Government of Canada Gouvernement du Canada

Screening Assessment

Naphthalene Sulfonic Acids and Salts (NSAs) Group

Chemical Abstracts Service Registry Numbers
1321-69-3
25322-17-2
25619-56-1
57855-77-3
60223-95-2
68425-61-6

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Synopsis

Pursuant to section 68 or 74 of the *Canadian Environmental Protection Act, 1999* (CEPA), the Minister of the Environment and the Minister of Health have conducted a screening assessment on six substances referred to collectively under the Chemicals Management Plan as the Naphthalene Sulfonic Acids and Salts Group. This screening assessment addresses the six substances listed in the table below.

Substances in the Naphthalene Sulfonic Acids and Salts Group

CAS RN[a]	Domestic Substances List name	Acronym
1321-69-3	Naphthalenesulfonic acid, sodium salt	NaNSA
25322-17-2	Naphthalenesulfonic acid, dinonyl-	DNNSA
25619-56-1	Naphthalenesulfonic acid, dinonyl-, barium salt	BaDNNSA
57855-77-3	Naphthalenesulfonic acid, dinonyl-, calcium salt	CaDNNSA
60223-95-2	Naphthalenedisulfonic acid, dinonyl-	DNNDSA
68425-61-6	Naphthalenesulfonic acid, bis(1-methylethyl)-, compd. with cyclohexanamine (1:1)	CDINSA

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All six substances in the NSAs Group are commercially produced and do not occur naturally in the environment. The six substances were included in surveys issued pursuant to section 71 of CEPA. According to information submitted, NaNSA was manufactured in a total quantity between 100 000 kg and 1 000 000 kg in 2015, and in 2011 less than 1000 kg of CaDNNSA was manufactured in Canada. The remaining substances in the group were not manufactured in Canada, but were imported in quantities between 1000 kg and 100 000 kg for each substance in either 2011 or 2015. In Canada, these substances have a variety of uses in fuels, lubricants, oil and natural gas extraction, paints and coatings, rubber materials, and water treatment.

The ecological risk of NaNSA was characterized using the ecological risk classification of organic substances (ERC), which is a risk-based approach that employs multiple metrics for both hazard and exposure, with weighted consideration of multiple lines of evidence for determining risk classification. Based on the outcome of the ERC analysis, NaNSA is considered unlikely to be causing ecological harm.

The other five substances in the NSAs Group were assessed for ecological risk based on a mixture of empirical data and results from models, which informed the fate and effects of these substances. These five NSAs are likely persistent, but not bioaccumulative. For the ecological assessment, the substances in the NSAs Group

were divided into two subgroups based on similarities in physical-chemical properties and hazard to aquatic organisms. The first subgroup, hereinafter referred to as the low solubility subgroup, includes DNNSA, BaDNNSA and CaDNNSA. The second subgroup, hereinafter referred to as the high solubility subgroup, includes DNNDSA and CDINSA. These two subgroups were considered separately for effects to aquatic organisms and ecological exposure. It was assumed that industrial uses were potentially interchangeable within each subgroup. The exposure scenarios examined in the ecological assessment included aquatic releases from lubricant oil blending, use of metal working fluids, formulation of paints and coatings, formulation of oil and gas products, formulation of fuels, and industrial use of paints. Exposure to sediment resulting from these releases, and exposure to soil via the application of biosolids to land were also considered. Low risk was identified from these five NSAs at current levels of exposure.

Considering all available lines of evidence presented in this screening assessment, there is low risk of harm to the environment from the six substances in the NSAs Group. It is concluded that the six substances in the NSAs Group do not meet the criteria under paragraphs 64(*a*) or (*b*) of CEPA as they are not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity or that constitute or may constitute a danger to the environment on which life depends.

With respect to human health, BaDNNSA and CDINSA were evaluated using the approach applied in the Rapid Screening of Substances with Limited General Population Exposure to determine if a substance requires further assessment on the basis of the potential for direct and indirect exposure of the general population. On the basis of this approach, the potential for exposure of the general population to BaDNNSA and CDINSA was considered to be negligible, indicating a low probability of risk to human health. Therefore, BaDNNSA and CDINSA are considered to be a low concern for human health at current levels of exposure.

For the four other substances, Canadians may be exposed to DNNSA, CaDNNSA and DNNDSA mainly through drinking water, while NaNSA is not released to the environment. In addition, DNNSA may be used as an antistatic agent in certain food packaging materials with potential for direct food contact. However, exposure from this food packaging use is expected to be negligible. The general population is not expected to be exposed to NaNSA, DNNSA or DNNDSA from the use of products available to consumers. The use of a general purpose aerosol lubricant containing CaDNNSA may result in intermittent inhalation and dermal exposures to this substance.

NaNSA was not identified as posing a high hazard to human health on the basis of classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity, or reproductive toxicity. Further investigation into the potential health effects of NaNSA was not pursued as exposure of the Canadian general population to this substance is not expected. The health effects data for

DNNSA, CaDNNSA and DNNDSA were limited; as such, a read-across approach was used to inform the health effects characterization of these substances. On the basis of laboratory studies conducted on structurally-related substances, the critical health effects of DNNSA, CaDNNSA, and DNNDSA are considered to be crystal formation in the kidneys and effects on the thyroid. Comparisons of levels of exposure to DNNSA or DNNDSA from environmental media to levels at which health effects occur result in margins that are considered adequate to address uncertainties in the health effects and exposure databases. Similarly, comparisons of levels of exposure to CaDNNSA from environmental media and from the use of a lubricant containing CaDNNSA to levels at which health effects occur result in margins that were considered adequate to address uncertainties in the health effects and exposure databases.

Considering all the information presented in this screening assessment, it is concluded that the six substances in the NSAs Group do not meet the criteria under paragraph 64(*c*) of CEPA as they are not entering the environment in a quantity or concentration or under conditions that constitute or may constitute a danger in Canada to human life or health.

It is therefore concluded that the six substances in the NSAs Group do not meet any of the criteria set out in section 64 of CEPA.

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1. Introduction

Pursuant to section 68 or 74 of the *Canadian Environmental Protection Act, 1999* (CEPA) (Canada 1999), the Minister of the Environment and the Minister of Health have conducted a screening assessment on six of seven substances, referred to collectively under the Chemicals Management Plan as the Naphthalene Sulfonic Acids and Salts (NSAs) Group, to determine whether these six substances present or may present a risk to the environment or to human health. Three substances were identified as priorities for assessment as they met categorization criteria under subsection 73(1) of CEPA (NaNSA, CDINSA)or were prioritized through other mechanisms (CaDNNSA) (ECCC, HC [modified 2017]). The remaining three substances (DNNSA, BaDNNSA and DNNDSA) were included because they were identified as priorities within the Identification of Risk Assessment Priorities approach (ECCC, HC 2015; Environment Canada, Health Canada 2014).

The seventh substance, naphthalenesulfonic acid, butyl-, sodium salt (Chemical Abstracts Service Registry Numbers (CAS RN[1]) 25638-17-9) was originally included in the NSAs Group. However, it was considered in the Ecological Risk Classification of Organic Substances (ERC) Science Approach Document (ECCC 2016a) and via the approach applied in the Rapid Screening of Substances with Limited General Population Exposure Screening Assessment (ECCC, HC 2018) was identified as being of low concern to both the environment and human health. As such, it is not further addressed in this report. The conclusion for this substance is provided in the Rapid Screening of Substances with Limited General Population Exposure Screening Assessment (ECCC, HC 2018). The six substances addressed in this screening assessment will hereinafter be referred to as the NSAs Group.

The ecological risk of one of the substances in the NSAs Group, NaNSA (CAS RN 1321-69-3), was characterized using ERC (ECCC 2016a; Appendix D), which is a risk-based approach that employs multiple metrics for both hazard and exposure, with weighted consideration of multiple lines of evidence for determining risk classification. The ERC identified NaNSA as having low potential to cause ecological harm (ECCC

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2016b), thus its ecological risk is not further discussed in this report, though its risk to human health is described.

For the ecological assessment, the substances in the NSAs Group were divided into two subgroups based on similarities in physical-chemical properties and hazard to aquatic organisms. The first subgroup, hereinafter referred to as the low solubility subgroup, includes DNNSA, BaDNNSA and CaDNNSA. The second subgroup, hereinafter referred to as the high solubility subgroup, includes DNNDSA and CDINSA. These two subgroups were considered separately for ecological exposure; it was assumed that within each subgroup there would be the potential for interchangeable industrial uses of the substances. This assessment primarily focusses on the naphthalene sulfonic acid anions of the substances in the group, rather than their associated cations. In particular, the cation of CDINSA, cyclohexanamine, is not addressed in this report, as it is included in a separate assessment (ECCC, HC 2019) where its ecological risk was characterized using ERC.

The risk to human health was assessed individually for each substance. BaDNNSA and CDINSA were considered under the approach applied in the Rapid Screening of Substances with Limited General Population Exposure Screening Assessment (ECCC, HC 2018). In the approach, the potential for direct exposure was evaluated on the basis of considerations such as evidence of the substance being present in a product used by the general population, and the potential for indirect exposure was adopted from the general approach reported in the Threshold of Toxicological Concern (TTC)-based Approach for Certain Substances science approach document (Health Canada 2016). On the basis of the evaluation of both direct and indirect exposure conducted as part of this approach, exposure of the general population to BaDNNSA and CDINSA was considered to be negligible. Therefore, BaDNNSA and CDINSA are considered to be a low concern for human health at current levels of exposure.

This screening assessment includes consideration of information on chemical properties, environmental fate, hazards, uses and exposures. Relevant data were identified up to April 2019, with additional targeted literature searches conducted up to December 2020, as well as information received from stakeholders up to April 2021. Empirical data from key studies as well as results from models were used to reach conclusions. When available and relevant, information presented in assessments from other jurisdictions was considered.

New research publications on the mode of action, ecotoxicity and bioaccumulation of NSAs became available in 2020 and 2021 after the draft screening assessment was published. As well, new information became available from the European Chemicals Agency (ECHA) on the inherent biodegradability of one of the analogues used in the assessment, C_9-rich DANSA. This new information has been included in this screening assessment.

This screening assessment was prepared by staff in the CEPA Risk Assessment Program at Health Canada and Environment and Climate Change Canada and incorporates input from other programs within these departments. The ecological and human health portions of this assessment have undergone external review or consultation. Comments on the technical portions relevant to the environment were received from Mr. Geoff Granville (GCGranville Consulting Corp.) and Dr. James Armitage (AES Environmental Services, Inc.). Comments on the technical portions relevant to human health were received from Ms. Theresa Lopez, Ms. Jennifer Flippin, and Dr. Joan Garey at Tetra Tech. The ERC science approach document (ECCC 2016a) was peer-reviewed and subject to a 60-day public comment period. The Rapid Screening of Substances with Limited General Population Exposure Screening Assessment (ECCC, HC 2018) was subject to a 60-day public comment period. Additionally, the draft of this screening assessment (published July 4, 2020) was subject to a 60-day public comment period. While external comments were taken into consideration, the final content and outcome of the screening assessment remain the responsibility of Health Canada and Environment and Climate Change Canada.

This screening assessment focuses on information critical to determining whether substances meet the criteria as set out in section 64 of CEPA by examining scientific information and incorporating a weight of evidence approach and precaution.[2] This screening assessment presents the critical information and considerations on which the conclusions are based.

2. Identity of substances

The CAS RN, *Domestic Substances List* (DSL) names, common names and acronyms for the six substances in the NSAs Group are presented in Table 2-1.

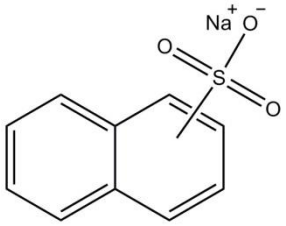
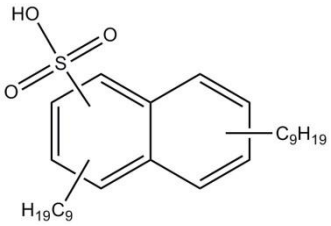
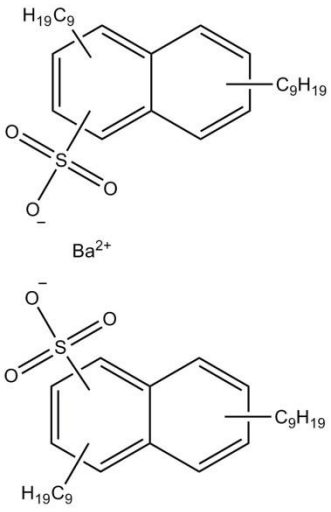
Each substance in this group is considered to be an Unknown or Variable composition Complex reaction products or Biological material (UVCB[3]) as the positions of both the sulfonate and the alkyl groups on the naphthalene are not specified. Furthermore, for

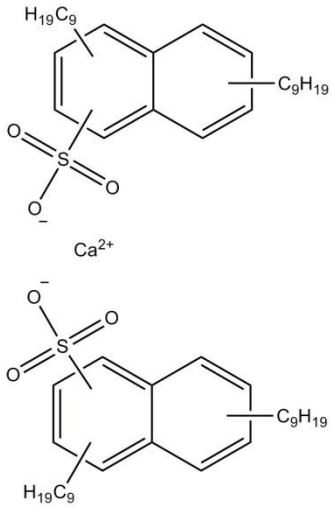
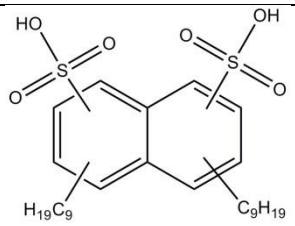
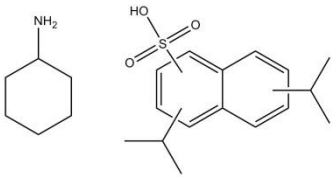
[2] A determination of whether one or more of the criteria of section 64 of CEPA are met is based upon an assessment of potential risks to the environment and/or to human health associated with exposures in the general environment. For humans, this includes, but is not limited to, exposures from ambient and indoor air, drinking water, foodstuffs, and products available to consumers. A conclusion under CEPA is not relevant to, nor does it preclude, an assessment against the hazard criteria specified in the *Hazardous Products Regulations*, which are part of the regulatory framework for the Workplace Hazardous Materials Information System for products intended for workplace use. Similarly, a conclusion based on the criteria contained in section 64 of CEPA does not preclude actions being taken under other sections of CEPA or other acts.

[3] UVCB is an acronym for Unknown or Variable composition, Complex reaction products or Biological materials. These materials are derived from natural sources or complex reactions. A UVCB is not an intentional mixture of discrete substances, and is considered a single substance. The complexity and variability of their compositions can make them difficult to fully and consistently characterize.

DNNSA, BaDNNSA, CaDNNSA and DNNDSA, the dinonyl alkyl groups may exist in both linear and branched forms. For simplicity, the exact geometry (linear or branched) is not shown in the representative structures.

Table 2-1. Substance identities

CAS RN (acronym)	DSL name (common name)	Representative chemical structure and molecular formula	Molecular weight (g/mol)
1321-69-3 (NaNSA)	Naphthalenesulfonic acid, sodium salt (sodium naphthalenesulfonate)	 $C_{10}H_8O_3SNa$	230.22
25322-17-2 (DNNSA)[a]	Naphthalenesulfonic acid, dinonyl- (dinonylnaphthalenesulfonic acid)	 $C_{28}H_{44}O_3S$	460.72
25619-56-1 (BaDNNSA)[a]	Naphthalenesulfonic acid, dinonyl-, barium salt (barium dinonylnaphthalenesulfonate)	 $C_{56}H_{88}O_6S_2Ba$	1058.75

CAS RN (acronym)	DSL name (common name)	Representative chemical structure and molecular formula	Molecular weight (g/mol)
57855-77-3 (CaDNNSA)[a]	Naphthalenesulfonic acid, dinonyl-, calcium salt (calcium dinonylnaphthalenesulfonate)	 $C_{56}H_{88}O_6S_2Ca$	961.50
60223-95-2 (DNNDSA)[b]	Naphthalenedisulfonic acid, dinonyl- (dinonylnaphthalenedisulfonic acid)	 $C_{28}H_{44}O_6S_2$	540.78
68425-61-6 (CDINSA)[b]	Naphthalenesulfonic acid, bis(1-methylethyl)-, compd. with cyclohexanamine (1:1) (cyclohexylammonium diisopropylnaphthalenesulfonate)	 $C_6H_{13}N.C_{16}H_{20}O_3S$	391.57

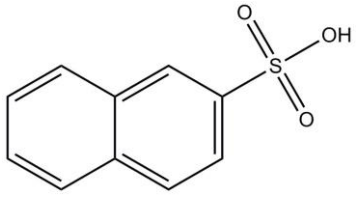
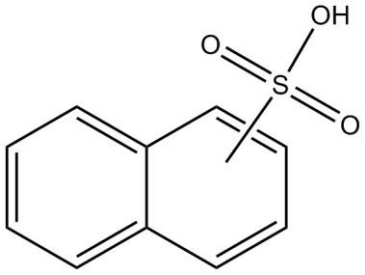
[a] This substance is included in the low solubility subgroup for the ecological assessment.
[b] This substance is included in the high solubility subgroup for the ecological assessment.

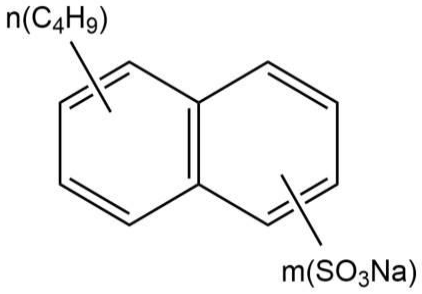
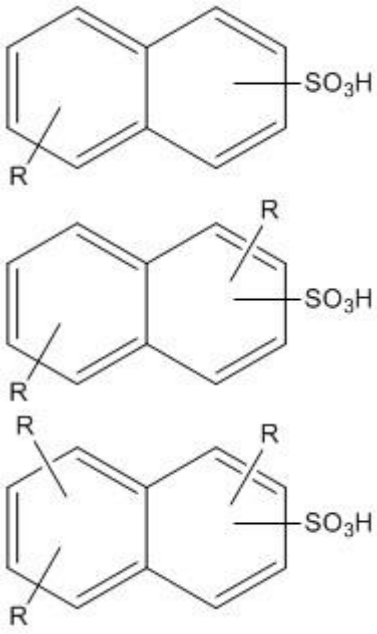
2.1 Selection of analogues and use of (Q)SAR models

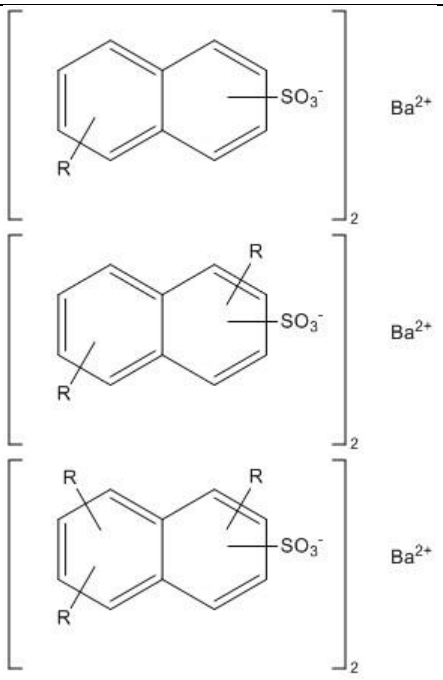
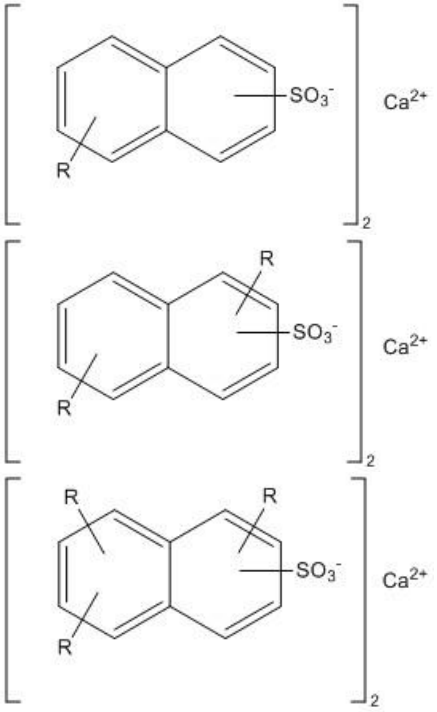
A read-across approach using data from analogues and the results of (quantitative) structure-activity relationship ((Q)SAR) models, where appropriate, has been used to inform the ecological and human health assessments. Analogues were selected that

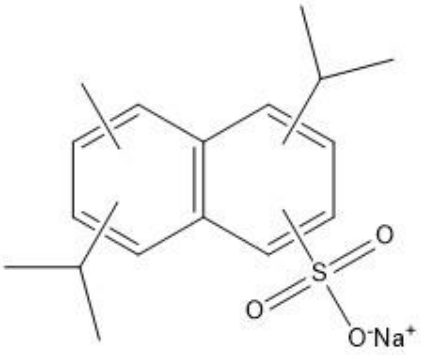
were structurally similar and/or functionally similar to substances within this group (for example, similar physical-chemical properties, toxicokinetics) and that had relevant empirical data that could be used to read across to substances with limited empirical data. The applicability of (Q)SAR models was determined on a case-by-case basis. Details of the read-across data and (Q)SAR models chosen to inform the ecological and human health assessments of the NSAs Group are further discussed in the relevant sections of this report, and in Appendix F. Information on the identities and chemical structures of the analogues used to inform this assessment is presented in Table 2-2. Table 2-3 provides an indication of the read-across data available for different parameters.

