Aticaprant

Cat. No.: HY-101718

CAS No.: 1174130-61-0

Molecular Formula: $C_{26}H_{27}FN_2O_2$

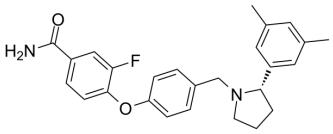
Molecular Weight: 418.5

Target: Opioid 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 : ≥ 100 mg/mL (238.95 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3895 mL	11.9474 mL	23.8949 mL
	5 mM	0.4779 mL	2.3895 mL	4.7790 mL
	10 mM	0.2389 mL	1.1947 mL	2.3895 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: ≥ 2.5 mg/mL (5.97 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (5.97 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.97 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Aticaprant (CERC-501) is a potent and centrally-penetrant kappa opioid receptor antagonist with a K_i of 0.807 nM.

IC_{50} & Target

Ki: 0.807 nM (kappa opioid)[1]

In Vitro

Aticaprant (CERC-501) binds with high affinity to the human kappa opioid receptor with a 30-fold higher affinity over the human mu opioid receptor and 190-fold higher affinity over the human delta opioid receptor. Aticaprant (CERC-501) shows

	no appreciable affinity for several non-opioid cell surface G-protein-coupled receptor targets, including monoaminergic, muscarinic, cholinergic, and adrenergic receptors or ion channel/transporter binding targets or the central benzodiazepine binding site[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Aticaprant (CERC-501) has a rapid absorption (t_{max}=1-2 h) and good oral bioavailability (F=25%). Oral Aticaprant (CERC-501) administration selectively and potently occupies central kappa opioid receptors (ED_{50}=0.33 mg/kg), without evidence of mu or delta receptor occupancy. LY2456302 potently blocks kappa-agonist-mediated analgesia and disruption of prepulse inhibition, without affecting mu-agonist-mediated effects at doses >30-fold higher. Aticaprant (CERC-501) produces antidepressant-like effects in the mouse forced swim test and enhances the effects of imipramine and citalopram. Aticaprant (CERC-501) reduces ethanol self-administration in alcohol-preferring rats[1]. Aticaprant (CERC-501) alleviates the nicotine withdrawal syndrome, as evidenced by decreased expression of nicotine withdrawal induced anxiety-related behavior, somatic signs, and CPA, and increased hotplate latency in nicotine withdrawn mice following pre-treatment[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Animal Administration [1]	Rats: Three male cannulated rats are administered a single 1 mg/kg intravenous (IV) and 10 mg/kg oral (PO) dose of Aticaprant (CERC-501) to determine the pharmacokinetic parameters. Plasma samples are collected at 0.08 (IV only), 0.25, 0.5, 1, 2, 4, 8, 12 and 24 h post-dose and analyzed by liquid chromatography coupled to tandem mass spectral detection to determine the concentrations of Aticaprant (CERC-501)[1]. Mice: Male mice are administered a single 10 mg/kg PO dose of Aticaprant (CERC-501) to determine the pharmacokinetic parameters. Plasma samples are collected at 0.5, 1, 2, 4, 8, and 24 h post-dose and analyzed by LCeMS/MS to determine the concentrations of Aticaprant (CERC-501). The plasma and brain binding of Aticaprant (CERC-501) is determined by equilibrium dialysis at 1 μM[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Neuron. 2022 Sep 29;S0896-6273(22)00863-7.
- J Neurosci. 2021 Nov 24;41(47):9827-9843.
- Neuropharmacology. 2020 Feb;163:107726.

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REFERENCES

[1]. Rorick-Kehn LM, et al. LY2456302 is a novel, potent, orally-bioavailable small molecule kappa-selective antagonist with activity in animal models predictive of efficacy in mood and addictive disorders. Neuropharmacology. 2014 Feb;77:131-44.

[2]. Jackson KJ, et al. Effects of orally-bioavailable short-acting kappa opioid receptor-selective antagonist LY2456302on nicotine withdrawal in mice. Neuropharmacology. 2015 Oct;97:270-4.

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA