1. PHYSICAL AND CHEMICAL PROPERTIES

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Batch Molecular Formula</td>
<td>$\text{C}<em>{16}\text{H}</em>{14}\text{N}<em>{2}\text{O}</em>{3}\text{S}$</td>
</tr>
<tr>
<td>Batch Molecular Weight</td>
<td>314.36</td>
</tr>
<tr>
<td>Physical Appearance</td>
<td>White solid</td>
</tr>
<tr>
<td>Solubility</td>
<td>DMSO to 100 mM</td>
</tr>
<tr>
<td>Storage</td>
<td>Store at RT</td>
</tr>
<tr>
<td>Batch Molecular Structure</td>
<td><img src="image" alt="Molecular Structure" /></td>
</tr>
</tbody>
</table>

2. ANALYTICAL DATA

- **HPLC:** Shows 99.7% purity
- **$^1$H NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:**
  - Carbon: 61.13
  - Hydrogen: 4.49
  - Nitrogen: 8.91
  - Found: 60.9
  - Calculated: 4.5
  - 8.93
Product Name: Valdecoxib
CAS Number: 181695-72-7
IUPAC Name: 4-(5-Methyl-3-phenylisoxazol-4-yl)benzenesulfonamide

Description:
Selective and potent COX-2 inhibitor (in vitro IC50 values are 0.005 and 140 μM for human recombinant COX-2 and COX-1 respectively). Displays potent anti-inflammatory activity in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C16H14N2O3S
Batch Molecular Weight: 314.36
Physical Appearance: White solid
Minimum Purity: >99%

Storage: Store at RT

Solubility & Usage Info:
DMSO 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: