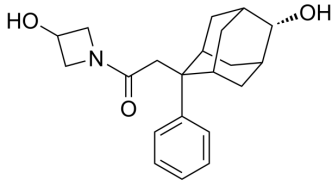
BMS-816336

Cat. No.:	HY-101930
CAS No.:	1009583-20-3
Molecular Formula:	$C_{21}H_{27}NO_3$
Molecular Weight:	341.44
Target:	11β-HSD
Pathway:	Metabolic Enzyme/Protease
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 : 300 mg/mL (878.63 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.9288 mL	14.6439 mL	29.2877 mL
	5 mM	0.5858 mL	2.9288 mL	5.8575 mL
	10 mM	0.2929 mL	1.4644 mL	2.9288 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: ≥ 7.5 mg/mL (21.97 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 7.5 mg/mL (21.97 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 7.5 mg/mL (21.97 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BMS-816336 is a novel, potent and orally bioavailable inhibitor against human 11β-hydroxysteroid dehydrogenase type 1 (11 β-HSD1) enzyme with an IC_{50} of 3.0 nM[1].

IC_{50} & Target

IC50: 3.0 nM (11β-HSD1)[1]

In Vitro

11β-HSD1 inhibition may be useful in the treatment of type II diabetes and other potential clinical utilities such as atheroprotection and cognitive protection. BMS-816336 (6n-2) inhibits 11β-HSD1 enzyme in HEK and 3T3L1 cells with IC_{50}s

	of 37.3 and 28.6 nM, respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	BMS-816336 represents a potential new treatment for type 2 diabetes, metabolic syndrome, and other human diseases modulated by glucocorticoid control. BMS-816336 (6n-2) exhibits a robust acute pharmacodynamic effect in cynomolgus monkeys (ED_{50}=0.12 mg/kg) and in DIO mice (1, 3, 10, 30, 100 mg/kg, 120 mintues). It is orally bioavailable (%F ranges from 20 to 72% in preclinical species) and has a predicted pharmacokinetic profile of a high peak to trough ratio and short half-life in humans[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Nonfasting diet-induced obese male mice[1]
Dosage:	1, 3, 10, 30, 100 mg/kg
Administration:	Oral, 120 mintues
Result:	ED_{50}=8.6 mg/kg and a plasma EC_{50} of 0.85 μM in this model[1].

REFERENCES

[1]. Ye XY, et al. Discovery of Clinical Candidate 2-((2S,6S)-2-Phenyl-6-hydroxyadamantan-2-yl)-1-(3'-hydroxyazetidin-1-yl)ethanone [BMS-816336], an Orally Active Novel Selective 11β-Hydroxysteroid Dehydrogenase Type 1 Inhibitor. J Med Chem. 2017 Jun 22;60(12):4932-4948.

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