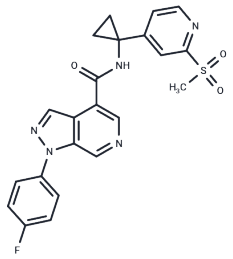
Data Sheet (Cat.No.T14899)

TargetMol

BI 639667

Chemical Properties



CAS No. : 1295298-26-8

Formula: C22H18FN5O3S

Molecular Weight: 451.47

Storage: Store at low temperature
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	BI 639667, a compound belonging to the azaindazole class, functions as a potent inhibitor of CCR1 activity, a property quantitatively demonstrated by its half-maximal inhibitory concentration (IC50) of 1.8 nM in standardized calcium flux assays.
Targets(IC50)	CCR
In vitro	**Methods**: Venlafaxine and paroxetine, which are marketed for the treatment of depression, were selected as positive drugs for affinity comparison. Molecular docking studies were performed using IL1R1 (PDB ID: 4gaf) and CCR1 antagonist 8 (BI 639667) to evaluate their binding energy with IL1R1, and further visualization was achieved through docking simulation with ILIRI. **Results**: BI 639667 exhibited the lowest binding energy; the root mean square deviation (RMSD) **Results** showed that the fluctuation of the system was within 0.1 nm, indicating that the system had strong stability. The solvent accessible surface area (SASA) showed that the binding of BI 639667 had little effect on the structure of IL1R1. Further calculations of the hydrogen bond contacts between BI 639667 and IL1R1 were consistent with the docking **Results**, and the complex was able to form stable hydrogen bonds. [2]

Solubility Information

Solubility	DMSO: 8 mg/mL (17.72 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween-80+45% Saline: 0.5 mg/mL (1.11 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.215 mL	11.0749 mL	22.1499 mL
5 mM	0.443 mL	2.215 mL	4.430 mL
10 mM	0.2215 mL	1.1075 mL	2.215 mL
50 mM	0.0443 mL	0.2215 mL	0.443 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

Harcken C, et al. Identification of novel azaindazole CCR1 antagonist clinical candidates. Bioorg Med Chem Lett. 2019 Feb 1;29(3):441-448.

Gao Y, et al. Exploring the diagnostic potential of IL1R1 in depression and its association with lipid metabolism. Front Pharmacol. 2025 Apr 24;16:1519287.