UNC9994 hydrochloride

Cat. No.: HY-111385

CAS No.: 2108826-33-9

Molecular Formula: $C_{21}H_{23}Cl_3N_2OS$

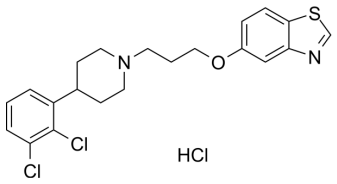
Molecular Weight: 457.84

Target: Dopamine Receptor; 5-HT Receptor; Arrestin

Pathway: GPCR/G Protein; Neuronal Signaling

Storage: 4°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 : 100 mg/mL (218.42 mM; ultrasonic and warming and heat to 80°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1842 mL	10.9208 mL	21.8417 mL
	5 mM	0.4368 mL	2.1842 mL	4.3683 mL
	10 mM	0.2184 mL	1.0921 mL	2.1842 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 (5.46 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (5.46 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (5.46 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

UNC9994 hydrochloride is a functionally selective, β-arrestin–biased dopamine D_2 receptor (D_2R) agonist that selectively activates β-arrestin recruitment and signaling. UNC9994 hydrochloride shows a binding affinity with a K_i of 79 nM for D_2R. UNC9994 hydrochloride is also an antagonist of G_i-regulated cAMP production and partial agonist for D2R/β-arrestin-2 interactions. UNC9994 hydrochloride shows antipsychotic-like activity[1].

IC_{50} & Target				
	D_3 Receptor 17 nM (Ki)	D_2 Receptor 79 nM (Ki)	D_4 Receptor 138 nM (Ki)	D_1 Receptor 4000 nM (Ki)
	5-HT_{2B} Receptor	5-HT_{1A} Receptor	5-HT_{2A} Receptor	5-HT_{2C} Receptor

	25 nM (Ki)	26 nM (Ki)	140 nM (Ki)	512 nM (Ki)

In Vitro

UNC9994 hydrochloride induces D_2-mediated β-arrestin-2 translocation with an EC_{50}s of 6.1 nM and 448 nM in Tango assay and DiscoveRx assay, respectively[1].

UNC9994 hydrochloride is an antagonist at $5HT_{2A}$ and $5HT_{2B}$ and an agonist at $5HT_{2C}$ and $5HT_{1A}$[1].

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

In Vivo

UNC9994 (2.0 mg/kg; i.p.; once) hydrochloride shows antipsychotic activity that is attenuated in β-arrestin-2 knockout mice [1].

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

Animal Model:	C57BL/6J wild-type and β-arrestin-2 knockout mice[1]
Dosage:	2.0 mg/kg, followed 30 min later with 6 mg/kg phencyclidine (PCP, i.p.)
Administration:	IP, once
Result:	Markedly inhibited PCP-induced hyperlocomotion in wild-type mice and the activity was completely abolished in β-arrestin-2 knockout mice.

REFERENCES

[1]. Allen JA, et al. Discovery of β-arrestin-biased dopamine D2 ligands for probing signal transduction pathways essential for antipsychotic efficacy. Proc Natl Acad Sci U S A. 2011 Nov 8;108(45):18488-93.

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