(1R,2R)-2-PCCA hydrochloride

Cat. No.: HY-100013A1

CAS No.: 1609563-71-4

Molecular Formula: $C_{30}H_{39}Cl_2N_3O$

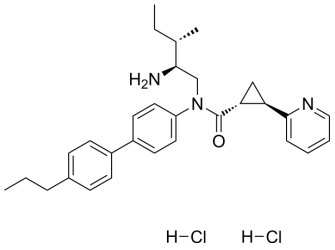
Molecular Weight: 529

Target: GPR88

Pathway: GPCR/G Protein

Storage: 4°C, stored under nitrogen

* In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (94.52 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8904 mL	9.4518 mL	18.9036 mL
	5 mM	0.3781 mL	1.8904 mL	3.7807 mL
	10 mM	0.1890 mL	0.9452 mL	1.8904 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (4.73 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (4.73 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

(1R,2R)-2-PCCA hydrochloride is a diastereomer of 2-PCCA, and acts as a potent GPR88 receptor agonist, with an EC_{50} of 3 nM in cell-free assay, and 603 nM in cell assay.

IC_{50} & Target

EC50: 3 nM (GPR88 receptor)[1], 603 nM (GPR88 receptor, in GPR88-22F cells)[2]

In Vitro

(1R,2R)-2-PCCA (Example 3) is a potent GPR88 receptor agonist, with an EC_{50} of 3 nM in cell-free assay, and 603 nM in cell assay[1][2]. (1R,2R)-2-PCCA inhibits GPR88-mediated cAMP production through a Gαi-coupled pathway, with an EC_{50} of 56 nM in HEK293 cells stably expressing the human GPR88 receptor and the GloSensor-22F cAMP construct[2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Nat Commun. 2022 May 2;13(1):2375.

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REFERENCES

[1]. Bi, Yingzhi, et al. Modulators of G Protein-Coupled Receptor 88. US 20110251204 A1.

[2]. Jin C, et al. Effect of Substitution on the Aniline Moiety of the GPR88 Agonist 2-PCCA: Synthesis, Structure-Activity Relationships, and Molecular Modeling Studies. ACS Chem Neurosci. 2016 Oct 19;7(10):1418-1432.

[3]. Jin C, et al. Synthesis, pharmacological characterization, and structure-activity relationship studies of small molecular agonists for the orphan GPR88 receptor. ACS Chem Neurosci. 2014 Jul 16;5(7):576-87.

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