# Aquatic toxicity of palladium: A grouping and readacross approach for some palladium substances and why others need separate assessments

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## INTRODUCTION

- Palladium (Pd) is used in catalysis and found in air, soil, and water
- Ecotoxicity Data: Limited data on algae, invertebrates, fish
- Alternative Assessment Approaches to facilitate ecotoxicological assessment

**Table 1:** Overview of key differences properties between read-across palladium substances and Palladium dinitrate, Palladium (II) di(4-oxopent-2-en-2-oate), and Palladium(II) Acetate. These distinctions explain the exclusion of the latter three Pd- compounds from the proposed grouping and read-across approach.

#### **Read-across Compounds**\*

Palladium dinitrate

Palladium (II) di(4-oxopent-2-en-2-oate)

Palladium (II) acetate

Туре	Inorganic	Inorganic	Organometallic (lipophile)	Organic metal salt
Ligand	e.g. Chloride; Ammonia	Nitrate	Acetylacetonate	Acetate
Expected aquatic respeciation	Respeciation to $Pd(OH)_2$	Hydrolysis to mixed aquato- nitrato species, ultimately forming Pd(OH) <sub>2</sub>	Slow and limited respeciation; retains molecular structure	Hydrolysis to mixed aquato-acetato species ultimately forming Pd(OH) <sub>2</sub>
Acute Toxicity (μg Pd/L (± sd)	Algae at 5.56 ± 2.6 μg/L Invertebrates at 50.6 ± 3.6 μg/L Fish at 267.8 ± 25.8 μg/L	Algae: 25.3 μg/L Invertebrate: 681.7 μg/L Fish: 46 516 μg/L	Algae: 28.3 μg/L Invertebrate: 75.9 μg/L Fish: 5.48 μg/L	Algae: 1.27 μg/L Invertebrate: 36 μg/L Fish: n.a.

## **STUDY OBJECTIVES**

- **Read-across:** Grouping Pd compounds by similar speciation
- Quantitative Ion Character-Activity Relationships (QICAR) modelling (Le Faucheur *et al.*, 2021)

## METHODS

- Literature Review (Klimisch score 1-2) and OECD/GLP compliant study reports from industry
- Collection of acute & chronic effective concentrations (EC50, EC10) of alga, invertebrates, and fish
- Identify outliers unsuitable for read-across
- Analyze Pd respeciation (freshwater) & establish grouping



#### Fig. 1: Boxplot of EC50 values grouped by algae (n =10), invertebrates (n=7), and fish (n=5). Outlier substances by IQR method depicted.



**Fig. 2:** Comparison of experimentally measured EC50 values (A) and QICAR modelled values (B) across three trophic levels for the grouped Pd compounds.

\* Read-across Compounds:

- simple inorganic Pd salts (e.g. Pd dichloride, Pd dihydroxide or Pd sulphate)
- tetraamminepalladium compounds
- tetra-and hexachloropalladium compounds
- mixed ammine/chloride salts (diamminedichloropalladium)

## **RESULTS & CONCLUSION**

#### 1. Toxicity Variations:

• Algae most sensitive species

#### • Outlier:

- Palladium (II) di(4-oxopent-2-en-2-oate) & Palladium dinitrate (Fig. 1)
- Palladium dinitrate (chronic; not shown)

### 2. Toxicity Variations:

• Prediction matches with measured values for algae and invertebrate, but conservative for fish (Fig. 2)

#### 3. Speciation Effects (Table 1):

- Grouped substances (inorganic Pd-salts): Respeciation in water to common Pd(OH)<sub>2</sub> species
- Palladium dinitrate: hydrolyzes to complexes with lower bioavailability & toxicity than grouped substances
- Palladium (II) di(4-oxopent-2-en-2-oate): limited respeciation; unique toxicity profile due to lipophilic mechanism
- Palladium (II) Acetate: speciation unclear, but comparable toxicity than grouped substances

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