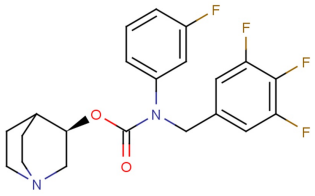
Data Sheet (Cat.No.T16990)

TargetMol
A DRUG SCREENING EXPERT

Tarafenacin

Chemical Properties



CAS No.:	385367-47-5
Formula:	C21H20F4N2O2
Molecular Weight:	408.39
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	Tarafenacin is a highly selective M3 muscarinic receptor antagonist (Ki= 0.19 nM), ~200 fold selectivity over the M2 receptor.
Targets(IC_{50})	Others: None
In vitro	SVT-40776 is highly selective for M(3) over M(2) receptors (Ki = 0.19 nmol.L(-1) for M(3) receptor affinity). SVT-40776 was the most potent in inhibiting carbachol-induced bladder contractions of the anticholinergic agents tested, without affecting atrial contractions over the same range of concentrations. SVT-40776 exhibited the highest urinary versus cardiac selectivity (199-fold). SVT-40776 has a much higher binding affinity (K(d) = 0.4 nM) to M5 mAChR than that of solifenacin (K(d) = 31 nM) with the same receptor. The calculated binding free energy change (-2.3 ± 0.3 kcal/mol) from solifenacin to SVT-40776 is in good agreement with the experimentally derived binding free energy change (-2.58 kcal/mol), suggesting that our modeled M5 mAChR structure and its complexes with the antagonists are reliable [1][2].
In vivo	SVT-40776 inhibited 25% of spontaneous bladder contractions at a very low dose (6.97 microg.kg(-1) i.v) in the guinea pig in vivo model, without affecting arterial blood pressure [1].

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.449 mL	12.243 mL	24.486 mL
5 mM	0.49 mL	2.449 mL	4.897 mL
10 mM	0.245 mL	1.224 mL	2.449 mL
50 mM	0.049 mL	0.245 mL	0.49 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Salcedo C, et al. In vivo and in vitro pharmacological characterization of SVT-40776, a novel M3 muscarinic receptor antagonist, for the treatment of overactive bladder. Br J Pharmacol. 2009 Mar;156(5):807-17.

2. Huang X, et al. Microscopic binding of M5 muscarinic acetylcholine receptor with antagonists by homology modeling, molecular docking, and molecular dynamics simulation. J Phys Chem B. 2012 Jan 12;116(1):532-41.

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