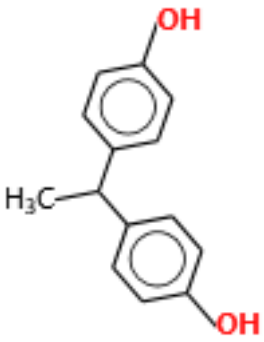
Read-across prediction report

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

Target information

Structural information	Numerical identifiers	Chemical names
SMILES: CC(c1ccc(O)cc1)c1ccc(O)cc1  Structure	CAS#: 2081-08-5 Other: N/A	"4,4'-ETHYLIDENEBISPHENOL" 1,1-Bis(4-hydroxyphenyl)ethane 4,4’-ethylidene bisphenol

Prediction summary

Predicted endpoint: Human Health Hazards -> Sensitisation -> Skin -> in Vivo -> LLNA -> EC3

Predicted value: Positive [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.

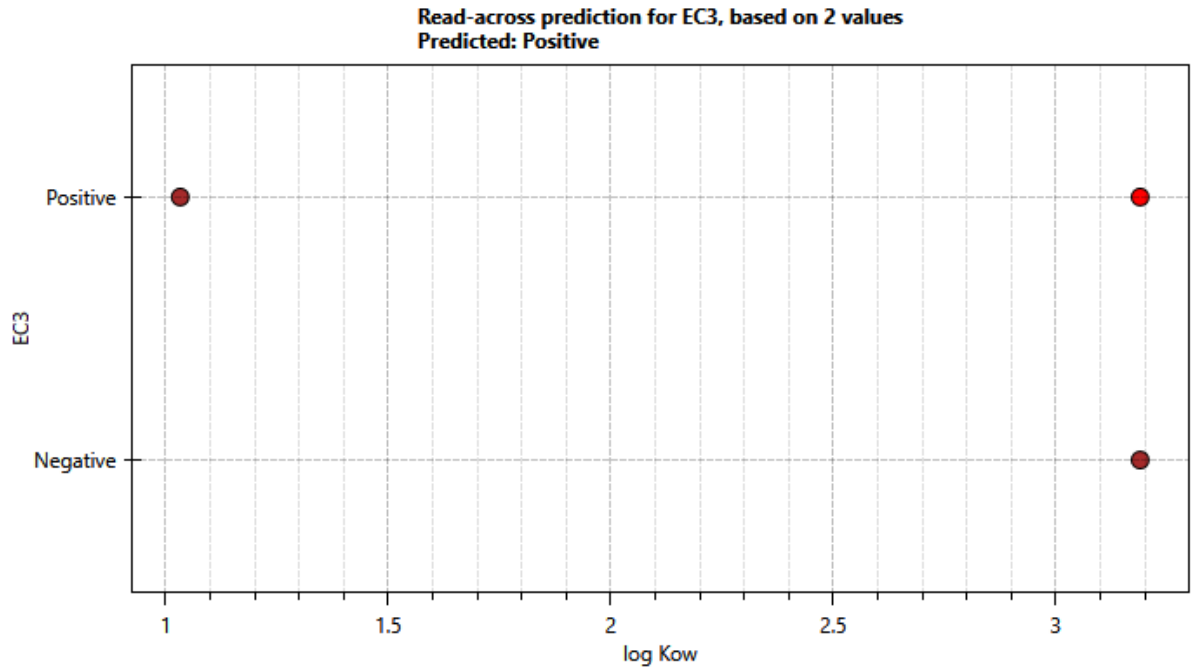
Prediction details

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

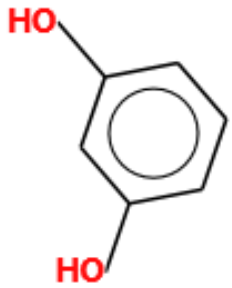
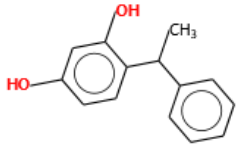
Applicability domain: In domain (DASS Overall domain: Positive)

Predicted endpoint: Human Health Hazards -> Sensitisation -> Skin -> in Vivo -> LLNA -> EC3

Prediction plot:



Values used for the prediction:

Structure	Experimental values used for the prediction (Maximal)	log Kow
CAS: 108-46-3 SMILES: Oc1cccc(O)c1 Name: resorcin 	Positive	1.03
CAS: 85-27-8 SMILES: CC(c1ccccc1)c1ccc(O)cc1O Name: 4-(1-phenylethyl)benzene-1,3-diol 	Negative	3.19

