



Certificate of Analysis

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Product Name: NS 398 Catalog No.: 0942 Batch No.: 2

CAS Number: 123653-11-2

IUPAC Name: N-[2-Cyclohexyloxy-4-nitrophenyl]methanesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{13}H_{18}N_2O_5S$

Batch Molecular Weight: 314.36

Physical Appearance: Pale cream crystalline solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.76$ (Ethyl acetate:Petroleum ether [2:8])

Melting Point: At 142°C

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 49.67 5.77 8.91 Found 49.67 5.87 8.59



Product Information

Print Date: Apr 28th 2015

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IUPAC Name: N-[2-Cyclohexyloxy-4-nitrophenyl]methanesulfonamide

Description:

Selective cyclooxygenase-2 inhibitor (IC $_{50}$ values are 3.8 and > 100 μ M for COX-2 and COX-1 respectively). Induces apoptosis in colorectal tumor cells and elevates COX-2 protein expression in vitro. Orally active and non-ulcerogenic analgesic and anti-inflammatory in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₃H₁₈N₂O₅S Batch Molecular Weight: 314.36

Physical Appearance: Pale cream crystalline solid

Minimum Purity: >99%

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:

Futaki *et al* (1993) NS-398, a novel non-steroidal anti-inflammatory drug with potent analgesic and antipyretic effects, which causes minimal stomach lesions. Gen.Pharmacol. **24** 105. PMID: 8482483.

Futaki *et al* (1994) NS-398, a new anti-inflammatory agent, selectively inhibits prostaglandin G/H synthase/cyclooxygenase (COX-2) activity *in vitro*. Prostaglandins **47** 55. PMID: 8140262.

Elder et al (2002) The MEK/ERK pathway mediates COX-2-selective NSAID-induced apoptosis and induced COX-2 protein expression in colorectal carcinoma cells. Int.J.Cancer 99 323. PMID: 11992399.

