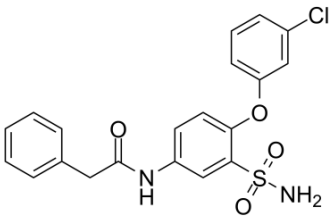
BAY-1797

Cat. No.:	HY-130605
CAS No.:	2055602-83-8
Molecular Formula:	$C_{20}H_{17}ClN_2O_4S$
Molecular Weight:	416.88
Target:	P2X Receptor
Pathway:	Membrane Transporter/Ion Channel
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 : 250 mg/mL (599.69 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3988 mL	11.9939 mL	23.9877 mL
	5 mM	0.4798 mL	2.3988 mL	4.7975 mL
	10 mM	0.2399 mL	1.1994 mL	2.3988 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: ≥ 2.08 mg/mL (4.99 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (4.99 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.99 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BAY-1797 is a potent, orally active, and selective P2X4 antagonist, with an IC_{50} of 211 nM against human P2X4. BAY-1797 displays no or very weak activity on the other P2X ion channels. BAY-1797 shows anti-nociceptive and anti-inflammatory effects[1].

IC_{50} & Target

IC50: 211 nM (human P2X4), >50 μM (human P2X1), >30 μM (human P2X23), 8.3 μM (human P2X3), 10.6 μM (human P2X7)[1]

In Vitro

BAY-1797 inhibits human, mouse, and rat P2X4 in 1321N1 cells with IC_{50}s of 108 nM, 112 nM, and 233 nM, respectively[1].

BAY-1797 exerts no measurable activity on hERG and carbonic anhydrase II (both IC_{50}>10 μM). BAY-1797 is also tested against a panel of off-targets, including G-protein coupled receptors (GPCRs), ion channels, kinases, and transporters at 10 μM. An inhibitory activity against the dopamine transporter (DAT, IC_{50} 2.17 μM) was revealed as the only hit[1].

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

In Vivo

BAY-1797 (12.5-50 mg/kg; p.o.) shows a significant induction of PGE2 levels in the inflamed paw in the mouse Complete Freund's Adjuvant (CFA) inflammatory pain model[1].

BAY-1797 (50 mg/kg; once daily for multiple p.o. administrations) induces a significant reduction of the ipsilateral paw load 24 and 48 h after CFA injection[1].

BAY-1797 treatment shows the AUC_{norm}, V_{ss} and $t_{1/2}$ are 1.06 kg h/L, 3.67 L/kg and 2.64 hours, respectively[1].

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

Animal Model:	Female adult C57BL/6N mice (CFA inflammatory pain model)[1]
Dosage:	12.5, 25, 50 mg/kg
Administration:	p.o.; once
Result:	Dose-dependently reduced PGE2 concentration in inflamed paw.

Animal Model:	Rat male Wistar[1]
Dosage:	1 mg/kg
Administration:	i.v. (Pharmacokinetic Analysis)
Result:	The AUC_{norm}, V_{ss} and $t_{1/2}$ were 1.06 kg h/L, 3.67 L/kg and 2.64 hours, respectively.

REFERENCES

[1]. Werner S, et al. Discovery and Characterization of the Potent and Selective P2X4 Inhibitor N-[4-(3-Chlorophenoxy)-3-sulfamoylphenyl]-2-phenylacetamide (BAY-1797) and Structure-Guided Amelioration of Its CYP3A4 Induction Profile. J Med Chem. 2019 Dec 26;62(24):11194-11217.

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