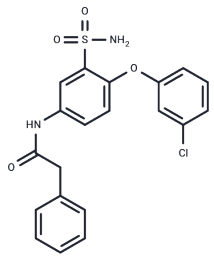
Data Sheet (Cat.No.T10466)

TargetMol

BAY-1797

Chemical Properties



CAS No. : 2055602-83-8

Formula: C20H17ClN2O4S

Molecular Weight: 416.88

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	BAY-1797 is an orally active and selective P2X4 antagonist (IC50: 211 nM against human P2X4) with anti-nociceptive and anti-inflammatory effects. BAY-1797 displays no or very weak activity on the other P2X ion channels.
Targets(IC50)	P2X Receptor
In vitro	BAY-1797 inhibits human, mouse, and rat P2X4 in 1321N1 cells (IC50s: 108 nM, 112 nM, and 233 nM). BAY-1797 exerts no measurable activity on hERG and carbonic anhydrase II (both IC50>10 μM). BAY-1797 (10 μM) is also tested against a panel of off-targets, including GPCRs, ion channels, kinases, and transporters. Inhibitory activity against the dopamine transporter (IC50: 2.17 μM) was revealed as the only hit.
In vivo	BAY-1797 (12.5-50 mg/kg; p.o.) significantly induces PGE2 levels in the inflamed paw in the mouse Complete Freund's Adjuvant (CFA) inflammatory pain model. At 50 mg/kg daily, BAY-1797 significantly reduces ipsilateral paw load 24 and 48 hours post-CFA injection. Pharmacokinetic parameters include AUCnorm of 1.06 kg h/L, Vss of 3.67 L/kg, and t1/2 of 2.64 hours.

Solubility Information

Solubility	DMSO: 250 mg/mL (599.69 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 5 mg/mL (11.99 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
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
50 mM	0.048 mL	0.2399 mL	0.4798 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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.