

Product Name: GLPG 0974

Catalog No.: 5621

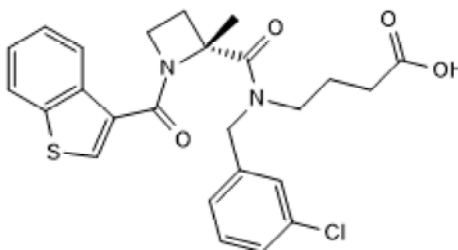
Batch No.: 2

CAS Number: 1391076-61-1

IUPAC Name: 4-[[[(2R)-1-(Benzo[b]thien-3-ylcarbonyl)-2-methyl-2-azetidiny]carbonyl][(3-chlorophenyl)methyl]amino]butanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₅ClN₂O₄S
Batch Molecular Weight: 485
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Dichloromethane:Methanol [9:1])
HPLC: Shows 98% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = +195 (Concentration = 1.01, Solvent = Chloroform)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.91	5.2	5.77
Found	62.14	5.22	5.85

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

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Description:

Potent FFA2 antagonist (IC₅₀ = 9 nM). Exhibits selectivity for FFA2 over FFA3. Inhibits acetate-induced human neutrophil migration in plasma or buffer. Also inhibits FFA2-induced expression of CD11b activation-specific epitope (AE) in human whole blood. Orally bioavailable.

Physical and Chemical Properties:

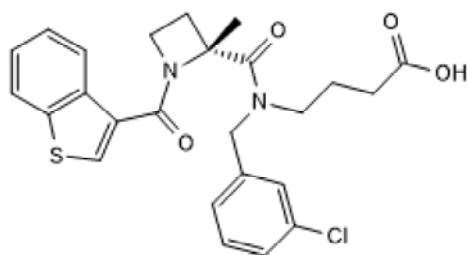
Batch Molecular Formula: C₂₅H₂₅ClN₂O₄S

Batch Molecular Weight: 485

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

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:

Pizzonero et al (2014) Discovery and optimization of an azetidine chemical series as a free fatty acid receptor 2 (FFA2) antagonist: from hit to clinic. *J.Med.Chem.* **57** 10044. PMID: 25380412.

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