

Product Name: BAY 8002

Catalog No.: 6817

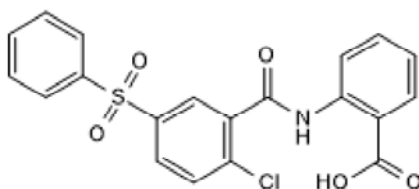
Batch No.: 1

CAS Number: 724440-27-1

IUPAC Name: 2-[[2-Chloro-5-(phenylsulfonyl)benzoyl]amino]benzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₁₄ClNO₅S
Batch Molecular Weight: 415.85
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 20 mM with gentle warming
 1eq. NaOH to 5 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.76	3.39	3.37
Found	57.81	3.36	3.54

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Potent dual MCT1/2 inhibitor (IC₅₀ values are 3, 8, and 12 nM at rat (C6), human (DLD-1) and mouse (4T1) MCT1 respectively; IC₅₀ values of Human MCT1, MCT2, and MCT4 isoforms recombinantly expressed in *X. laevis* oocytes are 1, 5 and >500 nM, respectively); suppress bidirectional lactate transport. Inhibits cellular SNARF-5 fluorescence change (IC₅₀ = 85 nM) in MCT1- expressing DLD-1 cells. Orally available.

Physical and Chemical Properties:

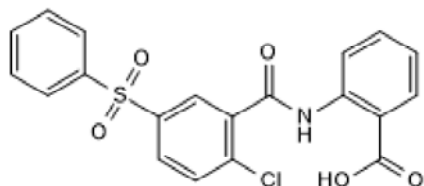
Batch Molecular Formula: C₂₀H₁₄ClNO₅S

Batch Molecular Weight: 415.85

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Quanz *et al* (2018) Preclinical efficacy of the novel monocarboxylate transporter 1 inhibitor BAY-8002 and associated markers of resistance. *Mol.Cancer Ther.* **17** 2285. PMID: 30115664.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 mM with gentle warming

1eq. NaOH to 5 mM with gentle warming

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.

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