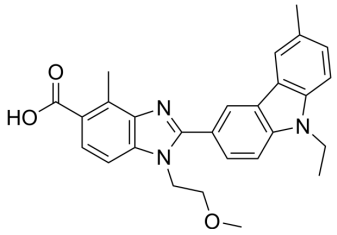
BAY-1316957

Cat. No.:	HY-111539
CAS No.:	1613264-40-6
Molecular Formula:	$C_{27}H_{27}N_3O_3$
Molecular Weight:	441.52
Target:	Prostaglandin Receptor
Pathway:	GPCR/G Protein
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 : 100 mg/mL (226.49 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.2649 mL	11.3245 mL	22.6490 mL
	5 mM	0.4530 mL	2.2649 mL	4.5298 mL
	10 mM	0.2265 mL	1.1325 mL	2.2649 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 5 mg/mL (11.32 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (4.71 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.71 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BAY-1316957 is a potent, selective and orally active prostaglandin E2 receptor subtype 4 (EP4-R) antagonist with an IC_{50} of 15.3 nM for human EP4-R. BAY-1316957 has excellent agent metabolism and pharmacokinetics properties, and can be used for endometriosis research[1].

IC_{50} & Target

human EP4-R
15.3 nM (IC_{50})

In Vitro	BAY-1316957 (Compound 32) shows high solubility and permeability using the Caco-2 cellular assay[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	BAY-1316957 (Compound 32; 0.2-5 mg/kg; oral administration; once) treatment significantly reduces mechanical allodynia in dmPGE2 pain model[1]. The pharmacokinetic parameters of BAY-1316957 (Compound 32) shows a low clearance, long half-life, and high bioavailability (F%=90%) in Wistar rats. Investigation of the metabolic pathways of BAY-1316957 (Compound 32) in human, rat, mouse, dog, and monkey hepatocytes revealed that the formation of the acyl glucuronide was also the common and predominant route of biotransformation, mainly catalyzed by UGT1A1 and to a lesser extent by UGT1A3[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male adult Sprague Dawley rats (220-265 g) injected with 16,16-dimethyl prostaglandin E2 (dmPGE2)[1]
Dosage:	0.2 mg/kg, 1 mg/kg, 5 mg/kg
Administration:	Oral administration; once
Result:	Significantly reduced paw withdrawal thresholds in dmPGE2 pain model.

REFERENCES

[1]. Bäurle S, et al. Identification of a Benzimidazolecarboxylic Acid Derivative (BAY 1316957) as a Potent and Selective Human Prostaglandin E2 Receptor Subtype 4 (hEP4-R) Antagonist for the Treatment of Endometriosis. J Med Chem. 2019 Mar 14;62(5):2541-2563.

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