Table 2-2. Analogue identities

CAS RN (acronym)	DSL or other name (common name)	Representative chemical structure and molecular formula	Molecular weight (g/mol)
120-18-3 (2-NSA)	2-Naphthalenesulfonic acid	 $C_{10}H_8O_3S$	208.23
68153-01-5	Naphthalenesulfonic acids	 $C_{10}H_8O_3S$	208.23

CAS RN (acronym)	DSL or other name (common name)	Representative chemical structure and molecular formula	Molecular weight (g/mol)
91078-64-7	Naphthalenesulfonic acids, branched and linear Bu derivs., sodium salts	 m = 1-2, n = 1-3	288.29 to 551.46
European Community Number[a, b] 939-714-0 (C_9-rich DANSA)	di C_8-C_{10}, branched, C_9 rich, alkylnaphthalene sulfonic acid (C_9-rich dialkylnaphthalenesulfonic acid)	 R = C_8-C_{10}	320.49 to 629.02

CAS RN (acronym)	DSL or other name (common name)	Representative chemical structure and molecular formula	Molecular weight (g/mol)
European Community Number[a, b] 939-718-2 (Ba- C_9-rich DANSA)	barium bis(di C_8-C_{10}, branched, C_9 rich, alkylnaphthalenesulfonate) (barium C_9-rich dialkylnaphthalenesulfonate)	 R = C_8-C_{10}	776.18 to 1393.39
European Community Number[a, b] 939-717-7 (Ca- C_9-rich DANSA)	calcium bis(di C_8-C_{10}, branched, C_9 rich, alkylnaphthalenesulfonate) (calcium C_9-rich dialkylnaphthalenesulfonate)	 R = C_8-C_{10}	678.24 to 1296.15

CAS RN (acronym)	DSL or other name (common name)	Representative chemical structure and molecular formula	Molecular weight (g/mol)
68909-82-0[b]	Naphthalenesulfonic acid, bis(1-methylethyl)-, Me derivs., sodium salts		328.40

Abbreviations: DANSA, dialkylnaphthalenesulfonate; N/A, Not Applicable
[a] This substance does not have a CAS RN or the CAS RN is unknown
[b] Molecular formula has not been included due to structural complexity

Table 2-3. Read-across data used to inform various parameters evaluated in this assessment

CAS RN for analogue (acronym)	Common name	Physical-chemical and ecological data	Health effects data
120-18-3 (2-NSA)	2-Naphthalenesulfonic acid	Phys/chem, Persistence	N/A[a]
68153-01-5	Naphthalenesulfonic acids	Ecotoxicity	N/A[a]
91078-64-7	Naphthalenesulfonic acids, branched and linear Bu derivs., sodium salts	Ecotoxicity	N/A[a]
68909-82-0	Naphthalenesulfonic acid, bis(1-methylethyl)-, Me derivs., sodium salts	Ecotoxicity	N/A[a]
EC No.[b] 939-714-0 (C_9-rich DANSA)	C_9-rich dialkylnaphthalenesulfonic acid	Water solubility, Persistence, Ecotoxicity	Reproductive and developmental toxicity, genotoxicity
EC No.[b] 939-718-2 (Ba- C_9-rich DANSA)	barium bis(di C_8-C_{10}, branched, C9 rich, alkylnaphthalenesulfonate)	Water solubility	Reproductive and developmental toxicity, genotoxicity
EC No.[b] 939-717-7 (Ca- C_9-rich DANSA)	calcium bis(di C_8-C_{10}, branched, C9 rich, alkylnaphthalenesulfonate)	Water solubility Ecotoxicity	Subacute toxicity, subchronic toxicity

Abbreviation: EC No., European Community Number; N/A, Not Applicable
[a] Health effects data are not needed for these substances as they are not being used as analogues in the human health assessment
[b] This substance does not have a CAS RN

3. Physical and chemical properties

Summaries of physical-chemical property data of the substances in the NSAs Group are presented in Table 3-1 and Table 3-2. Table 3-1 displays the selected physical-chemical property values for DNNDSA and DNNSA, which includes the dissociated organic DNNSA components of CaDNNSA and BaDNNSA. Table 3-2 displays the values for CDINSA and NaNSA. In these tables, values are the result of modelling programs, except where indicated. Modelled results were generated for both the linear and branched structural variations of DNNSA and DNNDSA, where applicable, and when the results differed, an average of the two values was calculated and used in the assessment.

All of these substances have very low acid dissociation constants (pK_a) and thus are expected to be completely ionized (that is, anionic) when in aqueous solutions at ambient pH of 6 to 9. Ionization occurs via loss of a hydrogen ion from each of the sulfonic acid moieties, resulting in a sulfonate anion (ACD/Percepta c1997-2017). However, since many of the QSAR-type models are based on fragment addition methods (for example, EPI Suite c2000-2012), they typically accept only the neutral form of a chemical as input. Therefore, only the un-ionized forms of these substances were modelled, where applicable. The physical-chemical properties of BaDNNSA and CaDNNSA were not modelled; rather they were read-across, as needed, from DNNSA, which represents their organic component. Similarly, the data displayed in Table 3-2 for CDINSA and NaNSA are for the neutral forms of their anions. The ionized forms of these substances are expected to be less volatile and to have lower Henry's law constants than the neutral forms that were modelled using EPI Suite.

Water solubilities of BaDNNSA, CaDNNSA and DNNDSA (Table 3-1) were measured by ECCC researchers (personal communication from the Aquatic Contaminants Research Division, Environment and Climate Change Canada (ECCC), to the Ecological Assessment Division, ECCC, June 2019, unreferenced). Unlike the Organisation for Economic Co-operation and Development (OECD) Shake Flask method (OECD 1995), the samples were shaken for three days, rather than 24 hours, and sonicated for 4 hours/day during those three days. However, only 100 mL of water was reported to have been used for 1 g of NSA solute (rather than for 0.1 g of solute as recommended), which may have contributed to the very low water solubilities obtained. In the European Chemicals Agency's REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) dossiers for DNNDSA and the analogue substances Ba- and Ca- C_9-rich DANSA (ECHA 2018 a,b,d), the reported measured water solubilities were several orders of magnitude higher (Table 3-1). For DNNDSA, few details about the water solubility study were available in its REACH dossier, other than it followed

OECD Test Guideline No. 105 (OECD 1995), though it states that the measurement was made at a pH of 1.1 to 2.1, at which an even lower water solubility would be expected (ACD/Percepta c1997-2017). The water solubility measurements for Ba- and Ca- C_9-rich DANSA were obtained in the pH range of 6.1 to 7.5 (ECHA 2018b, 2018d).

Several of the substances in the NSAs Group are expected to have surfactant properties, as they have hydrophobic alkyl chains with chain length between 8 and 18 (Farn 2006), as well as anionic sulfonate groups. However, given the absence of an alkyl group for NaNSA and the short alkyl groups for CDINSA, these two substances may exhibit surfactant properties only to a minimal extent. . In water, surfactants have the tendency to aggregate at the interface between two phases (for example, octanol and water) and, when concentrations are sufficiently high, form micelles. For these reasons, typical test methods used for studying the partitioning of substances (that is, log K_{ow}) as well as their water solubility, such as OECD 117 (HPLC method) and OECD 107 (shake flask method), do not typically give accurate or reliable results for surfactants (McWilliams and Payne 2011).

Due to the acidity and surface-active properties of most NSAs, the organic carbon-water partition coefficient (log K_{oc}) cannot be measured using standard methods, such as high performance liquid chromatography (HPLC) (ECHA 2018b). The log K_{oc} of DNNSA and CDINSA were selected based on the equation described in Abraham et al. (1994) and the model output from ACD/Percepta (c1997-2017). This approach uses polyparameter linear free energy relationships (ppLFER) to evaluate the equilibrium partitioning of organic compounds into water versus into organic matter. The ppLFER approach is considered to be more accurate for estimation of K_{oc} for polar compounds and compounds with specific interactions towards organic matter than other traditional methods. This is due to the consideration of multiple types of molecular interactions (with both water and/or organic matter) as contributions towards free energy changes (Nguyen et al. 2005). However, the ppLFER model for estimation of K_{oc} is not ideal, as it does not account for electrostatic interactions that would be present with ionized substances such as NSAs.

Table 3-1. Selected physical-chemical property values (averages of branched and linear structures, at standard temperature) for DNNSA, CaDNNSA, BaDNNSA, and DNNDSA

Property	DNNSA (CaDNNSA, BaDNNSA)[a]	DNNDSA	Reference(s)
Physical state	NA	solid	ECHA 2018a
Melting point (°C)	153	121[b]	Median of models (MPBPWIN 2010, TEST 2016); ECHA 2018a

Property	DNNSA (CaDNNSA, BaDNNSA)[a]	DNNDSA	Reference(s)
Vapour pressure (Pa)	1.03×10^{-10}	2.33×10^{-16}	Median of models (MPBPWIN 2010)
Henry's law constant ($Pa \cdot m^3/mol$)	2.82×10^{-3}	1.32×10^{-9}	HENRYWIN 2011 (bond method)
Water solubility (mg/L)	NA (DNNSA) 0.0039 (CaDNNSA) 0.011 (BaDNNSA)	2.00	unpublished ECCC internal report, Aquatic Contaminants Research Division, dated Apr. 26, 2019, unreferenced
Water solubility (mg/L)	0.23 (DNNSA)[b] 0.27 (CaDNNSA)[b] 0.21 (BaDNNSA)[b]	2.00×10^{3} [b,c]	Read-across from C_9-rich DANSA, Ca-C_9-rich DANSA, and Ba-C_9-rich DANSA (ECHA 2018b, 2018c, 2018d); ECHA 2018a
Water solubility of anion (mg/L), pH 5-9	0.003 (DNNSA) NA (CaDNNSA) NA (BaDNNSA)	0.18	ACD/Percepta c1997-2017
Log K_{ow} (dimensionless)	3.5[d]	<0.3	KOWWIN 2010; ECHA 2018a
Log K_{oc} (dimensionless)	5.09	1.1[d]	Abraham et al. 1994 and ACD/Percepta c1997-2017; KOCWIN 2010
D_{max} (nm)	NA	19.7	Simulation from ECHA 2018a
pK_{a1} (dimensionless)	0.4-0.7	-2.2-1.1	ACD/Percepta c1997-2017

Abbreviations: NA, Not Available

[a] Values for BaDNNSA and CaDNNSA are read-across from DNNSA, with the exception of water solubility

[b] Values are empirical data

[c] This value was found to be loading-rate dependent. Solubility varied from 2054 to 24 380 mg/L and was found to be on average 98.6% (ECHA 2018a).

[d] Values were estimated using the experimental value adjustment method in KOWWIN and KOCWIN, using the measured log K_{ow} value of DNNDSA as input.

Table 3-2. Selected physical-chemical property values (at standard temperature) for CDINSA and NaNSA

Property	CDINSA	NaNSA[a]	Reference(s) for CDINSA; NaNSA
Physical state	NA	Solid	ECHA 2019a
Melting point (°C)	164	115.5[b]	Median of models (MPBPWIN 2010, TEST 2016)
Vapour pressure (Pa)	5.07×10^{-7}	2.51×10^{-5}	Median of models (MPBPWIN 2010)
Henry's law constant ($Pa \cdot m^3/mol$)	9.42×10^{-5}	NR	HENRYWIN 2011 (bond method)
Water solubility (mg/L)	1.98×10^{2}	6.01×10^{4} [b]	Median of models (ACD/Percepta c1997-2017, WATERNT 2010, WSKOWWIN 2010, VCCLab 2005); experimental value (EPI Suite c2000-2012)
Log K_{ow} (dimensionless)	2.92	0.85[b]	Median of models (ACD/Percepta c1997-2017, ppLFER, VCCLab 2005, KOWWIN 2010); Median of experimental values (ACD/Percepta database)
Log K_{oc} (dimensionless)	3.28	NR	Abraham et al. 1994 and ACD/Percepta c1997-2017
pK_{a1} (dimensionless)	0.7	NR	ACD/Percepta c1997-2017

Abbreviations: NA, Not Available; NR, not required for this assessment
[a] Physical-chemical properties for NaNSA are read-across from empirical and/or modelled data for 2-NSA.
[b] Values are empirical data

4. Sources and uses

All six substances from the NSAs Group are commercially produced and do not occur naturally.

The six substances were included in surveys issued pursuant to section 71 of CEPA (Canada 2012; Canada 2017). Table 4-1 presents a summary of information reported on the total manufacture and total import quantities.

Table 4-1. Summary of information on Canadian manufacturing and imports of substances from the NSAs Group submitted in response to CEPA section 71 surveys

Common name	Total manufacture[a] (kg)	Total imports[a] (kg)	Reporting year	Survey reference
NaNSA	100 000 to 1 000 000	NR	2015	ECCC 2018
DNNSA	NR	10 000 to 100 000	2015	ECCC 2018
BaDNNSA	NR	37 975	2015	ECCC 2018
CaDNNSA	110	10 000 to 100 000	2011	Environment Canada 2013
DNNDSA	NR	1000 to 10 000	2015	ECCC 2018
CDINSA	NR	10 000 to 100 000	2011	Environment Canada 2013

Abbreviations: NR – not reported at a reporting threshold of 100 kg
[a] Values reflect quantities reported in response to CEPA section 71 surveys (Environment Canada 2013; ECCC 2018). See surveys for specific inclusions and exclusions (schedules 2 and 3).

Table 4-2 presents a summary of the non-confidential major uses of substances from the NSAs Group according to information submitted in response to CEPA section 71 surveys (Environment Canada 2013; ECCC 2018). The major uses reported for NaNSA are not included in Table 4-2 due to business confidentiality claims.

Table 4-2. Summary of Canadian uses of substances from the NSAs Group submitted in response to CEPA section 71 surveys

Major uses[a]	DNNSA	BaDNNSA	CaDNNSA	DNNDSA	CDINSA
Fuels and related products, mixtures or manufactured items	Y	Y	N	N	N
Lubricants and greases	N	Y	Y	N	N
Oil and natural gas extraction	Y	N	N	N	Y
Paints and coatings	Y	Y	N	Y	N
Rubber materials	Y	N	N	N	N
Water treatment	Y	N	N	N	N

Abbreviations: Y = yes, this use was reported for this substance; N = no, this use was not reported for this substance
[a] Non-confidential uses reported in response to CEPA section 71 surveys (Environment Canada 2013; ECCC 2018). See surveys for specific inclusions and exclusions (schedules 2 and 3).

In Canada, NaNSA is present as a formulant in registered pest control products (personal communication, email from the Pest Management Regulatory Agency, Health Canada, to the Existing Substances Risk Assessment Bureau, Health Canada, dated

January 2018; unreferenced). DNNSA may be used as an antistatic agent in the production of retention aids for use in the manufacture of paper and paperboard with potential for direct food contact (personal communication, email from the Food Directorate, Health Canada, to the Existing Substances Risk Assessment Bureau, Health Canada, dated January 2018; unreferenced). CaDNNSA may be used as a lubricant on equipment or machine parts where there is no contact of the lubricant with food (personal communication, email from the Food Directorate, Health Canada, to the Existing Substances Risk Assessment Bureau, Health Canada, dated August 2016; unreferenced). CaDNNSA is also used as a corrosion inhibitor in certain general purpose lubricants (SDS 2018).

In the United States, major uses of the substances in the NSAs Group include the manufacture of basic organic chemicals, petrochemicals, paints and coatings, petroleum lubricating oils and greases as well as activities in petroleum refineries, oil and gas drilling, extraction and support (Chemview c2013-). In the European Union, DNNDSA is reported to be used in paints and coatings (ECHA 2018a).

5. Releases to the environment

Potential releases of substances in this group to the environment may occur from industrial facilities that use these substances in lubricant oil blending, as metal working fluids, or in the formulation of oil and gas products, paints and coatings, fuels, or during the use of these products. Most of these uses would result in indirect releases to water bodies via wastewater treatment systems[4] (WWTSs). Additionally, indirect releases to soil may occur from the application of biosolids from WWTSs to land.

6. Environmental fate and behaviour

6.1 Environmental distribution

Due to the intended uses of the substances from the NSAs Group and their physical and chemical properties, releases of these substances are expected to be predominantly from industrial facilities via WWTSs.

[4] In this assessment, the term “wastewater treatment system” refers to a system that collects domestic, commercial and/or institutional household sewage and possibly industrial wastewater (following discharge to the sewer), typically for treatment and eventual discharge to the environment. Unless otherwise stated, the term wastewater treatment system makes no distinction of ownership or operator type (municipal, provincial, federal, indigenous, private, partnerships). Systems located at industrial operations and specifically designed to treat industrial effluents will be identified by the terms “on-site wastewater treatment systems” and/or “industrial wastewater treatment systems”.

NSAs are expected to be completely ionized (negatively charged) in the ambient environment, as discussed in Section 3, and most are expected to behave as surfactants (with the exceptions of NaNSA and CDINSA). As such, these substances are expected to have low vapour pressures and to partition to a greater extent to water than to air. When released to water, it is expected that some of these substances will partition to both the water column and to sediments given their varying physical-chemical properties such as their low to high water solubilities. DNNDSA and CDINSA have moderate to high water solubility and will likely remain mostly in the water column.

DNNSA and the DNNSA metal salts have low solubility in water and therefore would be expected to partition predominantly to sediment when released to water, and stay bound to soil particles when released to soil. The very high sorption of CaDNNSA and BaDNNSA to sediment has been confirmed in a sorption/desorption study with a composite sediment and sand (unpublished ECCC internal report, Aquatic Contaminants Research Division, dated Apr. 26, 2019; unreferenced) and also in a study involving CaDNNSA (Matten et al. 2020a). During the desorption phase of the experiment, aqueous concentrations of CaDNNSA and BaDNNSA were below method detection limits. Due to their low solubilities it was assumed that, at environmentally relevant concentrations, these NSAs will bind to sand or sediment irrespective of the organic carbon content of the substrate. In contrast, DNNDSA was detected in both sediment and water during the desorption phase of the experiment. DNNDSA also did not appear to sorb to sand (Matten et al. 2020a).

Based on the above information, it is expected that water, sediment, and soil will be the compartments of interest for hazard characterization for the NSAs Group.

6.2 Environmental persistence

No empirical biodegradation information on the substances in the NSAs Group was found, however some information was found on the biodegradation of analogue substances. The biodegradation of alkylnaphthalenesulfonates with branched alkyl groups ranging from isopropyl to isopentyl is described as “marginal at best” (Swisher 1987). However, alkylnaphthalenesulfonates with straight-chain alkyl groups had faster biodegradation, with the longer-chain substances degrading faster. Using a culture of *Escherichia coli*, Kölbel (1964) examined alkylnaphthalenesulfonates with *n*-butyl, *n*-hexyl, and *n*-octyl chains, and found that the derivatives with longer alkyl chains biodegraded more quickly (5-15 d) than those with shorter alkyl chains (24-30 d).

Data are available for several NSA analogue substances. 2-naphthalenesulfonic acid, a close analogue to NaNSA, was shown to biodegrade by >90% in a 28-day test following OECD test guideline (TG) 301 A (DOC die-away test) and was thus determined to be readily biodegradable (ECHA 2019a). For longer-chain NSAs, C_9-rich DANSA was used as read-across. It was found to biodegrade 14% to 17% in a 29-day CO_2 evolution test following OECD TG 301 B, and was thus determined to not be readily biodegradable

(ECHA 2018b). An inherent biodegradation study was also performed with C_9-rich DANSA, following a modification of OECD TG 310 (ECHA 2019a). The major modifications on the procedure were pre-adaptation of sludge during a 13-day period before the start of the test, and prolongation of the test period up to 56 days. No biodegradation (CO_2 evolution) was observed after 56 days, therefore C_9-rich DANSA was found to be not inherently biodegradable.

The reaction products of NSA with isobutanol, sodium salts, showed 0% biodegradation in a 28-day closed bottle test following OECD TG 301 D (ECHA 2018e). However, the study authors noted that the lack of biodegradation does not necessarily indicate that the substance is recalcitrant in nature; rather, the stringency of the closed bottle test procedures may possibly explain the recalcitrance (ECHA 2018e).

Biodegradation modelling was used as an additional line of evidence. Ultimate biodegradation half-life predictions from both CATALOGIC (2014) and BIOWIN (2010) are less than 182 days for representative structures of DNNSA and DNNDSA. However, CDINSA was predicted to have an ultimate half-life of greater than 3 years by CATALOGIC (2014), though in BIOWIN it was only “weeks to months”. Both models predicted that these substances are not readily biodegradable, which is consistent with the empirical data. Modelled data for the ultimate half-life of CDINSA are conflicting. There is also uncertainty in the half-life estimates given that the structures of the NSAs can vary (that is, may contain branched and linear alkyl groups), and since no empirical ultimate biodegradation data were available. Therefore, a range of biodegradation half-lives of 92 days to 200 days were used in the exposure modelling for soil (Section 7.2.8).

Based on the empirical data on NSA analogues and on branched alkylnaphthalenesulfonates presented above, the five NSAs with alkyl chains are likely to persist in the environment in water, soils and sediments, while NaNSA is not expected to persist in the environment.

Releases to air are not expected from the intended uses. As NSAs all have negligible vapour pressures and low Henry’s law constants, the likelihood of volatilization occurring from soil or surface waters is low, indicating that these substances will likely not be subject to long-range transport in air. DNNDSA is expected to be mobile in water, as it has high water solubility and minimal sorption to sand or sediments. However, its potential for long-range transport in water also depends on its half-life in water, which is unclear from the available data.

6.3 Potential for bioaccumulation

The octanol-water partition coefficient (log K_{ow}) may be used to inform the bioaccumulation of substances as it gives an indication of a substance’s ability to partition to fatty tissue. However, as the substances in this group are anionic

surfactants, they accumulate at the interface between the hydrophilic and hydrophobic regions of a log K_{ow} test. As a result, log K_{ow} does not provide an accurate measurement of their partitioning or bioaccumulation.

Experimental bioconcentration and bioaccumulation data for DNNDSA, CaDNNSA, and BaDNNSA and modelled data were used to characterize the bioaccumulation potential of NSAs. BCF values for DNNDSA following 8-week exposures in carp (*Cyprinus carpio*) at 0.1 mg/L and 1 mg/L were <2.0 L/kg and <0.19 L/kg respectively (Table 6-1), which indicate a low potential for bioaccumulation.

A study by Matten et al. (2021) examined the potential for DNNDSA, BaDNNSA and CaDNNSA to accumulate in the tissue of a freshwater oligochaete (*Tubifex tubifex*) and for CaDNNSA to accumulate in a freshwater mussel (*Lampsilis siliquoidea*). Worms *(T. tubifex)* were exposed to NSAs via spiked sediment for 28 days, whereas mussels were exposed via sand spiked with CaDNNSA for 25 days. Mussels were then removed from exposure to monitor their ability to depurate CaDNNSA over the following 28 days. For the sediment exposures, natural sediments containing 2% organic carbon were spiked to nominal concentrations of 200 µg/g dry weight (dw) or less (Matten et al. 2021). NSA concentrations were measured in whole body tissue samples of worms and separately in gill, foot, and remaining soft tissues (viscera) for mussels. The concentration of NSAs in worm tissue was greater than in mussels, most likely due to the endobenthic nature of the worms, their ingestion of sediment, and the ability of mussels to mitigate exposure by withdrawing their foot (Matten et al. 2021). Biota-sediment accumulation factors (BSAFs) could not be established from the mussel tests due to the exposure substrate (that is, sand) containing no organic carbon.

The kinetic bioaccumulation factor (BAF_k) and bioconcentration factor (BCF_k) were calculated for CaDNNSA with adult mussels using the uptake rate constants from sand or overlying water, respectively, divided by the depuration rate constants. Tissue concentrations were measured in the gills and the visceral mass. The BCF_ks were larger than the BAF_ks (Table 6-1), likely a result of experimental design. Specifically, frequent water changes during the uptake phase did not allow for CaDNNSA concentrations in sand and water to reach equilibrium (Matten et al. 2021).

The experimental data show mainly low levels of bioaccumulation of NSAs in fish and invertebrates. The only substance that appears to have bioaccumulated to any extent was DNNDSA. However, these BSAF values may not represent true bioaccumulation, as DNNDSA may have sorbed to the exterior of *T. tubifex*, due to its ionic nature. Therefore, these BSAF values for DNNDSA will not be further considered.On the basis of the limited experimental data, BaDNNSA, CaDNNSA and DNNDSA do not appear to be bioaccumulative. Using the data for BaDNNSA and CaDNNSA as read-across for DNNSA, and the data for DNNDSA as read-across for CDINSA, DNNSA and CDINSA are also not expected to be bioaccumulative.

Table 6-1. Summary of experimental bioaccumulation data for substances in the NSAs Group

Substance	Test organism	Experimental concentration (duration)	Value type (units)	Value	Reference
DNNDSA	Fish (*C. carpio*)	0.1 mg/L (8 weeks)	BCF (L/kg)	<2.0	ECHA 2018a
DNNDSA	Fish (*C. carpio*)	1 mg/L (8 weeks)	BCF (L/kg)	<0.19	ECHA 2018a
CaDNNSA	Mussel (*L. siliquoidea*)	5.86 ± 4.05 µg/L (mean value in water) (25 d)	BCF_k (L/kg)	14.1 to 16.4	Matten et al. (2021)
CaDNNSA	Mussel (*L. siliquoidea*)	73 µg/g dw (nominal concentration in sand) (25 d)	BAF_k (L/kg)	1.1 to 1.3	Matten et al. (2021)
CaDNNSA	Oligochaete worm (*T. tubifex*)	200 µg/g dw (nominal concentration in sediment) (28 d)	BSAF (unitless)	0.84 to 1.10	Matten et al. (2021)
BaDNNSA	Oligochaete worm (*T. tubifex*)	200 µg/g dw (nominal concentration in sediment) (28 d)	BSAF (unitless)	0.56 to 0.73	Matten et al. (2021)
DNNDSA	Oligochaete worm (*T. tubifex*)	200 µg/g dw (nominal concentration in sediment) (28 d)	BSAF (unitless)	3.30 to 4.42	Matten et al. (2021)

Abbreviations: BCF, bioconcentration factor; BAF_k, kinetic bioaccumulation factor; BSAF, biota-sediment accumulation factor

7. Potential to cause ecological harm

7.1 Ecological effects assessment

Limited experimental data are available for the toxicity of the substances under assessment, in all compartments. For this reason, analogue data are included in the ecological effects assessment.

7.1.1 Mode/mechanism of action

The manner in which a chemical interacts with biological macromolecules and exerts toxicity is relevant to the overall determination of its hazard potential. A difference in ecotoxicological potency can be seen between substances with a narcotic mode of action (MoA) and those with a non-narcotic MoA. In general, non-narcotic effects typically occur at lower tissue concentrations than narcotic effects.

Wallace et al. (2020) exposed embryonic frogs (*Silurana tropicalis)* in water overlaying sand spiked with a range of concentrations of CaDNNSA (17 µg/g to 1393 µg/g) over a 72 h period. A high percentage (94% to 100%) of individuals exposed to 96 mg/kg CaDNNSA or higher in sand had at least one malformation, including axial deformities and improperly coiled guts. The overall body length of embryos was shorter when exposed to 16.5 mg/kg CaDNNSA in sand or more. The EC_{50} value for malformations was estimated to be 40.5 mg/kg CaDNNSA in sand. The concentration of CaDNNSA in the overlying water corresponding to this EC_{50} value in sand was not reported, however, at 200 mg/kg CaDNNSA in sand the corresponding concentration in the water was 13.6 µg/L, therefore at the EC_{50} value, the concentration of CaDNNSA in water was lower than 13.6 µg/L.

S. tropicalis embryos exposed to 96 mg/kg CaDNNSA in sand were subject to targeted analyses for gene expression and metabolite levels. An overall decrease in the glutathione redox cycle was observed, including decreases in relative mRNA levels of enzymes (glutathione S-transferase (gst), glutathione reductase (gsr), glutathione peroxidase (gpx)) and decreases in the glutathione and glutathione disulfide metabolite concentrations. In addition, transcript levels of genes involved in antioxidant capacity and essential amino acid metabolites decreased significantly. It was hypothesized that the decreased body length observed in the *S. tropicalis* embryos may have been related to the decrease in essential amino acid metabolism (Wallace et al. 2020). It was also postulated that the overall decrease in the glutathione redox cycle and increased presence of malformations in embryos exposed to CaDNNSA suggested that cellular oxidative stress was occurring leading to disruptions in normal development (Wallace et al. 2020).

The identification of the ecotoxicological MoA as narcotic or non-narcotic was also investigated by using quantitative structure activity relationship (QSAR) models and calculations of critical body residue (CBR_{50})[5] and lethal activity (LA_{50})[6]. The calculations and summary of the QSAR data are provided in Appendix A.

Using a weight of evidence approach with the available data (Appendix Table A-3), NSAs are considered to have a non-narcotic MoA. The information on MoA informed the selection of an appropriate assessment factor (AF) for MoA (Okonski et al. 2021), as discussed later in this section.

7.1.2 Effects on aquatic organisms

Aquatic toxicity data for low solubility NSAs, including CaDNNSA and BaDNNSA, in fish and several invertebrate species are available from Matten et al. (2020a). In addition, fish, invertebrate and algae data are available for the analogue substance C_9-rich DANSA (ECHA 2018b). Toxicity data for DNNDSA, a high solubility NSA, are available for several invertebrate species from Matten et al. (2020a) and ECHA (2018a). Ecotoxicity modelling was not undertaken for NSAs as these substances are model-difficult as ionizable substances, with most having surfactant properties. The available aquatic toxicity data that were judged to be of reliable quality are described below and are summarized in Table 7-1 for low solubility NSAs and Table 7-2 for DNNDSA.

Fish, algae and invertebrate data were also reported by Greim et al. (1994) for the analogue substance naphthalene sulfonic acids (CAS RN 68153-01-5), as well as fish data for branched and linear butyl derivatives of naphthalene sulfonic acids, sodium salt (CAS RN 91078-64-7). No information was provided on test methods, however, and these data could not be found published elsewhere. Therefore, these data are included in Appendix B, but were not further considered here for critical toxicity value (CTV) selection.

Matten et al. (2020a) conducted early life-stage studies with fathead minnow (*Pimephales promelas)* eggs exposed to sediment and sand spiked with CaDNNSA, and sediment spiked with DNNDSA, with developmental and growth endpoints measured for 21 d (16 days post hatch (dph)). The exposure method followed OECD TG 210 (OECD 2013), where the eggs were suspended in a mesh cup in the water above spiked sediments or sand, except that the test was terminated at 16 dph instead

[5] Critical body residue (CBR_{50}) is defined as the tissue concentration of a substance associated with medial lethality. CBR_{50} is calculated in fish according to the equation: CBR_{50} = (BCF x LC_{50})/MW. A CBR_{50} greater than or equal to 2 mmol/kg indicates baseline narcosis, and a CBR_{50} less than 2 mmol/kg indicates an MoA more potent than baseline narcosis (McCarty and Mackay 1993).

[6] Lethal activity (LA_{50}) is an exposure-based toxicity metric, in which median lethality is expressed as a fraction of water saturation. The LA_{50} is calculated according to the equation: LA_{50}=LC_{50}/WS. An LA_{50} that ranges from greater than or equal to 0.01 to 1.0 indicates baseline narcosis. An LA_{50} of less than 0.01 indicates an MoA more potent than baseline narcosis (Mackay et al. 2014).

of 28 dph. No effects on hatch success and larval growth were observed when fathead minnow eggs were exposed to CaDNNSA and DNNDSA concentrations up to 246 µg/g dw and 798 µg/g dw, respectively, in spiked sediment (~2% organic carbon). These concentrations in sediment resulted in overlying water concentrations in these experiments of up to 5.89 x 10^4 µg/L for DNNDSA, however, the concentration of CaDNNSA in the overlying water was always below the method quantitation limit of 5.40 µg/L, likely due to sorption of CaDNNSA to the sediment. When CaDNNSA was associated with sand (0% organic carbon), this resulted in CaDNNSA concentrations in the overlying water of up to 260 µg/L, which caused decreases in hatch success, larval growth, biomass production, and overall survival of *P. promelas*, with effective concentration for 50% of the population (EC_{50}) values of 15.5 µg/L to 58.3 µg/L and a lethal concentration for 50% of the population (LC_{50}) value of 13.8 µg/L (Matten et al. 2020a).

Matten et al. (2020a) also conducted acute, aquatic exposures with the following freshwater species: the amphipod *Hyalella azteca*, the snail *Planorbella pilsbryi,* and larvae of the mussels *Lampsilis cardium* and *Lampsilis siliquoidea*. The first three species were exposed to BaDNNSA, CaDNNSA, and DNNDSA, while *L. siliquoidea* was exposed only to DNNDSA. The tests with mussel larvae (glochidia) were conducted according to the American Society of Testing and Materials method ASTM (2006), while the studies with juvenile *H. azteca* and mature snail were not conducted with standard methods. Test solutions were prepared as water soluble fractions, since the solubilities of the test substances were unknown. Each species was exposed to five concentrations of each NSA tested for 48 h (mussels) or 96 h. Measured test concentrations of BaDNNSA ranged from <2.88 x 10^{-3} mg/L to 20 mg/L, of CaDNNSA from 0.9 mg/L to 69 mg/L, and of DNNDSA from 2.1 mg/L to 1555 mg/L. CaDNNSA and BaDNNSA were one to two orders of magnitude more acutely hazardous to all of the above species than DNNDSA (Matten et al. 2020a, Tables 7-1 & 7-2).

Toxicity data were available for fish and daphnids for C_9-rich DANSA (ECHA 2018b), which appears to be a good analogue for DNNSA based on their similar structures. Due to its low solubility, water-accommodated fractions (WAFs) were used in testing. Measured concentrations were variable and not directly related to the applied loading rates. In an acute study following OECD TG 203, *Cyprinus carpio* were exposed to 5 nominal WAFs ranging from 4.6 mg/L to 100 mg/L, with measured concentrations ranging from 0.0088 mg/L to 0.33 mg/L. Exposure to C_9-rich DANSA induced no clinical or lethal effects in carp at an average exposure concentration of 0.28 mg/L, which is the no observed effect concentration (NOEC).

A 48 h *Daphnia magna* study with C_9-rich DANSA followed OECD TG 202 (ECHA 2018b). Measured concentrations ranged from 0.071 mg/L to 0.27 mg/L. The 48 h EC_{50} exceeded the average exposure concentration of 0.27 mg/L. Microscopic observation of the immobile daphnids showed test substance attached to their bodies. Therefore, it was assumed that the adverse effect was mechanical rather than caused by the toxicity

of the test substance, as the concentration measured in the highest WAF was higher but caused less effect (ECHA 2018b).

In two studies which followed OECD TG 201 (alga, growth inhibition test), *Raphidocelis subcapitata* (formerly known as *Selenastrum capricornutum* and *Pseudokirchneriella subcapitata*) was exposed to five concentrations of C_9-rich DANSA with measured concentrations of 0.039 mg/L to 1.8 mg/L in one test and 0.015 mg/L to 9.6 mg/L in the other (ECHA 2018b). The measured concentrations dropped significantly (17% to 76%) after 72 hours, due to adhesion to glassware. The most sensitive result from these two studies is a 72h EC_{10} of 0.16 mg/L for cell numbers (yield).

A static-renewal 21 d *Daphnia magna* reproduction test with Ca- C_9-rich DANSA was conducted according to OECD TG 211 (ECHA 2018b). Body length was significantly decreased at the two highest concentrations of 0.20 mg/L and 0.28 mg/L. The EC_{10} for reproduction was determined to be 2.7 mg/L nominal. This effect value was not given as a measured value, however, this concentration is bracketed by nominal concentrations of 2.2 mg/L and 4.6 mg/L which correspond to measured concentrations of 0.14 mg/L and 0.20 mg/L.

In a study which followed OECD TG 202 (*Daphnia* sp. acute immobilisation test) and EU Method C.2 (acute toxicity for *Daphnia*), juvenile *D. magna* offspring were exposed to five concentrations of DNNDSA prepared as water soluble fractions (ECHA 2018a). Test solutions, ranging from 50 mg/L to 234 mg/L, were only reported as nominal values; however, measured concentrations were reported to be 97% to 112% of the nominal values. The 48h EC_{50} for immobilization was 87 mg/L.

The substances from the NSAs Group have a range of physical-chemical properties; consequently, there are differences in how they behave in the environment, such as their sorption to organic matter in sediments, as previously discussed. There are also differences in their aquatic toxicities (Table 7-1; Table 7-2). For this reason, two CTVs were chosen: one for low solubility NSAs (DNNSA, CaDNNSA and BaDNNSA) and one for high solubility NSAs (DNNDSA and CDINSA). The most sensitive aquatic toxicity value for low solubility NSAs, including consideration of data for the analogue substance C_9-rich DANSA, was the 21 day EC_{50} of 0.014 mg/L CaDNNSA for survival of *P. promelas* hatchlings (Table 7-1). This value was selected as the aquatic critical toxicity value (CTV) for low solubility NSAs. A similar EC_{50} value was obtained for *S. tropicalis* hatchlings with CaDNNSA, as described in Section 7.1.1, however, this value was not further considered for the CTV since *S. tropicalis* is a tropical species not considered relevant to the Canadian environment. For high solubility NSAs, the most sensitive value was the 48 h EC_{50} for *D. magna* of 87 mg/L DNNDSA (Table 7-2), which was selected as the aquatic CTV for high solubility NSAs.

To derive the predicted no effect concentrations (PNECs), the CTVs were divided by assessment factors (AFs), employing the method described in Okonski et al. (2021). AFs account for various extrapolations and sources of uncertainty. An endpoint

standardization factor (F_{ES}) is considered for extrapolation from a short-term (acute) to a long-term (chronic) time-frame, from lethal effects (that is, mortality) to sublethal effects (for example, growth, reproduction), and from median effect levels (for example, EC_{50}) to low effect levels (for example, EC_{10}). The AF also accounts for the number of species and organism categories that are represented in the toxicity data set (species variation factor; F_{SV}), and whether the substance has a mode of action that is more toxic than baseline narcosis (mode of action factor, F_{MOA}). The final AF is derived by multiplying the F_{ES}, F_{SV} and the F_{MOA}.

The CTV for low solubility NSAs is from a chronic study with a median-effects lethal endpoint. However, sublethal effect endpoint values from this study were not significantly different than the lethal effects value, which happened to be the lowest value. For this reason, the F_{ES} was chosen to be 5 rather than 10 (Okonski et al. 2021). NSAs are considered to have a non-narcotic mode of action (Section 7.1.1), with the mode of action reflected in the toxicity datasets; therefore, the F_{MOA} is equal to 2 (Okonski et al. 2021). The aquatic toxicity dataset for low solubility NSAs and analogue substance C_9-rich DANSA includes 8 species, covering the 3 species categories (plants, invertebrates and vertebrates); therefore, a F_{SV} of 1 was used. The overall AF of 10 ($F_{ES} \times F_{SV} \times F_{MoA} = 5 \times 1 \times 2$) was applied to the CTV of 0.014 mg/L, resulting in an aquatic PNEC of 0.0014 mg/L for low solubility NSAs.

Table 7-1. Key aquatic toxicity studies considered in choosing a critical toxicity value for low solubility NSAs

Substance	Test organism	Endpoint	Value (mg/L)	Reference
BaDNNSA	Mussel (*L. cardium*)	48 h EC_{50} (larval viability)	0.47	Matten et al. 2020a
BaDNNSA	Snail (*P. pilsbryi*)	96 h LC_{50}	7.8	Matten et al. 2020a
CaDNNSA	Amphipod (*H. azteca*) (juvenile)	96 h LC_{50}	1.4	Matten et al. 2020a
CaDNNSA	Fish *(P. promelas)*	21 d LC_{50}	0.014	Matten et al. 2020a
C_9-rich DANSA	Fish (*C. carpio*)	96h LC_{50}	>0.28	ECHA 2018b
C_9-rich DANSA	Invertebrate (*D. magna*)	48h EC_{50}	>0.27	ECHA 2018b
Ca- C_9-rich DANSA	Invertebrate (*D. magna*)	21 d EC_{10}	0.14 – 0.20	ECHA 2018b
C_9-rich DANSA	Algae (*R. subcapitata*)	72h EC_{10} (yield)	0.16	ECHA 2018b

Abbreviations: LCx, Lethal concentration for x% of the population; ECx, Effect concentration for x% of the population; h, hours; d, days

Table 7-2 Key aquatic toxicity studies considered in choosing a critical toxicity value for high solubility NSAs

Substance	Test organism	Endpoint	Value (mg/L)	Reference
DNNDSA	Mussel (*L. siliquoidea*)	48 h EC_{50} (larval viability)	98.2	Matten et al. 2020a
DNNDSA	Mussel (*L. cardium*)	48 h EC_{50} (larval viability)	123	Matten et al. 2020a
DNNDSA	Amphipod (*H. azteca*) (juvenile)	96 h LC_{50}	> 662	Matten et al. 2020a
DNNDSA	Snail (*P. pilsbryi*)	96 h LC_{50}	123	Matten et al. 2020a
DNNDSA	Invertebrate (*D. magna*)	48h EC_{50}	87	ECHA 2018a

Abbreviations: LCx, Lethal concentration for x% of the population; ECx, Effect concentration for x% of the population; h, hours

The CTV for high solubility NSAs is an acute study with a median-effects endpoint; therefore, an F_{ES} of 10 was selected. The aquatic toxicity dataset for high solubility NSAs, which comprises studies with DNNDSA includes 5 species from only 1 species category (invertebrates); therefore, a F_{SV} of 10 was used (Okonski et al. 2021). NSAs

are considered to have a non-narcotic mode of action (Section 7.1.1), with the mode of action reflected in the toxicity datasets; therefore, the F_{MOA} is equal to 2 (Okonski et al. 2021). The overall AF of 200 ($F_{ES} \times F_{SV} \times F_{MoA} = 10 \times 10 \times 2$) was applied to the CTV of 87 mg/L, resulting in an aquatic PNEC of 0.435 mg/L for high solubility NSAs.

7.1.3 Effects on sediment-dwelling organisms

Matten et al. (2020b) studied the effects of DNNDSA, CaDNNSA, and BaDNNSA on two species of benthic invertebrates (the amphipod *H. azteca* and the worm *T. tubifex*) in chronic exposure tests in natural sediment with 2% organic carbon. Tests with *T. tubifex* used a nominal concentration range of 200 mg NSA/kg dw to 10 000 mg NSA/kg dw sediment, whereas tests with *H. azteca* used 100 mg NSA/kg dw to 2000 mg NSA/kg dw of sediment. The endpoints studied were mortality, growth, biomass, and juvenile production. The most sensitive effect values from these studies are included in Table 7-3. Effect values ranged from 89.4 mg/kg dw to 261 mg/kg dw. Tests similar to those described above were also conducted in sand with 0% OC, but are not discussed here, as the endpoints from the sediment studies are considered to be more representative of realistic environmental conditions.

When LC_{50} values were estimated based on concentrations of NSAs measured in overlying water (which can be an important route of exposure for *H. azteca*, BaDNNSA and CaDNNSA were 3 to 4 orders of magnitude more hazardous than DNNDSA (Matten et al. 2020b). The toxicity estimates based on the concentrations in overlying water are not further considered here as the substance concentrations in the overlying water varied considerably during the tests (between 21% and 91%), whereas the variation in concentrations in the sediment during the tests was lower (Matten et al. 2020b).

As the sediment toxicity values for both low solubility and high solubility NSAs were within the same order of magnitude, only one CTV was selected, and one PNEC derived. The CTV selected was the 28d EC_{10} of 89.4 mg/kg DNNDSA for juvenile production in *T. tubifex*. The PNEC was calculated by applying an AF to the sediment CTV. Since the CTV is a chronic study with a low-effects sublethal endpoint, an F_{ES} of one was chosen (Okonski et al. 2021). A F_{MoA} of 2 was used, as discussed in Section 7.1.1, and an F_{SV} of 20 was applied, as only one organism category, invertebrates, is represented. This gives an overall AF of 40, ($F_{ES} \times F_{SV} \times F_{MoA} = 1 \times 2 \times 20$), which results in a sediment PNEC of 2.24 mg/kg dw.

Table 7-3. Key sediment toxicity values considered in choosing a critical toxicity value for sediment (Matten et al. 2020b)

Common name	Test organism	Endpoint	Value (mg/kg dw)
BaDNNSA	*H. azteca*	28d LC_{10}	256
BaDNNSA	*T. tubifex*	28d EC_{10} (juvenile production)	124
CaDNNSA	*H. azteca*	28d EC_{10} (growth)	173
CaDNNSA	*T. tubifex*	28d EC_{25} (juvenile production)	307
DNNDSA	*H. azteca*	28d LC_{50}	>188
DNNDSA	*T. tubifex*	28d EC_{10} (juvenile production)	89.4

Abbreviations: dw: dry weight; LCx: Lethal concentration for x% of the population; ECx: Effect concentration for x% of the population

7.1.4 Effects on soil-dwelling organisms

Data on the soil toxicity of NSAs were very limited. Data were available for an earthworm study with the analogue substance naphthalenesulfonic acid, bis(1-methylethyl)-, Me derivs., sodium salts (CAS RN 68909-82-0) (ECHA 2019b), which appears to be a good analogue for CDINSA. Following the OECD test guideline for earthworm reproduction, adult earthworms (*Eisenia fetida*) were exposed to the test substance at nominal concentrations of 15.6 mg/kg dw to 500 mg/kg dw artificial soil, for 8 weeks. Table 7-4 summarizes the key (nominal) results from this study. There were no statistically significant differences in reproduction or body weight gain for treatment concentrations up to 250 mg/kg dw. However, at 500 mg/kg dw, reproduction (measured at 8 weeks) and body weight gain (measured at 28 days) were significantly reduced. No pathological symptoms or behavioural changes were observed over the test period.

As only one soil study was available, the data from this study were used to select a CTV and derive a PNEC for both low solubility and high solubility NSAs. The CTV selected for soil was the 8-week NOEC of 250 mg/kg dw for earthworm reproduction (Table 7-4). To calculate the PNEC, an overall assessment factor of 50 was applied to the CTV, which comprises an F_{ES} of 1, as no extrapolations were required to standardize this endpoint, a F_{MoA} of 2 and a F_{SV} of 50, as data for only one organism category and species were available. The overall AF of 100 ($F_{ES} \times F_{SV} \times F_{MoA} = 1 \times 2 \times 50$) was applied to the CTV of 250 mg/kg dw, resulting in a soil PNEC of 2.5 mg/kg dw.

