and bioaccumulation potential (described in Section 6). These endpoints are key components in evaluating a chemical's persistence and bioaccumulation potential.

Rationale: EPA review of experimental data indicates 1-docosanol is inherently biodegradable under aerobic conditions and expected to degrade under anaerobic conditions (Section 6.3.1). Read-across from a closely-related analog indicates low potential for bioaccumulation (Section 6.3.2).

Conclusion: Based on an initial screen of reasonably available information on persistence and bioaccumulation, EPA concludes that the screening-level review under 40 CFR 702.9(a)(2) does not support a finding that 1-docosanol meets the standard for a high-priority substance. The reasonably available persistence and bioaccumulation information described above provides sufficient information to support this finding.

8.3 Potentially Exposed or Susceptible Subpopulations

Approach: TSCA Section 3(12) states that the "term 'potentially exposed or susceptible subpopulation' means a group of individuals within the general population identified by the Administrator who, due to either greater susceptibility or greater exposure, may be at greater risk than the general population of adverse health effects from exposure to a chemical substance or mixture, such as infants, children, pregnant women, workers, or the elderly." EPA considered potentially exposed or susceptible subpopulations, such as infants, children, pregnant women, workers and the elderly. EPA identified workers engaged in the manufacturing, processing, distribution, use and disposal of 1-docosanol as a potentially exposed or susceptible subpopulation (described in more detail in Section 7). Consumers are also a potentially exposed subpopulation because of their use of paper products, paints and coatings, laundry and dishwashing products, and other products, as shown in Table 3.

Rationale: EPA did not identify hazard effects for this chemical that would make any population susceptible. EPA expects workers and consumers to have a higher exposure to 1-docosanol than the general population. Because of the chemical's low-concern hazard properties and reversibility of the effects, this exposure does not expose a significant increase in risk for consumers or workers.

Conclusion: Based on the Agency's understanding of the conditions of use and expected users such as potentially exposed or susceptible subpopulations, EPA concludes that the screening-level review under 40 CFR 702.9(a)(3) does not support a finding that 1-docosanol meets the standard for a high-priority substance. The conditions of use could result in increased exposures to certain populations. Even in light of this finding, the consistently low-concern hazard profile and reversible effects of 1-docosanol provides sufficient evidence to support a finding of low concern. The reasonably available information on conditions of use, hazard, and exposure described above provides sufficient information to support this finding.

8.4 Storage near Significant Sources of Drinking Water

Approach: In sections 6 and 7, EPA explains its evaluation of the elements of risk relevant to the storage of 1-docosanol near significant sources of drinking water. For this criterion, EPA focused primarily on the chemical substance's potential human health hazards, including to potentially exposed or susceptible subpopulations, and environmental fate properties, and explored a scenario of a release to a drinking water source. EPA also investigated whether the chemical was monitored for and detected in a range of environmental media. The requirement to consider storage near significant sources of drinking water is unique to prioritization under TSCA Section 6(b)(1)(A).

Rationale: In terms of health hazards, 1-docosanol is expected to present low concern to the general population, including potentially exposed or susceptible subpopulations, across a spectrum of endpoints.

In the event of an accidental release into a surface drinking water source, 1-docosanol is not water soluble (see Section 3) and it is not expected to persist (see Section 6.3.1) in the drinking water supply. In the event of an accidental release to land, its low water solubility and biodegradability (aerobic and anaerobic biodegradation are discussed in Section 6.3.1) reduces its potential for transport to surface drinking water sources and leaching into groundwater, including well water. Fate and transport evaluations indicate 1-docosanol is likely to partition into sediment (see Section 3),

predicted to biodegrade under aerobic and anaerobic conditions (see Section 6.3), and unlikely to bioaccumulate (see Section 6.3.2), minimizing the likelihood that the chemical would be present in sediment or groundwater to pose a longer-term drinking water contamination threat.

A sudden release of large quantities of the chemical near a drinking water source could have immediate effects on the usability of a surface drinking water source. If such a release were to occur, two primary factors would operate together to reduce concern. First, the chemical would be expected to present low concern to the general population, including susceptible subpopulations, across a spectrum of health endpoints (see Section 6). Second, 1-docosanol would degrade in aerobic and anaerobic environments (see Section 6.3). Together, these factors mean that any exposures to this chemical through drinking water sources would be short-lived, and that if ingestion were to take place, concern for adverse health effects would be low.

EPA also explored whether the chemical had been identified as a concern under U.S. environmental statutes in the past. EPA searched lists of chemicals and confirmed that 1-docosanol does not appear on these lists. The lists reviewed include EPA's List of Lists (https://www.epa.gov/sites/production/files/2015-03/documents/list_of_lists.pdf). EPA also searched the lists of chemicals included in the National Primary Drinking Water Regulations and the Unregulated Contaminant Monitoring Rule (UCMR) under the Safe Drinking Water Act (SDWA).

Conclusion: Based on a qualitative review of a potential release near a significant source of drinking water, EPA concludes that the screening-level review of 1-docosanol under 40 CFR 702.9(a)(4) does not support a finding that 1-docosanol meets the standard for a high-priority substance. The reasonably available information on storage near significant sources of drinking water described above provides sufficient information to support these findings.

8.5 Conditions of Use or Changes in Conditions of Use of the Chemical Substance

Approach: EPA evaluated the conditions of use for 1-docosanol and related potential exposures and hazards.

Rationale: EPA assessed the conditions of use of 1-docosanol (see Section 5 and Appendix A) and found it to have a broad range of conditions of use. EPA expects that even if the conditions of use were to expand beyond activities that are known, intended, or reasonably foreseen, the outcome of the screening review would likely not change and would not alter the Agency's conclusion of low concern. EPA bases this expectation on 1-docosanol's consistently low-concern hazard characteristics across the spectrum of hazard endpoints and regardless of a change in the nature or extent of its use and resultant increased exposures.

Conclusion: EPA's qualitative evaluation of potential risk does not support a finding that 1-docosanol meets the standard for a high-priority substance, based on its low-hazard profile under the current conditions of use. EPA concludes that even if conditions of use broaden, resulting in an increase in the frequency or amount of exposures, the analysis conducted to support the screening-level review under 40 CFR 702.9(a)(5) would not change significantly. In particular, the analysis of concern for hazard, which forms an important basis for EPA's findings, would not be impacted by a

change in conditions of use. Therefore, such changes would not support a finding that 1-docosanol meets the standard for a high-priority substance. The reasonably available information on conditions of use, or significant changes in conditions of use, described above provides sufficient information to support this finding.

8.6 The Volume or Significant Changes in Volume of the Chemical Substance Manufactured or Processed

Approach: EPA evaluated the current production volumes of 1-docosanol (Section 7.1) and related potential exposures (Section 7.2 through 7.4).

Rationale: EPA used reasonably available information on production volume (see Appendix A) in considering potential risk. It is possible that designation of 1-docosanol as a low priority substance could result in increased use and higher production volumes. EPA expects, however, that any changes in 1-docosanol's production volume would not alter the Agency's assessment of low concern given the chemical's low-concern hazard profile. EPA bases this expectation on 1-docosanol's consistently low-concern hazard characteristics across the spectrum of hazard endpoints. This expectation would apply, even with a significant change in the volume of the chemical manufactured or processed and resultant increased exposures.

Conclusion: Based on this screening criteria under 40 CFR 702.9(a)(6), EPA concludes that even if production volumes increase, resulting in an increase in the frequency or level of exposure, 1-docosanol does not meet the standard for a high-priority substance. The reasonably available information on production volume, or significant changes in production volume described above provides sufficient information to support this finding.

8.7 Other Considerations

EPA did not identify other considerations for the screening review to support the final designation of 1-docosanol as a low priority substance.

9. Final Designation

Based on a risk-based screening-level review of the chemical substance and relevant information received from the public and other information as appropriate and consistent with TSCA section 26(h), (i) and (j), EPA concludes that 1-docosanol does not meet the standard for a high-priority substance. The reasonably available information described above provides sufficient information to support this finding. Accordingly, EPA is designating 1-docosanol as a low-priority substance.

Appendix A: Conditions of Use Characterization

EPA gathered information on and related to conditions of use including uses of the chemical, products in which the chemical is used, types of users, and status (e.g., known, regulated).

A.1. CDR Manufacturers and Production Volume

The Chemical Data Reporting (CDR) rule (previously known as the Inventory Update Rule, or IUR), under TSCA section 8, requires manufacturers (including importers) to report information on the chemical substances they produce domestically or import into the U.S., generally above a reporting threshold of 25,000 lb. per site per year. According to the 2016 CDR database, 6 companies manufactured or imported 1-docosanol at 6 sites for reporting year 2015. Individual production volumes were withheld, but may be available in later releases of the 2016 CDR.

Table presents the historic production volume of 1-docosanol from the CDR (previously known as the Inventory Update Rule, or IUR) from 1986-2015. From 1986 to 1998 reporting years, aggregate production volume for 1-docosanol was between 1,000,000 and 10,000,000 lbs., and in 2002 aggregate production volume was less at 10,000 to 500,000 lbs. From 2011 to 2015 reporting years, aggregate production volume for 1-docosanol then increased to 1,000,000 to 10,000,000 lbs. In general, since 1986, production volume has remained relatively stable without significant increases or decreases, aside from a decrease in the 2002 reporting year.

Table A.1: 1986-2015 National Production Volume Data for 1-Docosanol (Non-Confidential Production Volume in Pounds)

1986	1990	1994	1998	2002	2006	2011	2012	2013	2014	2015
>1 M – 10M	>1 M – 10M	>1 M – 10M	>1 M – 10M	10 K – 500 K	1 M < 10 M	1 M – 10 M	1 M – 10 M	1 M – 10 M	1 M – 10 M	1 M – 10 M

Source(s):
EPA (2018a; 2017b; 2006; 2002)

Note(s):
K = Thousand; M = Million; NDR = No data reported

A.2. Uses

A.2.1 Methods for Uses

Section A.2 provides a list of known uses of 1-docosanol, organized by category of use. To compile the uses, EPA searched publicly available databases listed in Table A.2 and conducted additional internet searches to clarify uses. Search terms differed among databases because of different search term requirements for each database (i.e., some databases search by CASRN while others search by chemical name).

Table A.2: Sources Searched for Uses of 1-Docosanol

Title	Author and Year	Search Term(s)	Found Use Information? [1]
Sources searched for all use reports			
California Links to Pesticides Data	California Dept of Pesticide Regulation (2013)	629-96-9	No
Canada Chemicals Management Plan information sheets	Government of Canada (2018)	629-96-9; 1-docosanol	No
Chemical and Product Categories (CPCat)	CPCat (2019)	629-96-9	Yes
ChemView [2]	EPA (2018a)	629-96-9	Yes
Children's Safe Product Act Reported Data	Washington State Dept. of Ecology (2018)	629-96-9	No
Consumer Product Information Database (CPID)	DeLima Associates (2018a)	661-19-8	Yes
Danish surveys on chemicals in consumer products	Danish EPA (2018)	1-docosanol; Behenyl alcohol	No
Datamyne	Descartes Datamyne (2018)	1-docosanol	Yes
DrugBank	DrugBank (2018b)	661-19-8	Yes
European Chemicals Agency (ECHA) Registration Dossier	ECHA (2018)	661-19-8	Yes
eChemPortal [2]	OECD (2018)	661-19-8	No
Envirofacts [2]	EPA (2018b)	661-19-8	No
Functional Use Database (FUse)	EPA (2017a)	661-19-8	Yes
Kirk-Othmer Encyclopedia of Chemical Technology	Kirk-Othmer (2006)	1-docosanol; Behenyl alcohol	No
Non-Confidential 2016 Chemical Data Reporting (CDR)	EPA (2017b)	661-19-8	Yes
PubChem Compound	Kim et al. (2016)	661-19-8	Yes
Safer Chemical Ingredients List (SCIL)	EPA (2018d)	661-19-8	Yes

Table A.2: Sources Searched for Uses of 1-Docosanol			
Title	**Author and Year**	**Search Term(s)**	**Found Use Information?** [1]
Synapse Information Resources [2]	Synapse Information Resources (2009)	661-19-8	Yes
Resource Conservation and Recovery Act (RCRA)	EPA (2018c)	661-19-8; 1-docosanol	No
Scorecard: The Pollution Information Site	GoodGuide (2011)	661-19-8	No
Skin Deep Cosmetics Database	EWG (2018)	661-19-8	Yes
Toxics Release Inventory (TRI)	EPA (2018e)	661-19-8	No
TOXNET [2]	NLM (2018)	661-19-8	Yes
Ullmann's Encyclopedia of Industrial Chemistry	Ullmann's (2000)	1-docosanol; Behenyl alcohol	No
Additional sources identified from reasonably available information			
Manufacturer SDS	GlaxoSmithKline (2014)	Incidentally identified while researching into details of this chemical's uses and products.	Yes
Purdue University	Purdue University (2018)		
Note(s): 1. If use information was found in the resource, it will appear in Table unless otherwise noted. 2. This source is a group of databases; thus the exact resource(s) it led to will be cited instead of the database as whole.			

The U.S. Patent and Trademark Office has an online database that shows 384 patents referencing "1-docosanol" (USPTO 2018). Although patents could be useful in determining reasonably foreseen uses, it is difficult to confirm whether any of the patented technologies are currently in use. Uses inferred from patents containing 1-docosanol were not included in Table A.3. Note that the uses in Table A.3 that are covered under TSCA are included in Section 5, Table 3 of this document.

A.2.2 Uses of 1-Docosanol

Table A.3: Uses of 1-Docosanol		
Use	**Expected Users**	**Description of Use and References**
TSCA Conditions of Use: Manufacturing		
Agricultural additive manufacturing[1]	Industrial	Synapse Information Resources (2009) Synapse Information Resources lists use of 1-docosanol in manufacturing of agricultural additives. No further information on 1-docosanol use in this manufacturing process could be found. Expected user is not stated, but it is most likely industrial for agricultural additive manufacturing,
Basic organic chemical manufacturing	Industrial	EPA (2017b); CPCat (2019) CDR reported use of 1-docosanol as an intermediate in processing as a reactant in "all other basic organic chemical manufacturing." CPCat list the use of 1-docosanol in "all other chemical product and preparation manufacturing." No further information on 1-docosanol use in this manufacturing process could be found. Expected users are industrial based on identification in CDR's industrial processing and use report.
Food-contact metallic manufacturing[2]	Industrial	Synapse Information Resources (2009) Synapse Information Resources lists use of 1-docosanol as a surface lubricant in manufacturing of food-contact metallic articles. No further information on 1-docosanol use in this manufacturing process could be found. Expected user is not stated, but it is most likely industrial for food-contact metallic manufacturing.
Paint and coating manufacturing	Industrial	EPA (2017b) CDR reported use of 1-docosanol in processing – incorporation into formulation, mixture, or reaction product, in paint and coating manufacturing. No further information on 1-docosanol use in this manufacturing process could be found. Expected users are industrial based on identification in CDR's industrial processing and use report.

Table A.3: Uses of 1-Docosanol		
Use	**Expected Users**	**Description of Use and References**
Paper manufacturing	Industrial	EPA (2017b) CDR reported use of 1-docosanol in processing – incorporation into formulation, mixture, or reaction product, or surface active agent in paper manufacturing. No further information on 1-docosanol use in this manufacturing process could be found. Expected users are industrial based on identification in CDR's industrial processing and use report.
Petroleum lubricating oil and grease manufacturing	Industrial	EPA (2017b) CDR reported use of 1-docosanol in processing – incorporation into formulation, mixture, or reaction product, or additive, in petroleum lubricating oil and grease manufacturing. No further information on 1-docosanol use in this manufacturing process could be found. Expected users are industrial based on identification in CDR's industrial processing and use report.
Plastic material and resin manufacturing	Industrial	EPA (2017b) CDR reported use of 1-docosanol in processing – incorporation into formulation, mixture, or reaction product in plastic material and resin manufacturing. No further information on 1-docosanol use in this manufacturing process could be found. Expected users are industrial based on identification in CDR's industrial processing and use report.
Soap, cleaning compound, and toilet preparation manufacturing	Industrial	EPA (2017b) CDR reported use of 1-docosanol in processing – incorporation into formulation, mixture, or reaction product, or surface active agent in soap, cleaning compound, and toilet preparation manufacturing. No further information on 1-docosanol use in this manufacturing process could be found. Expected users are industrial based on identification in CDR's industrial processing and use report.

Table A.3: Uses of 1-Docosanol		
Use	**Expected Users**	**Description of Use and References**
Textiles, apparel, and leather manufacturing	Industrial	CPCat (2019); Synapse Information Resources (2009) CPCat list the use of 1-docosanol in textiles, apparel and leather manufacturing. Synapse Information Resources also list 1-docosanol use in manufacturing of textile and its use in synthetic fibers. No further information on 1-docosanol use in this manufacturing process could be found. Expected users are industrial based on CPCat's user classification.
TSCA Conditions of Use: Other Industrial Uses		
Anti-foaming agent	Industrial	CPCat (2019) CPCat lists the use of 1-docosanol as an anti-foaming agent. Expected users are industrial based on CPCat's user classification.
Lubricants, lubricant additive	Industrial	CPCat (2019) CPCat lists the use of 1-docosanol as a lubricant, or lubricant additive. Expected users are industrial based on CPCat's user classification.
Oil, resource extraction	Industrial	CPCat (2019); Synapse Information Resources (2009) Synapse Information Resources lists 1-docosanol use in oil well drilling. CPCat also lists the use of 1-docosanol in "oil and gas drilling, extraction, and support activities." Expected users are industrial based on CPCat's user classification.
Surfactant	Industrial	CPCat (2019) CPCat lists the use of 1-docosanol as a surfactant in fluid property modulation. Expected users are industrial based on CPCat's user classification.

Table A.3: Uses of 1-Docosanol		
Use	**Expected Users**	**Description of Use and References**
TSCA Conditions of Use: Home Care Products		
Laundry and dishwashing products	Consumer	EPA (2017b) CDR identified the use of 1-docosanol in laundry and dishwashing products. No information of its use in specific products could be found. Expected users are based on CDR's consumer/commercial classification.
Paints and coating	Consumer, commercial	EPA (2017b) CDR identified the use of 1-docosanol in paints and coatings. No information of its use in specific products could be found. The expected users are assumed to be consumer and commercial.
Window and door sealant	Consumer	DeLima Associates (2016a) CPID generally includes products for consumer use; therefore the expected user is a consumer.
TSCA Conditions of Use: Pesticides		
Pesticide ingredient[3]	Unknown	CPCat (2019); Purdue University (2018) CPCat lists the use of 1-docosanol as an "inert pesticide ingredient." Further information on the use of 1-docosanol in pesticides could not be found. The expected users are unknown, due to the limited availability of information.
TSCA Conditions of Use: Miscellaneous		
Paper products	Consumer, commercial	EPA (2017b) CDR identified the use of 1-docosanol in consumer and commercial paper products. No further information could be found on paper products containing 1-docosanol. Expected users are consumer and commercial based on inclusion in CDR's consumer and commercial use report.

Table A.3: Uses of 1-Docosanol		
Use	**Expected Users**	**Description of Use and References**
Plastics and rubber products	Consumer	EPA (2017b) CDR identified the use of 1-docosanol in commercial "plastic and rubber products not covered elsewhere." No further information could be found on plastic and rubber products containing 1-docosanol. Expected users are based on CDR's consumer/commercial classification.
Non-TSCA Uses		
Acne spot treatment	Consumer	DeLima Associates (2016d) CPID generally includes products for consumer use; therefore the expected user is a consumer.
After-shave	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Anti-aging cream	Consumer	DeLima Associates (2016f) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Anti-aging eye cream	Consumer	DeLima Associates (2016e) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Baby body lotion	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Baby body wash	Consumer	DeLima Associates (2018b) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Baby sunscreen	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Beauty or blemish (BB) cream	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.

Table A.3: Uses of 1-Docosanol		
Use	**Expected Users**	**Description of Use and References**
Body lotion	Consumer	DeLima Associates (2016g) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Body wash	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Color correcting (CC) cream	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Concealer	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Cuticle treatment	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Deodorant/ antiperspirant	Consumer	DeLima Associates (2017) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Eye liner	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Face wash/ scrub	Consumer	DeLima Associates (2015) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Facial cleanser	Consumer	DeLima Associates (2016b) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Facial moisturizer	Consumer	DeLima Associates (2016e) CPID generally includes products for consumer use; therefore the expected user is a consumer.

Table A.3: Uses of 1-Docosanol		
Use	**Expected Users**	**Description of Use and References**
Facial night cream	Consumer	DeLima Associates (2016c) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Hair conditioner	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Hair gel	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Hair relaxer	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Hair shampoo	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Hair spray	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Hair styling cream/ wax	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Hand cream/lotion	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Lip balm	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Lipstick	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.

Table A.3: Uses of 1-Docosanol		
Use	**Expected Users**	**Description of Use and References**
Makeup primer	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Mascara	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Pharmaceuticals	Unknown	Synapse Information Resources (2009) Synapse Information Resources lists 1-docosanol as a "raw material, consistency agent, emollient for pharmaceuticals" and its use in antihistamines. The expected users are unknown, due to the limited availability of information.
Skin facial mask	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Skin firming treatment	Consumer	DeLima Associates (2016d) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Skin foundation	Consumer	CPCat (2019) CPCat listed the use of 1-docosanol in two consumer available skin foundation products. Therefore the expected users is consumer.
Skin lightener	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Skin moisturizer	Consumer	DeLima Associates (2008) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Skin redness and pore reducer	Consumer	DeLima Associates (2016c) CPID generally includes products for consumer use; therefore the expected user is a consumer.

Table A.3: Uses of 1-Docosanol		
Use	**Expected Users**	**Description of Use and References**
Skin toner	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Sun-less tanner	Consumer	DeLima Associates (2016h) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Sunscreen	Consumer	DeLima Associates (2013) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Topical medications	Consumer	Drugbank (2018a); GlaxoSmithKline (2014) Drug Bank reports the use of 1-docosanol as a topical drug treatment for recurring herpes episodes of cold sores and fever blisters. It is currently available for purchase in the United States in two over-the-counter cream medications. Expected users are consumer, as the over-the-counter medications are currently available for consumer purchase.
Vapor rub	Consumer	EWG (2018) Skin Deep generally includes products for consumer use; therefore the expected user is a consumer.
Wrinkle treatment	Consumer	DeLima Associates (2016h) CPID generally includes products for consumer use; therefore the expected user is a consumer.
Children's Products CDR reports did not include any uses in children's products; however, uses in baby lotion, baby wipes, wash and sunscreen product intended for babies are found in this table.		
Recycling and Disposal In the 2016 CDR, five facilities reported that 1-docosanol was not recycled (e.g., not recycled, remanufactured, reprocessed, or reused), and one facility reported recycling information as CBI (EPA 2017b).		
Note(s): 1. Potentially a non-TSCA use, however, because information is insufficient to determine, it is assumed to be covered by TSCA. 2. TSCA product based on the assumption that the chemical is used in the manufacturing of products and not intended to be a component of food. 3. TSCA product based on assumption that it is a pesticide inert.		

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Appendix B: Hazard Characterization

Table B.1: Human Health Hazard

ADME

Source	Exposure Route	Species & Strain (if available)	Duration	Doses and Replicate Number	Effect	Study Details
4949228	Oral (gavage)	Chinchilla rabbits	24 hours	**Dose:** 25 mmol **Replicates:** 3	7.6% of the administered dose was excreted by glucuronide	**Methods:** • Test substance reported as CASRN 112-92-5 • Purity not reported • GLP compliance data not reported

Acute Mammalian Toxicity

Source	Exposure Route	Species & Strain (if available)	Duration	Doses and Replicate Number	Effect	Study Details
4949228, 4963011	Oral (gavage)	Sprague-Dawley rats	Single dose, observed for 14 days	**Dose:** 2000 mg/kg **Replicates:** 3 per sex	**LD_{50}** > 2000 mg/kg	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity not reported • OECD Guideline 423 • GLP compliant
4949228	Oral (gavage)	Sprague-Dawley rats	Single dose, observed for 14 days	**Doses**: 8250 and 10000 mg/kg **Replicates:** 5 per sex per dose	**LD_{50}** > 10000 mg/kg	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity not reported • OECD Guideline 423 • GLP compliant
4934050	Oral (gavage)	CF1 mice	Single dose, observed for 8 days	**Dose:** 1000 mg/kg **Replicate**: 10 mice	**LD_{50}** > 1000 mg/kg	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity not reported • GLP compliance data not reported
4949228	Dermal	New Zealand white rabbits	24 hour exposure, observed for 14 days	**Dose:** 8000 mg/kg **Replicates:** 4 animals	**LD_{50}** > 8000 mg/kg	**Methods:** • Test substance reported as CASRN 67762-27-0 • Purity not reported • Not GLP compliant

Table B.1: Human Health Hazard						
5094502	Inhalation	Sprague-Dawley rats	6 hour exposure, observed for 14 days	**Dose:** 0.00014 mg/L **Replicates:** 6 animals	**LC_{50} >** 0.00014 mg/L	**Methods:** • Test substance reported as CASRN 67762-27-0 • Purity not reported • Not GLP compliant
Repeated Dose Toxicity						
Source	**Exposure Route**	**Species & Strain (if available)**	**Duration**	**Doses and Replicate Number**	**Effect**	**Study Details**
4949228, 34905	Oral (gavage)	CD rats	26 weeks	**Doses:** 0, 10, 100, and 1000 mg/kg-day **Replicates:** 20 per sex per dose	**NOAEL:** 1000 mg/kg-day	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity: 98% • GLP compliant **Mortality Results:** • 1 male rat in 100 mg/kg group died from aspiration
34905	Oral (gavage)	Beagle dogs	26 weeks	**Doses**: 0, 20, 200, and 2000 mg/kg-day **Replicates:** 4 per sex per group	**NOAEL:** 2000 mg/kg-day	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity: 98% • GLP compliant
4949228	Oral	Wistar rats	45 days (males), 54 days (females)	**Doses:** 0, 100, 500, and 2000 mg/kg-day **Replicates:** 12 per sex per group	**NOAEL:** 2000 mg/kg-day	**Methods:** • Test substance reported as CASRN 112-92-5 • Purity: 99% • OECD Guideline 422 • GLP compliant
4949228, 4934169	Oral (gavage)	Sprague-Dawley rats	28 days	**Doses:** 0, 100, 500, and 1000 mg/kg-day **Replicates:** 10 per sex per group	**NOAEL:** 1000 mg/kg-day	**Methods:** • Test substance reported as CASRN 112-92-5 • Purity not reported • OECD Guideline 407 • GLP compliant

Table B.1: Human Health Hazard						
820061	Oral	Male Wistar rats	1 week- 3 months	**Doses:** 9400 – 28000 mg/kg-day **Replicates:** 15 total, 3-4 per timepoint	**LOAEL:** 28000 mg/kg-day based on hepatic structural changes in mitochondria	**Methods:** • Test substance reported as CASRN 112-92-5 • Purity not reported • GLP compliance not reported
Reproductive Toxicity						
Source	**Exposure Route**	**Species & Strain (if available)**	**Duration**	**Doses and Replicate Number**	**Effect**	**Study Details**
4949228, 4941207, 34906	Oral (gavage)	Sprague-Dawley rats	Males: 71 days premating, through mating Females: 15 days premating through GD17-20	**Doses:** 0, 10, 100, and 1000 mg/kg-day **Replicates:** 22 per sex per group	**NOAEL:** 1000 mg/kg-day	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity: 98% • ICH Harmonised Tripartite Guidelines for Detection of Toxicity to Reproduction for Medicinal Products • GLP compliant
Developmental Toxicity						
Source	**Exposure Route**	**Species & Strain (if available)**	**Duration**	**Doses and Replicate Number**	**Effect**	**Study Details**
4949228, 34906	Oral (gavage)	New Zealand white rabbits	GD 6-19	**Doses:** 0, 125, 500, and 2000 mg/kg-day **Replicates**: 19-20 pregnant rabbits per group	**NOAEL**: 2000 mg/kg-day	**Methods** • Test substance reported as CASRN 661-19-8 • Purity not reported • ICH Harmonised Tripartite Guidelines for Detection of Toxicity to Reproduction for Medicinal Products • GLP compliant

Table B.1: Human Health Hazard						
4949228, 34906	Oral (gavage)	Sprague-Dawley rats	Males: 71 days premating, through mating Females: 15 days premating through GD17-20	**Doses**: 0, 10, 100, and 1000 mg/kg-day **Replicates**: 22 per sex per group	**NOAEL:** 1000 mg/kg-day	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity: 98% • ICH Harmonised Tripartite Guidelines for Detection of Toxicity to Reproduction for Medicinal Products • GLP compliant
Cancer						
Source	**Effect**					**Study Details**
OncoLogic v8.0	High molecular weight aliphatic alcohols (C>20) are expected to be of low concern					**Methods:** The concern level is based on structure-activity relationships (SAR) analysis.
ISS v2.4[53]	Negative (Estimated) 1-Docosanol does not contain any structural features indicative of electrophilic potential.					**Methods:** Carcinogenicity alerts (genotoxic and non-genotoxic) by ISS profiler as available within the OECD Toolbox v4.3. **Results:** No alerts were identified for 1-docosanol

[53] Carcinogenicity alerts by ISS profiler comprises 55 structural alerts for genotoxic and non-genotoxic carcinogenicity. The alerts have been compiled upon existing knowledge of the mechanism of action of carcinogenic chemicals that have been published elsewhere (Benigni and Bossa (2011) *Chem Rev* 111: 2507-2536 and Benigni R et al. (2013) *Chem Rev.* 113: 2940-2957).

Table B.1: Human Health Hazard		
VEGA 1.1.4[54]	1-Docosanol was processed through all 4 models. ISS 1.0.2 and IRFMN/ISSCAN-GX 1.0.0 predicted the chemical to be non-carcinogenic with moderate reliability. IRFMN/Antares 1.0.0 predicted the chemical to be non-carcinogenic with good reliability.	**Methods:** VEGA 1.1.4 contains 4 models for carcinogenicity – CAESAR 2.1.9, ISS 1.0.2, IRFMN/Antares 1.0.0, IRFMN/ISSCAN-GX 1.0.0 **Results:** • CAESAR 2.1.9: Low reliability (1-Docosanol could be outside of the applicability domain (AD) of the model) • ISS 1.0.2: Moderate reliability • IRFMN/Antares 1.0.0: High reliability • IRFMN/ISSCAN-GX 1.0.0: Moderate reliability

[54] VEGA 1.1.4 contains 4 different models to facilitate an *in silico* assessment of carcinogenicity potential. The models are summarized in Golbamaki et al. (2016) J Environ Sci and Health Part C http://dx.doi.org/10.1080/10590501.2016.1166879 as well as in documentation that is downloadable from within the VEGA tool itself (https://www.vegahub.eu/).

- CAESAR 2.1.9 is a classification model for carcinogenicity based on a neural network.
- ISS 1.0.2 is a classification model based on the ISS ruleset (as described above for the OECD Toolbox).
- IRFMN/Antares 1.0.0 and IRFMN/ISSCAN-GX 1.0.0 are classification models based on a set of rules built with SARpy software (part of the same suite of VEGA tools https://www.vegahub.eu/) extracted from the Antares and ISSCAN-CGX datasets respectively.

Table B.1: Human Health Hazard						
Genotoxicity						
Source	**Test Type & Endpoint**	**Species & Strain (if available)**	**Metabolic Activation**	**Doses**	**Results**	**Study Details**
4941156, 34905, 4949228	Mammalian gene mutation assay (*in vitro*)	Chinese hamster lung fibroblast cells	With and without	**Doses**: 2, 7.5, 15, and 20 mg/mL	Negative	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity: 98% • GLP not reported
4941086, 34905	Mammalian chromosomal aberration assay (*in vitro*)	Chinese hamster lung fibroblast cells	With and without	**Doses:** Without metabolic activation 0, 0.6, 10, 20 µg/ml With metabolic activation: 0, 1.4, 10, 20 µg/ml	Negative	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity: 98% • GLP not reported
4941014, 34905	Gene mutation assay (*in vitro*)	Salmonella typhimurium strains TA 1535, TA 1538, TA 98, TA 100, TA 1537	With and without	**Doses:** 10, 100, 333.3, 666.6, and 1000 mg/plate	Negative	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity: 98% • GLP compliant
4949228	Gene mutation assay (*in vitro*)	Salmonella typhimurium strains TA98 and TA100	Yes	**Dose:** 0, 50, 150, 500, 1,000, 1,500 and 5,000 µg/plate	Negative	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity not reported • GLP compliant
4940922, 4949228, 34905	Mammalian gene mutation assay (*in vivo*)	NMRI Mice	NA	**Doses:** 0, 50, 150, and 500 mg/kg	Negative	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity: 98% • OECD Guideline 474 • GLP compliant

Table B.1: Human Health Hazard						
Neurotoxicity						
Source	**Exposure Route**	**Species & strain (if available)**	**Duration**	**Doses and replicate number**	**Effect**	**Study Details**
4949228, 34905	Oral (gavage)	CD rats	26 weeks	**Doses:** 0, 10, 100, and 1000 mg/kg-day **Replicates:** 20 per sex per dose	**NOAEL:** 1000 mg/kg-day	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity: 98% • GLP compliant **Results:** • No brain or spinal cord lesions observed
34905	Oral (gavage)	Beagle dogs	26 weeks	**Doses**: 0, 20, 200, and 2000 mg/kg-day **Replicates:** 4 per sex per group	**NOAEL:** 2000 mg/kg-day	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity: 98% • GLP compliant **Results:** • No histopathological lesions in the brain or spinal cord
Irritation						
Source	**Exposure Route**	**Species & Strain (if available)**	**Duration**	**Doses**	**Effect**	**Study Details**
4949228, 4963040	Dermal	New Zealand white rabbits	4 hours under semi-occlusive conditions	**Dose:** 0.5 g of undiluted test material **Replicates:** 3 Females	Negative	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity not reported • OECD Guideline 404 • GLP compliant

Table B.1: Human Health Hazard						
4949228, 4963041, 4963002	Ocular	New Zealand white rabbits	Single exposure, examined for 72 hours	**Dose:** 0.1 mL of undiluted test material **Replicates:** 1 Female, 2 Males	Moderate	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity not reported • OECD Guideline 405 • GLP compliant **Results:** • At 1 hour, all animals had slight conjunctival irritation • All effects were completely reversible by 72 hours
4949228, 4934050	Ocular	New Zealand white rabbits	Single exposure, examined for 48 hours	**Dose:** 50 µL of undiluted test material **Replicates:** 5 Rabbits	Low	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity not reported • GLP compliance not specified **Results:** • At 2 and 6 hours, there animals had conjunctival irritation • All effects were completely reversible by 24 hours

Table B.2: Environmental Hazard					
Aquatic Toxicity: Experimental					
Source	**Species & Strain (if available)**	**Duration**	**Doses and Replicate Number**	**Effect**	**Study Details**
49449228, 4962973	*Oncorhynchus mykiss*	96 hours	**Doses:** 0, 10, 100, and 1000 mg/L (nominal) **Replicates**: 7 organisms per vessel, 2 vessels per concentration	**LC_{50}** > 1000 mg/L	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity not reported • OECD Guideline 203 • GLP compliant
4962974, 4949228	*Daphnia magna*	48 hours	**Doses:** 0, 10, 30, 100, 300, 1000, 3000, and 10,000 mg/L (nominal)	**EC_{50}**: 1700 mg/L (NES)	**Methods:** • Test substance reported as CASRN 112-92-5 • Purity not reported • OECD Guideline 202 • GLP compliant
4949228, 4962964	*Scenedesmus subspicatus*	96 hours	**Doses:** 10, 30, 100, 300 mg/L unfiltered and 0.1, 0.3, 1.0, 3.0, 10.0 mg/L filtrate (nominal)	**EC_{50}**: 250 mg/L (unfiltered) **EC_{50}** > 10 mg/L (filtered) (NES)	**Methods:** • Test substance reported as CASRN 112-92-5 • Purity not reported • OECD Guideline 201 • GLP compliant
4949228	*Daphnia magna*	21 days	**Doses:** 0, 1,3, 10, 30, and 100 mg/L	**NOEC**: 0.98 mg/L **LOEC**: 2.94 mg/L based on slight mortality and reduced reproduction (NES)	**Methods:** • Test substance reported as CASRN 112-92-5 • Purity not reported • OECD Guideline 202 • GLP compliant

Table B.2: Environmental Hazard					
Aquatic Toxicity: Estimated					
Model	**Type**	**Duration**	**Species**	**Predicted Effect Level**	**Notes**
ECOSAR v2.0 (Class: Neutral Organics)	Estimate	96 hours	Freshwater fish	**LC_{50}**: 0.0006 mg/L	NES. Freshwater fish 96 hours LC50 = 0.00059 mg/L; Chemical may not be soluble enough to measure this predicted effect; the Log Kow of the chemical is greater than the endpoint specific cut-offs presented (max log Kow = 5), then no effects at saturation is expected.
ECOSAR v2.0 (Class: Neutral Organics)	Estimate	48 hours	Daphnia magna	**LC_{50}**: 0.0006 mg/L	NES. Daphnia magna 48 hours LC50 = 0.00060 mg/L; Chemical may not be soluble enough to measure this predicted effect; the Log Kow of the chemical is greater than the endpoint specific cut-offs presented (max log Kow = 5), then no effects at saturation is expected.
ECOSAR v2.0 (Class: Neutral Organics)	Estimate	96 hours	Green algae	**EC_{50}**: 0.005 mg/L	NES. Green Algae 96 hours EC50 = 0.0049 mg/L; Chemical may not be soluble enough to measure this predicted effect; the Log Kow of the chemical is greater than the endpoint specific cut-offs presented (max log Kow = 5), then no effects at saturation is expected.
ECOSAR v2.0 (Class: Neutral Organics)	Estimate	ChV	Freshwater fish	**EC_{50}**: 0.0001 mg/L	NES. Estimated ChV = 0.0001 mg/L. Chemical may not be soluble enough to measure this predicted effect; the Log Kow of the chemical is greater than the endpoint specific cut-offs presented (max log Kow = 8), then no effects at saturation is expected.
ECOSAR v2.0 (Class: Neutral Organics)	Estimate	ChV	Green algae	**EC_{50}**: 0.005 mg/L	NES. Estimated ChV = 0.005 mg/L. Chemical may not be soluble enough to measure this predicted effect; the Log Kow of the chemical is greater than the endpoint specific cut-offs presented (max log Kow = 8), then no effects at saturation is expected.

