Product Data Sheet

Product Name: RTI-13951-33
Cat. No.: GC31082

Chemical Properties

Cas. No.	2244884-08-8		
SMILES	COCC1=CC=C(C2=CC=C(N(C[C@@H](N)[C@@H](C)OC)C([C@H]3[C@H](C4=CC=CC=N4)C3)=O)C=C2)C=C1		
Formula	$C_{28}H_{33}N_3O_3$	M.Wt	459.58
Solubility	Soluble in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	RTI-13951-33		

Background

RTI-13951-33 is a potent, selective, and brain-penetrant GPR88 agonist, with an EC50 of 25 nM in GPR88 cAMP functional assay. RTI-13951-33 reduces alcohol reinforcement and intake behaviors in rats[1].

RTI-13951-33 is a potent, selective, and brain-penetrant GPR88 agonist, with an EC50 of 25 nM in GPR88 cAMP functional assay. RTI-13951-33 elevates [35S]-GTPγS binding (EC50□ 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; Ki, 2.29 μM), vesicular monoamine transporter (VMAT; Ki, 4.23 μM), and moderate affinity at serotonin transporter (SERT; Ki, 0.75 μM), however, RTI-13951-33 poorly inhibits SERT (IC50, 25.1 ± 2.7 μM)[1].

RTI-13951-33 (10 mg/kg, i.p.) has sufficient brain penetration, with t1/2 of 48 min and 87 min in rat plasma and brain[1].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].

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[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.

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