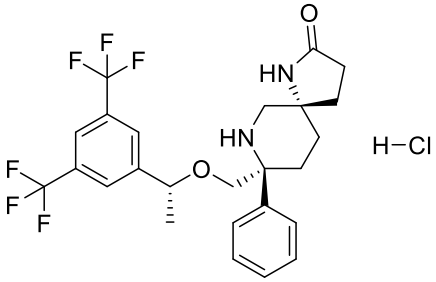
Product data sheet

MedKoo Cat#: 202470 Name: Rolapitant HCl CAS#: 858102-79-1 (HCl) Chemical Formula: $C_{25}H_{27}ClF_6N_2O_2$ Molecular Weight: 536.94	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
Rolapitant, also known as SCH-619734, is an orally bioavailable, centrally-acting, selective, neurokinin 1 receptor (NK1-receptor) antagonist with potential antiemetic activity.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
To be determined	To be determined	To be determined

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.86 mL	9.31 mL	18.62 mL
5 mM	0.37 mL	1.86 mL	3.72 mL
10 mM	0.19 mL	0.93 mL	1.86 mL
50 mM	0.04 mL	0.19 mL	0.37 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Kabil MF, Nasr M, Ibrahim IT, Hassan YA, El-Sherbiny IM. New repurposed rolapitant in nanovesicular systems for lung cancer treatment: Development, in-vitro assessment and in-vivo biodistribution study. Eur J Pharm Sci. 2022 Apr 1;171:106119. doi: 10.1016/j.ejps.2022.106119. Epub 2022 Jan 6. PMID: 34998905.

In vivo study

1. Kokhan VS, Anokhin PK, Abaimov DA, Shamakina IY, Soldatov VO, Deykin AV. Neurokinin-1 receptor antagonist rolapitant suppresses anxiety and alcohol intake produced by repeated withdrawal episodes. FEBS J. 2022 Aug;289(16):5021-5029. doi: 10.1111/febs.16400. Epub 2022 Feb 27. PMID: 35175687.
2. Duffy RA, Morgan C, Naylor R, Higgins GA, Varty GB, Lachowicz JE, Parker EM. Rolapitant (SCH 619734): a potent, selective and orally active neurokinin NK1 receptor antagonist with centrally-mediated antiemetic effects in ferrets. Pharmacol Biochem Behav. 2012 Jul;102(1):95-100. doi: 10.1016/j.pbb.2012.03.021. Epub 2012 Mar 31. PMID: 22497992.

7. Bioactivity
Biological target:

Rolapitant HCl is a NK1 receptor antagonist with a Ki of 0.66 nM. Rolapitant HCl does not interact with CYP3A4.

In vitro activity

Product data sheet

Rolapitant was loaded into various lipid nanovesicles (LNVs), and the LNVs were evaluated for particle size, zeta potential, entrapment efficiency (EE%), storage stability and surface morphology. The selected ethosomal and transethosomal vesicles displayed a particle size less than 400 nm, a positive charge, and EE% exceeding 90% for rolapitant, with a sustained release pattern over 15 days. The developed rolapitant-LNVs were able to reach the metastatic organs of lung cancer.

Reference: Eur J Pharm Sci. 2022 Apr 1;171:106119. https://pubmed.ncbi.nlm.nih.gov/34998905/

In vivo activity

This study utilized a male Wistar rat model of regular alcohol intake and subsequent withdrawl episodes. Upon intraperitoneal administration, rolapitant rapidly penetrated into specific rat brain regions implicated in the control of anxiety and reward. Rolapitant did not affect basal voluntary alcohol intake, but significantly suppressed anxiety-like behaviour and alcohol consumption following withdrawal episodes.

Reference: FEBS J. 2022 Aug;289(16):5021-5029. https://pubmed.ncbi.nlm.nih.gov/35175687/