



# Report



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

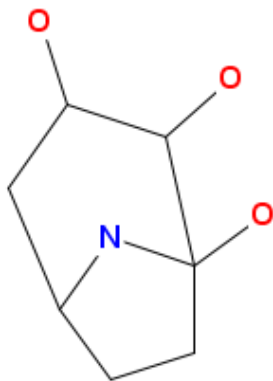
**Mutagenicity (Ames test) CONSENSUS model 1.0.2**

Core version: 1.2.4



## 1. Prediction Summary

### Prediction for compound Molecule 1



Prediction:

**Prediction is NON-Mutagenic with a consensus score of 0.25, based on 4 models.**

Compound: Molecule 1

Compound SMILES: OC2CC1NC(O)(CC1)C2(O)

Used models: 4

Predicted Consensus Mutagen activity: NON-Mutagenic

Mutagenic Score: 0.15

Non-Mutagenic Score: 0.25

Model Caesar assessment: NON-Mutagenic (low reliability)

Model ISS assessment: NON-Mutagenic (low reliability)

Model SarPy assessment: Mutagenic (moderate reliability)

Model KNN assessment: NON-Mutagen (moderate reliability)

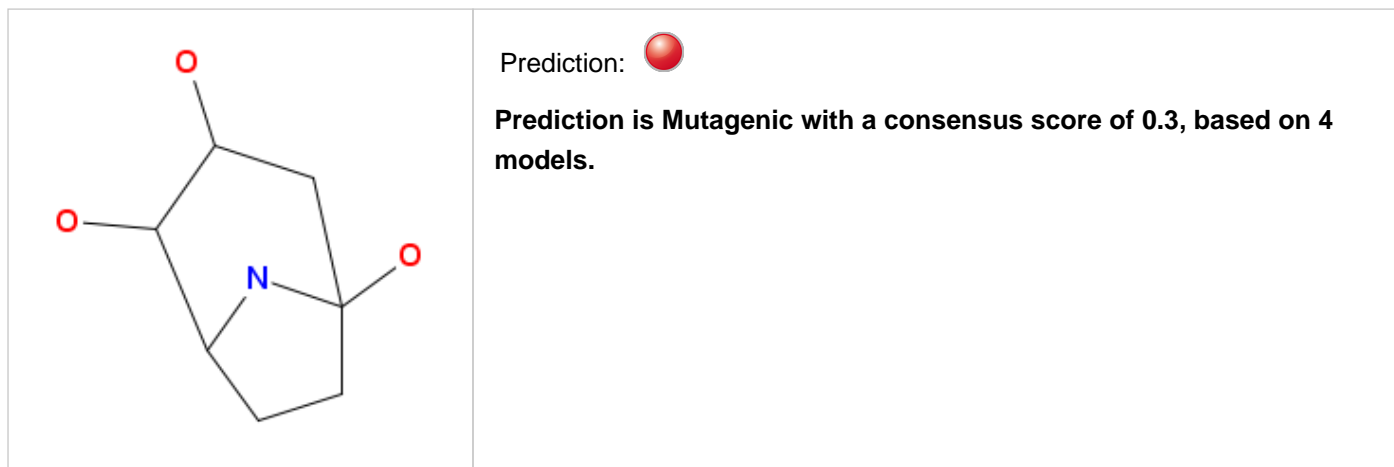
Remarks:

none



## 1. Prediction Summary

### Prediction for compound Molecule 1



Compound: Molecule 1

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

Used models: 4

Predicted Consensus Mutagen activity: Mutagenic

Mutagenic Score: 0.3

Non-Mutagenic Score: 0.2

Model Caesar assessment: Mutagenic (moderate reliability)

Model ISS assessment: NON-Mutagenic (low reliability)

Model SarPy assessment: Mutagenic (moderate reliability)

Model KNN assessment: NON-Mutagen (moderate reliability)

