

Certificate of Analysis

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Product Name: U 104

Catalog No.: 4540

Batch No.: 1

CAS Number: 178606-66-1

IUPAC Name: 4-[[[(4-Fluorophenyl)amino]carbonyl]amino]-benzesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₁₂FN₃O₃S

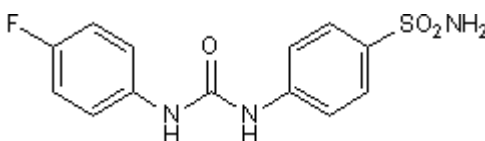
Batch Molecular Weight: 309.32

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.25 (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.48	3.91	13.58
Found	50.29	3.83	13.55

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

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IUPAC Name: 4-[[[(4-Fluorophenyl)amino]carbonyl]amino]-benzenesulfonamide

Description:

Potent carbonic anhydrase (CA) inhibitor (K_i values are 4.5, 45.1, 5080 and 9640 nM for CA XII, CA IX, CA I and CA II respectively in MDA-MB-231 cells). Inhibits tumor metastasis in the rat 4T1 metastasis model.

Physical and Chemical Properties:

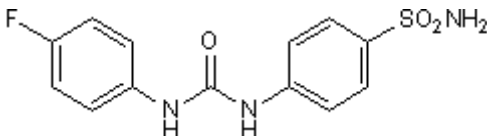
Batch Molecular Formula: $C_{13}H_{12}FN_3O_3S$

Batch Molecular Weight: 309.32

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO 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.

References:

Lou et al (2011) Targeting tumor hypoxia: suppression of breast tumor growth and metastasis by novel carbonic anhydrase IX inhibitors. *Cancer Res.* **71** 3364. PMID: 21415165.

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