

**Product Name:** Ki 16425

**Catalog No.:** 5056

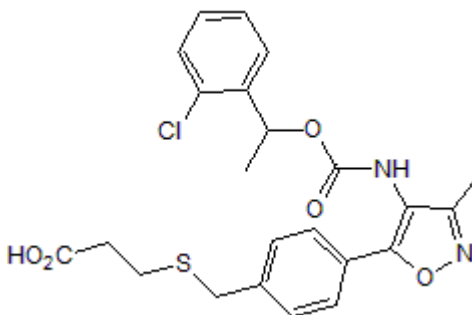
**Batch No.:** 1

**CAS Number:** 355025-24-0

**IUPAC Name:** 3-[[[4-[[[1-(2-Chlorophenyl)ethoxy]carbonyl]amino]-3-methyl-5-isoxazolyl]phenyl]methyl]thio]propanoic acid

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>23</sub>H<sub>23</sub>ClN<sub>2</sub>O<sub>5</sub>S  
**Batch Molecular Weight:** 474.96  
**Physical Appearance:** Off-white solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 100 mM  
 1eq. NaOH to 20 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 98.4% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon Hydrogen Nitrogen		
Theoretical	58.16	4.88	5.9
Found	58.12	4.85	6.02

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**Description:**

Antagonist of the lysophosphatidic acid receptors LPA<sub>1</sub> and LPA<sub>3</sub> (K<sub>i</sub> values are 0.25 and 0.36 μM respectively, in a GTPγS binding assay).

**Physical and Chemical Properties:**

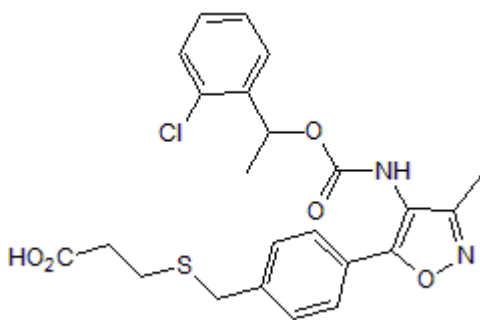
Batch Molecular Formula: C<sub>23</sub>H<sub>23</sub>ClN<sub>2</sub>O<sub>5</sub>S

Batch Molecular Weight: 474.96

Physical Appearance: Off-white solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 100 mM

1eq. NaOH 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.

**References:**

**Ohta *et al*** (2003) Ki16425, a subtype-selective antagonist for EDG-family lysophosphatidic acid receptors. *Mol.Pharmacol.* **64** 994. PMID: 14500756.

**Yamada *et al*** (2004) Lysophosphatidic acid (LPA) in malignant ascites stimulates motility of human pancreatic cancer cells through LPA<sub>1</sub>. *J.Biol.Chem.* **279** 6595. PMID: 14660630.

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