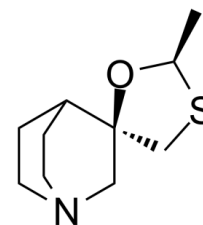


Data Sheet

Product Name:	(-)-Cevimeline (hydrochloride hemihydrate)
Cat. No.:	CS-3950
Molecular Formula:	C ₁₀ H ₁₇ NOS.HCl.1/2H ₂ O
Molecular Weight:	244.78
Target:	mAChR
Pathway:	GPCR/G Protein; Neuronal Signaling
Solubility:	10 mM in DMSO



HCl

0.5H₂O

BIOLOGICAL ACTIVITY:

Cevimeline hydrochloride hemihydrate, a novel muscarinic receptor agonist, is a candidate therapeutic drug for xerostomia in Sjogren's syndrome. IC₅₀ value: Target: mAChR The general pharmacol. properties of this drug on the gastrointestinal, urinary, and reproductive systems and other tissues were investigated in mice, rats, guinea pigs, rabbits, and dogs. The in vitro metab. of SNI-2011 was also evaluated with rat and dog liver microsomes. After oral administration, plasma concns. of SNI-2011 reached to C_{max} within 1 h in both species, suggesting that SNI-2011 was quickly absorbed, and then decreased with a t_{1/2} of 0.4-1.1 h. The bioavailability was 50% and 30% in rats and dogs, resp. Major metabolites in plasma were both S- and N-oxidized metabolites in rats and only N-oxidized metabolite in dogs, indicating that a large species difference was obsd. in the metab. of SNI-2011. Sex difference was also obsd. in the pharmacokinetics of SNI-2011 in rats, but not in dogs. In the in vitro study, chem. inhibition and pH-dependent studies revealed that the sulfoxidn. and N-oxidn. of SNI-2011 were mediated by cytochrome P 450 (CYP) and flavin-contg. monooxygenase (FMO), resp., in both species. In addn., CYP2D and CYP3A were mainly responsible for the sulfoxidn. in rat liver microsomes.

CAIndexNames:

(2R,3'R)-2-methyl-1'-azaspiro[[1,3]oxathiolane-5,3'-bicyclo[2.2.2]octane], hydrochloride, hydrate (2:2:1)

SMILES:

C[C@@H](SC1)O[C@@]21CN3CCC2CC3.Cl.[0.5H2O]

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

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