Print Date: Jan 16th 2023

Certificate of Analysis

www.tocris.com

Product Name: **BAY 1797** **Catalog No.: 7573** **Batch No.: 1**

CAS Number: 2055602-83-8

IUPAC Name: *N*-[3-(Aminosulfonyl)-4-(3-chlorophenoxy)phenyl]benzeneacetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{17}ClN_2O_4S$.

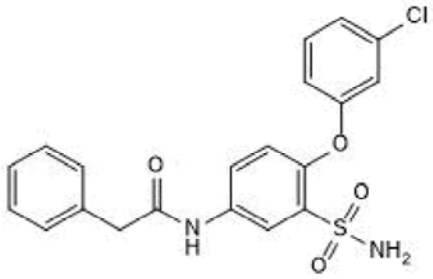
Batch Molecular Weight: 416.88

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.62	4.11	6.72
Found	57.69	4.05	6.62

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

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Description:

BAY 1797 is a selective purinergic $P2X_4$ receptor antagonist (IC_{50} values are 108, 112 and 233 nM for the human, mouse and rat $P2X_4$, respectively). It is selective for $P2X_4$ over $P2X_3$, $P2X_7$, and $P2X_1$ receptors (IC_{50} values are 8.3, 10.6 and >50 µM, respectively, for the human receptors). BAY 1797 dose-dependently reduces prostaglandin E_2 levels and exhibits anti-inflammatory and analgesic effects in an in vivo model of inflammatory pain. Orally active.

Physical and Chemical Properties:

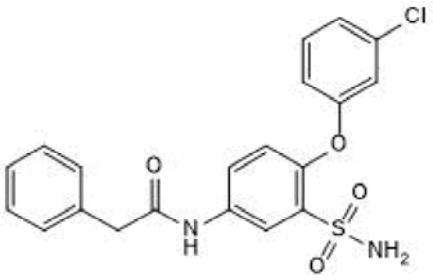
Batch Molecular Formula: $C_{20}H_{17}ClN_2O_4S$.

Batch Molecular Weight: 416.88

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the BAY 1797 probe summary on the SGC website.

References:

Werner *et al* (2019) Discovery and characterization of the potent and selective $P2X_4$ inhibitor *N*-[4-(3-chlorophenoxy)-3-sulfamoylphenyl] -2-phenylacetamide (BAY-1797) and structure-guided amelioration of its CYP3A4 induction profile. J.Med.Chem. ***62*** 11194. PMID: 31746599.