

Substance Profile for The Challenge
Benzenesulfonic acid, 2,2'-[(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-anthracenediyl)diimino]bis[5-(1,1-dimethylethyl)-, disodium salt
CAS No. 83006-67-1

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) required the Minister of Health and Minister of the Environment to categorize the approximately 23 000 substances on the Domestic Substances List (DSL). Categorization involved identifying those substances on the DSL that are a) considered to be persistent (P) and/or bioaccumulative (B), based on criteria set out in the *Persistence and Bioaccumulation Regulations* (Government of Canada, 2000), and “inherently toxic” (iT) to humans or other organisms, or b) that present, to individuals in Canada, the greatest potential for exposure (GPE).

Further to this activity, the Act requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that meet the categorization criteria. A screening assessment involves a scientific evaluation of available information for a substance to determine whether the substance meets the criteria set out in section 64 of CEPA 1999. Based on the results of a screening assessment, the Ministers can propose taking no further action with respect to the substance, adding the substance to the Priority Substances List (PSL) for further assessment or recommending the addition of the substance to the List of Toxic Substances in Schedule 1 of CEPA 1999 and, where applicable, the implementation of virtual elimination of releases to the environment.

A number of substances have been identified by the Ministers as high priorities for action based on the information obtained through the categorization process. This includes substances:

- that were found to meet all of the ecological categorization criteria, including persistence, bioaccumulation potential and inherent toxicity to aquatic organisms (PBiT), and that are known to be in commerce, or of commercial interest, in Canada, and/or
- that were found either to meet the categorization criteria for GPE or to present an intermediate potential for exposure (IPE), and were identified as posing a high hazard to human health based on available evidence on carcinogenicity, mutagenicity, developmental toxicity or reproductive toxicity.

Based on a consideration of the ecological and/or human health concerns associated with these substances, and the requirement under section 76.1 of CEPA 1999 for the Ministers to apply a weight of evidence approach and the precautionary principle when conducting

and interpreting the results of an assessment, sufficient data are currently available to conclude whether these substances meet the criteria under section 64 of CEPA 1999.

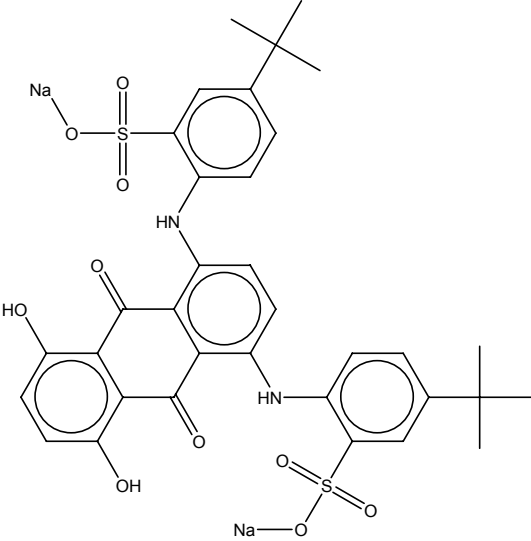
As such, the Ministers have issued a Challenge to industry and other interested stakeholders through publication in Canada Gazette Part I December 9, 2006 to submit, within the timelines stated in the Challenge section of this document, specific information that may be used to inform risk assessment and to develop and benchmark best practices for risk management and product stewardship.

The substance benzenesulfonic acid, 2,2'-[(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-anthracenediyl)diimino]bis[5-(1,1-dimethylethyl)-, disodium salt was identified as a high priority for action as it was found to be persistent, bioaccumulative and inherently toxic to aquatic organisms, and is believed to have commercial interest in Canada. The technical human health and ecological information that formed the basis for concern associated with this substance is contained in Appendices I and II, respectively.

Substance Identity

For the purposes of this document, this substance will be referred to as “ADIBSS” (“anthracenediyl **diimino benzenesulfonic acid, disodium salt**”), which has been derived from the inventory name Benzenesulfonic acid, 2,2'-[(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-anthracenediyl)diimino]bis[5-(1,1-dimethylethyl)-, disodium salt (NCI).

CAS Registry Number	83006-67-1
Inventory names	<ul style="list-style-type: none"> • Benzenesulfonic acid, 2,2'-[(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-anthracenediyl)diimino]bis[5-(1,1-dimethylethyl)-, disodium salt; • disodium 2,2'-[(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-anthrylene)diimino]bis[5-tert-butylbenzenesulphonate]; • 2,2'-[(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-anthrylene)diimino]bis[5-tert-butylbenzenesulfonate] de disodium
Chemical group	Discrete organics
Chemical sub-groups	Aromatic amines; alkyl benzene sulfonates
Chemical formula (EPIWIN)	C ₃₄ H ₃₂ N ₂ O ₁₀ S ₂ Na ₂

Chemical structure (EPIWIN)	
SMILES (EPIWIN)	<chem>c1cc(C(C)(C)C)cc(S(=O)(=O)O[Na])c1Nc2c3C(=O)c4c(O)ccc(O)c4C(=O)c3c(cc2)Nc5c(S(=O)(=O)O[Na])cc(C(C)(C)C)cc5</chem>
Molecular mass (EPIWIN)	738.74 g/mol

No reports of manufacture in or import into Canada of this substance at or above the reporting threshold of 100 kg in the 2005 calendar year were received in response to a Notice published under section 71 of CEPA 1999 (Environment Canada 2006a). However, the Declaration of Non-Engagement form associated with this Notice (Environment Canada 2006b) further invited any companies to identify themselves as stakeholders if they had an interest in a listed substance. One stakeholder identified themselves as having an interest in this substance.

THE CHALLENGE

Respecting direction under section 76.1 of CEPA 1999, and in the absence of additional relevant information as a result of this Challenge, the Ministers are predisposed to conclude, based on a screening assessment, that this substance satisfies the definition of toxic under section 64 of CEPA 1999. As such, the Ministers are prepared to then recommend to the Governor in Council that this substance be added to the List of Toxic Substances in Schedule 1 of CEPA 1999, with the intent of initiating the development of risk management measures taking into account socio-economic considerations.

If it is determined that the substance meets the virtual elimination criteria in subsection 77(4) of CEPA 1999, then subsequent risk management activities will be based on the objective of eliminating the release of any measurable quantity of the substance to the environment. In the absence of further information on existing management practices for a substance, actions would be proposed based on the assumption of worst-case practices. The management actions being considered for such substances at this time include prohibition through regulations, of the manufacture, use, sale, offer for sale and import of this substance, except for those activities controlled under the *Pest Control Products Act* and/or the *Food and Drugs Act*.

Exceptionally, should no information be identified to indicate that this substance is in commerce in Canada, the Ministers will conclude, based on a screening assessment, that this substance does not satisfy the definition of toxic under section 64 of CEPA 1999. However, given the properties of this substance, there is concern that new activities for the substance that have not been identified or assessed under CEPA 1999 could lead to the substance meeting the criteria set out in section 64 of the Act. Therefore it would be recommended that this substance be subject to the Significant New Activity provisions specified under subsection 81(3) of the Act, to ensure that any new manufacture, import or use of this substance in quantities greater than 100 kg/year is notified, and that ecological and human health risk assessments are conducted as specified in section 83 of the Act prior to the substance being introduced into Canada.

Section 71 Notice

Under the Challenge, information deemed necessary for improved decision making may be gathered by the Minister of Environment using section 71 of CEPA 1999. This information may be used for the purpose of assessing whether a substance is toxic or is capable of becoming toxic as defined under section 64 of CEPA 1999, or for the purpose of assessing whether to control, or the manner in which to control a substance.

The information mandated through the notices may relate to, among other things; quantity of the substance imported, manufactured, used, or released, concentrations, suppliers, customers, as well as types of uses of the substance.

Copies of the section 71 notice and guidance on how to comply with it are available from the Government of Canada Chemicals Portal (www.chemicalsubstanceschimiques.gc.ca), or from the contact provided below.

Opportunity to Submit Additional Information to Inform Screening Assessment

The Ministers of Health and Environment are inviting the submission of additional information for consideration during screening assessment of this substance. Data of the types described in the following paragraphs are considered most relevant, although other submitted information will be considered.

