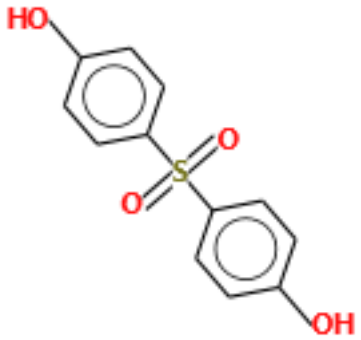
# Read-across prediction report

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

## Target information

| Structural information | Numerical identifiers | Chemical names |
|---|---|---|
| SMILES:<br>Oc1ccc(cc1)S(=O)(=O)c1ccc(O)cc1<br><br>Structure<br>  | CAS#: 80-09-1<br>Other: EC Number:2012505 | _Phenol,_4,4'-sulfonyldi-<br>"4,4'-sulfonyldiphenol"<br>4,4'-sulfonylbisphenol |



## 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.**

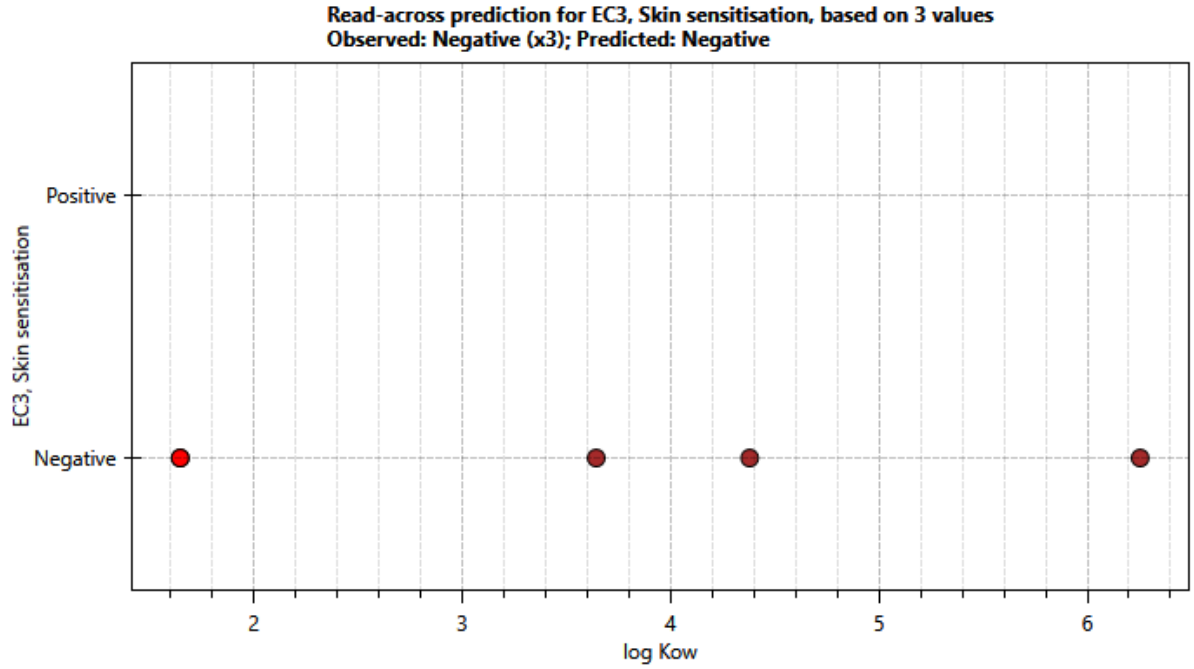
## Prediction details

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

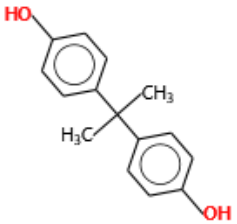
**Applicability domain:** In domain (DASS Overall domain: Negative-read-across)

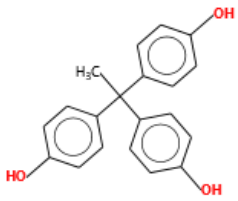
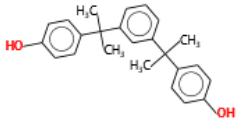
**Predicted endpoint:** Human Health Hazards -> Sensitisation -> Skin -> in Vivo -> GPMT <OR> LLNA -> EC3 <OR> Skin sensitisation

**Prediction plot:**




**Values used for the prediction:**

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

| | | |
|---|---|---|
| CAS: 27955-94-8<br>SMILES:<br>CC(c1ccc(O)cc1)(c1ccc(O)cc1)c1ccc(O)cc1<br>Name: tris(hydroxyphenyl)ethane<br>  | Negative | 4.38 |
| CAS: 13595-25-0<br>SMILES:<br>CC(C)(c1ccc(O)cc1)c1cccc(c1)C(C)(C)c1ccc(O)cc1<br>Name: 4,4'-(1,3-phenylenediisopropylidene)bisphenol<br>  | Negative | 6.25 |

**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

## Prediction protocol
(Inclusion criteria)

**Input:** CAS: 80-09-1

**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:** 187 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:** 170 chemicals with 365 experimental data

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

**Sub-category:** 170 chemicals with 170 experimental data

- Step 3:

**Profiler:** Substance type
**Target:** Discrete chemical; Mono constituent (predefined); Organic
**Selection:** Substances different from target are removed
**Sub-category:** 166 chemicals with 166 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:** 132 chemicals with 132 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:** 64 chemicals with 64 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:** 47 chemicals with 47 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:** 45 chemicals with 45 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:** 44 chemicals with 44 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:** 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

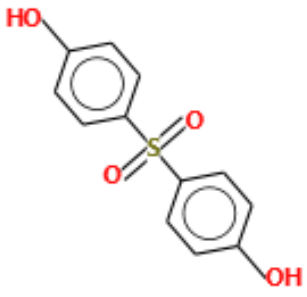
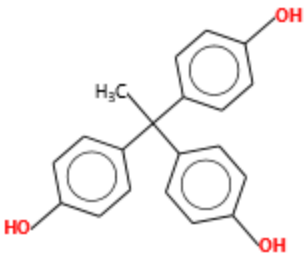
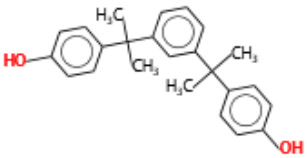
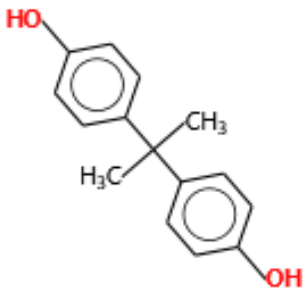
**Profilers result information:**

- 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# 80-09-1 |  | Sulfone<br>Aryl<br>Phenol |
| 2 CAS# 27955-94-8 |  | Aryl<br>Phenol |
| 3 CAS# 13595-25-0 |  | Aryl<br>Phenol |
| 4 CAS# 80-05-7 |  | Aryl<br>Phenol |

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