Table 7-4. Key soil toxicity values for naphthalenesulfonic acid, bis(1-methylethyl), Me derivs., sodium salts with the earthworm (*E. fetida)* (ECHA 2019b)

Endpoint	Value (mg/kg dw)
8 week EC_{50} (reproduction)	398
8 week NOEC (reproduction)	250
8 week LOEC (reproduction)	500[a]
8 week NOEC (mortality)	500

Abbreviations: dw: dry weight; NOEC: No observed effect concentration; LOEC: Lowest observed effect concentration; LCx: Lethal concentration for x% of the population; ECx: Effect concentration for x% of the population
[a] unbounded value

7.2 Ecological exposure assessment

As previously explained, the substances from the NSAs Group were divided into two subgroups. DNNSA, CaDNNSA, and BaDNNSA form the low solubility subgroup and CDINSA and DNNDSA form the high solubility subgroup. Aquatic exposure scenarios were prepared for these two subgroups.

The exposure scenarios are based on information reported for these substances in response to CEPA section 71 surveys (Environment Canada 2013; ECCC 2018). The exposure scenarios include aquatic releases from lubricant oil blending, use of metal working fluids, formulation of paints and coatings, formulation of oil and gas products, formulation of fuels and industrial use of paints. Scenarios for exposure to soil via the application of biosolids to land, and exposure in sediment via equilibrium in the water column were prepared as an extension of the aquatic scenarios. Each of these scenarios is described in more detail below. It was assumed that any of the substances within each subgroup could be substituted for another substance in the same subgroup for a given application, and therefore a company's usage quantity for a given application was summed within the subgroup. However, it was assumed that low solubility NSAs would not be substituted for high solubility NSAs and vice versa, if only one type of NSA was reported under the CEPA section 71 surveys for a given use.

An exposure scenario was not prepared for the use of lubricants and greases containing NSAs. It was determined that these uses would result in negligible environmental exposure, as these products are typically recycled or disposed at waste facilities according to provincial/territorial programs and are therefore not expected to be discharged to the environment.

An exposure scenario was also not prepared for the use of NSAs in oil and natural gas extraction products during oil field applications as the process waters and wastes are

generally not discarded to a sewer or the aquatic environment. Injection for well stimulation and deep well injection of the process water are the most common methods of disposal of this wastewater in North America (OECD 2012).

7.2.1 Measured concentrations in environmental media and wastewater

Limited data were found on measured environmental concentrations of NSAs in Canada. Sediment samples were collected from 12 river sites across southern Ontario and were analysed for CaDNNSA. The sites had a range of urban land use in their upstream catchment and were all less than 1 km downstream from a WWTS. Trace levels of CaDNNSA were found at 11 of the 12 sites. The highest concentration found was 2.8 mg/kg dw (Matten et al. 2020b).

DNNDSA, BaDNNSA and CaDNNSA were not detected in the effluent from four Canadian WWTSs, which had either primary treatment or lagoon treatment, at method detection limits of 0.46 µg/L to 3.6 µg/L (Personal communication, e-mail from CMP Research and Monitoring Section to Ecological Assessment Division, ECCC, dated July 15, 2019, unreferenced). Some metalworking facilities and oil and gas product formulation facilities discharge their effluents to these four WWTSs. However, it is not known whether these facilities use NSAs, or, assuming they do, if they may have discharged NSAs during periods when the WWTS sampling occurred.

7.2.2 Calculation of PECs and general assumptions

Aquatic predicted environmental concentrations (PECs) for each exposure scenario were calculated using the following equation:

$$\mathrm{PEC} = \frac{10^9 \text{ x } \mathrm{Q} \text{ x } \mathrm{L} \text{ x } (1 - \mathrm{R})}{\mathrm{D} \text{ x } \mathrm{N}}$$

Where,

PEC = Predicted Environmental Concentration (µg/L)

Q = Quantity used per site per year (kg/year)

L = Losses to wastewater (fraction)

R = WWTS removal efficiency (fraction)

D = Daily dilution volume (L/day)

N = number of days of release (days/year)

10^9 = conversion factor from kg to µg (µg/kg)

Due to the lack of measured data for NSAs, a range of WWTS removal efficiency rates were estimated using SimpleTreat 3.1 (2003) as well as professional judgement based on the sorption behaviour of the substances. A WWTS removal rate range of 0% to 20% was used for high solubility NSAs. For the low solubility NSAs that have stronger affinity to solids, a WWTS removal efficiency range of 85% to 95% was used. Ranges were used for the WWTS removal rates for low solubility and high solubility NSAs, to account for uncertainty with the actual removal rates and also for variability between the substances within each subgroup. Exposure estimates were prepared using both the lower end and upper end of the removal rate ranges to provide a range of possible PECs for each subgroup.

Daily dilution volumes were calculated by multiplying the effluent flow of WWTS or facilities discharging to a receiving water body by the dilution factor of the receiving water body. In all scenarios, aquatic PECs were derived using a dilution factor based on the 10^{th} percentile low flow of the receiving water body and capped at a maximum dilution factor of 10.

The aquatic PECs represent potential concentrations of the substances in the receiving water body near the discharge point of a WWTS. The PEC values are presented in each exposure scenario and a summary of key assumptions are provided in Appendix C. Potential releases via container cleaning and transport including loading and unloading are not considered in this assessment.

7.2.3 Exposure scenario 1: Lubricant oil-blending

On the basis of information reported for NSAs in response to CEPA section 71 surveys (Environment Canada 2013; ECCC 2018), one of the main uses of low solubility NSAs is as an additive in lubricants. Therefore, a scenario was developed to reflect the possible releases of low solubility NSAs to WWTS and water bodies from lubricant oil blending facilities in Canada. There are over 10 companies in Canada that manufacture and/or blend lubricant products, located in various regions across Canada.

The aquatic PEC for a generic representative blending facility was calculated based on compiled data from different sources. The scenario is based on import quantities from a number of companies, where an average value of these individual company import quantities was used as a representative facility usage quantity. It is assumed that a representative facility discharges its effluent via an off-site secondary, tertiary or lagoon WWTS. The daily dilution volume selected is a representative value for the lubricant oil-blending sector. Refer to Table C-1 in Appendix C for a summary of key assumptions.

The calculated generic aquatic PECs for this scenario range from 0.16 µg/L to 0.49 µg/L.

7.2.4 Exposure scenario 2: Use of metal working fluids

Based on information reported for the substances in response to CEPA section 71 surveys (Environment Canada 2013; ECCC 2018), low solubility NSAs are used as a corrosion inhibitor or anti-scaling agent in metalworking fluids used to coat metal parts. Therefore, a scenario was developed to reflect the possible releases of low solubility NSAs to WWTS from facilities that use metalworking fluids to coat metal parts.

Usage in metalworking fluids may occur in multiple facilities located across Canada, ranging in operation size and location. Specific information on the users of metalworking fluids containing NSAs is unknown. This scenario considers a generic situation where an industrial facility uses metalworking fluids containing low solubility NSAs throughout the year.

Parameters such as production capacity, emission factor, and days of release were based on data from the OECD (2011) emission scenario document on the use of metalworking fluids. The daily dilution volume selected is the 10th percentile value of a distribution of daily dilution volumes covering a variety of plants involved in activities requiring use of metalworking fluids. The facilities involved in these activities are assumed to have some on-site treatment of their wastewater in the form of an oil/water separator prior to releasing to the sewer system for further treatment at a WWTS. Refer to Table C-2 of Appendix C for a summary of assumptions used to calculate the PECs.

The resulting aquatic PECs from this scenario range from 0.42 µg/L to 1.3 µg/L.

7.2.5 Exposure scenario 3: Formulation of paints and coatings

According to information reported for NSAs in response to CEPA section 71 surveys (Environment Canada 2013; ECCC 2018), both high and low solubility NSAs are used as process regulators as well as oxidizing and reducing agents in the formulation of paints and coatings. This scenario considers the use of NSAs in the formulation of paints and coatings. Releases from these facilities are expected to enter WWTSbefore being released to the environment.

The scenario is based on the largest reported import quantity of NSAs by a formulation facility in this sector. The daily dilution volume selected is the 10th percentile value of a distribution of daily dilution volumes developed for the Canadian paints and coatings sector. A summary of key assumptions for this scenario is provided in Table C-3 of Appendix C.

The calculated aquatic PECs for high solubility NSAs in this scenario range from 1.8 µg/L to 2.3 µg/L, while PECs for low solubility NSAs range from 0.11 µg/L to 0.34 µg/L.

7.2.6 Exposure scenario 4: Formulation of oil and gas products

Based on information reported for NSAs in response to CEPA section 71 surveys (Environment Canada 2013; ECCC 2018), high solubility NSAs are used as processing aids in products used for oil and gas extraction. Therefore, this scenario looked at the release of high solubility NSAs to WWTS from the formulation of these products.

The estimated PECs considered a generic scenario where a facility is formulating products for oil and gas extraction and discharging to a secondary or tertiary WWTS. The daily dilution volume selected is the 10^{th} percentile value of a distribution of daily dilution volumes for a variety of Canadian industrial facilities. Refer to Table C-4 of Appendix C for a summary of key assumptions used to calculate the PEC.

The resulting PECs from this scenario range from 78 µg/L to 98 µg/L.

7.2.7 Exposure scenario 5: Formulation of fuels

On the basis of information reported for NSAs in response to CEPA section 71 surveys (Environment Canada 2013; ECCC 2018), low solubility NSAs are used as an additive in fuels. Therefore, a scenario was developed to reflect the possible releases of low solubility NSAs to water bodies from facilities in Canada where additives may be added to fuels.

The aquatic PEC for a generic representative blending facility was calculated based on compiled data from different sources. The scenario is based on import quantities from a number of companies, where an average value of these individual company import quantities was used as a representative usage quantity. It is assumed that a representative facility would have on-site treatment equivalent to a secondary treatment level and would afterwards discharge directly to the receiving water body. The daily dilution volume selected is a representative value for the fuel blending sector. Refer to Table C-5 in Appendix C for a summary of key assumptions.

The calculated generic aquatic PECs for this scenario range from 0.010 µg/L to 0.030 µg/L.

7.2.8 Exposure scenario 6: Industrial use of paints

According to information reported for NSAs in response to CEPA section 71 surveys (Environment Canada 2013; ECCC 2018)), as well as from the Canadian Vehicle Manufacturers' Association (CVMA) (personal communication, email from CVMA to Products Division, ECCC, dated August 2, 2019; unreferenced), high solubility NSAs are used in industrial paints, including in the automotive sector. Therefore, a scenario was developed to reflect the possible releases of high solubility NSAs to WWTSfrom facilities that use paints in automotive original equipment manufacturing (OEM).

OEM painting is automated and overspray is collected in waterwash booths of downdraft or crossdraft design where water is used almost exclusively to collect overspray in OEM (US EPA 1996). The US EPA generic scenario for automobile spray coating (US EPA 1996) was adapted to calculate the PEC for a site where painting occurs, using the following equation:

$$PEC = \frac{10^9 \times Q \times (1 - TE) \times (1 - R)}{D \times N}$$

Where,

Q = quantity used (kg/year)

TE = Average transfer efficiency for the spraying processes (fraction)

R = WWTS removal efficiency (fraction)

D = daily dilution volume (L/day)

N = number of release days (days/year)

The aquatic PEC was calculated based on compiled data from different sources. Parameters such as days of release were based on data from the US EPA generic scenario for automobile spray coating (US EPA 1996) while the transfer efficiency was based on the OECD emission scenario document on the coating industry (OECD 2009). Parameters such as discharge methods, on-site and off-site treatment systems, and wastewater flow were based on information representing relevant automotive manufacturing facilities in Canada. The use quantity is derived from the reported import quantity converted to a range, with the high end of the range used in the calculations (ECCC 2018). Refer to Appendix Table C-6 for a summary of key assumptions used to calculate the PECs.

The resulting aquatic PECs range from 120 µg/L to 190 µg/L.

7.2.9 Exposure in sediment

A sediment-water equilibrium partitioning approach was used to estimate the PEC of NSAs in bottom sediment. This approach is based on the European Chemicals Agency's guidance on environmental exposure estimation for suspended sediment (ECHA 2012) and on an equilibrium partitioning approach for bottom sediment described by the US EPA's National Center for Environmental Assessment (US EPA 2003). At equilibrium, the PEC in bottom sediment linearly correlates with the concentration in the aqueous phase of the overlying water. Characteristics of suspended and bottom sediments as suggested by Gobas (2007 and 2010) were used

in the estimation. The PEC in bottom sediment (in mg/kg) is calculated using the following equation:

$$PEC_{sediment} = 3\% \times K_{OC} \times \frac{C_{total}}{1 + 7.05 \times 10^{-6} kgOC / L \times K_{oc}}$$

Where,

C_{total} = total concentration in the water column (mg/L)

K_{oc} = organic carbon-water partition coefficient for suspended or bottom sediment (L/kgOC)

Ranges of PECs in bottom sediment, standardized to 3% organic carbon (a typical organic carbon content in bottom sediment for rivers and lakes in Canada), were estimated for scenarios 1 to 6 above. A log K_{OC} value of 1.1 was used as a representative value for higher solubility NSAs, while a log K_{OC} of 5.1 was used to represent the lower solubility NSAs. Sediment PECs are provided in Table 7-5. A summary of additional assumptions used are provided in Tables C-7 to C-12 of Appendix C. Note that the total concentration in the water column was calculated using the 50th percentile flows rather than 10th percentile flows. This was done in order to reflect a more average exposure period in receiving water bodies needed to reach equilibrium in sediment.

Table 7-5. PECs for sediment

Scenario	PEC (mg/kg)
1- Lubricant oil blending (low solubility NSAs)	0.19 – 0.56
2- Use of metalworking fluids (low solubility NSAs)	0.55 – 1.7
3a- Formulation of paints and coatings (high solubility NSAs)	<0.010
3b- Formulation of paints and coatings (low solubility NSAs)	0.23 – 0.68
4- Formulation of oil and gas products (high solubility NSAs)	<0.010
5- Formulation of fuels (low solubility NSAs)	0.020 – 0.059
6- Industrial use of paints (high solubility NSAs)	<0.010

7.2.10 Biosolids application to land

This scenario considered the application of NSAs to soil in the form of biosolids from WWTS. Soil PECs were calculated for scenarios 1 to 6 above as an extension of these aquatic scenarios.

The soil PEC after 10 years of biosolids application and considering biodegradation as a loss mechanism, is calculated by iterating the equations below. Degradation is assumed to be a first order reaction. Concentrations in soil were determined on a yearly basis immediately after application of biosolids and at the end of the year (after

biodegradation has occurred, but prior to the subsequent biosolids application) over a 10-year period.

At the beginning of the year (directly after biosolids application):

$$PEC_{beginning,t} = \frac{C_s \times A}{d \times \rho} + PEC_{end,t-1}$$

(note that $PEC_{beginning,1} = \frac{C_s \times A}{d \times \rho}$)

At the end of the year (after biodegradation):

$$PEC_{end,t} = PEC_{beginning,t} \times e^{\left(-0.693 \times \left(\frac{365}{biodeg}\right)\right)}$$

Where,

$PEC_{beginning}$ = Predicted Environmental Concentration in soil at the beginning of the year after application of biosolids (before biodegradation) (mg/kg)

PEC_{end} = Predicted Environmental Concentration in soil at the end of the year (after biodegradation), prior to subsequent application of biosolids (mg/kg)

t = Years of biosolids land application (y), varying from 1 to 10 years

C_s = Concentration of the substance in biosolids (mg/kg dw)

A = Annual biosolids land application rate (kg/m^2-y)

d = Soil mixing depth (m)

ρ = Dry soil density (kg/m^3)

Biodeg = Biodegradation half-life of the substance in soil (days)

A range of biodegradation half-lives of 92 days to 200 days was used for NSAs to reflect the variability in their potential biodegradation rates owing to differences in their structures. The concentration of NSAs in soil does not greatly increase over the 10-year period and soil concentrations are maximal after application (decreasing significantly afterwards over the year). The calculated PECs at the start of the 10th year for each scenario are provided in Table 7-6. A summary of key assumptions used are provided in Tables C-13 to C-18 of Appendix C.

Table 7-6. Soil PECs from biosolids application to land at the start of the 10th year

Scenario	PEC (mg/kg dw)
1- Lubricant oil blending (low solubility NSAs)	0.74 to 1.4
2- Use of metalworking fluids (low solubility NSAs)	0.63 to 0.92
3a- Formulation of paints and coatings (high solubility NSAs)	0 to 0.05
3b- Formulation of paints and coatings (low solubility NSAs)	0.16 to 0.24
4- Formulation of oil and gas products (high solubility NSAs)	0 to 2.0
5- Formulation of fuels	n/a*
6- Industrial use of paints (high solubility NSAs)	0 to 0.26

Abbreviations: dw, dry weight; n/a, not applicable

*: biosolids from industrial facilities discharging directly to the receiving environment following on-site treatment are not applied to land; it is assumed that facilities in this sector are direct dischargers

7.3 Characterization of ecological risk

The approach taken in this ecological screening assessment was to examine assessment information and develop conclusions using a weight-of-evidence approach and precaution. Evidence was gathered to determine the potential for substances in the NSAs Group to cause harm in the Canadian environment. Lines of evidence considered include those evaluated in this assessment that support the characterization of ecological risk in the Canadian environment. Reliable secondary or indirect lines of evidence were considered when available, including classifications of hazard or fate characteristics made by other regulatory agencies.

7.3.1 Ecological risk classification of organic substances (ERC)

NaNSA was identified as having a low potential to cause ecological harm via the ecological risk classification of organic substances (ERC) (ECCC 2016a). The ERC is a risk-based approach that considers multiple metrics for both hazard and exposure based on weighted consideration of multiple lines of evidence for determining risk classification. The approach is summarized in Appendix D. Critical data and considerations used to develop the substance-specific profile for NaNSA are available in ECCC (2016b).

On the basis of low hazard and low exposure classifications according to ERC, NaNSA was classified as having a low potential for ecological risk. It is therefore unlikely that this substance is resulting in concerns for the environment in Canada.

7.3.2 Risk quotient analysis

Risk quotient analyses were performed by comparing the various estimates of exposure (PECs; see the Ecological Exposure Assessment section) with ecotoxicity information

(PNECs; see the Ecological Effects Assessment section) to determine whether there is potential for ecological harm in Canada. Risk quotients (RQs) were calculated by dividing the PEC by the PNEC for relevant environmental compartments and associated exposure scenarios. Tables 7-7, 7-8 and 7-9 present RQs for aquatic, soil, and sediment compartments for the NSAs group, respectively.

Table 7-7. Risk quotient (RQ) calculations for aquatic industrial exposure scenarios for NSAs Group

Exposure scenario	Aquatic PEC (µg/L)	Aquatic PNEC (µg/L)	Aquatic RQ
Lubricant oil blending, low solubility NSAs	0.16 to 0.49	1.4	0.12 to 0.35
Use of metalworking fluids, low solubility NSAs	0.42 to 1.3	1.4	0.30 to 0.90
Formulation of paints and coatings, high solubility NSAs	1.8 to 2.3	435	<0.010
Formulation of paints and coatings, low solubility NSAs	0.11 to 0.34	1.4	0.081 to 0.24
Formulation of oil and gas products, high solubility NSAs	78 to 98	435	0.18 to 0.22
Formulation of fuels, low solubility NSAs	0.010 to 0.030	1.4	<0.010 to 0.021
Industrial use of paints, high solubility NSAs	120 to 190	435	0.28 to 0.44

Table 7-8. Risk quotient (RQ) calculations for sediment industrial exposure scenarios for NSAs Group

Exposure scenario	Sediment PEC (mg/kg dry wt)	Sediment PNEC (mg/kg dry wt)	Sediment RQ
Lubricant oil blending, low solubility NSAs	0.19 to 0.56	2.24	0.084 to 0.25
Use of metalworking fluids, low solubility NSAs	0.55 to 1.7	2.24	0.25 to 0.74
Formulation of paints and coatings, high solubility NSAs	<0.010	2.24	<0.010
Formulation of paints and coatings, low solubility NSAs	0.23 to 0.68	2.24	0.10 to 0.31
Formulation of oil and gas products, high solubility NSAs	<0.010	2.24	<0.010
Formulation of fuels, low solubility NSAs	0.020 to 0.059	2.24	<0.010 to 0.027

Exposure scenario	Sediment PEC (mg/kg dry wt)	Sediment PNEC (mg/kg dry wt)	Sediment RQ
Industrial use of paints, high solubility NSAs	<0.010	2.24	<0.01

Table 7-9. Risk quotient (RQ) calculations for soil industrial exposure scenarios for NSAs Group

Exposure scenario	Soil PEC (mg/kg)	Soil PNEC (mg/kg)	Soil RQ
Lubricant oil blending, low solubility NSAs	0.74 to 1.4	2.25	0.30 to 0.58
Use of metalworking fluids, low solubility NSAs	0.63 to 0.92	2.25	0.25 to 0.37
Formulation of paints and coatings, high solubility NSAs	0 to 0.05	2.25	0 to 0.020
Formulation of paints and coatings, low solubility NSAs	0.16 to 0.24	2.25	0.065 to 0.094
Formulation of oil and gas products, high solubility NSAs	0 to 2.0	2.25	0 to 0.82
Formulation of fuels, low solubility NSAs	n/a*	2.25	n/a*
Industrial use of paints, high solubility NSAs	0 to 0.26	2.25	0 to 0.11

Abbreviation: n/a, not applicable

*: biosolids from industrial facilities discharging directly to the receiving environment following on-site treatment are not applied to land; this is assumed to be the case for the facilities in this sector

The above RQs (Tables 7-7, 7-8, 7-9) are all below one, which indicates that NSAs have low to moderate potential to cause harm to aquatic, sediment or soil organisms as a result of their potential releases from industry. The parameter values used in the generic exposure scenarios employed a combination of different assumptions ranging from average to realistic worst case, to calculate the PECs. Site specific exposure analyses, which are not included in this screening assessment owing to confidential business information, were prepared for some of the exposure scenarios. These site-specific analyses had associated PECs which were similar or below those for the generic scenarios detailed here. These analyses add confidence that NSAs have low potential to cause harm to the environment at current exposure levels.