Data on the persistence, bioaccumulation, and potential for toxicity of the substance to organisms in different environmental media – Through the categorization exercise, available experimental data were collected up to December 2005. Where acceptable experimental data were not available, Quantitative Structure Activity Relationships (QSARs) or read across data were used to fill the data gaps. Since experimental data are preferred, interested parties have an opportunity to provide new or additional relevant experimental study information on the persistence, bioaccumulation, and potential for toxicity of this substance to organisms in different environmental media (air, water, sediment, soil). Efforts should focus on providing data for the endpoints for which quality experimental data does not already exist, as demonstrated by the information summarized in Appendix II of this document. As submitted data will be evaluated for completeness and robustness, it is recommended that stakeholders follow the guidance for test protocols and alternative approaches for test data, as described in Section 8 of the “Guidelines for the Notification and Testing of New Substances: Chemicals & Polymers”.¹

Data on the toxicity of the substance to human health - Through the categorization exercise, the high health priorities for action were those substances identified by various agencies as representing a high health hazard on the basis of potential to induce cancer, and/or adversely affect reproduction and development, two critical determinants of the health of Canadians of all ages. The hazard classifications used were those developed by national or international agencies in which large numbers of substances have been classified for endpoint-specific hazard based on original review and critical evaluation of data, assessments of weight of evidence and extensive peer review. Interested parties have an opportunity to provide new or additional relevant experimental study information on the toxicity of the substance to human health which could inform the screening assessment.

Responses to this part of the challenge for this substance should be received at the address provided below by November 13, 2007.

¹ “Guidelines for the Notification and Testing of New Substances: Chemicals & Polymers (version 2005)”, Government of Canada, available from http://www.ec.gc.ca/substances/nsb/eng/cp_guidance_e.shtml

Opportunity to Submit Additional Information on Current Uses and Existing Control Measures to Inform the Risk Management Approach for this Substance

The Ministers of Health and Environment are inviting the submission of additional information that is deemed beneficial by interested stakeholders, relating to the extent and nature of the management/stewardship of substances listed under the Challenge.

Organizations that may be interested in submitting additional information in response to this invitation include those that manufacture, import, export or use this substance whether alone, in a mixture, in a product or in a manufactured item.

Additional information is being invited in the following areas:

- Import, manufacture and use quantities
- Substance and product use details
- Releases to the environment and spill management
- Current and potential risk management and product stewardship actions
- Existing legislative or regulatory programs controlling/managing the substance
- Information to support the development of a regulatory impact assessment.

A questionnaire is available which provides a detailed template as an example for the submission of this information. Guidance on how to respond to the challenge questionnaire is also available. Interested stakeholders are invited to provide available additional information, recognizing that not all questions in the questionnaire may be relevant to a particular substance, use, or industrial sector.

Copies of the questionnaire and associated guidance are available from the Government of Canada Chemicals Portal (www.chemicalsubstanceschimiques.gc.ca), or from the contact provided below.

Responses to this part of the challenge for this substance should be received at the address provided below by November 13, 2007.

Request for Documents and Submission of Information

Documents and instructions may be requested from the following contact. Information in response to the above Challenge must be submitted to this address.

DSL Surveys Coordinator
Place Vincent Massey, 20th Floor
351 Saint Joseph Boulevard

Gatineau, QC, K1A 0H3
Tel.: 1-888-228-0530/819-956-9313
Fax: 1-800-410-4314 / 819-953-4936
E-mail: DSL.surveyco@ec.gc.ca

Appendix I
Human Health Information
to Support The Challenge for
Benzenesulfonic acid, 2,2'-[(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-
anthracenediyl)diimino]bis[5-(1,1-dimethylethyl)-, disodium salt
(ADIBSS)
CAS No. 83006-67-1

Introduction

Under the *Canadian Environmental Protection Act, 1999* (CEPA, 1999), Health Canada undertook to categorize substances on the Domestic Substances List (DSL) to identify those representing the greatest potential for human exposure (GPE) and those among a subset of substances considered persistent (P) and/or bioaccumulative (B) that are also considered to be “inherently toxic” to humans.

In order to efficiently identify substances that represent the highest priorities for screening assessment from a human health perspective, Health Canada developed and applied a Simple Exposure Tool (SimET) to the DSL to identify those substances that meet the criteria for GPE, Intermediate Potential for Exposure (IPE) or Low Potential for Exposure (LPE), and a Simple Hazard Tool (SimHaz) to identify those substances that pose a high or low hazard.

ADIBSS is considered to meet the criteria for LPE under SimET and does not meet the criteria for high hazard under SimHaz. This document summarizes the currently available information on which the SimET and SimHaz results are based.

Exposure Information from Health Related Components of DSL Categorization

SimET was developed and used to identify substances on the DSL considered to represent GPE. This approach was based on three lines of evidence: 1) the quantity in commerce in Canada, 2) the number of companies involved in commercial activities in Canada (i.e., number of notifiers), and 3) the consideration by experts of the potential for human exposure based on various use codes. The proposed approach was released for public comment in November 2003 and also enabled designation of substances as presenting an Intermediate (IPE) or Lowest Potential for Exposure (LPE), based on criteria for quantity and nature of use (Health Canada, 2003).

Results of the Application of SimET

ADIBSS has been determined to be LPE based on a consideration of the DSL nomination information listed below.

Nomination Information for DSL

Quantity in Commerce

The quantity reported to be manufactured, imported or in commerce in Canada during the calendar year 1986 was 1000 kg.

Number of Notifiers

The number of notifiers for the calendar years 1984-1986 was less than 4.

Use Codes and Description

The following DSL use codes have been identified for the substance:

85 Pigment, dye and printing ink

Hazard Information from Health Related Components of DSL Categorization

Simple Hazard Tool (SimHaz)

SimHaz is a tool that has been used to identify, among all of the approximately 23 000 substances on the DSL, those considered to present either high or low hazard to human health based on formalized weight of evidence criteria and/or peer review/consensus of experts. This tool has been developed through extensive compilation of hazard classifications of Health Canada and other agencies and consideration of their robustness based on availability of transparent documentation of both process and criteria (Health Canada, 2005).

Results of the Application of SimHaz

ADIBSS has not been classified for hazard by any of the agencies considered under the SimHaz tool and therefore does not meet the criteria for high hazard under SimHaz.

Uncertainties

SimET and SimHaz have been developed as robust tools for effectively identifying substances from the DSL considered to be human health related priorities for further consideration. It is recognized that they do not include a number of elements normally considered in a human health risk assessment such as a comprehensive characterization of exposure and hazard, a comparison of exposure metrics to hazard metrics and a detailed analysis of uncertainties.

References

Health Canada. 2003. Proposal for Priority Setting for Existing Substances on the Domestic Substances List under the Canadian Environmental Protection Act, 1999: Greatest Potential for Human Exposure.

http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/existsub/exposure/greatest_potential_human_exposure-risque_exposition_humaine_e.pdf

Health Canada. 2005. Proposed Integrated Framework for the Health-Related Components of Categorization of the Domestic Substances List under CEPA 1999.

http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/contaminants/existsub/framework-int-cadre_e.pdf

Appendix II
Ecological Information
to Support The Challenge for
Benzenesulfonic acid, 2,2'-[(9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1,4-
anthracenediyl)diimino]bis[5-(1,1-dimethylethyl)-, disodium salt
(ADIBSS)
CAS No. 83006-67-1

Introduction

The information in this document will form the basis of a screening assessment under section 74 of CEPA, 1999. Data relevant to an ecological screening assessment were identified in original literature, review documents, commercial and government databases prior to December 2005. Properties and characteristics may also have been estimated using Quantitative Structure Activity Relationship (QSAR) models. In addition, an industry survey was conducted for the year 2005 through a Canada Gazette Notice issued pursuant to section 71 of CEPA 1999 (Environment Canada, 2006a). This Notice requested data on the Canadian manufacture and import of the substance.

Physical and Chemical Properties

Experimental physico-chemical data for ADIBSS are not available. Table 1 contains modelled physico-chemical properties of this substance which are relevant to its environmental fate.

Table 1: Modelled physical-chemical properties for ADIBSS

Property	Value / Units	Reference
Boiling point (BP)	1144.78 °C	MPBPWIN v.1.41
Melting point (MP)	349.84 °C	MPBPWIN v.1.41
Henry's Law constant (HLC)	3.1×10^{-27} Pa · m ³ /mol (3.04×10^{-32} atm · m ³ /mol)	HENRYWIN v.3.10
log Koc	7.05	PCKOCWIN v.1.66
log Kow	5.32	KOWWIN v.1.67
Vapour pressure (VP)	5.09×10^{-32} Pa (3.82×10^{-34} mm Hg)	EPIWIN v.3.11
Water solubility (WS)	1.635×10^{-4} mg/L	WSKOWWIN v.1.41

Manufacture, Importation, and Uses

Manufacture and Importation

For the quantity reported to be manufactured, imported or in commerce in Canada during the calendar year 1986, refer to the Appendix I.

