



Report



Prediction and Applicability Domain analysis for models:

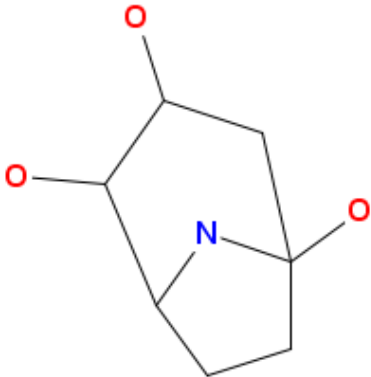




Mutagenicity (Ames test) model (SarPy/IRFMN) 1.0.7

Core version: 1.2.4



1. Prediction Summary

Prediction for compound Molecule 0

 The chemical structure of Molecule 0 is a bicyclic compound. It features a six-membered ring fused to a five-membered ring. The six-membered ring has two oxygen atoms (red) at the 1 and 4 positions. The five-membered ring contains a nitrogen atom (blue) at the 2 position and an oxygen atom (red) at the 5 position.	<p>Prediction:  Reliability:   </p> <p>Prediction is Mutagenic, but the result shows some critical aspects, which require to be checked:</p> <ul style="list-style-type: none">- only moderately similar compounds with known experimental value in the training set have been found- accuracy of prediction for similar molecules found in the training set is not optimal- some similar molecules found in the training set have experimental values that disagree with the predicted value <p>The following relevant fragments have been found: SM98; SM163</p>
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Compound: Molecule 0

Compound SMILES: OC2CC1(O)(NC(CC1)C2(O))

Experimental value: -

Predicted Mutagen activity: Mutagenic

No. alerts for mutagenicity: 1

No. alerts for non-mutagenicity: 1

Structural alerts: SM98; SM163

Reliability: the predicted compound could be out of the Applicability Domain of the model

Remarks:

none

3.1 Applicability Domain:

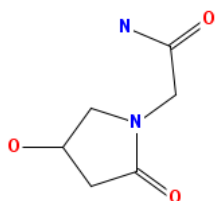
Similar Compounds, with Predicted and Experimental Values



	<p>Compound #1</p> <p>CAS: 112653-29-9 Dataset id: 2595 (Test set) SMILES: <chem>OCC(NC1CC(O)(CO)C(O)C(O)C1(O))CO</chem> Similarity: 0.805</p> <p>Experimental value: NON-Mutagenic Predicted value: NON-Mutagenic</p> <p>Alerts (found also in the target): SM163</p> <p>Alerts (not found in the target): SM169; SM182</p>
	<p>Compound #2</p> <p>CAS: 89911-79-5 Dataset id: 3770 (Training set) SMILES: <chem>O=NN(CC(O)C)CC(O)CO</chem> Similarity: 0.793</p> <p>Experimental value: Mutagenic Predicted value: Mutagenic</p> <p>Alerts (not found in the target): SM2; SM103</p>
	<p>Compound #3</p> <p>CAS: 2226-96-2 Dataset id: 248 (Training set) SMILES: <chem>ON1C(C)(C)CC(O)CC1(C)C</chem> Similarity: 0.792</p> <p>Experimental value: Mutagenic Predicted value: NON-Mutagenic</p> <p>Alerts (found also in the target): SM163</p> <p>Alerts (not found in the target): SM182</p>
	<p>Compound #4</p> <p>CAS: 122-20-3 Dataset id: 3709 (Training set) SMILES: <chem>OC(C)CN(CC(O)C)CC(O)C</chem> Similarity: 0.787</p> <p>Experimental value: NON-Mutagenic Predicted value: NON-Mutagenic</p> <p>Alerts (not found in the target): SM155; SM176</p>
	<p>Compound #5</p> <p>CAS: 110-97-4 Dataset id: 864 (Training set) SMILES: <chem>OC(C)CNCC(O)C</chem> Similarity: 0.782</p> <p>Experimental value: NON-Mutagenic Predicted value: Possible NON-Mutagenic</p>

3.1 Applicability Domain:

Similar Compounds, with Predicted and Experimental Values



Compound #6

CAS: 62613-82-5

Dataset id: 1784 (Training set)

SMILES: O=C(N)CN1C(=O)CC(O)C1

Similarity: 0.781

Experimental value: NON-Mutagenic

Predicted value: NON-Mutagenic

Alerts (not found in the target): SM156; SM176

3.2 Applicability Domain: Measured Applicability Domain Scores



Global AD Index

AD index = 0.728

Explanation: the predicted compound could be out of the Applicability Domain of the model.

