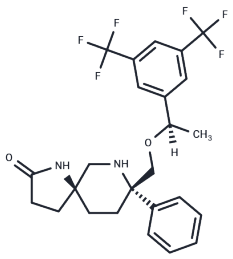
Data Sheet (Cat.No.T3716)

TargetMol

Rolapitant

Chemical Properties



CAS No. : 552292-08-7

Formula: C25H26F6N2O2

Molecular Weight: 500.48

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Rolapitant (SCH619734) Hydrochloride is the hydrochloride salt form of rolapitant, an orally bioavailable, centrally-acting, selective, neurokinin 1 receptor (NK1-receptor) antagonist with potential antiemetic activity. Upon oral administration, rolapitant competitively binds to and blocks the activity of the NK1-receptor in the central nervous system, thereby inhibiting the binding of the endogenous ligand, substance P (SP). This may prevent both SP-induced emesis and chemotherapy-induced nausea and vomiting (CINV). The interaction of SP with the NK1-receptor plays a key role in the induction of nausea and vomiting caused by emetogenic cancer chemotherapy. Compared to other NK1-receptor antagonists, rolapitant has both a more rapid onset of action and a much longer half-life.
Targets(IC50)	Neurokinin receptor
In vitro	Rolapitant has a high affinity for the human NK1 receptor with a Ki of 0.66 nM and high selectivity over the human NK2 and NK3 subtypes of more than 1000-fold. Rolapitant has a preferential affinity for human, guinea pig, gerbil, and monkey NK1 receptors over rat, mouse, and rabbit[1].
In vivo	Rolapitant reverses NK1 agonist-induced foot tapping in gerbils following both intravenous and oral administration up to 24 hours at a minimal effective dose (MED) of 0.1 mg/kg. Rolapitant is active at 0.1 and 1 mg/kg in both acute and delayed emesis models in ferrets, respectively which is the same as clinical data for other NK1 antagonists. The clinical efficacy of anti-emetics is highly correlated with efficacy in the ferret emesis model, suggesting rolapitant is a viable clinical candidate for this indication[1].
Kinase Assay	Rolapitant is made at a stock concentration of 1 mM in 100% DMSO. For most receptor binding studies, the stock solution is diluted with the final concentrations ranged from 0.1 to 3 μM. Radioligand concentrations for competition binding studies ranged from 0.5 to 1 nM. For species comparison studies, 150 pM [125I]-BHSP is incubated with varying concentrations of protein (10-50 μg) prepared from gerbil, rabbit and monkey striata, and from cells expressing cloned rat, mouse and guinea pig NK receptors[1].

Solubility Information

Solubility	DMSO: 142.8 mg/mL (285.33 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.9981 mL	9.9904 mL	19.9808 mL
5 mM	0.3996 mL	1.9981 mL	3.9962 mL
10 mM	0.1998 mL	0.999 mL	1.9981 mL
50 mM	0.040 mL	0.1998 mL	0.3996 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Duffy RA, et al. Rolapitant (SCH 619734): a potent, selective and orally active neurokininNK1 receptor antagonist with centrally-mediated antiemetic effects inferrets. Pharmacol Biochem Behav. 2012 Jul;102(1):95-100.

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