# Data Sheet

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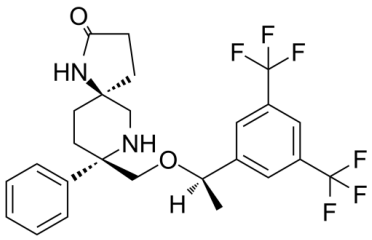
| **Product Name:** | Rolapitant |
| **Cat. No.:** | CS-6387 |
| **CAS No.:** | 552292-08-7 |
| **Molecular Formula:** | C25H26F6N2O2 |
| **Molecular Weight:** | 500.48 |
| **Target:** | Neurokinin Receptor |
| **Pathway:** | GPCR/G Protein; Neuronal Signaling |
| **Solubility:** | DMSO : ≥ 30 mg/mL (59.94 mM) |



## BIOLOGICAL ACTIVITY:

Rolapitant (SCH619734) is a potent, selective and orally active **neurokinin** NK1 receptor antagonist with a **$K_i$** of 0.66 nM. IC50 & Target: Ki: 0.66 nM (neurokinin)[1] **In Vitro:** Rolapitant has a high affinity for the human NK1 receptor with a $K_i$ of 0.66 nM and high selectivity over the human NK2 and NK3 subtypes of more than 1000-fold, as well as 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, consistent with clinical data for other NK1 antagonists. 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].

## PROTOCOL (Extracted from published papers and Only for reference)

**Kinase Assay:** [1]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 [$^{125}$I]-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].

## References:

[1]. 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.

## CAIndexNames:

1,7-Diazaspiro[4.5]decan-2-one, 8-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-8-phenyl-, (5S,8S)-

## SMILES:

C[C@@](C1=CC(C(F)(F)F)=CC(C(F)(F)F)=C1)([H])OC[C@@]2(C3=CC=CC=C3)CC[C@@](CCC4=O)(N4)CN2

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

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