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: 2081-08-5

Database(s) used:
- REACH Skin sensitisation database (normalised)
- Skin Sensitization

Selected endpoint: Human Health Hazards -> Sensitisation -> Skin -> in Vivo -> LLNA -> EC3

Categorisation:
Primary categorisation
Profiler: Protein binding alerts for skin sensitization by OASIS combined with Autoxidation simulator (not strict)
Target: No alert found (parent) AND Radical reactions >> Free radical formation >> Hydroperoxides (metabolites) AND Michael Addition >> Michael addition on quinoid type compounds >> Quinone methide(s)/imines; Quinoide oxime structure; Nitroquinones, Naphthoquinone(s)/imines (metabolites)
Selection: Hydroperoxides AND Quinone methide(s)/imines; Quinoide oxime structure; Nitroquinones, Naphthoquinone(s)/imines
Category: 58 chemicals with 94 experimental data

Sub-categorization steps
- Step 1: Data usage options are changed to: Maximal

Sub-category: 42 chemicals with 42 experimental data

- Step 2:

Profiler: Substance type
Target: Discrete chemical; Mono constituent (predefined); Organic
Selection: Substances different from target are removed
Sub-category: 41 chemicals with 41 experimental data

- Step 3:

Profiler: Protein binding alerts for skin sensitization by OASIS
Target: No alert found
Selection: Substances different from target are removed
Sub-category: 33 chemicals with 33 experimental data

- Step 4:

Profiler: Protein binding alerts for skin sensitization by OASIS combined with Autoxidation simulator
Target and metabolites: Michael Addition >> Michael addition on quinoid type compounds >> Quinone methide(s)/imines; Quinoide oxime structure; Nitroquinones, Naphthoquinone(s)/imines; No alert found; Radical reactions >> Free radical formation >> Hydroperoxides
Selection: Substances different from target are removed
Sub-category: 21 chemicals with 21 experimental data

- Step 5:
Profiler: Protein binding alerts for skin sensitization by OASIS combined with Skin metabolism simulator
Target and metabolites: Michael Addition >> Michael addition on quinoid type compounds >> Quinone methide(s)/imines; Quinoide oxime structure; Nitroquinones, Naphthoquinone(s)/imines; No alert found
Selection: Substances different from target are removed except No metabolites
Sub-category: 13 chemicals with 13 experimental data

- Step 6:
Profiler: Structure similarity
Target: [90%,100%]
Selection: Substances different from target are removed except [60%,70%); [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)
- Skin Sensitization

Profilers information:

- Substance type
- Protein binding alerts for skin sensitization by OASIS

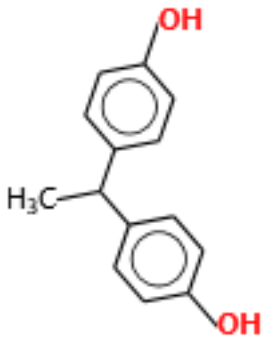
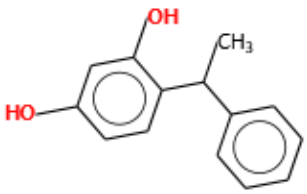
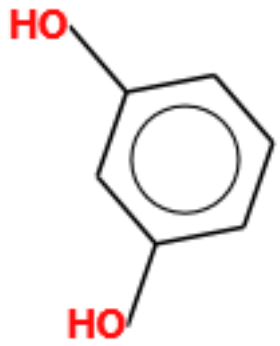
Profilers result information:

- Discrete chemical (Substance type)
- Organic (Substance type)
- Mono constituent (predefined) (Substance type)
- Michael Addition >> Michael addition on quinoid type compounds >> Quinone methide(s)/imines; Quinoide oxime structure; Nitroquinones, Naphthoquinone(s)/imines (Protein binding alerts for skin sensitization by OASIS)
- Radical reactions >> Free radical formation >> Hydroperoxides (Protein binding alerts for skin sensitization by OASIS)

Appendix: Specific report explanations

Specific information regarding the prediction

Table with profiling results for "Organic functional groups"

CAS	Structure	Results
1 CAS# 2081-08-5		Aryl Phenol
2 CAS# 85-27-8		Aryl Phenol
3 CAS# 108-46-3		Aryl Phenol

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