



# Report



**Prediction and Applicability Domain analysis for models:**

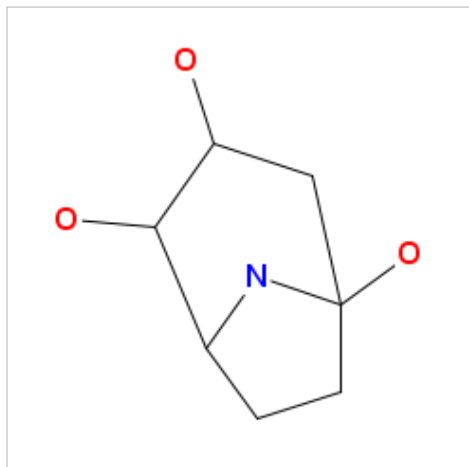
**Mutagenicity (Ames test) model (CAESAR) 2.1.13**

Core version: 1.2.4



## 1. Prediction Summary

### Prediction for compound Molecule 0



Prediction:

Reliability:

**Prediction is Mutagenic, but the result shows some critical aspects, which require to be checked:**

- only moderately similar compounds with known experimental value in the training set have been found
- some similar molecules found in the training set have experimental values that disagree with the predicted value

Compound: Molecule 0

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

Experimental value: -

Predicted Mutagen activity: Mutagenic

Structural alerts: -

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

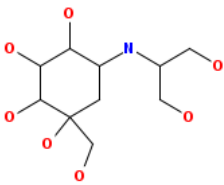
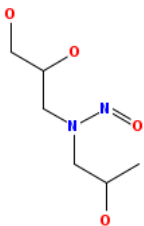
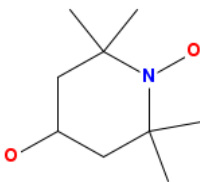
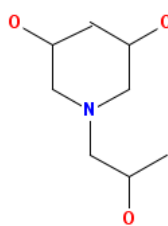
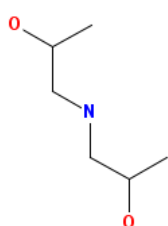
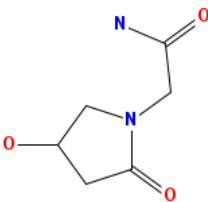
Remarks:

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>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): SA21 Alkyl and aryl N-nitroso groups</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: Mutagenic</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>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: NON-Mutagenic</p>
	<p>Compound #6</p> <p>CAS: 62613-82-5 Dataset id: 1784 (Training set) SMILES: <chem>O=C(N)CN1C(=O)CC(O)C1</chem> Similarity: 0.781</p> <p>Experimental value: NON-Mutagenic Predicted value: NON-Mutagenic</p>

## 3.2 Applicability Domain: Measured Applicability Domain Scores



### Global AD Index

AD index = 0.805

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 = 1

Explanation: accuracy of prediction for similar molecules found in the training set is good.

### 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.

### Model's descriptors range check

Descriptors range check = True

Explanation: descriptors for this compound have values inside the descriptor range of the compounds of the training set.

### 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.