Table B.3: Fate					
Environmental Fate: Experimental					
Source	**Endpoint**	**Duration**	**Doses and number of replicates**	**Results**	**Study Details**
4949228	CO biodegradation	28 days	**Dose:** 12.4 mg/L	Not biodegradable	**Methods:** • Test substance reported as CASRN 661-19-8 • Purity not reported • OECD Guideline 301B • GLP compliant **Degradation during test:** • 16% in 8 days • 23% in 10 days

Table B.3: Fate					
					• 29% in 14 days • 33% in 22 days • 37% in 28 days
4949228	Aerobic biodegradation	28 days	**Doses:** 2 and 5 mg/L	Inherently biodegradable	**Methods:** • Test substance reported as CASRN 112-92-5 • Purity not reported • OECD Guideline 301D • GLP compliance not reported **Results:** • 30% in 7 days • 52% in 14 days • 59% in 21 days • 69% in 28 days
4949228	Aerobic biodegradation	28 days	**Dose:** 100 mg/L	Inherently biodegradable	**Methods:** • Test substance reported as CASRN 112-92-5 • Purity not reported • OECD Guideline 301D • GLP compliance not reported **Results:** • 25% in 7 days • 52% in 14 days • 66% in 21 days • 67% in 28 days
4949228	Aerobic biodegradation	28 days	**Dose:** 20 mg/L	Inherently biodegradable	**Methods:** • Test substance reported as CASRN 112-92-5 • Purity not reported • OECD Guideline 301B • GLP compliant **Results:** • 10% in 8 days • 35% in 14 days • 39% in 20 days • 43% in 28 days

Table B.3: Fate					
4944275	Anaerobic biodegradation	28 days	**Dose**: 10 mg/L	Total biodegradation	**Methods:** • Test substance reported as CASRN 36653-82-4 • Purity: 98% • GLP compliance not reported **Degradation during test:** • 97.1% in 28 days
5094384	Anaerobic biodegradation	28 days	**Dose**: 1 mg/L	Total biodegradation	**Methods:** • Test substance reported as CASRN 36653-82-4 • Purity > 98% • GLP compliance not reported **Degradation during test:** • 90.1% in 28 days
4335934	Photolysis (indirect)	Not reported	Not specified	Readily photolyzes	**Methods:** • Test substance reported as CASRN 112-92-5 • Purity not reported • GLP compliance not reported **Results:** • Half-life of 5.7 hours in Narda Lagoon (brown) water • Half-life of 31.3 hours in distilled water
5094369	BCF	3 days	**Dose**: 50 µg/L **Replicates**: 5 Fish	56	**Methods:** • Test substance reported as CASRN 36653-82-4 • Purity: 95% • GLP compliance not reported

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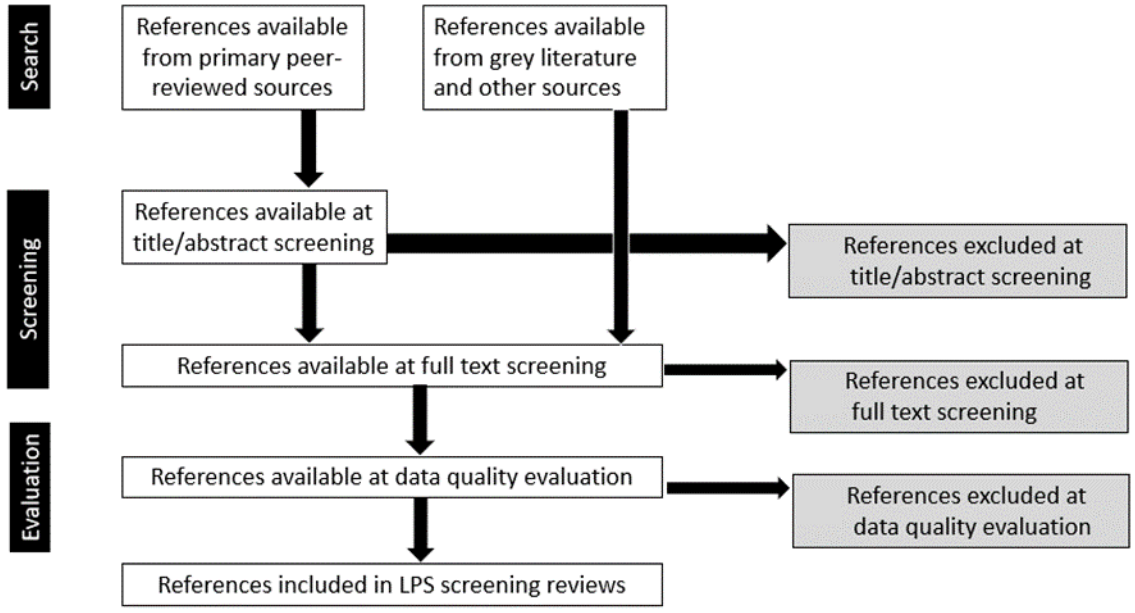
Appendix C: Literature Search Outcomes

C.1 Literature Search and Review

This section briefly describes the literature search and review process, search terms, and search outcomes for the hazard and fate screening of 1-docosanol. Search outcomes and reference details are provided on the candidate's HERO[55] project page.

EPA created a fit-for-purpose process to transparently document the literature search and review[56] of available hazard and fate information for low-priority substance (LPS) candidates. References from peer-reviewed primary sources, grey sources,[57] and other sources were identified, screened at the title/abstract and full text level, and evaluated for data quality based on discipline-specific criteria. An overview of the literature search and review process is illustrated in Figure C1.

Figure C.1: Overview of the Literature Search and Review Process



C.1.1 Search for Analog Data

To supplement the information on the candidate chemical, 1-docosanol, the following analogs were used for designation: alcohols, C16-18 (CASRN 67762-27-0); cetyl alcohol (CASRN 36653-82-4). Alcohols C16-18 and C18 unsaturated (CASRN 68002-94-8) was also searched but not used for designation. For

[55] The HERO low-priority substance candidate project pages are accessible to the public at https://hero.epa.gov/hero/.

[56] Discussed in the document "Approach Document for Screening Hazard Information for Low-Priority Substances Under TSCA."

[57] Grey literature and additional sources are the broad category of studies not found in standard, peer-reviewed literature database searches. This includes U.S. and international government agency websites, non-government organization (NGO) websites, and data sources that are difficult to find, or are not included, in the peer-reviewed databases, such as white papers, conference proceedings, technical reports, reference books, dissertations, and information on various stakeholder websites.

more details and justification on analogs, see section 6.1.1. Analogs were used to fill data gaps on endpoints for which 1-docosanol lacked quality data, such as aquatic toxicity, and to add to the weight of the scientific evidence. EPA collected reasonably available information for these endpoints by searching specific grey literature and other secondary sources, listed on Table C.1. If information related to the identified analogs were available in these sources, the references were screened and evaluated using the same process as references on 1-docosanol described above.[56] EPA also used read-across from the LPS candidates, 1-Octadecanol (CASRN 112-92-5) and 1-Eicosanol (CASRN 629-96-9). Although hazard information was only available for 1-octadecaonl, conditions of use information for 1-eicosanol was used for designation. The three LPS chemicals along with the analogs mentioned above fall under the fatty alcohols cluster in HERO.

Table C.1: Sources Used for Analog Search

Resource	URL
ATSDR	http://www.atsdr.cdc.gov/toxprofiles/index.asp
ChemID (EPA – HPVIS via ChemID)	http://chem.sis.nlm.nih.gov/chemidplus/
CIR	http://www.cir-safety.org/ingredients
ECHA	http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances
ECOTOX	https://cfpub.epa.gov/ecotox/quick_query.htm
EPA – ChemView (incl. TSCATS, RBP/HC, and HPV/HPVIS)	https://chemview.epa.gov/chemview
European Food Safety Authority (EFSA)	http://www.efsa.europa.eu/
FDA	https://www.fda.gov/default.htm
HERA	http://www.heraproject.com/RiskAssessment.cfm
NICNAS	http://www.nicnas.gov.au/
NITE (J-CHECK)	http://www.safe.nite.go.jp/jcheck/search.action?request_locale=en
NTP	https://ntpsearch.niehs.nih.gov/home
OECD/SIDS	https://hpvchemicals.oecd.org/UI/Search.aspx; http://webnet.oecd.org/hpv/ui/SponsoredChemicals.aspx

C.1.2 Search Terms and Results

EPA began the literature review process for the hazard screening of 1-docosanol by developing search terms. To gather publicly available information, specific search terms were applied for each discipline and across databases and grey literature sources. Table C.2 lists the search terms used in the database search of peer -reviewed literature for the fatty alcohols cluster including 1-docosanol. For grey literature and other secondary sources, Table C.3 lists the search terms used for the fatty alcohol LPS candidates and analogs.

Table C.2: Search Terms Used in Peer Reviewed Databases		
Discipline	**Database**	**Search terms[58]**
Human Health	PubMed	(112-92-5[rn] OR "1-Octadecanol" OR "Alcohol(C18)" OR "C18 alcohol" OR "n-Octadecanol" OR "Octadecan-1-ol" OR "octadecane-1-ol" OR "Octadecanol" OR "Octadecyl alcohol" OR "Stearic alcohol" OR "Stearol" OR "Stearyl alcohol" OR "Stenol" OR 661-19-8[rn] OR 30303-65-2[rn] OR "1-Docosanol" OR "Behenic alcohol" OR "Behenyl 80 Alcohol" OR "Behenyl alcohol" OR "Docosan-1-ol" OR "docosane-1-ol" OR "Docosanol" OR "Docosyl alcohol" OR "n-Docosanol" OR "Abreva" OR "IK 2" OR "IK.2" OR "Tadenan" OR 629-96-9[rn] OR "1-Eicosanol" OR "Arachidyl alcohol" OR "Eicosan-1-ol" OR "Eicosanol" OR "Icosanol" OR "n-Eicosanol" OR 143-28-2[rn] OR 593-47-5[rn] OR "(Z)-9-Octadecen-1-ol" OR "(Z)-Octadec-9-enol" OR "9-cis-Octadecenol" OR "9-Octadecen-1-ol" OR "9-Octadecenol" OR "Adol 85" OR "cis-9-Octadecen-1-ol" OR "cis-9-Octadecenyl alcohol" OR "Octadecenol" OR "Oleic alcohol" OR "Oleol" OR "Oleoyl alcohol" OR "Oleyl alcohol") "1-Hydroxyoctadecane" OR "1-Stearyl alcohol" OR "Alcohol stearylicus" OR "Decyl octyl alcohol" OR "Fatty alcohol(C18)" OR "n-1-Octadecanol" OR "n-Octadecyl alcohol" OR "Octadecanol, 1-" OR "Steraffine" OR "USP XIII stearyl alcohol" OR "Adol 62" OR "Adol 64" OR "Adol 68" OR "Aldol 62" OR "Alfol 18" OR "Alfol 18NF" OR "Atalco S" OR "Cachalot S 43" OR "Cachalot S-43" OR "CO 1895" OR "CO 1895F" OR "CO 1897" OR "CO-1895" OR "CO-1897" OR "Conol 1675" OR "Conol 30F" OR "Conol 30S" OR "Conol 30SS" OR "Crodacol S" OR "Crodacol S 70" OR "Crodacol S 95" OR "Crodacol S 95 NF" OR "Crodacol-S" OR "Dytol E-46" OR "Hainol 18 SS" OR "Hainol 18SS" OR "Hyfatol 18-95" OR "Hyfatol 18-98" OR "Kalchol 8098" OR "Kalcohl 80" OR "Kalcohl 8098" OR "Kalcohl 8099" OR "Kalcol 8098" OR "Lanette 18" OR "Lanette 18DEO" OR "Lanol S" OR "Laurex 18" OR "Lorol 28" OR "Lorol C 18" OR "Polaax" OR "Rofamol" OR "Sipol S" OR "Siponol S" OR "Siponol SC" OR "SSD AF" OR "Tego alkanol 18" OR "VLTN 6" OR "Conol 2265" OR "Hainol 22 S" OR "Hainol 22S" OR "Kalcohl 22080" OR "Kalcol 22080" OR "Lanette 22" OR "Lidavol" OR "NAA 422" OR "Nacol 22-97" OR "Nacol 22-98" OR "Stenol 1822" OR "Stenol 1822A" OR "Toho BH 65" OR "Arachic alcohol" "Arachidic alcohol" OR "Eicosyl alcohol" OR "Icosan-1-ol" OR "icosane-1-ol" OR "n-1-Eicosanol" OR "n-Eicosyl alcohol" OR "Pri-N-eicosyl alcohol" OR "Hainol 20 SS" OR "Hainol 20SS" OR "(Z)-9-Octadecenol" OR "9-Octadecen-1-ol, (9Z)-" OR "9-Octadecen-1-ol, (Z)-" OR "cis-Octadecen-1-ol" OR "cis-Delta9-Octadecenol" OR "HD oleyl alcohol 70/75" OR "HD oleyl alcohol 80/85" OR "HD oleyl alcohol 90/95" OR "HD oleyl alcohol CG" OR "Octadec-9-en-1-ol, (Z)-" OR "Octadeca-9-cis-en-1-ol" OR "Oleo alcohol" OR "Olive alcohol" OR "Adol 320" OR "Adol 330" OR "Adol 34" OR "Adol 340" OR "Adol 80" OR "Adol 85NF" OR "Adol 90" OR "Atalco O" OR "Cachalot O 1" OR "Cachalot O-1" OR "Cachalot O-15" OR "Cachalot O-3" OR "Cachalot O-8" OR "Crodacol A.10" OR "Crodacol O" OR "Crodacol-O" OR "Dermaffine" OR "H.D. eutanol" OR "HD-Eutanol" OR "HD-Ocenol 90/95" OR "HD-Ocenol 92/96" OR "HD-Ocenol K" OR "Lancol" OR "Loxanol 95" OR "Loxanol M" OR "Ocenol" OR "Ocenol 90/95" OR "Oceol" OR "Rikacol 90BHR" OR "Satol" OR "Sipol O" OR "Siponol OC" OR "Unjecol 110" OR "Unjecol 50" OR "Unjecol 70" OR "Unjecol 70N" OR "Unjecol 90" OR "Unjecol 90BHR" OR "Unjecol 90N" OR "Unjecol 90NR" OR "Vegecol 90B" OR "Witcohol 85" OR "Witcohol 85NF" OR "Witcohol 90" OR "Witcohol 90NF"
	Toxline	(112-92-5[rn] OR "1-Octadecanol" OR "Alcohol(C18)" OR "C18 alcohol" OR "n-Octadecanol" OR "Octadecan-1-ol" OR "octadecane-1-ol" OR "Octadecanol" OR "Octadecyl alcohol" OR "Stearic alcohol" OR "Stearol" OR "Stearyl alcohol" OR "Stenol" OR 661-19-8[rn] OR 30303-65-2[rn] OR "1-Docosanol" OR "Behenic alcohol" OR "Behenyl 80 Alcohol" OR "Behenyl alcohol" OR "Docosan-1-ol" OR "docosane-1-ol" OR "Docosanol" OR "Docosyl alcohol") AND (ANEUPL [org] OR BIOSIS [org] OR CIS [org] OR DART [org] OR EMIC [org] OR EPIDEM [org] OR HAPAB [org] OR HEEP [org] OR HMTC

[58] Additional language or syntax such as [tw], [rn], [org], and [nm] were added to search terms. These are unique to individual databases and must be applied to search terms so that the query can run properly.

Table C.2: Search Terms Used in Peer Reviewed Databases		
Discipline	**Database**	**Search terms[58]**
		[org] OR IPA [org] OR RISKLINE [org] OR MTGABS [org] OR NIOSH [org] OR NTIS [org] OR PESTAB [org] OR PPBIB [org]) AND NOT PubMed [org] AND NOT pubdart [org] ("n-Docosanol" OR "Abreva" OR "IK 2" OR "IK.2" OR "Tadenan" OR 629-96-9[rn] OR "1-Eicosanol" OR "Arachidyl alcohol" OR "Eicosan-1-ol" OR "Eicosanol" OR "Icosanol" OR "n-Eicosanol" OR 143-28-2[rn] OR 593-47-5[rn] OR "(Z)-9-Octadecen-1-ol" OR "(Z)-Octadec-9-enol" OR "9-cis-Octadecenol" OR "9-Octadecen-1-ol" OR "9-Octadecenol" OR "Adol 85" OR "cis-9-Octadecen-1-ol" OR "cis-9-Octadecenyl alcohol" OR "Octadecenol" OR "Oleic alcohol" OR "Oleol" OR "Oleoyl alcohol" OR "Oleyl alcohol") AND (ANEUPL [org] OR BIOSIS [org] OR CIS [org] OR DART [org] OR EMIC [org] OR EPIDEM [org] OR HAPAB [org] OR HEEP [org] OR HMTC [org] OR IPA [org] OR RISKLINE [org] OR MTGABS [org] OR NIOSH [org] OR NTIS [org] OR PESTAB [org] OR PPBIB [org]) AND NOT PubMed [org] AND NOT pubdart [org] ("1-Hydroxyoctadecane" OR "1-Stearyl alcohol" OR "Alcohol stearylicus" OR "Decyl octyl alcohol" OR "Fatty alcohol(C18)" OR "n-1-Octadecanol" OR "n-Octadecyl alcohol" OR "Octadecanol, 1-" OR "Steraffine" OR "USP XIII stearyl alcohol" OR "Adol 62" OR "Adol 64" OR "Adol 68" OR "Aldol 62" OR "Alfol 18" OR "Alfol 18NF" OR "Atalco S" OR "Cachalot S 43" OR "Cachalot S-43" OR "CO 1895" OR "CO 1895F" OR "CO 1897" OR "CO-1895" OR "CO-1897" OR "Conol 1675" OR "Conol 30F" OR "Conol 30S" OR "Conol 30SS" OR "Crodacol S" OR "Crodacol S 70" OR "Crodacol S 95" OR "Crodacol S 95 NF" OR "Crodacol-S" OR "Dytol E-46" OR "Hainol 18 SS" OR "Hainol 18SS" OR "Hyfatol 18-95" OR "Hyfatol 18-98" OR "Kalchol 8098" OR "Kalcohl 80" OR "Kalcohl 8098" OR "Kalcohl 8099" OR "Kalcol 8098" OR "Lanette 18" OR "Lanette 18DEO" OR "Lanol S" OR "Laurex 18" OR "Lorol 28" OR "Lorol C 18" OR "Polaax" OR "Rofamol" OR "Sipol S" OR "Siponol S" OR "Siponol SC" OR "SSD AF" OR "Tego alkanol 18" OR "VLTN 6" OR "Conol 2265" OR "Hainol 22 S" OR "Hainol 22S" OR "Kalcohl 22080" OR "Kalcol 22080" OR "Lanette 22" OR "Lidavol" OR "NAA 422" OR "Nacol 22-97" OR "Nacol 22-98" OR "Stenol 1822" OR "Stenol 1822A" OR "Toho BH 65" OR "Arachic alcohol" OR "Arachidic alcohol" OR "Eicosyl alcohol" OR "Icosan-1-ol" OR "icosane-1-ol" OR "n-1-Eicosanol" OR "n-Eicosyl alcohol" OR "Pri-N-eicosyl alcohol" OR "Hainol 20 SS" OR "Hainol 20SS" OR "(Z)-9-Octadecenol" OR "9-Octadecen-1-ol, (9Z)-" OR "9-Octadecen-1-ol, (Z)-" OR "cis-Octadecen-1-ol" OR "cis-Delta9-Octadecenol" OR "HD oleyl alcohol 70/75" OR "HD oleyl alcohol 80/85" OR "HD oleyl alcohol 90/95" OR "HD oleyl alcohol CG" OR "Octadec-9-en-1-ol, (Z)-" OR "Octadeca-9-cis-en-1-ol" OR "Oleo alcohol" OR "Olive alcohol" OR "Adol 320" OR "Adol 330" OR "Adol 34" OR "Adol 340" OR "Adol 80" OR "Adol 85NF" OR "Adol 90" OR "Atalco O" OR "Cachalot O 1" OR "Cachalot O-1" OR "Cachalot O-15" OR "Cachalot O-3" OR "Cachalot O-8" OR "Crodacol A.10" OR "Crodacol O" OR "Crodacol-O" OR "Dermaffine" OR "H.D. eutanol" OR "HD-Eutanol" OR "HD-Ocenol 90/95" OR "HD-Ocenol 92/96" OR "HD-Ocenol K" OR "Lancol" OR "Loxanol 95" OR "Loxanol M" OR "Ocenol" OR "Ocenol 90/95" OR "Oceol" OR "Rikacol 90BHR" OR "Satol" OR "Sipol O" OR "Siponol OC" OR "Unjecol 110" OR "Unjecol 50" OR "Unjecol 70" OR "Unjecol 70N" OR "Unjecol 90" OR "Unjecol 90BHR" OR "Unjecol 90N" OR "Unjecol 90NR" OR "Vegecol 90B" OR "Witcohol 85" OR "Witcohol 85NF" OR "Witcohol 90" OR "Witcohol 90NF") AND (ANEUPL [org] OR BIOSIS [org] OR CIS [org] OR DART [org] OR EMIC [org] OR EPIDEM [org] OR HAPAB [org] OR HEEP [org] OR HMTC [org] OR IPA [org] OR RISKLINE [org] OR MTGABS [org] OR NIOSH [org] OR NTIS [org] OR PESTAB [org] OR PPBIB [org]) AND NOT PubMed [org] AND NOT pubdart [org]
	TSCATS 1	(112-92-5 [rn] OR 661-19-8 [rn] OR 30303-65-2 [rn] OR 629-96-9 [rn] OR 143-28-2 [rn] OR 593-47-5 [rn]) AND (TSCATS [org]) AND NOT PubMed [org] AND NOT pubdart [org]
	WOS	TS=("112-92-5" OR "1-Octadecanol" OR "Alcohol(C18)" OR "C18 alcohol" OR "n-Octadecanol" OR "Octadecan-1-ol" OR "octadecane-1-ol" OR "Octadecanol" OR "Octadecyl alcohol" OR "Stearic

