Apinocaltamide

Cat. No.: HY-112723

CAS No.: 1838651-58-3

Molecular Formula: $C_{22}H_{18}F_3N_5O$

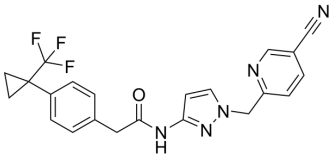
Molecular Weight: 425.41

Target: Calcium Channel

Pathway: Membrane Transporter/Ion Channel; Neuronal Signaling

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 125 mg/mL (293.83 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3507 mL	11.7534 mL	23.5067 mL
	5 mM	0.4701 mL	2.3507 mL	4.7013 mL
	10 mM	0.2351 mL	1.1753 mL	2.3507 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 (4.89 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (4.89 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.89 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Apinocaltamide (ACT-709478) is a potent, selective, orally active, and brain penetrating T-type calcium channel blocker. ACT-709478 is used in the research of generalized epilepsies[1].

IC_{50} & Target				
	$Ca_V1.2$	$Ca_V3.1$	$Ca_V3.2$	$Ca_V3.3$
	2410 nM (IC_{50})	6.4 nM (IC_{50})	18 nM (IC_{50})	7.5 nM (IC_{50})

In Vitro

Apinocaltamide (Compound 66b) blocks $Ca_v3.1$, $Ca_v3.2$, $Ca_v3.3$, $Ca_v1.2$ with IC_{50}s of 6.4, 18, 7.5 and 2410 nM, respectively.
Apinocaltamide blocks recombinant channel $hCa_v3.3$ potently with marked voltage-dependency (K_r≈1500 nM and K_i≈20 nM).
Apinocaltamide blocks currents through $hK_v11.1$-hERG channels with an IC_{50} of 5.5 μM[1].
Apinocaltamide also inhibits P450 enzymes with IC_{50}s of 14, 15, 22, 25, 51 and 52 μM for CYP2C8,CYP2D6 CYP2C9, CYP2C19, CYP3A4, and CYP2B6, respectively[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

Apinocaltamide (Compound 66b, 100, 300 mg/kg, p.o., measured 12 hours later) potently decreases the cumulative duration of absence-like seizures in mice[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male juvenile DBA/2J mice (22-24 days old)[1]
Dosage:	100, 300 mg/kg, 1 hour or 3 hours before exposure to the stimulus.
Administration:	P.O., for 12 hours
Result:	Decreased the cumulative duration of absence-like seizures over the next 12 h period by 93%.

REFERENCES

[1]. Bezençon O, et al. Discovery of a Potent, Selective T-type Calcium Channel Blocker as a Drug Candidate for the Treatment of Generalized Epilepsies. J Med Chem. 2017 Dec 14;60(23):9769-9789.

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