SAFER CONSUMER PRODUCTS

Proposal to Add *para*-Phenylenediamine (PPD) Derivatives to the Candidate Chemicals List

November 1, 2023

This meeting is being recorded

How to Participate

Questions and comments can be submitted in two ways:

- ✓ Question & Answer (Q&A) function
- ✓ Raise hand function

❖ For those calling in, dial *9 to raise your hand and dial *6 to unmute.

Agenda

Time	Topic	Details
9:05 – 9:10 AM	Welcome	**Ashley Alestra-Laursen,** Public Participation Specialist, Department of Toxic Substances Control
9:10 – 9:20 AM	Opening Remarks	**André Algazi,** Branch Chief, Chemical and Product Evaluation Team Branch, Safer Consumer Products Program
9:20 – 9:40 AM	Presentation on the Proposal to Add *para*-Phenylenediamine Derivatives to the Candidate Chemicals List	**Logan Hayes,** MS, Environmental Scientist, Safer Consumer Products Program **Lynn Nakayama Wong,** PhD, Staff Toxicologist, Safer Consumer Products Program
9:40 – end of comments	Question & Answer (Q&A), Public Comment Period	***The public comment period will last until 11:50 AM, or until there are no further public comments, whichever comes first.***
	Closing Remarks	***The workshop will end no later than 12 PM PDT.***

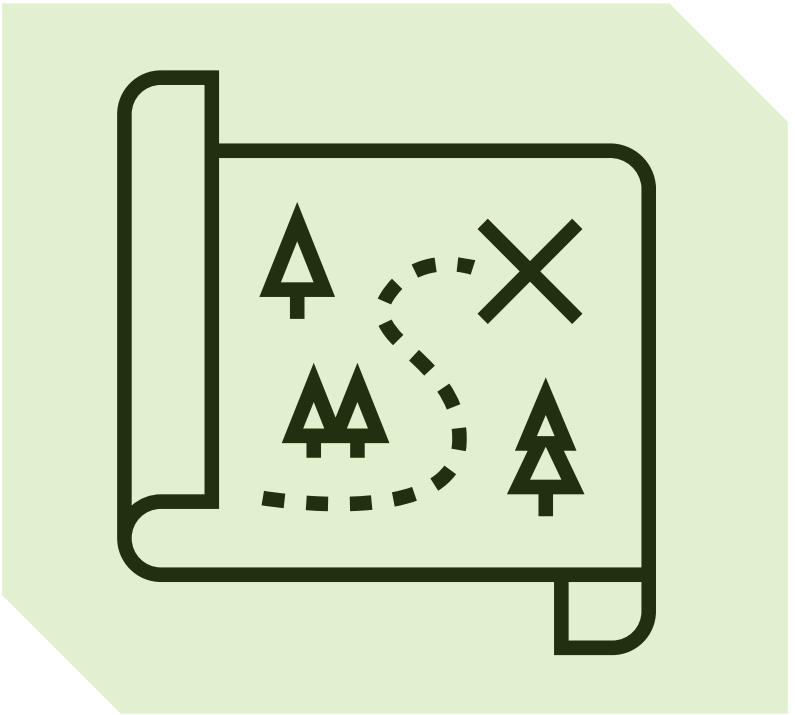
SAFER CONSUMER PRODUCTS (SCP)

Opening Remarks

André Algazi,
Chemical and Product Evaluation Team,
Branch Manager

Sneak Peek into Today's Presentation

- Introduction to the Safer Consumer Products (SCP) Program
- What will replace motor vehicle tires containing 6PPD?
- PPD derivatives proposed definition
- Exposure considerations
  - Water and sediment
- Hazard Traits
  - Wildlife Survival Impairment and Dermatotoxicity
- Conclusion
- Q&A / Comments

