Australian Government
Department of Health and Aged Care
Australian Industrial Chemicals Introduction Scheme

Phenylenediamines

Evaluation statement

26 June 2023

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AICIS evaluation statement

Subject of the evaluation

Phenylenediamines

Chemicals in this evaluation

Name	CAS registry number
1,4-Benzenediamine	106-50-3
1,2-Benzenediamine	95-54-5
1,3-Benzenediamine	108-45-2
1,4-Benzenediamine, dihydrochloride	624-18-0
1,2-Benzenediamine, dihydrochloride	615-28-1
1,3-Benzenediamine, dihydrochloride	541-69-5
1,3-Benzenediamine, sulfate (1:1)	541-70-8

Reason for the evaluation

Evaluation Selection Analysis indicated a potential environmental risk.

Parameters of evaluation

This evaluation considers the environmental risks associated with the industrial uses of 3 benzenediamines (also known as phenylenediamines) and 4 of their respective salts. These chemicals are listed on the Australian Inventory of Industrial Chemicals (the Inventory). These chemicals have been assessed for their risks to the environment according to the following parameters:

- Australian introduction volumes informed by industry-provided information
- Industrial uses listed below in the ‘Summary of introduction, use and end use’ section
- Expected emission into sewage treatment plants (STPs) following consumer and commercial use.

These chemicals have been assessed as a group because they are structurally similar and have similar functional uses. The salts of this group will dissolve under typical environmental conditions to form their respective chemical species.

Summary of evaluation

Summary of introduction, use and end use

The chemicals in this evaluation are used as dyes and intermediates in the following industrial products according to Australian and international use data:

- lubricant and grease products
- plastic and polymer products
- fabric, textile and leather products
- ink, toner, and colourant products
- photographic products
- other end uses not covered above (e.g. vulcanising accelerators and manufacture of corrosion inhibitors).

p-Phenylenediamine (PPD) and its hydrochloride salt also is used as a dye component in personal care products.

Due to regulations in Australia, the use of *m*-phenylenediamine (MPD), *o*-phenylenediamine (OPD) and their salts in personal care products is not permitted.

Most of the uses listed above are expected to result in limited environmental releases. The focus of this evaluation is PPD in hair dye products as this is the major industrial use that results in emissions of a phenylenediamine chemical to the environment.

Consolidated information provided by Accord Australia of their Members indicated approximately 4 tonnes of PPD is used in hair dye products in Australia annually. There is no information available on the use volumes of MPD and OPD in Australia.

Reported volumes from international jurisdictions indicate PPD, MPD and OPD are used in the European Union (EU) at up to 100 000, 10000 and 10 tonnes per year (t/year), respectively. Volumes of use in the USA are reported up to 45360, 22680 and 9071 t/year, respectively.

Environment

Summary of environmental hazard characteristics

Based on the information presented in this evaluation and according to the environmental hazard thresholds stated in the Australian Environmental Criteria for Persistent, Bioaccumulative and/or Toxic Chemicals (DCCEEW n.d.), the chemicals are:

- Persistent (P)
- Not Bioaccumulative (not B)
- Toxic (T).

Environmental hazard classification

These chemicals satisfy the criteria for classification according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) for environmental hazards as follows (UNECE 2017). This evaluation does not consider classification of physical and health hazards.

For PPD, OPD and their respective salts:

Environmental Hazard	Hazard Category	Hazard Statement
Hazardous to the aquatic environment (acute / short-term)	Aquatic Acute 1	H400: Very toxic to aquatic life
Hazardous to the aquatic environment (long-term)	Aquatic Chronic 1	H410: Very toxic to aquatic life with long lasting effects

For MPD and its dihydrochloride salt and sulfate salt:

Environmental Hazard	Hazard Category	Hazard Statement
Hazardous to the aquatic environment (acute / short-term)	Aquatic Acute 2	H401: Toxic to aquatic life
Hazardous to the aquatic environment (long-term)	Aquatic Chronic 1	H410: Very toxic to aquatic life with long lasting effects

Summary of environmental risk

The chemicals are categorised as persistent and toxic. Each has industrial uses or potential industrial uses as intermediates and dyes. Due to existing restrictions on the use of OPD and MPD in cosmetics in Australia, only PPD is expected to have potential for significant release to the aquatic environment, through its use in hair dye products. The annual Australian use volume of PPD in hair dyes is taken to be approximately 4 tonnes.

The toxic and persistent characteristics of PPD are due to the expected formation of recalcitrant or toxic degradants. PPD itself undergoes rapid primary degradation into degradants which, based on standard biodegradation tests, are not expected to mineralise in the environment. Based on the available information, there are no degradants that are expected to be both persistent and toxic. Identified degradants of PPD include *p*-benzoquinone and the trimer adduct Bandrowski’s base. The ultimate environmental fate of most PPD released to surface waters is expected to be sequestration into larger persistent macromolecules that are not harmful to the environment.

Due to these factors, and the relatively low annual volume of PPD used in emissive use patterns in Australia, current use of PPD is not expected to pose a significant risk to the environment in Australia. Due to their lower global use volumes, restricted use in personal care products, and lower apparent toxicity, the risks posed to the environment by OPD and MPD are expected to be lower than those posed by PPD. Therefore, their current use is not expected to pose a significant risk to the environment.

Conclusions

The conclusions of this evaluation are based on the information described in this statement.

The Executive Director is satisfied that the identified environment risks can be managed within existing risk management frameworks. This is provided that all requirements are met under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory.

Note: Obligations to report additional information about hazards under *Section 100 of the Industrial Chemicals Act 2019* apply.

Supporting information

Rationale

This evaluation considers the environmental risks associated with the industrial uses of phenylenediamines (benzenediamines) and their salts. The evaluation of these chemicals has been conducted as a group because of their structural similarity and known or potential applications as dye components.

PPD is widely used in the formulation of hair dyes. Hair dyes are released into sewers nationwide as a normal part of their use pattern. The use of PPD and its hydrochloride salt in these products has significant potential to result in environmental exposure through a common pathway involving release of the chemicals in treated effluents and biosolids produced by STPs.

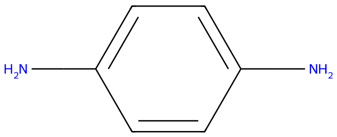
The ESA of PPD, MPD and OPD highlighted high production volume (HPV), and potential persistence and toxicity hazard characteristics, which are of concern for the environment. This evaluation includes further refinement of the risk characterisation of the chemicals in this group and a more in-depth assessment of the available environmental hazard and exposure information for these chemicals.

Chemical identity

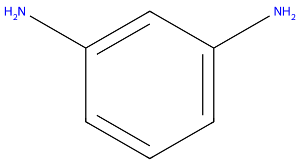
Phenylenediamines are a group of di-substituted benzenes. The chemicals are commonly manufactured through the hydrogenation of nitroaniline isomers (NCBIa; NCBIb; NCBIc n.d.).

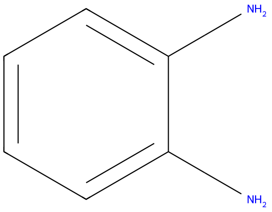
Reported purity of PPD exceeds 98% with the contaminants of OPD (<200 ppm), MPD (<200 ppm), *o*-aminophenol (<500 ppm) and aniline (<50 ppm) (Meyer and Fischer 2015). The purity of MPD and OPD are similarly reported to be above 98% containing phenylenediamine isomers, azobenzene and dinitrobenzene as impurities (NCBIb n.d.; REACHb n.d.).

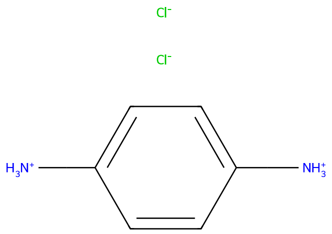
Chemical name	1,4-Benzenediamine
CAS RN	106-50-3
Synonyms	PPD *p*-phenylenediamine 1,4-phenylenediamine 4-aminoaniline
Molecular formula	C6H8N2
Molecular weight (g/mol)	108.14
SMILES	C1=CC(=CC=C1N)N
Chemical description	-
Structural formula:	



Chemical name	1,3-Benzenediamine
CAS RN	108-45-2
Synonyms	MPD *m*-phenylenediamine 1,3-phenylenediamine 3-aminoaniline
Molecular formula	C6H8N2
Molecular weight (g/mol)	108.14
SMILES	C1=CC(=CC(=C1)N)N
Chemical description	-
Structural formula:	

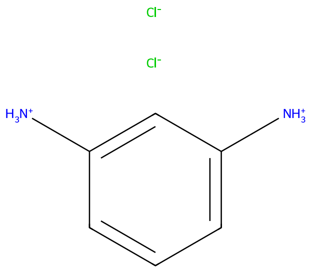


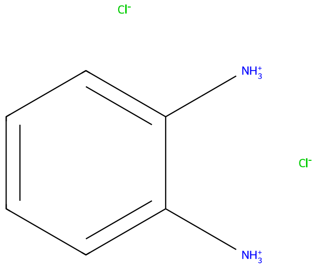
Chemical name	1,2-Benzenediamine
CAS RN	95-54-5
Synonyms	OPD *o*-phenylenediamine 1,2-phenylenediamine 2-aminoaniline
Molecular formula	C6H8N2
Molecular weight (g/mol)	108.14
SMILES	C1=CC=C(C(=C1)N)N
Chemical description	-
Structural formula:	

Chemical name	1,4-Benzenediamine, dihydrochloride
CAS RN	624-18-0
Synonyms	PPD HCl *p*-phenylenediamine dihydrochloride 1,4-phenylenediamine dihydrochloride 4-aminoaniline dihydrochloride
Molecular formula	C6H8N2.2ClH
Molecular weight (g/mol)	181.06
SMILES	C1=CC(=CC=C1[NH3+])[NH3+].[Cl-].[Cl-]
Chemical description	-
Structural formula:	

Chemical name	1,3-Benzenediamine, dihydrochloride
CAS RN	541-69-5
Synonyms	MPD HCl *m*-phenylenediamine dihydrochloride 1,3-phenylenediamine dihydrochloride 3-aminoaniline dihydrochloride
Molecular formula	C6H8N2.2ClH
Molecular weight (g/mol)	181.06
SMILES	C1=CC(=CC(=C1)[NH3+])[NH3+].[Cl-].[Cl-]
Chemical description	-

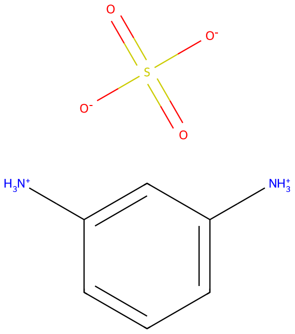
Structural formula:



Chemical name	1,2-Benzenediamine, dihydrochloride
CAS RN	615-28-1
Synonyms	OPD HCl *o*-phenylenediamine dihydrochloride 1,2-phenylenediamine dihydrochloride 2-aminoaniline dihydrochloride
Molecular formula	C6H8N2.2ClH
Molecular weight (g/mol)	181.06
SMILES	C1=CC=C(C(=C1)[NH3+])[NH3+].[Cl-].[Cl-]
Chemical description	-
Structural formula:	

Chemical name	1,3-Benzenediamine, sulfate (1:1)
CAS RN	541-70-8
Synonyms	*m*-phenylenediamine sulfate
	1,3-phenylenediamine sulfate
	3-aminoaniline sulfate
Molecular formula	C6H8N2.H2O4S
Molecular weight (g/mol)	206.22
SMILES	C1=CC(=CC(=C1)[NH3+])[NH3+].[O-]S(=O)(=O)[O-]
Chemical description	-

Structural formula:



Relevant physical and chemical properties

Measured physical and chemical property data for PPD, MPD and OPD were retrieved from the dossiers submitted under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation in the European Union (EU) (REACHa n.d.; REACHb n.d.; REACHc n.d.).

Henry's Law constants were calculated from measured values for water solubility and vapour pressure (US EPA 2017). Values for the pKa of the conjugate acid (pKaH) were retrieved from the CRC Handbook of Chemistry and Physics (Haynes 2010).

Chemical	PPD	MPD	OPD
Physical form	Solid	Solid	Solid
Melting point	142°C (exp.)	63.2°C (exp.)	101°C (exp.)
Boiling point	274°C (exp.)	284°C (exp.)	256°C (exp.)
Vapour pressure	0.01 Pa at 20°C (exp.)	0.038 Pa at 20°C (exp.)	0.108 Pa at 20°C (exp.)
Water solubility	31 g/L at 20°C (exp.)	429 g/L at 20°C (exp.)	39.3 g/L at 20°C (exp.)
Henry's law constant	3.488×10^{-5} Pa·m^3 /mol (calc.)	9.578×10^{-6} Pa·m^3 /mol (calc.)	2.972×10^{-4} Pa·m^3 /mol (calc.)
Ionisable in the environment?	Yes	Yes	Yes
pKaH	2.97, 6.31 (exp.)	2.50, 5.11 (exp.)	0.80, 4.57 (exp.)
log K_{OW}	-0.84 at 20°C (exp.)	-0.33 at 25°C (exp.)	0.15 at 25°C (exp.)

The pKaH values of PPD, MPD and OPD indicate that a proportion of the chemicals will be ionised under environmental conditions (pH = 4–9). For MPD and OPD the proportion of charged species will be negligible under neutral conditions (pH 7, <2% protonated species). For PPD a more significant proportion will be charged (~17% protonated species).

Introduction and use

Australia

Consolidated information provided by Accord Australasia of their Members indicated approximately 4 tonnes of PPD is used in hair dye products in Australia annually. PPD and its hydrochloride salt are present on the list of chemicals used as dyes in permanent and semi-permanent hair dyes in Australia (NICNAS 2007; NICNAS 2014a; NICNAS 2014b).

MPD and its sulfate salt were previously used in hair dye in Australia (NICNAS 2007). However, MPD and OPD (including all respective salts) are now prohibited in preparations for cosmetic use and skin colouration (including tattooing) under Schedule 10 of the Poisons Standard (TGA 2023).

International

The total registered use volumes for PPD, MPD and OPD in the European Economic Area are 10000–100000, 1000–10000 and 1–10 t/year, respectively (REACHa n.d.; REACHb n.d.; REACHc n.d.). In the United States of America (USA), PPD, MPD and OPD are on the US EPA HPV list (US EPA 2020b), with reported annual use volumes of 9071–45360, 4535–22680 and 453–9071 tonnes, respectively (US EPA 2020a). In Japan from 2012–2022, PPD, MPD and OPD were manufactured and/or imported in quantities of 1–2000, 925–1320 and 1553–2449 t/year, respectively (NITE 2020).

PPD is commonly used as a reactive component in oxidative permanent hair dyes for both household and professional salon use (Meyer and Fischer 2015). Hair dye products that contain PPD are designed to be mixed immediately before application to hair with an oxidizing agent, an alkaline substance and a coupling agent. Variation of the coupling agent generates different colours of dye (Compound Interest 2015). The Consumer Product Information Database (CPID) reports concentrations of PPD in hair dye kits of less than 5% (DeLima Associates), and in another study it was measured in concentrations up to 1.8% (w/w) (Al-Enezi and Aldawsari 2022).

PPD is used as a textile and leather dye, and as a photographic developing agent. In a study conducted in the United Arab Emirates, PPD was identified to have concentrations of 0.38–29.52% in black henna (Al-Suwaidi and Ahmed 2010). PPD is also used as an intermediate in the production of antioxidants, dyes, vulcanising accelerators and diisocyanates for polyurethanes (NCBIa n.d.; NICNAS 2014a; SWA n.d.).

Available information indicates that MPD is used as a component in hair, textile and leather dye. It is also used as an adhesive hardener, petroleum additive, vulcanising accelerator, in photographic developing, and in ion exchange resins. MPD is used as an intermediate in the production of antioxidants, polymers (epoxy resins, aramid fibres and rubber), dyes and corrosion inhibitors, and diisocyanates for polyurethane manufacturing (NCBIb n.d.; NICNAS 2013b; SPIN n.d.).

OPD is used as an intermediate in the manufacture of dyes, photographic developing agents, lubricants and corrosion inhibitors (NICNAS 2013a; SPIN n.d.).

PPD has non-industrial use as an active ingredient in pesticide products (US EPA n.d.). The use of this chemical as a pesticide additive is beyond the scope of this evaluation.

Existing Australian regulatory controls

Environment

The industrial use of the chemicals in this group are not subject to any specific national environmental regulations.

Public

Phenylenediamines are listed on the Poisons Standard as follows (TGA 2023):

Schedule 6

PHENYLENEDIAMINES including alkylated, arylated, halogenated and nitro derivatives not elsewhere specified in these Schedules:

(a) in preparations packed and labelled for photographic purposes; or

(b) in preparations packed and labelled for testing water **except** tablets containing 10 mg or less of diethyl-para-phenylenediamine or dimethyl-para-phenylenediamine in opaque strip packaging provided the directions for use include the statement, “Do not discard testing solutions into the pool”; or

(c) in hair dye preparations **except** when the immediate container and primary pack are labelled with the following statements:

(i) KEEP OUT OF REACH OF CHILDREN; and

(ii) WARNING – This product contains ingredients which may cause skin irritation to certain individuals. A preliminary test according to the accompanying directions should be made before use. This product must not be used for dyeing eyelashes or eyebrows; to do so may be injurious to the eye;

written in letters not less than 1.5 mm in height; or

(d) in eyelash and eyebrow tinting products when the immediate container and primary pack are labelled with the following statement:

WARNING – This product contains ingredients which may cause skin irritation to certain individuals, and when used for eyelash and eyebrow tinting may cause injury to the eye. A preliminary test according to the accompanying directions should be made before use;

written in letters not less than 1.5 mm in height.

Schedule 10 – Substances of such danger to health as to warrant prohibition of supply and use.

PHENYLENEDIAMINES, including alkylated, arylated, halogenated and nitro derivatives, in preparations for skin colouration, tattooing and dyeing of eyelashes or eyebrows **except** when included in Schedule 6.

1,2-BENZENEDIAMINE in preparations for cosmetic use and skin colouration (including tattooing).

1,3-BENZENEDIAMINE in preparations for cosmetic use and skin colouration (including tattooing)

International regulatory status

United Nations

The chemicals in this evaluation are not currently identified as persistent organic pollutants (UNEP 2001), ozone depleting substances (UNEP 1987), or hazardous substances for the purpose of international trade (UNEP and FAO 1998).

Canada

The maximum concentration of PPD and its salts in hair dye products after dilution with an oxidizer must not exceed 3% (Government of Canada 2019b).

OPD and its salts are present on the Health Canada List of Prohibited Cosmetic Ingredients (Government of Canada 2019a).

European Union

PPD and its salts maximum concentration applied to hair after mixing under oxidative conditions must not exceed 2% calculated as free base under the EU Cosmetics Regulation 1223/2009 Annex III (EC n.d.).

MPD and OPD, along with their salts, are prohibited in cosmetic products under the EU Cosmetics Regulation 1223/2009 Annex II (EC n.d.).

New Zealand

PPD and its salts maximum concentration applied to hair after mixing under oxidative conditions must not exceed 2% calculated as free base under the New Zealand Cosmetic Products Group Standard (NZ EPA 2020).

MPD and OPD, along with their salts, are prohibited in cosmetic products under the New Zealand Cosmetic Products Group Standard (NZ EPA 2020).

Asia

PPD and its salts maximum concentration applied to hair after mixing under oxidative conditions must not exceed 2% calculated as free base under the Association of South East Asian Nations (ASEAN) Cosmetic Directive Annex III (HSA 2022b).

MPD and OPD, along with their salts, are prohibited in cosmetic products under the ASEAN Cosmetic Directive Annex II (HSA 2022a).

Environmental exposure

PPD and its hydrochloride salt are expected to have the greatest potential for release to the environment due to their use in hair dye products. MPD and OPD are expected to have minimal potential for release due to their relatively non-emissive use patterns.

PPD and its hydrochloride salt have uses in personal care products, which are typically released to sewers in wastewater following use. Depending on degradation and partitioning processes of chemicals in STPs, some fraction of the quantity of chemicals in wastewater entering STPs can be emitted to:

- the air compartment
- rivers or oceans in treated effluent
- to soil by application of biosolids to agricultural land (Struijs 1996).

During the hair dyeing process PPD is oxidised to *para*-benzoquinone diimine (*p*-BQDI, CAS No. 4377-73-5) (Meyer and Fischer 2015). This reactive species reacts with the coupling agent present in the hair dye formulation to form coloured dye molecules. *p*-BQDI also readily self-couples to form dimeric, oligomeric and polymeric species (EC 2004). It is estimated that approximately 3–5% of PPD transforms to Bandrowski's base, a commonly observed trimer (Bessegato et al. 2018; França Stefoni et al. 2015; Meyer and Fischer 2015).

The proportion of PPD consumed during oxidative hair dyeing varies based on the coupling agent, method of application and duration that the formulation remains on the hair. Two studies were identified that measured the consumption of PPD during hair dyeing, finding that the quantity of unconsumed PPD ranged from 13.5–77% (Al-Enezi and Aldawsari 2022; Rastogi et al. 2006). Another study quantified the residual PPD present after use and rinsing of a hair dye product in a salon, finding 58 µg/L in the collected salon wash water (Bessegato et al. 2018).

The use of PPD and MPD in textile and leather dyeing is considered a site limited emission pathway as industrial coloured wastewater is managed under national trade waste guidelines (NWQMS 1994).

The chemicals in this evaluation are used to manufacture a variety of industrial chemical products including antioxidants, corrosion inhibitors, diisocyanates for polyurethanes, dyes, lubricants, photographic developing agents, polymers (epoxy resins, aramid fibres and rubber) and vulcanising accelerators. Manufacturing activity and clean-up of equipment may lead to localised release of these chemicals to wastewater, soil and air in small quantities. This is not expected to contribute to significant environmental exposure. Use of these chemicals as intermediates in the production of polymers is also not expected to cause significant environmental exposure as the process results in these chemicals being irreversibly bound within a polymer matrix.

Environmental fate

Dissolution, speciation and partitioning

Chemicals in this evaluation are expected to partition to water, soil and sediment when released to the environment from their industrial use.

In surface waters, the chemicals are in pH-dependent equilibrium between the neutral organic chemical and the protonated ammonium species. The pKa of PPD (pKa = 6.31) indicates that at pH 7 it will predominately exist in the neutral form (approximately 83%), although a significant proportion will exist as the charged ammonium species (approximately 17%). For OPD and MPD, the formation of the ammonium species is negligible at pH 7 (approximately 0.4% and 1.3%, respectively).

The phenylenediamine hydrochloride and sulfate salts in this evaluation are expected to dissociate in water to form the corresponding phenylenediamine, before undergoing pH-dependent speciation as described above.

The chemicals in this evaluation are readily soluble in water. Based on the calculated Henry’s Law constants, the chemicals in this group are very slightly volatile from water and moist soil. The ammonium species are expected to have low volatility and partition in negligible quantities from water to air. The calculated carbon soil adsorption coefficients (K_{OC}) of PPD, MPD and OPD (33.83, 33.83 and 34.52 L/kg, respectively) suggest these chemicals have very high mobility in soil (US EPA 2017).

Degradation

The chemicals in this evaluation have short primary half-lives but may form persistent degradants or adducts in aqueous environments. Phenylenediamines undergo rapid primary degradation in water through oxidative and photolytic mechanisms but undergo limited ultimate biodegradation in standard studies. Reaction of PPD primary degradants with other environmental organic substances is expected to form large, persistent compounds such as humic acids.

PPD and OPD are expected to undergo rapid primary degradation in STPs or surface waters through autoxidation. MPD will also degrade, but at a slower rate. One study measured the disappearance of PPD, OPD and MPD over 4 hours in static aerated well water at 25°C. At test substance concentrations of 2.5 mg/L, the primary degradation half-lives of PPD, OPD and MPD were 4.1 hours, 2.7 days and 13.4 days respectively. At 25 mg/L, the half-lives for PPD, OPD and MPD were 8.9 hours, 4.5 days and 33.6 days, respectively (REACHa n.d.; REACHb n.d.; REACHc n.d.).

The chemicals in this evaluation will undergo rapid primary photodegradation in sunlit surface waters. A photolysis study of MPD, OPD and PPD in water was conducted according to US EPA OTS 795.70, which measured test substance degradation by HPLC after sunlight irradiation in water for 40 minutes. Tests were run in both distilled water and water with dissolved humic acids. Control tests run without irradiation showed minimal degradation over the 40 minute test duration. Overall photolysis DT50s were calculated to be 0.12 days, 0.26 days and 0.51 days for PPD, OPD and MPD respectively (REACHa n.d.; REACHb n.d.; REACHc n.d.).

PPD, MPD and OPD will undergo rapid photo-oxidation by hydroxyl radicals in the atmosphere with calculated half-lives of 0.73, 0.64 and 0.73 hours respectively (US EPA 2017). This is unlikely to be a significant dissipation pathway in the environment as the chemicals have low volatility from surface waters.

The chemicals in this group are not readily biodegradable in standard biodegradation tests.

Several of the available biodegradation studies on PPD were conducted using concentrations in excess of PPD’s measured 3h microbial respiration EC50 of 13.4 mg/L (REACHa n.d.). There is also some evidence that the short-term degradants of PPD may be more toxic than the parent chemicals (Mishra et al. 2020). The results of these tests may therefore have been affected by the toxicity of the test substance or its primary degradants.

In a study conducted in accordance with OECD TG 301D, PPD degraded by 30% within 28 days as measured by biological oxygen demand (BOD) (REACHa n.d.). The test was conducted with a PPD concentration of 2 mg/L. Approximately 28% degradation was measured within the first 14 days of the test, with minimal degradation occurring thereafter. The test was extended to a total duration of 84 days, but no further degradation was measured, indicating lack of ultimate biodegradation under these test conditions.

An inherent biodegradation test was conducted with PPD according to OECD TG 302A (modified SCAS test) using a 15 mg/L test substance concentration. In this test method, degradation is measured over a series of 24h incubation cycles with the test substance recharged between measurements. No degradation of PPD was observed for the first 28 day cycles, with 14% degradation observed on the 29th day cycle (REACHa n.d.).

Additional ready biodegradability tests have been conducted according to OECD TG 301C for PPD, MPD and OPD, at 100 mg/L test substance concentrations. Minimal biodegradation was observed in each case (NITE 2020). In the study with PPD, the substance appeared to polymerise and precipitate out of solution during incubation, largely invalidating the test.

The available biotic and abiotic degradation studies available indicate that the chemicals in this group will have short primary half-lives in environmental surface waters, but may form degradants with limited ultimate biodegradation.

The oxidative transformation pathway of PPD has been studied (Meyer and Fischer 2015; REACHa n.d.). Chemical and electrochemical oxidation of PPD under laboratory conditions enables characterisation of degradants that may form under oxidative conditions in the environment. Initial one-electron oxidation gives a semibenzoquinone diimine radical cation that readily couples with other molecules of PPD to form dimers, oligomers and polymers, or undergoes further oxidation to form *p*-BQDI (Meyer and Fischer 2015). In surface waters or STPs, these reactive species may also react with phenols and anilines to form other multicyclic adducts. *p*-BQDI will also readily hydrolyse to form *p*-benzoquinone (CAS No.106-51-4) (Corbett 1969).

p-Benzoquinone is an industrial chemical previously assessed under the AICIS Evaluations framework (AICIS 2022). In that evaluation it was considered to be at least inherently biodegradable. *p*-Benzoquinone has complex reactivity; it is in redox equilibrium with hydroquinone, and it readily reacts with nucleophiles via conjugate addition to give substituted products (Katritzky et al. 2008). Addition of water gives 2-hydroxy-1,4-benzoquinone, which contributes to the formation of humic acids in the environment (AICIS 2022). Humic acids are highly oxygenated, aromatic macromolecules with varying compositions that are crucial, but highly persistent, environmental components (Grinhut et al. 2007).

Bioaccumulation

The chemicals in this evaluation have low potential to bioaccumulate in aquatic life.

The measured octanol-water partition coefficients of PPD, MPD and OPD (log K_{OW} of -0.84, -0.33 and 0.15 respectively) are below the Australian categorisation threshold for bioaccumulation hazards in aquatic organisms (log $K_{OW} \geq 4.2$), indicating low potential for bioaccumulation (DCCEEW n.d.).

Measured data indicates that PPD and MPD have low potential to bioconcentrate in fish. A study conducted on PPD in accordance with OECD TG 305C reported a lipid-normalised bioconcentration factor (BCF) value of 20–98 litres per kilogram (L/kg) wet weight (wwt) in *Cyprinus carpio* (carp) (NITE 2020). A test conducted using MPD (unspecified test guideline), reported a BCF value of 1.3–24 L/kg wwt in carp (NITE 2020). These values are below the Australian categorisation threshold for bioconcentration in aquatic organisms (BCF ≥2000) (DCCEEW n.d.).

Environmental transport

The chemicals in this evaluation are not expected to undergo long range transport based on their expected short primary half-lives in the environment.

Predicted environmental concentration (PEC)

Predicted environmental concentrations of the chemicals in this evaluation have not been determined. No Australian environmental monitoring data for these chemicals were available.

PPD is expected to be released to wastewater as a normal part of its use in commercial and domestic hair dyes. Based on available information, approximately 4 tonnes of PPD is taken to be used in hair dye products in Australia annually. Negligible environmental concentrations of PPD are expected given its rapid transformation, during use and subsequent STP treatment, to a number of adducts and degradant chemicals. A predicted environmental concentration for PPD has therefore not been determined.

OPD and MPD are expected to have low potential for release to the environment due to their use patterns. In an international monitoring study, MPD was detected at below the limits of detection in samples from effluents and surface water (<0.01 mg/L), sediments (<0.1 milligrams per kilogram (mg/kg) and biota (<0.5 mg/kg) (REACHc n.d.).

Environmental effects

Effects on aquatic life

Chemicals in this evaluation exhibit acute and chronic toxic effects at low concentrations in standard tests with aquatic organisms across multiple trophic levels.

There is evidence that the chemicals in this evaluation would undergo significant primary degradation within the timeframes of standard ecotoxicity tests. Tests using flow-through conditions are therefore considered the most relevant for characterising the toxicity of the parent chemicals. The outcomes of tests under static or semi-static conditions are likely to be significantly influenced by the formation of degradants.

Acute toxicity

The following measured median lethal concentration (LC50) and median effective concentration (EC50) values for model organisms across three trophic levels were retrieved from the Registration Dossiers for PPD, MPD and OPD under the EU REACH legislation (REACHa n.d.; REACHb n.d.; REACHc n.d.):

Taxon	Endpoint	Method
Fish	PPD: 96h LC50 = 3.9 mg/L	*Oncorhynchus mykiss* (rainbow trout) OECD TG 203 Flow-through
	PPD: 96h LC50 = 0.066 mg/L	*Oryzias latipes* (medaka) OECD TG 203 Semi-static
	MPD: 96h LC50 = 512 mg/L	Rainbow trout OECD TG 203 Flow-through
	OPD: 96h LC50 = 44 mg/L	*Pimephales promelas* (fathead minnow) OECD TG 203 Static
Invertebrate	PPD: 48h EC50 = 0.28 mg/L	*Daphnia magna* (water flea) OECD TG 202 Immobilisation Static
	MPD: 48h EC50 = 5.9 mg/L	Water flea OECD TG 202 Immobilisation Static
	OPD: 96h LC50 = 9.1 mg/L	*Gammarus fasciatus* (amphipods) OECD TG 202 Mortality Flow-through
Algae	PPD: 72h EC50 = 0.27 mg/L	*Raphidocelis subcapitata* (green algae) OECD TG 201 Growth rate Static
	MPD: 96h EC50 = 2.87 mg/L	Green algae OECD TG 201 equivalent Biomass Static
	OPD: 96h EC50 = 0.16 mg/L	Green algae OECD TG 201 equivalent Growth rate Static

Two additional fish acute toxicity studies according to OECD TG 203 have been conducted under static conditions for PPD (REACHa n.d.). These studies were conducted with *P. promelas* (fathead minnow), returning 96h LC50 values of 0.028 mg/L and 0.057 mg/L based on nominal test substance concentrations. One study was conducted with *O. latipes* (medaka) under semi-static conditions, returning an LC50 value of 0.066 mg/L based on time-weighted average (TWA) concentrations (see table above). These endpoints are significantly lower than the endpoint found using flow-through conditions with *O. mykiss* (see table above).

These studies likely do not represent the toxicity of the parent PPD substance, as maintenance of test substance concentrations was not demonstrated. In the two static tests conducted with fathead minnow, PPD could not be detected in solution at time zero in any vessel but those with the highest nominal test substance concentrations. In the semi-static test with medaka and 24h renewal of test medium, PPD concentrations declined to approximately 15% of nominal between each renewal. This study cited rapid degradation of PPD as the reason for loss of concentration. The generation of degradants is likely to have affected the test results. It is also noted that the test species are different between these tests, which may have had an effect depending on the species sensitivity.

Chronic toxicity

The following measured no-observed-effect concentrations (NOEC) and the 10th percentile effective concentration (EC10) for model organisms across two trophic levels were retrieved from the Registration Dossiers for PPD, MPD and OPD under EU REACH legislation (REACHa n.d.; REACHb n.d.; REACHc n.d.):

Taxon	Endpoint	Method
Invertebrate	PPD: 21d NOEC = 5.1 µg/L	*Daphnia magna* (water flea) OECD TG 211 Reproduction Semi-static
	MPD: 21d NOEC = 50 µg/L	Water flea OECD TG 211 Reproduction Semi-static
	OPD: 21d NOEC = 65 µg/L	Water flea OECD TG 211 equivalent Reproduction Semi-static
Algae	PPD: 72h EC10 = 71 µg/L	*Raphidocelis subcapitata* (green algae) OECD TG 201 Growth rate Static
	MPD: 96h NOEC = 915 µg/L	Green algae OECD TG 201 equivalent Growth rate Static

The PPD 21d endpoint with *Daphnia magna* summarised in the table above was calculated based on time-weighted average (TWA) test substance concentrations. Significant loss of test substance concentration was observed between each renewal, with the calculated TWA concentrations representing 40–66% of each of the nominal exposure concentrations. The study summary indicates that reproduction was the most sensitive endpoint, but that the dose-response relationship was not consistent, and less than 50% inhibition was observed up to the highest exposure concentration of 132 µg/L PPD. As for the static and semi-static acute tests, this endpoint may not adequately represent the toxicity of PPD due to the poor maintenance of test substance concentration and expected generation of degradant compounds.

Bandrowski's base and *p*-benzoquinone

There are some toxicity data available for *p*-benzoquinone and Bandrowski's base, two known degradants or adducts of PPD.

The industrial chemical *p*-benzoquinone was previously assessed as toxic under the AICIS Evaluations framework (AICIS 2022). Its lowest identified ecotoxicity endpoint was an acute 48h *Daphnia magna* EC50 of 0.059 mg/L, according to a study conducted under static conditions in accordance with OECD TG 202.

Bandrowski's base is likely less toxic to aquatic life than PPD. One fish embryo acute toxicity study currently being conducted with Bandrowski's base reported a preliminary LC50 value of 3.478 mg/L based on nominal concentrations (REACHa n.d.). Older literature suggests that saturated solutions of Bandrowski's base are not toxic to *D. magna* over 24h exposure, though the test methodology is not available (Zhakov 1960).

Effects on terrestrial life

The chemicals in this group are expected to be hazardous to terrestrial animals through oral and dermal exposure.

Further information on the effects of this chemical group on terrestrial organisms can be found in the Human Health IMAP Tier II assessments for:

- PPD and its dihydrochloride salt (NICNAS 2014a; 2014b)
- MPD and its dihydrochloride salt and sulfate salt (NICNAS 2013b; 2014c; 2017)
- OPD and its dihydrochloride salt (NICNAS 2014d).

Predicted no-effect concentration (PNEC)

Freshwater PNECs for PPD, MPD and OPD of 0.51, 5.0, 6.5 µg/L were derived from the measured invertebrate chronic ecotoxicity endpoints (21d NOEC = 0.0051, 0.050 and 0.065 mg/L) using an assessment factor of 10. This assessment factor was selected as reliable chronic and acute ecotoxicity data are available for the most sensitive trophic level.

Categorisation of environmental hazard

The categorisation of the environmental hazards of the assessed chemicals according to Australian Environmental Criteria for Persistent, Bioaccumulative and/or Toxic Chemicals is presented below:

Persistence

Persistent (P). Based on studies indicating lack of mineralisation and possible generation of persistent degradants, the chemicals in this group are categorised as Persistent.

Bioaccumulation

Not Bioaccumulative (Not B). Based on low measured log K_{OW} values and low measured bioconcentration factors (BCF) in fish, the chemicals in this group are categorised as Not Bioaccumulative.

Toxicity

Toxic (T). Based on available chronic ecotoxicity endpoints below 0.1 mg/L, chemicals in this group are categorised as Toxic.

Environmental risk characterisation

PPD and its hydrochloride salt are categorised as persistent and toxic based on the results of standard testing. These characteristics are expected to be due to the formation of recalcitrant or toxic degradants after the rapid primary degradation of the PPD parent substance.

PPD is a reactive component of permanent hair dyes. During use, a proportion of the PPD is rapidly oxidised into reactive intermediates, such as *p*-BQDI, by addition of an oxidising agent. In the concentrated hair dye mixture these intermediates undergo a side reaction with unoxidised PPD to form small amounts of conjugated multicyclic adducts, such as the trimer known as Bandrowski's base.

A large proportion of the PPD used in hair dyes remains unoxidised, and is diluted and released to wastewater after use. PPD is expected to undergo oxidation in oxygenated wastewater and surface waters, forming reactive intermediates as primary degradants. In diluted waters these intermediates may still oligomerise or react with other PPD present, producing the aforementioned adducts. However, they are also expected to react with phenolic substances in the environment, such as those present in dissolved organic carbon or humic acids, resulting in an effective sequestration of PPD into environmentally ubiquitous macromolecules. Alternatively, the intermediates will hydrolyse to *p*-benzoquinone.

The formation of reactive intermediates and/or other products is likely to influence the results of standard tests with PPD. The partial degradation of PPD in a ready biodegradability test suggests that some of the degradation products are resistant to degradation whilst others may be sufficiently toxic to microorganisms to halt respiratory activity during the test. The large disparity between toxicity tests under flow-through conditions and those conducted under static or semi-static conditions suggests that some degradant species are more toxic than the parent PPD; however, these studies cannot be used to directly characterise the toxicity of degradants as their identities and concentrations were not tracked.

Based on the available information, PPD degradants that are both persistent and toxic are not expected. There is evidence that Bandrowski's base is less toxic than PPD itself. *p*-Benzoquinone has been previously assessed under the AICIS evaluations framework and was found to be toxic, but not persistent or bioaccumulative. Reaction of PPD primary degradants with other environmental organic substances is expected to form large, persistent compounds such as humic acids that are not environmentally harmful.

Due to these factors, and the relatively low annual volume of PPD used in emissive use patterns in Australia, current use of PPD is not expected to pose a significant risk to the environment in Australia.

MPD and OPD are also categorised as persistent and toxic. Due to their lower global use volumes, restricted use in personal care products, and lower apparent toxicity, the risks posed to the environment by these chemicals are expected to be lower than those posed by PPD and its hydrochloride salt. Their current use is therefore not expected to pose a significant risk to the environment.

Insufficient ecotoxicity data are available to characterise the risks posed by release of these chemicals to the soil compartment.

Uncertainty

This evaluation was conducted based on a set of information that may be incomplete or limited in scope. Some relatively common data limitations can be addressed through use of conservative assumptions (OECD 2019) or quantitative adjustments such as assessment factors (OECD 1995). Others must be addressed qualitatively, or on a case by case basis (OECD 2019).

The most consequential areas of uncertainty for this evaluation are discussed below:

- There are no Australian monitoring data for the chemicals in this evaluation. The risk profiles of PPD, MPD and OPD may change should Australian monitoring data become available to indicate that these chemicals may be present in Australian surface waters, sediments, or soils at concentrations above the levels of concern.
- There are minimal ecotoxicity data on soil and sediment dwelling organisms available for the chemicals in this evaluation. The risk profile of PPD, MPD and OPD may change should new ecotoxicity data or exposure data become available to indicate that these chemicals are present in Australian soil and sediment above levels of concern.
- The identity and environmental effects of the degradation products of the chemicals in this evaluation are limited. If more information becomes available in the future to indicate that these degradants may have persistent, bioaccumulative and/or toxic (PBT) characteristics, the PBT categorisation of these chemicals may change.

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