

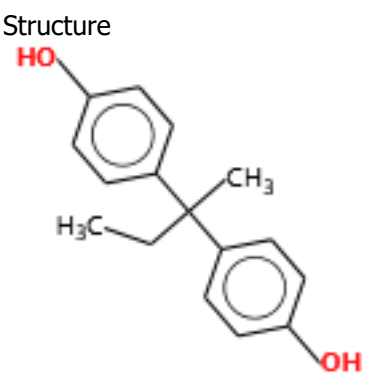
## Read-across prediction report

Toolbox version: 4.8

Date: 24 Oct 2025

Author(s):

Contact details:

Target information		
Structural information	Numerical identifiers	Chemical names
SMILES: <chem>CCC(C)(c1ccc(O)cc1)c1ccc(O)cc1</chem>  Structure 	CAS#: 77-40-7 Other: EC Number:2010251	2,2-Bis-(4-hydroxyphenyl)-butane 2,2-Bis(4-hydroxyphenyl)-n-butan = Bisphenol B 2,2-bis(4-hydroxyphenyl)butane

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

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

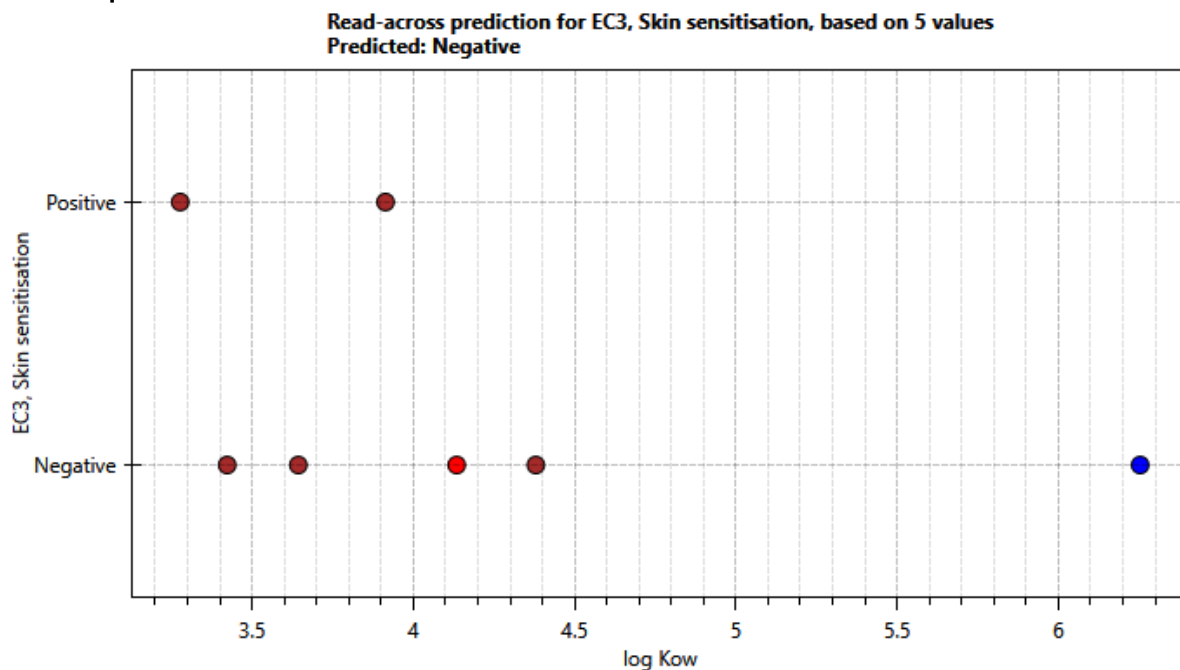
### Prediction details

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

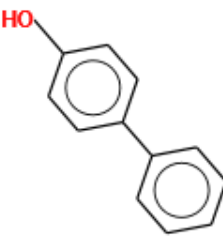
**Applicability domain:** In domain (DASS Overall domain: Negative-read-across)

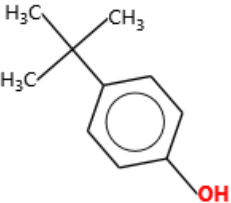
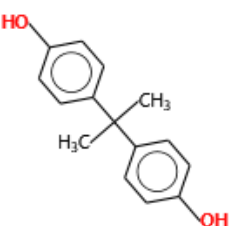
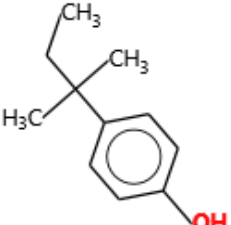
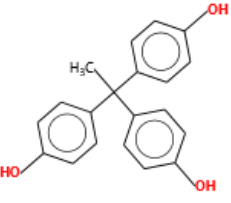
**Predicted endpoint:** Human Health Hazards -> Sensitisation -> Skin -> in Vivo -> GPMT <OR> LLNA -> EC3 <OR> Skin sensitisation

**Prediction plot:**



**Values used for the prediction:**

Structure	Experimental values used for the prediction (Maximal)	log Kow
CAS: 92-69-3 SMILES: <chem>Oc1ccc(cc1)-c1ccccc1</chem> Name: 4-biphenylol 	Positive	3.28

<p>CAS: 98-54-4 SMILES: <chem>CC(C)(C)c1ccc(O)cc1</chem> Name: Butylphen</p> 	Negative	3.42
<p>CAS: 80-05-7 SMILES: <chem>CC(C)(c1ccc(O)cc1)c1ccc(O)cc1</chem> Name: bisphenol</p> 	Negative	3.64
<p>CAS: 80-46-6 SMILES: <chem>CCC(C)(C)c1ccc(O)cc1</chem> Name: 4-tert-Amylphenol</p> 	Positive	3.91
<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><b>Calculation approach:</b> takes the highest mode value from the 5 nearest neighbours  <b>Active descriptor:</b> log Kow (calculated)  <b>Data usage:</b> 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: 77-40-7

**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:** Organic functional groups, Norbert Haider (checkmol) (not strict)

**Target:** Hydroxy compound AND Phenol AND Aromatic compound

**Selection:** Hydroxy compound AND Phenol AND Aromatic compound

**Category:** 295 chemicals with 482 experimental data

Sub-categorization steps

- Step 1: Filter data by metadata

**Target:** N/A

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

**Sub-category:** 257 chemicals with 472 experimental data

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

**Sub-category:** 257 chemicals with 257 experimental data

- Step 3:

**Profiler:** Substance type

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

**Selection:** Substances different from target are removed

**Sub-category:** 231 chemicals with 231 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:** 188 chemicals with 188 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:** 105 chemicals with 105 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:** 76 chemicals with 76 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:** 74 chemicals with 74 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:** 66 chemicals with 66 experimental data

- Step 9:

**Profiler:** Organic functional groups (US EPA)

**Target:** Aliphatic Carbon [-CH<sub>2</sub>-]; Aliphatic Carbon [-CH<sub>3</sub>]; Aliphatic Carbon [CH]; Aliphatic Carbon, two phenyl attach [-C-]; Aromatic Carbon [C]; Hydroxy, aromatic attach [-OH]; Oxygen, one aromatic attach [-O-]

**Selection:** Substances different from target are removed

**Sub-category:** 11 chemicals with 11 experimental data

- Step 10:

**Profiler:** Structure similarity

**Target:** [90%,100%]

**Selection:** Substances different from target are removed except [70%,80%); [50%,60%); [60%,70%); [80%,90%)

**Sub-category:** 7 chemicals with 7 experimental data

**Data gap filling:**

Calculation approach: takes the highest mode value from the 5 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](#)
- [Aquatic toxicity classification by ECOSAR](#)
- [Keratinocyte gene expression](#)

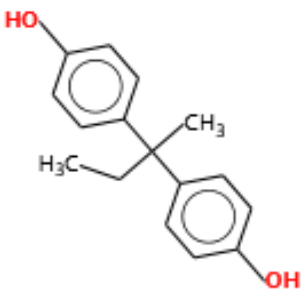
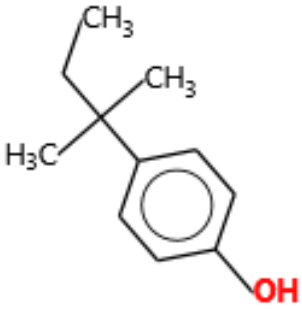
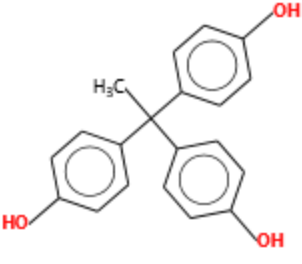
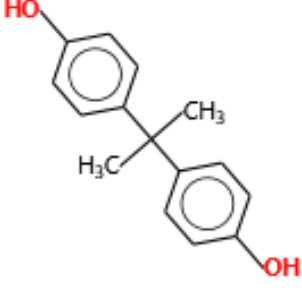
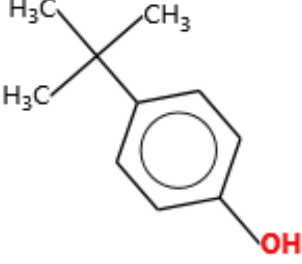
**Profilers result information:**

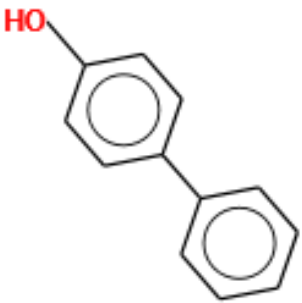
- [Phenols \(Acute toxicity\) \(US-EPA New Chemical Categories\)](#)
- [Discrete chemical \(Substance type\)](#)
- [Organic \(Substance type\)](#)
- [Mono constituent \(predefined\) \(Substance type\)](#)
- [Phenols, Poly \(Aquatic toxicity classification by ECOSAR\)](#)

## Appendix: Specific report explanations

Specific information regarding the prediction

Table with profiling results for "Organic functional groups"

CAS	Structure	Results
1 CAS# 77-40-7		Aryl Phenol
2 CAS# 80-46-6		Aryl Phenol Alkyl (hetero)arenes Alkyl-, alkenyl- and alkynyl (hetero)arenes
3 CAS# 27955-94-8		Aryl Phenol
4 CAS# 80-05-7		Aryl Phenol
5 CAS# 98-54-4		Aryl Phenol tert-Butyl Alkyl (hetero)arenes Alkyl-, alkenyl- and alkynyl (hetero)arenes

6 CAS# 92-69-3	 <p>The image shows the chemical structure of 4-phenylphenol, which consists of two benzene rings connected by a single bond. The top ring has a hydroxyl group (-OH) attached to it, highlighted in red. The bottom ring is a plain benzene ring.</p>	Aryl Phenol Biphenyl
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*Structural functionalities, different from the target are colored in red.*