

Certificate of Analysis

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Product Name: Niflumic acid Catalog No.: 4112 Batch No.: 1

CAS Number: 4394-00-7 EC Number: 224-516-2

IUPAC Name: 2-[3-(Trifluoromethyl)anilino]nicotinic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{13}H_9F_3N_2O_2$

Batch Molecular Weight: 282.22

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.33 3.27 9.93 Found 55.52 3.27 9.83



Product Information

Print Date: May 16th 2012

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IUPAC Name: 2-[3-(Trifluoromethyl)anilino]nicotinic acid

Description:

Nonsteroidal anti-inflammatory drug (NSAID); selectively inhibits COX-2. Also activates human TRPA1 inducibly expressed in HEK293 cells; displays agonist activity at GPR35.

Physical and Chemical Properties:

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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:

Ottolia and Toro (1994) Potentiation of large conductance KCa channels by niflumic, flufenamic and mefenamic acids. Biophys.J. 67 2272. PMID: 7535111.

Famaey (1997) In vitro and in vivo pharmacological evidence of selective cyclooxygenase-2 inhibition by nimesulide: an overview. Inflamm.Res. **46** 437. PMID: 9427063.

Hu et al (2010) Activation of TRPA1 channels by fenamate nonsteroidal anti-inflammatory drugs. Pflugers Arch. **459** 579. PMID: 19888597.

Deng et al (2012) Multiple tyrosine metabolites are GPR35 agonists. Sci.Rep. 2 373. PMID: 22523636.

