Screening Assessment for the Challenge

2-Naphthalenol, 1-[(2-methoxyphenyl)azo]-
(Solvent Red 1)
Chemical Abstracts Service Registry Number
1229-55-6

2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]-
(Solvent Orange 7)
Chemical Abstracts Service Registry Number
3118-97-6

1-Naphthalenol, 4-[(4-ethoxyphenyl)azo]-
(Solvent Red 3)
Chemical Abstracts Service Registry Number
6535-42-8

Environment Canada
Health Canada

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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 three monoazo solvent dyes, as follows:

- 2-Naphthalenol, 1-[(2-methoxyphenyl)azo]- (Solvent Red 1), Chemical Abstracts Service Registry Number 1229-55-6
- 2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]- (Solvent Orange 7), Chemical Abstracts Service Registry Number 3118-97-6
- 1-Naphthalenol, 4-[(4-ethoxyphenyl)azo]- (Solvent Red 3), Chemical Abstracts Service Registry Number 6535-42-8

These three monoazo solvent dyes were identified as high priorities for screening assessment and included in the Challenge because they were originally found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity to non-human organisms and were believed to be in commerce in Canada.

These substances were not considered to be high priorities 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 (DSL). Therefore, this assessment focuses primarily on information relevant to the evaluation of ecological risks.

These substances were previously used in Canada as colorant dyes—probably in textiles, fabric and paper based on use codes from the 1986 DSL. They are not naturally produced in the environment. No companies reported manufacturing, importing or using any of these substances in Canada above the reporting thresholds in 2006. In this assessment, the threshold of 100 kg was used to build scenarios and capture the potential quantity of these substances in use in Canada that would be below the threshold reporting value.

Based on certain assumptions and reported use patterns, when used, most of these substances are expected to end up in solid waste disposal sites and a significant proportion is estimated to be released to sewer water (17.4%). These three monoazo solvent dyes are not expected to be soluble in water; instead they are expected to partition to particles because of their hydrophobic nature. For these reasons, after release to water, these substances will likely end up mostly in sediments and, to a lesser extent, in agricultural soil that has been amended with sewage sludge. They are not expected to be volatile, hence not to be subject to long-range atmospheric transport.

Based on their physical and chemical properties, these three monoazo solvent dyes are expected to degrade slowly under aerobic conditions in the environment (in water, sediment and soil). Due to lack of experimental data relating to the bioaccumulation potential, a relatively close structural analogue of these three monoazo solvent dyes was used in the assessment and this resulted in the prediction that these substances have low potential to bioaccumulate in the environment. These substances are concluded to meet the persistence

criteria but not meet the bioaccumulation criteria as set out in the *Persistence and Bioaccumulation Regulations*. In addition, experimental toxicity data for chemical analogues suggest that these three monoazo solvent dyes do not cause acute harm to aquatic organisms exposed to low concentrations.

For this screening assessment, very conservative cumulative exposure scenarios were developed in which a single wastewater treatment plant was assumed to discharge these three monoazo solvent dyes after primary treatment into the aquatic environment. The predicted environmental concentrations in water were below the predicted no-effect concentration calculated for sensitive aquatic species.

It is concluded that Solvent Orange 7, Solvent Red 1 and Solvent Red 3 are not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity, or that constitute or may constitute a danger to the environment on which life depends.

Some of the substances in this group of monoazo dyes have been subjected to controls in other jurisdictions, based on concern for their hazardous properties, including carcinogenicity. Although the potential high hazard of Solvent Orange 7, Solvent Red 1 and Solvent Red 3 is recognized, on the basis of information which indicates that the substances are not manufactured in or imported into Canada in amounts above the reporting threshold, the likelihood of exposure in Canada is considered to be low; hence the risk to human health is likewise considered to be low and it is concluded that they are substances that are not entering the environment in a quantity or concentration or under conditions that constitute a danger in Canada to human life or health.

Based on available information, it is concluded that Solvent Orange 7, Solvent Red 1 do not meet any of the criteria set out in section 64 of CEPA 1999.

Because these substances are listed on the *Domestic Substances List*, their import and manufacture in Canada are not subject to notification under subsection 81(1). Given the hazardous properties of these substances, there is concern that new activities that have not been identified or assessed could lead to these substances meeting the criteria set out in section 64 of the Act. Therefore, it is recommended to amend the *Domestic Substances List*, under subsection 87(3) of the Act, to indicate that subsection 81(3) of the Act applies with respect to these substances so that new manufacture, import or use of these substances is notified and undergoes ecological and human health risk assessments.

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 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 those substances identified as high priorities.

Several substances that are being addressed simultaneously under the Challenge have been grouped together for risk assessment purposes. The grouping of these substances was conducted based on their shared chemical class (i.e., monoazo dyes), close structural similarities, common use patterns and the fact that their risk assessment conclusions are based on the same supporting data. Three monoazo solvent dyes (Solvent Red 1, Solvent Orange 7 and Solvent Red 3) are grouped together in this assessment.

The Challenge for these substances was published in the *Canada Gazette* on May 31, 2008 (Canada 2008). Substance profiles were released at the same time. The substance profiles presented the technical information available prior to December 2005 that formed the basis for categorization of these substances. As a result of the Challenge, submissions of information pertaining to the uses of the substances were received.

Although these three monoazo solvent dyes were determined to be high priorities for assessment with respect to the environment, they did not meet the criteria for GPE or IPE and high hazard to human health (Canada 2006b). Therefore, this assessment focuses principally on information relevant to the evaluation of ecological risks.

Screening assessments 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 CEPA 1999. Screening assessments examine scientific information and develop conclusions by incorporating a weight of evidence approach and precaution.

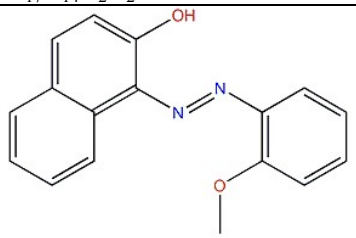
This screening assessment includes consideration of information on chemical properties, hazards, uses and exposure, including the additional information submitted under the Challenge. Data relevant to the screening assessment of this substance were identified in original literature, review and assessment documents, stakeholder research reports and from recent literature searches, up to December 2008. Key studies were critically evaluated; modelling results may have been used to reach conclusions. When available and relevant, information presented in hazard assessments from other jurisdictions was considered. 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 Programs at Health Canada and Environment Canada and incorporates input from other programs within these departments. This assessment has undergone external written peer review/consultation. Additionally, the draft of this screening assessment was subject to a 60-day public comment period. 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. The critical information and considerations upon which the assessment is based are summarized below.

Substance Identity

Three monoazo solvent dyes have been grouped together in this assessment. For the purposes of this document, when these three monoazo solvent dyes are discussed individually, they will be referred to by their common names: Solvent Red 1, Solvent Orange 7 and Solvent Red 3.

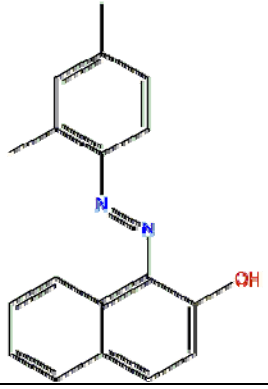
Table 1a. Substance identity for Solvent Red 1

Chemical Abstracts Service Registry Number (CAS RN)	**1229-55-6**
DSL name	**2-Naphthalenol, 1-[(2-methoxyphenyl)azo]-**
National Chemical Inventories (NCI) names[1]	*1-[(2-Methoxyphenyl)azo]-2-naphthol* (EINECS) *2-Naphthalenol, 1-[(2-methoxyphenyl)azo]-* (TSCA, DSL, AICS, PICCS, ASIA-PAC) *Solvent Red 1* (ENCS) *C.I. Solvent Red 001* (ECL) *NAPHTH-2-OL, 1-[(2-METHOXYPHENYL)AZO]-* (PICCS) *SUDAN RED 290* (PICCS)
Other names	*1-(o-Anisylazo)-2-naphthol; Anisole-2-azo-beta-naphthol; Brilliant Fat Scarlet R; (espace)C Red 2; C.I. Solvent Red 1;C.I. 12150; C.I. Food Red 16; Ceres Red G; Ceres Red G 102; Fat Red BG; Fat Red G; Fat Red RS; Fat Soluble Red S; Food Red 16;* *Lacquer Red V 2G; NSC 11232; NSC 45194; Oil Pink; Oil Red; Oil Red 113; Oil Red OG; Oil Scarlet 389; Oil Soluble Red S; Oil Vermilion; Oil Vermilion LP; Oleal Red G; Organol Vermilion; Orient Oil Red OG; Plastoresin Red FR; Resinol Red G; Sico Fat Red BG New; Silotras Red TG; Solvent Red 1;Somalia Red PG; Sudan R; Sudan Red 290; Sudan Red G*
Chemical group	Azo compounds
Chemical sub-class	Monoazo compounds
Chemical formula	$C_{17}H_{14}N_2O_2$
Chemical structure	
SMILES[2]	O(c(c(N=Nc(c(c(ccc1)cc2)c1)c2O)ccc3)c3)C
Molecular mass	278.31 g/mol