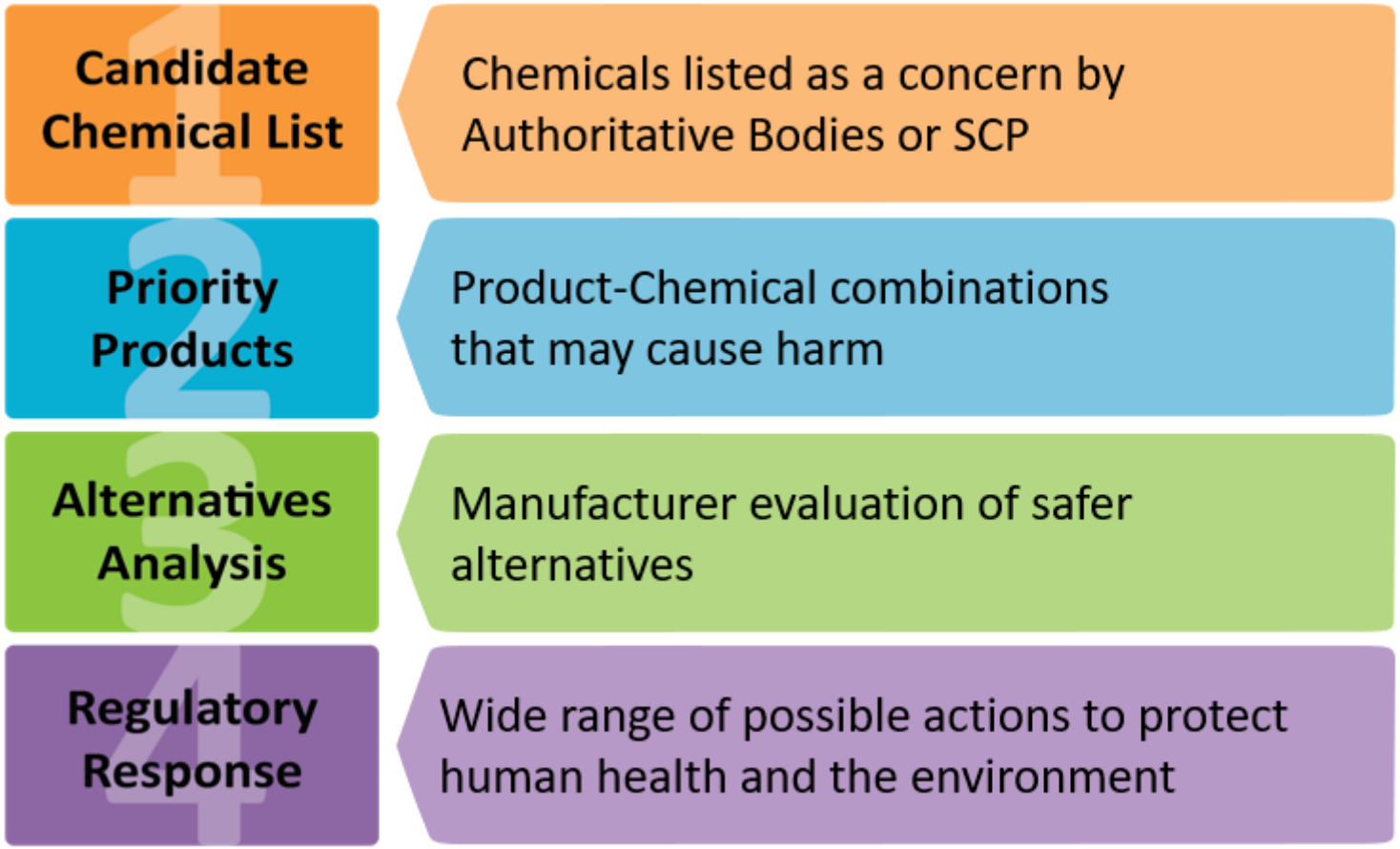


SCP Program's Mission and Goals

- **Mission:** advance the design, development, and use of products that are chemically safer for people and the environment
- **Goals:**
  - Reduce hazardous chemicals in consumer products
  - Increase adoption of green chemistry principles and safer alternatives to chemicals of concern in consumer products

California Code of Regulations, Title 22, Chapter 55 – Safer Consumer Products

Safer Consumer Products (SCP)



California Code of Regulations, Title 22, Chapter 55 – Safer Consumer Products

Safer Consumer Products (SCP)

Candidate Chemical List

Chemicals listed as a concern by Authoritative Bodies or SCP

Priority Products

Alternatives Analysis

Regulatory Response

- SCP may also add chemicals to the Candidate Chemicals List if they exhibit one or more hazard traits and/or environmental or toxicological endpoints by considering specific factors

California Code of Regulations, Title 22, section 69502.2(b) – Candidate Chemicals Identification

Safer Consumer Products (SCP)

Candidate Chemical List

Chemicals listed as a concern by Authoritative Bodies or SCP

Priority Products

Alternatives Analysis

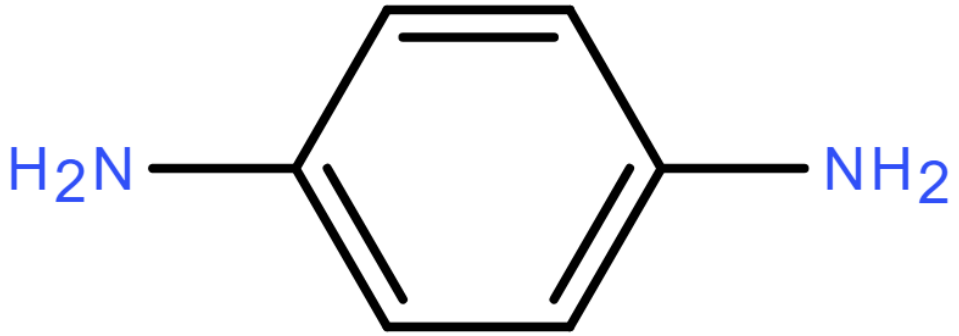
Regulatory Response

1. There are potential **exposures** to the chemical
2. There is potential for one or more of these exposures to contribute to or cause **adverse impacts**
3. SCP has considered the **extent and quality of information** that is available to substantiate the existence of these potential exposures and adverse impacts

California Code of Regulations, Title 22, section 69502.2(b) – Candidate Chemicals Identification

What will replace Motor Vehicle Tires containing 6PPD?

- Motor Vehicle Tires containing 6PPD are listed Priority Products as of October 1st, 2023
- PPD derivatives are viewed as the most effective, currently available, antiozonants for use in tires
- Other PPD derivatives have concerning hazard traits

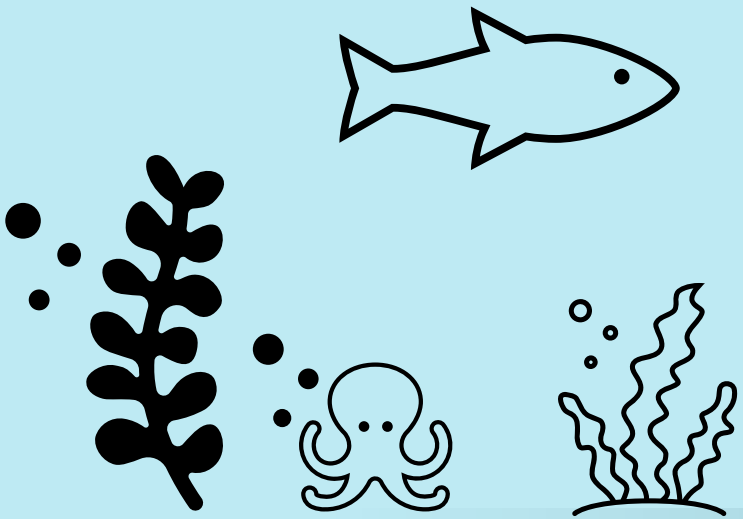


para-Phenylenediamine (PPD)

Toxicity of other PPD Derivatives

	6PPD	PPD	IPPD	44PD	7PPD	77PD
Acute fish toxicity	vH	vH	vH	vH	vH	vH
Acute invert. toxicity	vH	vH	vH	vH	vH	vH
Algal toxicity	vH	vH	H	vH	–	–

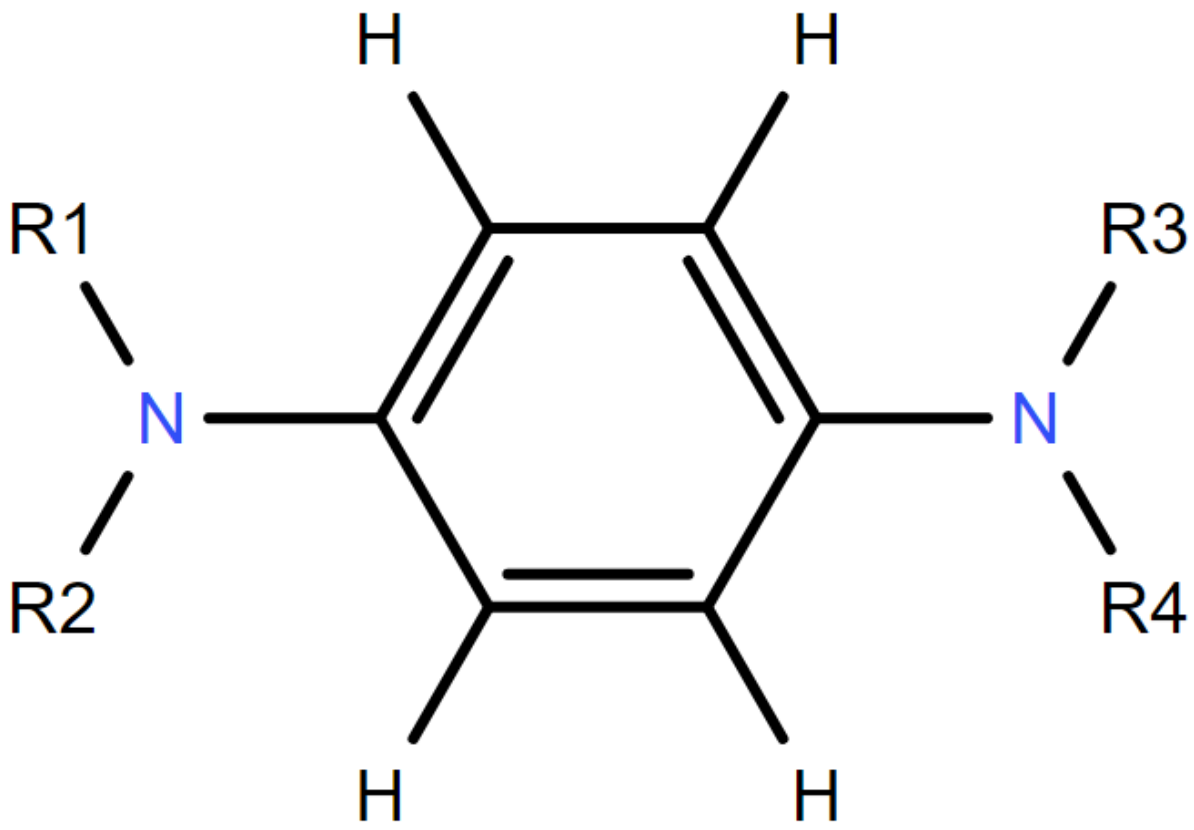
L	M	H	vH



Implications for Proposed Listing

Alternatives Analyses	Signal the need for strong scrutiny if PPD derivatives are included in the Alternatives Analyses for Motor Vehicle Tires containing 6PPD.
	IMPACT – More thorough evaluation of any PPD derivatives considered potential alternatives to 6PPD.
Regulatory Responses	SCP would have greater authority and flexibility when imposing regulatory responses if a PPD derivative is selected as the alternative to 6PPD.
	IMPACT – Promote determinations that are most protective for public health and the environment.
Priority Products	SCP could regulate consumer products containing any members of the broad class of PPD derivatives as Priority Products.
	IMPACT – Expanding the scope of product-chemical combinations SCP could regulate if there are potential for exposures and significant or widespread adverse impacts.

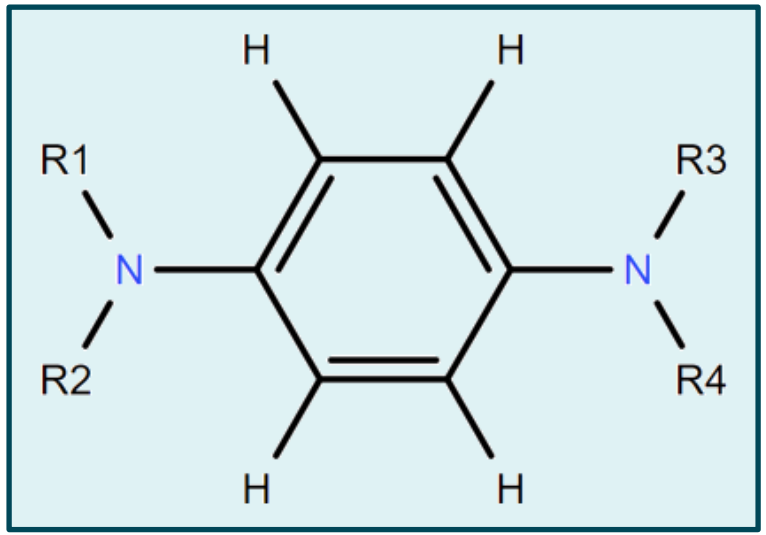
How do we propose to define the class of PPD derivatives?



PPD Derivatives - Definition

This chemical class comprises PPD and all its derivatives that:

- have one or two substituents on one or both **PPD nitrogen atoms**



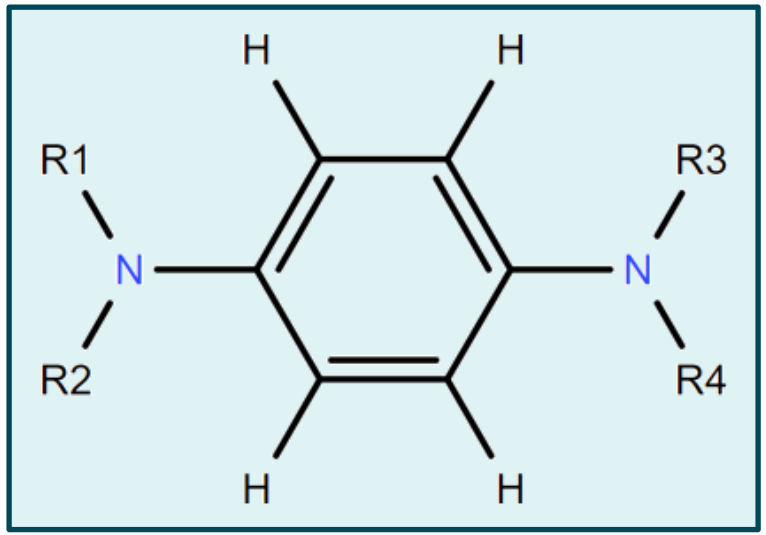
PPD derivative parent structure

PPD Derivatives - Definition

This chemical class comprises PPD and all its derivatives that:

- have one or two substituents on one or both **PPD nitrogen atoms**

- substitute any hydrogen in the PPD amine groups [**N**H2] with nitrogen or carbon only

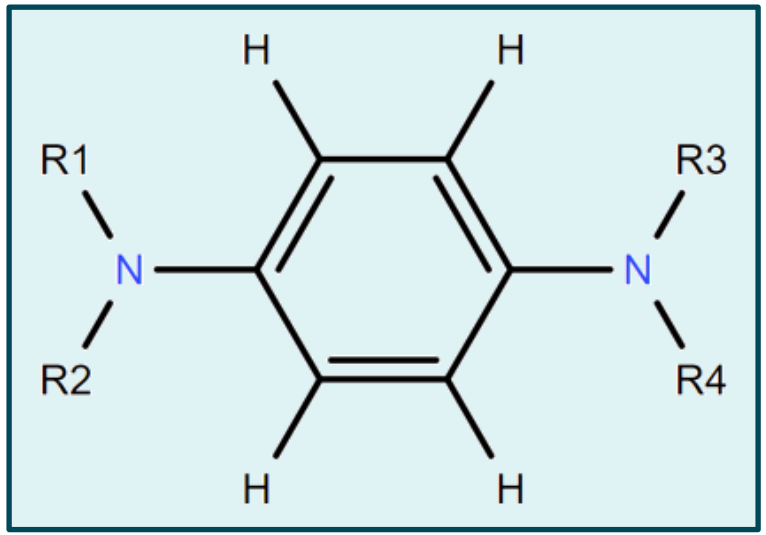


PPD derivative parent structure

PPD Derivatives - Definition

This chemical class comprises PPD and all its derivatives that:

- have one or two substituents on one or both **PPD nitrogen atoms**
- substitute any hydrogen in the PPD amine groups [**N**H2] with nitrogen or carbon only
- have a molecular weight of 1000 daltons (Da) or less. In multicomponent compounds, this applies only to those components that are PPD derivatives

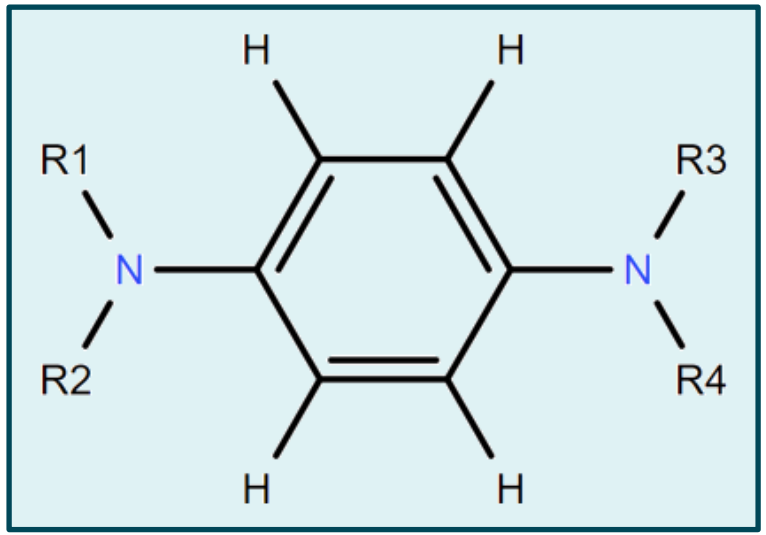


PPD derivative parent structure

PPD Derivatives - Exclusions

PPD derivatives do not:

- contain N-N double bonds or N-N triple bonds at either **PPD nitrogen atom**



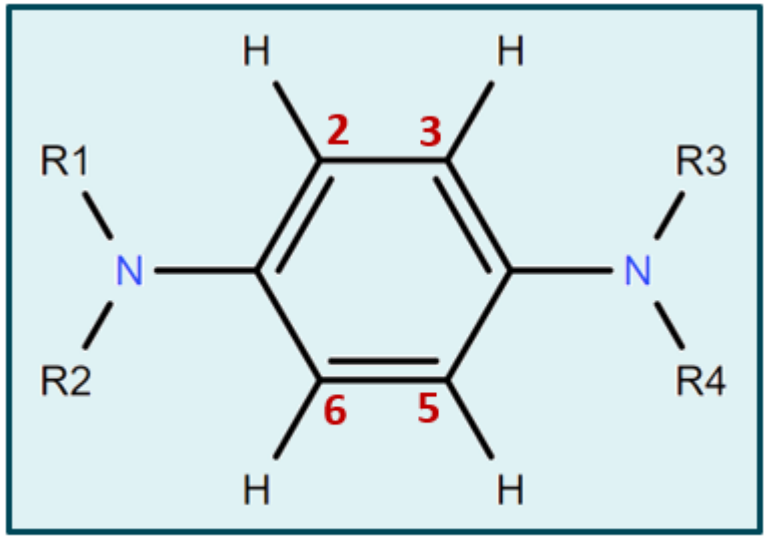
PPD derivative parent structure

PPD Derivatives - Exclusions

PPD derivatives do not:

- contain N-N double bonds or N-N triple bonds at either **PPD nitrogen atom**

- contain additional substituents or modifications to the PPD phenyl ring at the **2, 3, 5, or 6 positions**

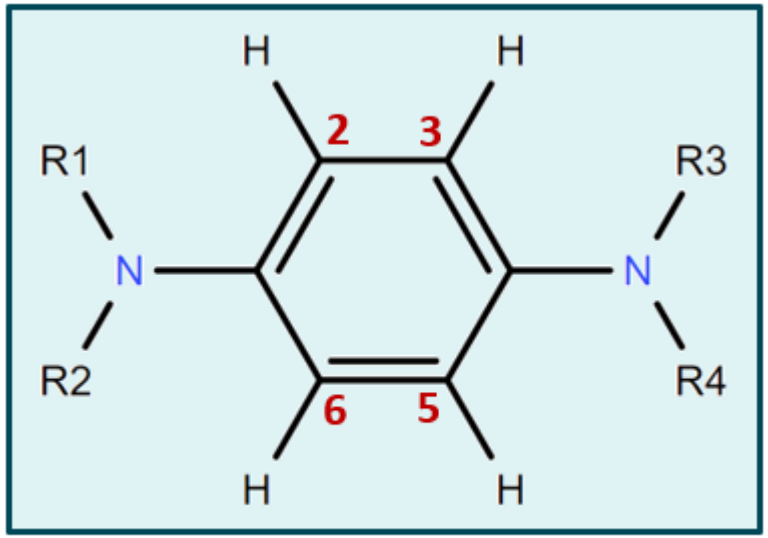


PPD derivative parent structure

PPD Derivatives - Exclusions

PPD derivatives do not:

- contain N-N double bonds or N-N triple bonds at either **PPD nitrogen atom**
- contain additional substituents or modifications to the PPD phenyl ring at the **2, 3, 5, or 6 positions**
- contain quaternary amines (i.e., quaternary ammonium cations) anywhere in the molecule



PPD derivative parent structure

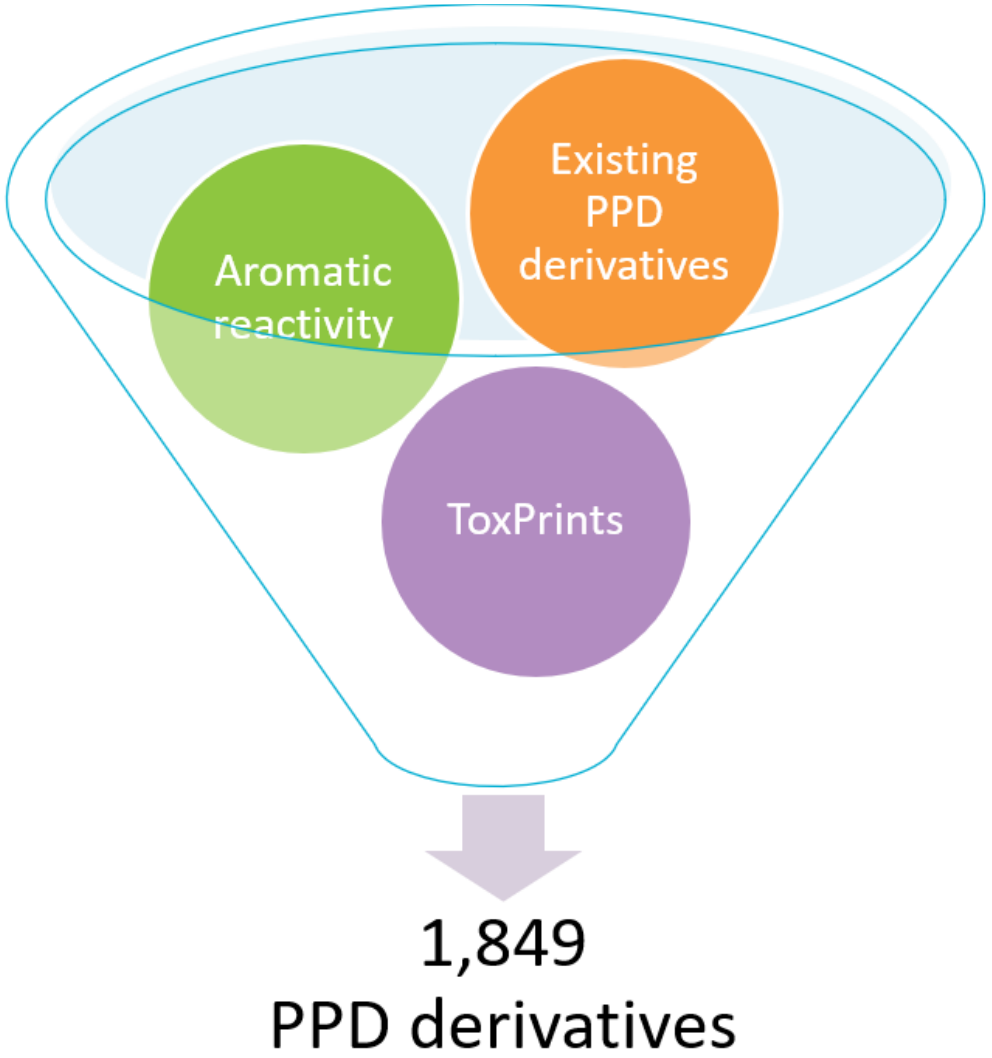
What we used to build the class

We generated a list of compounds by combining features from known PPD derivatives with other parameters to produce a class of chemicals:

1. **HCD's *Search* module** – substructure search using PPD as the parent structure

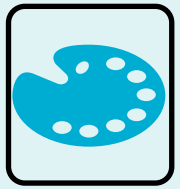
2. **Aromatic substitution reactivity** – effect of electron-donating and -withdrawing groups

3. **HCD's *ToxPrints* module** – removes QACs



[Hazard Comparison Dashboard (HCD), current version (U.S. EPA)]

Exposure: Production and Uses



PPD

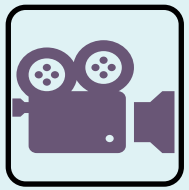
- Hair dye, photographic developing agent, chemical intermediate, vulcanization accelerator, rubber antioxidant

DPPD

- Antioxidant, polymerization inhibitor, copper degradation inhibitor, intermediate for dyes, drugs, plastics, and detergents

IPPD

- Antioxidant



PPPD

- Rubber, dyes, pharmaceuticals, photographic color production

44PD

- Used in gasoline as a gum inhibitor, antioxidant, and stabilizer

6PPD

- Antioxidant, antiozonant

7PPD

- Antioxidant, chemical reaction regulator

77PD

- Antioxidant

- 8 PPD derivatives are high-production volume (HPV) chemicals in the United States
- 100+ are reported to have been used in products

(HPV List, U.S. EPA), (CPDat, U.S. EPA)

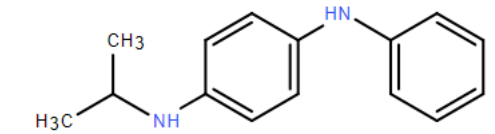
Exposure: PPDs are ubiquitous in the environment

