

Product Name: Celecoxib

Catalog No.: 3786

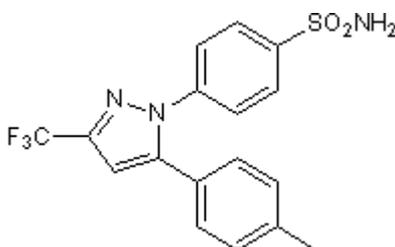
Batch No.: 1

CAS Number: 169590-42-5

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₄F₃N₃O₂S
Batch Molecular Weight: 381.37
Physical Appearance: White solid
Solubility: DMSO to 25 mM
 ethanol to 50 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.54	3.7	11.02
Found	53.72	3.7	11.03

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 15 and 0.04 μM for COX-1 and COX-2 respectively). Anti-inflammatory with shorter plasma half-life in vivo than SC 58121 (Cat. No. 2895). Displays chemopreventive activity in in vivo tumor models.

Physical and Chemical Properties:

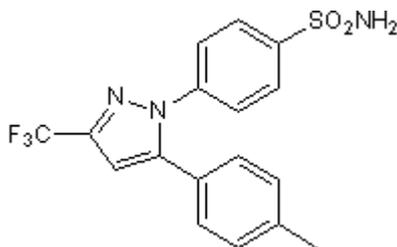
Batch Molecular Formula: C₁₇H₁₄F₃N₃O₂S

Batch Molecular Weight: 381.37

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 25 mM

ethanol to 50 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:

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)-1H-pyrazol-1-yl]benzenesulfonamide (SC-58635, celecoxib). *J.Med.Chem.* **40** 1347. PMID: 9135032.

DeWitt (1999) Cox-2-selective Inhibitors: the new super aspirins. *Mol.Pharmacol.* **55** 625. PMID: 10101019.

Harris *et al* (2000) Chemoprevention of breast cancer in rats by celecoxib, a cyclooxygenase 2 inhibitor. *Cancer Res.* **60** 2101. PMID: 10786667.

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