

Certificate of Analysis

www.tocris.com

Print Date: Jan 15th 2016

Product Name: (S)-(+)-lbuprofen Catalog No.: 2796 Batch No.: 1

CAS Number: 51146-56-6

IUPAC Name: (S)-α-Methyl-4-(2-methylpropyl)benzeneacetic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{13}H_{18}O_2$ Batch Molecular Weight: 206.28

Physical Appearance: White crystalline solid

Solubility: DMSO to 100 mM ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:

CO₂H

2. ANALYTICAL DATA

Melting Point:Between 51 - 52°CHPLC:Shows >99.9% purity¹H NMR:Consistent with structureMass Spectrum:Consistent with structure

Optical Rotation: $[\alpha]_D = +61.7$ (Concentration = 0.6, Solvent = Methanol)



Product Information

Print Date: Jan 15th 2016

www.tocris.com

Product Name: (S)-(+)-lbuprofen Catalog No.: 2796 Batch No.: 1

CAS Number: 51146-56-6

IUPAC Name: (S)-α-Methyl-4-(2-methylpropyl)benzeneacetic acid

Description:

Non-steroidal anti-inflammatory drug (NSAID) that inhibits cyclooxygenase 1 and cyclooxygenase 2 (IC $_{50}$ values are 12 and 80 μ M respectively). Active isomer of ibuprofen.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{13}H_{18}O_2$ Batch Molecular Weight: 206.28

Physical Appearance: White crystalline solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

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:

Kato *et al* (2001) Cyclooxygenase-1 and cyclooxygenase-2 selectivity of non-steroidal anti-inflammatory drugs: investigation using human peripheral monocytes. J.Pharm.Pharmacol. **53** 1679. PMID: 11804398.