QSAR Toolbox prediction for single chemical

Date: 7 Nov 2022
Author(s):
Contact details:

Target information

Structural information	Numerical identifiers	Chemical names
SMILES: CCCCC=CC=O Structure 	CAS#: 2463-63-0 Other: EC Number:3791712	2-Heptenal hept-2-enal

Prediction summary

Predicted endpoint: Gene mutation; No effect specified; Salmonella typhimurium; No duration specified; No guideline specified

Predicted value: Negative

Unit/scale: Gene mutation I

Data gap filling method: Read-across analysis

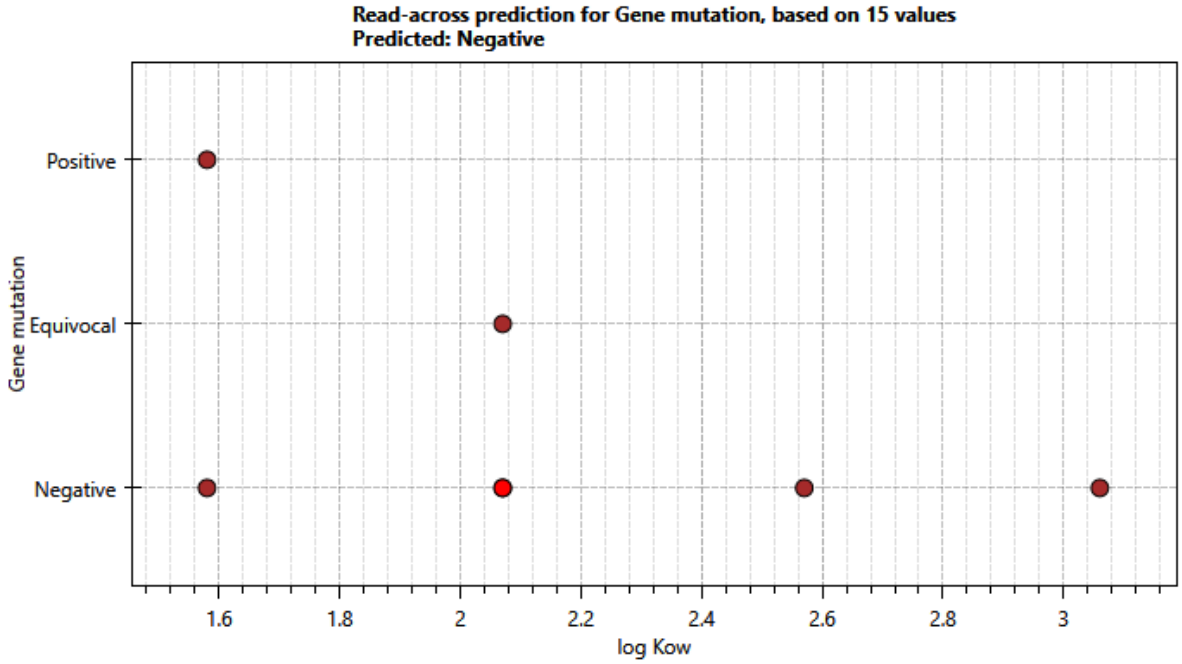
Summary: *manually editable field*
Not provided by the user

Prediction details (I)

Predicted value: Negative

Predicted endpoint (OECD Principle 1 - Defined endpoint): Human Health Hazards -> Genetic Toxicity -> Gene mutation -> Without S9 -> Salmonella typhimurium -> Bacterial Reverse Mutation Assay (e.g. Ames Test) -> in Vitro

Prediction plot:



Calculation approach (OECD principle 2 - Unambiguous algorithm): takes the highest mode value from the nearest 5 neighbours

Active descriptor: log Kow (calculated)

Data usage: All values*

*When multiple values are available for the same chemical, all of them are taken individually in prediction calculations

Prediction details (II)

Uncertainty of the prediction (OECD principle 4 - Uncertainty of the prediction):

The prediction is based on 15 values, 12 of them (80.0%) equal to predicted value

Prediction confidence is measured by the p-value: 0.000285

Strain coverage[1]:

-S9 : 2 strain(s) missing

+S9 : 2 strain(s) missing

Strain	-S9	+S9
TA 1535*	0/0	0/0
TA 1537*	0/0	0/0
TA 97*	0/0	0/0
TA 97A*	4/0	2/0
TA 98*	4/0	0/0
TA 100*	7/0	4/0
TA 102*	0/0	2/0
WP2 UvrA*	0/0	0/0
WP2 UvrA (pKM101)*	0/0	0/0
TA 104	6/2	4/0
TA100	0/2	0/0

Negative/Positive

*strain relevant for OECD TG 471

[1]The recommended combination of strains according to OECD TG 471 is S. typhimurium :

1. TA1535, and
2. TA1537 or TA97 or TA97a, and
3. TA98, and
4. TA100, and
5. TA102 or E. coli WP2 uvrA, or E. coli WP2 uvrA (pKM101)

Strain information comments: *manually editable field*

Not provided by the user

Mechanistic interpretation: *manually editable field*

Not provided by the user

Adequacy of the prediction: *manually editable field*

Not provided by the user

Target profiles (OECD principle 5 - Chemical and biological mechanisms)	
Profiles used for grouping/subcategorization	
No alert found (DNA alerts for AMES by OASIS) (primary grouping)	No alert found
DNA binding by OASIS (subcategorization)	AN2; AN2 >> Nucleophilic addition to alpha, beta-unsaturated carbonyl compounds; AN2 >> Nucleophilic addition to alpha, beta-unsaturated carbonyl compounds >> Alpha, Beta-Unsaturated Aldehydes; AN2 >> Schiff base formation; AN2 >> Schiff base formation >> Alpha, Beta-Unsaturated Aldehydes
in vitro mutagenicity (Ames test) alerts by ISS (subcategorization)	alpha,beta-unsaturated carbonyls
Organic functional groups (subcategorization)	Alkene; Allyl; apha,beta-Unsaturated aldehyde
Structure similarity (subcategorization)	[90%,100%]
log Kow (calculated): 2.07	

Analogue(s) selection

(OECD principle 3 - Applicability domain)

Database(s) used:

- Bacterial mutagenicity ISSSTY
- Genotoxicity OASIS

Category boundaries (applicability domain):

- Active descriptor(s) range:	
- log Kow: from 1.58 to 3.06	target chemical is in domain
- Response range:	
- Gene mutation: from Negative to Positive	

Profilers:

- No alert found (DNA alerts for AMES by OASIS) (primary grouping)	target chemical is in domain
- DNA binding by OASIS (subcategorization)	target chemical is in domain
- in vitro mutagenicity (Ames test) alerts by ISS (subcategorization)	target chemical is in domain
- Organic functional groups (subcategorization)	target chemical is in domain
- Structure similarity (subcategorization)	target chemical is in domain

Additional data pruning:

none

Manually eliminated data points:

none

Data matrix report
Options of data matrix report are listed in a separate excel file