1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{16}\text{H}_{12}\text{F}_{3}\text{NOS} \)

Batch Molecular Weight: 323.33

Physical Appearance: Off-white solid

Solubility:
- DMSO to 100 mM
- Ethanol to 100 mM

Storage: Store at +4°C

2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

\(^1\text{H NMR:}\)
Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>59.44</td>
<td>59.46</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>3.74</td>
<td>3.7</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>4.33</td>
<td>4.42</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
**Product Name:** NS 6180  
**CAS Number:** 353262-04-1  
**IUPAC Name:** 4-[[3-(Trifluoromethyl)phenyl]methyl]-2H-1,4-benzothiazin-3(4H)-one

### Description:
Potent $K_{Ca}^{3.1}$ channel blocker ($IC_{50}$ values are 9, 14 and 15 nM for rat, human and mouse erythrocyte $K_{Ca}^{3.1}$ channels respectively). Exhibits ~ 50% inhibition of $K_{Ca}^{1.1}$, $K_{Ca}^{1.3}$, and $K_{Ca}^{1.1}$ channels, noradrenaline and dopamine transporters, L-type Ca$^{2+}$ channels and melatonin receptors at a concentration of 10 $\mu$M. Potently inhibits IL-2 and IFN-$\gamma$ production in rat lymphocytes ($IC_{50}$ ~ 50 nM); reduces DBNS-induced experimental colitis in rats.

### Physical and Chemical Properties:
- **Batch Molecular Formula:** $C_{16}H_{12}F_{3}NOS$
- **Batch Molecular Weight:** 323.33
- **Physical Appearance:** Off-white solid
- **Minimum Purity:** >99%

### Storage:
Store at +4°C

### 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: