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
Storage: Store at RT
Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.7% purity
\( ^1H \) NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>47.83</td>
<td>2.76</td>
<td>10.46</td>
</tr>
<tr>
<td>Found</td>
<td>47.53</td>
<td>2.67</td>
<td>10.42</td>
</tr>
</tbody>
</table>

Certificate of Analysis

www.tocris.com

Product Name: SC 236
Catalog No.: 3919
Batch No.: 1
CAS Number: 170569-86-5
IUPAC Name: 4-[5-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide

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

Tocris Bioscience is an R&D Systems company
USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373
www.RnDSystems.com
**Product Name:** SC 236  
**Catalog No.:** 3919  
**Batch No.:** 1  

**Description:**  
Selective COX-2 inhibitor (IC50 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:**  
- **Batch Molecular Formula:** C19H11ClF3N3O2S  
- **Batch Molecular Weight:** 401.79  
- **Physical Appearance:** White solid  
- **Minimum Purity:** >99%  

**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:**