Information gathered from the CEPA section 71 Notice indicates that ADIBSS (CAS No. 83006-67-1) was not manufactured or imported into Canada in 2005 in a quantity meeting the 100 kg reporting threshold. One Canadian company identified themselves as having a stakeholder interest in the substance.

Elsewhere, this chemical was used in Sweden and Denmark throughout the years 1999-2004 (SPIN database); however, information on exact quantities of ADIBSS used and specific use patterns is not available.

Uses

For the use codes in Canada reported during the calendar year 1986, refer to Appendix I.

Information on use received through the S. 71 survey (Environment Canada, 2006a) has been claimed as confidential business information.

Releases, Fate, and Presence in the Environment

Releases

The substance ADIBSS is not naturally produced in the environment.

Since there were no reports of import or manufacture at or above the reporting threshold of 100 kg in 2006, releases of this substance to the Canadian environment are presumed to be very low.

Fate

Aquatic fate

The very high log K_{oc} value of ~7 (Table 1) indicates that if released into water, ADIBSS is expected to strongly adsorb to suspended solids and sediments. Volatilization from water surfaces is not expected based upon the extremely low estimated Henry's Law constant of 3×10^{-32} atm · m³/mol (Table 1). Thus, if water is a receiving medium, ADIBSS is expected to mainly partition to sediments and, in some extent, remain in water, as indicated by the results of Level III Fugacity modelling (Table 2).

Table 2: Results of the Level III fugacity modelling (EPIWIN V3.12) for ADIBSS

Receiving media	% in Air	% in Water	% in Soil	% in Sediment
Air (100%)	0.01	0.19	85.2	14.6
Water (100%)	0.00	1.26	0.00	98.7
Soil (100%)	0.00	0.00	99.8	0.19
Air, water, soil (33.3% each)	0.00	0.65	48.8	50.6

Terrestrial fate

If released into soil, this chemical is expected to have very high adsorptivity to soil and will be, therefore, virtually immobile in this environmental compartment based upon the estimated $\log K_{oc}$ of ~ 7 (Table 1). Volatilization from moist soil surfaces seems to be an unimportant fate process based upon a very low Henry's Law constant ($3 \times 10^{-32} \text{ atm} \cdot \text{m}^3/\text{mol}$, Table 1). This substance will not volatilize from dry soil surfaces based upon the estimated vapour pressure of $5.1 \times 10^{-32} \text{ Pa}$. Therefore, if soil is a receiving medium, ADIBSS is expected to remain exclusively in soil, which is illustrated by the results of Level III Fugacity modelling (Table 2).

Atmospheric fate

The extremely low value of a vapour pressure of $5.1 \times 10^{-32} \text{ Pa}$ (Table 1) indicates that ADIBSS is a non-volatile chemical, and it is expected to exist solely in the particulate phase in the ambient atmosphere. The exceptionally low Henry's Law constant of $3 \times 10^{-32} \text{ atm} \cdot \text{m}^3/\text{mol}$ (Table 1) also indicates that it will not volatilize from water to air. Therefore, if released to air, this chemical is not expected to remain in this environmental compartment. Considering the very high organic carbon partition coefficient of this chemical ($\log K_{oc} \approx 7$), it will mainly partition to soil and sediments, as indicated by the results of Level III Fugacity modelling (Table 2).

Therefore, it can be concluded that when ADIBSS is released to the environment, soil and sediment are expected to be the major media of concern, which is illustrated by the results of fugacity modelling (Table 2).

Presence in the Environment

No monitoring data relating to the presence of this substance in environmental media (air, water, soil, sediment) have yet been identified.

Evaluation of P, B, and iT Properties

Environmental Persistence

No experimental persistence data for air are available for ADIBSS. QSAR predictions show that once released to air, this chemical would be rapidly oxidized in this environmental compartment, as indicated by an atmospheric oxidation half-life value of 0.06 days (Table 3a), assuming an average atmospheric hydroxyl-radical concentration of $1.5 \times 10^6 \text{ molecule}/\text{cm}^3$.

This compound is not expected to react appreciably with other photo-oxidative species in the atmosphere such as O_3 and NO_3 , nor is it likely to degrade via direct photolysis. Therefore, it is expected that reactions with hydroxyl radicals will be the most important

fate process in the atmosphere for this chemical. With a half-life of 0.06 days via reactions with hydroxyl radical, this chemical is not persistent in air.

Table 3a: Predicted persistence values for ADIBSS

Medium	Fate Process	Degradation Value	Degradation Endpoint	Reference
Air	Atm. oxidation	0.0601	Half-life (days)	AOPWIN v1.91
Air	Ozone reaction	Non-reactive	Half-life (days)	AOPWIN v1.91
Water/soil	Biodegradation	182	Half-life (days)	BIOWIN v4.02, Ultimate survey
Water/soil	Biodegradation	0	Probability	BIOWIN v4.02, MITI non-linear probability
Water/soil	Biodegradation	0	Probability	BIOWIN v4.02, MITI linear probability

For estimation of biological degradation of ADIBSS in water, a QSAR-based weight-of-evidence approach (ESD, 2006a) was applied, using the models shown in Table 3a. Based on these results, the estimated timeframe for biodegradation of ADIBSS indicates that this chemical can be considered as persistent in water.

To extrapolate half-life in water to half-lives in soils and sediments, Boethling's extrapolation factors can be used: $t_{1/2 \text{ water}} : t_{1/2 \text{ soil}} : t_{1/2 \text{ sediment}} = 1 : 1 : 4$ (Boethling *et al.*, 1995). Applying the ultimate-survey half-life of 182 days (Table 3a) and Boethling's extrapolation factors, it may be concluded that in soil and sediments, ADIBSS half-lives are expected to be 182 days and ≈ 2 years, respectively. Therefore, this chemical is expected to be persistent in water, soil, and sediments.

The long-range transport potential (LRTP) of ADIBSS from its point of release to air is estimated to be low according to the model prediction presented in Table 3b. The TaPL3 model was used to estimate Characteristic Travel Distance (CTD), defined as the maximum distance traveled by 63% of the substance or, in other words, the distance that 37% of the substance may travel beyond.

Beyer *et al.* (2000) have proposed CTD of >2000 km as representing high LRTP, 700-2000 km – as moderate, and <700 km – as low LRTP. Based on the result (Table 3b), ADIBSS has low long-range transport potential, i.e. this substance is expected to remain primarily in areas close to its emission sources.

Table 3b: Model-predicted Characteristic Travel Distances (CTD) for ADIBSS

Characteristic Travel Distance	Reference
480 km	TaPL3, V. 2.10

Therefore, the empirical and modelled data demonstrate that ADIBSS meets the persistence criteria (half-lives in soil and water ≥ 182 days, in sediments ≥ 365 days) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000).

Potential for Bioaccumulation

Experimental data, such as octanol-water partition coefficient, as well as bioaccumulation and bioconcentration factors (BAF and BCF, respectively), are not available for ADIBSS. The modelled octanol-water partition coefficient ($\log K_{ow}=5.3$, Table 1) indicates that this chemical could potentially bioaccumulate in the organisms.

The Modified Gobas middle-trophic-level BAF model produced a BAF of approximately 53,000 L/kg (Table 4), indicating that ADIBSS has the potential to be highly bioaccumulative. The two BCF models – modified Gobas BCF and OASIS – produced BCF values of approximately 9,000 and 29,000 L/kg (Table 4), which provides a weight-of-evidence of high bioconcentration potential of this substance and supports the conclusion that ADIBSS could accumulate in the tissues of aquatic organisms and may biomagnify in the food web.

Table 4: Predicted bioaccumulation values for ADIBSS

Test Organism	Endpoint	Value (wet weight, L/kg)	Reference
Fish	BAF	53399	Gobas BAF T2MTL (Arnot & Gobas, 2003)
Fish	BCF	9280	Modified Gobas BCF 5% T2LTL (Arnot & Gobas, 2003)
Fish	BCF	28852	OASIS
Fish	BCF	10	BCFWIN v2.15

The very low BCF value of 10 (Table 4) is a default value recommended by the BCFWIN model for substances which are ionisable (i.e. it is not derived from the $\log K_{ow}$ /BCF relationship that BCFWIN typically uses for non-ionisable substances); therefore, this result is not a model-generated BCF calculated specifically for ADIBSS.

Thus, the weight of evidence indicates that the substance ADIBSS meets the bioaccumulation criteria ($BAF/BCF \geq 5000$) as set out in the Persistence and Bioaccumulation Regulations (Government of Canada, 2000).

