RTI-13951-33 hydrochloride

Cat. No.: HY-112612A

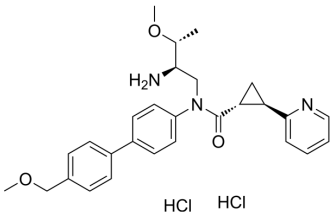
Molecular Formula: $C_{28}H_{35}Cl_2N_3O_3$

Molecular Weight: 532.5

Target: GPR88

Pathway: GPCR/G Protein

Storage: -20°C, sealed storage, away from moisture
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (93.90 mM; Need ultrasonic)
H_2O : 50 mg/mL (93.90 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.8779 mL	9.3897 mL	18.7793 mL
5 mM	0.3756 mL	1.8779 mL	3.7559 mL
10 mM	0.1878 mL	0.9390 mL	1.8779 mL

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

In Vivo

1. Add each solvent one by one: PBS
   Solubility: 100 mg/mL (187.79 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (3.91 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (3.91 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (3.91 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

RTI-13951-33 hydrochloride is a potent, selective, and brain-penetrant GPR88 agonist, with an EC_{50} of 25 nM in GPR88 cAMP functional assay. RTI-13951-33 hydrochloride reduces alcohol reinforcement and intake behaviors in rats[1].

IC_{50} & Target

EC50: 25 nM (GPR88)[1]

In Vitro

RTI-13951-33 is a potent, selective, and brain-penetrant GPR88 agonist, with an EC_{50} of 25 nM in GPR88 cAMP functional

	assay. RTI-13951-33 elevates [^{35}S]-GTPγS binding (EC_{50}, 535 nM) in mouse striatal membranes but not in membranes from GPR88 KO mice[1]. RTI-13951-33 has weak affinities at kappa opioid receptor (KOR; K_i, 2.29 μM), vesicular monoamine transporter (VMAT; K_i, 4.23 μM), and moderate affinity at serotonin transporter (SERT; K_i, 0.75 μM), however, RTI-13951-33 poorly inhibits SERT (IC_{50}, 25.1±2.7 μM)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	RTI-13951-33 (10 and 20 mg/kg, i.p.) dose-dependently decreases alcohol lever responses in a rat model of alcohol self-administration[1]. RTI-13951-33 (10 mg/kg, i.p.) has sufficient brain penetration, with $t_{1/2}$ of 48 min and 87 min in rat plasma and brain[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- bioRxiv. 2020 May.

See more customer validations on www.MedChemExpress.com

REFERENCES

[1]. Jin C, et al. Discovery of a Potent, Selective, and Brain-Penetrant Small Molecule that Activates the Orphan Receptor GPR88 and Reduces Alcohol Intake. J Med Chem. 2018 Aug 9;61(15):6748-6758.

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