

## Certificate of Analysis

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**Product Name:** Celecoxib

**Catalog No.:** 3786

**Batch No.:** 2

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:** C<sub>17</sub>H<sub>14</sub>F<sub>3</sub>N<sub>3</sub>O<sub>2</sub>S.

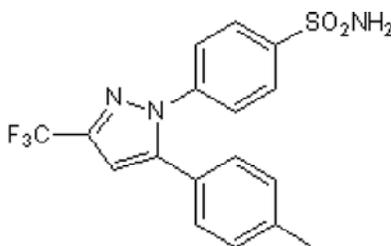
**Batch Molecular Weight:** 381.37

**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 99.9% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon Hydrogen Nitrogen		
Theoretical	53.54	3.7	11.02
Found	53.4	3.61	10.97

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

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**Description:**

Celecoxib is a selective cyclooxygenase-2 (COX-2) inhibitor (IC<sub>50</sub> values are 15 and 0.04 μM for COX-1 and COX-2 respectively). Celecoxib is an 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:**

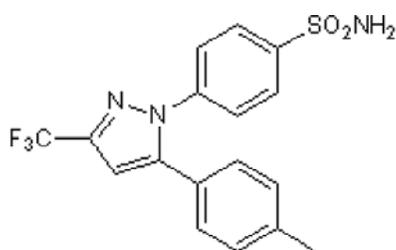
Batch Molecular Formula: C<sub>17</sub>H<sub>14</sub>F<sub>3</sub>N<sub>3</sub>O<sub>2</sub>S.

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:**

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

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

**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.

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