

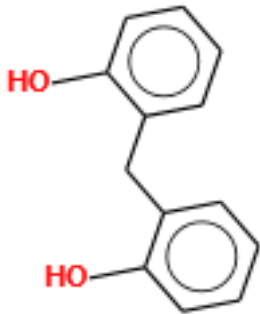
Read-across prediction report

Toolbox version: 4.8

Date: 24 Oct 2025

Author(s):

Contact details:

Target information		
Structural information	Numerical identifiers	Chemical names
SMILES: <chem>Oc1ccccc1Cc1ccccc1O</chem>	CAS#: 2467-02-9 Other: EC Number:2195782	2-(2-hydroxybenzyl)-phenol 2,2'-methanedioldiphenol 2,2'-Methylenebisphenol
 Structure		

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.

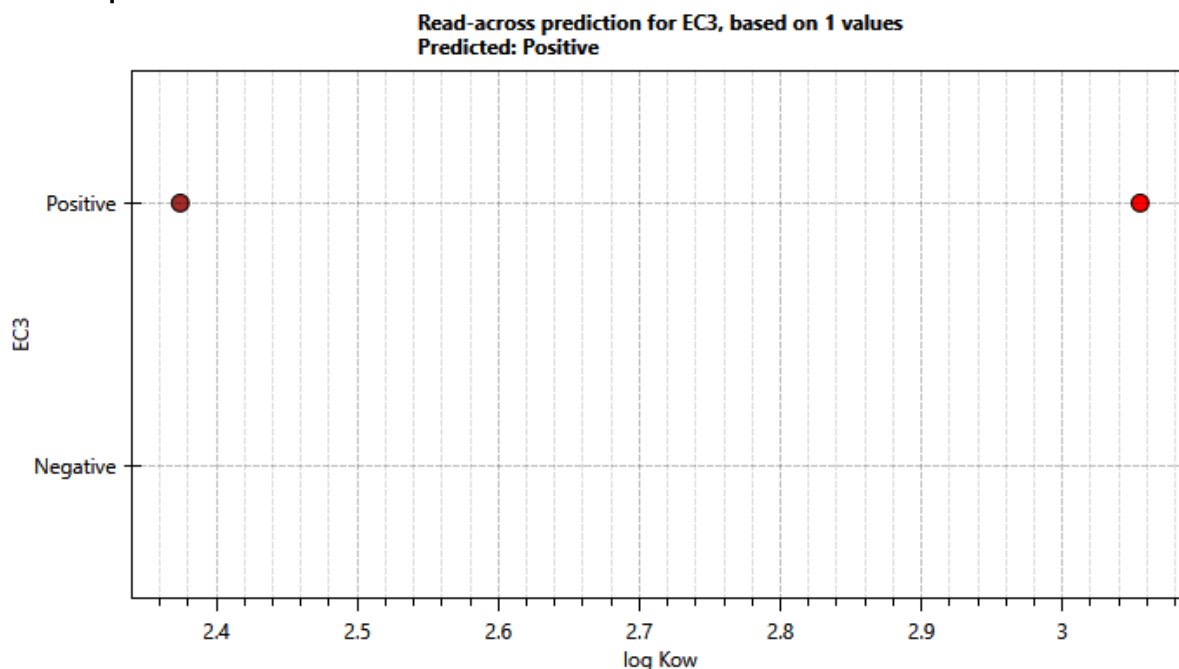
Prediction details

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

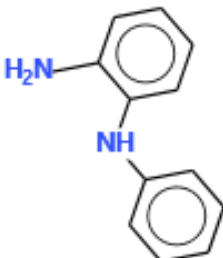
Applicability domain: In domain (DASS Overall domain: Positive)

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: 534-85-0 SMILES: <chem>Nc1cccc1Nc1cccc1</chem> Name: AMINODIPHENYLAMINE, 2- 	Positive	2.37

Calculation approach: takes the highest mode value from the 1 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: 2467-02-9

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 Michael Addition >> Michael addition on quinoid type compounds >> Quinone methide(s)/imines; Quinoide oxime structure; Nitroquinones, Naphthoquinone(s)/imines (metabolites)

Selection: Quinone methide(s)/imines; Quinoide oxime structure; Nitroquinones, Naphthoquinone(s)/imines

Category: 179 chemicals with 308 experimental data

Sub-categorization steps

- Step 1: Data usage options are changed to: Maximal

Sub-category: 130 chemicals with 130 experimental data

- Step 2:

Profiler: Substance type

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

Selection: Substances different from target are removed

Sub-category: 121 chemicals with 121 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: 108 chemicals with 108 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

Selection: Substances different from target are removed

Sub-category: 71 chemicals with 71 experimental data

- Step 5:

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: 8 chemicals with 8 experimental data

- Step 6:

Profiler: Structure similarity

Target: [90%,100%]

Selection: Substances different from target are removed except [50%,60%)

Sub-category: 2 chemicals with 2 experimental data

Data gap filling:

Calculation approach: takes the highest mode value from the 1 nearest neighbours, Active descriptor: log Kow (calculated), Data usage: Maximal value

References and explanations

Database information:

- [Skin Sensitization](#)

Profilers information:

- [Substance type](#)
- [Protein binding alerts for skin sensitization by OASIS](#)

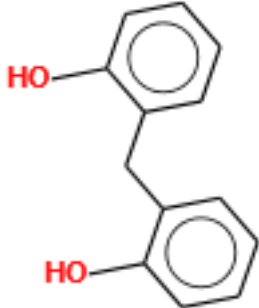
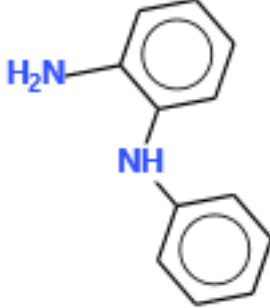
Profilers result information:

- [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 \(Protein binding alerts for skin sensitization by OASIS\)](#)

Appendix: Specific report explanations

Specific information regarding the prediction

Table with profiling results for "Organic functional groups"

CAS	Structure	Results
1 CAS# 2467-02-9		Aryl Phenol Precursors quinoid compounds
2 CAS# 534-85-0		Aryl Precursors quinoid compounds Amine, primary Amine, secondary Aniline

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