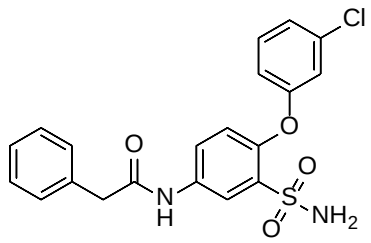
Product data sheet

MedKoo Cat#: 555698 Name: BAY-1797 CAS#: 2055602-83-8 Chemical Formula: $C_{20}H_{17}ClN_2O_4S$ Exact Mass: 416.0598 Molecular Weight: 416.88	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
BAY-1797 is an antagonist of the purinergic P2X4 receptor (IC50 = 0.211 µM for the human receptor). It is selective for P2X4 over P2X1, P2X3, and P2X7 receptors (IC50s = >50, 8.3, and 10.6 µM, respectively, for the human receptors), as well as a panel of G protein-coupled receptors (GPCRs), ion channels, kinases, and transporters at 10 µM. BAY-1797 (50 mg/kg) decreases intraplantar prostaglandin E2 (PGE2) levels and reduces non-evoked pain-related behavior in the dynamic weight bearing test in a mouse model of inflammatory pain induced by complete Freund's adjuvant (CFA).

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMF	30.0	71.96
DMSO	30.0	71.96
Ethanol	30.0	71.96

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.40 mL	11.99 mL	23.99 mL
5 mM	0.48 mL	2.40 mL	4.80 mL
10 mM	0.24 mL	1.20 mL	2.40 mL
50 mM	0.05 mL	0.24 mL	0.48 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

TBD

In vivo study

1. Werner S, Mesch S, Hillig RC, Ter Laak A, Klint J, Neagoe I, Laux-Biehlmann A, Dahllöf H, Bräuer N, Puetter V, Nubbemeyer R, Schulz S, Bairlein M, Zollner TM, Steinmeyer A. 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. doi: 10.1021/acs.jmedchem.9b01304. Epub 2019 Dec 11. PMID: 31746599.

7. Bioactivity
Biological target: BAY-1797 is a P2X4 antagonist with an IC50 of 211 nM.

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In vitro activity

TBD

In vivo activity

BAY-1797 demonstrated anti-inflammatory and anti-nociceptive effects in a mouse complete Freund's adjuvant (CFA) inflammatory pain model.

Reference: J Med Chem. 2019 Dec 26;62(24):11194-11217. https://pubs.acs.org/doi/abs/10.1021/acs.jmedchem.9b01304

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.