

Certificate of Analysis

Print Date: Jan 14th 2016

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Product Name: CID 5951923 Catalog No.: 4446 Batch No.: 1

CAS Number: 749872-43-3

IUPAC Name: 2-[Methyl(tetrahydro-1,1-dioxido-3-thienyl)amino]-2-oxoethyl (E)-3-(3-nitrophenyl)prop-2-enoate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{18}N_2O_7S$

Batch Molecular Weight: 382.39

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 97.1% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 50.26 4.74 7.32 Found 50.22 4.77 7.29



Product Information

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Description:

Inhibitor of Krüppel-like factor 5 (KLF5) transcription factor (IC $_{50}$ = 2.3 μ M). Selectively active against colon cancer cells in a panel of 60 different cancer cell lines.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₆H₁₈N₂O₇S Batch Molecular Weight: 382.39 Physical Appearance: Off-white solid

Minimum Purity: >97%

Batch Molecular Structure:

$$O_2N$$

Storage: Store at +4°C

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:

Bialkowska et al (2011) Identification of small-molecule inhibitors of the colorectal cancer oncogene Krüppel-like factor 5 expression by ultrahigh-throughput screening. Mol.Cancer Ther. 10 2043. PMID: 21885866.