

Certificate of Analysis

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Product Name: SC 58125

Catalog No.: 2895

Batch No.: 2

CAS Number: 162054-19-5

IUPAC Name: 5-(4-Fluorophenyl)-1-[4-(methylsulfonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazole

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₂F₄N₂O₂S

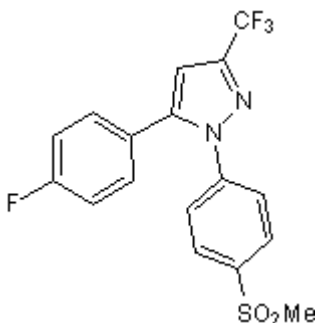
Batch Molecular Weight: 384.35

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.12	3.15	7.29
Found	52.86	2.96	7.21

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Selective cyclooxygenase 2 (COX-2) inhibitor (IC₅₀ values are 0.04 and >100 µM for COX-2 and COX-1 respectively). Anti-inflammatory; blocks edema and hyperalgesia in vivo following an inflammatory insult, without causing gastric mucosal damage. Also displays antitumor activity.

Physical and Chemical Properties:

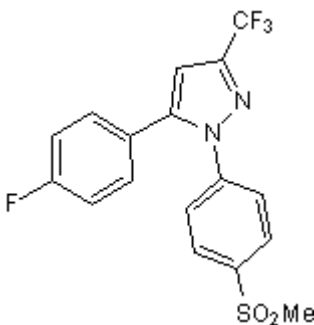
Batch Molecular Formula: C₁₇H₁₂F₄N₂O₂S

Batch Molecular Weight: 384.35

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 25 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:

Seibert et al (1994) Pharmacological and biochemical demonstration of the role of cyclooxygenase 2 in inflammation and pain. *Proc.Natl.Acad.Sci.USA* **91** 12013.

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.

Williams et al (2001) A cyclooxygenase-2 inhibitor (SC-58125) blocks growth of established colon cancer xenografts. *Neoplasia* **3** 428. PMID: 11687954.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956