- **13 PPD derivatives** and multiple quinones **have been detected in:**
  - Water (river, runoff, wastewater)
  - Sediment (urban river, estuary, coast, deep sea)
  - $PM_{2.5}$ and dust
  - Roadside soils

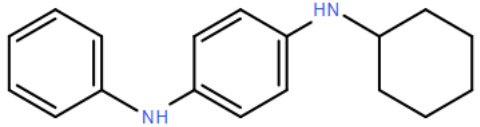
- Most exposure data is from China

If PPD derivatives were to replace 6PPD in tires, their worldwide use and emissions to the environment would increase

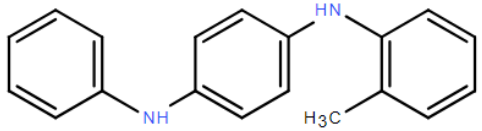
Exposure Highlight: Water



IPPD



CPPD



PTPD

Runoff[1]

Detected – CPPD, DPPD, DTPD, IPPD, 6PPD

River Water[2]

Detected – DPPD, DTPD, DNPD, 6PPD

Wastewater[3, 4]

Detected – DPPD, DTPD, IPPD, PTPD

[1]Cao et al. (2022), [2]Zhang et al. (2023), [3]Zhang et al. (2021), [4]Zhang et al. (2023)

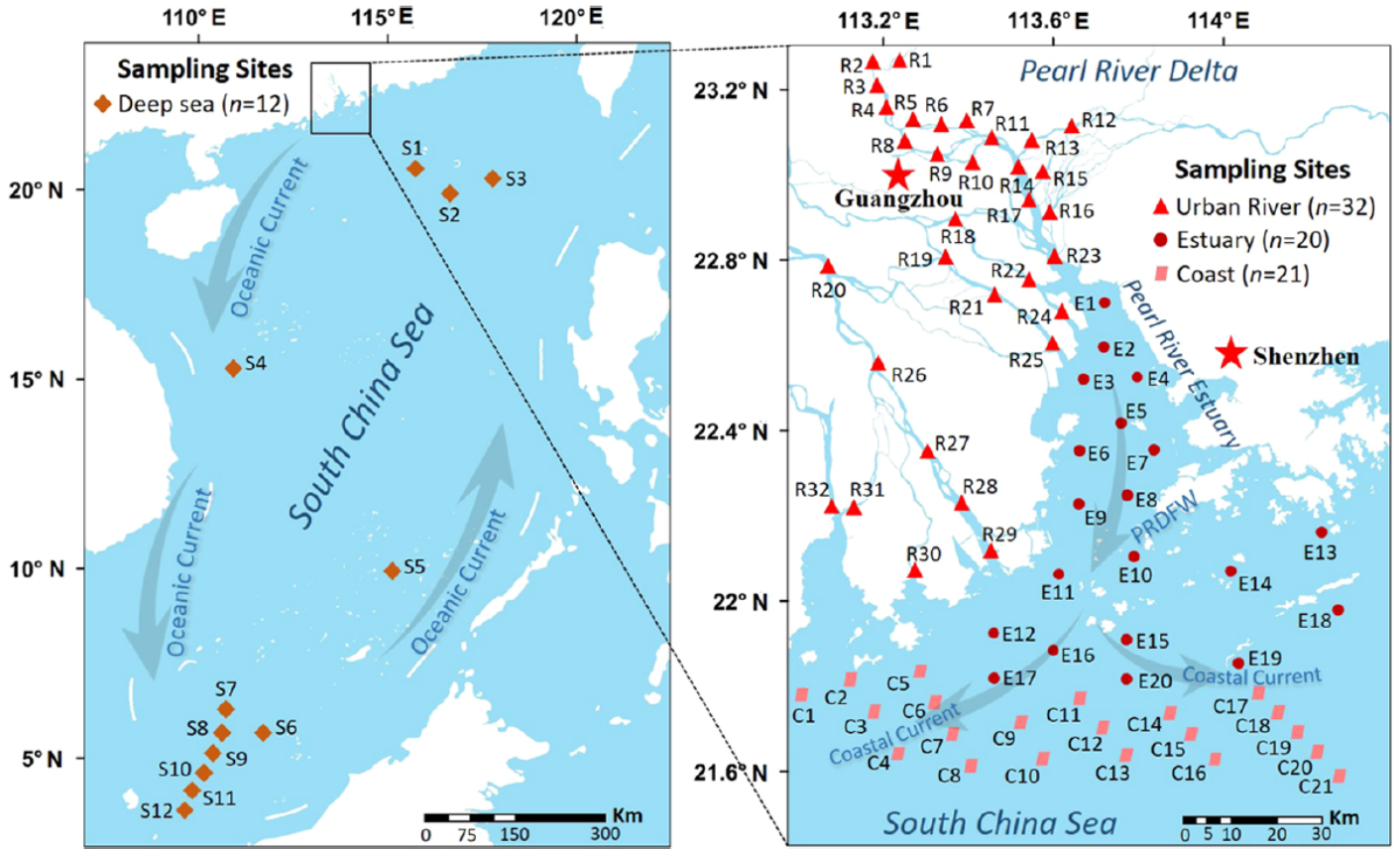
Exposure Highlight: Sediment

Pearl River Delta, China

- 8 of 8 PPD derivatives tested were detected in sediment

Pearl River Delta location	Median Total (ng/g, dw)	PPD Derivatives Detected
Urban River	39.7	8 of 8
Estuary	14.0	8 of 8
Coast	9.47	8 of 8
Deep-Sea	5.24	7 of 8

[Zeng et al. (2023)]



Σ[urban river] > Σ[estuary] > Σ[coast] > Σ[deep-sea]

Reliable Information for Adverse Impacts

- Evaluated structurally similar chemicals
- Extrapolated hazard information from "more-studied" PPD-derivatives
  - Empirical data from authoritative sources
    - U.S. EPA, FDA, CPSC, ECHA
  - U.S. EPA's Hazard Comparison Dashboard
    - Screening hazard scores based on various sources.
    - Quantitative Structure Activity Relationships (QSAR) Toxicity Estimation Software Tool (TEST)

Hazard Traits:

1) Wildlife Survival Impairment
2) Dermatotoxicity

Hazard Trait: Wildlife Survival Impairment

Acute aquatic toxicity

- Fish, invertebrates, algae
- Authoritative sources: ECHA, OECD

Hazard Endpoint	Description	L	M	H	vH	Total
Acute Aquatic Toxicity	n	196	293	501	715	1,705
	% of scores	11%	17%	29%	42%	100%

Hazard Trait: Dermatotoxicity

PPD is a strong sensitizer and may cause severe dermatitis

- Authoritative sources: ECHA's CLP, MAK Commission, Japan's NITE, Denmark

Hazard Endpoint	Description	L	M	H	vH	Total
Skin Sensitization	n	0	0	74	N/A	74
	% of scores	0%	0%	100%	N/A	100%

Summary of Findings

Candidate Chemical List

SCP may also add chemicals to the Candidate Chemicals List if they exhibit one or more hazard traits

Reliable Information

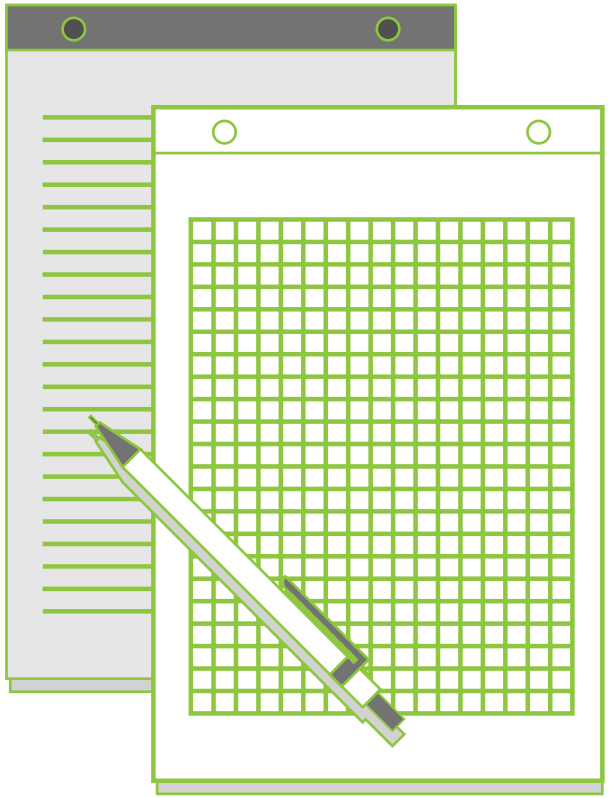
1. There are potential **exposures** to PPD derivatives — $PM_{2.5}$, dust, roadside soil, water, and sediment (for #1)
2. There is potential for one or more of these exposures to contribute to or cause **adverse impacts** — Wildlife Survival Impairment, Dermatotoxicity, or both (for #2)
3. SCP has considered the **extent and quality of information** that is available to substantiate the existence of these potential exposures and adverse impacts — Government reports, journal articles, and other scientific information (for #3)

California Code of Regulations, Title 22, section 69502.2(b) – Candidate Chemicals Identification

Extra Information for this Proposal

- For a detailed explanation, see the Technical Document for the Proposal to Add PPD Derivatives to the Candidate Chemicals List
- Our 45-day public comment period opened on October 2, 2023, and we will accept feedback until 11:59 PM PST on November 15, 2023
- Receive updates about the upcoming rulemaking by signing up for our SCP E-List
- Share a brief description of this proposal with the PPD Derivatives Summary Document
- Email us questions or comments at SaferConsumerProducts@dtsc.ca.gov

Other SCP Resources



- Workshop information—including this recording—will be available on our Workshops and Upcoming Events web page soon
- Celebrate the Safer Consumer Products Program's 10-year anniversary by visiting our Decade of Safer Consumer Products accomplishments page
- Visit the DTSC Green - YouTube Channel to learn more about other DTSC projects

Your feedback requested

1. Is our definition of PPD derivatives clear and unambiguous?

2. Have we demonstrated in a clear way how PPD derivatives meet the regulatory criteria for designation as a Candidate Chemical?

Question & Answer / Comment Period

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SAFER CONSUMER PRODUCTS (SCP)

Closing Remarks

Karl Palmer,
Deputy Director