Print Date: May 18th 2012

Certificate of Analysis

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Product Name: SC 236 **Catalog No.: 3919** **Batch No.: 1**

CAS Number: 170569-86-5

IUPAC Name: 4-[5-(4-chlorophenyl)-3-(trifluoromethyl)-1*H*-pyrazol-1-yl] benzenesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{11}ClF_3N_3O_2S$

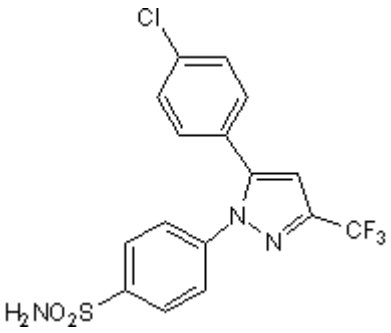
Batch Molecular Weight: 401.79

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	47.83	2.76	10.46
Found	47.53	2.67	10.42

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Description:

Selective COX-2 inhibitor (IC_{50} values are 0.005 and 17.8 µM for COX-2 and COX-1 respectively). Displays anti-inflammatory properties and potent antimetastatic activity against both experimental metastases and spontaneous metastases arising following primary tumor excision.

Physical and Chemical Properties:

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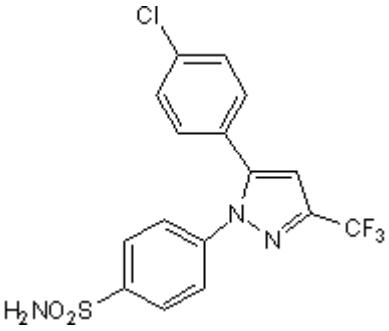
Batch Molecular Weight: 401.79

Physical Appearance: White 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:

Gierse *et al* (1996) A single amino acid difference between cyclooxygenase-1 (COX-1) and -2 (COX-2) reverses the selectivity of COX-2 specific inhibitors. J.Biol.Chem. ***271*** 15810. PMID: 8663121.

Penning *et al* (1997) Synthesis and biological evaluation of the 1,5-diarylpyrazole class of cyclooxygenase-2 inhibitors: identification of 4-[5-(4-Methylphenyl)-3-(trifluoromethyl)-1*H*-pyrazol-1-yl]benzenesulfonamide (SC-58635, Celecoxib). J.Med.Chem. ***40*** 1347. PMID: 9135032.

Roche-Nagle *et al* (2004) Antimetastatic activity of a cyclooxygenase-2 inhibitor. Br.J.Cancer ***91*** 359. PMID: 15213717.