

Table 1 Toxtree predictions

Name	Smiles	Toxtree (carcinogenicity&mutagenicity by ISS)	Toxtree (in vitro mutagenicity (AMES) by ISS)	Toxtree (in Vivo MN in rodents)
Calysteg in A3	<chem>O[C@H]1[C@@H](O)C2(O)CCC(N2)C1</chem>	Negative for genotox carcinogenicity Negative for nongenotox carcinogenicity	No alerts	QSA34*
Calysteg in A5	<chem>O[C@@H]1[C@@H](O)C[C@]2(O)CC[C@H]1N2</chem>	Negative for genotox carcinogenicity Negative for nongenotox carcinogenicity	No alerts	QSA34
Calysteg in B1	<chem>C1[C@H]2[C@@H](C[C@](N2)([C@H]([C@@H]1O)O)O)O</chem>	Negative for genotox carcinogenicity Negative for nongenotox carcinogenicity	No alerts	QSA34
Calysteg in B2	<chem>O[C@@H]1[C@@H](O)[C@H](O)[C@]2(O)CC[C@H]1N2</chem>	Negative for genotox carcinogenicity Negative for nongenotox carcinogenicity	No alerts	QSA34
Calysteg in B3	<chem>C1C[C@@]2([C@@H]([C@@H]([C@H]([C@H]1N2)O)O)O)O</chem>	Negative for genotox carcinogenicity Negative for nongenotox carcinogenicity	No alerts	QSA34
Calysteg in B4	<chem>O[C@H]1[C@@H](O)[C@H](O)[C@]2(O)CC[C@H]1N2</chem>	Negative for genotox carcinogenicity Negative for nongenotox carcinogenicity	No alerts	QSA34

* QSA34.H-acceptor-path3-H-acceptor

Table 2 VEGA predictions

Name	Smiles	Vega consensus (combined CAESAR, SarPy, ISS and kNN)
Calystegin A3	<chem>O[C@H]1[C@@H](O)C2(O)CCC(N2)C1</chem>	Non-mutagenic 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)
Calystegin A5	<chem>O[C@@H]1[C@@H](O)C[C@]2(O)CC[C@H]1N2</chem>	Mutagenic

		<p>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)</p>
Calystegin B1	<chem>C1[C@H]2[C@@H](C[C@](N2)([C@H]([C@@H]1O)O)O)O</chem>	<p>Non-mutagenic</p> <p>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)</p>
Calystegin B2	<chem>O[C@@H]1[C@@H](O)[C@H](O)[C@]2(O)CC[C@H]1N2</chem>	<p>Non-mutagenic</p> <p>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)</p>
Calystegin B3	<chem>C1C[C@@]2([C@@H]([C@@H]([C@H]([C@H]1N2)O)O)O)O</chem>	<p>Non-mutagenic</p> <p>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)</p>
Calystegin B4	<chem>O[C@H]1[C@@H](O)[C@H](O)[C@]2(O)CC[C@H]1N2</chem>	<p>Non-mutagenic</p> <p>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)</p>