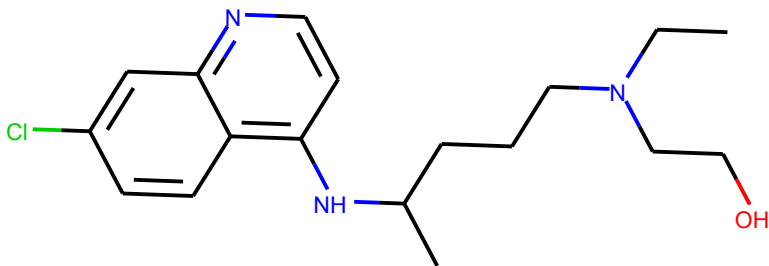


In Silico Predicted Toxic Properties

Molecule Depiction



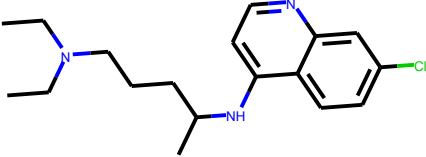
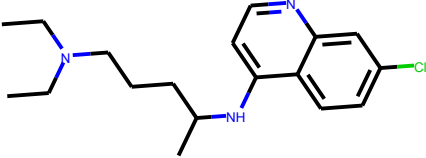
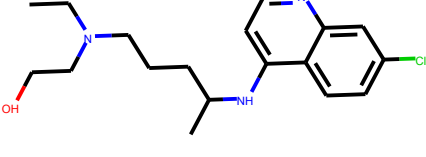
Mol

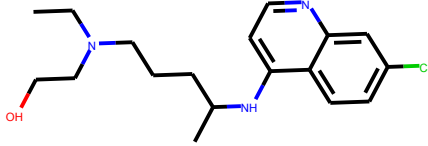
Molecule properties:

Property	Value
Num Aliphatic Carbocycles	0
Num Heteroatoms	5
Num Hydrogen Bond Acceptor	4
Num Aromatic Carbocycles	1
LogP	3.783
Num Rotatable Bonds	9
Num Aromatic Heterocycles	1
Num Lipinski HB Donor	2
Num Atoms	23
Num Lipinski HB Acceptor	4
Num Rings	2
Num Hydrogen bond Donor	2

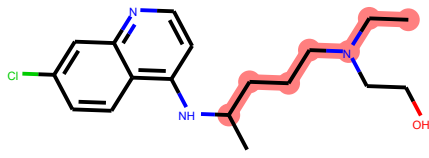
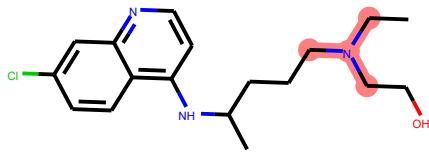
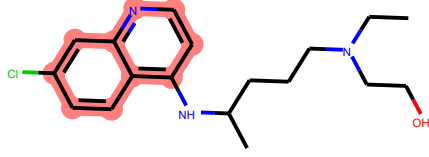
Property	Value
Num Aliphatic Rings	0
Num Aliphatic Heterocycles	0
Num Heterocycles	1
Mol Wt	335.176
Labute ASA	143.024
Num Aromatic Rings	2
Topological Polar SA	48.39

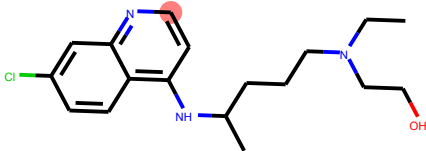
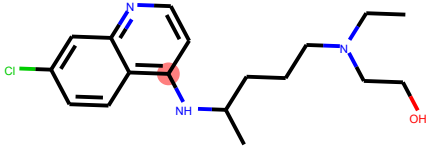
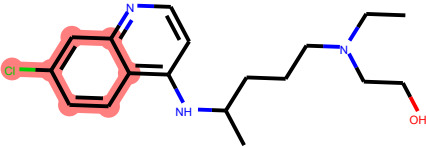
Potential Toxicity:

Index	Action	Injury	Confidence	Similar active compound in database
000	Antagonist of the constitutive androstane receptor (CAR) signaling pathway	Liver	0.993	
001	Differential cytotoxicity against isogenic chicken DT40 cell lines with known DNA damage response pathways - Rad54/Ku70 mutant cell line	Genotoxicity	1.0	
002	Differential cytotoxicity (isogenic chicken DT40 Rev3 mutant cell line)	Genotoxicity	0.996	

Index	Action	Injury	Confidence	Similar active compound in database
003	Differential cytotoxicity (isogenic chicken DT40 cell lines)	Genotoxicity	1.0	

Toxic substructure:

Index	Alert Name	Structure
000	PatWalters	
001	Covalent Bind With DNA	
002	Covalent Bind With DNA	

Index	Alert Name	Structure
003	Covalent Bind With DNA	
004	Covalent Bind With DNA	
005	Non genotoxic carcinogenicity	

Download full prediction result:

[download \(/static/4159892SummaryTable.csv.gz\)](/static/4159892SummaryTable.csv.gz)

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

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