

Screening Assessment for the Challenge

**Acetamide, *N*-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl]-
(Disperse Blue 79)**

**Chemical Abstracts Service Registry Number
12239-34-8**

**Environment Canada
Health Canada**

August 2009

Synopsis

Pursuant to section 74 of the *Canadian Environmental Protection Act, 1999* (CEPA 1999), the Ministers of the Environment and of Health have conducted a screening assessment on Acetamide, *N*-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl]- (Disperse Blue 79), Chemical Abstracts Service Registry Number 12239-34-8. This substance was identified as a high priority for screening assessment and included in the Challenge because it had been found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity to non-human organisms and is believed to be in commerce in Canada.

The substance Disperse Blue 79 was not considered to be a high priority for assessment of potential risks to human health, based upon application of the simple exposure and hazard tools developed by Health Canada for categorization of substances on the *Domestic Substances List*. Therefore, this assessment focuses on information relevant to the evaluation of ecological risks.

Disperse Blue 79 is an organic substance that is used in Canada and elsewhere as a blue colourant dye mainly in textiles and fabric. The substance is not naturally produced in the environment. Between 1 000 and 10 000 kg of Disperse Blue 79 were imported into Canada in 2006, for use as a colorant mainly in the chemical product manufacturing and textile and fabric finishing industries. The quantity of Disperse Blue 79 imported into Canada, along with the potentially dispersive uses of this substance, indicate that it could potentially be released into the Canadian environment.

Based on reported use patterns and certain assumptions, most of the substance is expected to end up in waste disposal sites (85.2%) and a significant proportion is, however, estimated to be released to sewer water (14.8%). Disperse Blue 79 is not expected to be soluble in water or to be volatile, but is expected to partition to particles because of its hydrophobic nature. For these reasons, after release to water, Disperse Blue 79 will likely end up mostly in sediments, and to a lesser extent, in agricultural soil that has been amended with sewage sludge. It is not expected to be significantly present in other media. It is also not expected to be subject to long-range atmospheric transport.

Based on its physical and chemical properties, Disperse Blue 79 is expected to be persistent in the environment (in water, sediment and soil). However, new experimental data relating to the bioaccumulation potential of a relatively close structural analogue suggest that this dye has a low potential to accumulate in the lipid tissues of organisms. The substance therefore meets the persistence criteria but does not meet the bioaccumulation criteria as set out in the *Persistence and Bioaccumulation Regulations*. In addition, experimental toxicity data for Disperse Blue 79 suggest that the substance does not harm aquatic organisms exposed to low concentrations.

For this screening assessment, two conservative exposure scenarios were selected in which an industrial operation (user of the dye) and consumer use of products containing this substance discharged Disperse Blue 79 into the aquatic environment. The

environmental concentrations predicted with this exposure scenario was similar to a previous concentration measured in the Canadian aquatic environment. Both the measured and predicted environmental concentrations in water were below the predicted no-effect concentration estimated for sensitive aquatic organisms.

This substance will be included in the upcoming *Domestic Substances List* inventory update initiative. In addition and where relevant, research and monitoring will support verification of assumptions used during the screening assessment.

Based on the information available, it is concluded that Disperse Blue 79 does not meet any of the criteria set out in section 64 of CEPA 1999.

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) (Canada 1999) requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that have met the categorization criteria set out in the Act to determine whether these substances present or may present a risk to the environment or human health. Based on the results of a screening assessment, the Ministers can propose to take no further action with respect to the substance, to add the substance to the Priority Substances List (PSL) for further assessment, or to recommend that the substance be added to the List of Toxic Substances in Schedule 1 of the Act and, where applicable, the implementation of virtual elimination.

Based on the information obtained through the categorization process, the Ministers identified a number of substances as high priorities for action. These include substances that

- met all of the ecological categorization criteria, including persistence (P), bioaccumulation potential (B) and inherent toxicity to aquatic organisms (iT), and were believed to be in commerce in Canada; and/or
- met the categorization criteria for greatest potential for exposure (GPE) or presented an intermediate potential for exposure (IPE), and had been identified as posing a high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity.

The Ministers therefore published a notice of intent in the *Canada Gazette*, Part I, on December 9, 2006 (Canada 2006a), that challenged industry and other interested stakeholders to submit, within specified timelines, specific information that may be used to inform risk assessment, and to develop and benchmark best practices for the risk management and product stewardship of these substances identified as high priorities.

The substance Disperse Blue 79 was identified as a high priority for assessment of ecological risk as it had been found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is believed to be in commerce in Canada. The Challenge for this substance was published in the *Canada Gazette* on February 16, 2008 (Canada 2008). A substance profile was released at the same time. The substance profile presented the technical information available prior to December 2005 that formed the basis for categorization of this substance. As a result of the Challenge, submissions of information pertaining to the physical and chemical properties, bioaccumulation, aquatic toxicity and uses of the substance were received.

Although Disperse Blue 79 was determined to be a high priority for assessment with respect to the environment, it did not meet the criteria for GPE or IPE, and was not identified as posing a high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental

toxicity or reproductive toxicity. Therefore, this assessment focuses principally on information relevant to the evaluation of ecological risks.

Screening assessments under CEPA 1999 focus on information critical to determining whether a substance meets the criteria for defining a chemical as toxic as set out in section 64 of the Act, where

- “64. [...] a substance is toxic if it is entering or may enter the environment in a quantity or concentration or under conditions that
- (a) have or may have an immediate or long-term harmful effect on the environment or its biological diversity;
 - (b) constitute or may constitute a danger to the environment on which life depends; or
 - (c) constitute or may constitute a danger in Canada to human life or health.”

Screening assessments examine scientific information and develop conclusions by applying a weight of evidence approach and precaution.

This screening assessment considers any new information on chemical properties, hazards, uses and exposure submitted under the Challenge. Data relevant to the screening assessment of this substance were identified in original literature, review documents, stakeholder research reports and from recent literature searches up to October 2008. Key studies were critically evaluated and generally only results from studies of good quality were used to reach conclusions, although other studies and modelling results may have been considered as part of the weight of evidence. When available and relevant, information presented in hazard assessments from other jurisdictions was also used. The screening assessment does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies and lines of evidence pertinent to the conclusion.

This screening assessment was prepared by staff in the Existing Substances Program at Health Canada and Environment Canada and it incorporates input from other programs within these departments. The assessment has undergone external written peer review. While external comments were taken into consideration, the final content and outcome of the screening risk assessment remain the responsibility of Health Canada and Environment Canada. Additionally, the draft of this screening assessment was subject to a 60-day public comment period. The critical information and considerations upon which the assessment is based are summarized below.

Substance Identity

For the purposes of this report, the substance Acetamide, *N*-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl] will be referred to as Disperse Blue 79. “Disperse Blue 79” is defined by the Colour Index (CII 2002–) as a mixture of two chemical abstracts service registry numbers (CAS RN 12239-34-8 and 3956-55-6). However, for the purposes of this document, the common name “Disperse Blue 79” refers exclusively to the CAS RN 12239-34-8. Information on substance identity is included in Table 1.

Table 1. Substance Identity

Chemical Abstracts Service Registry Number (CAS RN)	12239-34-8
DSL name	Acetamide, <i>N</i>-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl]-
Inventory names¹	Acetamide, <i>N</i> -[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-ethoxyphenyl]- (TSCA, DSL, AICS, PICCS, ASIA-PAC) 2,2'-[[5-acetamide-4-[(2-bromo-4,6-dinitrophenyl)azo]-2-ethoxyphenyl]imino]diethyl diacetate (EINECS) Disperse Blue 079 (ENCS) C.I. disperse blue 079 (ECL) 2,2'-[[5-acetamide-4-[(2-bromo-4,6-dinitrophenyl)azo]-2-ethoxyphenyl]imino]diethyl diacetate (PICCS) C.I. DISPERSE NAVY 29 (PICCS) C.I. DISPERSE NAVY 79 (PICCS)
Other names	<i>2-Acetamido-4-[N,N-bis(b-acetoxyethyl)amino]-5-ethoxy-2'-bromo-4',6'-dinitroazobenzene; 2'-Acetylamino-4'-[bis(acetoxyethyl)amino]-6-bromo-2,4-dinitro-5'-ethoxyazobenzene; 2-Bromo-4,6-dinitrophenylazo-2-acetamido-4-di-(2-acetoxyethyl)amino-5-ethoxybenzene; 4-(2-Bromo-4,6-dinitrophenylazo)-5-acetylamino-2-ethoxy-N,N-bis(b-acetoxyethyl)aniline; C.I. 11345; C.I. disperse blue 079; C.I. Disperse Blue 079; C.I. DISPERSE NAVY 29 ; C.I. DISPERSE NAVY 79; Disperse Blue 2GL; Disperse Blue 079; Disperse Blue HGL; Disperse Navy Blue 2GL; Eastman Polyester Navy Blue 2R-LSW; Foron Navy 2GL; Foron Navy Blue S 2GL; Foron Navy S 2GL; Foron Navy S 2GLI; Miketon Polyester Navy Blue GLSF; Navy Blue 2GL; Ostacet Navy Blue S-G; p-Acetophenetidide, 5'-[bis(2-hydroxyethyl)amino]-2'-[(2-bromo-4,6-dinitrophenyl)azo]-, diacetate; p-Acetophenetidide, 5'-[bis(2-hydroxyethyl)amino]-2'-[(2-bromo-4,6-dinitrophenyl)azo]-, diacetate (ester); Samaron Marine Blue G; Samaron Navy Blue G; Serilene Navy Blue 2GN-LS; Terasil Navy GRL; Tulasteron Fast Navy Blue 2G-D; Tulasteron Navy Blue 2GDN</i>
Chemical group	Discrete organics
Chemical sub-group	Monoazo dye

Chemical formula	C ₂₄ H ₂₇ BrN ₆ O ₁₀
Chemical structure	
SMILES²	<chem>N(=O)(=O)c1c(c(cc1N(=O)(=O))Br)N=Nc2cc(cc(c2NC(=O)C)N(CCOC(=O)C)CCOC(=O)C)OCC</chem>
Molecular mass	639.42 g/mol

¹ NCI 2006; AICS (Australian Inventory of Chemical Substances); ASIA-PAC (Asia-Pacific Substances Lists); ECL (Korean Existing Chemicals List); EINECS (European Inventory of Existing Chemical Substances); ENCS (Existing and New Chemical Substances); PICCS (Philippine Inventory of Chemicals and Chemical Substances); TSCA (Toxic Substances Control Act Chemical).

²Simplified Molecular Line Input Entry System

Physical and Chemical Properties

Few experimental data are available for Disperse Blue 79. At the Environment Canada-sponsored Quantitative Structure-Activity Relationship (QSAR) Workshop in 1999 (Environment Canada 2000), modelling experts identified many structural classes of pigments and dyes as “difficult to model” using QSARs. The physical and chemical properties of many of the structural classes of dyes and pigments (including acid and disperse dyes) are not amenable to model prediction because they are considered “out of the model domain of applicability” (e.g., structural and/or property parameter domains). Therefore, to determine the potential utility, the domains applicability of QSAR models to dyes and pigments are evaluated on a case-by-case basis. It is generally considered inappropriate to use QSAR models to predict the physical and chemical properties of Disperse Blue 79. Consequently, a number of analogues were identified and "read-across" data has been used to determine the approximate physical and chemical properties in Table 2. These properties were subsequently used for further modeling and lines of evidence in this assessment.

An analogue is a chemical which is structurally similar to the substance under assessment and is therefore expected to have similar physical-chemical properties, behaviour in the environment and/or toxicity. Where there are experimental data for a given parameter for an analogue substance, these can be used directly or with adjustment as an estimate of that parameter value for the substance under assessment.

In order to find acceptable analogues, a review of data for several disperse azo dyes was performed (Anliker *et al.* 1981, Anliker and Moser 1987, Baughman and Perenich 1988, ETAD 1995, Brown 1992, Yen *et al.* 1989, Sijm *et al.* 1999). These compounds have structural similarities to Disperse Blue 79 but also share other important attributes that contribute to their suitability as analogues. This includes properties affecting their fate in the environment such as high molecular weights (generally >300 g/mol), similar cross sectional diameters (1.31 – 2.03 nm) solid particulate structures, decomposition at greater than 74 °C (to 240 °C), and “dispersibility” in water (i.e. not truly soluble). The presence of the ethanolamine grouping on the azo dye is meant to increase the dispersibility in water (Bomberger and Boughton 1984). In addition, they have limited solubility in n-octanol, a negligible vapour pressure and are stable under environmental conditions as they are designed to be so.

Table 2 contains experimental, analogue as well as read-across experimental and modelled physical-chemical properties of Disperse Blue 79 that are relevant to its environmental fate.

Table 2. Physical and chemical properties for Disperse Blue 79 and relevant chemical analogues.

Property	Type ¹	Value	Temperature (°C)	Reference
Physical state		Powder		Canada 2008
Melting point ² (°C)	Experimental	157		PhysProp 2006
	Read-across for disperse azo dyes	117 to 175, 74 to 236		Anliker and Moser 1987, Baughman and Perenich 1988
	Analogue Disperse Blue 79:1	≥138-153		Sandoz Chemicals 1989, Yen <i>et al.</i> 1989
Boiling point ³ (°C)	Not Applicable			
Density (kg/m ³)	Not Available			
Vapour pressure (Pa)	Experimental	4.53×10^{-7}		Clariant 1996
	Read-across for disperse azo dyes	$5.33 \times (10^{-12} \text{ to } 10^{-5})$ (4×10^{-14} to 4×10^{-7} mm Hg)	25	Baughman and Perenich 1988
Henry's Law constant (Pa·m ³ /mol)	Read-across ⁴	10^{-8} to 10^{-1} (10^{-13} to 10^{-6} atm·m ³ /mol)		Baughman and Perenich 1988
Log K _{ow} (Octanol-water partition coefficient) (dimensionless)	Experimental	4.1		Clariant 1996
	Experimental	4.3		Brown 1992
	Analogue	4.44, 4.8		Sijm <i>et al.</i>

Property	Type ¹	Value	Temperature (°C)	Reference
	Disperse Blue 79:1			1999, Yen et al. 1989
	Read-across for disperse azo dyes	1.79 to 5.1		Baughman and Perenich 1988
	Analogue dye	2.5		Anliker <i>et al.</i> 1981; Anliker and Moser 1987
	Analogue Disperse Orange 30	4.2		Brown 1992
Log K _{oc} (Organic carbon partition coefficient) (dimensionless)	Read-across, calculated ⁵	3.4 to 4.2		Baughman and Perenich 1988
Water solubility (mg/L)	Experimental	0.0054	25	Clariant 1996
	Experimental	0.02		Brown 1992
	Experimental	0.000938	15-25	Baughman and Perenich 1988
	Read-across for disperse azo dyes	<0.01		Anliker and Moser 1987
		1.2×10^{-5} to 35.5 (4×10^{-11} to 1.8×10^{-4} mol/L)		Baughman and Perenich 1988
		substantially water insoluble		ETAD 1995
	Analogue Disperse Blue 79:1	0.0052, 0.022	25	Baughman and Perenich 1988, Sijm <i>et al.</i> 1999

Property	Type ¹	Value	Temperature (°C)	Reference
	Analogue Disperse Orange 30	0.07		Brown 1992
n-octanol solubility (mg/L)	Read-across for disperse azo dyes	81-2100	20	Anliker and Moser 1987
pK _a (Acid dissociation constant) (dimensionless)	Modelled	13.3 for acid form 3.25 for base form		ACD/pK _a DB 2005

¹ These extrapolated values used for Disperse Blue 79 are based on evidence on disperse dyes submitted to Environment Canada under the New Substance Notification Regulations (ETAD 1995) and available evidence from other disperse dye analogues found in literature.

² The phrase melting point is used but this may be better referred to as a decomposition point because disperse dyes are known to char at high temperatures (greater than 200°C) rather than melt.

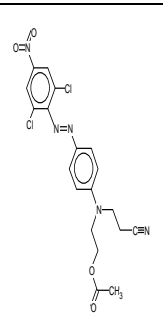
³ Boiling point is generally not applicable for disperse dyes. For powder dyes, charring or decomposition occurs at high temperatures instead of boiling. For liquids and pastes, boiling will only occur for the solvent component while the unevaporated solid will decompose or char (ETAD 1995).

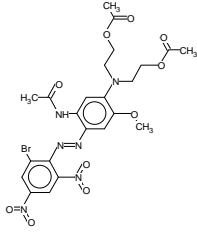
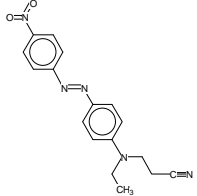
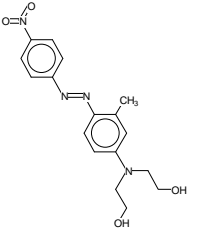
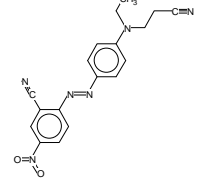
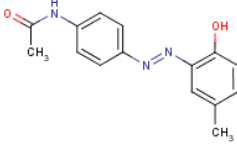
⁴ Solubilities of several disperse dyes at 25 and 80°C were used by Baughman and Perenich (1988) to calculate Henry's Law constants for these dyes. These values are presented here as a range to illustrate the expected Henry's Law constant for Disperse Blue 79.

⁵ Log K_{oc} values are based on calculations by Baughman and Perenich (1988) using a range of measured solubilities for commercial dyes and an assumed melting point of 200°C.

Structural disperse azo analogues to Disperse Blue 79 are presented in Table 3 below. Certain physico-chemical properties (see Table 2), empirical bioaccumulation data (Table 6) and empirical toxicity data (see Table 7) of these analogues were used in support of the weight of evidence and proposed decisions in this SAR. Specifically, data were obtained for the structural analogues: Disperse Orange 30, Disperse Blue 79:1, Disperse Red 17, Disperse Red 73, Disperse Orange 25 and Disperse Yellow 3 (Table 3a).

Table 3a. Structural analogues for Disperse Blue 79.

	CAS RN	Common Name	DSL name ¹	Structure of analogue	Available empirical data
i.	5261-31-4	Disperse Orange 30	Propanenitrile, 3-[[2-(acetyloxy)ethyl][4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]amino]-		Bioaccumulation, aquatic toxicity

ii.	3618-72-2	Disperse Blue 79:1	Acetamide, N-[5-[bis[2-(acetyloxy)ethyl]amino]-2-[(2-bromo-4,6-dinitrophenyl)azo]-4-methoxyphenyl]-		Melting point, log K _{ow} , water solubility, aquatic toxicity
iii	31482-56-1	Disperse Orange 25	3-(Ethyl(4-((4-nitrophenyl)azo)phenyl)amino)propanenitrile		Aquatic toxicity
iv	3179-89-3	Disperse Red 17	Ethanol, 2,2'-((3-methyl-4-(2-(4-nitrophenyl)diazenyl)phenyl)imino)bis-		Aquatic toxicity
v	16889-10-4	Disperse Red 73	2-((4-((2-Cyanoethyl)ethylamino)phenyl)azo)-5-nitrobenzonitrile		Aquatic toxicity
vi	2832-40-8	Disperse Yellow 3	4-(2-Hydroxy-5-methylphenylazo)acetanilide		Aquatic toxicity

¹ Source: National Chemical Inventories (NCI) 2007; Canadian Domestic Substances List (DSL).

It should be noted that there are several uncertainties associated with the use of physico-chemical-toxicological and bioaccumulation data available for the substances presented in Table 3a. All these substances belong to the same chemical class (disperse azo dyes with their characteristic azo bond) and are used for similar industrial purposes. However, there are differences between these substances associated with their unique functional groups (see Table 3b below) and for some their molecular size (especially for Disperse Orange 25 and Disperse Red 17 and 73). As a result, these analogues have empirical water solubilities that range over three orders of magnitude from 10⁻⁵ to 0.07 mg/L. Due

to this variability, caution should be exercised in attributing too much weight to these values as it would be preferable to utilise empirical water solubility and log K_{ow} specific to the substance Disperse Blue 79 (Table 2). However the analogue data presented can be considered as part of the weight of evidence for the evaluation of this substance.

Table 3b. Comparisons of structural analogues with Disperse Blue 79.

	CAS RN	Common Name	Molecular mass (g/mol)	structure similarity ¹ (%)	Minimum-maximum cross-sectional diameter (nm) ²
i	3618-72-2	Disperse Blue 79:1	625.39	96.19	1.43-2.03
ii	5261-31-4	Disperse Orange 30	450.28	74.83	1.75-1.98
iii	31482-56-1	Disperse Orange 25	323.35	NA	1.37-1.95
iv	3179-89-3	Disperse Red 17	344.36	NA	1.41-1.86
v	16889-10-4	Disperse Red 73	348.36	NA	1.31-1.93
vi	2832-40-8	Disperse Yellow3	269.31	NA	1.59-1.70

¹ ChemID Plus 2008, value presented if >60% similar

² CPOP (2008)

Sources

Disperse Blue 79 is not naturally produced in the environment.

Recent information was collected through industry surveys conducted for the years 2005 and 2006 under Canada Gazette Notices issued pursuant to section 71 of CEPA 1999 (Canada 2006b and 2008). These Notices required submission of data on the Canadian manufacture and import of the substance. For 2006, data were also required on use quantities of Disperse Blue 79.

No manufacture of Disperse Blue 79 was reported, above the threshold of 100 kg/year for the 2006 calendar year. However, less than four companies reported importing Disperse Blue 79 into Canada in 2006 and collectively they imported between 1 000 and 10 000 kg of the substance (Canada 2008). One company reported using between 1 000 and 10 000 kg of Disperse Blue 79 in 2006. In the Declaration of Stakeholder-Interest form associated with the section 71 survey for 2006, one company reported a stakeholder interest in this substance despite not meeting mandatory reporting requirements (Canada 2008).

The quantity reported under the *Domestic Substances List* (DSL) to be manufactured, imported or in commerce in Canada during the calendar year 1986 was 10 100 kg (Environment Canada 1988).

This substance has been listed as a European Union (EU) low production volume chemical substance, indicating that production within the EU is estimated to be between 10 and 1000 tonnes per year (ESIS 2008). The production volume of Disperse Blue 79 in the United States was 10,000 – 500,000 pounds in 1994 and 2002 and 500,000 – 1,000,000 pounds in 1998 (US EPA 2007). The Substances in Preparation in Nordic Countries (SPIN) database states that this substance was in use in Denmark from 2002 to 2006 and in Sweden from 1999 to 2006 (SPIN 2008).

Uses

Information on uses for the 2006 calendar year was gathered from responses to the CEPA 1999 section 71 survey Notice (Canada 2008).

In 2006, an importer of Disperse Blue 79 indicated that its business activity was chemical product manufacturing and that the substance was sold to four other companies (Canada 2008). According to additional research, these four companies are in the textile industry and produce apparel, cord, laces and webbing for domestic and foreign markets. Textiles used by these companies include cotton, polyester, spandex, wool, fleece, interlocks and other fabrics (Industry Canada 2008a).

The DSL use code, “Colourant - pigment/stain/dye/ink”, was identified for the substance during the development of DSL nomination (1984-1986) (Environment Canada 1988).

Review of the available scientific and technical information indicates that Disperse Blue 79 is primarily a textile dye. It is bright navy blue in colour and is suitable for thermosol dyeing and printing (Epochem 2008). Disperse Blue 79 may be used on polyester, acetate, nylon and wool/polyester blends (CII 2002).

Releases to the Environment

Mass flow tool

To estimate potential releases of the substance to the environment at different stages of its life cycle, a Mass Flow Tool was developed (Environment Canada 2008a). Empirical data concerning releases of specific substances to the environment are seldom available. Therefore, for each identified type of use of the substance, the proportion and quantity of release to the different environmental media are estimated, as are the proportion of the substance chemically transformed or sent for waste disposal. Unless specific information on the rate or potential for release of the substance from landfills and incinerators is available, the Mass Flow Tool does not quantitatively account for releases to the environment from disposal.

Assumptions and input parameters used in making the release estimates are based on information obtained from a variety of sources including responses to regulatory surveys, Statistics Canada, manufacturers' websites and technical databases and documents. Of particular relevance are emission factors, which are generally expressed as the fraction of a substance released to the environment, particularly during its manufacture, processing, and use associated with industrial processes. Sources of such information include emission scenario documents, often developed under the auspices of the Organization for Economic Cooperation and Development (OECD), and default assumptions used by

different international chemical regulatory agencies. It is noted that the level of uncertainty in the mass of substance and quantity released to the environment generally increases towards the end of the life-cycle.

Based on Statistics Canada information and an analysis by Industry Canada (2008b), it is proposed that Disperse Blue 79 may be imported in manufactured articles (principally textiles). A ratio of textiles manufactured in Canada / textiles imported into Canada of 30/70 has been used to estimate the amount of dye imported in textiles (Environment Canada 2008b). This import quantity was included in the Mass Flow Tool calculations.

Table 4. Estimated releases and losses of Disperse Blue 79 to environmental media, chemical transformation and transfers to waste disposal sites, based on the Mass Flow Tool.

Fate	Proportion of the mass (%)¹	Major life cycle stage involved²
Releases to receiving media:		
To soil	0.0	n/a ³
To air	0.0	n/a
To sewer ⁴	14.8	Formulation, consumer use,
Chemically transformed	0.0	n/a
Transferred to waste disposal sites (e.g., landfill, incineration)	85.2	Formulation, waste disposal

¹ For Disperse Blue 79, information from the following OECD emission scenario documents was used to estimate releases to the environment and distribution of the substance as summarized in this table: OECD 2004, 2007. Values presented for release to environmental media do not account for possible mitigation measures that may be in place in some locations (e.g., partial removal by sewage treatment plants). Specific assumptions used in derivation of these estimates are summarized in Environment Canada 2008b.

² Applicable stage(s): production-formulation-industrial use-consumer use-service life of article/product-waste disposal.

³ Not applicable

⁴ Wastewater before any form of treatment

Results indicate that Disperse Blue 79 can be expected to be found largely in waste management sites (85.2%), due to the eventual disposal of manufactured items containing it. Mass Flow Tool calculations do not quantitatively account for releases of the substance to the environment from waste disposal sites (such as landfills, incinerators) unless specific information on the rate or potential for release is available. No such information has been identified for Disperse Blue 79. A small fraction of solid waste is incinerated which is expected to result in transformation of the substance. Based largely on information contained in OECD emission scenario documents for processing and uses associated with this type of substance, it is estimated that 14.8% of Disperse Blue 79 may be released to sewers.

Based on the above, sewer water is the medium receiving the greatest proportion of Disperse Blue 79 emitted during product processing. It is anticipated that the majority of the substance bound in products will be sent to landfills for disposal.

Environmental Fate

As indicated by the results of the Mass Flow Tool (Table 4), the substance Disperse Blue 79 is expected to be released to waste water effluents during industrial processing and use. The moderate log K_{ow} (experimental 4.1 and 4.3; analogue 2.5 to, 4.8) and high log K_{oc} (read-across: 3.4 to 4.2) values (see Table 2) indicate that this substance may have affinity for solids. However, the log K_{oc} is a calculated value (see footnote 3 below Table 2) and the adsorption potential of solid particulate dye structures is generally not well understood, therefore the degree of adsorption of Disperse Blue 79 is uncertain.

Disperse Blue 79 is expected to be mostly found in sediment or soil, and is not expected to be subject to long-range atmospheric transport.

Disperse Blue 79 does not biodegrade fast (see Table 5 below). It may inadvertently be applied to agricultural soils and pasture lands in Canada as a component of biosludge which is commonly used for soil enrichment. Moreover, it may also be released from coloured textiles deposited in landfills.

In solution Disperse Blue 79 can behave as either an acid or as a base. With an estimated pK_a for the acid of 13.3 and for the base of 3.25 (see Table 2), dissolved forms of Disperse Blue 79 are not expected to ionize in water at environmentally relevant pHs. Disperse Blue 79 is a powder with a limited water solubility (see Table 2). Because of its low solubility when released into water, this substance is expected to behave as a colloidal dispersion (Yen et al. 1991). Thus, this substance will be mostly present as a solid or adsorbed to suspended particles and to sink eventually to bed sediments where it is expected to remain in a relatively biologically unavailable form. It has been concluded by Yen et al. (1989) that disperse dyes tend to accumulate extensively in sediments and biota unless they are degraded at rates comparable to uptake. Razo-Flores *et al.* (1997) have stated that due to the recalcitrant nature of azo dyes in the aerobic environment, they eventually end up in anaerobic sediments due to sediment burial, shallow aquifers and in groundwater. Yen et al. (1991) observed that some azobenzene dye analogues were transformed under anaerobic conditions in sediment via hydrolysis and reduction, and concluded that most azo dyes would likely not persist in anaerobic sediment systems. In buried sediment, Disperse Orange 30 may undergo anaerobic degradation. Weber and Adams (1995) reported that Disperse Blue 79 was initially transformed rapidly in sediments under anoxic conditions but then the transformation was slow.

The rate of volatilization from water is proportional to the Henry's law constant (Baughman and Perenich 1988). The low to negligible read-across Henry's Law constant value (10^{-8} to 10^{-1} Pa·m³/mol, read-across data in Table 2) and the low experimental (4.53×10^{-7} Pa Table 2) and the low to negligible read-across vapour pressure ($5.33 \times (10^{-12}$ to $10^{-5})$ Pa, read-across data in Table 2). Transfer to or transport in air due to the loss of

this substance from moist and dry soil surfaces is not likely to be important for this substance as indicated by very low vapour pressure of Disperse Blue 79. This behaviour is consistent with the physical state (solid particle) of Disperse Blue 79 which does not make it a likely candidate for volatilization.

Persistence and Bioaccumulation Potential

Persistence

No experimental biological degradation data for Disperse Blue 79 have been identified. According to the Ecological and Toxicological Association of Dyes and Organic Pigments Manufacturers, with some exceptions, dyes are considered essentially non-biodegradable under aerobic conditions (ETAD 1995). Repeated evaluation of ready and inherent biodegradability using accepted screening tests (see OECD Guidelines for Testing Chemicals) have confirmed this speculation based on other chemicals (Pagga and Brown 1986; ETAD 1992). Based on the chemical structure of Disperse Blue 79, there is no reason to suspect that biodegradation will be other than that described for dyes generally (ETAD 1995).

Some disperse azo dyes have been shown to undergo relatively rapid anaerobic degradation in sediment at depths where anoxic conditions persist (Yen *et al.* 1991, Baughman and Weber 1994, Weber and Adams 1995). Disperse dyes enter the aquatic system mostly as a dispersion of fine suspended particles, eventually settling to the aerobic layers of surface sediment where they will persist until sediment burial creates reducing conditions. The rate of sediment deposition and the extent of bioturbation varies from site to site and thus it is very difficult to ascertain the residence time of dyes in aerobic sediment layers. It is likely however, that in many cases this is greater than 365 days. Once under anaerobic or reducing conditions, azo dyes may undergo rapid degradation to substituted aromatic amine constituents as demonstrated by Yen *et al.* (1991) who measured reduction half-life values in compacted sediments at room temperature of 2.9 hours to 2.0 days for an azobenzene dyes. However, in deep anoxic sediment, these biodegradation transformation products are not expected to present a high degree of exposure potential to most aquatic organisms, and therefore they are not likely to present an ecological concern.

Since no experimental biodegradation data are available for Disperse Blue 79, a QSAR-based weight-of-evidence approach (Environment Canada 2007) was applied using the degradation models shown in Table 5 below. Although the expected release of Disperse Blue 79 will be to wastewater, its residence time in the water column may be short before finally sinking to the sediment bed due to its low solubility and behaviour as a colloidal dispersion. However, given the lack of data regarding this issue, persistence was primarily examined using predictive QSAR models for biodegradation in water. The following analysis applies primarily to the portion of this substance that is present in the environment in the dissolved form, recognizing that a significant proportion would also

likely exist in dispersed form as solid particles. Disperse Blue 79 does not contain functional groups expected to undergo hydrolysis in aerobic environments (dyes are designed to be stable in aqueous conditions). Table 5 summarizes the results of available QSAR models for biodegradation in water.

Table 5. Modelled data for biodegradation of Disperse Blue 79

Model	Model Basis	Medium	Value	Interpretation	Extrapolated half-life (days)	Extrapolation Reference and/or Source
BIOWIN1* v4.1 (2000)	Linear probability	water (aerobic)	-0.340	Does not biodegrade fast	n/a	
BIOWIN2* v4.1 (2000)	Non-linear probability	water (aerobic)	0.00	Does not biodegrade fast	n/a	
BIOWIN3* v4.1 (2000)	Expert Survey (ultimate biodegradation)	water (aerobic)	0.9239	Recalcitrant	180	US EPA 2002
BIOWIN4* v4.1 (2000)	Expert Survey (primary biodegradation)	water (aerobic)	2.95	Weeks	15	US EPA 2002
BIOWIN5* v4.1 (2000)	MITI linear probability	water (aerobic)	-0.24	Does not biodegrade fast	n/a	
BIOWIN6* v4.1 (2000)	MITI non-linear probability	water (aerobic)	0.00	Does not biodegrade fast	n/a	
BIOWIN Overall Conclusion ¹	BIOWIN 3 + BIOWIN 5	water (aerobic)	no	Not readily biodegradable	n/a	
CATABOL v. 5.100 (c2004–2008)	% BOD (OECD 301C)	water (aerobic)	14.6	Persistent (<20%)	> 182	Aronson <i>et al.</i> 2006

*BIOWIN 1–6 are outputs obtained from the predictive model BIOWIN (2000). BIOWIN estimates aerobic biodegradability of organic chemicals using six different models.

¹ Based on outcome of BIOWIN 3 and BIOWIN 5.

The results from Table 5 show that the majority of the probability models (BIOWIN 1, 2, 5, 6) suggest this substance does not biodegrade rapidly. In fact, all probability results are less than 0.3, the cut-off suggested by Aronson *et al.* (2006) identifying substances as having a half-life >60 days (based on the MITI probability models). The half-life from the primary survey model (BIOWIN 4) result of weeks is suggested to mean approximately 15 days (US EPA 2002, Aronson *et al.* 2006); however, the nature of the degradation products is unknown. The ultimate survey model (BIOWIN 3) result of recalcitrant is suggested to mean 180 days by the US EPA 2002, Aronson *et al.* 2006). However a structural analogue (Disperse Blue 79:1) in feed sludge was degraded by an average of 98.2% over 15 days by anaerobic digestion in a study conducted by Gardner *et al.* (1989). Cruz and Buitron (2001) also presented high biotransformation by anaerobic

biofilter of Disperse Blue 79 with efficiencies of decolorization of over 95% within 72 hours. The overall conclusion from BIOWIN (2000) is that this substance is not readily biodegradable in water.

CATABOL predicted 14.6 % biodegradation based on the OECD 301 readily biodegradation test (%BOD) which has been suggested as meaning likely persistent (Aronson and Howard 1999) and having a half-life in water of >182 days.

When the results of the probability models, the overall BIOWIN conclusion and ultimate degradation models are considered, there is model consensus suggesting that the half-life in water is >182 days, which is consistent with what would be expected for a chemical used as a disperse dye (i.e., manufactured to be relatively insoluble and durable). Using a ratio of 1:1:4 for a water:soil:sediment half-life extrapolation (Boethling et al. 1995), the half-life in soil should be >182 days and the half-life in aerobic sediments should be >365 days.

Based on the results of predictive modelling (principally for ultimate degradation) and expert judgement (ETAD 1995), Disperse Blue 79 meets the persistence criteria for water and soil (half life in soil and water ≥ 182 days) as well as sediments (half life in sediments ≥ 365 days) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

No experimental bioaccumulation experimental data are available for Disperse Blue 79.

In the absence of experimental and modelled data for Disperse Blue 79 itself, bioconcentration factors (BCFs) for structural analogues were used to estimate Disperse Blue 79's potential for bioaccumulation. A bioconcentration study submitted for a relatively close structural analogue of Disperse Blue 79 suggests that it is unlikely to accumulate in fish (Shen and Hu 2008). This test was performed according to OECD Guidelines for Testing of Chemicals, Test No. 305B-1996, Bioconcentration: Semi-Static Fish Test. The bioconcentration of Disperse Orange 30 in zebra fish (*Brachydanio rerio*) was determined in a 28-day semi-static test with a test medium renewal every two days. An exposure test at a nominal concentration of 20 mg/L (mean measured concentration 0.028 - 0.28 mg/L) was performed in accordance with the result of the fish acute toxicity test to check the bioconcentration potential of the test substance. Samples from both test solutions and test organisms were taken daily from the 26th day to the last day during the 28-day exposure test period. Samples were prepared by extracting the lipid component from the test fish. The measured concentration of test substance, fish lipid content and BCF calculation are reported in Table 6.

Table 6. Measured concentration of Disperse Orange 30, fish lipid content and BCF calculation

	Sampling Time
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		The 26 th day	The 27 th day	The 28 th day
Treatments (20 mg/L)	Measured concentration of the test substance in extracted solutions (mg/L)	<0.028	<0.028	<0.028
	Content of the test substance in the fish lipids (mg)	<1.68	<1.68	<1.68
	Fish total weight (g)	2.07	2.13	2.53
	Concentration of the test substance in the fish C _f (mg/kg)	<0.81	<0.79	<0.66
	Measured concentration of the test substance in the water C _w (mg/L)	0.028 ~ 0.28	0.028 ~ 0.28	0.028 ~ 0.28
	Fish lipid content (%)	0.81	0.57	1.25
	BCF	<100	<100	<100
	Average BCF	<100		

The Shen and Hu (2008) study has been reviewed and considered acceptable (see Appendix 1). Lack of detection in fish extracts (<0.028 mg/L) suggests a limited solubility in lipids and/or limited potential to partition into fish tissue from aqueous systems. However, there is some uncertainty associated with limit bounded values in any study because the absolute value is not known. But given the structure and likely behavior of disperse dyes in aqueous systems, the low BCF result would be expected. Most disperse dyes, as their name suggests, exist as fine dispersible particles with limited truly soluble fractions. Solubility, however, can be increased by adding polar functional groups to the molecule. Disperse Blue 79 does not contain any polar functional groups expected to be ionic at a relevant environmental pH. Therefore, given a melting point of 157°C (experimental data in table 2) and a log K_{ow} of 4.2 (median of experimental data in Table 2), the predicted water solubility (WSKOWIN 2000) corrected for melting point and log K_{ow} is ~0.08 mg/L which is within the aqueous detection limit in the study and comparable to the experimental value of 0.02 mg/L reported by Brown 1992. Assuming that the concentration in solution in the test was equal to the water solubility value of 0.081 mg/L and using the fish concentration of 0.81 mg/kg as a worst case estimate, the BCF may be calculated to be <100.

While the above study serves as primary evidence to support Disperse Blue 79's lack of bioaccumulation potential, other research corroborates this conclusion. Anliker *et al.* (1981) reported experimental fish bioaccumulation values for 18 disperse monoazo dyes, performed according to test methods specified by the Japanese Ministry of International Trade and Industry (MITI). Expressed on the basis of wet body weight of the fishes, these log bioaccumulation factors (BAFs) ranged from 0.00 to 1.76 (Anliker *et al.* 1981). A lack of reporting of chemical registry numbers and chemical structures limited the utility of this study for read-across purposes to Disperse Blue 79. However, follow-up studies, which provided the chemical structures for the disperse dyes tested, confirmed low bioaccumulation potential for ten nitroazo dyes, with reported log bioaccumulation factors ranging from 0.3 to 1.76 (Anliker and Moser 1987; Anliker *et al.* 1988). Studies available from MITI also support low bioaccumulation potential for disperse azo dyes. Reported BCFs for three disperse azo dyes (CAS# 40690-89-9, 61968-52-3 and 71767-

67-4) tested at a concentration of 0.01 mg/L were in the range of <0.3 to 47 (MITI 1992). An accumulation study by Brown (1987) also showed that none of the twelve disperse dyes tested accumulated during an eight week study with carp.

A high, median experimental log K_{ow} value of 4.2 for Disperse Blue 79 (Table 2) is the only line of evidence that suggests Disperse Blue 79 may have a high potential for bioaccumulation. In spite of the high K_{ow} values for Disperse Blue 79 and other disperse azo dyes, evidence for bioaccumulation of such dyes is lacking (Anliker *et al.* 1981, Anliker and Moser 1987, MITI 1992). Authors who have measured high log K_{ows} and concomitant low bioaccumulation factors for disperse azo dyes suggest the low accumulation factors may be due in some cases to their low absolute fat solubility (Brown 1987) or their relatively high molecular weight (typically 450-550) which may make transport across fish membranes difficult (Anliker *et al.* 1981, Anliker and Moser 1987). It is also likely that the lack of bioavailability and limited capacity to partition under BCF test conditions limits accumulation in fish lipids.

It has been stated by ETAD (1995) that the molecular characteristics indicating the absence of bioaccumulation are a molecular weight of >450 g/mol and a cross-sectional diameter of >1.05 nm. Recent investigation by Dimitrov *et al.* (2002), Dimitrov *et al.* (2005) and the BBM (2008) suggests that the probability of a molecule crossing cell membranes as a result of passive diffusion declines significantly with increasing maximum cross-sectional diameter (D_{max}). The probability of passive diffusion lowers appreciably when cross-sectional diameter is > ~1.5 nm and more significantly for molecules having a cross-sectional diameter of >1.7 nm. Sakuratani *et al.* (2008) have also investigated the effect of cross-sectional diameter on passive diffusion from a test set of about 1200 new and existing chemicals also observing that substances not having a very high bioconcentration potential often have a D_{max} >2.0 nm and an effective diameter (D_{eff}) >1.1 nm.

Disperse Blue 79 has a molecular weight of 639.42 g/mol (see Table 1) and its molecular structure is relatively uncomplicated; the later characteristic in particular indicates a potential bioaccumulation capability. In addition, an Environment Canada (2007) report points out that there is no clear evidence for establishing strict molecular size cut-offs for assessing bioaccumulation potential. However, the report does not dispute the notion that a reduction in uptake rate can be associated with increasing cross-sectional diameter as demonstrated by Dimitrov *et al.* (2002, 2005). The maximum diameter of Disperse Blue 79 and its conformers ranges from 1.69 to 2.045 nm (BBM 2008) suggesting that a potential for a significantly reduced uptake rate from water and in vivo bioavailability exists with this dye.

In a study by Maguire and Tkacz (1991), no dyes (including Disperse Blue 79) were detected in the approximately 600 fish extracts analysed. However Disperse Blue 79 was detected in water and sediment at the same location where the fish were collected. Although this is not a bioaccumulation study it does suggest a possible low trophic magnification potential of Disperse Blue 79.

Results of bioaccumulation modeling have not been used in this assessment of Disperse Blue 79. Environment Canada considers many higher molecular weight pigments and non-soluble dye classes, including disperse azo dyes as difficult to model and thus the results are generally unreliable. Predicted and/or empirically determined properties of disperse dyes related to bioaccumulation (e.g., log K_{ow}) can be of uncertain relevance or associated with a high degree of error, which reduce the utility of model predictions of BCF and BAF. In addition, disperse azo dyes generally fall outside of bioaccumulation model domains of applicability.

Based on a lack of observed accumulation in bioconcentration tests with Disperse Orange 30 and other related disperse azo dyes, and Disperse Blue 79's large molecular size which likely limits its partitioning behavior, Disperse Blue 79 is expected to have a low potential for bioaccumulation. Therefore, considering analogue BCF evidence, and structural and bioavailability considerations, Disperse Blue 79 does not meet the bioaccumulation criteria (BCF or BAF ≥ 5000) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential to Cause Ecological Harm

Ecological Effects Assessment

A - In the Aquatic Compartment

Few empirical ecotoxicity data were identified for Disperse Blue 79. According to a study submitted to Environment Canada on behalf of ETAD (Brown 1992), a 96-hour LC_{50} of 340 mg/L for zebra fish, a 48-hour EC_{50} of 4.5 mg/L for *Daphnia magna*, a 72-hour EC_{50} (for growth) for *Scenedesmus subspicatus* have been obtained experimentally (Table 7a). However, the original study has not been provided to allow verification of its reliability. Another experimental study on the toxicity of effluent containing Disperse Blue 79 reported an LC_{50} (48 hours) for Mysid shrimp of 35% (Reife 1989). However, this study did not provide the LC_{50} value in terms of the concentration of Disperse Blue 79 and therefore these results could not be included in Table 7a or used in the risk quotient analysis. A summary of a fish toxicity study conducted by BASF (1990) was also submitted to Environment Canada by ETAD in August 2008. An assessment of the reliability of the study using a robust study summary was conducted and the results indicated that the study was unreliable due to lack of details (Appendix 1). Another acute toxicity study was submitted to Environment Canada (Table 7a) in August 2008. An assessment of the reliability of this study using a robust study summary was undertaken with the result that the study was deemed to be of "low confidence" due to lack of details (Appendix 1).

Table 7a. Empirical data for aquatic toxicity of Disperse Blue 79

Test organism	Type of	Duration	End	Reliability of	Value	Reference
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	test	(hours)	point	the study	(mg/L)	
Golden orfe	Acute	96	LC ₅₀ ¹	Unreliable	>100 - <220	BASF 1990
Rainbow trout	Acute	96	LC ₅₀	Low confidence	>100	SafePharm laboratories Ltd 1990.
Zebra fish	Acute	96	LC ₅₀	Not Available	340	Brown 1992
<i>Daphnia magna</i>	Acute	48	EC ₅₀ ²	Not Available	4.5	
<i>Scenedesmus subspicatus</i>	Acute	72	EC ₅₀	Not Available	9.5	
<i>Bacteria</i>	Acute	n/a	IC ₅₀ ³	Not Available	>100	

¹ LC₅₀ – The median concentration of a substance that is estimated to be lethal to 50% of the test organisms.

² EC₅₀ – The median concentration of a substance that is estimated to cause some toxic sublethal effect on 50% of the test organisms.

³ IC₅₀ – The median concentration of a substance that is estimated to cause inhibition to growth 50% of the test organisms.

Environment Canada also received ecotoxicological data for a structurally similar analogue substance through the New Substance Notification Regulations. Ecotoxicological data were provided with this notification. The results for the 96hr static toxicity test with Rainbow trout (*Oncorhynchus mykiss*) revealed that the LC₅₀ for this species is 505 mg/L (Table 7b). The test was conducted according to OECD guideline No. 203. The Material Safety Data Sheets (MSDS) of the notified substance also contained information on bacterial toxic effects. The results indicate an activated sludge respiration inhibition EC₅₀ > 100 mg/L. Based on the available ecotoxicity information, the notified substance is expected to be of low concern for toxic effects to aquatic organisms. Reliability of the study was assessed using a robust study summary and is considered to be satisfactory (Appendix 1).

In another study, a summary of which was submitted to Environment Canada on behalf of ETAD (Brown 1992), 11 disperse dyes were tested on the following organisms: zebra fish, *Daphnia magna*, algae and bacteria. One of the disperse dyes tested was Disperse Blue 79 (Table 7a). Of the remainder of the disperse dyes tested by Brown (1992), four are azo analogues of Disperse Blue 79 (Brown 1992). These are Disperse Red 73, Disperse Orange 30, Disperse Orange 25, and Disperse Red 17 (Table 7b). The four analogues showed moderate to low toxicity to zebra fish (96 hr LC₅₀=17 to 710 mg/L). Moderate toxicity was also presented for algae growth (EC₅₀ for growth = 6.7 to 54 mg/L) and no toxicity was detected for bacteria (IC₅₀>100 mg/L). The experimental details for the dyes tested were not provided, greatly limiting evaluation of these studies (Brown 1992). However, these data were considered usable and are included in this

Screening Assessment as part of the weight of evidence. Lastly, an analogue, Disperse Blue 79:1, had a chronic 122-day no effect concentration (NOEC) for rainbow trout of > 0.0048 mg/L (Table 7). Reliability of this study was assessed as high (Appendix 1). However, this value was not used to calculate the predicted no effect concentration because the value is a hypothesis-based unbounded result. These analogue values would also therefore suggest that Disperse Blue 79 is not highly hazardous to aquatic organisms (i.e., acute LC₅₀ are >1 mg/L).

