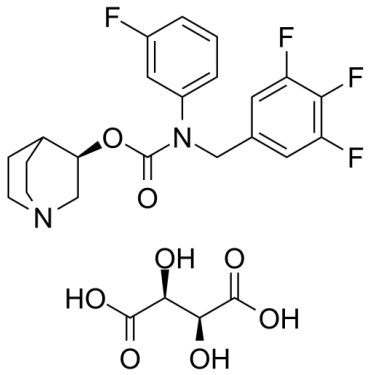
Data Sheet

Product Name:	Tarafenacin (D-tartrate)
Cat. No.:	CS-2113
CAS No.:	1159101-48-0
Molecular Formula:	C25H26F4N2O8
Molecular Weight:	558.48
Target:	mAChR
Pathway:	GPCR/G Protein; Neuronal Signaling
Solubility:	DMSO : ≥ 100 mg/mL (179.06 mM)



BIOLOGICAL ACTIVITY:

Tarafenacin D-tartrate (SVT-40776 D-tartrate) is a highly selective M3 muscarinic receptor antagonist (Ki= 0.19 nM), ~200 fold selectivity over M2 receptor. IC50 value: 0.19 nM (Ki) [1] Target: M3 muscarinic receptor 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 anti-cholinergic agents tested, without affecting atrial contractions over the same range of concentrations. SVT-40776 exhibited the highest urinary versus cardiac selectivity (199-fold) [1]. 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 reeptor. 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 [2]. in vivo: In the guinea pig in vivo model, SVT-40776 inhibited 25% of spontaneous bladder contractions at a very low dose (6.97 microg.kg(-1) i.v), without affecting arterial blood pressure [1].

References:

[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.

CAIndexNames:

Carbamic acid, N-(3-fluorophenyl)-N-[(3,4,5-trifluorophenyl)methyl]-, (3R)-1-azabicyclo[2.2.2]oct-3-yl ester, (2S,3S)-2,3-dihydroxybutanedioate (1:1)

SMILES:

O=C(O[C@H]1CN2CCC1CC2)N(C3=CC=CC(F)=C3)CC4=CC(F)=C(F)C(F)=C4.O[C@@H]([C@@H](C(O)=O)O)C(O)=O

Caution: Product has not been fully validated for medical applications. For research use only.

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