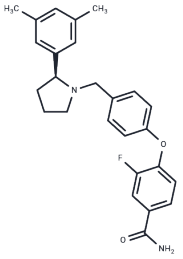
Data Sheet (Cat.No.TQ0082)

TargetMol

Aticaprant

Chemical Properties



CAS No. : 1174130-61-0

Formula: C26H27FN2O2

Molecular Weight: 418.5

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Aticaprant (CERC-501) is a potent and centrally-penetrant antagonist of the kappa-opioid receptor (Ki: 0.807 nM).[2]
Targets(IC50)	Opioid Receptor
In vitro	Aticaprant(CERC-501) binds with a high affinity to the human kappa opioid receptor with a 30-fold higher affinity over the human mu-opioid receptor and a 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 [1].
In vivo	**METHODS**: Mice were given Aticaprant(CERC-501) (0.1 to 3 mg/kg, intraperitoneal injection) 30 minutes before the alcohol deprivation effect (ADE) test and naltrexone (0.3 or 1 mg/kg, intraperitoneal injection) 10 minutes before the test to observe the effect of aticaprant on the ADE effect. **RESULTS** 0.3 mg/kg of Aticaprant(CERC-501) and 1 mg/kg of naltrexone reduced the ADE alcohol intake of mice at 4 hours. [1]
Animal Research	Three male cannulated rats are administered a single 1 mg/kg intravenous (IV) and 10 mg/kg oral (PO) dose of Aticaprant 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). Male mice are administered a single 10 mg/kg PO dose of Aticaprant to determine the pharmacokinetic parameters. Plasma samples are collected at 0.5, 1, 2, 4, 8, and 24 h post-dose and analyzed by LCMS/MS to determine the concentrations of Aticaprant. The plasma and brain binding of Aticaprant is determined by equilibrium dialysis at 1 μM [1].

Solubility Information

Solubility	DMSO: 100 mg/mL (238.95 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 4 mg/mL (9.56 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one.*

In vivo Formulation	*Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.3895 mL	11.9474 mL	23.8949 mL
5 mM	0.4779 mL	2.3895 mL	4.779 mL
10 mM	0.2389 mL	1.1947 mL	2.3895 mL
50 mM	0.0478 mL	0.2389 mL	0.4779 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Zhou Y, et al. Aticaprant (Clinically Developed Kappa-Opioid Receptor Antagonist) Combined With Naltrexone Prevents Alcohol "Relapse" Drinking. J Pharm Pharmacol (Los Angel). 2022 May;9(1):10.13188/2327-204x.1000032.
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.