Table C.2: Search Terms Used in Peer Reviewed Databases		
Discipline	**Database**	**Search terms[58]**
		alcohol" OR "Stearol" OR "Stearyl alcohol" OR "Stenol" OR "661-19-8" OR "30303-65-2" OR "1-Docosanol" OR "Behenic alcohol" OR "Behenyl 80 Alcohol" OR "Behenyl alcohol" OR "Docosan-1-ol" OR "docosane-1-ol" OR "Docosanol" OR "Docosyl alcohol" OR "n-Docosanol" OR "Abreva" OR "IK 2" OR "IK.2" OR "Tadenan" OR "629-96-9" OR "1-Eicosanol" OR "Arachidyl alcohol" OR "Eicosan-1-ol" OR "Eicosanol" OR "Icosanol" OR "n-Eicosanol" OR "143-28-2" OR "593-47-5" OR "(Z)-9-Octadecen-1-ol" OR "(Z)-Octadec-9-enol" OR "9-cis-Octadecenol" OR "9-Octadecen-1-ol" OR "9-Octadecenol" OR "Adol 85" OR "cis-9-Octadecen-1-ol" OR "cis-9-Octadecenyl alcohol" OR "Octadecenol" OR "Oleic alcohol" OR "Oleol" OR "Oleoyl alcohol" OR "Oleyl alcohol" OR "Adol 85NF" OR "Arachic alcohol" OR "Decyl octyl alcohol" OR "Eicosyl alcohol" OR "Icosan-1-ol" OR "Ocenol" OR "Satol" OR "Witcohol 85") AND ((WC=("Toxicology" OR "Endocrinology & Metabolism" OR "Gastroenterology & Hepatology" OR "Gastroenterology & Hepatology" OR "Hematology" OR "Neurosciences" OR "Obstetrics & Gynecology" OR "Pharmacology & Pharmacy" OR "Physiology" OR "Respiratory System" OR "Urology & Nephrology" OR "Anatomy & Morphology" OR "Andrology" OR "Pathology" OR "Otorhinolaryngology" OR "Ophthalmology" OR "Pediatrics" OR "Oncology" OR "Reproductive Biology" OR "Developmental Biology" OR "Biology" OR "Dermatology" OR "Allergy" OR "Public, Environmental & Occupational Health") OR SU=("Anatomy & Morphology" OR "Cardiovascular System & Cardiology" OR "Developmental Biology" OR "Endocrinology & Metabolism" OR "Gastroenterology & Hepatology" OR "Hematology" OR "Immunology" OR "Neurosciences & Neurology" OR "Obstetrics & Gynecology" OR "Oncology" OR "Ophthalmology" OR "Pathology" OR "Pediatrics" OR "Pharmacology & Pharmacy" OR "Physiology" OR "Public, Environmental & Occupational Health" OR "Respiratory System" OR "Toxicology" OR "Urology & Nephrology" OR "Reproductive Biology" OR "Dermatology" OR "Allergy")) OR (WC="veterinary sciences" AND (TS="rat" OR TS="rats" OR TS="mouse" OR TS="murine" OR TS="mice" OR TS="guinea" OR TS="muridae" OR TS=rabbit* OR TS=lagomorph* OR TS=hamster* OR TS=ferret* OR TS=gerbil* OR TS=rodent* OR TS="dog" OR TS="dogs" OR TS=beagle* OR TS="canine" OR TS="cats" OR TS="feline" OR TS="pig" OR TS="pigs" OR TS="swine" OR TS="porcine" OR TS=monkey* OR TS=macaque* OR TS=baboon* OR TS=marmoset*)) OR (TS=toxic* AND (TS="rat" OR TS="rats" OR TS="mouse" OR TS="murine" OR TS="mice" OR TS="guinea" OR TS="muridae" OR TS=rabbit* OR TS=lagomorph* OR TS=hamster* OR TS=ferret* OR TS=gerbil* OR TS=rodent* OR TS="dog" OR TS="dogs" OR TS=beagle* OR TS="canine" OR TS="cats" OR TS="feline" OR TS="pig" OR TS="pigs" OR TS="swine" OR TS="porcine" OR TS=monkey* OR TS=macaque* OR TS=baboon* OR TS=marmoset* OR TS="child" OR TS="children" OR TS=adolescen* OR TS=infant* OR TS="WORKER" OR TS="WORKERS" OR TS="HUMAN" OR TS=patient* OR TS=mother OR TS=fetal OR TS=fetus OR TS=citizens OR TS=milk OR TS=formula OR TS=epidemio* OR TS=population* OR TS=exposure* OR TS=questionnaire OR SO=epidemio*)) OR TI=toxic* OR TS=metaboli* OR TS=biotransform* OR ((TS="breakdown" OR TS="break-down") AND (TS=product OR TS=products))) Indexes=SCI-EXPANDED, CPCI-S, CPCI-SSH, BKCI-S, BKCI-SSH, CCR-EXPANDED, IC Timespan=All years TS=("1-Hydroxyoctadecane" OR "1-Stearyl alcohol" OR "Alcohol stearylicus" OR "Fatty alcohol(C18)" OR "Steraffine" OR "USP XIII stearyl alcohol" OR "Adol 62" OR "Adol 64" OR "Adol 68" OR "Aldol 62" OR "Alfol 18" OR "Alfol 18NF" OR "Atalco S" OR "Cachalot S 43" OR "Cachalot S-43" OR "CO 1895" OR "CO 1895F" OR "CO 1897" OR "CO-1895" OR "CO-1897" OR "Conol 1675" OR "Conol 30F" OR "Conol 30S" OR "Conol 30SS" OR "Crodacol S" OR "Crodacol S 70" OR "Crodacol S 95" OR "Crodacol S 95 NF" OR "Crodacol-S" OR "Dytol E-46" OR "Hainol 18 SS" OR "Hainol 18SS" OR "Hyfatol 18-95" OR "Hyfatol 18-98" OR "Kalchol 8098" OR "Kalcohl 80" OR "Kalcohl 8098" OR "Kalcohl 8099" OR "Kalcol 8098" OR "Lanette 18" OR "Lanette 18DEO" OR "Lanol S" OR "Laurex 18" OR "Lorol 28" OR "Lorol C 18" OR "Polaax" OR "Rofamol" OR "Sipol S" OR "Siponol S" OR "Siponol SC" OR

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Discipline	**Database**	**Search terms[58]**
		"SSD AF" OR "Tego alkanol 18" OR "VLTN 6" OR "Conol 2265" OR "Hainol 22 S" OR "Hainol 22S" OR "Kalcohl 22080" OR "Kalcol 22080" OR "Lanette 22" OR "Lidavol" OR "NAA 422" OR "Nacol 22-97" OR "Nacol 22-98" OR "Stenol 1822" OR "Stenol 1822A" OR "Toho BH 65" OR "Arachidic alcohol" OR "icosane-1-ol" OR "n-1-Eicosanol" OR "Hainol 20 SS" OR "Hainol 20SS" OR "(Z)-9-Octadecenol" OR "cis-Octadecen-1-ol" OR "cis-Delta9-Octadecenol" OR "HD oleyl alcohol 70/75" OR "HD oleyl alcohol 80/85" OR "HD oleyl alcohol 90/95" OR "HD oleyl alcohol CG" OR "Octadec-9-en-1-ol, (Z)-" OR "Octadeca-9-cis-en-1-ol" OR "Oleo alcohol" OR "Olive alcohol" OR "Adol 320" OR "Adol 330" OR "Adol 34" OR "Adol 340" OR "Adol 80" OR "Adol 90" OR "Atalco O" OR "Cachalot O 1" OR "Cachalot O-1" OR "Cachalot O-15" OR "Cachalot O-3" OR "Cachalot O-8" OR "Crodacol A.10" OR "Crodacol O" OR "Crodacol-O" OR "Dermaffine" OR "H.D. eutanol" OR "HD-Eutanol" OR "Lancol" OR "Loxanol 95" OR "Loxanol M" OR "Oceol" OR "Rikacol 90BHR" OR "Sipol O" OR "Siponol OC" OR "Unjecol 110" OR "Unjecol 50" OR "Unjecol 70" OR "Unjecol 70N" OR "Unjecol 90" OR "Unjecol 90BHR" OR "Unjecol 90N" OR "Unjecol 90NR" OR "Vegecol 90B" OR "Witcohol 85NF" OR "Witcohol 90" OR "Witcohol 90NF") Indexes=SCI-EXPANDED, CPCI-S, CPCI-SSH, BKCI-S, BKCI-SSH, CCR-EXPANDED, IC Timespan=All years
Environmental Hazard	WOS	TS=("112-92-5" OR "1-Octadecanol" OR "Alcohol(C18)" OR "C18 alcohol" OR "n-Octadecanol" OR "Octadecan-1-ol" OR "octadecane-1-ol" OR "Octadecanol" OR "Octadecyl alcohol" OR "Stearic alcohol" OR "Stearol" OR "Stearyl alcohol" OR "Stenol" OR "661-19-8" OR "30303-65-2" OR "1-Docosanol" OR "Behenic alcohol" OR "Behenyl 80 Alcohol" OR "Behenyl alcohol" OR "Docosan-1-ol" OR "docosane-1-ol" OR "Docosanol" OR "Docosyl alcohol" OR "n-Docosanol" OR "Abreva" OR "IK 2" OR "IK.2" OR "Tadenan" OR "629-96-9" OR "1-Eicosanol" OR "Arachidyl alcohol" OR "Eicosan-1-ol" OR "Eicosanol" OR "Icosanol" OR "n-Eicosanol" OR "143-28-2" OR "593-47-5" OR "(Z)-9-Octadecen-1-ol" OR "(Z)-Octadec-9-enol" OR "9-cis-Octadecenol" OR "9-Octadecen-1-ol" OR "9-Octadecenol" OR "Adol 85" OR "cis-9-Octadecen-1-ol" OR "cis-9-Octadecenyl alcohol" OR "Octadecenol" OR "Oleic alcohol" OR "Oleol" OR "Oleoyl alcohol" OR "Oleyl alcohol" OR "Adol 85NF" OR "Arachic alcohol" OR "Decyl octyl alcohol" OR "Eicosyl alcohol" OR "Icosan-1-ol" OR "Ocenol" OR "Satol" OR "Witcohol 85") AND ((WC=("Agriculture, Dairy & Animal Science" OR "Biodiversity Conservation" OR "Biology" OR "Developmental Biology" OR "Ecology" OR "Entomology" OR "Environmental Sciences" OR "Environmental Studies" OR "Fisheries" OR "Forestry" OR "Limnology" OR "Marine & Freshwater Biology" OR "Microbiology" OR "Mycology" OR "Oceanography" OR "Ornithology" OR "Plant Sciences" OR “Reproductive Biology” OR "Zoology")) OR (SU=("Agriculture" OR "Biodiversity & Conservation" OR “Developmental Biology” OR "Entomology" OR "Environmental Sciences & Ecology" OR "Fisheries" OR "Forestry" OR "Marine & Freshwater Biology" OR "Microbiology" OR "Mycology" OR "Plant Sciences" OR “Reproductive Biology” OR "Zoology" OR "Oceanography")) OR (TI=toxic*) OR (TS=(ecotox* OR environment* OR phytotox* OR pollut* OR "A. platyrhynchos" OR "agnatha" OR "agnathan" OR "alligator" OR "alligators" OR "amphibian" OR "amphibians" OR "amphipod" OR "amphipoda" OR "amphipods" OR "Anas platyrhynchos" OR "annelid" OR "annelida" OR "annelids" OR "Antilocapridae" OR "apidae" OR "Aplodontidae" OR "Apoidea" OR "aquatic" OR "archiannelid" OR "archiannelida" OR "Arvicolinae" OR "aves" OR "avian" OR "avians" OR "badger" OR "badgers" OR "barnacle" OR "barnacles" OR "bass" OR "bear" OR "bears" OR "beaver" OR "beavers" OR "bee" OR "bees" OR "bird" OR "birds" OR "bivalve" OR "bivalves" OR "bleak" OR "bluegill" OR "bluegills" OR "bluehead" OR "bobwhite" OR "bobwhites" OR "Bovidae" OR "C. carpio" OR "caiman" OR "Canidae" OR "carp" OR "Castoridae" OR "catfish" OR "cephalopod" OR "cephalopoda" OR "cephalopods" OR "Cervidae" OR "chicken" OR "chickens" OR "chiselmouth" OR "clam" OR "clams" OR "cockle" OR "cockles" OR "cod" OR "copepod" OR "copepoda" OR "copepods" OR "coturnix" OR "crab" OR "crabs" OR "crappie" OR "crappies" OR "crayfish" OR "croaker" OR "crocodile" OR "crocodiles" OR "crustacea" OR "crustacean" OR "crustaceans" OR "Cyprinus carpio" OR "D. magna" OR "D. rerio" OR

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Discipline	**Database**	**Search terms[58]**
		"dace" OR "Danio rerio" OR "daphnia" OR "Daphnia magna" OR "darter" OR "darters" OR "Dasypodidae" OR "Dicotylidae" OR "Didelphidae" OR "Dipodidae" OR "dog" OR "dogs" OR "dogfish" OR "duck" OR "duckling" OR "ducklings" OR "ducks" OR "earthworm" OR "earthworms" OR "ec50" OR "ec50s" OR "echinoderm" OR "echinoderms" OR "eel" OR "eels" OR "elasmobranch" OR "Equidae" OR "Erethizontidae" OR "Felidae" OR "ferret" OR "fish" OR "fisher" OR "fishers" OR "fishes" OR "flagfish" OR "flatworm" OR "flatworms" OR "flounder" OR "frog" OR "frogs" OR "galaxias" OR "gallus" OR "gastropod" OR "gastropoda" OR "gastropods" OR "Geomyidae" OR "goldfish" OR "gourami" OR "gouramy" OR "Green Algae" OR "grunion" OR "guppies" OR "guppy" OR "haddock" OR "hagfish" OR "haplodrili" OR "Harvest mice " OR "Harvest mouse" OR "herring" OR "Heteromyidae" OR "honeybee" OR "honeybees" OR "hooknose" OR "inanga" OR "killifish" OR "L. idus" OR "L. macrochirus" OR "lamprey" OR "lampreys" OR "lc50" OR "lc50s" OR "leech" OR "lemming" OR "Lepomis macrochirus" OR "Leporidae" OR "lethal concentration" OR "Leuciscus idus" OR "lizard" OR "lizards" OR "lobster" OR "lobsters" OR "macroinvertebrate" OR "macroinvertebrates" OR "mallard" OR "mallards" OR "marten" OR "medaka" OR "menhaden" OR "Microtus" OR "milkfish" OR "mink" OR "minnow" OR "minnows" OR "mollusc" OR "molluscs" OR "mollusk" OR "mollusks" OR "molly" OR "mrigal" OR "mudfish" OR "mudsucker" OR "mulles" OR "mullet" OR "mummichog" OR "mummichogs" OR "mussel" OR "mussels" OR "Mustelidae" OR "Myocastoridae" OR "Mysid shrimp" OR "newt" OR "newts" OR "northern pike" OR "O. latipes" OR "O. mykiss" OR "Ochotonidae" OR "octopi" OR "octopus" OR "oligochaeta" OR "oligochaete" OR "Oncorhynchus mykiss" OR "Onychomys" OR "opossum" OR "Oryzias latipes" OR "oyster" OR "oysters" OR "P. promelas" OR "P. reticulata" OR "P. subcapitata" OR "perch" OR "Peromyscus" OR "Pimephales promelas" OR "pinfish" OR "pinfishes" OR "planaria" OR "planarian" OR "Poecilia reticulata" OR "polychaeta" OR "polychaete" OR "polychaetes" OR "Procyonidae" OR "Pseudokirchneriella subcapitata" OR "puffer" OR "puffers" OR "pumpkinseed" OR "pumpkinseeds" OR "pupfish" OR "quahog" OR "quahogs" OR "quail" OR "quails" OR "rasbora" OR "rasboras" OR "Reithrodontomys" OR "reptile" OR "reptiles" OR "rohu" OR "S. erythrophthalmus" OR "S. quadricauda" OR "S. subspicatus" OR "salamander" OR "salamanders" OR "salmon" OR "scallop" OR "scallops" OR "Scardinius erythrophthalmus" OR "Scenedesmus quadricauda " OR "Scenedesmus subspicatus" OR "Sciuridae" OR "sea anemone" OR "sea anemones" OR "sea cucumber" OR "sea cucumbers" OR "sea urchin" OR "sea urchins" OR "seabass" OR "seabream" OR "shark" OR "sharks" OR "shiner" OR "shiners" OR "shrimp" OR "Sigmodon" OR "Sigmodontinae" OR "silverside" OR "silversides" OR "skunk" OR "skunks" OR "snake" OR "snakehead" OR "snakes" OR "songbird" OR "songbirds" OR "Soricidae" OR "squid" OR "starfish" OR "stickleback" OR "sticklebacks" OR "sting ray" OR "sting rays" OR "sucker" OR "suckers" OR "Suidae" OR "sunfish" OR "Talpidae" OR "teleost" OR "teleostei" OR "teleosts" OR "terrapin" OR "terrapins" OR "tilapia" OR "tilapiaz" OR "toad" OR "toadfish" OR "toadfishes" OR "toads" OR "tortoise" OR "tortoises" OR "trout" OR "tubificid" OR "tubificidae" OR "tubificids" OR "turkey" OR "turkeys" OR "turtle" OR "turtles" OR "Ursidae" OR "vole" OR "walleye" OR "walleyes" OR "water flea" OR "water fleas" OR "waterbird" OR "waterbirds" OR "waterfowl" OR "waterfowls" OR "weakfish" OR "weasel" OR "whelk" OR "whelks" OR "wildlife"))) Indexes=SCI-EXPANDED, CPCI-S, CPCI-SSH, BKCI-S, BKCI-SSH, CCR-EXPANDED, IC Timespan=All years
	Toxline	Same as human health strategy synonyms only
	TSCATS 1	Same as human health strategy CASRN only
	Proquest	TITLE=("112-92-5" OR "143-28-2" OR "30303-65-2" OR "593-47-5" OR "629-96-9" OR "661-19-8" OR "1-Docosanol" OR "1-Eicosanol" OR "1-Hydroxyoctadecane" OR "1-Octadecanol" OR "1-Stearyl alcohol" OR "9-Octadecen-1-ol" OR "9-Octadecenol" OR "9-cis-Octadecenol" OR "Abreva" OR "Adol 85" OR "Alcohol C18" OR "Aldol 62" OR "Arachic alcohol" OR "Arachidic alcohol" OR "Arachidyl alcohol" OR "Behenic alcohol" OR "Behenyl 80 Alcohol" OR "Behenyl alcohol" OR "C18 alcohol" OR

