Seltorexant hydrochloride

Cat. No.: HY-109012A

CAS No.: 1293284-49-7

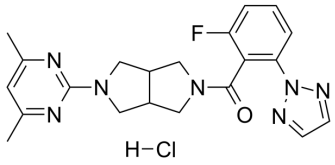
Molecular Formula: $C_{21}H_{23}ClFN_7O$

Molecular Weight: 443.91

Target: Orexin Receptor (OX Receptor)

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

H_2O : 100 mg/mL (225.27 mM; Need ultrasonic)
DMSO : 83.33 mg/mL (187.72 mM; Need ultrasonic)

Preparing Stock Solutions

Mass / Solvent / Concentration	1 mg	5 mg	10 mg
1 mM	2.2527 mL	11.2635 mL	22.5271 mL
5 mM	0.4505 mL	2.2527 mL	4.5054 mL
10 mM	0.2253 mL	1.1264 mL	2.2527 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: ≥ 2.08 mg/mL (4.69 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (4.69 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.69 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Seltorexant hydrochloride (JNJ-42847922 hydrochloride) is an orally active, high-affinity, and selective OX2R antagonist (pK_i values of 8.0 and 8.1 for human and rat OX2R). Seltorexant hydrochloride crosses the blood-brain barrier and quickly occupies OX2R binding sites in the rat brain[1].

IC_{50} & Target

human OX2R	rat OX2R
8.0 (pKi)	8.1 (pKi)

In Vivo

Seltorexant hydrochloride (JNJ-42847922 hydrochloride) (3-30 mg/kg; p.o.) dose-dependently induces and prolongs sleep in

male Sprague-Dawley rats[1].
The sleep-promoting effects of Seltorexant hydrochloride (30 mg/kg; p.o.; per day for 7 days) are maintained upon 7-day repeated dosing in rats[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male Sprague-Dawley rats (350-450 g)[1]
Dosage:	30 mg/kg
Administration:	p.o.; per day for 7 days
Result:	The reduced sleep onset (non–rapid eye movement (NREM) latency) and the increased NREM sleep duration were maintained upon 7-day repeated dosing with JNJ-42847922. The prolongation of NREM sleep time was due to a significant increase in NREM bout duration throughout the treatment period assessed on D1 and D7. Rapid eye movement (REM) sleep was only marginally affected on D4 of treatment, resulting in a small but significant reduction in REM sleep latency and an increase in REM sleep duration.

CUSTOMER VALIDATION

- Bioorg Chem. 2022 Jun;123:105779.

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REFERENCES

[1]. Bonaventure P, et al. Characterization of JNJ-42847922, a Selective Orexin-2 Receptor Antagonist, as a Clinical Candidate for the Treatment of Insomnia. J Pharmacol Exp Ther. 2015 Sep;354(3):471-82.

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