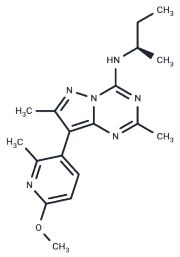
Data Sheet (Cat.No.T16475)

TargetMol

Pexacerfont

Chemical Properties



CAS No. : 459856-18-9

Formula: C18H24N6O

Molecular Weight: 340.42

Storage: Store at low temperature
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	Pexacerfont (BMS-562086) is a selective antagonist of the corticotropin-releasing factor receptor (IC50: 6.1±0.6 nM for the human CRF1 receptor).
Targets(IC50)	CRFR
In vitro	Pexacerfont shows an effective and specific inhibitory effect (IC50=6.1 ± 0.6 nM) toward the human CRF1 receptor. It also has greater than 1000-fold lower affinity (IC50>1000 nM) for the CRF-binding protein and biogenic amine receptors[1].
In vivo	Pexacerfont is active in rats (1-10 mg/kg, orally) in the defensive withdrawal and elevated plus-maze models of anxiety. The CLp of Pexacerfont was higher in rats (17.9 mL/kg per min) and dogs (11.6 mL/kg per min) than in chimpanzees (2.0 mL/kg per min). The plasma Pexacerfont concentrations exhibited a multiexponential decline in rats, dogs, and chimpanzees after the intravenous bolus dose. Assuming the value of CLp of Pexacerfont approximates the value of CLb in these three species, Pexacerfont has an estimated hepatic extraction ratio of 0.32, 0.38, and 0.08 in rats, dogs, and chimpanzees, respectively (calculated by dividing CLp by respective hepatic blood flow, 55.2, 30.9, and 25.5 mL/kg per min for rats, dogs, and chimpanzees). The assumption that CLb is equal to CLp is reasonable at least in rats, where the blood to the plasma concentration ratio of BMS-562086-equivalent radioactivity was 0.95 at 1 h postdose[1].

Solubility Information

Solubility	DMSO: 45 mg/mL (132.19 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: 2 mg/mL (5.88 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. 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	2.9375 mL	14.6877 mL	29.3755 mL
5 mM	0.5875 mL	2.9375 mL	5.8751 mL
10 mM	0.2938 mL	1.4688 mL	2.9375 mL
50 mM	0.0588 mL	0.2938 mL	0.5875 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 L, et al. In vitro and in vivo metabolism and pharmacokinetics of BMS-562086, a potent and orally bioavailable corticotropin-releasing factor-1 receptor antagonist. Drug Metab Dispos. 2012 Jun;40(6):1093-103.