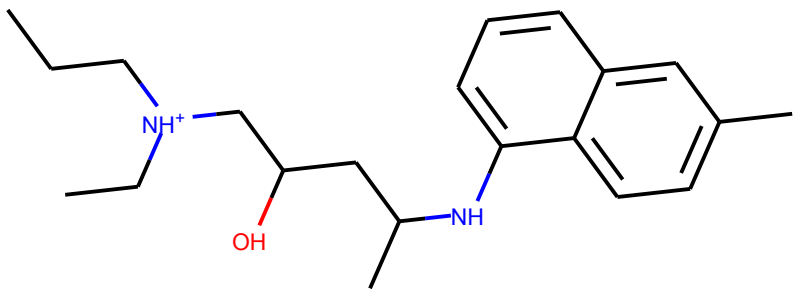


In Silico Predicted Toxic Properties

Molecule Depiction



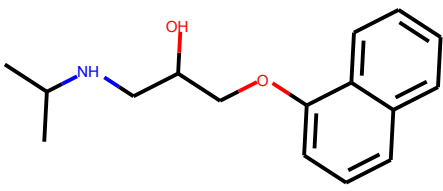
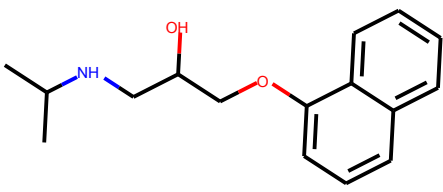
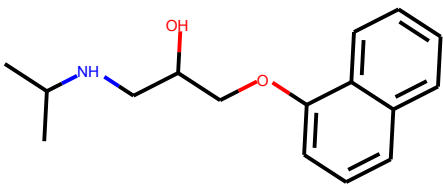
Mol

Molecule properties:

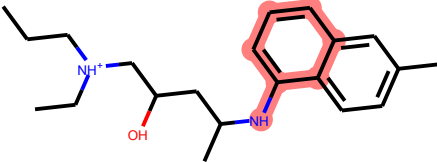
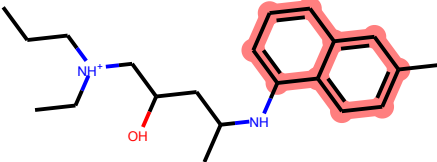
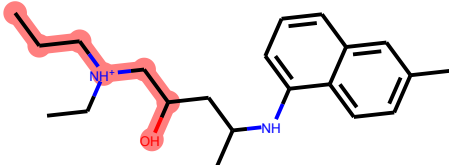
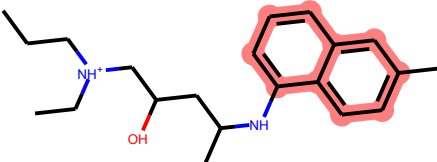
Property	Value
Num Aliphatic Carbocycles	0
Num Heteroatoms	3
Num Hydrogen Bond Acceptor	2
Num Aromatic Carbocycles	2
LogP	3.014
Num Rotatable Bonds	9
Num Aromatic Heterocycles	0
Num Lipinski HB Donor	3
Num Atoms	24
Num Lipinski HB Acceptor	3
Num Rings	2
Num Hydrogen bond Donor	3

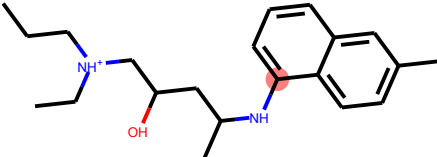
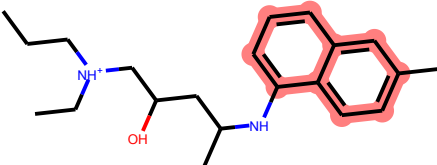
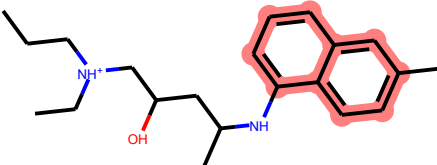
Property	Value
Num Aliphatic Rings	0
Num Aliphatic Heterocycles	0
Num Heterocycles	0
Mol Wt	329.259
Labute ASA	146.231
Num Aromatic Rings	2
Topological Polar SA	36.7

Potential Toxicity:

Index	Action	Injury	Confidence	Similar active compound in database
000	Differential cytotoxicity (isogenic chicken DT40 cell lines)	Genotoxicity	0.994	
001	Differential cytotoxicity (isogenic chicken DT40 Rev3 mutant cell line)	Genotoxicity	0.99	
002	Differential cytotoxicity against isogenic chicken DT40 cell lines with known DNA damage response pathways - Rad54/Ku70 mutant cell line	Genotoxicity	0.994	

Toxic substructure:

Index	Alert Name	Structure
000	Alert from Top200 Drug	 <chem>CCN(CC)CC[C@H](O)CC[C@H](Nc1ccc2ccccc2c1C)C</chem>
001	Potential electrophilic agents	 <chem>CCN(CC)CC[C@H](O)CC[C@H](Nc1ccc2ccccc2c1C)C</chem>
002	PatWalters	 <chem>CCN(CC)CC[C@H](O)CC[C@H](Nc1ccc2ccccc2c1C)C</chem>
003	Covalent Bind With DNA	 <chem>CCN(CC)CC[C@H](O)CC[C@H](Nc1ccc2ccccc2c1C)C</chem>

Index	Alert Name	Structure
004	Covalent Bind With DNA	
005	Genotoxic carcinogenicity mutagenicity	
006	Hepatotoxicity	

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[Run another prediction \(/moltox\)](/moltox)

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