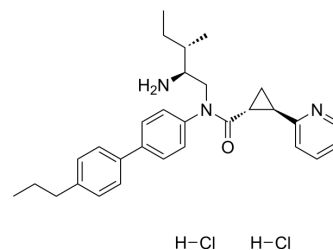


## (1R,2R)-2-PCCA hydrochloride

Cat. No.:	HY-100013A1
CAS No.:	1609563-71-4
Molecular Formula:	C <sub>30</sub> H <sub>39</sub> Cl <sub>2</sub> N <sub>3</sub> O
Molecular Weight:	528.56
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 (94.60 mM; Need ultrasonic)					
	Preparing Stock Solutions	Solvent Concentration	Mass			
			1 mg	5 mg	10 mg	
			1 mM	1.8919 mL	9.4597 mL	18.9193 mL
			5 mM	0.3784 mL	1.8919 mL	3.7839 mL
10 mM	0.1892 mL	0.9460 mL	1.8919 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 <sub>50</sub> of 3 nM in cell-free assay, and 603 nM in cell assay.
IC <sub>50</sub> & Target	EC <sub>50</sub> : 3 nM (GPR88 receptor) <sup>[1]</sup> , 603 nM (GPR88 receptor, in GPR88-22F cells) <sup>[2]</sup>
In Vitro	(1R,2R)-2-PCCA (Example 3) is a potent GPR88 receptor agonist, with an EC <sub>50</sub> of 3 nM in cell-free assay, and 603 nM in cell assay <sup>[1][2]</sup> . (1R,2R)-2-PCCA inhibits GPR88-mediated cAMP production through a Gai-coupled pathway, with an EC <sub>50</sub> of 56 nM in HEK293 cells stably expressing the human GPR88 receptor and the GloSensor-22F cAMP construct <sup>[2]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

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

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## REFERENCES

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- [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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**Caution: Product has not been fully validated for medical applications. For research use only.**

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