Ecological Effects

In the Aquatic Compartment

Experimental aquatic ecotoxicity data are not available for ADIBSS. Therefore, QSAR models were used for estimation of ecotoxicity. Table 5 contains the prediction that was considered reliable and was used in the QSAR weight-of-evidence approach for aquatic toxicity (ESD, 2006a). This acute LC50 value of 0.007 mg/L indicates that ADIBSS has a potential for very high toxicity to aquatic organisms.

Table 5: Modelled aquatic toxicity values for ADIBSS

Organism	Duration	Endpoint	Toxicity value (mg/L)	Model
Fish	Acute	LC50	0.007*	ECOSAR (Neutral Organic SAR)

*Pivotal iT value for categorization

Since the acute LC50 value is well below 1 mg/L, it may be concluded that ADIBSS is expected to pose high (acute or immediate) hazard for aquatic organisms exposed to the chemical in water.

In Other Media

No effects studies for non-aquatic non-mammalian organisms were found for this compound.

Potential to Cause Ecological Harm

Evidence that a substance is highly persistent and bioaccumulative as defined in the Persistence and Bioaccumulation Regulations of CEPA 1999 (Government of Canada, 2000) together with evidence of commercial activity provides a significant indication of its potential to be entering the environment under conditions that may have harmful long term ecological effects (ESD, 2006b). Substances that are persistent remain in the environment for a long time after being released, increasing the potential magnitude and duration of exposure. Substances that have long half-lives in mobile media (air and water) and partition into these media in significant proportions, have the potential to cause widespread contamination. Releases of small amounts of bioaccumulative substances may lead to high internal concentrations in exposed organisms. Highly bioaccumulative and persistent substances are of special concern, since they may biomagnify in food webs, resulting in very high internal exposures, especially for top predators. Evidence that a substance is both highly persistent and bioaccumulative, when taken together with other information (such as evidence of toxicity at relatively low concentrations, and evidence of uses and releases) may therefore be sufficient to indicate that the substance has the potential to cause ecological harm.

The information collected to date suggests that ADIBSS has the potential to cause ecological harm if it were to be released in the Canadian environment. Once released into the environment, because of its resistance to degradation, it could remain in water, sediment, and/or soil for a long time. As it persists in the environment, and because of its lipophilic character, it could bioaccumulate and possibly be biomagnified in trophic food chains. It has also demonstrated relatively high toxicity to aquatic organisms. However, the lack of importation or manufacture of ADIBSS in Canada at significant volumes suggests very low releases of this chemical into the Canadian environment.

Uncertainties

Based on information collected, there is some uncertainty about the precise use patterns of ADIBSS. In addition, information on concentrations in the Canadian environment is currently lacking.

Neither experimental data for the key physico-chemical properties (e.g. K_{ow} , water solubility, Henry's Law constant), nor experimental data on ecotoxicity, degradation, and bioaccumulation are currently available for ADIBSS. Therefore, uncertainties exist in the conclusions reached in this document because P, B, and iT evaluations are based on model data.

Regarding toxicity, based on the predicted partitioning behaviour of this chemical, the significance of soil and sediments as important media of exposure cannot be appropriately addressed because no ecotoxicological data are available for these two environmental compartments.

The experimental or predicted concentrations, associated with inherent toxicity for aquatic organisms, may have an additional source of uncertainty in some situations, e.g. where these concentrations exceed the solubility of the chemical in water (either experimental or predicted). Given that concentrations for both the toxicity and water solubility often vary considerably (up to several orders of magnitude), it is acknowledged that these uncertainties exist.

There is also uncertainty associated with basing the overall conclusion that ADIBSS may be causing ecological harm, solely on information relating to its persistence, bioaccumulation, relative toxicity, and use pattern. Typically quantitative risk estimates (i.e., risk quotients or probabilistic analyses) are important lines of evidence when evaluating a substance's potential to cause environmental harm. However when risks for persistent and bioaccumulative substances such as ADIBSS are estimated using such quantitative methods, they are highly uncertain and are likely to be underestimated (ESD, 2006b). Given that long term risks associated with persistent and bioaccumulative substances cannot at present be reliably predicted, quantitative risk estimates have limited relevance. Furthermore, since accumulations of such substances may be widespread and are difficult to reverse, a conservative response to uncertainty (that avoids underestimation of risks) is justified.

References

AOPWIN v1.91. 2000. U.S. Environmental Protection Agency.
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