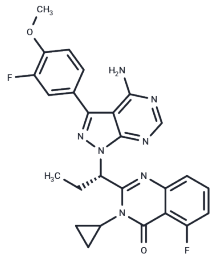
Data Sheet (Cat.No.T60196)

TargetMol®
YOUR TARGET MOLECULES

IHMT-PI3Kδ-372 S-isomer

Chemical Properties



CAS No. : 2429889-61-0

Formula: C26H23F2N7O2

Molecular Weight: 503.5

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	IHMT-PI3Kδ-372 S-isomer is a potent and selective PI3Kδ inhibitor with an IC50 of 14 nM. IHMT-PI3Kδ-372 S-isomer shows high selectivity over other class I PI3Ks (5683 fold) and other protein kinases. IHMT-PI3Kδ-372 can be uesd for chronic obstructive pulmonary disease (COPD) research.
Targets(IC50)	PI3K
In vitro	IHMT-PI3Kδ-372 (S)-18 (0.03-3 μM; 1 hour; Raji cells) treatment inhibits PI3Kδ-mediated AKT T308 phosphorylation in Raji cells with an EC50 value of 67 nM. IHMT-PI3Kδ-372 (S)-18 shows moderate inhibition of CYP2C9 (IC50 of 2.7 μM) and no apparent inhibition against CYP1A2, CYP2B6, CYP2C19, and CYP3A4 (IC50s > 10 μM)[1].
In vivo	IHMT-PI3Kδ-372 (S)-18; 1-5 mg/kg; inhalation; daily; for 28 days) improves lung function and reduced the inflammatory patterns characteristic of COPD. The lung function parameters such as forced expiratory volume in the first second (FEV1), forced vital capacity (FVC), and peak expiratory flow (PEF) are improved dose-dependently. The abnormally high level of leukocytes including the alveolar macrophages, neutrophils, and lymphocytes are also reduced. IHMT-PI3Kδ-372 (S)-18 decreases the inflammatory cell infiltration in a dose-dependent manner. In rats, inhalation of 5 mg/kg dose of IHMT-PI3Kδ-372 (S)-18 displays a half-life of 2.3 h, low exposure of 66 ng/mL, and high clearance of 348.5 mL/min/kg in plasma but high exposure of 5599 ng/g (6 h after inhalation) in lung tissue. IHMT-PI3Kδ-372 (S)-18 is stable in human, rat, and mouse liver microsomes, while it has moderate stability in monkey and dog liver microsomes[1].

Solubility Information

Solubility	DMSO: 50 mg/mL (99.3 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.9861 mL	9.9305 mL	19.861 mL
5 mM	0.3972 mL	1.9861 mL	3.9722 mL
10 mM	0.1986 mL	0.993 mL	1.9861 mL
50 mM	0.0397 mL	0.1986 mL	0.3972 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.

Reference

Li F, et al. Discovery of (S)-2-(1-(4-Amino-3-(3-fluoro-4-methoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl)propyl)-3-cyclopropyl-5-fluoroquinazolin-4(3H)-one (IHMT-PI3Kδ-372) as a Potent and Selective PI3Kδ Inhibitor for the