7.3.3 Consideration of the lines of evidence

To characterize the ecological risk of the NSAs Group, technical information for various lines of evidence was considered (as discussed in the relevant sections of this report) and qualitatively weighted. The key lines of evidence supporting the assessment

conclusion are presented in Table 7-10, with an overall discussion of the weight of evidence provided in section **Error! Reference source not found.**. The level of confidence refers to the combined influence of data quality and variability, data gaps, causality, plausibility and any extrapolation required within the line of evidence. The relevance refers to the impact the line of evidence has when determining the potential to cause harm in the Canadian environment. Qualifiers used in the analysis ranged from low to high, with the assigned weight having five possible outcomes.

Table 7-10. Weighted lines of key evidence considered to determine the potential for NSAs to cause harm in the Canadian environment

Line of evidence	Level of confidence[a]	Relevance in assessment[b]	Weight assigned[c]
Similarity in analogue chemical structure for read-across purposes - C_9-rich DANSA and Ca- C_9-rich DANSA to DNNSA, BaDNNSA and CaDNNSA	High	High	High
Physical-chemical properties	Low	Moderate	Low-Moderate
Environmental distribution	Moderate	Moderate	Moderate
Persistence in the environment	Low	High	Moderate
Long-range transport	Moderate	Low	Low-Moderate
Bioaccumulation in aquatic organisms	Moderate	Moderate	Moderate
Mode of action and/or other non-apical[d] data	Moderate	High	Moderate-High
PNECs for aquatic organisms, low solubility NSAs	High	High	High
PNEC for aquatic organisms, high solubility NSAs	Moderate	High	Moderate-High
PNEC for soil-dwelling organisms	Low	High	Moderate
PNEC for sediment-dwelling organisms	Moderate	High	Moderate-High
PECs in water	Moderate	High	Moderate-High
PECs in soil	Moderate	High	Moderate-High
PECs in sediment	Moderate	High	Moderate-High
RQs for water	Moderate	High	Moderate-High
RQs for soil	Low	High	Moderate
RQs for sediment	Moderate	High	Moderate-High

[a] Level of confidence is determined according to data quality, data variability, data gaps (that is, are the data fit for purpose).
[b] Relevance refers to the impact of the evidence in the assessment.
[c] Weight is assigned to each line of evidence according to the overall combined weights for level of confidence and relevance in the assessment.
[d] Non-apical endpoints refer to endpoints other than mortality, growth, reproduction (that is, those endpoints identified with population-level effects).

7.3.4 Weight of evidence for determining potential to cause harm to the Canadian environment

The physical-chemical properties and other parameter values selected for NSAs were informed by a combination of experimental, modelled, and read-across data, depending on availability of information. The weight of evidence supporting the selected parameters varied depending on the source (that is, experimentally obtained versus modelled) and reflect the limited dataset.

Given the uncertainty associated with the modelling of these substances, which are ionizing and have surfactant properties, the risk assessment was based on read-across and empirical evidence where possible, and ranges of values were used in the exposure assessment, to mitigate the impact of these uncertainties on the overall assessment.

Environmental persistence was informed using empirical data for other naphthalene sulfonic acids, analogue substances, as well as modelling. The empirical biodegradation and modelled data indicate that NSAs, other than NaNSA, are likely to persist in the environment long enough to cause chronic effects.

No empirical information was available on whether NSAs undergo long-range transport in the environment. Given their physical-chemical properties (that is, negligible vapour pressure, low Henry's law constants), it is not expected that NSAs will undergo long-range transport in air. High solubility NSAs are expected to be mobile in water, however their potential for long-range transport in water also depends on their half-lives in water, which are not known.

Limited empirical data were available for bioaccumulation of NSAs. These data indicate that DNNDSA, CaDNNSA and BaDNNSA do not appear to be bioaccumulative. Therefore, DNNSA, which is structurally similar to CaDNNSA and BaDNNSA, and CDINSA, which is structurally similar to DNNDSA, are also unlikely to be bioaccumulative. The limited empirical data, and lack of empirical data for DNNSA and CDINSA, means that there is only moderate confidence that these substances are not likely to bioaccumulate to a considerable degree.

The mode of action characterization was informed by one empirical study, as well as modelled data. This resulted in moderate confidence in the determination of the MoA of NSAs. The PNECs for aquatic (high solubility NSAs), sediment and soil organisms were determined using small datasets, resulting in low to moderate confidence in these PNECs. There is high confidence in the aquatic PNEC for low solubility NSAs, as a relatively large toxicity dataset of good quality data was available, including chronic data for all trophic levels.

The reliability of the PECs considers a number of factors, including the WWTS removal rate, physical-chemical property data, the usage quantity, the industrial emission factor, and the daily dilution water volume of the receiving environment.

Due to the limitations in the available data, the confidence in the PECs is moderate.

The RQs and other information discussed above indicate that the NSAs Group has low potential to cause ecological harm in Canada. While exposure of the environment to the NSAs Group is not of concern at current levels, the low solubility NSAs (DNNSA, BaDNNSA and CaDNNSA) are considered to have an environmental effect of concern on the basis of their potential effects on aquatic organisms. Therefore, there may be a concern if exposure levels were to increase.

7.3.5 Sensitivity of conclusion to key uncertainties

Substances with ionizing and surfactant properties such as NSAs, as well as being UVCBs, pose a challenge for risk assessment due to their physical-chemical properties and toxicities being difficult to measure in empirical studies. They are also challenging from a modelling perspective, which adds uncertainty to the assessment conclusions. Reliance on empirical or modelled physical chemical properties that are of questionable validity for these substances (such as log K_{ow}) was minimized as much as possible. As well, a range of values were used for relevant parameters in the exposure scenarios, such as for WWTS removal rates and biodegradation half-life values, to compensate for the lack of certainty in these values, as well as to account for possible differences in values between different NSAs. As such, additional information about these properties would likely have a low impact on the conclusion.

Usage quantities used in the exposure scenarios were based on information obtained through CEPA section 71 surveys. As there was limited information on the use quantities, import quantities were used for the calculations in the exposure scenarios. Additionally, information was lacking on the clients of the importers of these substances. In the absence of complete data, a number of assumptions were made in order to derive PEC values. For example, it was assumed that reported quantities from two survey years (2011 and 2015) are reflective of quantities used in the current year. In addition, when relevant, due to the lack of facility-relevant use quantities, it was assumed that the total import quantity reported by a company could be used at each of its facilities. There was limited information on percent composition of products containing NSAs, so this parameter was derived from relevant material safety data sheets (MSDS) as well as OECD Emission Scenario Documents. Assumptions were also made about the treatment technologies at industrial facilities. In addition, it was assumed that any of the substances within each subgroup (that is, low solubility, high solubility) could be substituted for another for a given application. However, it was assumed that low solubility NSAs would not be substituted for high solubility NSAs and vice versa, if only one type of NSA was reported under the CEPA section 71 surveys for

a given usage. Better industrial usage and composition data would have increased the certainty in the PECs.

8. Potential to cause harm to human health

BaDNNSA and CDINSA were considered under the approach applied in the Rapid screening of substances with limited general population exposure screening assessment (ECCC, HC 2018). In the approach, Health Canada determined if the substances required further evaluation of potential to cause harm to human health on the basis of the potential for direct and indirect exposure to the general population. The potential for direct exposure was evaluated on the basis of considerations such as evidence of the substance being present in a product used by the general population, and the potential for indirect exposure was adopted from the general approach reported in the Threshold of Toxicological Concern (TTC)-based Approach for Certain Substances science approach document (Health Canada 2016). On the basis of the evaluation of both direct and indirect exposure conducted as part of this approach, exposure of the general population to BaDNNSA and CDINSA was considered to be negligible. Therefore, BaDNNSA and CDINSA are considered to be a low concern for human health at current levels of exposure. Additional details with regards to data and considerations used in the TTC-based approach are presented in the science approach document (Health Canada 2016).

8.1 Exposure assessment

8.1.1 Environmental media and food

NaNSA

No reports of measured concentrations of NaNSA in environmental media or dust in Canada or elsewhere were identified. The only uses reported in response to CEPA section 71 surveys (Environment Canada 2013; ECCC 2018) were industrial; on the basis of available information including that which was obtained through follow-up communication with an industry stakeholder, it was determined these uses would not result in exposure for the general population (personal communication, email from a stakeholder to the Existing Substances Risk Assessment Bureau, Health Canada, dated August 2018; unreferenced) (Section 7.3.1).

DNNSA, CaDNNSA and DNNDSA

As described in Section 7.2, trace levels of CaDNNSA (up to 2.8 µg/g dw) were found in sediment samples at 11 of 12 river sites across southern Ontario (Matten et al. 2020b). Neither DNNSA nor DNNDSA were identified to be present in environmental media in

Canada or elsewhere. DNNDSA and CaDNNSA (as well as BaDNNSA) were not detected in the effluent from four Canadian wastewater treatment systems (WWTSs), which had either primary treatment or lagoon treatment, at method detection limits of 0.46 µg/L to 3.6 µg/L (Personal communication, e-mail from CMP Research and Monitoring Section to Ecological Assessment Division, ECCC, dated July 15, 2019, unreferenced). DNNSA, CaDNNSA, and DNNDSA were not identified to be present in dust in Canada or elsewhere.

As indicated in section 6.1, these substances are expected to partition mainly to water, soil and sediment when released to the environment, on the basis of their physical-chemical properties, and current uses in Canada indicate that water, sediment and soil are compartments of interest in the environment. According to information reported for the substances in response to CEPA section 71 surveys (Environment Canada 2013; ECCC 2018), and communication with the Canadian Vehicle Manufacturers' Association (CVMA) (personal communication, email from CVMA to Products Division, ECCC, dated August 2, 2019; unreferenced), these substances are used in industrial settings in Canada and may be released to the environment through treated wastewater and biosolids. The highest predicted environmental concentrations (PECs) for water were 190 µg/L and 1.3 µg/L for high solubility NSAs and low solubility NSAs, respectively. These PECs were associated with possible releases of high solubility NSAs to wastewater treatment systems (WWTS) from facilities that use paints in automotive original equipment manufacturing (OEM) and low solubility NSAs to WWTSs from facilities that use metalworking fluids to coat metal parts (Section 7.2). As a conservative approach, intakes of DNNSA, CaDNNSA and DNNDSA by the general population via drinking water were estimated based on the highest PECs for industrial-release scenarios; these PECs are representative of the highest potential concentrations of the substances in the receiving body of water near the discharge point of a wastewater treatment system (WWTS). Maximal estimates of daily intake from drinking water ranged from 0.023 µg/kg bw/day (9 to 13 year olds and 14 to 18 year olds) to 0.17 µg/kg bw/day (0 to 5 months, formula fed) for DNNSA and CaDNNSA and from 3.3 µg/kg bw/day (9 to 13 year olds and 14 to 18 year olds) to 25 µg/kg bw/day (0 to 5 months, formula fed) for DNNDSA. Exposure from soil is considered to be negligible, and exposure from air is not expected (Appendix E).

Exposure through food to DNNSA from its use as an antistatic agent in the production of a retention aid in the manufacture of paper and paperboard with direct food contact is expected to be negligible (personal communication, emails from the Food Directorate, Health Canada, to the Existing Substances Risk Assessment Bureau, Health Canada, dated October 2018 and April 2019; unreferenced). The highest estimated intake from drinking water (0.17 µg/kg bw/day; 0 to 5 months, formula fed) is carried forward for risk characterization (Appendix E).

Exposure to CaDNNSA through food from its potential use as a lubricant on equipment or machine parts is not expected since there is no contact of the lubricant with food (personal communication, email from the Food Directorate, Health Canada, to the

Existing Substances Risk Assessment Bureau, Health Canada, dated August 2016; unreferenced).

8.1.2 Products available to consumers

NaNSA, DNNSA and DNNDSA

NaNSA, DNNSA and DNNDSA were not identified in products available to consumers in Canada and therefore exposure of the general population to these substances from the use of products available to consumers is not expected.

CaDNNSA

CaDNNSA is present as a corrosion inhibitor (1-5%) in a general purpose aerosol lubricant (SDS 2018). This product is expected to be used by the general population on an intermittent basis, leading to potential exposure via the inhalation and dermal routes. Table 8-1 summarizes the estimated exposures to CaDNNSA from the use of the aerosol lubricant on a per event basis. Details of the parameters used in the exposure estimation are presented in Appendix F.

Table 8-1. Estimated exposures to CaDNNSA from the use of a general purpose aerosol lubricant (per event)

Product scenario (age group)	Product concentration	Inhalation exposure[a] (mg/kg bw)	Dermal exposure[a] (mg/kg bw)	Combined inhalation and dermal exposure[a] (mg/kg bw)
General purpose aerosol lubricant, intermittent exposure (adult, aged 19 years or older)	5%[b]	2.2×10^{-3}	1.1×10^{-2}	1.4×10^{-2}

[a] Dermal and inhalation absorption was assumed to be 100% (that is, equivalent to oral absorption)
[b] The maximum concentration shown on the SDS was used to estimate exposures

8.2 Health effects assessment

NaNSA

NaNSA was not identified as posing a high hazard to human health on the basis of classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity, or reproductive toxicity. It is also not on the European Chemicals Agency's List, or Candidate List of Substances of Very High Concern for Authorisation (ECHA 2018f). Further investigation of health effects is not warranted given that the general Canadian population is not expected to be exposed to this substance.

DNNSA, CaDNNSA, and DNNDSA

A US EPA screening level hazard characterization document of several dinonylnaphthalene substances is available as part of the US HPV Challenge program, which includes DNNSA and CaDNNSA (US EPA 2012). Both DNNSA and CaDNNSA were evaluated as a sub-category, with data being available for oral, inhalation and dermal acute toxicity, as well as eye and skin irritancy and sensitivity. However, no data were identified for repeat-dose, reproductive, or developmental toxicity, or for genotoxicity or carcinogenicity.

A REACH dossier for DNNDSA with empirical data on acute toxicity is available (ECHA 2018a). The other health effects data available for DNNDSA in the REACH dossier are based on read-across from C_9-rich DANSA, Ca- C_9-rich DANSA and Ba- C_9-rich DANSA (ECHA 2018b, 2018c, 2018d).

DNNSA, CaDNNSA and DNNDSA share similar chemical structures; each has a naphthalene ring with one or two sulfonic acid substituents and two C_9 alkyl chains, which may exist in branched or linear configurations. CaDNNSA is an alkaline earth metal salt of DNNSA; it is assumed to dissociate into the DNNSA anion and metal cation upon ingestion and absorption, and is expected to manifest similar toxicological effects to DNNSA. As the overall empirical toxicological database for these substances is limited (no repeat-dose or genotoxicity data available), and given their overall structural similarities, the health effects assessment of DNNSA, CaDNNSA and DNNDSA will be presented together and a read-across approach will be used (DNNDSA is considered sufficiently similar to DNNSA and CaDNNSA for the purpose of read-across, despite differences in water solubility). See Appendix G for details.

For characterization of human health effects for DNNSA, CaDNNSA and DNNDSA, C_9-rich DANSA, Ca- C_9-rich DANSA and Ba- C_9-rich DANSA were used as analogues. These three C_9-rich DANSA substances are considered appropriate analogues as they are mixtures of the corresponding C_8 to C_{10} naphthalenesulfonic acids that contain either DNNSA or CaDNNSA as a major component; the mono- and tri-

alkylnaphthalenesulfonic acid components (that is, with only one or three alkyl substituents) within these DANSA substances are also considered appropriate analogues due to their structural similarity with DNNSA, CaDNNSA and DNNDSA.

Genotoxicity

C_9-rich DANSA (ECHA 2018b) and Ba- C_9-rich DANSA (ECHA 2018d) were both negative for mutagenicity in the Ames test for all *S. typhimurium* and *E. coli* strains up to the highest tested concentration (5000 µg/plate), with and without metabolic activation. Cytotoxicity was observed at 1000 µg/plate and above for C_9-rich DANSA, and at 333 µg/plate and above for Ba- C_9-rich DANSA.

A mouse lymphoma thymidine kinase assay showed that Ba- C_9-rich DANSA is negative for mutagenicity in mammalian cells up to the highest tested concentration (90 µg/mL) with and without metabolic activation, with cytotoxicity observed from 50 µg/mL (with activation) and 70 µg/mL (without activation) and above (ECHA 2018d). Ba- C_9-rich DANSA was negative for clastogenicity in a chromosome aberration study up to a maximum concentration of 250 µg/mL with and without metabolic activation (ECHA 2018d).

No genotoxicity studies were found for Ca- C_9-rich DANSA.

In addition, QSAR predictive modelling did not produce any structural alerts for genotoxicity for representative structures of these substances (Derek Nexus 2018; Leadscope Model Applier 2018; TIMES 2016).

On the basis of these findings, DNNSA, CaDNNSA and DNNDSA are deemed not likely to be genotoxic.

No carcinogenicity studies for C_9-rich DANSA or its salts are available.

Repeat dose toxicity

In a 14-day repeat dose study, male and female adult Wistar rats (n=3 for each sex and dose) were given 0, 80, 250 or 750 mg/kg bw/day Ca- C_9-rich DANSA in dimethylsulfoxide by oral gavage (ECHA 2018c). Findings included non-significant higher inorganic phosphate levels, alkaline phosphatase (ALP) and alanine aminotransferase (ALT) activities, and lower total protein level in females at the highest tested dose, with no overt adverse effects observed at any dose. The NOAEL established by the study authors is 750 mg/kg bw/day (the highest dose tested). Compared to an OECD guideline 28-day repeat dose study, this study used a lower number of animals per sex and dose, had a shorter duration and fewer examined parameters.

In a 90-day repeat dose study, male and female adult Wistar rats (n=10 for each sex and dose) were given 0, 100, 300 or 1000 mg/kg bw/day Ca- C_9-rich DANSA in corn oil by oral gavage (ECHA 2018c). At 1000 mg/kg bw/day, 6 females died and necropsy revealed effects on the gastrointestinal tract (GIT) (for example, ulceration, squamous epithelial hyperplasia, hyperkeratosis and thickening of the forestomach lining, mucosal atrophy and erosion, and distended intestines), bone marrow atrophy and a small thymus. At 1000 mg/kg bw/day, significant changes in biochemical parameters were observed: alanine aminotransferase (ALT) activity (decreased in males, increased in females), cholesterol (decreased in males and females), phosphate (increased in males), bile acid (decreased in males), albumin (decreased in females), potassium (decreased in females) and calcium (increased in females). At 300 mg/kg bw/day and 1000 mg/kg bw/day, surviving animals showed irreversible significant reduced mean body weight gains with increased food consumption, ulcerative and inflammatory effects of the GIT, significant changes in relative or absolute weights of the thymus (decreased in males and females), liver (decreased in males, increased in females), kidney (increased in males and females), and adrenal gland (increased in males and females). In addition, significant changes in haematology parameters were observed: clotting time (decreased in males and females), neutrophils (increased in females), lymphocytes, platelets and reticulocytes (decreased in females). Histopathological findings at 300 mg/kg bw/day and 1000 mg/kg bw/day revealed increased lymphocytolysis and lymphoid depletion in the thymus of males and females, an increase in thyroid follicular cell hypertrophy in males, and an increase in the presence of alveolar macrophages in the lungs of males. Furthermore, vaginal atrophy and inactive uteri were observed in females at 300 mg/kg bw/day. Thus, the NOAEL for Ca- C_9-rich DANSA is established at 100 mg/kg bw/day based on effects on body and organ weight changes, and alterations in the GIT and hematopoietic system observed at 300 mg/kg bw/day.

Repeat dose studies were conducted for C_9-rich DANSA and Ba- C_9-rich DANSA in the form of combined repeat dose/reproduction-developmental toxicity screening tests, and results are presented in the next section.

No repeat dose studies for other routes of exposure (that is, dermal or inhalation) were identified.

No long-term repeat dose studies were identified.

Developmental and reproductive toxicity

In a combined repeat dose toxicity study with a reproduction / developmental toxicity screening test, male and female adult Wistar rats (n=10 for each sex and dose) were given 0, 95, 298 or 893 mg/kg bw/day C_9-rich DANSA (analytical doses) in propylene glycol by oral gavage (ECHA 2018b). Males were exposed for 31 days while females were exposed for 41-52 days. Surviving pups were sacrificed on day 5-7 of lactation. At 893 mg/kg bw/day, five animals were sacrificed in extremis. Surviving adult males exhibited lower mean body weight or body weight gains throughout the mating period

compared to controls. Males in the highest dose group also showed a statistically significant higher mean white blood cell count. Additionally, both adult males and females exhibited higher ALT and alkaline phosphatase (ALP) activities and lower cholesterol levels than controls. Histopathological findings were noted in the GIT, thymus, lungs and liver of the surviving adult animals. Microscopic findings observed in early sacrifices were generally similar in nature and severity as those recorded for surviving animals. At 298 mg/kg bw/day, higher ALP activity in adult females and lower cholesterol level in adult males were observed, with one female in extremis sacrificed on day 27 post-coitum. At 893 mg/kg bw/day, female pups at lactation day 4 exhibited significant lower mean body weights compared to controls, which could not be attributed to maternal neglect or as secondary effects due to changes in maternal body weight and food consumption. However, no other developmental parameters examined in this study were adversely affected (that is, gestation index and duration, parturition, maternal care and early postnatal pup development consisting of mortality, clinical signs and macroscopy). No reproductive toxicity was observed in any of the examined parameters in adult males and female rats (that is, mating, fertility and conception indices, pre-coital time, spermatogenesis and numbers of corpora lutea and implantation sites). Thus, the NOAEL for parental toxicity is 95 mg/kg bw/day based on changes in clinical biochemistry at 298 mg/kg bw/day and systemic toxicity at 893 mg/kg bw/day, while the NOAEL for developmental effects is 298 mg/kg bw/day based on changes in pup mean body weight at 893 mg/kg bw/day. The NOAEL for reproductive effects is 893 mg/kg bw/day due to the absence of effects at the highest tested dose.

In a combined repeat dose toxicity study with the reproduction / developmental toxicity screening test, male and female adult Wistar rats (n=10 for each sex and dose) were given 0, 17, 55 or 165 mg/kg bw/day (corrected for UVCB final purity) of Ba- C_9 rich DANSA by oral gavage (ECHA 2018d). Males were exposed for 29 days, while females were exposed for 42-55 days. Surviving pups were sacrificed on days 5-7 of lactation. In the adults exposed to 165 mg/kg bw/day of Ba- C_9-rich DANSA, a statistically non-significant increase in the incidence of tubular crystals in the kidneys was observed in one male and one female, along with minimal or slight degrees of tubular dilatation, epithelial hypertrophy and granular casts in the female. In addition, females experienced reversible lower motor activity, and had a slight increase in hypertrophy and hyperplasia of the thyroid gland epithelium. There were no treatment-related effects in any of the reproductive (that is, mating, fertility and conception indices, pre-coital time, spermatogenesis and numbers of corpora lutea and implantation sites) or developmental (that is, gestation index and duration, parturition, maternal care and early postnatal pup development consisting of mortality, clinical signs, body weight and macroscopy) parameters examined in the adults or offspring. Thus, the NOAEL for parental toxicity is 55 mg/kg bw/day based on effects in the kidney and the thyroid at 165 mg/kg bw/day, while the NOAEL for reproductive and developmental toxicity is 165 mg/kg bw/day due to the absence of effects at the highest tested dose.

No reproductive or developmental toxicity studies for Ca- C_9-rich DANSA are available.

8.3 Characterization of risk to human health

BaDNNSA and CDINSA

BaDNNSA and CDINSA were considered under the approach applied in the Rapid Screening of Substances with Limited General Population Exposure Screening Assessment (ECCC, HC 2018). On the basis of the evaluation of both direct and indirect exposure conducted as part of this approach, exposure of the general population to BaDNNSA and CDINSA was considered to be negligible. Therefore, BaDNNSA and CDINSA were considered to be a low concern for human health at current levels of exposure.

NaNSA

The general population is not expected to be exposed to NaNSA through environmental media, food, or from the use of products available to consumers. On the basis of these considerations, the risk to human health is considered to be low.

DNNSA, CaDNNSA and DNNDSA

As the health effects data of DNNSA, CaDNNSA and DNNDSA were limited, a read-across approach using health effects data from the analogues C_9-rich DANSA, Ca- C_9-rich DANSA and Ba- C_9-rich DANSA was used. On the basis of available information on analogues, DNNSA, CaDNNSA and DNNDSA are deemed not likely to be genotoxic. Long term repeat dose studies were not identified for DNNSA, CaDNNSA, DNNDSA or their analogues; however, a NOAEL of 100 mg/kg bw/day was established based on effects on body and organ weight changes, and alterations in the GIT observed in experimental animals at 300 mg/kg bw/day in a 90-day oral study conducted with Ca-C_9-rich DANSA. A NOAEL of 55 mg/kg bw/day was identified based on kidney and thyroid effects (tubular crystals in the kidneys and hyperplasia/ hypertrophy of the thyroid epithelium) observed at the next dose of 165 mg/kg bw/day in parental animals in a reproductive / developmental toxicity screening test conducted with the analogue Ba- C_9-rich DANSA.

The NOAEL of 55 mg/kg bw/day from the reproductive / developmental toxicity screening test is considered protective of effects observed in studies with longer exposure durations, and was used to characterize risk from daily oral exposures to CaDNNSA, DNNSA and DNNDSA in environmental media, and from intermittent exposures to CaDNNSA via inhalation and dermal routes from the use of a general purpose aerosol lubricant. Table 8-2 provides all relevant exposure and hazard values for the NSAs Group, as well as resultant margins of exposure for determination of risk.

Table 8-2. Relevant exposure and hazard values for the NSAs Group, as well as margins of exposure, for determination of risk

Exposure scenario (age group)	Substance(s)	Systemic exposure (mg/kg bw/day)	Critical effect level (mg/kg bw/day)	Critical health effect endpoint	MOE
Environmental media (formula-fed infants, aged 0-5 months)	DNNSA and CaDNNSA	1.7×10^{-4} (daily)	55 (NOAEL for analogue: Ba- C_9-rich DANSA)	Tubular crystals in the kidneys and hyperplasia/ hypertrophy of the thyroid epithelium	320 000
Environmental media (formula-fed infants, aged 0-5 months)	DNNDSA	2.5×10^{-2} (daily)	55 (NOAEL for analogue: Ba- C_9-rich DANSA)	Tubular crystals in the kidneys and hyperplasia/ hypertrophy of the thyroid epithelium	2200
General purpose aerosol lubricant, combined inhalation and dermal exposure[a] (adult, aged 19 years or older)	CaDNNSA	1.4×10^{-2} (per event)	55 (NOAEL for analogue: Ba- C_9-rich DANSA)	Tubular crystals in the kidneys and hyperplasia/ hypertrophy of the thyroid epithelium	3900

Abbreviation: MOE, margin of exposure

[a] Dermal and inhalation absorption was assumed to be 100% (that is, equivalent to oral absorption)

Comparison of the daily (CaDNNSA, DNNSA, and DNNDSA) and per event (CaDNNSA) exposure estimates to the critical effect level resulted in margins of exposure (MOEs) of between 2200 and 320 000. The calculated margins are considered adequate to address uncertainties in the health effects and exposure databases.

8.4 Uncertainties in evaluation of risk to human health

The key sources of uncertainty are presented in the table below.

Table 8-3. Sources of uncertainty in the risk characterization

Key source of uncertainty	Impact
Data on the presence of DNNSA, CaDNNSA and DNNDSA in environmental media are unavailable.	+/-
The use of an aerosol lubricant containing CaDNNSA is associated with potential inhalation and dermal exposure; however, there are no route-specific inhalation or dermal toxicity studies on CaDNNSA or its analogues. Characterization of risk from inhalation and dermal exposures to CaDNNSA is based on route-to-route extrapolation.	+/-
Substance-specific empirical health effects data, including chronic hazard studies, for DNNSA, CaDNNSA and DNNDSA, and their analogues, were limited or unavailable.	+/-
The available health effects data for the analogues are limited and were accessible only as robust summaries submitted in REACH dossiers.	+/-
The UVCB nature of the analogues creates uncertainty in identifying which component is driving the observed health effects.	+/-

+ = uncertainty with potential to cause over-estimation of exposure/risk; - = uncertainty with potential to cause under-estimation of exposure/risk; +/- = unknown potential to cause over or under estimation of risk.

9. Conclusion

Considering all available lines of evidence presented in this screening assessment, there is low risk of harm to the environment from the six substances in the NSAs Group. It is concluded that the six substances in the NSAs Group do not meet the criteria under paragraphs 64(*a*) or (*b*) of CEPA as they are not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity or that constitute or may constitute a danger to the environment on which life depends.

Considering all the information presented in this screening assessment, it is concluded that the six substances in the NSAs Group do not meet the criteria under paragraph 64(*c*) of CEPA as they are not entering the environment in a quantity or concentration or under conditions that constitute or may constitute a danger in Canada to human life or health.

It is therefore concluded that the six substances in the NSAs Group do not meet any of the criteria set out in section 64 of CEPA.

References

Abraham MH, Chadha HS, Whiting GS, Mitchell RC. 1994. Hydrogen bonding. 32. An analysis of water-octanol and water-alkane partitioning and the Δlog *P* parameter of seiler. J Pharm Sci. 83(8):1085-1100.

ACD/Percepta [prediction module]. c1997-2017. Toronto (ON): Advanced Chemistry Development, Inc.

Alberta Environment. 2009. Guidelines for the application of municipal wastewater sludges to agricultural lands [PDF]. Edmonton (Alberta): Alberta Environment. [accessed 2018 December 11].

[ASTER] Assessment Tools for the Evaluation of Risk. 1999. Duluth (MN): US Environmental Protection Agency, Mid-Continent Ecology Division. [restricted access].

[ASTM] (American Standards for Testing of Materials). 1997. Standard guide for determination of the bioaccumulation of sediment-associated contaminants by benthic invertebrates. E 1688-97a. Philadelphia, PA.

[ASTM] (American Standards for Testing of Materials). 2006. Standard Guide for Conducting Toxicity Tests with Freshwater Mussels E2455-06. ASTM International, West Conshohocken, PA. [cited in Matten et al. 2020a]

BIONIC Model. 2016. Ver. 2.0. A mechanistic mass balance model for predicting bioconcentration factors (BCFs) of ionizable organic chemicals in fish. Model developed by: James Armitage and Frank Wania (University of Toronto, Canada), Trevor Brown (Dalhousie University, Canada), Don Mackay (Trent University, Canada), John Arnot (ARC Arnot Research and Consulting, Canada).

[BIOWIN] Biodegradation Probability Program for Microsoft Windows [estimation model]. 2010. Ver. 4.10. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation.

Canada. 1999. *Canadian Environmental Protection Act, 1999*. S.C. 1999, c.33. Canada Gazette Part III, vol. 22, no. 3.

Canada, Dept. of the Environment. 2012. *Canadian Environmental Protection Act, 1999*: *Notice with respect to certain substances on the Domestic Substances List* [PDF]. Canada Gazette, Part I, vol. 146, no. 48, Supplement.

Canada, Dept. of the Environment. 2017. *Canadian Environmental Protection Act, 1999: Notice with respect to substances included as part of the 2017 Inventory Update* [PDF]. Canada Gazette, Part 1, vol. 151, no. 2.

CATALOGIC [environmental fate and ecotoxicity model]. 2014. Ver. 5.11.15. Bourgas (BG): University "Prof. Dr. Assen Zlatarov", Laboratory of Mathematical Chemistry.

ChemView [database]. 2013- . Search results for CAS RNs 25322-17-2, 25619-56-1, 57855-77-3, 60223-95-2 and 68425-61-6. Washington (DC): US Environmental Protection Agency. [updated 2018 Oct 26; accessed 2018 Sep 19].

[ConsExpo Web] Consumer Exposure Web Model. 2016. Bilthoven (NL): Rijksinstituut voor Volksgezondheid en Milieu [National Institute for Public Health and the Environment].

Derek Nexus [toxicity prediction module]. 2018. Ver. 6.0.1 Leeds (UK): Lhasa Limited. [restricted access].

[ECCC] Environment and Climate Change Canada. 2016a. Science approach document: ecological risk classification of organic substances. Ottawa (ON): Government of Canada.

[ECCC] Environment and Climate Change Canada. 2016b.Suporting documentation: data used to create substance-specific hazard and exposure profiles and assign risk. Gatineau (QC). ECCC. Information in support of the science approach document: ecological risk classification of organic substances. Available from: eccc.substances.eccc@canada.ca.

[ECCC] Environment and Climate Change Canada. 2018. DSL Inventory Update data collected under the *Canadian Environmental Protection Act, 1999*, section 71: *Notice with respect to substances included as part of the 2017 Inventory Update.* Data prepared by: Environment Canada, Health Canada; Existing Substances Program.

[ECCC, HC] Environment and Climate Change Canada, Health Canada. 2015. Identification of Risk Assessment Priorities: Results of the 2015 Review. [accessed 2020 Mar 5]

[ECCC, HC] Environment and Climate Change Canada, Health Canada. [modified 2017 Mar 12]. Categorization. Ottawa (ON): Government of Canada. [accessed 2018 Nov 14].

[ECCC, HC] Environment and Climate Change Canada, Health Canada. 2018. Rapid screening of substances with limited general population exposure. Ottawa (ON): Government of Canada.

[ECCC, HC] Environment and Climate Change Canada, Health Canada. 2019. Draft screening assessment - Sulfamic acid, cyclohexyl-, monosodium salt (sodium cyclamate) and Cyclohexanamine (cyclohexylamine). Ottawa (ON): Government of Canada.

[ECHA] European Chemicals Agency. 2012. Guidance on information requirements and chemical safety assessment. Ver. 2.1. Helsinki (FI): European Chemicals Agency. (Environmental exposure estimation; Chapter R.16).

[ECHA] European Chemicals Agency. 2016. Guidance on information requirements and chemical safety assessment. Chapter R.16: Environmental exposure estimation, Version 3.0. Helsinki (FI): ECHA.

[ECHA] European Chemicals Agency. 2018a. Registration dossier: Dinonylnaphthalenedisulphonic acid; CAS RN 60223-95-2. Helsinki (FI): ECHA. [accessed 2018 Dec 4].

[ECHA] European Chemicals Agency. 2018b. Registration dossier: di C8-C10, branched, C9 rich, alkylnaphthalene sulphonic acid; EC number 939-714-0. Helsinki (FI): ECHA. [accessed 2018 Dec 3].

[ECHA] European Chemicals Agency. 2018c. Registration dossier: calcium bis(di C8-C10, branched, C9 rich, alkylnaphthalene sulphonic acid); EC number 939-717-7. Helsinki (FI): ECHA. [accessed 2018 Sep 4].

[ECHA] European Chemicals Agency. 2018d. Registration dossier: barium bis (di C8-C10, branched, C9 rich, alkylnaphthalene sulphonic acid); EC number 939-718-2. Helsinki (FI): ECHA. [accessed 2018 Aug 22].

[ECHA] European Chemicals Agency. 2018e. Registration dossier: Naphthalene sulfonic acid, reaction products with isobutanol, sodium salts; EC number 947-977-8. Helsinki (FI): ECHA. [updated 13 June 2018].

[ECHA] European Chemicals Agency. 2018f. Candidate List of Substances of Very High Concern for Authorisation [Internet]. Helsinki (FI): European Chemicals Agency. [accessed 2018 Dec 3].

[ECHA] European Chemicals Agency. 2019a. Registration dossier: 2-Naphthalenesulfonic acid; CAS RN 120-18-3. Helsinki (FI): ECHA. [updated 2019 March 7; accessed 2019 May 2].

[ECHA] European Chemicals Agency. 2019b. Registration dossier: Naphthalene sulfonic acid, bis(1-methylethyl)-, Me derivs., sodium salts; CAS RN 68909-82-0. Helsinki (FI): ECHA. [updated 14 July 2019].

Environment Canada. 2013. DSL Inventory Update data collected under the *Canadian Environmental Protection Act, 1999*, section 71: *Notice with respect to certain substances on the Domestic Substances List.* Data prepared by: Environment Canada, Health Canada; Existing Substances Program.

Environment Canada, Health Canada. 2014. Approach for identification of chemicals and polymers as risk assessment priorities under Part 5 of the *Canadian Environmental Protection Act, 1999* (CEPA 1999). Ottawa (ON): Government of Canada. [accessed 5 March 2020]

[EPI Suite] Estimation Program Interface Suite for Microsoft Windows [estimation model]. c2000-2012. Ver. 4.11. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation.

Farn RJ (Ed.). 2006. Chemistry and Technology of Surfactants [PDF]. Blackwell Publishing Ltd. U.K. [cited in ECCC 2015].

Gobas F. 2007. Development and review of a generic water–sediment modelling framework for organic chemicals. Burnaby (BC): Simon Fraser University, Faculty of Environment. Report prepared for Environment Canada.

Gobas F. 2010. Comments on approach to sediment exposure approach. Burnaby (BC): Simon Fraser University, Faculty of Environment. Report prepared for Environment Canada.

Gobas FAPC, Mayer P, Parkerton TF, Burgess RM, van de Meent D, Gouin T. 2018. A chemical activity approach to exposure and risk assessment of chemicals. Environ. Toxicol. Chem. 37(5): 1235-51.

Greim H, Ahlers J, Bias R, Broecker B, Hollander H, Gelbke H-P, Klimisch H-J, Mangelsdorf I, Paetz A, Schong N, et al. 1994. Toxicity and ecotoxicity of sulfonic acids: Structure-activity relationships. Chemosphere 28(12): 2203-2236.

Health Canada. 1998. Exposure factors for assessing total daily intake of priority substances by the general population of Canada. Unpublished report. Ottawa (ON): Health Canada, Environmental Health Directorate.

Health Canada. 2015. Food Consumption Table derived from Statistics Canada, Canadian Community Health Survey, Cycle 2.2, Nutrition (2004), Share file. Ottawa (ON).

Health Canada. 2016. Science approach document: threshold of toxicological concern (TTC)-based approach for certain substances. Ottawa (ON): Government of Canada.

[HENRYWIN] Henry's Law Constant Program for Microsoft Windows [estimation model]. 2011. Ver. 3.20. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation.

Kim M, Guerra P, Theocharides M, Barclay K, Smyth SA and Alaee M. 2013. Polybrominated diphenyl ethers in sewage sludge and treated biosolids: effect factors and mass balance. Water Res. 47: 6496-6505.

[KOCWIN] Organic Carbon Partition Coefficient Program for Microsoft Windows [estimation model]. 2010. Ver. 2.00. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation.

Kölbel H, Kurzendörfer P, Zahiruddin M. 1964. Constitution and properties of surfactants. IV. Influence of structure on the aerobic biodegradation of anionic surfactants. Tenside 1: 7-18. [Cited in: Swisher 1987].

Kosswig K. 2012. Surfactants. In Ullmann's Encyclopedia of Industrial Chemistry. Vol. 35. Weinheim: Wiley-VCH Verlag GmbH & Co. p. 431-505.

[KOWWIN] Octanol-Water Partition Coefficient Program for Microsoft Windows [estimation model]. 2010. Ver. 1.68. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation.

Leadscope Model Applier [prediction module]. 2016. Ver. 2.1. Columbus (OH): Leadscope, Inc. [restricted access].

Lee Y, Chen L, Fang H, Hu J, Zhang P, inventors; Dow Global Technologies LLC, assignee. 2011 July 21. Alkyd coating formulations. World Intellectual Property Organization WO 085520.

McCarty LS, Mackay D. 1993. Enhancing ecotoxicological modeling and assessment: critical body residues and modes of toxic action. Environ Sci Technol. 27(9): 1719-1728.

McWilliams P, Payne G. 2011. Bioaccumulation potential of surfactants: a review. Royal Society of Chemistry and the European Oilfield Speciality Chemicals Association. [accessed September 2018].

Mackay D, McCarty LS, and Arnot JA. 2014. Relationships between exposure and dose in aquatic toxicity tests for organic chemicals. Environ. Toxicol. Chem. 33(9): 2038-46.

Mansouri K, Abdelaziz A, Rybacka A, Roncaglioni A, Tropsha A, Varnek A, Zakharov A, Worth A, Richard AM, Grulke CM. 2016. CERAPP: Collaborative estrogen receptor activity prediction project. Environ Health Perspect. 124:1023-1033.

Mansouri K, Kleinstreuer N, Abdelaziz AM, Alberga D, Alves VM, Andersson PL, Andrade CH, Bai F, Balabin I, Ballabio D, et al. 2020. CoMPARA: Collaborative modeling project for androgen receptor activity. Environ Health Perspect. 128:2.

Matten, KJ, Parrott, JL, Bartlett, AJ, Gillis, PL, Milani D, Toito J, Balakrishnan VK, Prosser RS. 2020a. Toxicity of dinonylnaphthalene sulfonates to *Pimephales promelas* and epibenthic invertebrates. Sci Total Environ. 741: 140260.

Matten KJ, Bartlett, AJ, Milani D, Gillis, PL, Parrott, JL, Toito J, Balakrishnan VK, Prosser RS. 2020b. The influence of organic carbon on the toxicity of sediment-associated dinonylnaphthalene sulfonic acids to the benthic invertebrates *Tubifex tubifex* and *Hyalella azteca*. Environ Poll. 267: 115604.

Matten, KJ, Gillis, PL, Milani D, Parrott, JL, Bartlett, AJ, Toito J, Balakrishnan VK, Prosser RS. 2021. Bioaccumulation of sediment-associated dinonylnaphthalene sulfonates in the freshwater mussel *Lampsilis siliquoidea* and oligochaete *Tubifex tubifex*. Chemosphere. 264: 128391.

[MPBPWIN] Melting Point Boiling Point Program for Microsoft Windows [estimation model]. 2010. Ver. 1.43. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation.

[MSDS] Material Safety Data Sheet. 2015. TRETOLITE™ DMO46X DEMULSIFIER. Calgary, AB: Baker Hughes Canada Co. [accessed 22 June 2021].

Nguyen TH, Goss K-U, Ball WP. 2005. Critical Review: Polyparameter linear free energy relationships for estimating the equilibrium partition of organic compounds between water and the natural organic matter in soils and sediments. Environ Sci Technol. 39(4): 913-924.

[OECD] Organisation for Economic Co-operation and Development. 1995. OECD Guideline for the testing of chemicals, Test No. 105: water solubility. Paris (FR): OECD, Environment Directorate. [accessed 27 Dec 2020].

[OECD] Organisation for Economic Co-operation and Development. 2004. Emission scenario document on lubricants and lubricant additives [PDF]. Paris (FR): OECD, Environment Directorate. (Series on Emission Scenario Documents No. 10; Report No.: ENV/JM/MONO(2004)21, JT00174617). [accessed 2018 Dec 19].

[OECD] Organisation for Economic Co-operation and Development. 2005. SIDS initial assessment report: Linear Alkylbenzene Sulfonates (LAS) [PDF]. SIAM [SIDS Initial Assessment Meeting]: 20: 2005 April: Paris, France. [accessed 2018 November].

[OECD] Organisation for Economic Co-operation and Development. 2009. Emissions Scenario Document on Coating Industry (Paints, Laquers, and Varnishes) [PDF]. Paris (FR): OECD, Environment Directorate. (Series on Emission Scenario Documents No. 22; Report No. ENV/JM/MONO(2009)24). [accessed 2019 January].

[OECD] Organization for Economic Co-operation and Development. 2011. Emission Scenario Document on the use of Metalworking Fluids [PDF]. Paris (FR): OECD, Environment Directorate. (Series on Emission Scenario Documents No. 28, Report No. ENV/JM/MONO(2011)18). [accessed 2019 January].

[OECD] Organization for Economic Co-operation and Development. 2012. Emission Scenario Document on Chemicals used in oil well production [PDF]. Paris (FR): OECD, Environment Directorate. (Series on Emission Scenario Documents No. 31, Report No. ENV/JM/MONO(2012)7). [accessed 2019 March].

[OECD] Organisation for Economic Co-operation and Development. 2013. OECD Guideline for the testing of chemicals, Test No. 210: Fish early-life stage toxicity test. Paris (FR): OECD, Environment Directorate. [accessed 27 Dec 2020].

[OECD] QSAR Toolbox [Read-across tool]. 2014. Version 3.3. Paris (FR): Organisation for Economic Co-operation and Development, Laboratory of Mathematical Chemistry.

OECD QSAR Toolbox. [read across tool]. 2017. Ver.4.1. Paris (FR): Organisation for Economic Co-operation and Development, Laboratory of Mathematical Chemistry.

Okonski AI, MacDonald DB, Potter K, Bonnell M. 2021. Deriving predicted no-effect concentrations (PNECs) using a novel assessment factor method. Human and Ecological Risk Assessment. DOI:10.1080/10807039.2020.1865788

[PDS] Product Data Sheet. 2011. Stadis ® 450. Cheshire, U.K.: Innospec Ltd. [accessed Feb 2021]

[RIVM] Rijksinstituut voor Volksgezondheid en Milieu [National Institute for Public Health and the Environment]. 2009. The ConsExpo spray model – Modelling and experimental validation of the inhalation exposure of consumers to aerosols from spray cans and trigger sprays [PDF]. Bilthoven (NL): RIVM. Report No.: 320104005/2009. [accessed 2019 Feb 11].

[RIVM] Rijksinstituut voor Volksgezondheid en Milieu [National Institute for Public Health and the Environment]. 2014. General fact sheet: General default parameters for estimating consumer exposure – Updated version 2014 [PDF]. Bilthoven (NL): RIVM. Report No.: 090013003. [accessed 2019 Feb 11].

[RIVM] Rijksinstituut voor Volksgezondheid en Milieu [National Institute for Public Health and the Environment]. 2018. Cleaning products fact sheet: Default parameters for estimating consumer exposure – Updated version 2018 [PDF]. Bilthoven (NL): RIVM. Report No.: 2016-0179. [accessed 2019 Feb 11].

SimpleTreat [sewage treatment plant removal model]. 2003. Ver. 3.1. Bilthoven (NL): Rijksinstituut voor Volksgezondheid en Milieu (RIVM) [National Institute for Public Health and the Environment]. RIVM, Laboratory for Ecological Risk Assessment, PO Box 1, 3720 BA Bilthoven, The Netherlands.

[SDS] Safety Data Sheet. 2004. Stadis (R) 450. [accessed June 2021]. Cheshire, England: The Associated Octel Co. Ltd. [accessed 22 June 2021]

[SDS] Safety Data Sheet. 2018. Termin-8R [PDF]. Toronto (ON): Spectra Products [accessed 2019 Feb 11].

[SDS] Safety Data Sheet. 2019. MOBIL DTE 26. Spring, TX: Exxon Mobil Corp. [accessed 22 Jun 2021]Statistics Canada. 2004. Canadian Community Health Survey, Cycle 2.2: General Health Component. Share File

Swisher, RD. 1987. Surfactant Biodegradation, 2nd ed. Marcel Dekker Inc., New York.

[TEST] Toxicity Estimation Software Tool. 2016. Ver. 4.2. Washington (DC): US Environmental Protection Agency.

[TIMES] Tissue MEtabolism Simulator [prediction module]. 2018. Ver. 2.27.19. Bourgas (BG): University “Prof. Dr. Assen Zlatarov”, Laboratory of Mathematical Chemistry.

[US EPA] US Environmental Protection Agency. 1996. Generic scenario for automobile spray coating. Draft report. Washington (DC): US EPA, Office of Pollution Prevention and Toxics.

[US EPA] US Environmental Protection Agency. 2003. Exposure and human health reassessment of 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) and related compounds. Washington (DC): US EPA, National Center for Environmental Assessment. Report No.: EPA/600/P-00/001Cb. Part I: Estimating exposure to

dioxin-like compounds; Volume 3: Site-specific assessment procedures; Chapter 4: Estimating exposure media concentrations. 148 pages.

[US EPA] US Environmental Protection Agency. 2011. Exposure factors handbook. Washington (DC): US EPA, National Center for Environmental Assessment, Office of Research and Development. [accessed 2018 Feb 20].

[US EPA] US Environmental Protection Agency. 2012. Screening level hazard characterization of high production volume chemicals: Dinonylnaphthalene category. Washington (DC): US EPA, Office of Pollution Prevention and Toxics. [accessed 2018 Feb 20].

[VCCLab] Virtual Computational Chemistry Laboratory. ALOGPS [non-Java interface]. 2005. Ver. 2.1. Munich (DE): VCCLab. [Tetko IV, Gasteiger J, Todeschini R, Mauri A, Livingstone D, Ertl P, Palyulin VA, Radchenko EV, Zefirov NS, Makarenko AS, et al. 2005. Virtual computational chemistry laboratory - design and description. J Comput Aid Mol Des. 19:453-463.].

Wallace SJ, Leclerc AJA, Prosser R, de Solla, SR, Balakrishnan V, Langlois VS. 2020. Sub-lethal effects of calcium dinonylnaphthalenesulfonate on Western clawed frog embryos. Comp Biochem Physiol - Part D. 34: 100658.

[WATERNT] Water Solubility Program [estimation model]. 2010. Ver. 1.01. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation.

Williams JH. 1999. Regulations on additions of sludge-borne metals to soil and their adaptation to local conditions. In L'Hermite P (editor): Treatment and use of sewage sludge and liquid agricultural wastes, 243-250. London (GB): Commission of the European Communities.

[WSKOWWIN] Water Solubility for Organic Compounds Program for Microsoft Windows [estimation model]. 2010. Ver. 1.42. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation.

Appendix A. Summary of data for determination of ecotoxicological mode of action

Table A-1. Data for calculation of Critical Body Residue (CBR) and Lethal Activity for low solubility NSAs

Endpoint	Result	Data type, Reference
Molecular Weight (MW)	460.71 mg/mmol[a]	--
Melting Point (MP)	153 °C (426 K)	Modelled, median of MPBPWIN 2010 and TEST 2016
Water solubility (WS)	0.23 mg/L at 20 °C	Experimental analogue data, ECHA 2018b
Octanol-Water Partition Coefficient (log K_{ow})	3.5	Modelled, KOWWIN with EVA
Bioconcentration factor (BCF)	16 L/kg (CaDNNSA) with mussel *L. siliquoidea*	Experimental (no fish data available), Matten et al. 2021
Ecotoxicity	BaDNNSA: mussel (*L. cardium*) 48 h EC_{50} (larval viability) = 0.47 mg/L CaDNNSA: Fish embryos (*P. promelas*) 21d LC_{50} = 0.014 mg/L	Experimental (no acute fish data available), Matten et al. 2020a

[a] molecular weight of dissociated molecule of CaDNNSA or BaDNNSA

CBR calculations, Low Solubility NSAs

$CBR_{50\,(BaDNNSA)} = (BCF \times LC_{50}) \div MW$

$= (16\ L/kg \times 0.47\ mg/L) \div 460.71\ mg/mmol$

$= 0.016\ mmol/kg$

$CBR_{50\,(CaDNNSA)} = (BCF \times LC_{50}) \div MW$

$= (16\ L/kg \times 0.014\ mg/L) \div 460.71\ mg/mmol$

$= 0.00049\ mmol/kg$

Table A-2. Data for calculation of Critical Body Residue (CBR) for high solubility NSAs based on DNNDSA

Endpoint	Result	Data type, Reference
Molecular Weight (MW)	540.78 mg/mmol	--
Water Solubility (WS)	2000 mg/L	Experimental, ECHA 2018a
Octanol-Water Partition Coefficient (log K_{ow})	<0.3 L/kg	Experimental, ECHA 2018a
Bioconcentration factor (BCF)	<2.0 L/kg (*C. carpio*)	Experimental, ECHA 2018a
Ecotoxicity	*Daphnia magna* 48 h EC_{50} = 87 mg/L	experimental (no fish data available), ECHA 2018a

CBR calculation, High Solubility NSAs (DNNDSA)

CBR_{50} = (BCF × LC_{50}) ÷ MW

= (2 L/kg × 87 mg/L) ÷ 540.78 mg/mmol

= 0.32 mmol/kg

Lethal activity (LA)

For high solubility NSAs (DNNDSA), the log K_{ow} < 2, so the LA cannot be calculated.

For low solubility NSAs, log K_{ow} ≥ 2, therefore LA can be calculated. No acute fish ecotoxicity data were available, so calculation is based on the available data, as summarized in Table A-1.

$$LA_{50} = LC_{50} \times (F \div WS) \text{ (for solids)}$$

where F is the fugacity ratio (dimensionless) and is calculated using melting point (MP, in K) and temperature (T, in K) from the water solubility test or prediction as follows:

$$F = e^{(-6.79 \times [(MP \div T)-1])} \text{ (Gobas et al. 2018)}$$

$LA_{50\ (BaDNNSA)}$ = LC_{50} x (F ÷ WS)

= 0.47 mg/L x (0.047 ÷ 0.23 mg/L)

= 0.10

$LA_{50\ (CaDNNSA)}$ = LC_{50} x (F ÷ WS)

= 0.014 mg/L x (0.047 ÷ 0.23 mg/L)

= 0.003

Table A-3. Weight of evidence for determining mode of action

Line of evidence	Result	MoA indication
Embyonic frog study (Wallace et al. 2020)	Reduced body lengths, malformations, significant decreases in transcript levels of genes involved in antioxidant capacity and essential amino acid metabolism	Non-narcotic
CBR_{50}	0.016 to 0.32 mmol/kg (<< 2 mmol/kg for acute baseline narcosis) 0.00049 (chronic) << 0.2 mm/kg for chronic baseline narcosis	Non-narcotic
LA_{50}	0.1 for BaDNNSA, 0.003 for CaDNNSA (but not based on acute fish data, and solubility for analogue) N/A (high solubility NSAs)	Inconclusive: narcotic (LA > 0.01) and non-narcotic for low solubility NSAs (noting uncertainty with the data)
Verhaar Aquatic Toxicity Classification (OECD QSAR Toolbox 2017)	Class 5 (Not possible to classify according to these rules)	Inconclusive
TEST (2016)	Metabolite predictions in most cases were not possible. Others predicted to be narcotics with high error associated with the predictions.	Inconclusive
ASTER (1999)	Narcotic	Narcotic
OECD QSAR Toolbox (2017) OASIS MoA	Reactive unspecified	Non-narcotic
OECD QSAR Toolbox (2017) In vitro/in vivo	In vivo alert - H-acceptor-path 3-H-acceptor	Non-narcotic

Line of evidence	Result	MoA indication
mutagenicity predictions (Ames & Micronucleus)		
Additional Evidence	All parent NSAs and their major metabolites predicted by CATALOGIC (2014), are predicted by CoMPARA and CERAPP models (Mansouri et al. 2020, 2016) to be androgen receptor (AR) binders and AR antagonists. DNNSA and a majority of NSA metabolites also predicted to be estrogen receptor binders.	Non-narcotic

Abbreviations: CBR, critical body residue; LA, lethal activity; MoA, mode of action; N/A, not applicable

Appendix B. Additional ecological effects data

Table B-1. Additional analogue aquatic ecological effects data (Greim et al. 1994)

Common name (CAS RN)	Test organism	Endpoint[a]	Value (mg/L)
Naphthalene sulfonic acids (68153-01-5)	Fish (Unspecified)	96h LC_{50}	100 to 500
Naphthalene sulfonic acids (68153-01-5)	Invertebrate (*D. magna*)	24h EC_{50}	85
Naphthalene sulfonic acids (68153-01-5)	Invertebrate (*D. magna*)	48h EC_{50}	34
Naphthalene sulfonic acids (68153-01-5)	Algae (Unspecified)	96h EC_{10}	73.3
Naphthalene sulfonic acids (68153-01-5)	Algae (Unspecified)	96h EC_{50}	54.3
Branched and linear butyl derivatives of naphthalene sulfonic acids, sodium salts (91078-64-7)	Fish (Unspecified)	48h LC_{0}	20
Branched and linear butyl derivatives of naphthalene sulfonic acids, sodium salts (91078-64-7)	Fish (Unspecified)	48h LC_{100}	100

Abbreviations: LCx, Lethal concentration for x% of the population; ECx, Effect concentration for x% of the population
[a] Endpoints not specified for invertebrate and algae studies.

Appendix C. Ecological exposure assessment: Summary of assumptions

Table C-1. Summary of assumptions for calculating aquatic PECs for scenario 1: Lubricant oil blending

Variable name	Value	Units	Additional comments
Quantity	1500	kg/year	ECCC (2013, 2018), average quantity of low solubility NSAs used by lubricant blending facilities based on reported import quantities in response to CEPA section 71 surveys . If a company reported multiple low solubility NSAs, the sum of their quantities was used in the calculation of the average. It is assumed that the entire quantity imported by a company could be used at a single facility.
Emission factor	0.25	Percent	OECD (2004), this is the worst-case emission factor for a lubricant blending plant.
Days of release	50	Days/year	OECD (2004), number of days is determined by converting the total yearly quantity of low solubility NSAs used at a facility to the quantity of product formulated at the facility per year, and then converting the product tonnage to number of days. This conversion was based on the maximum concentration (1%) of NSA within a lubricant based on information for one product (SDS 2019).
Removal rate (on-site)	0	Percent	None.
Removal rate (off-site)	85 - 95	Percent	Removal rate was varied between 85 and 95 percent to account for the uncertainty and variability between low solubility NSAs, based on SimpleTreat estimates and other considerations.
Daily dilution volume	22 982 400	L/day	Daily dilution volumes are calculated by multiplying the effluent flow of WWTS by the dilution factor (DF) of the receiving water body. Maximum DF of 10 is used when actual DF is greater than 10. This value corresponds to a representative value for the lubricant oil-blending sector in Canada.

Table C-2. Summary of assumptions for calculating aquatic PEC for scenario 2: Use of metalworking fluids

Variable name	Value	Units	Additional comments
Quantity	161.24	kg/year	OECD (2011), estimate of the mass of low solubility NSAs handled at a facility, determined using the geometric mean volume of oil based metalworking fluid handled at a facility (16 124 L/year), density of the metalworking fluid (1 kg/L), and representative concentration of low solubility NSAs in metalworking fluids (1%[a]).
Emission factor	11	Percent	OECD (2011), emission factor associated with metalworking fluids varies between 11 and 100%, which includes releases from residual oil cleaning on metal surfaces, raw materials handling, finishing and other processes. The lowest emission factor of 11% was used.
Days of release	247	Days/year	OECD (2011), it is assumed that the default number of release days for facilities using metalworking fluids is equal to the default days of operation.
Removal rate (on-site)	25	Percent	OECD (2011) indicates that the majority of sites using metalworking fluids use on-site wastewater treatment prior to discharging effluents to WWTS. This value was estimated given the phys-chem properties and internal compilation of information compiled on industrial wastewater treatment systems.
Removal rate (off-site)	85 to 95	Percent	Removal rate was varied between 85 and 95 percent to account for the uncertainty and variability between low solubility NSAs, based on SimpleTreat estimates and other considerations.
Daily dilution volume	6 430 000	L/day	Daily dilution volumes are calculated by multiplying the effluent flow of WWTS by the dilution factor (DF) of the receiving water body. Maximum DF of 10 is used when actual DF is greater than 10. This value corresponds to the 10th percentile of the distribution of daily dilution volumes for lagoons, secondary, and tertiary WWTS associated with facilities using metalworking fluid in Canada.

[a] Although information was identified indicating that a concentration of NSA up to 10% in metal working fluids could occur, the majority of lubricant products were reported containing less than 1% NSA. Therefore, a value of 1% was

determined to be a suitable generic value. Nonetheless, in order to verify whether a risk could be identified if a product with higher NSA content was used, an additional scenario considering quantities equivalent to the use of a metal working fluid containing 10% NSA was developed using site-specific information. This scenario did not indicate a concern (RQs ≤0.6) (details not included here).

Table C-3. Summary of assumptions for calculating aquatic PEC for scenario 3: Formulation of paints and coatings

Variable name	Value	Units	Additional comments
Quantity	1000 to 10 000	kg/year	ECCC (2013 and 2018), the highest import quantity reported to CEPA section 71 surveys by any company. Value is presented as a range due to confidentiality, however reported value was used in the calculations.. It is assumed that the entire quantity imported by a company could be used at a single facility. This quantity is applicable to both low and high solubility NSAs.
Emission factor	0.505	Percent	OECD (2009), emission factor associated with standard batch manufacture of aqueous coatings when raw materials are used in powder form.
Days of release	300	Days/year	EC (2003), number of release days for facilities formulating paints and coatings.
Removal rate (on-site)	0	Percent	None.
Removal rate (off-site, high solubility NSAs)	0 to 20	Percent	Removal rate was varied between 0 and 20 percent to account for the uncertainty and variability between high solubility NSAs, based on SimpleTreat estimates and other considerations.
Removal rate (off-site, low solubility NSAs)	85 to 95	Percent	Removal rate was varied between 85 and 95 percent to account for the uncertainty and variability between low solubility NSAs, based on SimpleTreat estimates and other considerations.
Daily dilution volume	10 000 000 to 100 000 000	L/day	Daily dilution volumes are calculated by multiplying the effluent flow of WWTS by the dilution factor (DF) of the receiving water body. The value used in the calculations corresponded to the 10th percentile value of the distribution of daily dilution volumes for paints and coatings formulation facilities in Canada, which considers lagoons, secondary

Variable name	Value	Units	Additional comments
			and tertiary WWTS. Value is presented as a range to avoid back calculation of specific quantity.

Table C-4. Summary of assumptions for calculating aquatic PEC for scenario 4: Formulation of oil and gas products

Variable name	Value	Units	Additional comments
Quantity	10 000	kg/year	ECCC (2013 and 2018), the highest import quantity of high solubility NSAs reported in response to CEPA section 71 surveys was converted to a range of 1000 to 10 000 kg/year and the upper end of the rangeis used in the calculations. It is assumed that the entire quantity imported by a company could be used at any of its facilities.
Emission factor	0.3	Percent	EC (2003), while 2% is the determined emission factor from EC (2003) for the given use quantity, based on the expected cleaning processes of vessels used for formulation, a value of 0.3% is judged as being more appropriate. It is expected that solvents may be used in the cleaning of vessels, and therefore 2% would overestimate the releases to wastewater.
Days of release	60	Days/year	EC (2003), number of days is determined by converting the total yearly quantity of high solubility NSAs used at a facility to the quantity of product formulated at the facility per year, and then converting the product tonnage to number of days. This conversion was based on the concentration of 30% of NSA within an oil and gas extraction product (MSDS 2015).
Removal rate (on-site)	0	Percent	None.
Removal rate (off-site)	0 to 20	Percent	Removal rate was varied between 0 and 20 percent to account for the uncertainty and variability between high solubility NSAs, based on SimpleTreat estimates and other considerations.

Variable name	Value	Units	Additional comments
Daily dilution volume	5 120 000	L/day	Daily dilution volumes are calculated by multiplying the effluent flow of WWTS by the dilution factor (DF) of the receiving water body. Maximum DF of 10 is used when actual DF is greater than 10. This value corresponds to the 10th percentile of the distribution of daily dilution volumes for lagoons, secondary and tertiary WWTS associated with a variety of industrial facilities in Canada.

Table C-5. Summary of assumptions for calculating aquatic PEC for scenario 5: Formulation of fuels

Variable name	Value	Units	Additional comments
Quantity	800	kg/year	ECCC (2018), average quantity of low solubility NSAs used by facilities formulating fuels based on reported import quantities in response to CEPA section 71 surveys. If a company reported multiple low solubility NSAs, the sum of their quantities was used in the calculation of the average. It is assumed that the entire quantity imported by a company could be used at a single facility.
Emission factor	0.3	Percent	EC (2003), emission factor for the mineral oil and fuel industry.
Days of release	300	Days/year	EC (2003), number of days is determined by converting the total yearly quantity of high solubility NSAs used at a facility to the quantity of product formulated at the facility per year, and then converting the product tonnage to number of days using relevant reference. This conversion was based on the concentration of 20% of NSA within an additive which is added to fuels at 5 mg/L based on information for one product (SDS 2004, PDS 2011).
Removal rate (on-site)	85 to 95	Percent	Removal rate was varied between 85 and 95 percent to account for the uncertainty and variability between high solubility NSAs, based on SimpleTreat estimates and other considerations.

Variable name	Value	Units	Additional comments
Removal rate (off-site)	0	Percent	None
Daily dilution volume	40 390 000	L/day	For direct dischargers, daily dilution volumes are calculated by multiplying the effluent flow of the facility by the dilution factor (DF) of the receiving water body. Maximum DF of 10 is used when actual DF is greater than 10. This value corresponds to a representative value for the fuel formulation sector in Canada.

Table C-6. Summary of assumptions for calculating aquatic PECs for scenario 6: Industrial use of paints

Variable name	Value	Units	Additional comments
Quantity	1000	kg/year	ECCC (2018), the highest import quantity of high solubility NSAs reported in response to CEPA section 71 survey was converted to a range of 100 to 1000 kg/year and the upper end of the range was used in the calculations. It is assumed that the entire quantity will be used at a single facility.
Transfer efficiency	65	Percent	OECD (2009), this is the average transfer efficiency for spraying processes used in the manufacture of original automotive equipment.
Days of release	21	Days/year	OECD (2009), US EPA (1996), number of days is determined by converting the total yearly quantity of high solubility NSAs used at a facility to the quantity of product used at the facility per year, and then converting the product tonnage to number of days. This conversion was based on the maximum concentration (1.5%) (Lee et al. 2011) of surfactant within a coating formulation based on patent information.
Removal rate (on-site)	0 to 20	Percent	Removal rate was varied between 0 and 20 percent to account for the uncertainty and variability between high solubility NSAs, based on SimpleTreat estimates and other

Variable name	Value	Units	Additional comments
			considerations. Assumed to be same efficiency as in off-site wastewater treatment system.
Removal rate (off-site)	0 to 20	Percent	Removal rate was varied between 0 and 20 percent to account for the uncertainty and variability between high solubility NSAs, based on SimpleTreat estimates and other considerations.
Daily dilution volume (for aquatic calculation)	86 969 000	L/day	Daily dilution volumes are calculated by multiplying the effluent flow of WWTS by the dilution factor (DF) of the receiving water body. Maximum DF of 10 is used when actual DF is greater than 10. This value corresponds to the daily dilution volume associated to a selected Canadian facility based on the 10th percentile flow of the receiving water body.

Table C-7. Summary of assumptions for calculating sediment PEC for scenario 1: Lubricant oil blending

Variable name	Value	Units	Additional comments
Daily dilution volume	40 176 000	L/d	Daily dilution volumes are calculated by multiplying the effluent flow of WWTS by the dilution factor (DF) of the receiving water body. Maximum DF of 10 is used when actual DF is greater than 10. This value corresponds to a representative value for the lubricant oil-blending sector in Canada, based on the 50th percentile flow of the receiving water body.
Total concentration in the water column (C_{total})	0.09 to 0.28	µg/L	Aquatic concentrations calculated using the daily dilution volume above. Other inputs are the same as for the aquatic scenario.

Table C-8. Summary of assumptions for calculating sediment PEC for scenario 2: Use of metalworking fluids

Variable name	Value	Units	Additional comments
Daily dilution volume	9 731 600	L/d	Daily dilution volumes are calculated by multiplying the effluent flow of WWTS by the dilution factor (DF) of the receiving water body.

Variable name	Value	Units	Additional comments
			Maximum DF of 10 is used when actual DF is greater than 10. This value corresponds to the 10th percentile of the distribution of daily dilution volumes based on 50th percentile flows of receiving water bodies for lagoons, secondary, and tertiary WWTS associated with facilities using metalworking fluid in Canada.
Total concentration in the water column (C_{total})	0.28 to 0.83	µg/L	Aquatic concentrations calculated using the daily dilution volume above. Other inputs are the same as for the aquatic scenario.