Similar molecules with known experimental value

Similarity index = 0.797

Explanation: only moderately similar compounds with known experimental value in the training set have been found.

Accuracy of prediction for similar molecules

Accuracy index = 0.669

Explanation: accuracy of prediction for similar molecules found in the training set is not optimal.

Concordance for similar molecules

Concordance index = 0.662

Explanation: some similar molecules found in the training set have experimental values that disagree with the predicted value.

Atom Centered Fragments similarity check

ACF index = 1

Explanation: all atom centered fragment of the compound have been found in the compounds of the training set.

Symbols explanation:



The feature has a good assessment, model is reliable regarding this aspect.



The feature has a non optimal assessment, this aspect should be reviewed by an expert.



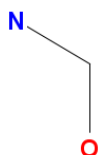
The feature has a bad assessment, model is not reliable regarding this aspect.

4.1 Reasoning: Relevant Chemical Fragments and Moieties



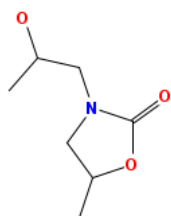
(Molecule 0) Reasoning on fragments/structural alerts - 1 of 2:

Fragment found: SM98



Sarpy alert n. 98 for Mutagenicity, defined by the SMARTS: C(O)N

Following, the most similar compounds from the model's dataset having the same fragment.

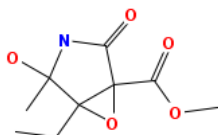


CAS: 3375-84-6
Dataset id: 1637 (Test set)
SMILES: O=C1OC(C)CN1CC(O)C
Similarity: 0.774

Experimental value: NON-Mutagenic
Predicted value: Mutagenic

Alerts (found also in the target): SM98

Alerts (not found in the target): SM94; SM155; SM156; SM176



CAS: 142438-63-9
Dataset id: 2715 (Training set)
SMILES: O=C(OC)C12(OC2(CC)(C(O)(NC1(=O))C))
Similarity: 0.724

Experimental value: Mutagenic
Predicted value: Mutagenic

Alerts (found also in the target): SM98

Alerts (not found in the target): SM27; SM92; SM97; SM182; SM202



CAS: 142438-62-8
Dataset id: 2394 (Training set)
SMILES: O=C(OC)C12(OC2(C)(C(O)(NC1(=O))C))
Similarity: 0.721

Experimental value: Mutagenic
Predicted value: Mutagenic

Alerts (found also in the target): SM98

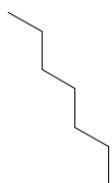
Alerts (not found in the target): SM27; SM92; SM97; SM182; SM202

4.1 Reasoning: Relevant Chemical Fragments and Moieties



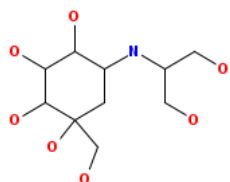
(Molecule 0) Reasoning on fragments/structural alerts - 2 of 2:

Fragment found: SM163



Sarpy alert n. 163 for NON-Mutagenicity, defined by the SMARTS: CCCCCC

Following, the most similar compounds from the model's dataset having the same fragment.

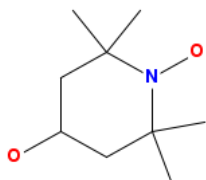


CAS: 112653-29-9
Dataset id: 2595 (Test set)
SMILES: OCC(NC1CC(O)(CO)C(O)C(O)C1(O))CO
Similarity: 0.805

Experimental value: NON-Mutagenic
Predicted value: NON-Mutagenic

Alerts (found also in the target): SM163

Alerts (not found in the target): SM169; SM182

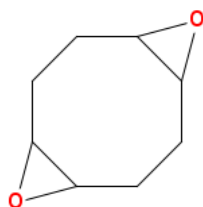


CAS: 2226-96-2
Dataset id: 248 (Training set)
SMILES: ON1C(C)(C)CC(O)CC1(C)C
Similarity: 0.792

Experimental value: Mutagenic
Predicted value: NON-Mutagenic

Alerts (found also in the target): SM163

Alerts (not found in the target): SM182



CAS: 286-75-9
Dataset id: 1286 (Training set)
SMILES: O1C2CCC3OC3(CCC12)
Similarity: 0.755

Experimental value: NON-Mutagenic
Predicted value: Mutagenic

Alerts (found also in the target): SM163

Alerts (not found in the target): SM97