Zegocractin

Cat. No.: HY-101942

CAS No.: 1713240-67-5

Molecular Formula: $C_{19}H_{11}ClF_3N_3O_3$

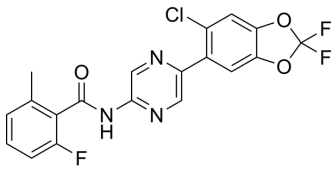
Molecular Weight: 421.76

Target: CRAC Channel

Pathway: Membrane Transporter/Ion Channel

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 : ≥ 100 mg/mL (237.10 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3710 mL	11.8551 mL	23.7102 mL
	5 mM	0.4742 mL	2.3710 mL	4.7420 mL
	10 mM	0.2371 mL	1.1855 mL	2.3710 mL

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

In Vivo

1. Add each solvent one by one: 70% PEG300 >> 30% (20% SBE-β-CD in saline)
   Solubility: 10 mg/mL (23.71 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: 2.08 mg/mL (4.93 mM); Suspended solution; Need ultrasonic and warming
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.08 mg/mL (4.93 mM); Suspended solution; Need ultrasonic and warming
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.93 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Zegocractin (CM-4620) is a calcium-release activated calcium-channel (CRAC channel) inhibitor, with IC_{50}s of 119 nM and 895 nM for Orai1/STIM1 and Orai2/STIM1 channels, respectively[1].

IC_{50} & Target

IC50: 119 nM (Orai 1/STIM1), 895 nM (Orai 1/STIM1)[1]

In Vitro	It is determined that Zegocractin (compound 1) inhibits Orai 1/STIM1 channels with an IC_{50} of 119 nM, and Orai2/STIM1 channels with an IC_{50} of 895 nM. It is more potent on Orai1 than Orai2-type CRAC channels. In human PBMCs, Zegocractin potently inhibits release of multiple cytokines which play important roles in T cells (IC_{50}s, IFN γ: 138 nM, IL-4: 879 nM, IL-6: 135 nM, IL-1β: 240 nM, IL-10: 303 nM, TNFα: 225 nM, IL-2: 59 nM, IL-17 120 nM)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Mouse PACs are treated with CRAC inhibitors Zegocractin or GSK-7975A and monitored for their rate of Calcium uptake. Both CRAC inhibitors reduce the rate of store-operated Calcium entry into the ER to 50% of controllevels upon treatment with 700 nM of inhibitor. Zegocractin blocks 100% of reuptake at 10 mM[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Nat Aging. 2023 Jun 5.
- Nat Commun. 2023 Mar 8;14(1):1286.
- Life Sci. 2021 Jun 5;119699.
- bioRxiv. 2023 Jun 6.
- Humboldt university. 2023 Jan 27.

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REFERENCES

[1]. ARYL SULFONOHYDRAZIDES. WO2016/138472Al.

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