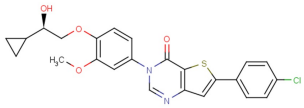
Data Sheet (Cat.No.T14678)

TargetMol
A DRUG SCREENING EXPERT

BMS-819881

Chemical Properties



CAS No.:	1197420-05-5
Formula:	C24H21ClN2O4S
Molecular Weight:	468.95
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	BMS-819881 is a melaninconcentrating hormone receptor 1 (MCHR1) antagonist, which binds rat MCHR1 with a Ki of 7 nM and it also is selective and potent for CYP3A4 activity with an EC50 of 13 μM.
Targets(IC_{50})	CYP3A4: 13 μM (EC50) rat MCHR1: 7 nM (ki)
In vitro	BMS-819881 (Compound 27) is 99.8% binds to rat serum proteins and rat MCHR1 Ki is 7 nM. When BMS-819881 is screened for cytochrome P450 (CYP) activity, EC50 values for CYP1A2, CYP2C9, CYP2C19, CYP2D6 are >40 μM; however, the CYP3A4 EC50 is 13 μM. The percent of BMS-819881 binds to serum proteins is species dependent ranging from 99.8%, 99.6%, and 99.3%, respectively, for rat, dog, and monkey. FLIPR-based assays establish that BMS-819881 is a potent and highly selective MCHR1 functional antagonist. BMS-819881 (Kb=32 nM) effectively blocks MCH stimulated Ca2+ mobilization in heterologous cells overexpressing MCHR1 but fails to inhibit MCH mediated Ca2+ mobilization of cells expressing MCHR2 at 10 μM. No activity is observed upon screening BMS-819881 at 10 μM versus a panel of 20 GPCRs associated with feeding homeostasis [1].
In vivo	BMS-819881 has moderate terminal elimination half-life (t1/2=5.7 h, 32±8 h, and 14±3 h for rat (1 mg/kg, iv), dog (1 mg/kg, iv), and cynomologous monkey (1 mg/kg, iv))[1].

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.132 mL	10.662 mL	21.324 mL
5 mM	0.426 mL	2.132 mL	4.265 mL
10 mM	0.213 mL	1.066 mL	2.132 mL
50 mM	0.043 mL	0.213 mL	0.426 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Washburn WN, et al. Identification of a nonbasic melanin hormone receptor 1 antagonist as an antiobesity clinical candidate. J Med Chem. 2014 Sep 25;57(18):7509-22.

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