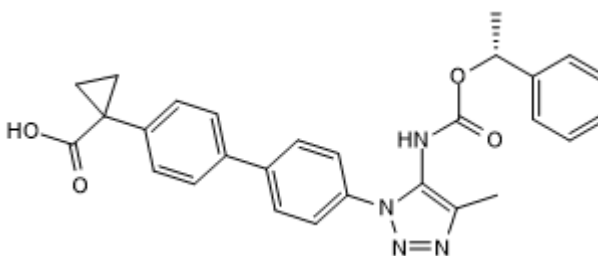


Product Name: Ro 6842262 **Catalog No.:** 5913 **Batch No.:** 1
CAS Number: 1396006-71-5
IUPAC Name: 1-[4'-[4-Methyl-5-[[[(1*R*)-1-phenylethoxy]carbonylamino]-1*H*-1,2,3-triazol-1-yl]][1,1'-biphenyl]-4-yl]cyclopropanecarboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₂₆N₄O₄·½H₂O
Batch Molecular Weight: 487.03
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 20 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.65 (Ethyl acetate)
HPLC: Shows 98.9% purity
Chiral HPLC: Shows 99.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = +15.9 (Concentration = 1, Solvent = Methanol)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	69.05	5.48	11.5
Found	69.1	5.42	11.41

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

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Description:

Potent LPA₁ antagonist (IC₅₀ = 25 nM). Exhibits >1,200-fold selectivity for LPA₁ over LPA₃. Attenuates NHLF human lung fibroblast cell proliferation and contraction in vitro. Also reduces plasma histamine levels in mouse LPA-challenge model. Orally bioavailable.

Physical and Chemical Properties:

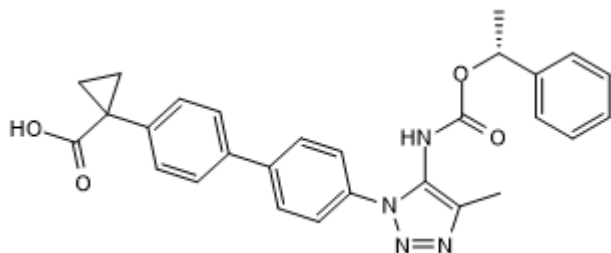
Batch Molecular Formula: C₂₈H₂₆N₄O₄ · ¼H₂O

Batch Molecular Weight: 487.03

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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:

Qian et al (2012) Discovery of highly selective and orally active lysophosphatidic acid receptor-1 antagonists with potent activity on human lung fibroblasts. *J.Med.Chem.* **55** 7920. PMID: 22894757.

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