Product Name: S 18886 Catalog No.: 5568 Batch No.: 1
CAS Number: 165538-40-9
IUPAC Name: (6R)-6-[(4-Chlorophenyl)sulfonyl]amino]-5,6,7,8-tetrahydro-2-methyl-1-naphthalenepropanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{22}ClNO_4S$
Batch Molecular Weight: 407.91
Physical Appearance: White solid
Solubility: DMSO to 100 mM ethanol to 20 mM with gentle warming
Storage: Store at -20°C

2. ANALYTICAL DATA

HPLC: Shows 98.3% purity
Chiral HPLC: Shows 99.2% purity
$^1$H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: $[\alpha]_D = +29$ (Concentration = 1, Solvent = DMSO)
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>58.89</td>
<td>5.44</td>
<td>3.43</td>
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<tr>
<td>Found</td>
<td>58.9</td>
<td>5.41</td>
<td>3.33</td>
</tr>
</tbody>
</table>
Product Information

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CAS Number: 165538-40-9

IUPAC Name: (6R)-6-[[4-Chlorophenylsulfonyl]amino]-5,6,7,8-tetrahydro-2-methyl-1-naphthalenepropanoic acid

Description:
Potent thromboxane A₂ (TP) inhibitor (IC₅₀ = 16.4 nM). Inhibits U 46619 (Cat. No. 1932) induced human platelet aggregation and contraction of isolated rabbit saphenous vein in vitro. Also inhibits U 46619 induced increase in tracheal pressure in guinea pigs. Orally available.

Physical and Chemical Properties:
Batch Molecular Formula: C₂₀H₂₂ClNO₅S
Batch Molecular Weight: 407.91
Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:
DMSO to 100 mM
ethanol to 20 mM with gentle warming

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: