JNJ-54717793

Cat. No.: HY-134188

CAS No.: 1628843-99-1

Molecular Formula: $C_{22}H_{18}F_4N_6O$

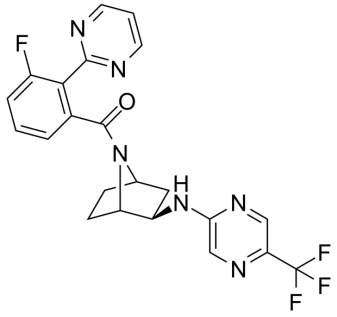
Molecular Weight: 458.41

Target: Orexin Receptor (OX Receptor)

Pathway: GPCR/G Protein; Neuronal Signaling

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 240 mg/mL (523.55 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.1815 mL	10.9073 mL	21.8145 mL
5 mM	0.4363 mL	2.1815 mL	4.3629 mL
10 mM	0.2181 mL	1.0907 mL	2.1815 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: ≥ 6 mg/mL (13.09 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 6 mg/mL (13.09 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

JNJ-54717793, as a brain penetrant, is an orally active, selective and high affinity orexin-1 receptor (OX1R) antagonist (plasma EC_{50}=85 ng/mL). The K_i values of JNJ-54717793 for hOX1R (human OX1R) and hOX2R are 16 nM and 700 nM, respectively. JNJ-54717793 is a potent compound of anxiety disorders[1][2].

IC_{50} & Target

human OX1R	human OX2R	OX_1 Receptor
16 nM (Ki)	700 nM (Ki)	85 ng/mL (EC50)

In Vivo

JNJ-5471779 (30 mg/kg; p.o.; 6 hours) significantly reduces the latency for rapid eye movement (REM) sleep and prolongs the time spent in REM sleep[2].

JNJ-5471779 (3~30 mg/kg; p.o.) attenuates bradycardia responses[2].

JNJ-5471779 (5mg/kg; p.o.) shows low clearance[1].

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

Animal Model:	OX2R KO mice[2]
Dosage:	30 mg/kg
Administration:	P.o.
Result:	Significantly reduced the latency for rapid eye movement (REM) sleep and prolonged the time spent in REM sleep.

Animal Model:	Rat[2]
Dosage:	3~30 mg/kg
Administration:	P.o.
Result:	Attenuated bradycardia responses.

Animal Model:	Mouse[1]
Dosage:	5.0 mg/kg (Pharmacokinetic Analysis)
Administration:	P.o.
Result:	Clearance was found to be low.

REFERENCES

[1]. Préville C, et al. Substituted Azabicyclo[2.2.1]heptanes as Selective Orexin-1 Antagonists: Discovery of JNJ-54717793. ACS Med Chem Lett. 2020;11(10):2002-2009. Published 2020 Apr 27.

[2]. Bonaventure P, et al. Evaluation of JNJ-54717793 a Novel Brain Penetrant Selective Orexin 1 Receptor Antagonist in Two Rat Models of Panic Attack Provocation. Front Pharmacol. 2017;8:357. Published 2017 Jun 9.

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