

Product Name: Ki 16425

Catalog No.: 5056

Batch No.: 2

CAS Number: 355025-24-0

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₃ClN₂O₅S.¾H₂O

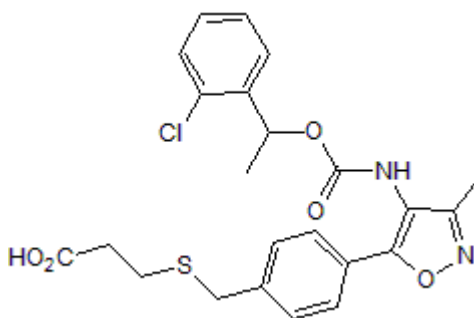
Batch Molecular Weight: 488.47

Physical Appearance: 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% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.55	5.06	5.73
Found	56.65	4.85	5.99

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Description:

Antagonist of the lysophosphatidic acid receptors LPA₁ and LPA₃ (K_i values are 0.25 and 0.36 μM respectively, in a GTPγS binding assay). Blocks LPA-induced dephosphorylation of Yes-associated protein (YAP) and WW domain-containing transcription regulator protein 1 (TAZ), inhibiting the Hippo signaling pathway, in HEK293A cells.

Physical and Chemical Properties:

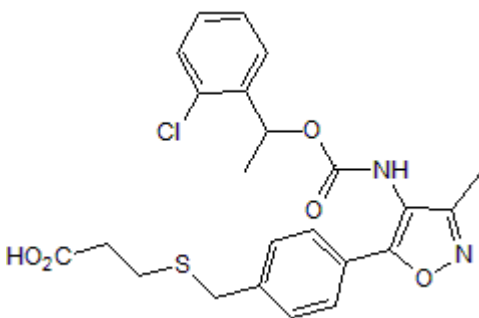
Batch Molecular Formula: C₂₃H₂₃ClN₂O₅S.¾H₂O

Batch Molecular Weight: 488.47

Physical Appearance: 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 LPA₁. *J.Biol.Chem.* **279** 6595. PMID: 14660630.

Yu et al (2012) Regulation of the Hippo-YAP pathway by G-protein-coupled receptor signaling. *Cell* **150** 780. PMID: 22863277.

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