Product Name: NS 398
CAS Number: 123653-11-2
IUPAC Name: N-[2-Cyclohexyloxy-4-nitrophenyl]methanesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{13}H_{18}N_{2}O_{5}S \)
Batch Molecular Weight: 314.36
Physical Appearance: Pale cream crystalline solid
Solubility: DMSO to 100 mM
Storage: Store at RT

2. ANALYTICAL DATA

TLC: \( R_f = 0.76 \) (Ethyl acetate:Petroleum ether [2:8])
Melting Point: At 142°C
HPLC: Shows 100% purity
\(^1\)H NMR: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>49.67</td>
<td>49.67</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.77</td>
<td>5.87</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>8.91</td>
<td>8.59</td>
</tr>
</tbody>
</table>
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Description:
Selective cyclooxygenase-2 inhibitor (IC₅₀ values are 3.8 and > 100 μM for COX-2 and COX-1 respectively). Induces apoptosis in colorectal tumor cells and elevates COX-2 protein expression in vitro. Orally active and non-ulcerogenic analgesic and anti-inflammatory in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C₁₃H₁₉N₂O₅S
Batch Molecular Weight: 314.36
Physical Appearance: Pale cream crystalline 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: