

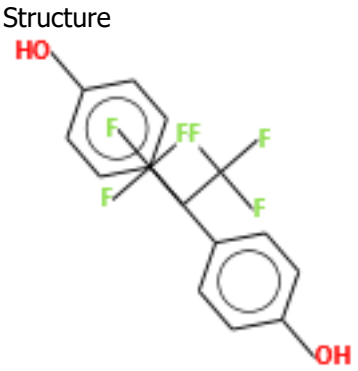
Read-across prediction report

Toolbox version: 4.8

Date: 24 Oct 2025

Author(s):

Contact details:

Target information		
Structural information	Numerical identifiers	Chemical names
SMILES: <chem>Oc1ccc(cc1)C(c1ccc(O)cc1)(C(F)(F)F)C(F)(F)F</chem> Structure 	CAS#: 1478-61-1 Other: EC Number:2160367	"4,4'- (hexafluoroisopropylidene)_diph enol" "4,4'- (hexafluoroisopropylidene)diphe nol" 4-[1,1,1,3,3,3-hexafluoro-2-(4- hydroxyphenyl)propan-2- yl]phenol

Prediction summary
Predicted endpoint: Human Health Hazards -> Sensitisation -> Skin -> in Vivo -> GPMT <OR> LLNA -> EC3 <OR> Skin sensitisation Predicted value: Negative [Skin sensitisation II (ECETOC)] Data gap filling method: Read-across analysis, Automated workflow for EC3 from LLNA or Skin sensitization from GPMT assays for defined approaches (SS AW for DASS) Applicability domain: In domain

Detailed information on analogues and data used for data gap filling is included in the attached Data matrix.

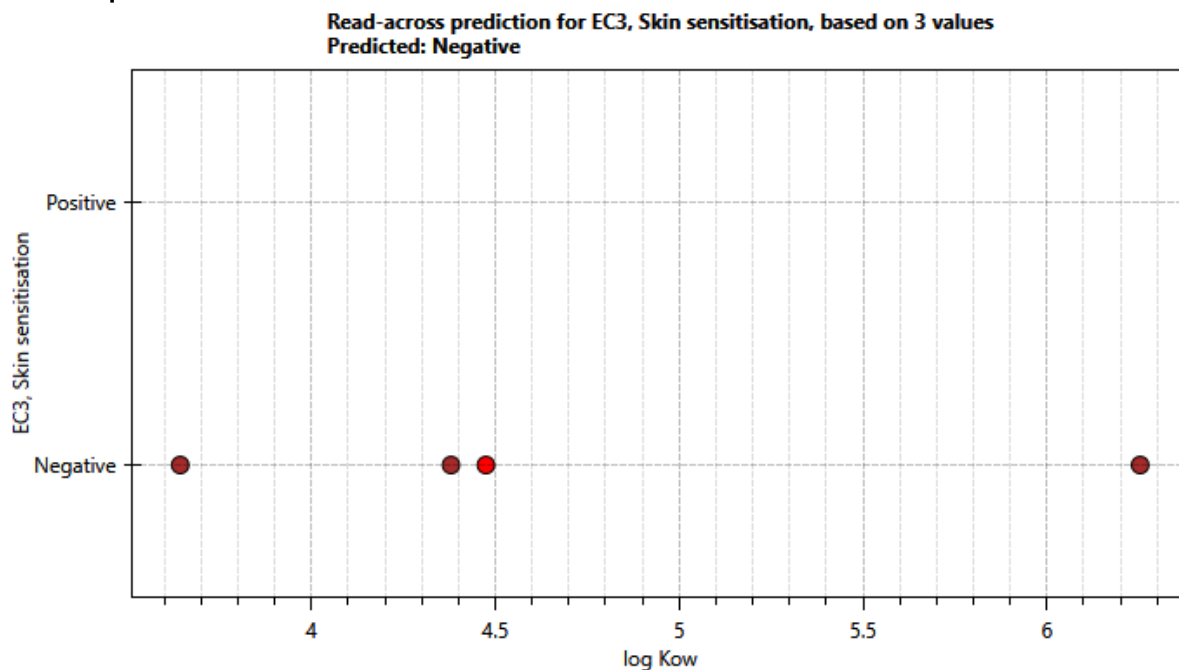
Prediction details

Predicted value: Negative [Skin sensitisation II (ECETOC)]

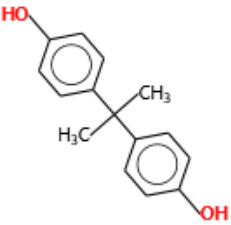
Applicability domain: In domain (DASS Overall domain: Negative-read-across)

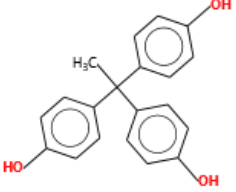
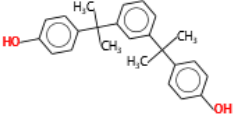
Predicted endpoint: Human Health Hazards -> Sensitisation -> Skin -> in Vivo -> GPMT <OR> LLNA -> EC3 <OR> Skin sensitisation

