

**Product Name:** CID 5951923

**Catalog No.:** 4446

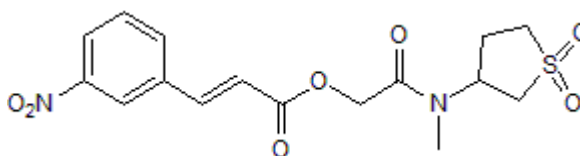
**Batch No.:** 1

**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<sub>16</sub>H<sub>18</sub>N<sub>2</sub>O<sub>7</sub>S  
**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  
**<sup>1</sup>H 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

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**Description:**

Inhibitor of Krüppel-like factor 5 (KLF5) transcription factor (IC<sub>50</sub> = 2.3 µM). Selective for colon cancer cells in a panel of 60 different cancer cell lines.

**Physical and Chemical Properties:**

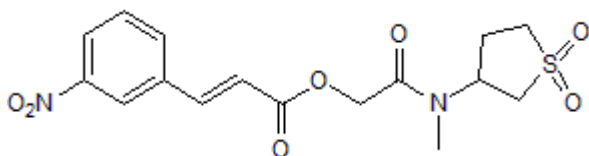
Batch Molecular Formula: C<sub>16</sub>H<sub>18</sub>N<sub>2</sub>O<sub>7</sub>S

Batch Molecular Weight: 382.39

Physical Appearance: Off-white solid

**Minimum Purity:** >97%

**Batch Molecular Structure:**



**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.

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