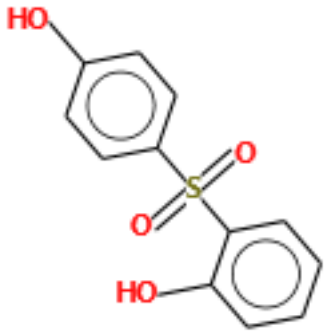
Read-across prediction report

Toolbox version: 4.8
Date: 24 Oct 2025
Author(s):
Contact details:

Target information

Structural information	Numerical identifiers	Chemical names
SMILES: Oc1ccc(cc1)S(=O)(=O)c1ccccc1O Structure 	CAS#: 5397-34-2 Other: EC Number:2264211	2-[(4-hydroxyphenyl)sulfonyl]phenol 2,4'-Dihydroxydiphenyl sulfone 2,4'-sulfonyldiphenol

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.

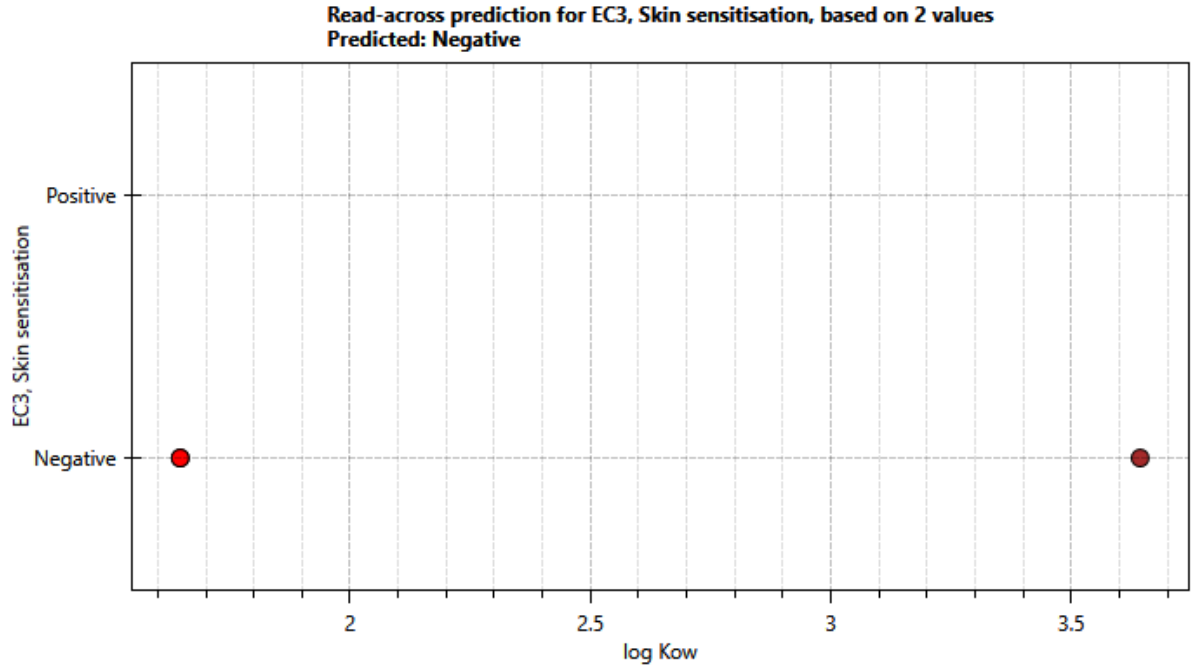
Prediction details

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

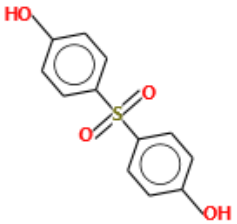
Applicability domain: In domain (DASS Overall domain: Negative-read-across)

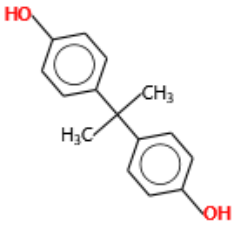
Predicted endpoint: Human Health Hazards -> Sensitisation -> Skin -> in Vivo -> GPMT <OR> LLNA -> EC3 <OR> Skin sensitisation

Prediction plot:



Values used for the prediction:

Structure	Experimental values used for the prediction (Maximal)	log Kow
CAS: 80-09-1 SMILES: Oc1ccc(cc1)S(=O)(=O)c1ccc(O)cc1 Name: BISPHENOL S 	Negative	1.65

CAS: 80-05-7 SMILES: CC(C)(c1ccc(O)cc1)c1ccc(O)cc1 Name: bisphenol 	Negative	3.64

Calculation approach: takes the highest mode value from the 2 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

Prediction protocol
(Inclusion criteria)

Input: CAS: 5397-34-2

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: Aromatic compound; Hydroxy compound; Phenol; Sulfone
Selection: Substances different from target are removed
Sub-category: 9 chemicals with 9 experimental data

- Step 10:
Profiler: Structure similarity
Target: [90%,100%]
Selection: Substances different from target are removed except [70%,80%); [50%,60%)
Sub-category: 3 chemicals with 3 experimental data

Data gap filling:
Calculation approach: takes the highest mode value from the 2 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

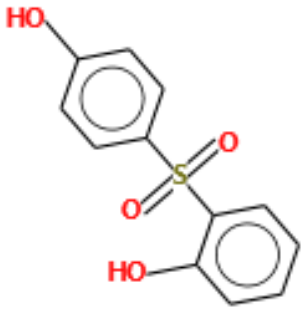
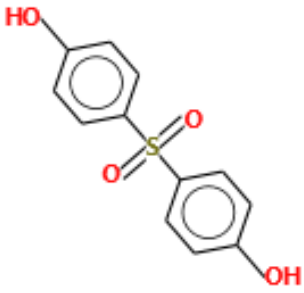
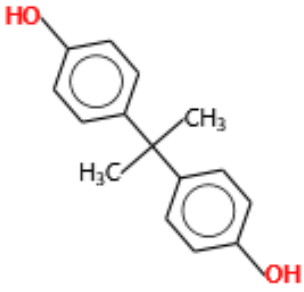
Profilers result information:

- 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# 5397-34-2		Sulfone Aryl Phenol
2 CAS# 80-09-1		Sulfone Aryl Phenol
3 CAS# 80-05-7		Aryl Phenol

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