

Product Name: Zileuton

Catalog No.: 3308

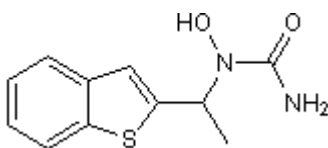
Batch No.: 1

CAS Number: 111406-87-2

IUPAC Name: *N*-(1-Benzo[*b*]thien-2-ylethyl)-*N*-hydroxyurea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₁H₁₂N₂O₂S
Batch Molecular Weight: 236.29
Physical Appearance: white solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows >99.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.92	5.12	11.85
Found	55.86	5.07	11.89

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

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Description:

Orally active 5-lipoxygenase (5-LOX) inhibitor that inhibits LTB₄ synthesis (IC₅₀ values are 0.56, 2.3 and 2.6 μM in dog, rat and human blood respectively). Inhibits antigen-induced contraction of tracheal strips in vitro (IC₅₀ = 6 μM) and exhibits antiasthmatic activity in vivo. Also weakly inhibits CYP1A2 (K_i = 66 - 98 μM).

Physical and Chemical Properties:

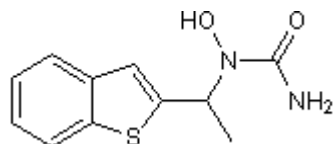
Batch Molecular Formula: C₁₁H₁₂N₂O₂S

Batch Molecular Weight: 236.29

Physical Appearance: white solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

McMillan et al (1992) Pre-clinical pharmacology of ICI D2138, a potent orally-active non-redox inhibitor of 5-lipoxygenase. *Br.J.Pharmacol.* **107** 1042. PMID: 1334748.

Malo et al (1994) The 5-lipoxygenase inhibitory activity of zileuton in in vitro and in vivo models of antigen-induced airway anaphylaxis. *Pulm.Pharmacol.* **7** 73. PMID: 8081074.

Lu et al (2003) Mechanism-based inhibition of human liver microsomal cytochrome P450 1A2 by zileuton, a 5-lipoxygenase inhibitor. *Drug Metab.Dispos.* **31** 1352. PMID: 14570767.

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.

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