(R)-BMS-816336

Cat. No.: HY-101930B

CAS No.: 1009583-83-8

Molecular Formula: $C_{21}H_{27}NO_3$

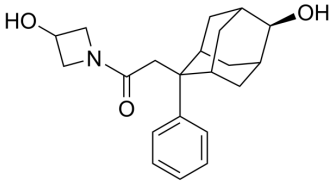
Molecular Weight: 341.44

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

(R)-BMS-816336 (Compound 6n-1) is a potent and orally active inhibitor of human, mouse and cynomolgus monkey 11β-hydroxysteroid dehydrogenase type 1 (11β-HSD1) enzyme with IC_{50}s of 14.5 nM, 50.3 nM and 16 nM, respectively [1].

IC_{50} & Target

IC50: 14.5 nM (Human 11β-HSD1), 50.3 nM (Mouse 11β-HSD1) and 16 nM (Cynomolgus monkey 11β-HSD1)[1]

In Vivo

During the in vivo studies of BMS-816336 (Compound 6n-2) in animals, its enantiomer (R)-BMS-816336 (Compound 6n-1) in the plasma samples, together with trace amount of Ketone A are detected. The interconversion of BMS-816336 and (R)-BMS-

816336 take place via the intermediate Ketone A through physiological oxidation and reduction process. In vivo studies in rat, dog, and cynomolgus monkey, the plasma ratios of (R)-BMS-816336/BMS-816336 decrease in the order: dog ≫ rat >cynomolgus monkey[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

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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