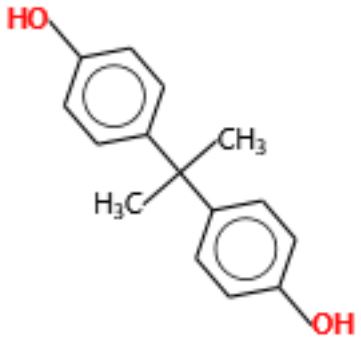
Read-across prediction report

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

Target information

Structural information	Numerical identifiers	Chemical names
SMILES: CC(C)(c1ccc(O)cc1)c1ccc(O)cc1 Structure  	CAS#: 80-05-7 Other: EC Number:2012458	"bisphenol a" "phenol, 4,4'-(1-methylethylidene)bis-;2,2-bis (4'-hydroxyphenyl) propane;bisphenol a;diphenylolpropane;bis-phenol a;bisphenol;phenol, 4,4 -(1-methylethylidene)bis-;phenol, 4,4-(1-methylethylidene)bis-;4,4'-isopropylidenediphenol;bisphenol a (bpa);4,4'-propane-2,2-diyldiphenol;bisphenola(4,4?isopropylidenediphenol);4,4'-(1-methylethylidene)bisphenol;phenol, 4,4'-isopropylidenedi-;2,2-bis(4-hydroxyphenyl)propane" 2,2-bis (4'-hydroxyphenyl) propane

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.

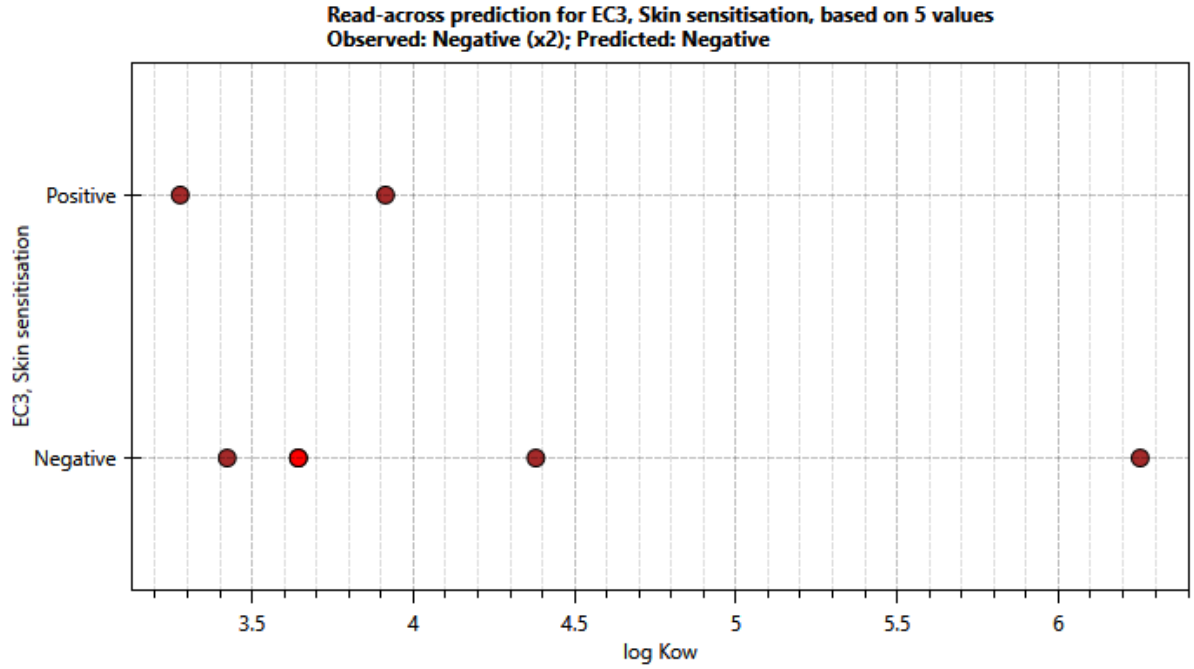
Prediction details

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

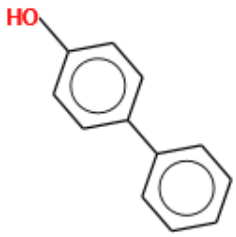
Applicability domain: In domain (DASS Overall domain: Negative-read-across)

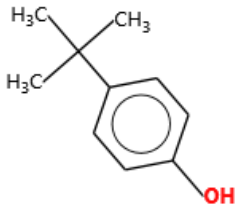
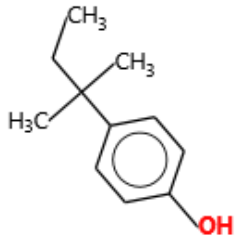
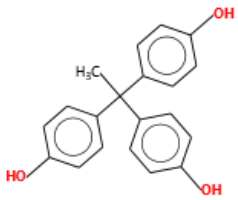
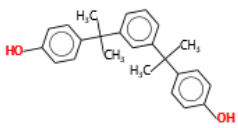
Predicted endpoint: Human Health Hazards -> Sensitisation -> Skin -> in Vivo -> GPMT <OR> LLNA -> EC3 <OR> Skin sensitisation

