Product Data Sheet

CID 2745687

Cat. No.: HY-107537 CAS No.: 264233-05-8 Molecular Formula: $C_{17}H_{19}F_{2}N_{5}O_{2}S$ Molecular Weight: 395.43

Target: GPR35

Pathway: GPCR/G Protein

Storage: Powder -20°C 3 years

4°C 2 years

In solvent -80°C 6 months

> -20°C 1 month

SOLVENT & SOLUBILITY

In Vitro DMSO: 125 mg/mL (316.11 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.5289 mL	12.6445 mL	25.2889 mL
	5 mM	0.5058 mL	2.5289 mL	5.0578 mL
	10 mM	0.2529 mL	1.2644 mL	2.5289 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (5.26 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	CID 2745687 acts as a specific, reversible and competitive GPR35 antagonist with a K_i of 12.8 $nM^{[1]}$.
In Vitro	For ERK1/2 phosphorylation with 1 μ M Pamoic acid as the agonist, the CID 2745687 (CID2745687) K _i is 18 nM ^[1] . CID 2745687 (CID-2745687) is a potent antagonist in β -arrestin-2 interaction assays only at human GPR35 ^[2] . Using the BRET-based GPR35- β -arrestin-2 interaction assay and an EC ₈₀ concentration of Zaprinast (20 μ M) as agonist, CID 2745687 behaved as a moderately potent, concentration-dependent antagonist at human GPR35 with pIC ₅₀ =6.70±0.09 ^[2] . CID 2745687 (pIC ₅₀ =6.27±0.08) fully reverses the agonist action of Cromolyn disodium ^[2] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	CID 2745687 (CID2745687; 1 mg/kg; administrated orally every day for the last 4 weeks), a specific GPR35 antagonist, reverses Lodoxamide-mediated anti-fibrotic effects ^[3] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Six-week-old male C57BL/6 mice ^[3]
Dosage:	1 mg/kg
Administration:	Oral administration, every day for 4 weeks
Result:	Inhibited Lodoxamide-mediated protective effects.

REFERENCES

- [1]. Pingwei Zhao, et al. Targeting of the orphan receptor GPR35 by pamoic acid: a potent activator of extracellular signal-regulated kinase and β -arrestin2 with antinociceptive activity. Mol Pharmacol. 2010 Oct;78(4):560-8.
- [2]. Laura Jenkins, et al. Antagonists of GPR35 display high species ortholog selectivity and varying modes of action. J Pharmacol Exp Ther. 2012 Dec;343(3):683-95.
- [3]. Mi-Jeong Kim, et al. Lodoxamide Attenuates Hepatic Fibrosis in Mice: Involvement of GPR35. Biomol Ther (Seoul). 2019 Jun 13;28(1):92-97.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

Tel: 609-228-6898

Fax: 609-228-5909

E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA