

Certificate of Analysis

Print Date: Jan 15th 2016

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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:361.43Physical 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

1H 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

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Product Information

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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: C₂₃H₂₃NO₃ Batch Molecular Weight: 361.43 Physical Appearance: Beige solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at RT

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.

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.

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