

## Certificate of Analysis

**Product Name:** SC 57461A

**Catalog No.:** 3107

**Batch No.:** 2

**CAS Number:** 423169-68-0

**IUPAC Name:** *N*-methyl-*N*-[3-[4-(phenylmethyl)phenoxy]propyl]-β-alanine hydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>20</sub>H<sub>25</sub>NO<sub>3</sub>.HCl

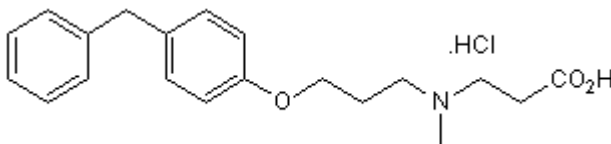
**Batch Molecular Weight:** 363.88

**Physical Appearance:** White solid

**Solubility:** water to 25 mM  
DMSO to 100 mM

**Storage:** Desiccate at +4°C

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**HPLC:** Shows 99.7% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	66.01	7.2	3.85
Found	66.21	7.26	3.84

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**Description:**

Potent and selective inhibitor of LTA<sub>4</sub> hydrolase. Does not inhibit other enzymes of the arachidonic acid cascade including COX-1, COX-2, LTC<sub>4</sub> synthase and 5-lipoxygenase. Potently inhibits LTB<sub>4</sub> production in whole blood (IC<sub>50</sub> = 49 nM). Orally active.

**Physical and Chemical Properties:**

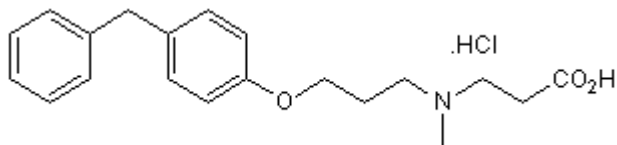
Batch Molecular Formula: C<sub>20</sub>H<sub>25</sub>NO<sub>3</sub>·HCl

Batch Molecular Weight: 363.88

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Desiccate at +4°C

**Solubility & Usage Info:**

water to 25 mM  
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.

**References:**

**Penning *et al*** (2002) Synthesis of potent leukotriene A<sub>4</sub> hydrolase inhibitors. Identification of 3-[methyl[3-[4-(phenylmethyl)phenoxy]propyl]amino]propanoic acid. *J.Med.Chem.* **45** 3482. PMID: 12139459.

**Askonas *et al*** (2002) Pharmacological characterization of SC-57461A (3-[methyl[3-[4-(phenylmethyl)phenoxy]propyl]amino]propanoic acid HCl), a potent and selective inhibitor of leukotriene A<sub>4</sub> hydrolase I: in vitro studies. *J.Pharmacol.Exp.Ther.* **300** 577. PMID: 11805219.

**Kachur *et al*** (2002) Pharmacological characterization of SC-57461A (3-[methyl[3-[4-(phenylmethyl)phenoxy]propyl]amino]propanoic acid HCl), a potent and selective inhibitor of leukotriene A<sub>4</sub> hydrolase II: in vivo studies. *J.Pharmacol.Exp.Ther.* **300** 583. PMID: 11805220.

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