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

[2] Simplified Molecular Line Input Entry System

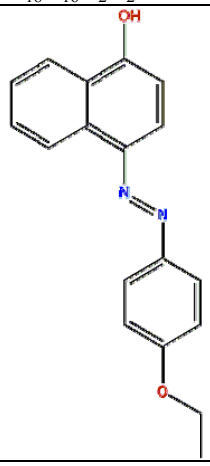
Table 1b. Substance identity for Solvent Orange 7

Chemical Abstracts Service Registry Number (CAS RN)	**3118-97-6**
DSL name	**2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]-**
National Chemical Inventories (NCI) names[1]	*1-(2,4-Dimethylphenylazo)napht-2-ol* (DSL) *1-(2,4-dimethylphenylazo)-2-naphthol* (EINECS) *1-(2,4-dimethylphenylazo)-2-naphtol* (EINECS) *Solvent Orange 7* (ENCS, PICCS) *1-[(2,4-Dimethylphenyl)azo]-2-naphthalenol* (ECL) *C.I. SOLVENT ORANGE 7, (SUNDAN RED)* (PICCS) *SUDAN RED* (PICCS)
Other names	*AF Red No. 5; Brasilazina Oil Scarlet 6G; C.I. 12140; C.I. Solvent Orange 7; Calco Oil Scarlet BL; Ceres Orange RR; Cerisol Scarlet G; Ext D and C Red No. 14; Fast Oil Orange II; Fat Scarlet 2G; FD and C Red No. 32; Grasan Orange 3R; Japan Red 5; Japan Red 505; Japan Red No.5; Lacquer Orange VR; NSC 10457; Oil Orange 2R; Oil Orange KB; Oil Orange N Extra; Oil Orange R; Oil Orange X; Oil Orange XO; Oil Red XO; Oil Scarlet; Oil Scarlet 371; Oil Scarlet 6; Oil Scarlet BL; Oil Scarlet YS; Red 505; Red No. 5; Resin Scarlet 2R; Somalia Orange 2R; Somalia Orange A 2R; Sudan 2; Sudan II; Sudan orange; Sudan Orange RPA; Sudan Orange RRA*
Chemical group	Azo compounds
Chemical sub-class	Monoazo compounds
Chemical formula	$C_{18}H_{16}N_2O$
Chemical structure	
SMILES[2]	Oc(ccc(c1ccc2)c2)c1N=Nc(c(cc(c3)C)C)c3
Molecular mass	276.34 g/mol

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

[2] Simplified Molecular Line Input Entry System

Table 1c. Substance identity for Solvent Red 3

Chemical Abstracts Service Registry Number (CAS RN)	**6535-42-8**
DSL name	**1-Naphthalenol, 4-[(4-ethoxyphenyl)azo]-**
National Chemical Inventories (NCI) names[1]	*Solvent Red 3* (ENCS, PICCS) *C.I. Solvent Red 003* (ECL) *C.I. Solvent Red 3, (1-NAPHTHALENOL, 4-[(4-ETHOXYPHENYL)AZO]-* (PICCS) *1-Naphthalenol, 4-[(4-ethoxyphenyl)azo]-* (TSCA, AICS, PICCS, ASIA-PAC) *4-[(4-ethoxyphenyl)azo]naphthol* (EINECS)
Other names	*C Ext. Brown 3; C.I. 12010; Ceres Brown B; Fat Brown B; Oil Brown PB; Oleal Brown 4BG; Orient Oil Brown BB* *4-[(4-Ethoxyphenyl)azo]-1-naphthol; C.I. Solvent Red 3; 4-[(4-ehoxyphenyl)azo]naphtol*
Chemical group	Azo compounds
Chemical sub-class	Monoazo compounds
Chemical formula	$C_{18}H_{16}N_2O_2$
Chemical structure	
SMILES[2]	O(c(ccc(N=Nc(c(c(c(O)c1)ccc2)c2)c1)c3)c3)CC
Molecular mass	294.34 g/mol

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

[2] Simplified Molecular Line Input Entry System

Physical and Chemical Properties

There are only limited experimental data available for these three monoazo solvent dyes.

At the Environment Canada-sponsored Quantitative Structure-Activity Relationship (QSAR) Workshop in 1999, invited modelling experts identified many structural classes of pigment and dyes as "difficult to model" using QSARs (Environment Canada 2000). The physical and chemical properties of many of the structural classes of dyes and pigments 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 of applicability of QSAR models to dyes and pigments are reviewed on a case-by-case basis.

It is generally considered inappropriate to use QSAR models to predict the physical and chemical properties of these three monoazo solvent dyes. Consequently, a number of analogues were identified and "read-across" data have 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.

To find acceptable analogues, a review of data for several 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 these three monoazo solvent dye, 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, solid particulate structures, decomposition at greater than 220 ^{o}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.

To predict environmental fate and effects of Solvent Red 1, Solvent Orange 7 and Solvent Red 3, experimental data for the following monoazo dyes were considered for this assessment:

- Disperse Orange 30 (for bioaccumulation prediction)
- Disperse Orange 30, Disperse Red 17, Disperse Red 73, Disperse Orange 25, and Disperse Yellow 3 (for inherent toxicity prediction)

These monoazo dyes were selected using a combination of criteria: structural similarity, similar key physical and chemical properties, and expert judgment. Although not all parameter values were available for each chemical, the available physical and chemical property values (see Table 2), empirical bioaccumulation data (see Table 6) and empirical toxicity data (see Table 7) for these dyes were used in support of the weight of evidence decisions in this screening assessment report. Key experimental studies with these monoazo dyes were critically reviewed for validity. The reviews (Robust Study Summaries) can be found in Appendix I.

Table 2 contains physical and chemical property values of Solvent Red 1, Solvent Orange 7 and Solvent Red 3 and the other azo chemicals mentioned above, which are relevant to assessing their environmental fate. Information in the table may be represented as 1) a range or single value for a specific substance or 2) a range of values from reading across the data for a series of like substances.

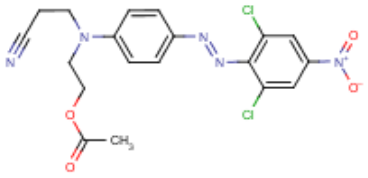
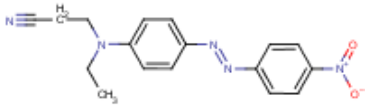
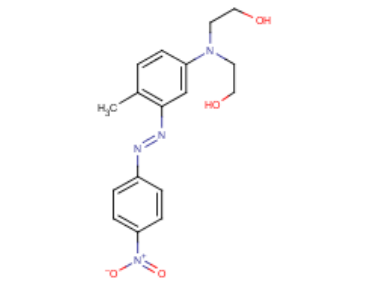
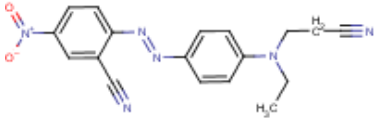
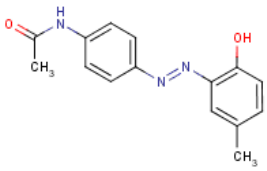
Table 2. Physical and chemical properties for Solvent Red 1, Solvent Orange 7, Solvent Red 3, Disperse Orange 30, and the "read-across" of azo substances

