Lemborexant

Cat. No.: HY-16725

CAS No.: 1369764-02-2

Molecular Formula: $C_{22}H_{20}F_2N_4O_2$

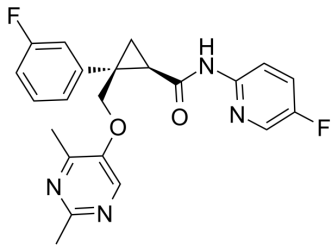
Molecular Weight: 410.42

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 : 250 mg/mL (609.13 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.4365 mL	12.1826 mL	24.3653 mL
5 mM	0.4873 mL	2.4365 mL	4.8731 mL
10 mM	0.2437 mL	1.2183 mL	2.4365 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.09 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (5.07 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.07 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Lemborexant (E-2006) is a reversible, competitive and orally active dual antagonist of the orexin OX1 and OX2 receptors with IC_{50} values of 6.1 nM and 2.6 nM, respectively. Lemborexant can be treated insomnia[1].

IC_{50} & Target

OX1	OX2
6.1 nM (IC_{50})	2.6 nM (IC_{50})

In Vitro

A high-fat and high-calorie meal has been found to delay the time to peak levels by 2 hours. Its plasma protein binding in

	vitro is 94%. Lemborexant is metabolized primarily by CYP3A4 and to a lesser extent by CYP3A5[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Lemborexant is administered orally to pregnant rats during the period of organogenesis in 2 studies at doses of 60, 200, and 600 mg/kg/day or 20, 60, and 200 mg/kg/day, which are approximately 6 to >300 times the maximum recommended human dose (MRHD) based on AUC. Lemborexant causes maternal toxicity, manifests by decreased body weight and food consumption, decreases mean fetal body weight, an increased number of dead fetuses, and skeletal, external and visceral malformations (omphalocele, cleft palate, and membranous ventricular septal defect) at >300 times the MRHD based on AUC[2]. Lemborexant causes maternal toxicity that consisted of decreased body weight and food consumption and toxicity to offspring consisting of decreased pup body weights, decreases femur length, and decreases acoustic startle responses at 206 times the MRHD based on AUC. The no observed adverse effect levels (NOAEL) of 100 mg/kg/day is approximately 93 times the MRHD based on AUC[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- bioRxiv. 2020 May.

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REFERENCES

[1]. OREXIN RECEPTOR ANTAGONIST PROVEN EFFECTIVE FOR BOTH SLEEP ONSET AND SLEEP MAINTENANCE IN CLINICAL DEVELOPMENT PROGRAM OF MORE THAN 2,000 PATIENTS. 2019.

[2]. HIGHLIGHTS OF PRESCRIBING INFORMATION

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