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Discipline	**Database**	**Search terms[58]**
		"cis-9-Octadecen-1-ol" OR "cis-9-Octadecenyl alcohol" OR "Decyl octyl alcohol" OR "Docosan-1-ol" OR "docosane-1-ol" OR "Docosanol" OR "Docosyl alcohol") TITLE=("Eicosan-1-ol" OR "Eicosanol" OR "Eicosyl alcohol" OR "Fatty alcohol C18" OR "Icosanol" OR "Lanette 18" OR "Lanette 22" OR "n-Docosanol" OR "n-Eicosanol" OR "n-Octadecanol" OR "n-Octadecyl alcohol"OR "Octadecan-1-ol" OR "octadecane-1-ol" OR "Octadecanol" OR "Octadecanol, 1-" OR "Octadecenol" OR "Octadecyl alcohol" OR "Oleic alcohol" OR "Oleo alcohol" OR "Oleol" OR "Oleoyl alcohol" OR "Oleyl alcohol" OR "Olive alcohol" OR "Stearic alcohol" OR "Stearol" OR "Stearyl alcohol" OR "Stenol" OR "Tadenan" OR "Witcohol 85") SUBJECT=("112-92-5" OR "143-28-2" OR "30303-65-2" OR "593-47-5" OR "629-96-9" OR "661-19-8" OR "1-Docosanol" OR "1-Eicosanol" OR "1-Hydroxyoctadecane" OR "1-Octadecanol" OR "1-Stearyl alcohol" OR "9-Octadecen-1-ol" OR "9-Octadecenol" OR "9-cis-Octadecenol" OR "Abreva" OR "Adol 85" OR "Alcohol C18" OR "Aldol 62" OR "Arachic alcohol" OR "Arachidic alcohol" OR "Arachidyl alcohol" OR "Behenic alcohol" OR "Behenyl 80 Alcohol" OR "Behenyl alcohol" OR "C18 alcohol" OR "cis-9-Octadecen-1-ol" OR "cis-9-Octadecenyl alcohol" OR "Decyl octyl alcohol" OR "Docosan-1-ol" OR "docosane-1-ol" OR "Docosanol" OR "Docosyl alcohol") SUBJECT=("Eicosan-1-ol" OR "Eicosanol" OR "Eicosyl alcohol" OR "Fatty alcohol C18" OR "Icosanol" OR "Lanette 18" OR "Lanette 22" OR "n-Docosanol" OR "n-Eicosanol" OR "n-Octadecanol" OR "n-Octadecyl alcohol"OR "Octadecan-1-ol" OR "octadecane-1-ol" OR "Octadecanol" OR "Octadecanol, 1-" OR "Octadecenol" OR "Octadecyl alcohol" OR "Oleic alcohol" OR "Oleo alcohol" OR "Oleol" OR "Oleoyl alcohol" OR "Oleyl alcohol" OR "Olive alcohol" OR "Stearic alcohol" OR "Stearol" OR "Stearyl alcohol" OR "Stenol" OR "Tadenan" OR "Witcohol 85") ABSTRACT=("112-92-5" OR "143-28-2" OR "30303-65-2" OR "593-47-5" OR "629-96-9" OR "661-19-8" OR "1-Docosanol" OR "1-Eicosanol" OR "1-Hydroxyoctadecane" OR "1-Octadecanol" OR "1-Stearyl alcohol" OR "9-Octadecen-1-ol" OR "9-Octadecenol" OR "9-cis-Octadecenol" OR "Abreva" OR "Adol 85" OR "Alcohol C18" OR "Aldol 62" OR "Arachic alcohol" OR "Arachidic alcohol" OR "Arachidyl alcohol" OR "Behenic alcohol" OR "Behenyl 80 Alcohol" OR "Behenyl alcohol" OR "C18 alcohol" OR "cis-9-Octadecen-1-ol" OR "cis-9-Octadecenyl alcohol" OR "Decyl octyl alcohol" OR "Docosan-1-ol" OR "docosane-1-ol" OR "Docosanol" OR "Docosyl alcohol") ABSTRACT=("Eicosan-1-ol" OR "Eicosanol" OR "Eicosyl alcohol" OR "Fatty alcohol C18" OR "Icosanol" OR "Lanette 18" OR "Lanette 22" OR "n-Docosanol" OR "n-Eicosanol" OR "n-Octadecanol" OR "n-Octadecyl alcohol"OR "Octadecan-1-ol" OR "octadecane-1-ol" OR "Octadecanol" OR "Octadecanol, 1-" OR "Octadecenol" OR "Octadecyl alcohol" OR "Oleic alcohol" OR "Oleo alcohol" OR "Oleol" OR "Oleoyl alcohol" OR "Oleyl alcohol" OR "Olive alcohol" OR "Stearic alcohol" OR "Stearol" OR "Stearyl alcohol" OR "Stenol" OR "Tadenan" OR "Witcohol 85") TITLE=("(Z)-9-Octadecen-1-ol" OR "(Z)-Octadec-9-enol" OR "9-Octadecen-1-ol, (Z)-" OR "Octadec-9-en-1-ol, (Z)-") SUBJECT=("(Z)-9-Octadecen-1-ol" OR "(Z)-Octadec-9-enol" OR "9-Octadecen-1-ol, (Z)-" OR "Octadec-9-en-1-ol, (Z)-") 5 – still returned above – not searched ABSTRACT=("(Z)-9-Octadecen-1-ol" OR "(Z)-Octadec-9-enol" OR "9-Octadecen-1-ol, (Z)-" OR "Octadec-9-en-1-ol, (Z)-")

Table C.2: Search Terms Used in Peer Reviewed Databases		
Discipline	**Database**	**Search terms[58]**
		TITLE=("Alcohol stearylicus" OR "n-1-Octadecanol" OR "Steraffine" OR "USP XIII stearyl alcohol" OR "Atalco S" OR "Alfol 18" OR "Alfol 18NF" OR "Cachalot S 43" OR "Cachalot S-43" OR "Conol 1675" OR "Conol 30F" OR "Conol 30S" OR "Conol 30SS" OR "Crodacol S" OR "Crodacol S 70" OR "Crodacol S 95" OR "Crodacol S 95 NF" OR "Crodacol-S" OR "Dytol E-46" OR "Hainol 18 SS" OR "Hainol 18SS" OR "Hyfatol 18-95" OR "Hyfatol 18-98" OR "Kalchol 8098" OR "Kalcohl 80" OR "Kalcohl 8098" OR "Kalcohl 8099" OR "Kalcol 8098" OR "Lanol S" OR "Laurex 18" OR "Lorol 28" OR "Lorol C 18" OR "Polaax" OR "Rofamol" OR "Sipol S" OR "Siponol S" OR "Siponol SC" OR "Tego alkanol 18" OR "VLTN 6" OR "Conol 2265" OR "Hainol 22 S" OR "Hainol 22S" OR "Kalcohl 22080" OR "Kalcol 22080" OR "Lidavol" OR "Nacol 22-97" OR "Nacol 22-98" OR "Stenol 1822" OR "Stenol 1822A" OR "Toho BH 65" OR "Icosan-1-ol" OR "icosane-1-ol" OR "n-1-Eicosanol" OR "n-Eicosyl alcohol" OR "Pri-N-eicosyl alcohol" OR "Hainol 20 SS" OR "Hainol 20SS" OR "cis-Octadecen-1-ol" OR "cis-Delta9-Octadecenol" OR "HD oleyl alcohol 70/75" OR "HD oleyl alcohol 80/85" OR "HD oleyl alcohol 90/95" OR "HD oleyl alcohol CG" OR "Octadeca-9-cis-en-1-ol" OR "(Z)-9-Octadecenol" OR "9-Octadecen-1-ol, (9Z)-" OR "Atalco O" OR "Cachalot O 1" OR "Cachalot O-1" OR "Cachalot O-15" OR "Cachalot O-3" OR "Cachalot O-8" OR "Crodacol A.10" OR "Crodacol O" OR "Crodacol-O" OR "Dermaffine" OR "H.D. eutanol" OR "HD-Eutanol" OR "HD-Ocenol 90/95" OR "HD-Ocenol 92/96" OR "HD-Ocenol K" OR "Lanette 18DEO" OR "Lancol" OR "Loxanol 95" OR "Loxanol M" OR "Ocenol" OR "Ocenol 90/95" OR "Oceol" OR "Rikacol 90BHR" OR "Satol" OR "Sipol O" OR "Siponol OC" OR "Unjecol 110" OR "Unjecol 50" OR "Unjecol 70" OR "Unjecol 70N" OR "Unjecol 90" OR "Unjecol 90BHR" OR "Unjecol 90N" OR "Unjecol 90NR" OR "Vegecol 90B" OR "Witcohol 85NF" OR "Witcohol 90" OR "Witcohol 90NF") ABSTRACT=("Alcohol stearylicus" OR "n-1-Octadecanol" OR "Steraffine" OR "USP XIII stearyl alcohol" OR "Atalco S" OR "Alfol 18" OR "Alfol 18NF" OR "Cachalot S 43" OR "Cachalot S-43" OR "Conol 1675" OR "Conol 30F" OR "Conol 30S" OR "Conol 30SS" OR "Crodacol S" OR "Crodacol S 70" OR "Crodacol S 95" OR "Crodacol S 95 NF" OR "Crodacol-S" OR "Dytol E-46" OR "Hainol 18 SS" OR "Hainol 18SS" OR "Hyfatol 18-95" OR "Hyfatol 18-98" OR "Kalchol 8098" OR "Kalcohl 80" OR "Kalcohl 8098" OR "Kalcohl 8099" OR "Kalcol 8098" OR "Lanol S" OR "Laurex 18" OR "Lorol 28" OR "Lorol C 18" OR "Polaax" OR "Rofamol" OR "Sipol S" OR "Siponol S" OR "Siponol SC" OR "Tego alkanol 18" OR "VLTN 6" OR "Conol 2265" OR "Hainol 22 S" OR "Hainol 22S" OR "Kalcohl 22080" OR "Kalcol 22080" OR "Lidavol" OR "Nacol 22-97" OR "Nacol 22-98" OR "Stenol 1822" OR "Stenol 1822A" OR "Toho BH 65" OR "Icosan-1-ol" OR "icosane-1-ol" OR "n-1-Eicosanol" OR "n-Eicosyl alcohol" OR "Pri-N-eicosyl alcohol" OR "Hainol 20 SS" OR "Hainol 20SS" OR "cis-Octadecen-1-ol" OR "cis-Delta9-Octadecenol" OR "HD oleyl alcohol 70/75" OR "HD oleyl alcohol 80/85" OR "HD oleyl alcohol 90/95" OR "HD oleyl alcohol CG" OR "Octadeca-9-cis-en-1-ol" OR "(Z)-9-Octadecenol" OR "9-Octadecen-1-ol, (9Z)-" OR "Atalco O" OR "Cachalot O 1" OR "Cachalot O-1" OR "Cachalot O-15" OR "Cachalot O-3" OR "Cachalot O-8" OR "Crodacol A.10" OR "Crodacol O" OR "Crodacol-O" OR "Dermaffine" OR "H.D. eutanol" OR "HD-Eutanol" OR "HD-Ocenol 90/95" OR "HD-Ocenol 92/96" OR "HD-Ocenol K" OR "Lanette 18DEO" OR "Lancol" OR "Loxanol 95" OR "Loxanol M" OR "Ocenol" OR "Ocenol 90/95" OR "Oceol" OR "Rikacol 90BHR" OR "Satol" OR "Sipol O" OR "Siponol OC" OR "Unjecol 110" OR "Unjecol 50" OR "Unjecol 70" OR "Unjecol 70N" OR "Unjecol 90" OR "Unjecol 90BHR" OR "Unjecol 90N" OR "Unjecol 90NR" OR "Vegecol 90B" OR "Witcohol 85NF" OR "Witcohol 90" OR "Witcohol 90NF") SUBJECT=("Alcohol stearylicus" OR "n-1-Octadecanol" OR "Steraffine" OR "USP XIII stearyl alcohol" OR "Atalco S" OR "Alfol 18" OR "Alfol 18NF" OR "Cachalot S 43" OR "Cachalot S-43" OR "Conol 1675" OR "Conol 30F" OR "Conol 30S" OR "Conol 30SS" OR "Crodacol S" OR "Crodacol S 70" OR "Crodacol S 95" OR "Crodacol S 95 NF" OR "Crodacol-S" OR "Dytol E-46" OR "Hainol 18 SS" OR "Hainol 18SS" OR "Hyfatol 18-95" OR "Hyfatol 18-98" OR "Kalchol 8098" OR "Kalcohl 80" OR "Kalcohl

Table C.2: Search Terms Used in Peer Reviewed Databases		
Discipline	**Database**	**Search terms[58]**
		8098" OR "Kalcohl 8099" OR "Kalcol 8098" OR "Lanol S" OR "Laurex 18" OR "Lorol 28" OR "Lorol C 18" OR "Polaax" OR "Rofamol" OR "Sipol S" OR "Siponol S" OR "Siponol SC" OR "Tego alkanol 18" OR "VLTN 6" OR "Conol 2265" OR "Hainol 22 S" OR "Hainol 22S" OR "Kalcohl 22080" OR "Kalcol 22080" OR "Lidavol" OR "Nacol 22-97" OR "Nacol 22-98" OR "Stenol 1822" OR "Stenol 1822A" OR "Toho BH 65" OR "Icosan-1-ol" OR "icosane-1-ol" OR "n-1-Eicosanol" OR "n-Eicosyl alcohol" OR "Pri-N-eicosyl alcohol" OR "Hainol 20 SS" OR "Hainol 20SS" OR "cis-Octadecen-1-ol" OR "cis-Delta9-Octadecenol" OR "HD oleyl alcohol 70/75" OR "HD oleyl alcohol 80/85" OR "HD oleyl alcohol 90/95" OR "HD oleyl alcohol CG" OR "Octadeca-9-cis-en-1-ol" OR "(Z)-9-Octadecenol" OR "9-Octadecen-1-ol, (9Z)-" OR "Atalco O" OR "Cachalot O 1" OR "Cachalot O-1" OR "Cachalot O-15" OR "Cachalot O-3" OR "Cachalot O-8" OR "Crodacol A.10" OR "Crodacol O" OR "Crodacol-O" OR "Dermaffine" OR "H.D. eutanol" OR "HD-Eutanol" OR "HD-Ocenol 90/95" OR "HD-Ocenol 92/96" OR "HD-Ocenol K" OR "Lanette 18DEO" OR "Lancol" OR "Loxanol 95" OR "Loxanol M" OR "Ocenol" OR "Ocenol 90/95" OR "Oceol" OR "Rikacol 90BHR" OR "Satol" OR "Sipol O" OR "Siponol OC" OR "Unjecol 110" OR "Unjecol 50" OR "Unjecol 70" OR "Unjecol 70N" OR "Unjecol 90" OR "Unjecol 90BHR" OR "Unjecol 90N" OR "Unjecol 90NR" OR "Vegecol 90B" OR "Witcohol 85NF" OR "Witcohol 90" OR "Witcohol 90NF")
Fate	WOS	TS=("112-92-5" OR "1-Octadecanol" OR "Alcohol(C18)" OR "C18 alcohol" OR "n-Octadecanol" OR "Octadecan-1-ol" OR "octadecane-1-ol" OR "Octadecanol" OR "Octadecyl alcohol" OR "Stearic alcohol" OR "Stearol" OR "Stearyl alcohol" OR "Stenol" OR "661-19-8" OR "30303-65-2" OR "1-Docosanol" OR "Behenic alcohol" OR "Behenyl 80 Alcohol" OR "Behenyl alcohol" OR "Docosan-1-ol" OR "docosane-1-ol" OR "Docosanol" OR "Docosyl alcohol" OR "n-Docosanol" OR "Abreva" OR "IK 2" OR "IK.2" OR "Tadenan" OR "629-96-9" OR "1-Eicosanol" OR "Arachidyl alcohol" OR "Eicosan-1-ol" OR "Eicosanol" OR "Icosanol" OR "n-Eicosanol" OR "143-28-2" OR "593-47-5" OR "(Z)-9-Octadecen-1-ol" OR "(Z)-Octadec-9-enol" OR "9-cis-Octadecenol" OR "9-Octadecen-1-ol" OR "9-Octadecenol" OR "Adol 85" OR "cis-9-Octadecen-1-ol" OR "cis-9-Octadecenyl alcohol" OR "Octadecenol" OR "Oleic alcohol" OR "Oleol" OR "Oleoyl alcohol" OR "Oleyl alcohol" OR "Adol 85NF" OR "Arachic alcohol" OR "Decyl octyl alcohol" OR "Eicosyl alcohol" OR "Icosan-1-ol" OR "Ocenol" OR "Satol" OR "Witcohol 85") AND TS=(adsorp* OR aerob* OR anaerob* OR bioaccumulat* OR bioavail* OR bioconcentrat* OR biodegrad* OR biomoni* OR biotrans* OR degrad* OR dispers* OR fish* OR hydroly* leach* OR migrat* OR partic* OR partition* OR persisten* OR photoly* OR volatil* OR abiotic OR absorb OR absorption OR accumulation-rate OR aerosol OR aerosols OR air OR anoxic OR atm-m3/mol OR biomagnification OR biosolids OR biota OR breakdown-product OR breakdown-products OR chelation OR coagulation complexation OR decay-rate OR diffusion-coefficient OR dissolution OR dust OR effluent OR environmental-fate OR evaporation-from-water OR excretion OR flocculation OR flux OR fugacity OR gas-phase-mass-transfer OR ground-water OR groundwater OR half-life OR henry's-law OR incinerate OR incineration OR indoor-outdoor-ratio OR influent OR ingestion OR intake OR kinetics OR liquid-phase-mass-transfer OR mass-transfer-coefficient OR microcosm OR modified-state-space OR particle-size OR particulate OR pathway OR pathways OR penetration-factor OR penetration-ratio OR photostability OR placenta OR plasma OR plume OR point-source OR point-sources OR pore-water OR pretreatment-program OR redox OR sediment OR serum OR sewage-treatment OR sludge OR soil OR subsurface-intrusion OR surface-water-concentration OR time-weighted-average OR transfer OR transformation OR trophic-magnification OR vapor OR wait-time OR wastewater-treatment OR weight-fraction OR wildlife OR BAF OR BCF OR BSAF OR BSAFs OR KAW OR Kd OR KOA OR KOC OR POTW OR SES OR WWTP OR ((OECD OR OPPTS OR OCSPP) AND (Guideline OR guidelines))) Indexes=SCI-EXPANDED, CPCI-S, CPCI-SSH, BKCI-S, BKCI-SSH, CCR-EXPANDED, IC Timespan=All years

Table C.3: Search Terms Used in Grey Literature and Additional Sources	
Chemical	**Search terms**
Fatty alcohol cluster (1-Octadecanol; 1-Docosanol; 1-Eicosanol)	Searched as a string or individually depending on source: "112-92-5" OR "1-Octadecanol" OR "Alcohol(C18)" OR "C18 alcohol" OR "n-Octadecanol" OR "Octadecan-1-ol" OR "octadecane-1-ol" OR "Octadecanol" OR "Octadecyl alcohol" OR "Stearic alcohol" OR "Stearol" OR "Stearyl alcohol" OR "Stenol" OR "1-Hydroxyoctadecane" OR "Decyl octyl alcohol" OR "Fatty alcohol(C18)" "661-19-8" OR "30303-65-2" OR "1-Docosanol" OR "Behenic alcohol" OR "Behenyl 80 Alcohol" OR "Behenyl alcohol" OR "Docosan-1-ol" OR "docosane-1-ol" OR "Docosanol" OR "Docosyl alcohol" OR "n-Docosanol" OR "Abreva" OR "IK 2" OR "IK.2" OR "Tadenan" "629-96-9" OR "1-Eicosanol" OR "Arachidyl alcohol" OR "Eicosan-1-ol" OR "Eicosanol" OR "Icosanol" OR "n-Eicosanol" OR "Eicosyl alcohol" OR "Icosan-1-ol" "143-28-2" OR "593-47-5" OR "(Z)-9-Octadecen-1-ol" OR "(Z)-Octadec-9-enol" OR "9-cis-Octadecenol" OR "9-Octadecen-1-ol" OR "9-Octadecenol" OR "Adol 85" OR "cis-9-Octadecen-1-ol" OR "cis-9-Octadecenyl alcohol" OR "Octadecenol" OR "Oleic alcohol" OR "Oleol" OR "Oleoyl alcohol" OR "Oleyl alcohol"
Analogs searched	alcohols, C16-18 (CASRN 67762-27-0); cetyl alcohol (CASRN 36653-82-4); alcohols, C16-18 and C-18 unsatd. (CASRN 68002-94-8)

After the search terms were applied, more than 2,700 references were returned by all search efforts across peer-reviewed databases and grey literature sources. The total number of references include database results, additional strategies, and analog searches for the fatty alcohol cluster including 1-Docosanol. All references from the search efforts were screened and evaluated through the LPS literature search and review process.[56] Of these, 48 references were included for data evaluation and used to support the designation of 1-docosanol as LPS. The included hazard and fate references are listed in the bibliography of Appendix B.

C.2 Excluded Studies and Rationale

This section lists the excluded references, by HERO ID, found to be off-topic or unacceptable for use in the hazard screening of 1-docosanol. The excluded references are organized by discipline (human health hazard, environmental hazard, and fate), presented along with a rationale based on exclusion criteria. The criteria[56] was used to determine off-topic references in the title/abstract or full text screening and to determine unacceptable references in the data quality evaluation are provided in the form of questions.

C.2.1 Human Health Hazard Excluded References

For the screening review of 1-docosanol, EPA excluded a total of 2163 references when assessing human health hazard. Off-topic references (e.g., studies that did not contain information relevant to human health) were excluded at either title/abstract screening (see Table C.4), or full-text screening (see Table C.5). Unacceptable references (e.g., studies that did not meet data quality metrics) were excluded at full-text screening (see Tables C.6 and C.7). Off-topic and unacceptable references are displayed next to the corresponding exclusion criteria.

Table C.4: Off-Topic References Excluded at Title/Abstract Screening for Human Health Hazard									
Reference excluded (HERO ID) because the reference did NOT contain information needs[59] relevant to human health hazard									
1022420	4936774	4934150	4929473	4929337	1617954	4936986	4936291	4929536	4929422
1023649	4936932	4934151	4929500	4929338	1629199	4936987	4936292	4929573	4929423
1036897	4936933	4934152	4929502	4929341	1689817	4936988	4936297	4929574	4929424
1048762	4936934	4934153	4929503	4929343	1786996	4936989	4936298	4929576	4929425
1054609	4936937	4934157	4929505	4929344	1796863	4936990	4936299	4929577	4929426
1055722	4936938	4934159	4929507	4929347	1799769	4936991	4936301	4929578	4929427
1066804	4936939	4934160	4929509	4929366	1799943	4936992	4936304	4929579	4929428
1083310	4936940	4934162	4929510	4929367	1921479	4936993	4936306	4929580	4929429
1180326	4936941	4934164	4929512	4929368	1922729	4936994	4936307	4929581	4929430
1182858	4936942	4934165	4929513	4929371	1942034	4936996	4936309	4929582	4929431
1183605	4936944	4934166	4929516	4929372	1942090	4936998	4936311	4929583	4929432
1184441	4936945	4934167	4929518	4929373	2013215	4936999	4936312	4929586	4929433
1201393	4936946	4934168	4929519	4929375	2052484	4937312	4936315	4929587	4929453
1298180	4936947	4934170	4929520	4929376	2114411	4937317	4936316	4929589	4929455
1314409	4936948	4934171	4929522	4929378	2114490	4937334	4936317	4929590	4929456
1332580	4936950	4934172	4929523	4929379	2115523	4937372	4936321	4929593	4929457
1333586	4936952	4934193	4929524	4929380	2142633	4940070	4936322	4929594	4929460
1335600	4936953	4934194	4929525	4929381	218703	4940374	4936324	4929595	4929461
1335601	4936955	4934195	4929527	4929382	2198513	4940381	4936325	4929597	4929462
1454877	4936977	4934197	4929529	4929415	2239576	4940417	4936327	4929598	4929463
1535286	4936978	4936279	4929530	4929416	2241165	4940470	4936328	4929599	4929464
1609897	4936979	4936282	4929531	4929417	2279749	4940481	4936329	4929600	4929465
1610348	4936981	4936283	4929532	4929418	2553466	4940529	4936330	4929602	4929466
1615034	4936982	4936285	4929533	4929419	2582663	4940580	4936331	4929603	4929467
1615229	4936984	4936289	4929534	4929420	2592724	4940594	4936332	4929604	4929468
1616488	4936985	4936290	4929535	4929421	2598412	4940647	4936335	4929605	4929469
4229640	4943454	4936421	4930662	4934104	2630975	4940681	4936336	4929606	4929471
4307605	4943484	4936424	4931196	4934106	2676957	4940685	4936337	4929607	4929472
4360860	4943496	4936425	4931197	4934107	2736581	4940742	4936342	4929609	4936523
4407501	4943511	4936426	4931198	4934110	2751190	4940747	4936343	4929611	4936524

[59] The information needs for human health hazard includes a list of study characteristics pertaining to the study population/test organism, types of exposures and routes, use of controls, type and level of effects. A complete list of the information needs is provided in Table A1 of the "Approach Document for Screening Hazard Information for Low-Priority Substances Under TSCA". These information needs helped guide the development of questions for title/abstract and full-text screening.

Table C.4: Off-Topic References Excluded at Title/Abstract Screening for Human Health Hazard									
4415125	4943518	4936427	4931199	4934111	2778777	4940787	4936344	4929612	4936526
4657051	4943598	4936428	4931200	4934112	2778903	4940812	4936345	4929614	4936528
4683785	4943603	4936429	4931201	4934113	2792512	4941754	4936346	4929615	4936529
4702660	4943606	4936430	4931202	4934114	2850268	4941773	4936347	4929616	4936530
4702949	4943610	4936431	4931203	4934115	2850717	4941805	4936348	4929617	4936532
4703541	4943637	4936432	4931735	4934117	2861607	4941851	4936350	4929618	4936533
4704266	4943666	4936434	4931835	4934119	2886973	4941853	4936352	4929619	4936534
4754296	4943687	4936437	4932655	4934121	2902056	4941863	4936353	4929620	4936535
4755704	4943690	4936438	4932656	4934122	2960467	4941903	4936354	4929622	4936537
4824314	4943830	4936439	4932658	4934123	2997327	4941910	4936355	4929624	4936538
4837527	4943831	4936440	4932660	4934124	3006582	4941933	4936356	4929625	4936539
4837631	4943993	4936442	4932663	4934149	3036421	4941942	4936357	4929627	4936540
4854956	4944012	4936443	4932667	4936501	3036831	4941953	4936358	4929628	4936541
4861399	4944044	4936444	4932668	4936502	3037540	4941954	4936359	4929629	4936544
4862450	4944047	4936447	4932669	4936504	3037597	4941955	4936360	4929630	4936618
4864847	4944080	4936448	4932673	4936505	3038125	4941964	4936362	4929632	4936635
4867770	4944097	4936449	4932674	4936508	3038131	4941965	4936363	4929633	4936643
4885573	4944184	4936450	4932675	4936510	3038686	4941975	4936364	4929634	4936719
4923332	4944189	4936451	4932679	4936514	3038849	4941976	4936365	4929635	4936733
4929232	4944247	4936453	4932684	4936515	3039428	4942009	4936366	4929637	4936737
4929233	4944248	4936455	4932692	4936516	3039460	4942011	4936367	4929638	4936752
4929234	4944254	4936456	4932693	4936518	3039499	4942017	4936369	4929639	4929281
4929236	4944264	4936457	4932694	4936520	3039606	4942021	4936370	4929641	4929282
4929238	4944289	4936458	4932698	4936521	3039656	4942070	4936371	4929642	4929284
4929239	4944309	4936463	4934038	4936522	3040053	4942179	4936373	4929643	4929285
4929240	4944342	4936464	4934039	4929274	3040498	4942209	4936375	4929644	4929286
4929241	4944375	4936467	4934041	4929275	3041004	4942245	4936376	4929646	4929287
4929243	4944388	4936468	4934042	4929276	3041038	4942401	4936378	4929647	4929288
4929244	4944395	4936470	4934043	4929277	3041115	4942465	4936381	4929651	4929289
4929245	4944412	4936472	4934044	4929278	3046658	4942474	4936383	4929653	4929290
4929247	4944423	4936474	4934046	4929279	3047306	4942478	4936384	4929654	4929291
4929248	4944425	4936475	4934048	4929280	3047450	4942481	4936386	4929655	4929314
4929249	4944494	4936477	4934049	4934085	3060406	4942488	4936389	4930607	4929315
4929250	4944528	4936478	4934051	4934088	3120107	4942500	4936390	4930608	4929316

Table C.4: Off-Topic References Excluded at Title/Abstract Screening for Human Health Hazard									
4929251	4944562	4936481	4934052	4934090	3153771	4942677	4936394	4930609	4929317
4929254	4944567	4936482	4934053	4934091	3220885	4942740	4936395	4930611	4929318
4929255	4944634	4936483	4934057	4934080	3270232	4942806	4936396	4930613	4929320
4929256	4944653	4936484	4934059	4934081	3329064	4942896	4936397	4930614	4929321
4929257	4949200	4936485	4934060	4934084	3347947	4943090	4936398	4930616	4929322
4929258	495881	4936486	4934063	4936497	3360098	4943094	4936399	4930617	4929324
4929259	615565	4936488	4934064	4936499	3489777	4943105	4936400	4930620	4929325
4929260	658179	4936489	4934065	4936500	3539765	4943173	4936401	4930622	4929326
4929261	659153	4936490	4934066	698371	3539879	4943205	4936404	4930623	4929327
4929262	662088	4936492	4934070	791097	3605567	4943212	4936406	4930624	4929328
4929265	662407	4936493	4934072	846220	3716876	4943244	4936407	4930626	4929329
4929266	669806	4936494	4934075	4929270	3769616	4943252	4936408	4930627	4929330
4929267	673420	4936495	4934076	4929271	3784853	4943259	4936409	4930628	4929331
4929269	697436	4936496	4934077	4929273	3817669	4943373	4936410	4930629	4929332
4080833	4943430	4936418	4930655	4934101	3846363	4943419	4936413	4930651	4929333
4146230	4943436	4936419	4930657	4934102	3859469	4943424	4936414	4930652	4929334
4220986	4943444	4936420	4930660	4934103	3859486	4943426	4936415	4930653	4934092
4080205	4943428	4936416	4930654	4934097					
Reference excluded (HERO ID) because the reference primarily contained *in silico* data									
1580276	4929640								

Table C.5: Screening Questions and Off-Topic References Excluded at Full Text Screening for Human Health Hazard		
Question	**Off-topic if answer is:**	**References excluded (HERO ID)**
Does the reference contain information pertaining to a low- priority substance candidate?	No	4949221 660848 1333463 1580238 1815447 3039801 4929246 4934082 4936487 4940326 4940347

Table C.5: Screening Questions and Off-Topic References Excluded at Full Text Screening for Human Health Hazard		
Question	**Off-topic if answer is:**	**References excluded (HERO ID)**
		4942963 1320113 2143371 3039802 3041821 4929335 4929458 4929636 4934093 4934095 4936295 4936338 4936392 4936935 4936951 4936956 4940327 4941960 4942074 4944059 4949204 4949218 4949229 4962993 4963012 4963038 4949225 1976706 4929237 4929283 4932648 4932654 4932657 4934067 4934118

Table C.5: Screening Questions and Off-Topic References Excluded at Full Text Screening for Human Health Hazard		
Question	**Off-topic if answer is:**	**References excluded (HERO ID)**
		4934154 4934161 4934198 4936310 4940935 4941653 4942034 4942038 4942469 4943035 4943918 4945110 4945111 4945112
What type of source is this reference?	Review article or book chapter that contains only citations to primary literature sources	4949221 660848 1333463 1580238 1815447 3039801 4929246 4934082 4936487 4940326 4940347 4942963
What kind of evidence does this reference primarily contain?	*In silico* studies that DO NOT contain experimental verification	
The following question apply to HUMAN evidence only		
Does the reference report an exposure route that is or is presumed to be by an inhalation, oral, or dermal route?	No	4929283 4929526 4930618
Does the reference report both test substance exposure(s) AND related health outcome(s)?	No	4929283

Table C.5: Screening Questions and Off-Topic References Excluded at Full Text Screening for Human Health Hazard		
Question	**Off-topic if answer is:**	**References excluded (HERO ID)**
If the reference reports an exposure to a chemical mixture, are measures of the test substance or related metabolite(s) reported independently of other chemicals?	No	4944301
Note: If the paper does not pertain to mixtures, choose "Not Applicable".	No	N/A.
The following question apply to ANIMAL evidence only		
Does the reference report an exposure route that is by inhalation, oral, or dermal route?	No	4963003 4963007 4963008 4963007 4963008 32772 4929621 4930658 4932652
Does the reference report both test substance-related exposure(s) AND related health outcome(s)?	No	4963007 4963008 4929621 4949218 1616835 4929506
Does the reference report the duration of exposure?	No	4963007 4963008 4934118 4949225 4949226
Does the reference report an exposure to the test substance only (i.e. no mixtures with the exception of aqueous solutions and reasonable impurities and byproducts)?	No	4963007 4963008 4949225 1621193 1629232 2744702 3037827

Table C.5: Screening Questions and Off-Topic References Excluded at Full Text Screening for Human Health Hazard		
Question	**Off-topic if answer is:**	**References excluded (HERO ID)**
		4942469 4943827 4962997 4963009 4963038 4930658
Does the paper report a negative control that is a vehicle control or no treatment control?	No[60]	4963007 4963008 4949225 2744702 3037827 4942469 4930658 4949226 4929621 4949218 4932652 4963003
The following questions apply to MECHANISTIC/ALTERNATIVE TEST METHODS evidence only		
Does the reference report a negative control that is a vehicle control or no treatment control?	No	4949226
Does the reference report an exposure to the test substance only (i.e. no mixtures with the exception of aqueous solutions and reasonable impurities and byproducts)?	No	1617542 2232626 4934067
For genotoxicity studies only: Does the study use a positive control?	No	4949226

[60] Except for acute mammalian toxicity and skin and eye irritation studies, where the use of a negative control may not be required (e.g., OECD 403 Acute Inhalation Toxicity Guidelines).

Table C.6: Data Quality Metrics and Unacceptable References Excluded at Data Quality Evaluation for Human Health Hazard – Animal		
Data Quality Metric	**Unacceptable if:**	**References excluded (HERO ID)**
Metric 1: Test Substance Identity	• The test substance identity cannot be determined from the information provided (e.g., nomenclature was unclear and CASRN or structure were not reported). **OR** • For mixtures, the components and ratios were not characterized or did not include information that could result in a reasonable approximation of components.	4963010 58939
Metric 2: Negative and Vehicle Controls	A concurrent negative control group was not included or reported. **OR** The reported negative control group was not appropriate (e.g., age/weight of animals differed between control and treated groups).	4962996 4963006
Metric 3: Positive Controls	When applicable, an appropriate concurrent positive control (i.e., inducing a positive response) was not used.	N/A.
Metric 4: Reporting of Doses/Concentrations	Doses/concentrations were not reported and could not be calculated using default or reported estimates of body weight and diet/water intake (e.g., default intake values are not available for pregnant animals).	2454784 4930615 4936314 4962994 4962995 4963042 58939
Metric 5: Exposure Duration	The duration of exposure was not reported. **OR** The reported exposure duration was not suited to the study type and/or outcome(s) of interest (e.g., <28 days for repeat dose).	2454784 4930615 4936314 4936469 4963006 58939
Metric 6: Test Animal Characteristics	The test animal species was not reported. **OR** The test animal (species, strain, sex, life-stage, source) was not appropriate for the evaluation of	4936382 4963006 58939

Table C.6: Data Quality Metrics and Unacceptable References Excluded at Data Quality Evaluation for Human Health Hazard – Animal		
Data Quality Metric	**Unacceptable if:**	**References excluded (HERO ID)**
	the specific outcome(s) of interest (e.g., genetically modified animals, strain was uniquely susceptible or resistant to one or more outcome of interest).	
Metric 7: Number of Animals Per Group	The number of animals per study group was not reported. **OR** The number of animals per study group was insufficient to characterize toxicological effects (e.g., 1-2 animals in each group).	4963000 4963001 58939
Metric 8: Outcome Assessment Methodology	The outcome assessment methodology was not sensitive for the outcome(s) of interest (e.g., evaluation of endpoints outside the critical window of development, a systemic toxicity study that evaluated only grossly observable endpoints, such as clinical signs and mortality, etc.).	4930615 4936314 4936469
Metric 9: Reporting of Data	Data presentation was inadequate (e.g., the report does not differentiate among findings in multiple exposure groups). **OR** Major inconsistencies were present in reporting of results.	4930615 4962995 4963006 58939 4929652

Table C.7: Data Quality Metrics and Unacceptable References Excluded at Data Quality Evaluation for Human Health Hazard – In Vitro		
Data Quality Metric	**Unacceptable if:**	**References excluded (HERO ID)**
Metric 1: Test Substance Identity	The test substance identity or description cannot be determined from the information provided (e.g., nomenclature was unclear and CASRN or structure were not reported). **OR** For mixtures, the components and ratios were not characterized or did not include information that could result in a reasonable approximation of components.	N/A.

Table C.7: Data Quality Metrics and Unacceptable References Excluded at Data Quality Evaluation for Human Health Hazard – In Vitro		
Data Quality Metric	**Unacceptable if:**	**References excluded (HERO ID)**
Metric 2: Negative Controls	A concurrent negative control group was not included or reported. **OR** The reported negative control group was not appropriate (e.g., different cell lines used for controls and test substance exposure).	N/A.
Metric 3: Positive Controls	A concurrent positive control or proficiency group was not used.	N/A.
Metric 4: Assay Type	The assay type was not reported. **OR** The assay type was not appropriate for the study type or outcome of interest (e.g., *in vitro* skin corrosion protocol used for *in vitro* skin irritation assay).	N/A.
Metric 5: Reporting of Concentration	The exposure doses/concentrations or amounts of test substance were not reported.	N/A.
Metric 6: Exposure Duration	No information on exposure duration(s) was reported. **OR** The exposure duration was not appropriate for the study type and/or outcome of interest (e.g., 24 hours exposure for bacterial reverse mutation test).	4963005 4963043
Metric 7: Metabolic Activation	No information on the characterization and use of a metabolic activation system was reported. **OR** The exposure duration was not appropriate for the study type and/or outcome of interest (e.g., 24 hours exposure for bacterial reverse mutation test).	N/A.
Metric 8: Test Model	The test model was not reported **OR** The test model was not routinely used for evaluation of the specific outcome of interest.	N/A.

Table C.7: Data Quality Metrics and Unacceptable References Excluded at Data Quality Evaluation for Human Health Hazard – In Vitro		
Data Quality Metric	**Unacceptable if:**	**References excluded (HERO ID)**
Metric 9: Outcome Assessment Methodology	The outcome assessment methodology was not reported. **OR** The assessment methodology was not appropriate for the outcome(s) of interest (e.g., cells were evaluated for chromosomal aberrations immediately after exposure to the test substance instead of after post-exposure incubation period).	N/A.

C.2.2 Environmental Hazard

For the screening review of LPS candidate 1-docosanol EPA excluded a total of 1815 references when assessing environmental hazard. Off-topic environmental hazard references excluded at title/abstract screening are listed in Table C.8, and those excluded at full-text screening are listed in Table C.9. References in Table C.10 represent unacceptable studies based on specific data quality metrics for environmental hazard. Off-topic and unacceptable references are displayed next to the corresponding exclusion criteria.

Table C.8: Off-Topic References Excluded at Title/Abstract Screening for Environmental Hazard									
Reference excluded (HERO ID) because the reference did NOT contain information needs[61] relevant to environmental hazard									
4936344	4944097	4942715	4941853	4931198	4081878	4940679	4943671	4942244	4936923
4936346	4944100	4942716	4941854	4931199	4084200	4940680	4943673	4942245	4936927
4936347	4944101	4942717	4941855	4931202	4146230	4940681	4943678	4942288	4936959
4936350	4944103	4942718	4941856	4931735	4236566	4940685	4943683	4942289	4936961
4936353	4944111	4942721	4941857	4932648	4239751	4940688	4943684	4942290	4936965
4936389	4944112	4942722	4941858	4932650	4244979	4940692	4943687	4942294	4936973
4936444	4944116	4942723	4941859	4932652	4307605	4940695	4943690	4942297	4937003
4936448	4944117	4942724	4941861	4932654	4335934	4940702	4943691	4942298	4937013
4936449	4944120	4942726	4941862	4932655	4366990	4940709	4943692	4942301	4937016
4936450	4944121	4942727	4941864	4932656	4395162	4940712	4943697	4942302	4937017
4936453	4944123	4942733	4941865	4932657	4407501	4940715	4943699	4942303	4937019
4936457	4944124	4942738	4941867	4932658	4408854	4940722	4943700	4942350	4937021

[61] The information needs for environmental hazard includes a list of study characteristics pertaining to the test organism/species, type and level of effects, and use of controls. A complete list of the information needs is provided in Table A2 of the "Approach Document for Screening Hazard Information for Low-Priority Substances Under TSCA". These information needs helped guide the development of questions for title/abstract and full-text screening.

Table C.8: Off-Topic References Excluded at Title/Abstract Screening for Environmental Hazard									
4936458	4944125	4942745	4941890	4932660	4415125	4940724	4943703	4942351	4937030
4936464	4944126	4942751	4941893	4932661	4428588	4940729	4943704	4942354	4937038
4936467	4944129	4942753	4941894	4932663	4433785	4940730	4943707	4942355	4937040
4936468	4944130	4942777	4941895	4932666	4559854	4940732	4943708	4942356	4937047
4936932	4944131	4942778	4941896	4932667	4567128	4940741	4943709	4942358	4937073
4936933	4944135	4942779	4941897	4932668	4585086	4940742	4943710	4942359	4937074
4936934	4944137	4942782	4941898	4932669	4657051	4940747	4943713	4942360	4937081
4936938	4944138	4942783	4941899	4932673	4658174	4940754	4943714	4942361	4937087
4936939	4944142	4942785	4941900	4932674	4660710	4940759	4943715	4942362	4937098
4936940	4944143	4942800	4941901	4932675	4699816	4940762	4943717	4942363	4937106
4936941	4944169	4942801	4941902	4932679	4703541	4940767	4943718	4942364	4937109
4936942	4944170	4942802	4941903	4932680	4704266	4940770	4943721	4942365	4937112
4936944	4944173	4942806	4941904	4932682	4730460	4940772	4943723	4942367	4937187
4936945	4944175	4942807	4941905	4932684	4824309	4940773	4943725	4942391	4937188
4936946	4944177	4942808	4941906	4932691	4824314	4940781	4943726	4942392	4937190
4936947	4944179	4942810	4941907	4932692	4837527	4940782	4943759	4942393	4937197
4936948	4944184	4942811	4941908	4932693	4837631	4940784	4943762	4942394	4937205
4936950	4944186	4942813	4941909	4932694	4854956	4940787	4943766	4942395	4937207
4936952	4944189	4942842	4941914	4932698	4855089	4940788	4943795	4942396	4937214
4936953	4944190	4942843	4941915	4934038	4855197	4940791	4943798	4942397	4937221
4936978	4944196	4942845	4941916	4934039	4861399	4940794	4943799	4942399	4937234
4936979	4944197	4942850	4941918	4934041	4862450	4940795	4943800	4942400	4937267
4936982	4944198	4942851	4941919	4934042	4864847	4940798	4943804	4942401	4937272
4936985	4944203	4942854	4941920	4934043	4866029	4940799	4943805	4942403	4937278
4936986	4944204	4942855	4941922	4934044	4867770	4940800	4943807	4942404	4937283
4936987	4944205	4942856	4941923	4934046	4873855	4940801	4943808	4942405	4937294
4936990	4944206	4942858	4941925	4934049	4875163	4940802	4943812	4942406	4937299
4936991	4944209	4942861	4941927	4934050	4883397	4940806	4943815	4942410	4937300
4936993	4944238	4942862	4941928	4934051	4885804	4940812	4943816	4942411	4937301
4936996	4944242	4942863	4941929	4934052	4929232	4940814	4943819	4942412	4937302
4936998	4944243	4942864	4941930	4934053	4929234	4940817	4943820	4942413	4937303
4937334	4944245	4942866	4941931	4934057	4929251	4940821	4943822	4942463	4937304
4937372	4944246	4942867	4941932	4934059	4929254	4940826	4943827	4942464	4937305
4940070	4944247	4942869	4941934	4934060	4929255	4940828	4943830	4942465	4937306

Table C.8: Off-Topic References Excluded at Title/Abstract Screening for Environmental Hazard									
4941863	4944248	4942872	4941936	4934063	4929256	4940834	4943831	4942466	4937309
4941910	4944252	4942896	4941937	4934064	4929261	4940835	4943838	4942467	4937310
4941933	4944253	4942922	4941938	4934065	4929265	4940842	4943841	4942468	4937311
4941942	4944254	4942929	4941940	4934066	4929266	4940849	4943842	4942469	4937312
4941954	4944255	4942956	4941941	4934067	4929269	4940863	4943845	4942470	4937313
4941955	4944257	4942957	4941943	4934072	4929274	4940871	4943849	4942471	4937314
4941964	4944259	4942960	4941945	4934075	4929275	4940875	4943852	4942472	4937315
4941965	4944260	4942961	4941946	4934076	4929276	4940877	4943853	4942474	4937316
4941975	4944264	4942963	4941947	4934077	4929277	4940879	4943854	4942476	4937317
4941976	4944268	4942966	4941948	4934080	4929281	4940884	4943888	4942478	4937318
4942009	4944275	4942967	4941949	4934081	4929282	4940885	4943891	4942483	4937319
4942011	4944277	4942968	4941950	4934082	4929284	4940886	4943893	4942484	4937320
4942017	4944279	4942969	4941951	4934083	4929289	4940893	4943894	4942485	4937321
4942021	4944281	4942972	4941953	4934084	4929315	4940895	4943896	4942486	4937322
4942070	4944289	4942979	4941956	4934085	4929317	4940935	4943901	4942487	4937323
4942179	4944295	4942980	4941957	4934088	4929321	4941653	4943902	4942488	4937324
4942209	4944296	4942982	4941958	4934090	4929322	4941661	4943903	4942489	4937325
4942481	4944301	4942983	4941959	4934091	4929326	4941663	4943905	4942490	4937326
4942740	4944303	4942984	4941961	4934092	4929340	4941665	4943906	4942491	4937327
4943090	4944304	4942987	4941962	4934093	4929341	4941667	4943908	4942492	4937328
4943105	4944306	4942988	4941963	4934094	4929343	4941677	4943910	4942493	4937329
4936446	4944307	4942993	4941966	4934097	4929347	4941691	4943912	4942494	4937330
4936935	4944308	4942996	4941967	4934099	4929366	4941717	4943918	4942495	4937331
4936951	4944309	4942997	4941969	4934101	4929367	4941718	4943921	4942498	4937332
4936956	4944310	4943002	4941970	4934102	4929373	4941719	4943968	4942499	4937333
4940069	4944314	4943005	4941971	4934103	4929375	4941720	4943969	4942500	4937336
4941960	4944315	4943006	4941972	4934104	4929376	4941723	4943973	4942501	4937337
4942038	4944316	4943008	4941974	4934106	4929382	4941727	4943980	4942552	4937338
4942074	4944317	4943009	4942001	4934107	4929418	4941741	4943983	4942553	4937339
4943035	4944319	4943012	4942002	4934108	4929422	4941749	4943992	4942554	4937341
32772	4944320	4943013	4942003	4934110	4929427	4941750	4943993	4942555	4937342
34905	4944321	4943014	4942004	4934111	4929431	4941752	4943994	4942556	4937343
34906	4944322	4943025	4942005	4934112	4929462	4941753	4943995	4942559	4937344
59200	4944325	4943026	4942006	4934113	4929467	4941754	4944000	4942560	4937347

Table C.8: Off-Topic References Excluded at Title/Abstract Screening for Environmental Hazard									
194837	4944326	4943027	4942007	4934114	4929473	4941755	4944001	4942562	4937348
495881	4944327	4943028	4942008	4934115	4929502	4941756	4944003	4942563	4937349
513717	4944329	4943029	4942010	4934117	4929503	4941758	4944004	4942564	4937350
613226	4944331	4943031	4942012	4934118	4929506	4941764	4944005	4942566	4937352
658179	4944332	4943032	4942013	4934119	4929508	4941765	4944006	4942568	4937353
660848	4944334	4943033	4942014	4934121	4929510	4941767	4944009	4942569	4937354
662407	4944335	4943034	4942015	4934122	4929516	4941768	4944012	4942573	4937356
664147	4944342	4943036	4942018	4934123	4929518	4941769	4944013	4942599	4937357
669806	4944344	4943042	4942019	4934124	4929519	4941770	4944015	4942600	4937358
673420	4944345	4943060	4942020	4934149	4929528	4941773	4944019	4942601	4937359
688977	4944348	4943063	4942022	4934150	4929533	4941777	4944025	4942602	4937360
697436	4944349	4943065	4942023	4934151	4929534	4941804	4944032	4942603	4937362
698371	4944350	4943068	4942025	4934152	4929535	4941805	4944034	4942604	4937364
699391	4944351	4943069	4942027	4934153	4929573	4941806	4944035	4942606	4937365
791097	4944352	4943071	4942028	4934154	4929577	4941807	4944038	4942609	4937366
820061	4944354	4943072	4942029	4934157	4929578	4941809	4944039	4942613	4937367
1023649	4944359	4943073	4942031	4934159	4929579	4941810	4944040	4942614	4937368
1038607	4944370	4943075	4942032	4934160	4929580	4941811	4944042	4942615	4937369
1043433	4944375	4943085	4942033	4934161	4929582	4941814	4944043	4942616	4937371
1048762	4944388	4943086	4942034	4934162	4929583	4941815	4944044	4942617	4937373
1054985	4944391	4943087	4942035	4934164	4929585	4941817	4944047	4942619	4937374
1055722	4944395	4943088	4942036	4934165	4929586	4941818	4944054	4942620	4937375
1062474	4944397	4943089	4942037	4934166	4929587	4941819	4944057	4942621	4937376
1066804	4944399	4943092	4942039	4934167	4929588	4941820	4944059	4942622	4937381
1066911	4944404	4943093	4942041	4934168	4929594	4941821	4944066	4942623	4937382
1107881	4944406	4943094	4942042	4934170	4929595	4941823	4944068	4942625	4937385
1180326	4944408	4943095	4942044	4934171	4929604	4941825	4944069	4942626	4937418
1183605	4944409	4943098	4942045	4934172	4929605	4941826	4944074	4942627	4940289
1184441	4944412	4943100	4942047	4934193	4929606	4941833	4944075	4942629	4940290
1184956	4944413	4943103	4942048	4934194	4929607	4941835	4944077	4942633	4940291
1193690	4944416	4943129	4942049	4934195	4929612	4941836	4944079	4942636	4940295
1201393	4944418	4943132	4942050	4934196	4929614	4941848	4944080	4942637	4940296
1206833	4944419	4943133	4942051	4934197	4929616	4941849	4944092	4942638	4940297
1230933	4944422	4943135	4942052	4934198	4929618	4941850	4940344	4942639	4940305

Table C.8: Off-Topic References Excluded at Title/Abstract Screening for Environmental Hazard									
1232514	4944423	4943138	4942053	4936285	4929619	4941851	4940347	4942640	4940307
1293111	4944424	4943139	4942054	4936291	4929624	4941852	4940349	4942641	4940314
1311549	4944425	4943140	4942056	4936297	4929626	4942680	4940355	4942644	4940321
1313686	4944430	4943143	4942057	4936298	4929629	4942681	4940361	4942668	4940323
1314409	4944457	4943144	4942058	4936306	4929641	4942683	4940363	4942670	4940325
1332580	4944460	4943148	4942059	4936309	4929642	4942686	4940364	4942671	4940326
1333463	4944462	4943171	4942060	4936311	4929644	4942687	4930626	4942673	4940327
1333586	4944488	4943173	4942061	4936312	4929647	4942689	4930627	4942674	4940328
1335600	4944490	4943174	4942062	4936315	4929649	4942690	4930651	4942675	4940331
1335601	4944494	4943176	4942063	4936316	4930613	4930654	4930653	4942677	4940332
1342169	4944512	4943177	4942064	4936321	4930617	4931196	4942678	4940335	4940342
1445642	4944514	4943186	4942065	4936322	4930620	4931197	4942679	4942210	4936705
1447796	4944517	4943187	4942067	4936324	3044660	4940481	4943549	4942211	4936713
1452217	4944518	4943190	4942068	4936325	3046658	4940484	4943550	4942213	4936717
1454619	4944523	4943191	4942069	4936329	3047256	4940529	4943555	4942214	4936719
1454877	4944524	4943193	4942071	4936336	3047306	4940540	4943556	4942215	4936722
1462603	4944525	4943194	4942072	4936337	3060406	4940542	4943561	4942216	4936733
1463310	4944528	4943199	4942075	4936342	3120107	4940544	4943562	4942217	4936737
1509821	4944531	4943200	4942077	4936343	3220885	4940548	4943563	4942218	4936742
1522006	4944532	4943201	4942078	4936355	3457657	4940549	4943565	4942219	4936747
1580238	4944533	4943204	4942079	4936358	3479045	4940557	4943597	4942220	4936748
1580276	4944539	4943205	4942080	4936360	3480260	4940558	4943598	4942223	4936750
1609897	4944543	4943212	4942081	4936362	3481353	4940565	4943600	4942224	4936759
1610348	4944545	4943242	4942082	4936365	3491553	4940577	4943603	4942225	4936770
1615229	4944546	4943244	4942084	4936373	3539879	4940580	4943604	4942227	4936774
1616835	4944549	4943247	4942085	4936376	3586858	4940593	4943606	4942228	4936824
1617954	4944552	4943249	4942087	4936386	3586922	4940594	4943607	4942229	4936825
1621193	4944554	4943250	4942088	4936400	3605567	4940602	4943608	4942231	4936826
1623806	4944562	4943252	4942089	4936401	3695872	4940614	4943610	4942232	4936830
1629199	4944563	4943255	4942090	4936406	3696986	4940615	4943611	4942233	4936834
1629232	4944566	4943258	4942091	4936407	3747323	4940618	4943616	4942235	4936883
1631061	4944567	4943259	4942095	4936413	3817669	4940620	4943628	4942236	4936890
1716948	4944568	4943260	4942096	4936420	3846363	4940625	4943630	4942237	4936891
1734012	4944569	4943308	4942098	4936421	3849146	4940635	4943633	4942238	4936905

Table C.8: Off-Topic References Excluded at Title/Abstract Screening for Environmental Hazard									
1796863	4944577	4943309	4942099	4936426	3859486	4940638	4943637	4942239	4936908
1799769	4944581	4943317	4942100	4936432	3999151	4940645	4943664	4942240	4936909
1799943	4944626	4943319	4942101	4936437	4079260	4940647	4943666	4942242	4936914
1813008	4944628	4943326	4942102	4936439	4080205	4940650	4943667	4942243	4936917
1815447	4944630	4943354	4942103	4936440	4080833	4940654	4943670	4942151	4936608
1921479	4944633	4943361	4942104	4936442	2850268	4944719	4943457	4942152	4936618
1922729	4944634	4943365	4942105	4936475	2866384	4944720	4943484	4942153	4936621
1938473	4944635	4943366	4942106	4936477	2869405	4944722	4943485	4942154	4936622
1951523	4944637	4943370	4942107	4936478	2886973	4949200	4943488	4942180	4936623
1952548	4944639	4943371	4942108	4936486	2889553	4949230	4943489	4942182	4936639
1963069	4944641	4943373	4942110	4936487	2890731	4949231	4943490	4942185	4936643
1976706	4944642	4943375	4942113	4936488	2902056	4949232	4943493	4942187	4936649
2043010	4944644	4943376	4942114	4936495	2904241	4940367	4943494	4942189	4936650
2048152	4944645	4943378	4942115	4936496	2960467	4940369	4943495	4942190	4936656
2114411	4944647	4943382	4942116	4936497	2990387	4940370	4943496	4942192	4936658
2114490	4944648	4943383	4942117	4936500	2997327	4940371	4943501	4942193	4936676
2115509	4944651	4943385	4942118	4936501	3006582	4940372	4943502	4942195	4936677
2115523	4944653	4943387	4942119	4936502	3036831	4940373	4943503	4942196	4936678
2142633	4944654	4943391	4942121	4936504	3037597	4940374	4943506	4942200	4936681
2232626	4944655	4943419	4942123	4936505	3038125	4940377	4943508	4942201	4936690
2239576	4944657	4943421	4942124	4936514	3038131	4940378	4943510	4942202	4936692
2241165	4944658	4943422	4942127	4936516	3038849	4940381	4943511	4942204	4936695
2241600	4944659	4943424	4942128	4936520	3039606	4940417	4943513	4942205	4936697
2279749	4944661	4943426	4942129	4936523	3041004	4940470	4943518	4942206	4936698
2291292	4944665	4943427	4942130	4936524	3041038	4940471	4943522	4942207	4936702
2309936	4944666	4943428	4942131	4936526	3041821	4940474	4943524	4942141	4936552
2592724	4944668	4943430	4942132	4936529	2744702	4944702	4943437	4942142	4936557
2667123	4944673	4943431	4942133	4936532	2751190	4944704	4943438	4942144	4936580
2700015	4944690	4943432	4942135	4936533	2778777	4944706	4943444	4942145	4936585
2700017	4944694	4943433	4942136	4936534	2778903	4944710	4943449	4942146	4936594
2710254	4944697	4943435	4942138	4936538	2792512	4944711	4943451	4942148	4936597
2733844	4944701	4943436	4942140	4936539	2809961	4944712	4943452	4942150	4936604
2832359	4944713	4943454							

Table C.8: Off-Topic References Excluded at Title/Abstract Screening for Environmental Hazard									
Reference excluded (HERO ID) because the reference did NOT present quantitative environmental hazard data									
N/A.									

Table C.9: Screening Questions and Off-Topic References Excluded at Full Text Screening for Environmental Hazard		
Question	**Off-topic if answer is:**	**References excluded (HERO ID)**
Does the reference contain information pertaining to a low- priority substance candidate?	No	4949229 4962967 4962970 2017579 4949218 4955546
What type of source is this reference?	Review article or book chapter that contains only citations to primary literature sources	4955546 4955547
Is quantitative environmental hazard data presented?	No	4962968
Is this primarily a modeling/simulation study? [Note: select "No" if experimental verification was included in the study]	Yes	4962969
Is environmental hazard data presented for standard or non-standard aquatic or terrestrial species (fish, invertebrates, microorganisms, non-mammalian terrestrial species)?	No	N/A.
Is exposure measured for the target substance or is the test substance a mixture (except for reasonable impurities, byproducts, and aqueous solutions) or formulated product?	Mixture	N/A.
	Formulated Product	N/A.
Does the reference report a duration of exposure?	No	N/A.
Does the reference report a negative control that is a vehicle control or no treatment control?	No	4962968 4962971 4962972
Does the reference include endpoints in the information needs?	No	N/A.

Table C.10: Data Quality Metrics and Unacceptable References Excluded at Data Quality Evaluation for Environmental Hazard		
Question	**Unacceptable if:**	**References excluded (HERO ID)**
Metric 1: Test Substance Identity	The test substance identity or description cannot be determined from the information provided (e.g., nomenclature was unclear, CASRN or structure were not reported, substance name/ description does not match CASRN). **OR**	N/A.

Table C.10: Data Quality Metrics and Unacceptable References Excluded at Data Quality Evaluation for Environmental Hazard		
Question	**Unacceptable if:**	**References excluded (HERO ID)**
	For mixtures, the components and ratios were not characterized or did not include information that could result in a reasonable approximation of components.	
Metric 2: Negative Controls	A concurrent negative control group was not included or reported.	4949228
Metric 3: Experimental System	The experimental system (e.g., static, semi-static, or flow-through regime) was not described.	4949228
Metric 4: Reporting of Concentrations	Test concentrations were not reported.	4949228
Metric 5: Exposure Duration	The duration of exposure was not reported. **OR** The reported exposure duration was not suited to the study type and/or outcome(s) of interest (e.g., study intended to assess effects on reproduction did not expose organisms for an acceptable period of time prior to mating).	N/A.
Metric 6: Test Organism Characteristics	The test species was not reported. **OR** The test species, life stage, or age was not appropriate for the outcome(s) of interest.	N/A.
Metric 7: Outcome Assessment Methodology	The outcome assessment methodology was not reported.	4949228
Metric 8: Reporting of Data	Data presentation was inadequate. **OR** Major inconsistencies were present in reporting of results.	4949228

C.2.3 Fate

For the screening review of LPS candidate 1-docosanol, EPA excluded a total of 980 references when assessing environmental fate. Off-topic fate references excluded at title/abstract screening are listed in Table C.11, and those excluded at full-text screening are listed in Table C.12. References in Table C.13 represent unacceptable studies based on specific data quality metrics for fate. Off-topic and unacceptable references are displayed next to the corresponding exclusion criteria.

Table C.11: Off-Topic References Excluded at Initial Screening for Fate									
Reference excluded (HERO ID) because the reference did NOT contain information needs[62] relevant to environmental fate									
453473	4937086	4937018	4936663	4929274	4407501	4940371	4944628	4936975	4936554
495881	4937087	4937019	4936664	4929276	4408854	4940784	4949230	4936977	4936555
603694	4937088	4937020	4936665	4929278	4410598	4941653	4738938	4936984	4936556
613226	4937090	4937021	4936666	4929279	4415125	4941769	4754296	4936985	4936557
658179	4937091	4937022	4936667	4929281	4426138	4941770	4755704	4936989	4936558
662407	4937092	4937023	4936668	4929282	4426912	4941809	4771899	4936990	4936560
664147	4937094	4937024	4936669	4929283	4428588	4941820	4783131	4936994	4936561
680131	4937097	4937025	4936670	4929286	4433785	4941825	4789397	4936998	4936563
697436	4937098	4937026	4936671	4929289	4437674	4941852	4824309	4937002	4936564
698371	4937099	4937027	4936672	4929291	4559854	4942193	4853263	4937003	4936565
699391	4937100	4937028	4936673	4929315	4580424	4942216	4854956	4937005	4936566
791097	4937101	4937029	4936675	4929317	4580873	4942294	4855089	4937006	4936568
852358	4937102	4937030	4936676	4929318	4580879	4942355	4864847	4937007	4936569
913357	4937104	4937031	4936677	4929322	4660710	4942362	4885573	4937008	4936570
994977	4937105	4937032	4936678	4929324	4683785	4942465	4890357	4937009	4936571
1043433	4937106	4937033	4936679	4929325	4699816	4942467	4890737	4937011	4936572
1055722	4937107	4937034	4936680	4929326	4702763	4942473	4891667	4937012	4936573
1062474	4937108	4937035	4936681	4929329	4703541	4942474	4891705	4937013	4936574
1066804	4937109	4937036	4936682	4929331	4704411	4942476	4904245	4937014	4936575
1083310	4937110	4937037	4936683	4929332	4711530	4942478	4911351	4937015	4936576
1107298	4937111	4937038	4936684	4929337	4722086	4942483	4923332	4937016	4936577
1107881	4937112	4937039	4936685	4929338	4737333	4942484	4929234	4937017	4936578
1108876	4937113	4937040	4936686	4929343	4929243	4929255	4929266	4929270	4929251
1128044	4937175	4937041	4936687	4929367	4929245	4929257	4929269	4929273	4929254
1170843	4937177	4937042	4936690	4929368	4929248	4929261	4929249	4929265	4936399
1177731	4937178	4937043	4936692	4929371	3039499	4937291	4936594	4936881	4936404
1180326	4937179	4937044	4936693	4929372	3039656	4937292	4936595	4936882	4936407
1182858	4937181	4937045	4936694	4929375	3040053	4937294	4936596	4936883	4936409
1184441	4937182	4937046	4936695	4929378	3040498	4937295	4936597	4936884	4936410
1184748	4937183	4937047	4936696	4929380	3044660	4937296	4936600	4936885	4936413

[62] The information needs for fate includes a list of study characteristics pertaining to the associated media and exposure pathways, associated processes, and use of controls. A complete list of the information needs is provided in Table A3 of the "Approach Document for Screening Hazard Information for Low-Priority Substances Under TSCA". These information needs helped guide the development of questions for title/abstract and full-text screening.

Table C.11: Off-Topic References Excluded at Initial Screening for Fate									
1184956	4937184	4937048	4936697	4929381	3046658	4937297	4936601	4936886	4936416
1185903	4937185	4937049	4936698	4929382	3047450	4937298	4936602	4936887	4936421
1193690	4937186	4937050	4936699	4929415	3055188	4937299	4936603	4936888	4936425
1202190	4937187	4937051	4936701	4929416	3060406	4937311	4936604	4936889	4936427
1204628	4937188	4937052	4936702	4929417	3120107	4937329	4936605	4936890	4936429
1230933	4937190	4937053	4936703	4929418	3153771	4937338	4936606	4936891	4936432
1298180	4937191	4937054	4936704	4929423	3270232	4937351	4936607	4936904	4936442
1311549	4937192	4937055	4936705	4929424	3280834	4937358	4936608	4936905	4936443
1333586	4937193	4937056	4936706	4929426	3329064	4937369	4936609	4936906	4936446
1342169	4937194	4937057	4936707	4929427	3347947	4937375	4936610	4936908	4936448
1445642	4937195	4937058	4936708	4929428	3475488	4937387	4936611	4936909	4936449
1458431	4937197	4937059	4936709	4929432	3479045	4937388	4936613	4936910	4936455
1462820	4937198	4937060	4936710	4929460	3489777	4937389	4936614	4936911	4936456
1509821	4937200	4937061	4936711	4929462	3539765	4937390	4936615	4936913	4936470
1535286	4937201	4937062	4936712	4929465	3539879	4937391	4936616	4936914	4936478
1609897	4937202	4937063	4936713	4929469	3586922	4937392	4942486	4936915	4936482
1610348	4937203	4937064	4936714	4929472	3605567	4937394	4942498	4936917	4936483
1615034	4937205	4937065	4936715	4929473	3702436	4937395	4942556	4936918	4936485
1615229	4937206	4937066	4936716	4929510	3715419	4937396	4942564	4936920	4936490
1616488	4937207	4937071	4936717	4929513	3759848	4937397	4942617	4936921	4936492
1617542	4937208	4937072	4936718	4929515	3762169	4937398	4942619	4936922	4936496
1631061	4937209	4937073	4936719	4929516	3769616	4937400	4942722	4936923	4936505
1689817	4937211	4937074	4936720	4929522	3817669	4937401	4942872	4936924	4936510
1716948	4937212	4937075	4936721	4929524	3841811	4937402	4943035	4936925	4936514
1729158	4937213	4937076	4936722	4929525	3846363	4937404	4943133	4936926	4936518
1734002	4937214	4937077	4936724	4929527	3857405	4937405	4943139	4936927	4936521
1734012	4937215	4937078	4936725	4929532	3859223	4937407	4943177	4936928	4936522
1754231	4937217	4937079	4936726	4929533	3859469	4937408	4943489	4936929	4936524
1786996	4937218	4937080	4936727	4929577	3859473	4937409	4943633	4936930	4936526
1799943	4937219	4937081	4936728	4929586	3859478	4937410	4943838	4936931	4936528
1921479	4937220	4937082	4936730	4929587	3859479	4937411	4943845	4936952	4936530
1939967	4937221	4937083	4936731	4929594	3859480	4937413	4943902	4936957	4936532
1942034	4937222	4937084	4936732	4929595	3859481	4937414	4943995	4936959	4936533
1942090	4937223	4937085	4936733	4929615	3859482	4937415	4944004	4936960	4936534

Table C.11: Off-Topic References Excluded at Initial Screening for Fate									
1951523	4937226	4936617	4936734	4929627	3999151	4937416	4944025	4936961	4936537
1952548	4937227	4936618	4936735	4930609	4080205	4937417	4944039	4936962	4936539
1963069	4937228	4936619	4936736	4930617	4081878	4937418	4944074	4936963	4936540
1964008	4937230	4936620	4936737	4930618	4146230	4937419	4944079	4936964	4936541
1968320	4937231	4936621	4936738	4930620	4220986	4937420	4944111	4936965	4936544
1970937	4937233	4936622	4936740	4930622	4229640	4937421	4944189	4936967	4936545
1970938	4937234	4936623	4936741	4930623	4239751	4940294	4944252	4936968	4936546
2013215	4937235	4936624	4936742	4930624	4244979	4940296	4944260	4936969	4936547
2043010	4937236	4936625	4936743	4931198	4352480	4940298	4944275	4936970	4936548
2052484	4937237	4936626	4936745	4931199	4360860	4940299	4944306	4936971	4936550
2112446	4937238	4936627	4936747	4931203	4366990	4940300	4944404	4936972	4936551
2114411	4937239	4936629	4936748	4931735	4395162	4940349	4944424	4936973	4936553
2115523	4937240	4936631	4936750	4932692	4402780	4940364	4944525	4936974	4936347
2115821	4937241	4936632	4936751	4932693	2886973	4937274	4936579	4936827	4936348
2241165	4937242	4936635	4936752	4932694	2902056	4937275	4936580	4936828	4936350
2241600	4937244	4936636	4936753	4934041	2907786	4937276	4936581	4936829	4936352
2279749	4937246	4936637	4936754	4934077	3036421	4937277	4936582	4936830	4936353
2394777	4937248	4936638	4936755	4934097	3036831	4937278	4936583	4936831	4936363
2408288	4937250	4936639	4936756	4934152	3037540	4937280	4936585	4936832	4936365
2551884	4937251	4936640	4936757	4934159	3037597	4937282	4936586	4936833	4936367
2553466	4937252	4936642	4936758	4934195	3037827	4937283	4936587	4936834	4936369
2558636	4937253	4936643	4936759	4936282	3038125	4937284	4936589	4936835	4936371
2592724	4937254	4936645	4936760	4936291	3038131	4937285	4936590	4936836	4936381
2630975	4937255	4936646	4936761	4936292	3038686	4937286	4936591	4936837	4936394
2667123	4937257	4936648	4936762	4936299	3038849	4937287	4936592	4936839	4936398
2676957	4937259	4936649	4936764	4936301	3039428	4937289	4936593	4936880	4936328
2684969	4937260	4936650	4936765	4936304	2700017	4937266	4936655	4936770	4936331
2700012	4937261	4936651	4936766	4936309	2736581	4937267	4936656	4936771	4936335
2700013	4937263	4936652	4936767	4936311	2751190	4937268	4936657	4936772	4936336
2700015	4937265	4936654	4936768	4936327	2792512	4937269	4936658	4936774	4936337
2879992	4937272	4936661	4936824	4936343	2850717	4937270	4936659	4936822	4936342
2884409	4937273	4936662	4936826	4936346	2869405	4937271	4936660	4936823	
Reference excluded (HERO ID) because the reference did NOT present quantitative environmental fate data									
N/A.									

Table C.12: Screening Questions and Off-Topic References Excluded at *Full Text Screening* for Fate		
Question	**Off-topic if answer is:**	**References excluded (HERO ID)**
Does the reference contain information pertaining to a low- priority substance candidate?	No	2048152 3101649 3457657 4657051 4936345 4936552 4936628 4936825 4937103 4937290 4942968 4949225 4955546 1922729 4867770 4936919
What type of source is this reference?	Review article or book chapter that contains only citations to primary literature sources	4955546
Is quantitative fate data presented?	No	4867770 4949229
Is this primarily a modeling/simulation study? [Note: Select "Yes" only if there is no experimental verification]	Yes	N/A.

Table C.13: Data Quality Metrics and Unacceptable References Excluded at Data Quality Evaluation for Fate		
Data quality metric	**Unacceptable if:**	**References excluded (HERO ID)**
Metric 1: Test Substance Identity	The test substance identity or description cannot be determined from the information provided (e.g., nomenclature was unclear and CASRN or structure were not reported). **OR** For mixtures, the components and ratios were not characterized or did not include information that could result in a reasonable approximation of components.	N/A.
Metric 2: Study Controls	The study did not include or report crucial control groups that consequently made the study unusable (e.g., no positive control for a biodegradation study reporting 0% removal).	4934169 4949222

Table C.13: Data Quality Metrics and Unacceptable References Excluded at Data Quality Evaluation for Fate		
Data quality metric	**Unacceptable if:**	**References excluded (HERO ID)**
	OR The vehicle used in the study was likely to unduly influence the study results.	4955550
Metric 3: Test Substance Stability	There were problems with test substance stability, homogeneity, or preparation that had an impact on concentration or dose estimates and interfered with interpretation of study results.	4934169 4949222 4949228
Metric 4: Test Method Suitability	The test method was not reported or not suitable for the test substance. **OR** The test concentrations were not reported. **OR** The reported test concentrations were not measured and the nominal concentrations reported greatly exceeded the substances water solubility, which would greatly inhibit meaningful interpretation of the outcomes.	4934169 4949222
Metric 5: Testing Conditions	Testing conditions were not reported and the omission would likely have a substantial impact on study results. **OR** Testing conditions were not appropriate for the method (e.g., a biodegradation study at temperatures that inhibit the microorganisms).	4934169 4949228 4955550
Metric 6: System Type and Design- Partitioning	Equilibrium was not established or reported, preventing meaningful interpretation of study results. **OR** The system type and design (e.g. static, semi-static, and flow-through; sealed, open) were not capable of appropriately maintaining substance concentrations, preventing meaningful interpretation of study results.	4949222
Metric 7: Test Organism-Degradation	The test organism, species, or inoculum source were not reported, preventing meaningful interpretation of the study results.	4934169 4949228 4955550
Metric 8: Test Organism-Partitioning	The test organism information was not reported. **OR** The test organism is not routinely used and would likely prevent meaningful interpretation of the study results.	N/A.
Metric 9: Outcome Assessment Methodology	The assessment methodology did not address or report the outcome(s) of interest.	4934169
Metric 10: Data Reporting	Insufficient data were reported to evaluate the outcome of interest or to reasonably infer an outcome of interest. **OR**	4955550

Table C.13: Data Quality Metrics and Unacceptable References Excluded at Data Quality Evaluation for Fate		
Data quality metric	**Unacceptable if:**	**References excluded (HERO ID)**
	The analytical method used was not suitable for detection or quantification of the test substance. **OR** Data indicate that disappearance or transformation of the parent compound was likely due to some other process.	
Metric 11: Confounding Variables	There were sources of variability and uncertainty in the measurements and statistical techniques or between study groups.	4934169 4949222 4949228
Metric 12: Verification or Plausibility of Results	Reported value was completely inconsistent with reference substance data, related physical chemical properties, or otherwise implausible, suggesting that a serious study deficiency exists (identified or not).	4949228 4955550