TOCRIS bioscience

Print Date: Jan 16th 2012

# Certificate of Analysis

www.tocris.com

**Product Name: BAY-X 1005** **Catalog No.: 3541** **Batch No.: 1**

CAS Number: 128253-31-6

IUPAC Name: (*R*)-α-Cyclopentyl-4-(2-quinolinylmethoxy)benzeneacetic acid

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{23}H_{23}NO_3$

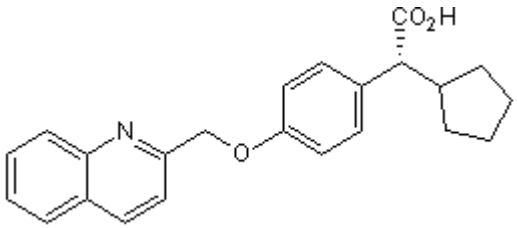
**Batch Molecular Weight:** 361.43

**Physical Appearance:** Beige solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at RT

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**TLC:** $R_f$ = 0.2 (Ethyl acetate:Petroleum ether [1:2])

**HPLC:** Shows >99.9% purity

**Chiral HPLC:** Shows 100% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** $[\alpha]_D$ = -41.2 (Concentration = 1, Solvent = Chloroform)

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 76.43 | 6.41 | 3.88 |
| Found | 76.2 | 6.44 | 3.9 |

**Product Name: BAY-X 1005** **Catalog No.: 3541** **Batch No.: 1**

CAS Number: 128253-31-6

IUPAC Name: (*R*)-α-Cyclopentyl-4-(2-quinolinylmethoxy)benzeneacetic acid

**Description:**

5-lipoxygenase activating protein (FLAP) inhibitor. Inhibits the synthesis of leukotrienes $B_4$ and $C_4$ in animal models; inhibits synthesis of leukotriene $B_4$ in A23187-stimulated leukocytes ($IC_{50}$ values are 0.026, 0.039 and 0.22 μM for rat, mice and human leukocytes respectively). Displays anti-inflammatory activity. Orally active.

**Physical and Chemical Properties:**

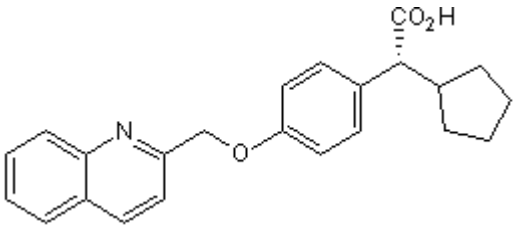
Batch Molecular Formula: $C_{23}H_{23}NO_3$

Batch Molecular Weight: 361.43

Physical Appearance: Beige solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**




**Storage:** Store at RT

**Solubility & Useage 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.

**References:**

**Muller-Peddinghaus** *et al* (1993) BAY X1005, a new inhibitor of leukotriene synthesis: in vivo inflammation pharmacology and pharmacokinetics. J.Pharmacol.Exp.Ther. ***267*** 51. PMID: 8229782.

**Fruchtmann** *et al* (1993) In vitro pharmacology of BAY X1005, a new inhibitor of leukotriene synthesis. Agents Actions ***38*** 188. PMID: 8213345.

**Hatzelmann** *et al* (1994) Mode of action of the leukotriene synthesis (FLAP) inhibitor BAY X 1005: implications for biological regulation of 5-lipoxygenase. Agents Actions ***43*** 64. PMID: 7741044.