

Product Name: S4

Catalog No.: 5577

Batch No.: 1

CAS Number: 1330061-67-0

IUPAC Name: 4-[[[(3,5-Dimethylphenyl)amino]carbonyl]amino]phenyl sulfamate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₇N₃O₄S·¼H₂O

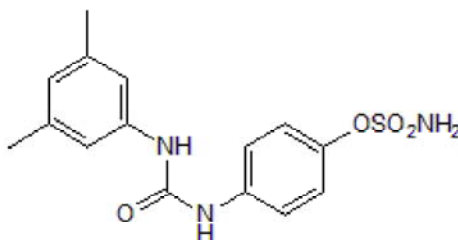
Batch Molecular Weight: 339.88

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 20 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.41 (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.01	5.19	12.36
Found	53.02	5.04	12.28

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

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:

High affinity and selective CA IX and CA XII inhibitor (K_i values are 2, 7, 547 and 5600 nM for CA XII, IX, II and I, respectively). Inhibits migration and proliferation of breast cancer cells in vitro. Inhibits lung metastasis in mice bearing breast tumor xenografts, without affecting primary tumor.

Physical and Chemical Properties:

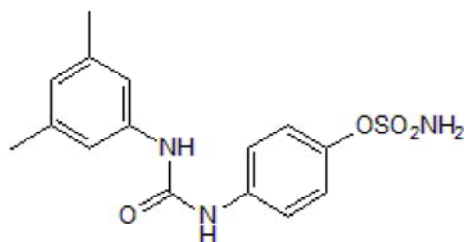
Batch Molecular Formula: $C_{15}H_{17}N_3O_4S \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 339.88

Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:



References:

Gieling *et al* (2012) Antimetastatic effect of sulfamate carbonic anhydrase IX inhibitors in breast carcinoma xenografts. *J.Med.Chem.* **55** 5591. PMID: 22621623.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 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.

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