Chemicals	Type[1]	Value	Temperature (°C)	Reference
Melting point (ºC)[2]				
Solvent Red 1	Experimental	183.00	--	PhysProp 2006
Solvent Orange 7	Experimental	166.00	--	PhysProp 2006
Disperse Orange 30	Experimental	126.9–128.5		ETAD 2005
	Read-across for azo disperse dyes	117–225		Anliker and Moser 1987
	Read-across for azo dyes	74–236		Baughman and Perenich 1988
Boiling point (ºC)[3]				
Not applicable				
Vapour pressure (Pa)				
	Read-across for azo dyes	5.33×10^{-12} to 5.33×10^{-5} (4×10^{-14} to 4×10^{-7} mm Hg)	25	Baughman and Perenich 1988
Henry's Law constant ($Pa \cdot m^3/mol$)				
Solvent Orange 7	Experimental (derived)	2.78×10^{-6} (2.74×10^{-11} $atm \cdot m^3/mol$)	--	Hine and Mookerjee 1975
	Read-across for azo dyes[4]	10^{-8} to 10^{-1} (10^{-13} to 10^{-6} $atm \cdot m^3/mol$)		Baughman and Perenich 1988
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)				
Solvent Red 1	(derived from Disperse Orange 30)[5]	4.27		EPIWIN 2007
Solvent Orange 7	(derived from Disperse Orange 30)[5]	5.28		EPIWIN 2007
Solvent Red 3	(derived from Disperse Orange 30)[5]	4.06		EPIWIN 2007
Analogue (Disperse Orange 30)	Experimental	4.2		Brown 1992
	Read-across for azo dyes	2.05–4.2		Baughman and Perenich 1988
	Read-across for azo disperse dyes	> 2 – 5.1		Anliker et al. 1981 Anliker and Moser 1987
Log K_{oc} (Organic carbon-water partition coefficient) (dimensionless)				
	Read-across for azo dyes, calculated[6]	3.4–4.2		Baughman and Perenich 1988
Water solubility (mg/L)				
Solvent Red 1	Experimental	0.0003	15–25	Baughman and Weber 1991
Solvent Red 3	Experimental	< 1		Study Submission 2008
Analogue (Disperse	Experimental	0.07		Brown 1992

Orange 30)				
	Read-across for azo disperse dyes	< 0.01		Anliker and Moser 1987
	Read-across for azo dyes	1.2×10^{-5} to 35.5 (4×10^{-11} to 1.8×10^{-4} mol/L)		Baughman and Perenich 1988
n-octanol solubility (mg/L)				
Analogue (Disperse Orange 30)	Experimental	576		ETAD 2005
	Read-across for azo disperse dyes	81–2430	20	Anliker and Moser 1987
pK_a (Acid dissociation constant) (dimensionless)				
	Read-across for azo disperse dyes	8.1–13.5 (acid form)		ACD/pK_aDB 2005

[1] The extrapolated values used for the monoazo solvent dyes are based on available evidence from other dye analogues found in literature.
[2] The phrase "melting point" is used, but this may be better referred to as a decomposition point because dyes are known to char at high temperatures (greater than 200°C) rather than melt.
[3] Boiling point is generally not applicable for 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 azo 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 the monoazo solvent dyes.
[5] An experimental value adjustment method was applied using EPISUITE to derive a log Kow from an experimental measure, with consideration of the structural differences.
[6] 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.

Table 3a. Chemical structures and other information available for a few monoazo dyes

CAS RN (Common Name)	Structure of Analogue	Molecular Mass (g/mol)	Minimum-Maximum D_{max} (nm) [1]	Available Empirical Data
5261-31-4 (Disperse Orange 30)		450.28	1.75–1.98	Melting point, vapour pressure, log k_{ow}, water solubility, aquatic toxicity,
31482-56-1 (Disperse Orange 25)		323.35	1.37–1.95	Aquatic toxicity
3179-89-3 (Disperse Red 17)		344.36	1.41–1.86	Aquatic toxicity
16889-10-4 (Disperse Red 73)		348.36	1.31–1.93	Aquatic toxicity
2832-40-8 (Disperse Yellow 3)		269.31	1.59--1.90	Aquatic toxicity

[1] Based on range of maximum diameters (D_{max}) for conformers calculated using CPOPs (2008).

Structural comparisons between the three monoazo solvent dyes being assessed and the dyes listed in Table 3a are presented in Table 3b, below. The greater the percent of structural similarity between azo compounds, the more reliable the information may be to predict the environmental fate and aquatic toxicity. .

Table 3b. Structural comparisons between the three monoazo solvent dyes being assessed and Disperse Orange 30, Disperse Red 17, Disperse Red 73, Disperse Orange 25, and Disperse Yellow 3.

Monoazo Dyes	**% Similarity [1] (comparing to the monoazo dyes in the left column)**		
	Solvent Red 1	**Solvent Orange 7**	**Solvent Red 3**
5261-31-4 (Disperse Orange 30)	59.79 %	57.99 %	62.24 %
31482-56-1 (Disperse Orange 25)	71.97 %	69.01 %	74.17 %
3179-89-3 (Disperse Red 17)	69.64 %	68.83 %	71.08 %
16889-10-4 (Disperse Red 73)	67.06 %	66.27 %	69.80 %
2832-40-8 (Disperse Yellow 3)	76.64 %	77.36 %	76.61 %

[1] The structural similarities were calculated by Artificial Intelligence Expert System (AIES 2003-2005).

Sources

None of the three monoazo solvent dyes are naturally produced in the environment.

During development of the Domestic Substances List (DSL), the following quantities of the three monoazo solvent dyes were reported as being manufactured, imported or in commerce in Canada during the 1986 calendar year (Environment Canada 1988):

- Solvent Red 1: 1000–10 000 kg
- Solvent Orange 7: 1000–10 000 kg
- Solvent Red 3: 10 000–100 000 kg

Recent information was collected through an industry survey conducted for the 2005 and 2006 calendar years under *Canada Gazette* notices issued pursuant to section 71 of CEPA 1999 (Canada 2006b and Canada 2008). The notices required submission of data on the Canadian manufacture and import of the substance. In the notice for the 2006 survey, data were also required on the use quantities of these three monoazo solvent dyes.

For the 2005 calendar year, no manufacture of any of these three monoazo solvent dyes was reported above the 100 kg/year threshold, in response to a CEPA section 71 survey notice. However, one company reported importing between 100 and 1000 kg of Solvent Red 3 into Canada (Canada 2008).

For the 2006 calendar year, no manufacture or importing of any of these three monoazo solvent dyes, above the 100 kg/year threshold, was reported in response to a CEPA section 71 survey

notice (Canada 2008). In the Declaration of Stakeholder Interest form associated with the section 71 survey,

- two companies reported a stakeholder interest in Solvent Red 1;
- one company reported a stakeholder interest in Solvent Orange 7; and
- five companies reported a stakeholder interest in Solvent Red 3.

Given that no information on manufacture, import or use of these monoazo solvent dyes was reported for 2006, a mass of 100 kg was used throughout this screening assessment to build scenarios and conservatively capture the potential quantity of each dye in use in Canada below the threshold reporting value.

Solvent Orange 7 and Solvent Red 3 are in the European Inventory of Existing Commercial Chemical Substances (EINECS) but have not been reported by European Union industry as either high or low production volume chemicals (ESIS 2008). Solvent Red 1 has been identified as a low production volume (LPV) chemical, indicating that production within the European Union is estimated to be between 10 and 1000 tonnes per year (ESIS 2008). These three monoazo solvent dyes were used in Sweden, Denmark, Finland and Norway between 2000 and 2006. Use quantities of Solvent Red 1 in Denmark range from 5800 to 7100 kg and are unreported for the other countries and substances (SPIN 2008). In the United States, the national aggregate production volume for Solvent Orange 7 was 10 000–500 000 pounds in both the 1990 and 1994 reporting cycles under the US Environmental Protection Agency's Inventory Update Reporting Program. Reports were not available for the other substances and reporting cycles (1986, 1998 and 2002) (US EPA 2002).

Products containing these monoazo solvent dyes may enter the country even if they are not identified as such in the section 71 survey because they may be imported unknowingly in manufactured items, or in quantities below the 100-kg reporting threshold for the survey. Given the use of these substances in other countries, it is possible that the substances are entering the Canadian market as components of manufactured items and consumer products.

Uses

Information on uses for the 2005 and 2006 calendar years was gathered in response to the CEPA section 71 notices (Canada 2006b and 2008).

Solvent Red 1

No recent information on the use of this substance in Canada has been identified. The following DSL use codes were identified for the substance during the DSL nomination period (1984–1986): Colourant - pigment/stain/dye/ink; Formulation component; Pigment, Dye and Printing Ink; Textile, Primary Manufacture (Environment Canada 1988).

While there have been no reports of its current use in Canada, Solvent Red 1 may be used internationally to colour paints, printing inks, plastics, oils, fats, waxes, biological stains and smoke for military and other purposes (Biocompare 1999–2009; CII 2002; NLM 2006). The

use of Solvent Red 1 as a colorant in spices has also been reported; however this substance is currently not on the list of permitted food colorants in the European Union, the United States or Canada (ESA 2008; European Community 1994; Canada 2009; US FDA 2007). Solvent Red 1, also known as C.I. 12150, may be found in cosmetic products including lip balm (CII 2002; TheFind c2007–2008); however, Solvent Red 1 has been banned for use in cosmetics or hair dyes in the European Union owing to a lack of available safety data and is not on the list of approved colour additives for cosmetics in the United States (EU 2005, EU 2008a, EC 2006, US FDA 2007).

Solvent Orange 7

No recent information on the use of this substance in Canada has been identified. The following DSL use codes were identified for the substance during the DSL nomination (1984–1986): Fragrance/perfume/deodorizer/flavouring agent; Lubricating agent/lubricant additive/mould release agent; Textile, Primary Manufacture (Environment Canada 1988).

While there have been no reports of its current use in Canada, Solvent Orange 7 may be used internationally to colour oils, fats, waxes, candles, inks, soaps, detergents, plastics, polystyrene (CII 2002) and biological stains (Premier Diagnostics 2001). In the United States, Solvent Orange 7 was previously approved for use in food (under the name FD&C Red No. 32) as well as drugs and cosmetics for external use (Ext. D&C Red No. 14); however these permitted uses were delisted in 1958 and 1966, respectively (Marmion 2007; US FDA 2003). Currently Solvent Orange 7 is not a permitted food or cosmetic colorant in the European Union (ESA 2008; EU 2008a).

Solvent Red 3

No recent information on the use of this substance in Canada has been identified. The following DSL use codes were identified for the substance during the DSL nomination (1984–1986): Colourant - pigment/stain/dye/ink; Fragrance/perfume/deodorizer/flavouring agent; Pigment, Dye and Printing Ink; Soap and Cleaning Products; Textile, Primary Manufacture (Environment Canada 1988).

While there have been no reports of its current use in Canada, Solvent Red 3 may be used internationally in plastics, inks, petroleum and fat products (CII 2002). Use of Solvent Red 3 in lubricants, including gear oil, has been reported in Norway (SPIN 2008). Solvent Red 3 may have been previously used in hair dyes in Europe; however, this use of Solvent Red 3 was prohibited in the European Union on September 23, 2008 owing to a lack of available safety data (EU 2008b).

Releases to the Environment

Mass Flow

Empirical data concerning releases of specific substances to the environment are seldom available. Therefore, to estimate potential releases of a substance to the environment at different stages of its life cycle, a Mass Flow Tool was developed (Environment Canada 2008a). For each identified type of use of the substance, the proportion and quantity of release to the different environmental media are estimated, as is 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 off-site releases to the environment from waste disposal sites.

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 Organisation for Economic Co-operation 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.

Since there were no reports of use, import or manufacture of Solvent Red 1, Solvent Orange 7 or Solvent Red 3 in Canada in 2006 at or above the 100 kg reporting thresholds specified in the CEPA section 71 notice (Environment Canada 2006), releases of these substances to the Canadian environment were expected to be very low. The Mass Flow Tool was nevertheless applied to estimate the fraction of these monoazo solvent dyes that could be released to the environment. Although there is uncertainty about the extent of current use in textile applications, this use has been assumed for Mass Flow Tool calculations, because it is considered to represent a reasonable worst-case (relatively high release) scenario for these monoazo solvent dyes.

Based on Statistics Canada information and an analysis by Industry Canada (2008), it is recognized that dyes may be imported in manufactured articles. Following this proposal, a ratio of the amount of textiles manufactured in Canada relative to the amount of imported textiles of 30:70 has been used to estimate the amount of dye imported in finished textiles (Industry Canada 2008; Environment Canada 2008b). This import quantity was included in the Mass Flow Tool calculations as well as in the exposure scenarios.

Table 4. Estimated releases and losses of azo dyes to environmental media, chemical transformation during life cycle and transfer to waste disposal sites, based on the Mass Flow Tool.

Fate	Proportion of the Mass (%)[1]	Major Life Cycle Stage Involved[2]
Releases to receiving media:		
To soil	0.0	n/a[3]
To air	0.0	n/a
To sewer[4]	17.4	Formulation, consumer use
Chemically transformed	0.0	n/a
Transferred to waste disposal sites (e.g., landfill, incineration)	82.6	Formulation, waste disposal

[1] For azo dyes, 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: Textile manufacturing wool mills (OECD 2004); and Adhesive formulation (OECD 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 from the Mass Flow Tool indicate that these three monoazo solvent dyes can be expected to be found largely in waste management sites (82.6%), due to the eventual disposal of manufactured items containing them. No information of any kind has been identified on the rate or potential for release of any of these substances, therefore the Mass Flow Tool calculations can not quantitatively account for the substances that may be released to the environment from waste disposal sites (such as landfills and incinerators).

Based largely on information contained in OECD emission scenario documents for processing and uses associated with this type of substance, it is estimated that 17.4% of these three monoazo solvent dyes may be released to sewers.

Based on the above Mass Flow Tool estimation, sewer water is the medium receiving the greatest proportion of these three monoazo solvent dyes emitted during product processing and use.

Environmental Fate

As indicated by the results of the Mass Flow Tool (Table 4), these three monoazo solvent dyes would be expected to be released to wastewater effluents during industrial processing and down-the-drain uses. The high log K_{ow} values (modelled data of 4.1 to 5.3 for three monoazo solvent dyes, 4.2 for Disperse Orange 30, and 2 to 5.1 for read across) and high log K_{oc} values (read-across of 3.4 to 4.2) (see Table 2) indicate that these three monoazo solvent dyes would have affinity for solids. However, the log K_{oc} is a calculated value (see footnote 3 below Table

2) and the adsorption potential of particulate dye structures is generally not well understood; therefore the degree to which this particular behaviour applies to the monoazo solvent dyes is uncertain.

According to aerobic biodegradation models, these three monoazo dyes are expected to biodegrade slowly (see Table 5 below). These substances may be applied to agricultural soils and pasture lands in Canada as a component of biosludge which is commonly used for soil enrichment (Environment Canada 2006). Moreover, they may also be released from coloured products deposited in landfills.

Given a pKa range from 8.1 to 13.5 (acid form; read-across of azo disperse dyes), the expected low water solubility of these three monoazo solvent dyes (Table 5) , and the particulate state, it is unlikely that ionization will have a significant impact on the partitioning or water solubilities of these substances. Instead, when released into water, these three monoazo solvent dyes are expected to be mostly present as a particulate solid or adsorbed to suspended particles and eventually sink to surface bed sediments where they are expected to remain in a relatively biologically unavailable form. 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, shallow aquifers and in groundwater.

The rate of volatilization from the surface of water is proportional to the Henry's Law constant (Baughman and Perenich 1988). Baughman and Perenich (1988) stated that volatilization from aquatic systems would not be an important loss process for dyes, which agreed with the low to negligible experimental data (2.78×10^{-6} Pa•m^3/mol for Solvent Orange 7) and read-across Henry's Law constant value (10^{-8} to 10^{-1} Pa•m^3/mol, Table 5). Transport in air due to the loss of these substances from moist and dry soil surfaces is not likely to be important, as indicated by very low read-across vapour pressures for azo dyes (5.33×10^{-12} to 5.33×10^{-5} Pa) (Table 5). These data are consistent with the physical state (solid particle) of these three monoazo solvent dyes, which makes them unlikely candidates for volatilization.

Persistence and Bioaccumulation Potential

Environmental Persistence

No experimental degradation data for these three monoazo solvent dyes 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 1996) have confirmed this for other dye chemicals (Pagga and Brown 1986; ETAD 1992). Based on the chemical structure of these three monoazo solvent dyes, there is no reason to suspect that their biodegradation will be other than that of dyes generally (ETAD 1995).

Solvent 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 vary 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 are likely to undergo degradation to substituted aromatic amine constituents. However, in anoxic sediment these biodegradation transformation products are not expected to present a high degree of exposure potential to most aquatic and benthic organisms, and therefore they are not likely to present a signifiicant ecological concern.

Given the expected release of these three monoazo solvent dyes into wastewater, persistence in water was primarily examined using predictive QSAR models for aerobic biodegradation. These models are considered acceptable for use in this situation as they are based on chemical structure and the monoazo structure is represented in the training sets of all the BIOWIN models used, thereby increasing the reliability of the predictions (Environment Canada 2007). The following analysis applies primarily to the portion of a substance that is present in the environment in the dissolved form, recognizing that the majority would likely exist in dispersed form as solid particles. These three monoazo solvent dyes do 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 degradation of three monoazo solvent dyes in water.

Table 5. Modelled data for aerobic biodegradation of Solvent Red 1, Solvent Orange 7 and Solvent Red 3 in water

Fate Process	Model and Model Basis	Model Output	Expected Half-life (days)
WATER			
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 3: Expert Survey (ultimate biodegradation)	2.19–2.28 (biodegrades relatively slowly)	> 182
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 5: MITI linear probability	0.07–0.19 (biodegrades very slowly)	> 182
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 6: MITI non-linear probability	0.0 (biodegrades very slowly)	> 182
Biodegradation (aerobic)	CATABOL c2004–2008 % BOD (biological oxygen demand)	0 (biodegrades very slowly)	> 182

The results in Table 5 for the aerobic biodegradation models BIOWIN 3, 5, 6 and CATABOL, suggest that all three of these monoazo solvent dyes biodegrade slowly with a half-life that is likely to be greater than 182 days. Both of the BIOWIN 5 and 6 probability results are much less than 0.3, the cut-off suggested by Aronson et al. (2006) to identify substances as having a half-life > 60 days (based on the MITI probability models). Furthermore, both of the other

ultimate degradation models, BIOWIN3 and CATABOL, predict that these dyes will degrade slowly in water.

When the results of the probability and the other degradation models are considered, there is model consensus suggesting that the ultimate biodegradation half-life in water is > 182 days. This finding is consistent with what would be expected for these chemical structures (i.e., few degradable functional groups, solid sparingly soluble particle).

Using an extrapolation ratio of 1:1:4 for a water:soil:sediment biodegradation half-life (Boethling et al. 1995), the ultimate degradation half-life in aerobic soil should be > 182 days and the half-life in aerobic sediments should be > 365 days. This suggests that these three monoazo solvent dyes are expected to be persistent in soil and sediment.

Based on modelled ultimate degradation data (Table 5) and expert judgment (ETAD 1995), it is concluded that these three monoazo solvent dyes meet the persistence criteria in water, soil and sediment (half-lives in soil and water ≥ 182 days and half-life in sediment ≥ 365 days) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

No experimental bioaccumulation experimental data are available for any of these three monoazo solvent dyes.

Many water insoluble dye classes, including solvent azo dyes, are considered difficult to model and thus the results are generally unreliable. Predicted and/or empirically determined properties of dyes related to bioaccumulation (e.g., log K_{ow}) can be of uncertain relevance or associated with a high degree of error, which reduces the utility of model predictions of BCF and BAF. In addition, monoazo solvent dyes generally fall outside of bioaccumulation model domains of applicability. As a result, in this assessment, bioaccumulation modelling has not been used to evaluate the bioaccumulation potentials of Solvent Red 1, Solvent Orange 7 or Solvent Red 3.

In this case, Disperse Orange 30 was considered as an acceptable surrogate for assessing the bioaccumulation potential of the monoazo dyes. The structural differences between three monoazo solvent dyes and Disperse Orange 30 have been noted (see Tables 2 and 3). However because of the physical and chemical property similarities among monoazo dyes, some structural difference is not anticipated to result in significant variation in the environmental behaviour of these particulate substances. Furthermore, using an experimental value adjustment method in the KOWWIN model of EPISUITE, these three monoazo solvent dyes were estimated to have modelled log Kow values (4.27 for Solvent Red 1; 5.28 for Solvent Orange 7; 4.06 for Solvent Red 3), which are relatively close to the experimental value of Disperse Orange 30 (4.2). Therefore, in the absence of substance-specific experimental and applicable modelled data, the empirical bioconcentration factors (BCFs) for Disperse Orange 30 were used to predict bioaccumulation potentials of these three monoazo solvent dyes.

A bioconcentration study submitted for Disperse Orange 30 suggests that it is unlikely to accumulate in fish (Shen and Hu 2008). This test was performed according to OECD guidelines (OECD 1996). 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 a 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 Day 26 to Day 28 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 concentrations of Disperse Orange 30, fish lipid content and BCF calculation

		Sampling Time		
		Day 26	Day 27	Day 28
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 is considered acceptable (see Appendix 1). The very low level 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 "true" value is not known. But given the structure and likely behavior of these three monoazo solvent dyes and Disperse Orange 30 in aqueous systems, the low BCF result is expected.

Most hydrophobic dyes exist as fine dispersible particles with limited truly soluble fractions. Solubility, however, can be increased by adding polar (especially ionic) functional groups to the molecule. While these monoazo dyes contain some of these solubilizing functional groups (phenol groups), available pKa estimates suggest that significant ionization will not occur under typical conditions in surface waters (pH 6–8). Assuming that the concentration in solution in the test was equal to the lower bound of the measured concentration in water (i.e.,

0.028 mg/L), and using the highest fish concentration of 0.81 mg/kg, the BCF may be conservatively estimated to be < 100.

While the above study serves as primary evidence to indicate that these monoazo solvent dyes lack 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 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 these monoazo solvent dyes. However, follow-up studies, which provided the chemical structures for the disperse dyes tested, confirmed low bioaccumulation potential for ten nitro-substituted azo 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 RNs 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.

High modelled log K_{ow} values for Solvent Red 1 (4.27), Solvent Orange 7 (5.28), Solvent Red 3 (4.06), and the read-across for the azo dyes (2~5.1) (Table 5) are the only line of evidence that suggests these 3 monoazo solvent dyes may have a high potential for bioaccumulation. In spite of the high K_{ow} values for Disperse Orange 30 and the other azo compounds, evidence for bioaccumulation of disperse azo dyes is lacking (Anliker et al. 1981; Anliker and Moser 1987; Anliker et al. 1988; MITI 1992). Authors who have measured high log K_{ow}s and concomitant low bioaccumulation factors for disperse azo dyes suggest that the low accumulation factors may be due to their low absolute fat solubility (Brown 1987) or relatively high molecular weight, 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, 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.

These three monoazo solvent dyes have molecular weights less than 300 g/mol, indicating that they may have some potential for bioaccumulation. However, the cross-sectional diameters

(1.35 to 1.73 nm) suggest that a potential for a significantly reduced uptake rate from water and reduced in vivo bioavailability exists with these dyes.

Based on bioconcentration tests with azo substances that showed a lack of observed accumulation, as well as on the large molecular sizes of the three monoazo solvent dyes (cross-sectional diameters of 1.35 to 1.73 nm) that likely limit their partitioning behaviour, these substances are expected to have low potentials for bioaccumulation. It is therefore concluded that Solvent Red 1, Solvent Orange 7 and Solvent Red 3 do not meet the bioaccumulation criteria (BCF, BAF $\geq$ 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

There are no experimental data available for aquatic toxicity for any of these three monoazo solvent dyes; hence the assessment of ecological effects was based on the empirical data for Disperse Orange 30, with consideration of toxicity data for some other monoazo substances (see Table 3).

A study submitted on behalf of ETAD provides acute ecotoxicity data in fish, invertebrates, algae and bacteria for Disperse Orange 30 (Brown 1992). A 96-hour LC_{50} of 710 mg/L for zebra fish, a 48-hour EC_{50} of 5.8 mg/L for *Daphnia magna*, and a 72-hour EC_{50} (for growth) of 6.7 mg/L for *Scenedesmus subspicatus* have been reported based on toxicity studies using Disperse Orange 30 (Table 7a). However, the original studies have not been provided to allow verification of their reliability.

Another result for Disperse Orange 30 was submitted to Environment Canada as a voluntary data submission. An LC_{50} for rainbow trout (*Oncorhynchus mykiss*) was established as > 700mg/L (Sandoz 1975). An evaluation was conducted based on the robust study summary provided in the submission and it was concluded that the study (Sandoz 1975) was unacceptable (see Appendix 1).

An experimental study on the toxicity of an effluent containing Disperse Orange 30 reported an LC_{50} (48 hours) for mysid shrimp when the whole effluent is diluted by 46% (Reife 1989). However this study did not present the LC_{50} as a concentration of Disperse Orange 30 and therefore these results could not be included in Table 7a or used in the risk quotient analysis.

An acute toxicity study with Disperse Orange 30 using rainbow trout was submitted to Environment Canada (Table 7a) (Safepharm Laboratories Ltd. 1990). An assessment of the reliability of the study using a robust study summary was conducted and 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 Orange 30

Test Organism	Type of Test	Duration (hours)	Endpoint	Reliability of the Study	Value (mg/L)	Reference
Rainbow trout	Acute	48	LC_{50}[1]	Unacceptable	> 700	Sandoz 1975
Rainbow trout	Acute	96	LC_{50}	Low confidence	> 100	Safepharm Laboratories Ltd 1990
Zebra fish	Acute	96	LC_{50}	Not Available	710	Brown 1992
Daphnia magna	Acute	48	EC_{50}[2]	Not Available	5.8	
Scenedesmus subspicatus	Acute	72	EC_{50}	Not Available	6.7	
Bacteria	Acute	n/a	IC_{50}[3]	Not Available	> 100	

[1] LC_{50} – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.
[2] EC_{50} – The concentration of a substance that is estimated to cause some toxic sublethal effect on 50% of the test organisms.
[3] IC_{50} – The concentration of a substance that is estimated to cause inhibition to growth 50% of the test organisms.

Ecotoxicological data for a disperse azo dye was received through the *New Substance Notification Regulations* (Environment Canada 1995). The notified substance had the molecular weight (471.46) and the chemical structure similar to Disperse Orange 30. Ecotoxicological data were provided with this notification. The results for the 96-hr static toxicity test with rainbow trout revealed that the LC_{50} 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 activated sludge respiration inhibition EC_{50} > 1000 mg/L (Table 7b). 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. Aquatic toxicity data for four of the monoazo chemicals listed in Tables 3a and 3b are presented in Table 7b below.

In this study there were some disperse dyes (non-azo compounds) which had toxicity levels reported as < 1mg/L for algae. However it was reported by Brown (1992) that algae growth inhibition was due largely to light absorption by the dyes rather than as a result of chemical activity. 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 as part of the weight of evidence as they are in agreement with other data and concur with the expected range of ecotoxicity values for these structures.

Table 7b. Empirical data for aquatic toxicity of other monoazo substances

Chemical	Test Organism	Endpoint	Value (mg/L)	Reference
Analogous disperse azo dye	Rainbow trout	LC_{50}[1]	505	Environment Canada 1995
	Bacteria	EC_{50}[2]	> 100	
Disperse Red 73	Zebra fish	LC_{50}	17	Brown 1992
	Daphnia magna	EC_{50}	23	
	Scenedesmus subspicatus	EC_{50}	> 10	
	Bacteria	IC_{50}[3]	> 100	
Disperse Red 17	Zebra fish	IC_{50}	103	Brown 1992
	Daphnia magna	LC_{50}	98	
	Scenedesmus subspicatus	EC_{50}	7	
	Bacteria	EC_{50}	> 100	
Disperse Orange 25	Zebra fish	IC_{50}	268	Brown 1992
	Daphnia magna	LC_{50}	110	
	Scenedesmus subspicatus	EC_{50}	54	
	Bacteria	EC_{50}	> 100	
Disperse Yellow 3	Fathead minnow	LC_{50}	> 180	Little and Lamb 1973

[1] LC_{50} − The concentration of a substance that is estimated to be lethal to 50% of the test organisms.
[2] EC_{50} − The concentration of a substance that is estimated to cause some toxic sublethal effect on 50% of the test organisms.
[3] IC_{50} − The concentration of a substance that is estimated to cause inhibition to growth on 50% of the test organisms.

In general, due to their very low water 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 Orange 30 and several similar analogues are consistent with this expectation, indicating EC_{50s}/LC_{50}s in the 5.8–710 mg/L range, with *Daphnia magna* being the most sensitive organisms tested (EC_{50}s/LC_{50}s from 5.8 to 100mg/L). Although interpretation of results from these tests is complicated by the fact that the reported effect values (i.e., EC_{50}s and LC_{50}s) are likely to be much greater than the solubility of the substances tested and are likely the result of "indirect" toxic effects, the analogue data available do indicate that the toxicity of the three monoazo solvent dyes being assessed is likely to be low.

A range of aquatic toxicity predictions for the three monoazo solvent dyes being assessed and analogues were also obtained from QSAR models. However, as with bioaccumulation, these QSAR ecotoxicity predictions for these dyes are not considered reliable because of the potential error associated with input parameters and the unique nature of both disperse and solvent dyes, such as physical state, structural and/or physical and chemical properties which fall outside of the models' domain of applicability.

The available empirical ecotoxicity information from Disperse Orange 30 and a few other monoazo substances indicates that Solvent Red 1, Solvent Orange 7, and Solvent Red 3 are not likely to be highly hazardous to aquatic organisms.

B - In Other Environmental Compartments

Since these three monoazo solvent dyes are expected to accumulate in sediment and 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 these solvent dyes, it would be desirable to have toxicity data for sediment and soil organisms. However, no suitable ecological effects studies were found for these chemicals in media other than water. The toxicity potential is also likely to be low in sediment- and soil-dwelling species, however, considering the lack of bioaccumulation potential and bioavailability as well as the physical and chemical makeup of these three monoazo solvent dyes, although this cannot be substantiated due to lack of suitable whole organism toxicity data.

Ecological Exposure Assessment

No data concerning concentrations of these three monoazo solvent dyes in water in Canada have been identified. Environmental concentrations are, therefore, estimated from available information, including estimated substance quantities (using the reporting threshold quantities of 100 kg), release rates and characteristics of receiving water bodies.

The Mass Flow Tool identified releases to water (sewer) from formulation use and from consumer use of products containing these substances (Table 4). To address releases from industrial activities, Environment Canada's Industrial Generic Exposure Tool – Aquatic (IGETA) was applied to estimate a conservative substance concentration of 0.0020 mg/L in a generic watercourse receiving industrial effluents (Environment Canada 2008c). The generic scenario is designed to provide these estimates based on conservative assumptions regarding the amount of chemical processed and released, the number of processing days, the sewage treatment plant removal rate, and the size of the receiving watercourse. The tool models an industrial-release scenario based on loading data, from sources such as industrial surveys and knowledge of the distribution of industrial discharges in the country, and calculates a predicted environmental concentration (PEC).

The PEC for all three monoazo solvent dyes was calculated based on a use quantity of 100 kg of each substance for a single facility (this corresponds to the reporting threshold for the section 71 notice, which was not met by any reporter in 2006). To make the assessment more conservative and to account for potential additive releases from industrial facilities located in the same area and releasing through a single sewage treatment plant (STP), quantities of these three monoazo solvent dyes were added; therefore a cumulative use quantity of 300 kg was used for modelling. The cumulative release quantity was estimated with IGETA, where it was assumed that 16% was being released over a period of 250 days (to represent industrial activities on an annual basis), with primary removal rate at an STP of 60% and release into a small receiving watercourse with a flow of 0.4 m^3/s. The equation and inputs used to calculate the PEC in the receiving watercourse are described in Environment Canada (2008d).

As these monoazo solvent dyes can be found in consumer products, Mega Flush, Environment Canada's spreadsheet model for estimating down-the-drain releases from consumer uses, was applied to estimate the potential substance concentration in multiple water bodies receiving

sewage treatment plant effluents to which 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 substance(s) used and released by consumers.

A scenario was run assuming a total consumer use quantity of 1000 kg/year (representing the cumulative quantity of these three monoazo solvent dyes at the reporting threshold of 300 kg as the cumulative use quantity and taking into consideration the ratio of 30/70 of textiles manufactured in Canada / imported textiles, assuming that all 300 kg could be used in the colouring sector. All other default parameters were used for this scenario. The overall effect of these parameters is to make this scenario conservative.

Characterization of Ecological Risk

The approach taken in this ecological screening assessment was to examine available scientific information and develop conclusions based on a weight-of-evidence approach and precaution as required under CEPA 1999.

Based on the available information, these three monoazo solvent dyes are predicted to be persistent in water, soil and sediment but are expected to have low bioaccumulation potential. The lack of reports of manufacture and the likely very low importation quantities of these substances into Canada, along with information on physical and chemical properties indicate a low potential for releases into the Canadian environment. If released into the environment, it is expected that these substances will be mainly discharged to surface waters where ultimately they are expected to be transferred to sediment.

Based on the toxicity data of other monoazo dyes, Solvent Red 1, Solvent Orange 7, and Solvent Red 3 are also expected to have only moderate potential for acute toxicity to aquatic organisms.

A predicted no-effect concentration (PNEC) was estimated based on the lowest nominal acute effect concentration (EC_{50}) for Disperse Orange 30 (see Table 7a). The critical toxicity value was the 96-hour EC_{50} to *D. magna* for Disperse Orange 30 of 5.8 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 for these three monoazo solvent dyes is 0.058 mg/L.

When compared to the conservative cumulative PEC calculated above using IGETA, the resulting risk quotient for industrial discharges (PEC/PNEC) is 0.0020/0.058 = 0.035. Therefore, concentrations of any of these three monoazo solvent dyes in surface waters in Canada appear unlikely to cause adverse effects on populations of aquatic organisms. Given that IGETA provides a conservative estimate of exposure, the results indicate a low potential for ecological harm resulting from local exposure to a point source industrial release

For exposure resulting from down-the-drain releases through consumer uses (conservative scenario), Mega Flush results estimate that the cumulative PEC will not exceed the PNEC at any sites (i.e., all risk quotients < 1) (Environment Canada 2008f). This indicates that down-the-drain consumer releases of these three monoazo solvent dyes combined are not expected to cause harm to aquatic organisms.

Therefore these substances are unlikely to be causing ecological harm in Canada.

Uncertainties in Evaluation of Ecological Risk

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 biodegradation model outputs confirmed that these three monoazo solvent dyes are not likely to biodegrade quickly, and meet the persistence criteria as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000). 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) could be biologically available. Although the degradation products are not expected to be biologically available because they form only in relatively deep anoxic sediment, this issue is a source of uncertainty in the toxicity assessment of these three monoazo solvent dyes.

An area of uncertainty for these three monoazo solvent dyes is associated with the use of "read-across" physical and chemical properties as well as toxicity data from analogues. While the chemicals identified (Disperse Orange 30, Disperse Orange 25, Disperse Red 17, Disperse Red 73 and Disperse Yellow 3), share many similarities with these three monoazo solvent dyes, including being azo dyes with high molecular weights, having solid particulate structures that decompose at greater than 220 ^{o}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 these three monoazo solvent dyes 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 these three monoazo solvent dyes.

Uncertainties are also present due to the lack of information on environmental concentrations in Canada for these three monoazo solvent dyes. However the lack of reports of manufacturing and import into Canada, expected high fixation rates during industrial processing and the anticipated high removal rate in wastewater treatment plants suggests low releases of these substances into the Canadian environment. When developing the exposure scenarios, assumptions about their applications were based on reported DSL use codes as well as the traditional uses of solvent dyes. Among a variety of potential uses, the application with the greatest potential for releases to the environment (i.e., textile manufacturing) was chosen for predicting the environmental concentrations of these three monoazo solvent dyes in the assessment.

Uncertainties are also associated with the fraction of the substances that is assumed to be released during use (i.e., during industrial activities and use of consumer products). These

uncertainties were addressed by making conservative assumptions in each of the modelling exercises.

The lack of experimental toxicity data for aquatic organisms is an additional source of uncertainty. Based on the available data of an analogue and low water solubilities, these three monoazo solvent dyes are not highly hazardous to aquatic organisms.

Also, regarding ecotoxicity, based on the predicted partitioning behaviour of the dyes, 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, although the water column may not be the medium of primary long-term concern based on partitioning estimates.

Potential to Cause Harm to Human Health

Some of the substances in this group of monoazo dyes have been subjected to controls in other jurisdictions, based on concern for their hazardous properties (e.g., carcinogenicity, genotoxicity). Although data is not comprehensive for each substance, given the similarities in chemical structures, it is considered likely that Solvent Orange 7, Solvent Red 1 and Solvent Red 3 would exhibit similar toxicological properties, i.e., undergo enzymatic reductive cleavage into component aromatic amine metabolites which have carcinogenic and genotoxic properties (Chen, 2006, Xu et al., 2007).

However, based on the results of a survey under section 71 of CEPA 1999, Solvent Orange 7, Solvent Red 1 and Solvent Red 3 are not believed to be manufactured in or imported into Canada in quantities above the reporting limits. Therefore, the likelihood of exposure in Canada is considered to be small; hence the risk to human health is likewise considered to be low.

Conclusion

Based on the information presented in this screening assessment, it is concluded that Solvent Red 1, Solvent Orange 7 and Solvent Red 3 are not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity or that constitute or may constitute a danger to the environment on which life depends.

Although the potential high hazard of Solvent Orange 7, Solvent Red 1 and Solvent Red 3 is recognized, on the basis of information which indicates that the substances are not manufactured in or imported into Canada in amounts above the reporting threshold, it is concluded that they are substances that are not entering the environment in a quantity or concentration or under conditions that constitute a danger in Canada to human life or health.

It is concluded that Solvent Red 1, Solvent Orange 7 and Solvent Red 3 do not meet the definition of toxic as set out in section 64 of CEPA 1999. These dyes meet the criteria for persistence but do not meet the criteria for bioaccumulation as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Considerations For Follow-up

In light of the potential high hazard of substances which metabolize to aromatic amines that may be of concern for carcinogenicity, including these substances, additional activity (e.g., research, monitoring and surveillance, assessment) to characterize the risk to human health in Canada of this broader group will be undertaken.

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Appendix I - Robust Study Summaries for key studies

There are limited experimental data for Solvent Red 1, Solvent Orange 7 and Solvent Red 3. Robust study summaries for the other monoazo dyes referred in the assessment are provided as follows.

Robust Study Summaries Form and Instructions: Aquatic B				
No	**Item**	**Weight**	**Yes/No**	**Specify**
1	**Reference:** Shen G, Hu S. 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	not applicable[1]	Y	5261-31-4
3	Substance identity: chemical name(s)	not applicable	Y	Propanenitrile, 3-[[2-(acetyloxy)ethyl][4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]amino]-
4	Chemical composition of the substance	not applicable		
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?	not applicable		No Radiolabelled test substance was used in the study.
	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 a nonstandard method was used	not applicable		OECD standard method was used as identified in item 9.
11	GLP (good laboratory practice)	3	N	
	Test organism			
12	Organism identity: name	not applicable	Y	*zebra fish, Brachydanio rerio*
13	Latin or both Latin and 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 +/- 0.18 cm and mean body weight 0.32 +/-0.06 g
16	Sex	1	N	
17	Number of organisms per replicate	1	Y	7
18	Organism loading rate	1	Y	20 mg/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)	not applicable	Y	Laboratory
21	Exposure pathways (food, water, both)	not applicable	Y	Water
22	Exposure duration	not	Y	28 days

		applicable		
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 was 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	Water concentration < 0.028 mg/L; Organism concentration < 0.82 mg/kg-bw
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 metal toxicity - pH, DOC/TOC, water hardness, temperature)	3	Y	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?	not applicable		Solubilizer was not used in the study.
	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)?	not applicable		No Radiolabelled test substance was used in the study.
	Results			
43	Endpoints (BAF, BCF) and values	not applicable	Y	BCF < 100
44	Was 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?	not applicable	Y	Method 1
45	Was BAF/BCF derived from a 1) tissue sample or 2) whole organism?	not applicable	Y	Method 2

46	Was 1) average or 2) maximum BAF/BCF used?	not applicable	Y	Method 1
47	***Score*: %**	***36/46 x 100 = 78.26***		
48	***EC reliability code*:**	***2***		
49	***Reliability category (high, satisfactory, low)*:**	***Satisfactory***		
50	***Comments***	*The present procedure is based on semi-static conditions (renewal of test solutions every 2 days). Therefore, test chemicals with very low water solubility, such as Disperse Orange 30, can also be characterized as to their bioconcentration potential without adding solvents or other auxiliary substances which may affect the results.*		

[1] Not applicable – this information may or may not have been provided in the study, however it is not accounted into the total weight for the robust study summary, or not considered due to the other similar consideration in the same category.

