Elcubragistat

Cat. No.: HY-117632

CAS No.: 1446817-84-0

Molecular Formula: $C_{20}H_{22}F_9N_3O_2$

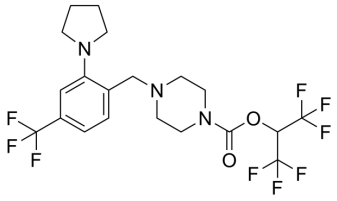
Molecular Weight: 507.39

Target: MAGL

Pathway: Metabolic Enzyme/Protease

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 (492.72 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9709 mL	9.8544 mL	19.7087 mL
	5 mM	0.3942 mL	1.9709 mL	3.9417 mL
	10 mM	0.1971 mL	0.9854 mL	1.9709 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 (4.10 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.08 mg/mL (4.10 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.10 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Elcubragistat (ABX-1431) is a highly potent, selective, and orally available, CNS-penetrant monoacylglycerol lipase (MAGL) inhibitor with an IC_{50} of 14 nM.

IC_{50} & Target

IC50: 14 nM (human MGLL)[1]

In Vitro

Elcubragistat (ABX-1431) is a potent human MGLL inhibitor (IC_{50}=0.014 μM) with >100-fold selectivity against ABHD6 and >200-fold selectivity against PLA2G7. Elcubragistat inhibits human PC3 cells with an IC_{50} of 0.0022 μM. In the cell-based

	assay, >100-fold selectivity for MGLL over ABHD6 (IC_{50}=0.253 μM) and PLA2G7 (IC_{50}=494 μM) is maintained[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Elcubragistat (ABX-1431) inhibits MGLL activity in rodent brain (ED_{50}=0.5-1.4 mg/kg), increases brain 2-AG concentrations, and suppresses pain behavior in the rat formalin pain model[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Cell Assay [1]	Human prostate cancer PC3 cells are grown in F-12K medium supplemented with 10% fetal bovine serum at 37°C with 5% CO_2 to 80% confluency in 100 mm dishes. ABX-1431 is added to cells to give final concentration of 0.1-10 μM compound in serum free media. Cells are incubated for 30 min. Cells are washed, harvested, and lysed by probe sonication. Cell lysates (2mg/mL) are treated with JW912 (1μM) and analyzed by SDS-PAGE and in-gel fluorescence scanning[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Animal Administration [1]	Rats[1] Elcubragistat is administered in a volume of 5 mL/kg. Male ICR mice or male Sprague Dawley rats 6 to 12 weeks are administered single oral doses of Elcubragistat (0.5-32 mg/kg for mice and 0.03-10 mg/kg for rats). Four hours after Elcubragistat administration, animals are anesthetized. Following blood collection, animals are killed by decapitation and brains are removed, hemisected and frozen in liquid nitrogen for analysis[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Nat Commun. 2022 Feb 25;13(1):1058.

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REFERENCES

[1]. Cisar JS, et al. Identification of ABX-1431, a Selective Inhibitor of Monoacylglycerol Lipase and Clinical Candidate for Treatment of Neurological Disorders. J Med Chem. 2018 Oct 25;61(20):9062-9084.

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