

Certificate of Analysis

Print Date: Feb 25th 2019

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Product Name: BI 01383298 Catalog No.: 6518 Batch No.: 1

CAS Number: 2227549-00-8

IUPAC Name: 1-[(3,5-Dichlorophenyl)sulfonyl]-*N*-[(4-fluorophenyl)methyl]-4-piperidinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₁₉Cl₂FN₂O₃S

Batch Molecular Weight: 445.34 **Physical Appearance:** White solid

Solubility: DMSO to 50 mM Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: R_f = 0.45 (Ethyl acetate:Petroleum ether [2:3])

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 51.24 4.3 6.29 Found 51.24 4.24 6.46

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

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Product Information

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IUPAC Name: 1-[(3,5-Dichlorophenyl)sulfonyl]-*N*-[(4-fluorophenyl)methyl]-4-piperidinecarboxamide

Description:

Potent and selective inhibitor of human SLC13A5 (Na+/citrate cotransporter; $IC_{50} = 56$ nM in HEK cells overexpressing hSLC13A5 and 24 nM in HepG2 cells with endogenous SLC13A5 expression). Displays >1000-fold selectivity over other family members.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₉H₁₉Cl₂FN₂O₃S

Batch Molecular Weight: 445.34 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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 BI01383298 probe summary on the SGC website.

References:

Peters (2017) Flipping a citrate switch on liver cancer cells. J.Biol.Chem. 292 13902. PMID: 28821606.