Robust Study Summary Form: Aquatic iT				
No	**Item**	**Weight**	**Yes/No**	**Specify**
1	Reference: Sandoz 1975. Data for Batch 5 substances collected under the Canadian Environmental Protection Act, 1999, Section 71: *Notice with respect to certain Batch 5 Challenge substances.* Submitted to Environment Canada. Submission ID: #157 - Acute fish tox (Rainbow trout) 48 hr			
2	Substance identity: CAS RN	not applicable[1]	Y	5261-31-4
3	Substance identity: chemical name(s)	not applicable	Y	
4	Chemical composition of the substance	not applicable		
5	Chemical purity	1	N	
6	Persistence/stability of test substance in aquatic solution reported?	1	N	
Method				
7	Reference	1	Y	See item 9
8	OECD, EU, national, or other standard method?	not applicable		The modified method was used in the study.
9	Justification of the method/protocol if a nonstandard method was used	2	Y	Modified Routine Bioassay Method
10	GLP (good laboratory practice)	3	N	
Test organism				
11	Organism identity: name	not applicable	Y	*Rainbow trout, Salmo giardneri*
12	Latin or both Latin and common names reported?	1	Y	Both
13	Life cycle age / stage of test organism	1	N	
14	Length and/or weight	1	Y	70 mm and 3 g
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)	not applicable	Y	Acute
20	Experiment type (laboratory or field)	not applicable	Y	Laboratory
21	Exposure pathways (food, water, both)	not applicable	Y	Water
22	Exposure duration	not applicable	Y	48-hrs
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	
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 metal toxicity - pH,	3	N	

	DOC/TOC, water hardness, temperature)			
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?	not applicable		
34	If solubilizer/emulsifier was used, was its ecotoxicity reported?	not applicable		
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 the organism's health (e.g., when mortality in the control > 10%) or physical effects (e.g., "shading effect")?	not applicable		
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	Y	20°C
43	Was toxicity value below the chemical's water solubility?	3	N	
Results				
44	Toxicity values (specify endpoint and value)	not applicable	Y	48-hr LC_{50} > 700 mg/L. This value shall be interpreted as the loading rate.
45	Other endpoints reported - e.g., BCF/BAF, LOEC/NOEC (specify)?	not applicable	N	
46	Other adverse effects (e.g., carcinogenicity, mutagenicity) reported?	not applicable	N	
47	***Score*: %**		***9/42 x 100 = 21.43***	
48	***EC reliability code*:**		***4***	
49	***Reliability category (high, satisfactory, low)*:**		***Low***	
50	***Comments***			

[1] Not applicable – this information may or may be provided in the study, however it does not contribute in the total weight accounted for the robust study summary, or not considered due to the other similar consideration in the same category.

Robust Study Summary Form: Aquatic iT				
No	**Item**	**Weight**	**Yes/No**	**Specify**
1	Reference: Environment Canada. 1995. New Substances Notification submission. NSN#: 3791			
2	Substance identity: CAS RN	not applicable	Y	Confidential information
3	Substance identity: chemical name(s)	not applicable	Y	
4	Chemical composition of the substance	not applicable		
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	OECD
9	Justification of the method/protocol if a nonstandard method was used	not applicable		OECD standard method was used in the study,
10	GLP (good laboratory practice)	3	Y	
Test organism				
11	Organism identity: name	not applicable	Y	*Rainbow trout*
12	Latin or both Latin and common names reported?	1	Y	
13	Life cycle age / stage of test organism	1	Y	Mean length 51 mm and mean weight 1.54 g
14	Length and/or weight	1	Y	See above
15	Sex	1	N	
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)	not applicable	Y	Acute
20	Experiment type (laboratory or field)	not applicable	y	Laboratory
21	Exposure pathways (food, water, both)	not applicable	y	Water
22	Exposure duration	not applicable	y	96-hrs
23	Negative or positive controls (specify)	1	Y	3
24	Number of replicates (including controls)	1	Y	2
25	Nominal concentrations reported?	1	Y	320–3200 mg/L
26	Measured concentrations reported?	3	N	
27	Food type and feeding periods during the long-term tests	not applicable		not applicable in the acute study
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 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?	not applicable		Solubilizer was not used in the study.
34	If solubilizer/emulsifier was used, was its ecotoxicity reported?	not applicable		Solubilizer was not used in the study.
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 the organism's health (e.g., when mortality in the control > 10%) or physical effects (e.g., "shading effect")?	not applicable	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	N	Although the water solubility was unknown, it is anticipated to be lower than the reported toxicity value.
Results				
44	Toxicity values (specify endpoint and value)	not applicable	Y	96-hr LC_{50} > 505 mg/L. This value shall be interpreted as a loading rate.
45	Other endpoints reported - e.g., BCF/BAF, LOEC/NOEC (specify)?	not applicable	N	
46	Other adverse effects (e.g., carcinogenicity, mutagenicity) reported?	not applicable	N	
47	***Score*: %**	***31/42 x 100 = 73.81***		
48	***EC reliability code*:**	***2***		
49	***Reliability category (high, satisfactory, low)*:**	***Satisfactory***		
50	***Comments***			

[1] Not applicable – this information may or may be provided in the study, however it does not contribute in the total weight accounted for the robust study summary, or not considered due to the other similar consideration in the same category.

Robust Study Summary Form: Aquatic iT				
No	**Item**	**Weight**	**Yes/No**	**Specify**
1	Reference: Safepharm Laboratories Ltd. 1990. Acute toxicity to rainbow trout. Project number 47/781. Challenge submission ID#11347.			
2	Substance identity: CAS RN	not applicable	Y	5261-31-4
3	Substance identity: chemical name(s)	not applicable	Y	
4	Chemical composition of the substance	not applicable		
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?	not applicable		Item 9 was taken into account for the total weight.
9	Justification of the method/protocol if a nonstandard method was used	2	N	
10	GLP (good Llboratory practice)	3	N	
Test organism				
11	Organism identity: name	not applicable	Y	*Rainbow trout (Salmo Gairdneri)*
12	Latin or both Latin and common names reported?	1	Y	Both
13	Life cycle age / stage of test organism	1	N	
14	Length and/or weight	1	Y	4.8 $\pm$ 0.4 cm and 1.40 $\pm$ 0.41 g
15	Sex	1	N	
16	Number of organisms per replicate	1	Y	3-10
17	Organism loading rate	1	Y	0.70 g-bw/L
18	Food type and feeding periods during the acclimation period	not applicable		not applicable in the acute test
Test design / conditions				
19	Test type (acute or chronic)	not applicable	Y	Acute
20	Experiment type (laboratory or field)	not applicable	Y	Laboratory
21	Exposure pathways (food, water, both)	not applicable	Y	Water
22	Exposure duration	not applicable	Y	96 hrs
23	Negative or positive controls (specify)	1	Y	Negative
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	not applicable		not applicable in the acute test
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 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?	not applicable		Solubilizer was not used in the study.
33	If solubilizer/emulsifier was used, was its concentration reported?	not applicable		
34	If solubilizer/emulsifier was used, was its ecotoxicity reported?	not applicable		
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 the organism's health (e.g., when mortality in the control >10%) or physical effects (e.g., "shading effect")?	not applicable	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?	not applicable		
41	Was pH of the test water within the range typical for the Canadian environment (6 to 9)?	1	N	No pH was reported.
42	Was temperature of the test water within the range typical for the Canadian environment (5 to 27°C)?	1	Y	14 $\pm$ 1 °C
43	Was toxicity value below the chemical's water solubility?	3	N	Water solubility for this substance was 0.07 mg/L
Results				
44	Toxicity values (specify endpoint and value)	not applicable	Y	96-hr LC_{50} > 100 mg/L. This value shall be interpreted as the loading rate.
45	Other endpoints reported - e.g., BCF/BAF, LOEC/NOEC (specify)?	not applicable	N	
46	Other adverse effects (e.g., carcinogenicity, mutagenicity) reported?	not applicable	N	
47	***Score*: %**		***16/37 x 100 = 43.24***	
48	***EC reliability code*:**		***3***	
49	***Reliability category (high, satisfactory, low)*:**		***Low***	
50	***Comments***			

[1] Not applicable – this information may or may be provided in the study, however it does not contribute in the total weight accounted for the robust study summary, or not considered due to the other similar consideration in the same category.

Appendix II – PBT Model Inputs Summary Table

Note: Solvent Red 1, Solvent Orange 7 and Solvent Red 3 are not in commerce in Canada. They are dyes which have been identified as not amenable to model prediction because these chemicals are considered “out of the model domain of applicability”. Therefore, BIOWIN and CATABOL are only applied to predict the persistence half-life for Solvent Red 1, Solvent Orange 7 or Solvent Red 3. The required input for these models is structural coding information which can be obtained by using the SMILES (Simplified Molecular Input Line Entry System) string.