Table C-9. Summary of assumptions for calculating sediment PEC for scenario 3: Formulation of paints and coatings

Variable name	Value	Units	Additional comments
Daily dilution volume	10 000 000 to 100 000 000	L/d	Daily dilution volumes are calculated by multiplying the effluent flow of WWTS by the dilution factor (DF) of the receiving water body. Maximum DF of 10 is used when actual DF is greater than 10. This value corresponds to the 10th percentile of the distribution of daily dilution volumes based on 50th percentile flows of receiving water bodies for lagoons, secondary, and tertiary WWTS associated with paints and coatings facilities in Canada.
Total concentration in the water column (C_{total})	0.11 to 2.3	µg/L	Aquatic concentrations calculated using the daily dilution volumes above. Other inputs are the same as for the aquatic scenario. Although calculations are done separately, this range is for both the low and high solubility NSAs.

Table C10. Summary of assumptions for calculating sediment PEC for scenario 4: Formulation of oil and gas products

Variable name	Value	Units	Additional comments
Daily dilution volume	29 384 000	L/d	Daily dilution volumes are calculated by multiplying the effluent flow of WWTS by the dilution factor (DF) of the receiving water body. Maximum DF of 10 is used when actual DF is greater than 10. This value

Variable name	Value	Units	Additional comments
			corresponds to the 10th percentile of the distribution of daily dilution volumes based on 50th percentile flows of receiving water bodies for secondary and tertiary WWTS associated with all industrial facilities in Canada.
Total concentration in the water column (C_{total})	14 to 17	µg/L	Aquatic concentrations calculated using the daily dilution volumes above. Other inputs are the same as for the aquatic scenario.

Table C11. Summary of assumptions for calculating sediment PEC for scenario 5: Formulation of fuels

Variable name	Value	Units	Additional comments
Daily dilution volume	40 390 000	L/d	For direct dischargers, daily dilution volumes are calculated by multiplying the effluent flow of the facility by the dilution factor (DF) of the receiving water body. Maximum DF of 10 is used when actual DF is greater than 10. This value corresponds to a representative value for the fuel formulation sector in Canada.
Total concentration in the water column (C_{total})	0.010 to 0.030	µg/L	Aquatic concentrations calculated using the daily dilution volumes above. Other inputs are the same as for the aquatic scenario.

Table C-12. Summary of assumptions for calculating sediment PEC for scenario 6: Industrial use of paints

Variable name	Value	Units	Additional comments
Daily dilution volume (for calculation of C_{total} in sediment calculation)	86 969 000	L/d	Daily dilution volumes are calculated by multiplying the effluent flow of WWTS by the dilution factor (DF) of the receiving water body. Maximum DF of 10 is used when actual DF is greater than 10. This value corresponds to the daily dilution volume associated to a selected Canadian facility, based on the 50th percentile flow of the receiving water body.
Total concentration in the water column (C_{total})	2.3 to 3.6	µg/L	Aquatic concentrations calculated using the daily dilution volumes above. Other inputs are the same as for the aquatic scenario.

Table C-13. Summary of assumptions applicable to all soil PEC calculations

Variable name	Value	Units	Comments
Fraction of removal via sorption in WWTS for low solubility NSAs ($R_{sorption}$)	85 to 95	Percent	Removal rate was varied between 85 and 95 percent to account for the uncertainty and variability between low solubility NSAs, based on SimpleTreat estimates and other considerations. It was assumed that all removal was via sorption.
Fraction of removal via sorption in WWTS for high solubility NSAs ($R_{sorption}$)	0 to 20	Percent	Removal rate was varied between 00 and 20 percent to account for the uncertainty and variability between high solubility NSAs, based on SimpleTreat estimates and other considerations. It was assumed that all removal was via sorption.
Biosolids generation rate (BP)	104	mg/L	Default value based on field data of several secondary treatment systems, Kim et al. (2013); used to calculate concentration of substance in biosolids (C_s).
Annual biosolids land application rate (A)	0.83	kg/m^2-yr	In Canada, the maximum land application rate of biosolids is regulated by provinces/territories and varies. The highest rate occurs in Alberta and is used as a default value (Alberta Environment 2009).
Number of years for biosolids land application (N)	10	Yr	A period of 10 consecutive years is suggested by the European Chemicals Agency (ECHA 2016) for calculating exposure in soils to which biosolids are applied.
Soil mixing depth (d)	0.2	m	Default value. A soil mixing depth of 20 cm is suggested by the European Chemicals Agency (ECHA 2016) for calculating exposure in soils to which biosolids are applied.
Dry soil density (ρ)	1200	kg/m^3	Default value reported for soil density (dry) by Williams (1999).
Biodegradation half-life in soil	92 to 200	days	CATALOGIC (2014).

Table C-14. Summary of assumptions for calculating soil PEC for scenario 1: Lubricant oil blending

Variable name	Value	Units	Comments
Concentration of substance in biosolids (C_s)	266 to 298	mg/kg dw	C_s is determined by the following equation: $$C_s = \frac{Q_d * R_{sorption} * 10^{12}}{F * BP}$$ Where Q_d (kg/day) is the daily mass of substance released to WWTS, $R_{sorption}$ is the fraction of substance removed via sorption, F is the flow of selected WWTS in L/day, and BP is the biosolids generation rate per litre of wastewater in mg/L. See values below and in Table C-13.
Daily mass of substance released to WWTS (Q_d)	0.075	kg/d	Q_d is calculated from the annual quantity of the substance at the facility multiplied by the emission factor (from aquatic scenario); used to calculate concentration of substance in biosolids (C_s).
Flow of WWTS (F)	2 298 240	L/d	This value is based on the same daily dilution volume as in the aquatic scenario and assumes a dilution factor (DF) of 10; used to calculate concentration of substance in biosolids (C_s).

Table C-15. Summary of assumptions for calculating soil PEC for scenario 2: Use of metalworking fluids

Variable name	Value	Units	Comments
Concentration of substance in biosolids (C_s)	171 to 191	mg/kg dw	C_s is determined by the following equation: $$C_s = \frac{Q_d * R_{sorption} * 10^{12}}{F * BP}$$ Where Q_d (kg/day) is the daily mass of substance released to WWTS, $R_{sorption}$ is the fraction of substance removed via sorption, F is the flow of selected WWTS in L/day, and BP is the biosolids generation rate per litre of wastewater in mg/L. See values below and in Table C-13.

Daily mass of substance released to WWTS (Q_d)	0.054	kg/d	Q_d is calculated from the annual quantity of the substance at the facility multiplied by the emission factor (from aquatic scenario); used to calculate concentration of substance in biosolids (C_s).
Flow of WWTS (F)	2 572 400	L/d	This value is based on the 10th percentile of the distribution of daily dilution volumes for secondary, and tertiary WWTS associated with facilities using metalworking fluid in Canada and assumes a dilution factor of 10; used to calculate concentration of substance in biosolids (C_s).

Table C-16. Summary of assumptions for calculating soil PEC for scenario 3: Formulation of paints and coatings

Variable name	Value	Units	Comments
Concentration of substance in biosolids (C_s)	0 to 49	mg/kg dw	C_s is determined by the following equation: $$C_s = \frac{Q_d * R_{sorption} * 10^{12}}{F * BP}$$ Where Q_d (kg/day) is the daily mass of substance released to WWTS, $R_{sorption}$ is the fraction of substance removed via sorption, F is the flow of selected WWTS in L/day, and BP is the biosolids generation rate per litre of wastewater in mg/L. See values below and in Table C-13.
Daily mass of substance released to WWTS (Q_d)	0.025	kg/d	Q_d is calculated from the annual quantity of the substance at the facility multiplied by the emission factor (from aquatic scenario); used to calculate concentration of substance in biosolids (C_s).
Flow of WWTS (F)	4 728 300	L/d	This value is based on the 10th percentile of the distribution of daily dilution volumes for secondary, and tertiary WWTS associated with paints and coatings formulation facilities in Canada and assumes a dilution factor of 10; used to calculate concentration of substance in biosolids (C_s).

Table C-17. Summary of assumptions for calculating soil PEC for scenario 4: Formulation of oil and gas products

Variable name	Value	Units	Additional Comments
Concentration of substance in biosolids (C_s)	0 - 424	mg/kg dw	C_s is determined by the following equation: $$C_s = \frac{Q_d * R_{sorption} * 10^{12}}{F * BP}$$ Where Q_d (kg/day) is the daily mass of substance released to WWTS, $R_{sorption}$ is the fraction of substance removed via sorption, F is the flow of selected WWTS in L/day, and BP is the biosolids generation rate per litre of wastewater in mg/L. See values below and in Table C-13.
Daily mass of substance released to WWTS (Q_d)	0.5	kg/d	Q_d is calculated from the annual quantity of the substance at the facility multiplied by the emission factor (from aquatic scenario); used to calculate concentration of substance in biosolids (C_s).
Flow of WWTS (F)	2 269 700	L/d	This value is based on the 10th percentile of the distribution of daily dilution volumes for secondary, and tertiary WWTS associated with a variety of industrial facilities in Canada and assumes a dilution factor of 10; used to calculate concentration of substance in biosolids (C_s).

Table C18. Summary of assumptions for calculating soil PEC for scenario 6: Industrial use of paints

Variable name	Value	Units	Comments
Concentration of substance in biosolids (C_s)	0 - 55	mg/kg dw	C_s is determined by the following equation: $$C_s = \frac{Q_d * R_{sorption} * 10^{12}}{F * BP}$$ Where Q_d (kg/day) is the daily mass of substance released to WWTS, $R_{sorption}$ is the fraction of substance removed via sorption, F is the flow of selected WWTS in L/day, and BP is the biosolids generation rate per litre of

Variable name	Value	Units	Comments
			wastewater in mg/L. See values below and in Table C-13.
Daily mass of substance released to WWTS (Q_d)	0.25 – 0.31	kg/d	Q_d is calculated from the annual quantity of the substance at the facility; used to calculate concentration of substance in biosolids (C_s).
Flow of WWTS (F)	8 696 900	L/d	This value is based on the daily dilution volume used in the aquatic scenario and assuming a dilution factor of 10; used to calculate concentration of substance in biosolids (C_s).

Appendix D. The Ecological Risk Classification of organic substances (ERC) approach

The ERC is a risk-based approach that considers multiple metrics for both hazard and exposure based on weighted consideration of multiple lines of evidence for determining risk classification. The various lines of evidence are combined to discriminate between substances of lower or higher potency (hazard) and lower or higher potential for exposure in various media. This approach reduces the overall uncertainty with risk characterization compared to an approach that relies on a single metric in a single medium (for example, median lethal concentration [LC_{50}]) for characterization. The following paragraphs in this section summarize the approach, which is described in detail in ECCC (2016a,b).

Data on physical-chemical properties, fate (chemical half-lives in various media and biota, partition coefficients, and fish bioconcentration), acute fish ecotoxicity, and chemical import or manufacture volume in Canada were collected from the scientific literature, available empirical databases (for example, OECD QSAR Toolbox 2014), and from responses to surveys conducted under section 71 of CEPA, or they were generated using selected quantitative structure-activity relationship (QSAR) or mass-balance fate and bioaccumulation models. These data were used as inputs to other mass-balance models or to complete the substance hazard and exposure profiles.

Hazard profiles were based principally on metrics regarding mode of toxic action, chemical reactivity, food web-derived internal toxicity thresholds, bioavailability, and chemical and biological activity. Exposure profiles were also composed of multiple metrics, including potential emission rate, overall persistence and long-range transport potential. Hazard and exposure profiles were compared to decision criteria to classify the hazard and exposure potentials for each organic substance as low, moderate or high. Additional rules were applied (for example, classification consistency, margin of exposure) to refine the preliminary classifications of hazard or exposure.

A risk matrix was used to assign a low, moderate or high classification of potential risk for each substance based on its hazard and exposure classifications. ERC classifications of potential risk were verified using a two-step approach. The first step adjusted the risk classification outcomes from moderate or high, to low for substances that had a low estimated rate of emission to water after wastewater treatment, representing a low potential for exposure. The second step reviewed low risk potential classification outcomes using relatively conservative, local-scale (that is, in the area immediately surrounding a point-source of discharge) risk scenarios, designed to be protective of the environment, to determine whether the classification of potential risk should be increased.

ERC uses a weighted approach to minimize the potential for both over and under classification of hazard and exposure and subsequent risk. The balanced approaches

for dealing with uncertainties are described in greater detail in ECCC (2016). The following describes two of the more substantial areas of uncertainty. Error in empirical or modeled acute toxicity values could result in changes in classification of hazard, particularly metrics relying on tissue residue values (that is, mode of toxic action), many of which are predicted values from (Q)SAR models (OECD QSAR Toolbox 2014). However, the impact of this error is mitigated by the fact that overestimation of median lethality will result in a conservative (protective) tissue residue value used for critical body residue (CBR) analysis. Error of underestimation of acute toxicity will be mitigated through the use of other hazard metrics such as structural profiling of mode of action, reactivity and/or estrogen binding affinity. Changes or errors in chemical quantity could result in differences in classification of exposure as the exposure and risk classifications are highly sensitive to emission rate and use quantity. The ERC classifications thus reflect exposure and risk in Canada based on what is considered to be the current use quantity and may not reflect future trends.

Appendix E. Potential human exposures to DNNSA, CaDNNSA, and DNNDSA in environmental media and food

Table E-1. Estimated daily intake of DNNSA and CaDNNSA (µg/kg bw/day) by various age groups

Route of Exposure	0 to 5 months, formula fed[a]	6 to 11 months[b]	1 year[c]	2 to 3 years[d]	4 to 8 years[e]	9 to 13 years[f]	14 to 18 years[g]	19 years or older[h]
Drinking Water[i]	0.17	0.11	0.043	0.037	0.030	0.023	0.023	0.027
Food	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Total Intake	0.17[j]	0.11	0.043	0.037	0.030	0.023	0.023	0.027

Abbreviations: N/A, not applicable

[a] Assumed to weigh 6.3 kg (Health Canada 2015) and drink 0.826 L of water per day (Health Canada 1998). It is assumed that infants younger than 1 year old consume drinking water through formula exclusively, and that infants younger than 1 year old who are breastfed do not consume any drinking water.

[b] Assumed to weigh 9.1 kg (Health Canada 2015) and drink 0.764 L of water per day (Health Canada 1998). It is assumed that infants younger than 1 year old consume drinking water through formula exclusively, and that infants younger than 1 year old who are breastfed do not consume any drinking water.

[c] Assumed to weigh 11 kg (Health Canada 2015) and drink 0.36 L of water per day (Health Canada 1998).

[d] Assumed to weigh 15 kg (Health Canada 2015) and drink 0.43 L of water per day (Health Canada 1998).

[e] Assumed to weigh 23 kg (Health Canada 2015) and drink 0.53 L of water per day (Health Canada 1998).

[f] Assumed to weigh 42 kg (Health Canada 2015) and drink 0.74 L of water per day (Health Canada 1998).

[g] Assumed to weigh 62 kg (Health Canada 2015) and drink 1.09 L of water per day (Health Canada 1998).

[h] Assumed to weigh 74 kg (Health Canada 2015) and drink 1.53 L of water per day (Health Canada 1998).

[i] A maximum concentration of 1.3 µg/L of DNNSA and CaDNNSA (low solubility NSAs) in wastewater was used in estimating drinking water intake of these substances.

[j] Maximum total intake from all routes of exposure

Table E-2. Estimated daily intake of DNNDSA (µg/kg bw/day) by various age groups

Route of Exposure	0 to 5 months, formula fed[a]	6 to 11 months[b]	1 year[c]	2 to 3 years[d]	4 to 8 years[e]	9 to 13 years[f]	14 to 18 years[g]	19 years or older[h]
Drinking Water[i]	25	16	6.2	5.4	4.4	3.3	3.3	3.9
Food	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Total Intake	25[j]	16	6.2	5.4	4.4	3.3	3.3	3.9

Abbreviations: N/A, not applicable

[a] Assumed to weigh 6.3 kg (Health Canada 2015) and drink 0.826 L of water per day (Health Canada 1998). It is assumed that infants younger than 1 year old consume drinking water through formula exclusively, and that infants younger than 1 year old who are breastfed do not consume any drinking water.

[b] Assumed to weigh 9.1 kg (Health Canada 2015) and drink 0.764 L of water per day (Health Canada 1998). It is assumed that infants younger than 1 year old consume drinking water through formula exclusively, and that infants younger than 1 year old who are breastfed do not consume any drinking water.

[c] Assumed to weigh 11 kg (Health Canada 2015) and drink 0.36 L of water per day (Health Canada 1998).

[d] Assumed to weigh 15 kg (Health Canada 2015) and drink 0.43 L of water per day (Health Canada 1998).

[e] Assumed to weigh 23 kg (Health Canada 2015) and drink 0.53 L of water per day (Health Canada 1998).

[f] Assumed to weigh 42 kg (Health Canada 2015) and drink 0.74 L of water per day (Health Canada 1998).
[g] Assumed to weigh 62 kg (Health Canada 2015) and drink 1.09 L of water per day (Health Canada 1998).
[h] Assumed to weigh 74 kg (Health Canada 2015) and drink 1.53 L of water per day (Health Canada 1998).
[i] A maximum concentration of 190 µg/L of DNNDSA (high solubility NSA) in wastewater was used in estimating drinking water intake of these substances.
[j] Maximum total intake from all routes of exposure

Appendix F. Parameters used to estimate human exposure to CaDNNSA from the use of a general purpose aerosol lubricant

Exposure estimates for a general purpose aerosol lubricant containing up to 5% of CaDNNSA were estimated using ConsExpo Web (ConsExpo Web 2016). The user was assumed to be an adult aged 19 years or older, with a body weight of 74 kg and an inhalation rate of 15.1 m^3/day (Health Canada 2015). Unless otherwise specified, default parameters for the ConsExpo Web model for a penetrating spray lubricant were selected from the General Fact Sheet (RIVM 2014), Cleaning Product Fact Sheet (RIVM 2018) and ConsExpo spray model documentation (RIVM 2009). Absorption from inhalation and dermal routes was conservatively assumed to be 100%.

Table F-1. Exposure parameters and assumptions for a general purpose aerosol lubricant, inhalation and dermal scenarios

Exposure scenario and route of exposure	Parameters used in ConsExpo Web
General purpose aerosol lubricant, inhalation	Model: Exposure to spray – spraying Spray duration: 10 seconds (based on product instructions from manufacturer) Exposure duration: 60 minutes (RIVM 2018) Weight fraction: 0.05 (SDS 2018) Room volume: 34 m^3 (default for garage, RIVM 2014) Room height: 2.5 m (RIVM 2014) Ventilation rate: 1.5/h (default for garage, RIVM 2014)

Exposure scenario and route of exposure	Parameters used in ConsExpo Web
	Mass generation rate: 1.5 g/s (for penetrating spray in a spray can, RIVM 2009) Airborne fraction: 0.2 (RIVM 2018) Density non-volatile: 1.8 g/cm^3 (RIVM 2018) Inhalation cut off diameter: 15 µm (RIVM 2018) Aerosol diameter distribution type: log-normal (median diameter: 23.3 µm, arithmetic coefficient of variation: 1.3, maximum diameter: 50 µm; RIVM 2009)
General purpose aerosol lubricant, dermal	Model: Direct product contact – constant rate Exposed area: 2185 cm^2 (hands and forearms; Statistics Canada 2004 and US EPA 2011) Weight fraction: 0.05 (SDS 2018) Contact rate: 100 mg/min (RIVM 2018) Release duration: 10 seconds (same as spray duration)

Appendix G. Summary table of read-across for health effects endpoints

Table G-1. Considerations for analogues of DNNSA, CaDNNSA and DNNDSA

Consideration	Rationale
1) Chemical structure. Emphasis was placed on analogues that contained a naphthalene ring core, one or more alkyl chains, and one or two sulfonate groups.	Analogues that have similar chemical structure and/or are metabolized through similar pathways to similar degradation products are expected to have similar toxicity profiles. Analogues found that have known toxic metabolites which are not expected to result from the metabolism of the target were not considered.
2) Similar metabolites (predicted or observed). Using OASIS TIMES models for autooxidation and rat *in vivo* and *in vitro* metabolism all analogues and substances of interest produced similar metabolic profiles.	Analogues that have similar chemical structure and/or are metabolized through similar pathways to similar degradation products are expected to have similar toxicity profiles. Analogues found that have known toxic metabolites which are not expected to result from the metabolism of the target were not considered.
3) Similar physical-chemical properties. Emphasis was placed on chemical structures with similar molecular weight, water solubility, and vapour pressure.	Analogues with similar physical-chemical properties may potentially share similar toxicological profiles and bioavailability.
4) Availability of health effects data	Only analogues with hazard data of sufficient quality and coverage of routes and durations of exposure relevant to exposure scenarios were considered applicable for read-across purposes.

Table G-2. Summary table of health effects

Chemical name	DNNSA	CaDNNSA	DNNDSA
Acute toxicity[a, b]	Oral LD_{50} > 5000 mg/kg bw Inhalation LC_{50} > 200 mg/L Dermal LD_{50} > 2000 mg/kg bw	Oral LD_{50} > 5000 mg/kg bw Inhalation LC_{50} > 18 mg/L Dermal LD_{50} > 20000 mg/kg bw	Oral LD_{50} = 2035 mg/kg bw Dermal LD_{50} > 1100 mg/kg bw
Genotoxicity	Ames: negative [read-across from C_9-rich DANSA] TK: negative Chr. Ab: negative [read-across from Ba- C_9-rich DANSA]	Ames: negative TK: negative Chr. Ab: negative [read-across from Ba- C_9-rich DANSA]	Ames: negative [read-across from C_9-rich DANSA] TK: negative Chr. Ab: negative [read-across from Ba- C_9-rich DANSA]
Short term oral studies	NOAEL= 55 mg/kg bw/day [read-across from Ba- C_9-rich DANSA repro/devo study]	NOAEL= 55 mg/kg bw/day [read-across from Ba- C_9-rich DANSA repro/devo study]	NOAEL= 55 mg/kg bw/day [read-across from Ba- C_9-rich DANSA repro/devo study]
Sub-chronic oral studies	NOAEL= 100 mg/kg bw/day [read-across from Ca- C_9-rich DANSA]	NOAEL= 100 mg/kg bw/day [read-across from Ca- C_9-rich DANSA]	NOAEL= 100 mg/kg bw/day [read-across from Ca- C_9-rich DANSA]
Reproductive and developmental	NOAEL= 165 mg/kg bw/day [read-across	NOAEL= 165 mg/kg bw/day [read-across	NOAEL= 165 mg/kg bw/day [read-across

Chemical name	DNNSA	CaDNNSA	DNNDSA
toxicity oral studies	from Ba- C_9-rich DANSA]	from Ba- C_9-rich DANSA]	from Ba- C_9-rich DANSA]
Carcinogenicity	Not available	Not available	Not available

Abbreviations: LD_{50}, the lethal dose required to kill 50% of the population; LC_{50}, the lethal concentration required to kill 50% of the population; TK, tyrosine kinase; Chr. Ab, chromosome aberration

[a] US EPA 2012

[b] ECHA 2018a