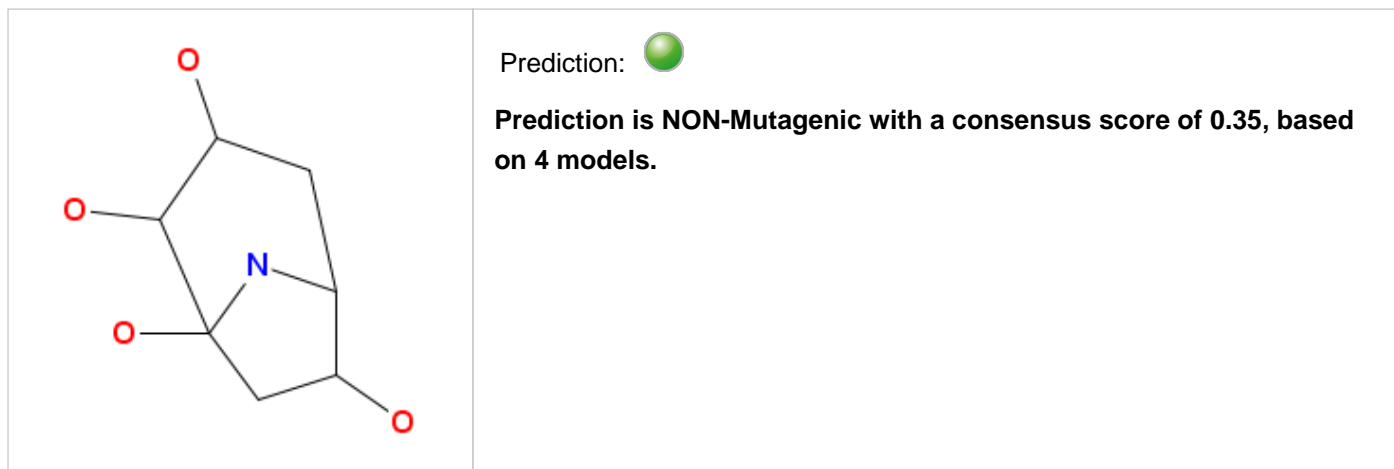
Remarks:

none



## 1. Prediction Summary

### Prediction for compound Molecule 2



Compound: Molecule 2

Compound SMILES: OC2CC1NC(O)(CC1(O))C2(O)

Used models: 4

Predicted Consensus Mutagen activity: NON-Mutagenic

Mutagenic Score: 0.15

Non-Mutagenic Score: 0.35

Model Caesar assessment: NON-Mutagenic (moderate reliability)

Model ISS assessment: NON-Mutagenic (low reliability)

Model SarPy assessment: Mutagenic (moderate reliability)

Model KNN assessment: NON-Mutagen (moderate reliability)

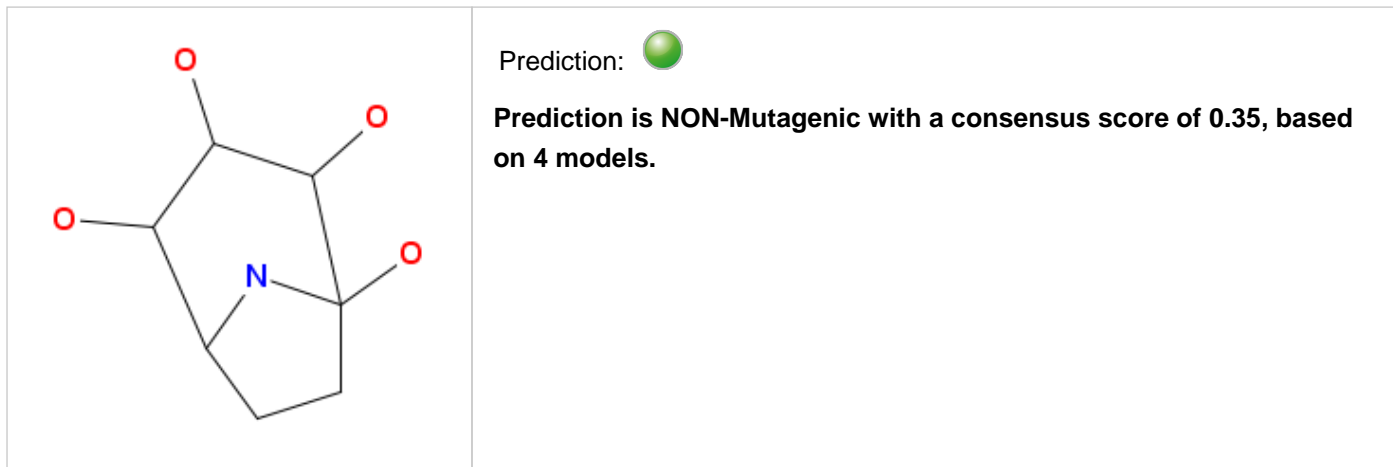
Remarks:

none



## 1. Prediction Summary

### Prediction for compound Molecule 3



Compound: Molecule 3

Compound SMILES: OC2C(O)C(O)C1(O)(NC2(CC1))

Used models: 4

Predicted Consensus Mutagen activity: NON-Mutagenic

Mutagenic Score: 0.15

Non-Mutagenic Score: 0.35

Model Caesar assessment: NON-Mutagenic (moderate reliability)

Model ISS assessment: NON-Mutagenic (low reliability)

Model SarPy assessment: Mutagenic (moderate reliability)

Model KNN assessment: NON-Mutagen (moderate reliability)

Remarks:

none