Prediction plot:



Values used for the prediction:

Structure	Experimental values used for the prediction (Maximal)	log Kow
CAS: 80-05-7 SMILES: <chem>CC(C)(c1ccc(O)cc1)c1ccc(O)cc1</chem> Name: bisphenol 	Negative	3.64

<p>CAS: 27955-94-8 SMILES: <chem>CC(c1ccc(O)cc1)(c1ccc(O)cc1)c1ccc(O)cc1</chem> Name: tris(hydroxyphenyl)ethane</p> 	Negative	4.38
<p>CAS: 13595-25-0 SMILES: <chem>CC(C)(c1ccc(O)cc1)c1ccc(c1)C(C)(C)c1ccc(O)cc1</chem> Name: 4,4'-(1,3-phenylenediisopropylidene)bisphenol</p> 	Negative	6.25
<p>Calculation approach: takes the highest mode value from the 3 nearest neighbours Active descriptor: log Kow (calculated) Data usage: Maximal value* *When multiple values are available for the same chemical, their maximal value is taken in prediction calculations</p>		

Prediction protocol (Inclusion criteria)

Input: CAS: 1478-61-1

Database(s) used:

- REACH Skin sensitisation database (normalised)
- Skin Sensitization

Selected endpoint: Human Health Hazards -> Sensitisation -> Skin -> in Vivo -> GPMT <OR> LLNA -> EC3 <OR> Skin sensitisation

Categorisation:

Primary categorisation

Profiler: US-EPA New Chemical Categories (not strict)

Target: Phenols (Acute toxicity)

Selection: Phenols (Acute toxicity)

Category: 188 chemicals with 371 experimental data

Sub-categorization steps

- Step 1: Filter data by metadata

Target: N/A

Selection: Data with metadata: "Qualifier = >" have been removed

Sub-category: 171 chemicals with 365 experimental data

- Step 2: Data usage options are changed to: Maximal

Sub-category: 171 chemicals with 171 experimental data

- Step 3:

Profiler: Substance type

Target: Discrete chemical; Mono constituent (predefined); Organic

Selection: Substances different from target are removed

Sub-category: 167 chemicals with 167 experimental data

- Step 4:

Profiler: Protein binding alerts for skin sensitization by OASIS

Target: No alert found

Selection: Substances different from target are removed

Sub-category: 133 chemicals with 133 experimental data

- Step 5:

Profiler: Protein binding alerts for skin sensitization by OASIS combined with Autoxidation simulator

Target and metabolites: No alert found

Selection: Substances different from target are removed

Sub-category: 65 chemicals with 65 experimental data

- Step 6:

Profiler: Protein binding alerts for skin sensitization by OASIS combined with Skin metabolism simulator

Target and metabolites: No alert found

Selection: Substances different from target are removed

Sub-category: 48 chemicals with 48 experimental data

- Step 7:

Profiler: Protein binding potency GSH

Target: Not possible to classify according to these rules (GSH)

Selection: Substances different from target are removed

Sub-category: 46 chemicals with 46 experimental data

- Step 8:

Profiler: Keratinocyte gene expression

Target: Not possible to classify according to these rules

Selection: Substances different from target are removed

Sub-category: 45 chemicals with 45 experimental data

- Step 9:

Profiler: Organic functional groups, Norbert Haider (checkmol)

Target: Alkyl fluoride; Alkyl halide; Aromatic compound; Halogen derivative; Hydroxy compound; Phenol

Selection: Substances different from target are removed

Sub-category: 8 chemicals with 8 experimental data

- Step 10:

Profiler: Structure similarity

Target: [90%,100%]

Selection: Substances different from target are removed except [60%,70%); [50%,60%); [70%,80%)

Sub-category: 4 chemicals with 4 experimental data

Data gap filling:

Calculation approach: takes the highest mode value from the 3 nearest neighbours, Active descriptor: log Kow (calculated), Data usage: Maximal value

References and explanations

Database information:

- [REACH Skin sensitisation database \(normalised\)](#)

Profilers information:

- [US-EPA New Chemical Categories](#)
- [Substance type](#)
- [Protein binding potency GSH](#)
- [Protein binding alerts for skin sensitization by OASIS](#)
- [Keratinocyte gene expression](#)

Profilers result information:

- [Phenols \(Acute toxicity\) \(US-EPA New Chemical Categories\)](#)
- [Discrete chemical \(Substance type\)](#)
- [Organic \(Substance type\)](#)
- [Mono constituent \(predefined\) \(Substance type\)](#)

Appendix: Specific report explanations

Specific information regarding the prediction

Table with profiling results for "Organic functional groups"

CAS	Structure	Results
1 CAS# 1478-61-1		Alkyl halide Aryl Phenol Perfluorocarbon derivatives
2 CAS# 27955-94-8		Aryl Phenol
3 CAS# 13595-25-0		Aryl Phenol
4 CAS# 80-05-7		Aryl Phenol

Structural functionalities, different from the target are colored in red.