Table 7b. Empirical data for aquatic toxicity of Disperse Blue 79 analogues

Common Name or CAS#	Test Organism	End point	Value (mg/L)	Reference
Analogue to disperse azo dye	Rainbow trout	LC ₅₀ ¹	505	Environment Canada 1995
Disperse Red 73	Zebra fish	LC ₅₀	17	Brown 1992
	<i>Daphnia magna</i>	EC ₅₀	23	
	<i>Scenedesmus subspicatus</i>	EC ₅₀	>10	
	<i>Bacteria</i>	IC ₅₀ ³	>100	
Disperse Orange 30	Zebra fish	LC ₅₀	710	Brown 1992
	<i>Daphnia magna</i>	EC ₅₀ ²	5.8	
	<i>Scenedesmus subspicatus</i>	EC ₅₀	6.7	
	<i>Bacteria</i>	IC ₅₀ ³	>100	
Disperse Red 17	Zebra fish	IC ₅₀ ³	103	Brown 1992
	<i>Daphnia magna</i>	LC ₅₀	98	
	<i>Scenedesmus subspicatus</i>	EC ₅₀ ²	7	
	<i>Bacteria</i>	EC ₅₀	>100	
Disperse Orange 25	Zebra fish	IC ₅₀ ³	268	Brown 1992
	<i>Daphnia magna</i>	LC ₅₀	110	
	<i>Scenedesmus subspicatus</i>	EC ₅₀ ²	54	
	<i>Bacteria</i>	EC ₅₀	>100	
Disperse Blue 79:1	Rainbow trout	NOEC ⁴ (122 days)	>0.0048	Cohle and Mihalik 1991
Disperse Yellow 3	Fathead minnow	LC ₅₀	>180	Little and Lamb 1973

¹ LC₅₀ – The median concentration of a substance that is estimated to be lethal to 50% of the test organisms.

² EC₅₀ – The median concentration of a substance that is estimated to cause some toxic sublethal effect on 50% of the test organisms.

³ IC₅₀ – The median concentration of a substance that is estimated to cause inhibition to growth 50% of the test organisms.

⁴ NOEC The concentration at which no effects have been observed.

In general, due to their low solubility (<1 mg/L) disperse dyes are expected to have a low acute ecological impact (Hunger 2003). The results of empirical toxicity studies with both Disperse Blue 79 and several analogues are consistent with this expectation,

indicating LC₅₀s in the 4.5 to 340 mg/L range with *Daphnia* being the most sensitive organisms tested. Although interpretation of results from these tests is complicated by the fact that the lowest effect values are more than 100-fold greater than the estimated solubility of the substance (i.e., approximately 0.02 mg/L), the data available do indicate that the toxicity of Disperse Blue 79 is likely to be low.

A range of aquatic toxicity predictions for Disperse Blue 79 were also obtained from the various QSAR models considered for Disperse Blue 79 and its analogues. However, as with bioaccumulation, these QSAR ecotoxicity predictions for Disperse Blue 79 are not considered reliable because of the unique nature of disperse dyes, such as specifically structural and/or physico-chemical properties which fall outside of the models' domain of applicability.

The available empirical ecotoxicity information for Disperse Blue 79 and analogues of Disperse Blue 79 thus indicate that it is not likely to be highly hazardous to aquatic organisms.

B - In Other Environmental Compartments

Since Disperse Blue 79 may potentially enter soil from biosludge which is commonly used for soil enrichment as well as from the disposal of products that degrade and release Disperse Blue 79, it would be desirable to obtain toxicity data for soil organisms. Although no suitable ecological effects studies were found for this compound in soil, considering the toxicity data for aquatic organisms as well as the lack of bioaccumulation potential and its low bioavailability, potential for toxicity to soil-dwelling organisms is likely to be low. For the same reasons the toxicity potential is also likely to be low for sediment dwelling species, although this cannot be substantiated due to lack of whole organism sediment toxicity data for Disperse Blue 79 or suitable analogues.

Ecological Exposure Assessment

Environmental monitoring data relating to the presence of Disperse Blue 79 in the Canadian environment (water, suspended solids and sediment) have been identified (Table 8). This substance has been shown previously to be present in water, suspended solids and sediment downstream of textile mills in Canada (Maguire and Tkacz 1991). The upper concentration of Disperse Blue 79 in water in the Maguire and Tkacz (1991) study is three times the water solubility reported by Clariant (1996), 18 times greater than the water solubility reported by Baughman and Perenich (1988) and similar to the water solubility referenced by Brown (1992) (Table 2).

Table 8. Concentrations of Disperse Blue 79 in the environment

Medium	Location; year	Concentration	Reference
Water	Yamaska River,	0.0019 to 0.0171 mg/L	Maguire and Tkacz 1991

Suspended Solids	Qc, 1985-1987	0.0008 to 0.0033mg/L	
Sediment		0.1 to 4.2mg/kg (dw)	

dw = dry weight

The Mass Flow Tool predicted releases to the water (sewers) from formulation use of this substance (Table 4). To address releases from industrial activities, Environment Canada's Industrial Generic Exposure Tool – Aquatic (IGETA) was also employed to estimate the substance concentration (worst-case) in a generic water course receiving industrial effluents. The equation and inputs used to calculate the predicted environmental concentration (PEC) in the receiving water course are described in the Environment Canada (2008c). The environmental concentration predicted with Environment Canada's Industrial Generic Exposure Tool – Aquatic (IGETA) assuming that 10,000 kg (the upper bound of the range of possible use quantities) was used at one facility was 0.0334 mg/L (Environment Canada 2008d). Conservative assumptions were made regarding receiving water body, by assuming the chemical is released to a very small river. A removal rate in a sewage treatment plant was modelled using ASTreat 1.0 (ASTreat 2006) and was equal to 68.8%. This is of similar range as the removal rate of 78% presented for 5 disperse dyes in ETAD (1992). The ASTreat (2006) removal rate was the most conservative modelled value for removal rates and therefore was included in the IGETA model.

To address down-the-drain releases from consumer uses, Environment Canada's spreadsheet model (Mega Flush) was used. Using Mega Flush, potential substance concentrations are estimated in multiple water bodies receiving sewage treatment plant (STP) effluents to which consumer products containing the substance may have been released (Environment Canada 2008e). The spreadsheet model is designed to provide these estimates based on conservative assumptions regarding the amount of chemical used and released by consumers. By default, primary and secondary STP removal rates are assumed to be of 0%, fraction released during use of 100%, the consumer use of the substance is assumed to extend over 365 days/year, and the flow rate used for receiving water bodies at all sites is a low-end (10th percentile) value. These estimates are made for approximately 1000 release sites across Canada, which account for most of the major STPs in Canada. These parameter values are considered to result in a very conservative scenario.

The equation and inputs used in Mega Flush to calculate the PEC of Disperse Blue 79 in the receiving water bodies are described in Environment Canada (2008f). The mass flow tool was used to predict releases to water (sewers) from formulation use and from consumer use of products containing this substance. A scenario was run assuming a total consumer use quantity of 20 780 kg/year (Environment Canada 2008b). This consumer use quantity was estimated conservatively using the total mass of substance reportedly imported into Canada by less than four companies based on information from the s. 71 survey, and applying the 30/70 ratio for dyes in textiles manufactured / imported in Canada. A 10% loss of dye was then assumed for the total amount of the substance being used by consumers (Øllgaard *et al.* 1998). That is, 2078 kg of Disperse Blue 79 were predicted to be released to water, as a result of loss to sewers during the laundering of

articles that contain this dye. Primary and secondary STP removal rates of 0% were used. These assumptions result in a very conservative scenario. Using this scenario, the Mega Flush tool estimates that the PEC in the receiving water bodies ranges from 0.00026 to 0.0032 mg/L.

Characterization of Ecological Risk

A predicted no-effect concentration (PNEC) was estimated based on the effect concentration (EC_{50}) to the aquatic invertebrate (*Daphnia magna*). The 96-hour EC_{50} for Disperse Blue 79 was 4.5 mg/L (Table 7a) based on nominal concentrations. A factor of 100 was then applied to account for extrapolating from acute to chronic (long-term) toxicity and from laboratory results for one species to other potentially sensitive species in the field. The resulting PNEC is 0.045mg/L.

When it is compared to the conservative PEC presented above, the resulting risk quotient for industrial discharges ($PEC/PNEC$) is $0.0171/0.045 = 0.38$. Furthermore a risk quotient based on the PEC from the IGETA model (0.033 mg/L) would also be below 1. Therefore, concentrations of Disperse Blue 79 in surface waters in Canada appear unlikely to cause adverse effects to aquatic organisms. Given that we used the highest detected levels of this substance in Canada and that this concentration is similar to the level predicted by the IGETA model, the results indicate a low potential for ecological harm resulting from local exposure to point source industrial releases to the aquatic environment.

For exposure resulting from down-the-drain releases through consumer uses (conservative scenario), MegaFlush results estimate that the PEC will not exceed the PNEC at any sites (i.e. all risk quotients < 1). This indicates that down-the-drain consumer releases of Disperse Blue 79 are not expected to harm aquatic organisms.

Based on the available information, Disperse Blue 79 is expected to be persistent in water, soil and sediment; it is however expected to have a low bioaccumulation potential. The low importation quantities of Disperse Blue 79 into Canada, along with information on physical and chemical properties and its uses, indicate a low to moderate potential for releases into the Canadian environment. If released into the environment, it is expected that Disperse Blue 79 will be mainly discharged to surface waters where ultimately it is expected to be transferred to sediment. It is also expected to have only a low to moderate potential for toxicity to aquatic organisms. Risk quotients for aquatic exposures indicate that Disperse Blue 79 concentrations likely do not exceed concentrations associated with effects, even when using conservative scenarios and assumptions. Therefore Disperse Blue 79 is unlikely to be causing harm to populations of aquatic organisms in Canada.

Uncertainties in Evaluation of Ecological Risk

An area of uncertainty for Disperse Blue 79 is associated with the use of read-across data for physical and chemical properties, as well as toxicity data from analogues. While the

chemicals identified (Disperse Blue 79:1, Disperse Orange 30, Disperse Orange 25, Disperse Red 17, Disperse Red 73 and Disperse Yellow 3), share many similarities with Disperse Blue 79, including being azo dyes with high molecular weights, similar cross sectional diameters, having solid particulate structures that decompose at greater than 74 °C (to 240 °C), and being “dispersible” in water (i.e., not truly soluble), they do have some differences in functional groups. These differences in chemical structure add uncertainty because the properties and toxicity of Disperse Blue 79 may be somewhat different. However, it was reasoned that the similarities were sufficient to include the data from analogues to contribute to the weight of evidence in the assessment of Disperse Blue 79.

The persistence assessment is limited by the absence of biodegradation data, which necessitated generation of model predictions. Although all model prediction has some degree of error, the aerobic biodegradation model outputs confirmed the expected persistence of Disperse Blue 79 given its uses and structural characteristics. In addition, the persistence assessment is limited by the uncertainty about the rate and extent to which degradation occurs in anaerobic sediments and whether the degradation products (e.g., amines) would be biologically available. Nevertheless, it is clear that anaerobic degradation of the bioavailable portion azo dyes in sediments to constitutive amines is much faster (half-lives in the order of days) than aerobic biodegradation. Although the degradation products are not expected to be biologically available because they form only in relatively deep anoxic sediment and can be irreversibly bound to sediment through nucleophilic addition and oxidative radical coupling (Colon *et al.* 2002, Weber *et al.* 2001), this issue is a source of uncertainty in the assessment of Disperse Blue 79.

Uncertainties are also present due to the lack of bioaccumulation studies for this substance. However, based on a lack of accumulation in bioconcentration tests with Disperse Orange 30 and other related disperse azo dyes, and Disperse Blue 79's large molecular size which likely limits its partitioning behavior, Disperse Blue 79 is expected to have a low potential for bioaccumulation.

The experimental concentrations associated with toxicity for aquatic organisms may have an additional source of uncertainty when these concentrations exceed the solubility of the chemical in water (either experimental or predicted). Despite this, the available data indicate that Disperse Blue 79 is not highly hazardous to aquatic organisms.

There are uncertainties regarding the degradation products of this dye. This risk assessment did not evaluate the ecological risk of these breakdown compounds which have been known to form under anaerobic conditions (Weber and Adams 1995). One breakdown product of Disperse Blue 79 has been found in the Canadian environment by Maguire and Tkacz (1991).

Uncertainties are also associated with the fraction of the substance that is released during use and with the fraction that is removed in sewage treatment plants. These uncertainties were addressed by making conservative assumptions using best model estimates.

Regarding ecotoxicity, based on the predicted partitioning behaviour of this chemical, the significance of soil and sediment as important media of exposure is not well addressed by the effects data available. Indeed, the only effects data identified apply primarily to pelagic aquatic exposures.

Conclusion

Based on the information presented in this screening assessment, it is concluded that Disperse Blue 79 is 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.

