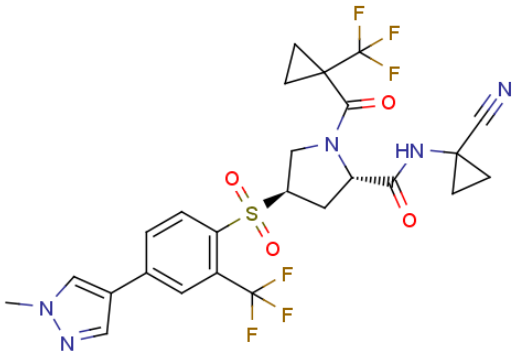
Name: Petesicatib

Cat#: EX-A3136

Chemical Structure of Petesicatib:



Chemical Name	(2S,4R)-N-(1-cyanocyclopropyl)-4-((4-(1-methyl-1H-pyrazol-4-yl)-2-(trifluoromethyl)phenyl)sulfonyl)-1-(1-(trifluoromethyl)cyclopropane-1-carbonyl)pyrrolidine-2-carboxamide

Molecular Weight	603.54	Storage	2 years -20°C powder 6 months -80°C in solvent Away from light
Formula	C25H23F6N5O4S		
CAS No.	1252637-35-6	Synonyms	RG-7625; RO-5459072

Target: Cathepsin
Pathway: Metabolic Enzyme/Protease

Solubility (25°C) *	In vitro	DMSO	>50 mg/mL
		Ethanol	N/A
		Water	N/A
	In vivo （should be freshly prepared each time）	1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.08 mg/mL (3.45 mM); Clear solution 2. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (3.45 mM); Clear solution	

* <1 mg/ml means slightly soluble or insoluble.
* Please note that Selleck tests the solubility of all compounds in-house, and the actual solubility may differ slightly from published values. This is normal and is due to slight batch-to-batch variations.

Preparing Stock Solutions(In vitro):

Mass / Volume / Concentration	1 mg	5 mg	10 mg
1 mM	1.6569 mL	8.2845 mL	16.5689 mL
5 mM	0.3314 mL	1.6569 mL	3.3138 mL
10 mM	0.1657 mL	0.8284 mL	1.6569 mL

*The above data is based on the product molecular weight 603.54.

Biological Activities:

Description	Petesicatib is a cathepsin S inhibitor, used in research of immune diseases.

References	[1]. Theron, Michel et al. "Pharmacodynamic Monitoring of RO5459072, a Small Molecule Inhibitor of Cathepsin S." Frontiers in immunology vol. 8 806. 17 Jul. 2017. [2]. Kratochwil, Nicole A et al. "Population pharmacokinetic analysis of RO5459072, a low water-soluble drug exhibiting complex food-drug interactions." British journal of clinical pharmacology vol. 87,9 (2021): 3550-3560. [3].Rubén Alvarez Sánchez, et al. Novel proline derivatives. US20100267722A1.