Prediction plot:



Values used for the prediction:

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

CAS: 98-54-4 SMILES: CC(C)(C)c1ccc(O)cc1 Name: Butylphen 	Negative	3.42
CAS: 80-46-6 SMILES: CCC(C)(C)c1ccc(O)cc1 Name: 4-tert-Amylphenol 	Positive	3.91
CAS: 27955-94-8 SMILES: CC(c1ccc(O)cc1)(c1ccc(O)cc1)c1ccc(O)cc1 Name: tris(hydroxyphenyl)ethane 	Negative	4.38
CAS: 13595-25-0 SMILES: CC(C)(c1ccc(O)cc1)c1cccc(c1)C(C)(C)c1ccc(O)cc1 Name: 4,4'-(1,3-phenylenediisopropylidene)bisphenol 	Negative	6.25

Calculation approach: takes the highest mode value from the 5 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: 80-05-7

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: 294 chemicals with 483 experimental data

Sub-categorization steps

- Step 1: Filter data by metadata

Target: N/A
Selection: Data with metadata: "Qualifier = >" have been removed
Sub-category: 256 chemicals with 473 experimental data

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

Sub-category: 256 chemicals with 256 experimental data

- Step 3:

Profiler: Substance type
Target: Discrete chemical; Mono constituent (predefined); Organic
Selection: Substances different from target are removed
Sub-category: 230 chemicals with 230 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: 187 chemicals with 187 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: 104 chemicals with 104 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: 75 chemicals with 75 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: 73 chemicals with 73 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: 65 chemicals with 65 experimental data

- Step 9:
Profiler: Organic functional groups (US EPA)
Target: Aliphatic Carbon [-CH2-]; Aliphatic Carbon [-CH3]; 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: 10 chemicals with 10 experimental data

- Step 10:
Profiler: Structure similarity
Target: [90%,100%]
Selection: Substances different from target are removed except [70%,80%); [50%,60%); [60%,70%)
Sub-category: 6 chemicals with 6 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

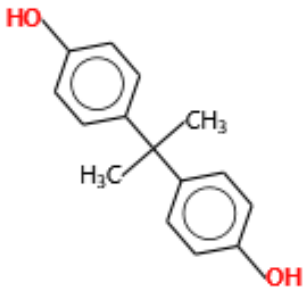
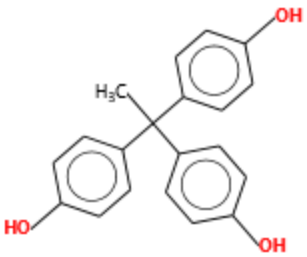
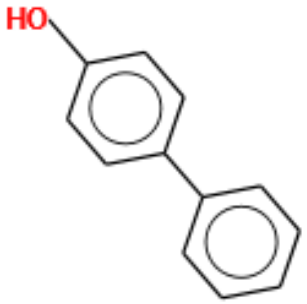
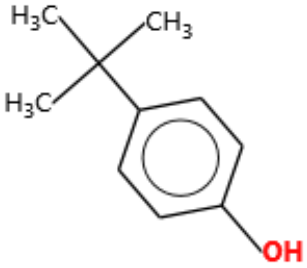
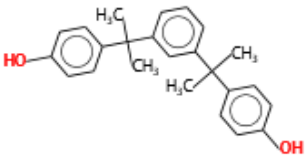
Profilers result information:

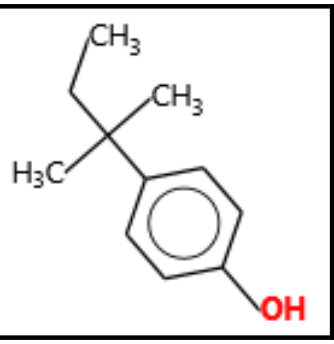
- Phenols (Acute toxicity) (US-EPA New Chemical Categories)
- Discrete chemical (Substance type)
- Organic (Substance type)
- Mono constituent (predefined) (Substance type)
- Phenols, Poly (Aquatic toxicity classification by ECOSAR)

Appendix: Specific report explanations

Specific information regarding the prediction

Table with profiling results for "Organic functional groups"

CAS	Structure	Results
1 CAS# 80-05-7		Aryl Phenol
2 CAS# 27955-94-8		Aryl Phenol
3 CAS# 92-69-3		Aryl Phenol Biphenyl
4 CAS# 98-54-4		Aryl Phenol tert-Butyl Alkyl (hetero)arenes Alkyl-, alkenyl- and alkynyl (hetero)arenes
5 CAS# 13595-25-0		Aryl Phenol

6 CAS# 80-46-6		Aryl Phenol Alkyl (hetero)arenes Alkyl-, alkenyl- and alkynyl (hetero)arenes

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