It is therefore concluded that Disperse Blue 79 does not meet the definition of toxic as set out in section 64 of CEPA 1999. Additionally, Disperse Blue 79 meets the criteria for persistence but does not meet the criteria for bioaccumulation potential as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

References

- ACD/pK_aDB [Prediction Module]. 2005. Version 9.04. Toronto (ON): Advanced Chemistry Development. Available from: http://www.acdlabs.com/products/phys_chem_lab/pka/
- Anliker R, Clarke EA, Moser P. 1981. Use of the partition coefficient as an indicator of bioaccumulation tendency of dyestuffs in fish. *Chemosphere* 10(3): 263-274.
- Anliker R, Moser P. 1987. The limits of bioaccumulation of organic pigments in fish: their relation to the partition coefficient and the solubility in water and octanol. *Ecotoxicol Environ Safety* 13:43-52.
- Anliker R, Moser P, Poppinger D. 1988. Bioaccumulation of dyestuffs and organic pigments in fish. Relationships to hydrophobicity and steric factors. *Chemosphere* 17(8): 1631-1644.
- Aronson D, Howard PH. 1999. Evaluating potential POP/PBT compounds for environmental persistence. North Syracuse (NY): Syracuse Research Corp., Environmental Science Centre. Report No.: SRC-TR-99-020.
- Aronson D, Boethling B, Howard P, W Stiteler W. 2006. Estimating biodegradation half-lives for use in chemical screening. *Chemosphere* 63: 1953-1960.
- ASTreat v.1.0, A software program developed by The Procter & Gamble Company for sewage treatment plant removal predictions, revised and released 2006, available from Dr. Drew C. McAvoy, The Procter & Gamble Company, P.O. Box 538707, Cincinnati, OH 45253-8707, USA, Tel: (513) 634-7603, Email: mcavoy.dc@pg.com
- BASF. 1990. Bericht über die Prüfung der akuten Toxizität an der Goldorfe (*Leuciscus idus* L., Goldvariante). Submitted by ETAD to Environment Canada on August 13, 2008 via e-mail.
- Baughman GL, Perenich TA. 1988. Fate of dyes in aquatic systems: I. Solubility and partitioning of some hydrophobic dyes and related compounds. *Environ Toxicol Chem* 7(3):183-199.
- Baughman GL, Weber EJ. 1994. Transformation of dyes and related compounds in anoxic sediment: kinetics and products. *Environ Sci Technol* 28(2): 267-276.
- [BBM] Baseline Bioaccumulation Model. 2008. Gatineau (QC): Environment Canada, Existing Substances Division. [Model based on Dimitrov et al 2005]. [cited 2008-11-21]. Available upon request.
- [BIOWIN] Biodegradation Probability Program for Windows [Estimation Model]. 2000. Version 4.1. Washington (DC): US Environmental Protection Agency, Office of Pollution Prevention and Toxics; Syracuse (NY): Syracuse Research Corporation. Available from: www.epa.gov/oppt/exposure/pubs/episuite.htm
- Boethling RS, Howard PH, Beauman JA, Larosche ME. 1995. Factors for intermedia extrapolations in biodegradability assessment. *Chemosphere* 30(4): 741-752.
- Bomberger D.C. and R.L. Boughton. 1984. *Wastes from manufacture of dyes and pigments: Volume 1. Azo dyes and pigments (benzidine and its congeners subsector)* (1984), p. 94 EPA-600/2-84-111a.
- Brown D. 1987. Effects of colorants in the aquatic environment. *Ecotoxicol Environ Safety* 13:139-47.
- Brown D (ICI Group Environmental Laboratory, Brixham, UK). 1992. Environmental assessment of dyestuffs. Prepared for Ecological and Toxicological Association of the Dyes and Organic Pigments

Manufacturers, Basel, Switzerland. ETAD ecological sub-committee project E3020. Submitted to Environment Canada.

Canada. 1999. *Canadian Environmental Protection Act, 1999*. S.C., 1999, c. 33, Canada Gazette. Part III, vol. 22, no. 3. Available from: <http://canadagazette.gc.ca/partIII/1999/g3-02203.pdf>

Canada. 2000. *Canadian Environmental Protection Act: Persistence and Bioaccumulation Regulations*, P.C. 2000-348, 23 March, 2000, SOR/2000-107, Canada Gazette. Part II, vol. 134, no. 7, p. 607–612. Available from: <http://canadagazette.gc.ca/partII/2000/20000329/pdf/g2-13407.pdf>

Canada, Dept. of the Environment, Dept. of Health. 2006a. *Canadian Environmental Protection Act, 1999: Notice of intent to develop and implement measures to assess and manage the risks posed by certain substances to the health of Canadians and their environment*. Canada Gazette, Part I, vol. 140, no. 49, p. 4109–4117. Available from: <http://canadagazette.gc.ca/partI/2006/20061209/pdf/g1-14049.pdf>

Canada, Dept. of the Environment, Dept. of Health. 2006b. *Canadian Environmental Protection Act, 1999: Notice with respect to selected substances identified as priority for action*. Canada Gazette, Part I, vol. 140, no. 9, p. 435–459. Available from: <http://canadagazette.gc.ca/partI/2006/20060304/pdf/g1-14009.pdf>

Canada, Dept. of the Environment, Dept. of Health. 2008. *Canadian Environmental Protection Act, 1999: Notice of fifth release of technical information relevant to substances identified in the Challenge*. Canada Gazette, Part I, vol. 147, no. 7. Available from: <http://canadagazette.gc.ca/partI/2008/20080216/html/notice-e.html#d101>

[CATABOL] Probabilistic assessment of biodegradability and metabolic pathways [Computer Model]. c2004–2008. Version 5.10.2. Bourgas (BG): Bourgas Prof. Assen Zlatarov University, Laboratory of Mathematical Chemistry. Available from: <http://oasis-lmc.org/?section=software&swid=1>.

Clariant. 1996. IUCLID dataset for C.I. Disperse Blue 79 (CAS No 12239-34-8).

Cohle P, Mihalik R. 1991. Early life stage toxicity of C.I. Disperse Blue 79:1 purified preecake to rainbow trout (*Oncorhynchus mykiss*) in a flow-through system. Final report. ABC Laboratories Inc. Columbia MO.

Colón D, Weber EJ and Baughman GL. 2002. Sediment-associated reactions of aromatic amines. 2. QSAR development. *Environ Sci Technol* 36:2443-2450.

ChemID Plus. [Database on the Internet]. 2008. <http://chem.sis.nlm.nih.gov/chemidplus/> Accessed on October 1, 2008.

[CII] Color Index International [database on the Internet]. 2002. 4th ed. Research Triangle Park (NC): American Association of Textile Chemists and Colorists. [cited August 2008]. Available from: <http://www.colour-index.org/>

[CPOPs] Canadian POPs Model. 2008. Gatineau (QC): Environment Canada, Existing Substances Division; Bourgas (BG): Bourgas Prof. Assen Zlatarov University, Laboratory of Mathematical Chemistry. [Model developed based on Mekenyan et al. 2005]. Available upon request.

Cruz A, Buitrón G, 2001. Biodegradation of Disperse Blue 79 using sequenced anaerobic/aerobic biofilters, *Water Sci. Technol.* **44** (2001) (4), pp. 159–166

Dimitrov S, Dimitrova N, Parkerton T, Comber M, Bonnell M, Mekenyan O. 2005. Base-line model for identifying the bioaccumulation potential of chemicals. *SAR QSAR Environ Res* 16(6):531–554.

Dimitrov SD, Dimitrova NC, Walker JD, Veith GD, Mekenyan OG. 2002. Predicting bioconcentration factors of highly hydrophobic chemicals. Effects of molecular size*. Pure Appl. Chem. 74(10):1823-1830.

Environment Canada. 1988. Data relating to the Domestic Substances List (DSL) 1984-1986, collected under CEPA, 1988, s. 25(1). Based on Reporting for the Domestic Substances List [guide] 1988. Data prepared by: Environment Canada.

Environment Canada. 1995. Acute fish toxicity test submission in fulfillment of new substances notification regulations. Submitted to New Substances Branch, Environment Canada under New Substance Notification Program.

Environment Canada. 2000. Chemicals Evaluation Division. *Environmental Categorization for Persistence, Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substances List Using QSARs. Final Report*. Environment Canada. July.

Environment Canada. 2007. Review of the limitations and uncertainties associated with use for molecular size information when assessing bioaccumulation potential. Unpublished Final Report. Gatineau (QC): Environment Canada, Existing Substances Division.

Environment Canada. 2008a. Guidance for conducting ecological assessments under CEPA, 1999: science resource technical series, technical guidance module: Mass Flow Tool. Preliminary draft working document. Gatineau (QC): Environment Canada, Existing Substances Division.

Environment Canada. 2008b. Assumptions, limitations and uncertainties of the mass flow tool for Disperse Blue 79, CAS RN 12239-34-8. Internal draft document. Gatineau (QC): Environment Canada, Existing Substances Division. Available on request.

Environment Canada. 2008c. Guidance for conducting ecological assessments under CEPA, 1999: science resource technical series, technical guidance module: the Industrial Generic Exposure Tool – Aquatic (IGETA). Working document. Gatineau (QC): Environment Canada, Existing Substances Division.

Environment Canada. 2008d. IGETA report: CAS RN 12239-34-8, 2008-07-21. Unpublished report. Gatineau (QC): Environment Canada, Existing Substances Division.

Environment Canada. 2008e. Guidance for conducting ecological assessments under CEPA, 1999: science resource technical series, technical guidance module: Mega Flush consumer release scenario. Preliminary draft working document. Gatineau (QC): Environment Canada, Existing Substances Division.

Environment Canada. 2008f. Mega Flush report: CAS RN 12239-34-8, 2008-08-12. Unpublished report. Gatineau (QC): Environment Canada, Existing Substances Division.

Epochem. 2008. Product: Dyestuffs and Pigments. [cited 2008 Oct 11]. Available from: <http://www.epochem.com/products/dyesDisperse.htm>

[ESIS] European Substances Information System [database on the Internet]. [date unknown]. Version 5. European Chemical Bureau (ECB). [cited August 2008]. Available from: <http://ecb.jrc.it/esis>

[ETAD] Ecological and Toxicological Association of Dyes and Organic Pigments Manufacturers. 1992. Draft Guidelines for the Assessment of Environmental Exposure to Dyestuffs.

[ETAD] Ecological and Toxicological Association of Dyes and Organic Pigments Manufacturers Canadian Affiliates, Dayan J, Trebitz H, consultants. 1995. Health and environmental information on dyes used in Canada. Unpublished report submitted to Environment Canada, New Substances Division.

Gardner DA, Holsworth TJ, Shaul GM, Dostal KA, Betowski LD. 1989. Aerobic and anaerobic treatment of C.I. Disperse Blue 79. Risk Reduction Engineering Laboratory Office of Research and Development, US EPA. EPA/600/2-89/051a.

Hunger K, editor. 2003. Industrial dyes; chemistry, properties, applications. Weinheim (DE): WILEY-VCH Verlag GmbH & Co. KGaA.

Industry Canada. 2008a. Canadian Company Capabilities.
<http://strategis.ic.gc.ca/app/ccc/srch/cccBscSrch.do?lang=eng&prtl=1&app=1>

Industry Canada. 2008b. Textile and Fabric Finishing [NAICS 31331]: 2004-2007 and Fabrics Coating 2004-2007. [NAICS 31332]: 2004-2007. Prepared by: Apparel and Textiles Directorate, Service Industries and Consumer Products Branch, Industry Canada, Enquiries B John (Jazz) Szabo, 613-957-1242, szabo.john@ic.gc.ca

Little, LW, Lamb LC, III. 1973. Acute Toxicity of 46 Selected Dyes to the Fathead Minnow, *Pimephales promelas*. Dyes and the Environment - Reports on Selected Dyes and Their Effects, Vol.1, American Dye Manufacturers Institute, Inc.:130

Maguire RJ, Tkacz RJ. 1991. Occurrence of Dyes in the Yamaska River, Québec. Water Pollution Research Journal of Canada, 26(2): 145-161.

[MITI] Ministry of International Trade & Industry (Jpn), Basic Industries Bureau, Chemical Products Safety Division. 1992. Biodegradation and bioaccumulation data of existing chemicals based on the CSCL Japan. Tokyo (Jpn): Japan Chemical Industry Ecology-Toxicology & Information Centre.

[NCI] National Chemical Inventories [database on CD-ROM]. 2006. Columbus (OH): American Chemical Society. [cited 2006 Dec 11]. Available from: <http://www.cas.org/products/cd/nci/index.html>

[OECD] Organisation for Economic Co-operation and Development. 2004. Draft emission scenario on textile manufacturing wool mills [Internet]. Paris (FR): OECD, Environment Directorate. Report No.: ENV/JM/EEA(2004)8/1/REV, JT00175156. [cited 2008 August]. Available from: <http://www.oecd.org/dataoecd/2/47/34003719.pdf>

[OECD] Organisation for Economic Co-operation and Development. 2007. Emission scenario document on adhesive formulation [Internet]. Final report. Paris (FR): OECD, Environment Directorate. (Series on Emission Scenario Documents). [Cited 2008 August]. Available from: <http://ascouncil.org/news/adhesives/docs/EPAFormulation.pdf>

Øllgaard H, Frost L, Galster J, Hansen OC. 1998. Survey of azo-colorants in Denmark, Consumption, use, health and environmental aspects Miljøprojekt no. 509, Danish Technological Institute, Environment, Ministry of Environment and Energy, Denmark, Danish Environmental Protection Agency, November, 1998.

Pagga U, Brown D. 1986. The degradation of dyestuffs: Part II Behaviour of dyestuffs in aerobic biodegradation tests. Chemosphere, 15, 4, 479-491.

[PhysProp] Interactive PhysProp Database [database on the Internet]. 2006. Syracuse (NY): Syracuse Research Corporation. [cited 2006 Mar] Available from: <http://www.syrres.com/esc/physdemo.htm>

Razo-Flores E, Luijten M, Donlon B, Lettinga G, Field J. 1997. Biodegradation of selected azo dyes under methanogenic conditions. Wat. Sci. Tech 36(6-7): 65-72.

Reife A. 1989. Reduction of toxic wastewaters in disperse azo dye manufacture. American Association of textile chemists and colorists. International Conference and Exhibition.

Safepharm Laboratories Ltd. 1990. Acute toxicity to rainbow trout. Project number 47/918. Challenge submission ID#11347.

Sakuratani Y, Noguchi Y, Kobayashi K, Yamada J, Nishihara T. 2008. Molecular size as a limiting characteristic for bioconcentration in fish. : J Environ Biol. 29(1):89-92

Sandoz Chemicals. 1989. Material Safety Data sheet of Foron Navy S-2GRL Purified presscakes.

Shen Genxiang, Hu Shuangqing (Environmental Testing Laboratory, Shanghai Academy of Environmental Sciences, Shanghai, China). 2008. Bioconcentration Test of C.I. Disperse Orange 30 in Fish. Prepared for Dystar in the name of Ecological and Toxicological Association of the Dyes and Organic Pigments Manufacturers (ETAD) Basel, Switzerland. Report No. S-070-2007. Submitted to Environment Canada in April 2008. Challenge Submission ID#8351

Sijm DTHM, Schuurmann G, deVries PJ, Opperhuizen A. 1999. Aqueous solubility, octanol solubility, and octanol/water partition coefficient of nine hydrophobic dyes. Environ Toxicol Chem 18(6): 1109-1117.

[SPIN] Substances in Preparations in Nordic Countries [database on the Internet]. 2008. Copenhagen (DK): Nordic Council of Ministers. [cited 2008] Available from: <http://195.215.251.229/Dotnetnuke/Home/tabid/58/Default.aspx>

[US EPA] US Environmental Protection Agency. 2002. PBT Profiler Methodology [Internet]. Washington (DC): US EPA, Office of Pollution Prevention and Toxics. [cited 2008 August]. Available from: <http://www.pbtprofiler.net/methodology.asp>

[US EPA] US Environmental Protection Agency. 2007. Inventory Update Reporting, Past IUR Data, Non-confidential Production Volume Information submitted by companies under the 1986, 1990, 1994, 1998, and 2002 Inventory Update Reporting Regulation, CAS RN 52697-38-8 [Internet]. Washington (DC): US EPA; [cited 2007 Feb 28]. Available from: <http://www.epa.gov/oppt/iur/tools/data/2002-vol.htm>

Weber EJ, Adams RL. 1995. Chemicals and sediment-mediated reduction of the azo dye DisperseBlue 79. Environ. Sci. Tech. 29:1163-1170.

Weber EJ, Colón D, Baughmann GL. 2001. Sediment-Associated Reactions of Aromatic Amines. 1. Elucidation of sorption mechanisms. Environ Sci Technol 35:2470-2475.

Yen CC, Perenich TA, Baughman GL. 1989. Fate of dyes in aquatic systems II. Solubility and octanol/water partition coefficients of disperse dyes. Environ Toxicol Chem 8 (11): 981-986.

Yen CC, Perenich TA, Baughman GL. 1991. Fate of commercial disperse dyes in sediments. Environ Toxicol Chem 10:1009-1017.

Appendix I - Robust Study Summaries for Key studies

Robust Study Summaries Form: Aquatic B				
No	Item	Weight	Yes/No	Specify
1	Reference: Shen, Genxiang and Hu, Shuangqing. 2008. Bioconcentration Test of C.I. Disperse Orange 30 in Fish. Prepared by Environmental Testing Laboratory, Shanghai Academy of Environmental Sciences, Shanghai, China for Dystar in the name of Ecological and Toxicological Association of the Dyes and Organic Pigments Manufacturers (ETAD) Basel, Switzerland. Report No. S-070-2007. Submitted to Environment Canada in April 2008. Challenge Submission ID#8351			
2	Substance identity: CAS RN	n/a	Y	5261-31-4
3	Substance identity: chemical name(s)	n/a	Y	Propanenitrile, 3-[[2-(acetyloxy)ethyl][4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]amino]-
4	Chemical composition of the substance	2	N	
5	Chemical purity	1	N	
6	Persistence/stability of test substance in aquatic solution reported?	1	N	
7	If test material is radiolabelled, were precise position(s) of the labelled atom(s) and the percentage of radioactivity associated with impurities reported?	2	n/a	
	Method			
8	Reference	1	Y	OECD guidelines for the testing of chemicals No 305B-1996
9	OECD, EU, national, or other standard method?	3	Y	OECD
10	Justification of the method/protocol if not a standard method was used	2		
11	GLP (Good Laboratory Practice)	3	N	
	Test organism			
12	Organism identity: name	n/a	Y	zebra fish, <i>Brachydanio rerio</i>
13	Latin or both Latin & common names reported?	1	Y	both
14	Life cycle age / stage of test organism	1	N	
15	Length and/or weight	1	Y	Mean body length 3.91+/-0.18cm and mean body weight 0.32+/-0.06g
16	Sex	1	N	
17	Number of organisms per replicate	1	Y	7
18	Organism loading rate	1	Y	20mg/L
19	Food type and feeding periods during the acclimation period	1	Y	Fed a commercial fish diet until one day before start of test
	Test design / conditions			
20	Experiment type (laboratory or field)	n/a	Y	Laboratory
21	Exposure pathways (food, water, both)	n/a	Y	Water
22	Exposure duration	n/a	Y	28 days
23	Number of replicates (including controls)	1	Y	
24	Concentrations	1	Y	20 mg/L
25	Food type/composition and feeding periods during the test	1	Y	Fish were fed two hours before water renewal
26	If BCF/BAF derived as a ratio of chemical concentration in the organism and in water, was experiment duration equal to or longer than the time required for the chemical concentrations to reach steady state?	3	Y	28 days

27	If BCF/BAF derived as a ratio of chemical concentration in the organism and in water, were measured concentrations in both water and organism reported?	3	Y	
28	Were concentrations in the test water measured periodically?	1	Y	On three separate days
29	Were the exposure media conditions relevant to the particular chemical reported? (e.g., for the metal toxicity - pH, DOC/TOC, water hardness, temperature)	3	Y	Yes every second day
30	Photoperiod and light intensity	1	Y	12:12
31	Stock and test solution preparation	1	Y	
32	Analytical monitoring intervals	1	Y	Every second day for dissolved oxygen, pH and temperature
33	Statistical methods used	1	Y	
34	Was solubilizer/emulsifier used, if the chemical was unstable or poorly soluble?	n/a	N	
	Information relevant to the data quality			
35	Was the test organism relevant to the Canadian environment?	3	Y	
36	Were the test conditions (pH, temperature, DO, etc.) typical for the test organism?	1	Y	
37	Does system type and design (static, semi-static, flow-through; sealed or open; etc.) correspond to the substance's properties and organism's nature/habits?	2	Y	Semi-static
38	Was pH of the test water within the range typical for the Canadian environment (6 to 9)?	1	Y	7.22-7.84
39	Was temperature of the test water within the range typical for the Canadian environment (5 to 27°C)?	1	Y	22-23
40	Was lipid content (or lipid-normalized BAF/BCF) reported?	2	Y	
41	Were measured concentrations of a chemical in the test water below the chemical's water solubility?	3	N	
42	If radiolabelled test substance was used, was BCF determination based on the parent compound (i.e. not on total radiolabelled residues)?	3	n/a	
	Results			
43	Endpoints (BAF, BCF) and values	n/a	n/a	BCF<100
44	BAF or BCF determined as: 1) the ratio of chemical concentration in the organism and in water, or 2) the ratio of the chemical uptake and elimination rate constants	n/a	n/a	1
45	Whether BAF/BCF was derived from a 1) tissue sample or 2) whole organism?	n/a	n/a	2
46	Whether 1) average or 2) maximum BAF/BCF was used?	n/a	n/a	1
47	Score: ... %	75.0		
48	EC Reliability code:	2		
49	Reliability category (high, satisfactory, low):	Satisfactory Confidence		
50	Comments	The present procedure is based on semi-static conditions (renewal of test solutions every 2 days). Therefore, test chemical with very low water solubility Disperse Blue 79, can also be characterized as to their bioconcentration potential without adding solvents or other auxiliary substances which may affect the results.		

Robust Study Summaries Form: Aquatic iT				
No	Item	Weight	Yes/No	Specify
1	Reference: Environment Canada. 1995. Acute fish toxicity test submission in fulfillment of new substances notification regulations to New Substances Branch, Environment Canada under New Substance Notification Program.			
2	Substance identity: CAS RN	n/a	N	
3	Substance identity: chemical name(s)	n/a	Y	
4	Chemical composition of the substance	2	N	
5	Chemical purity	1	N	
6	Persistence/stability of test substance in aquatic solution reported?	1	N	
Method				
7	Reference	1	Y	OECD 203
8	OECD, EU, national, or other standard method?	3	Y	
9	Justification of the method/protocol if not a standard method was used	2		not applicable
10	GLP (Good Laboratory Practice)	3	Y	
Test organism				
11	Organism identity: name	n/a	Y	<i>Rainbow trout</i>
12	Latin or both Latin & common names reported?	1	Y	
13	Life cycle age / stage of test organis	1	Y	mean length 51mm and mean weight 1.54
14	Length and/or weight	1	Y	see above
15	Sex	1		not applicable
16	Number of organisms per replicate	1	Y	10
17	Organism loading rate	1	Y	
18	Food type and feeding periods during the acclimation period	1	Y	

Test design / conditions				
19	Test type (acute or chronic)	n/a	Y	acute
20	Experiment type (laboratory or field)	n/a	y	lab
21	Exposure pathways (food, water, both)	n/a	y	water
22	Exposure duration	n/a	y	96hrs
23	Negative or positive controls (specify)	1	Y	3
24	Number of replicates (including controls)	1	Y	2
25	Nominal concentrations reported?	1	Y	320 to 3200 mg/L
26	Measured concentrations reported?	3	N	
27	Food type and feeding periods during the long-term tests	1		not applicable
28	Were concentrations measured periodically (especially in the chronic test)?	1	N	
29	Were the exposure media conditions relevant to the particular chemical reported? (e.g., for the metal toxicity - pH, DOC/TOC, water hardness, temperature)	3	Y	
30	Photoperiod and light intensity	1	Y	
31	Stock and test solution preparation	1	Y	
32	Was solubilizer/emulsifier used, if the chemical was poorly soluble or unstable?	1	N	
33	If solubilizer/emulsifier was used, was its concentration reported?	1		
34	If solubilizer/emulsifier was used, was its ecotoxicity reported?	1		
35	Analytical monitoring intervals	1	Y	
36	Statistical methods used	1	Y	
Information relevant to the data quality				
37	Was the endpoint directly caused by the chemical's toxicity, not by organism's health (e.g. when mortality in the control >10%) or physical effects (e.g. 'shading effect')?	n/a	Y	
38	Was the test organism relevant to the Canadian environment?	3	Y	
39	Were the test conditions (pH, temperature, DO, etc.) typical for the test organism?	1	Y	
40	Does system type and design (static, semi-static, flow-through; sealed or open; etc.) correspond to the substance's properties and organism's nature/habits?	2	Y	
41	Was pH of the test water within the range typical for the Canadian environment (6 to 9)?	1	Y	
42	Was temperature of the test water within the range typical for the Canadian environment (5 to 27°C)?	1	Y	
43	Was toxicity value below the chemical's water solubility?	3		unknown water solubility

Results				
44	Toxicity values (specify endpoint and value)	n/a	n/a	96hr LC50=505mg/L
45	Other endpoints reported - e.g. BCF/BAF, LOEC/NOEC (specify)?	n/a	N	
46	Other adverse effects (e.g. carcinogenicity, mutagenicity) reported?	n/a	N	
47	Score: ... %			77.5
48	EC Reliability code:			2
49	Reliability category (high, satisfactory, low):			Satisfactory Confidence
50	Comments			

Robust Study Summaries Form: Aquatic iT				
No	Item	Weight	Yes/No	Specify
1	Reference: BASF 1990. Bericht über die Prüfung der akuten Toxizität an der Goldorfe (Leuciscus idus L., Goldvariante. Submitted by ETAD to Environment Canada, August 2088			
2	Substance identity: CAS RN	n/a		
3	Substance identity: chemical name(s)	n/a		
4	Chemical composition of the substance	2	N	
5	Chemical purity	1	N	
6	Persistence/stability of test substance in aquatic solution reported?	1	N	
Method				
7	Reference	1	N	
8	OECD, EU, national, or other standard method?	3	N	
9	Justification of the method/protocol if not a standard method was used	2	N	
10	GLP (Good Laboratory Practice)	3		
Test organism				
11	Organism identity: name	n/a	Y	Golden orfe
12	Latin or both Latin & common names reported?	1	Y	
13	Life cycle age / stage of test organism	1	N	
14	Length and/or weight	1	N	
15	Sex	1	N	
16	Number of organisms per replicate	1	N	
17	Organism loading rate	1	N	
18	Food type and feeding periods during the acclimation period	1	N	

Test design / conditions				
19	Test type (acute or chronic)	n/a	Y	Acute
20	Experiment type (laboratory or field)	n/a	N	
21	Exposure pathways (food, water, both)	n/a	N	
22	Exposure duration	n/a	Y	96HRS
23	Negative or positive controls (specify)	1	N	
24	Number of replicates (including controls)	1	N	
25	Nominal concentrations reported?	1	N	
26	Measured concentrations reported?	3	N	
27	Food type and feeding periods during the long-term tests	1		n/a
28	Were concentrations measured periodically (especially in the chronic test)?	1	N	
29	Were the exposure media conditions relevant to the particular chemical reported? (e.g., for the metal toxicity - pH, DOC/TOC, water hardness, temperature)	3	N	
30	Photoperiod and light intensity	1	N	
31	Stock and test solution preparation	1	N	
32	Was solubilizer/emulsifier used, if the chemical was poorly soluble or unstable?	1	N	
33	If solubilizer/emulsifier was used, was its concentration reported?	1	N	
34	If solubilizer/emulsifier was used, was its ecotoxicity reported?	1	N	
35	Analytical monitoring intervals	1	N	
36	Statistical methods used	1	N	
Information relevant to the data quality				
37	Was the endpoint directly caused by the chemical's toxicity, not by organism's health (e.g. when mortality in the control >10%) or physical effects (e.g. 'shading effect')?	n/a	N	
38	Was the test organism relevant to the Canadian environment?	3	Y	
39	Were the test conditions (pH, temperature, DO, etc.) typical for the test organism?	1	N	
40	Does system type and design (static, semi-static, flow-through; sealed or open; etc.) correspond to the substance's properties and organism's nature/habits?	2	N	
41	Was pH of the test water within the range typical for the Canadian environment (6 to 9)?	1	N	
42	Was temperature of the test water within the range typical for the Canadian environment (5 to 27°C)?	1	N	
43	Was toxicity value below the chemical's water solubility?	3		

Results				
44	Toxicity values (specify endpoint and value)	n/a		LC50=>100<220mg/L
45	Other endpoints reported - e.g. BCF/BAF, LOEC/NOEC (specify)?	n/a		NOEC=100mg/L
46	Other adverse effects (e.g. carcinogenicity, mutagenicity) reported?	n/a		
47	Score: ... %			9.5
48	EC Reliability code:			4
49	Reliability category (high, satisfactory, low):			Not Satisfactory
50	Comments	Not enough data submitted to properly assess the reliability of this study.		

Robust Study Summaries Form: Aquatic iT				
No	Item	Weight	Yes/No	Specify
1	Reference: Cohle P, R Mihalik R. 1991. Early life stage toxicity of C.I. Disperse Blue 79:1 purified preecake to rainbow trout (<i>Oncorhynchus mykiss</i>) in a flow-through system. Final report. ABC Laboratories Inc. Columbia MO.			
2	Substance identity: CAS RN	n/a		
3	Substance identity: chemical name(s)	n/a		Disperse Blue 79:1
4	Chemical composition of the substance	2		n/a
5	Chemical purity	1	Y	96.61
6	Persistence/stability of test substance in aquatic solution reported?	1	N	
Method				
7	Reference	1	Y	
8	OECD, EU, national, or other standard method?	3	Y	
9	Justification of the method/protocol if not a standard method was used	2		n/a
10	GLP (Good Laboratory Practice)	3	Y	
Test organism				
11	Organism identity: name	n/a		Rainbow trout
12	Latin or both Latin & common names reported?	1	Y	
13	Life cycle age / stage of test organis	1	Y	
14	Length and/or weight	1	Y	
15	Sex	1		n/a
16	Number of organisms per replicate	1	Y	20
17	Organism loading rate	1	Y	0.36 to 4.8ug/L
18	Food type and feeding periods during the acclimation period	1	Y	

Test design / conditions				
19	Test type (acute or chronic)	n/a	Y	chronic
20	Experiment type (laboratory or field)	n/a	Y	lab
21	Exposure pathways (food, water, both)	n/a	Y	water
22	Exposure duration	n/a	Y	122 days
23	Negative or positive controls (specify)	1	Y	control and carrier blank
24	Number of replicates (including controls)	1	Y	2
25	Nominal concentrations reported?	1	Y	5
26	Measured concentrations reported?	3	Y	
27	Food type and feeding periods during the long-term tests	1	Y	
28	Were concentrations measured periodically (especially in the chronic test)?	1	Y	
29	Were the exposure media conditions relevant to the particular chemical reported? (e.g., for the metal toxicity - pH, DOC/TOC, water hardness, temperature)	3	Y	
30	Photoperiod and light intensity	1	Y	
31	Stock and test solution preparation	1	Y	
32	Was solubilizer/emulsifier used, if the chemical was poorly soluble or unstable?	1	Y	
33	If solubilizer/emulsifier was used, was its concentration reported?	1	Y	
34	If solubilizer/emulsifier was used, was its ecotoxicity reported?	1	Y	no tox value but however is was used as a control
35	Analytical monitoring intervals	1	Y	
36	Statistical methods used	1	Y	
Information relevant to the data quality				
37	Was the endpoint directly caused by the chemical's toxicity, not by organism's health (e.g. when mortality in the control >10%) or physical effects (e.g. 'shading effect')?	n/a	Y	
38	Was the test organism relevant to the Canadian environment?	3	Y	
39	Were the test conditions (pH, temperature, DO, etc.) typical for the test organism?	1	Y	
40	Does system type and design (static, semi-static, flow-through; sealed or open; etc.) correspond to the substance's properties and organism's nature/habits?	2	Y	flow through
41	Was pH of the test water within the range typical for the Canadian environment (6 to 9)?	1	Y	
42	Was temperature of the test water within the range typical for the Canadian environment (5 to 27°C)?	1	Y	

43	Was toxicity value below the chemical's water solubility?	3		n/a
Results				
44	Toxicity values (specify endpoint and value)	n/a	n/a	NOEC>0.005mg/L
45	Other endpoints reported - e.g. BCF/BAF, LOEC/NOEC (specify)?	n/a		
46	Other adverse effects (e.g. carcinogenicity, mutagenicity) reported?	n/a		
47	Score: ... %			97.6
48	EC Reliability code:			1
49	Reliability category (high, satisfactory, low):			High Confidence
50	Comments			

Robust Study Summaries Form: Aquatic iT				
No	Item	Weight	Yes/No	Specify
1	Reference: Safepharm laboratories Ltd. 1990. Acute toxicity to rainbow trout. Project number 47/918			
2	Substance identity: CAS RN	n/a	Y	12239-34-8
3	Substance identity: chemical name(s)	n/a	N	
4	Chemical composition of the substance	2	N	
5	Chemical purity	1	N	
6	Persistence/stability of test substance in aquatic solution reported?	1	N	
Method				
7	Reference	1	N	
8	OECD, EU, national, or other standard method?	3	N	
9	Justification of the method/protocol if not a standard method was used	2	N	
10	GLP (Good Laboratory Practice)	3		n/a
Test organism				
11	Organism identity: name	n/a		Rainbow trout
12	Latin or both Latin & common names reported?	1	Y	
13	Life cycle age / stage of test organis	1	Y	
14	Length and/or weight	1	Y	
15	Sex	1		n/a
16	Number of organisms per replicate	1	Y	10-Feb
17	Organism loading rate	1	Y	0.78g bodyweight/L
18	Food type and feeding periods during the acclimation period	1		n/a since acute test
Test design / conditions				

19	Test type (acute or chronic)	n/a		acute
20	Experiment type (laboratory or field)	n/a		lab
21	Exposure pathways (food, water, both)	n/a		water
22	Exposure duration	n/a		96hrs
23	Negative or positive controls (specify)	1	Y	positive
24	Number of replicates (including controls)	1	Y	two at definitive study
25	Nominal concentrations reported?	1	Y	3
26	Measured concentrations reported?	3	N	
27	Food type and feeding periods during the long-term tests	1		n/a
28	Were concentrations measured periodically (especially in the chronic test)?	1	N	
29	Were the exposure media conditions relevant to the particular chemical reported? (e.g., for the metal toxicity - pH, DOC/TOC, water hardness, temperature)	3	Y	
30	Photoperiod and light intensity	1	N	
31	Stock and test solution preparation	1	N	
32	Was solubilizer/emulsifier used, if the chemical was poorly soluble or unstable?	1	N	
33	If solubilizer/emulsifier was used, was its concentration reported?	1		n/a
34	If solubilizer/emulsifier was used, was its ecotoxicity reported?	1		n/a
35	Analytical monitoring intervals	1	Y	
36	Statistical methods used	1	N	
Information relevant to the data quality				
37	Was the endpoint directly caused by the chemical's toxicity, not by organism's health (e.g. when mortality in the control >10%) or physical effects (e.g. 'shading effect')?	n/a	Y	
38	Was the test organism relevant to the Canadian environment?	3	Y	
39	Were the test conditions (pH, temperature, DO, etc.) typical for the test organism?	1	Y	
40	Does system type and design (static, semi-static, flow-through; sealed or open; etc.) correspond to the substance's properties and organism's nature/habits?	2		n/a
41	Was pH of the test water within the range typical for the Canadian environment (6 to 9)?	1	N	no pH given
42	Was temperature of the test water within the range typical for the Canadian environment (5 to 27°C)?	1	Y	
43	Was toxicity value below the chemical's water solubility?	3	N	Water solubility for this substance ranged from 0.0009 to 0.02

Results				
44	Toxicity values (specify endpoint and value)	n/a		96Hrs LC50 > 100mg/L
45	Other endpoints reported - e.g. BCF/BAF, LOEC/NOEC (specify)?	n/a	N	
46	Other adverse effects (e.g. carcinogenicity, mutagenicity) reported?	n/a	N	
47	Score: ... %		43.6	
48	EC Reliability code:		3	
49	Reliability category (high, satisfactory, low):		Low Confidence	
50	Comments			

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