Product Name: GR 113808
Catalog No.: 1322
Batch No.: 3
CAS Number: 144625-51-4
IUPAC Name: 1-methyl-1H-indole-3-carboxylic acid, [1-[2-[(methylsulfonyl)amino]ethyl]-4-piperidinyl]methyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{19}\text{H}_{27}\text{N}_{3}\text{O}_{4}\text{S} \cdot \frac{1}{4}\text{H}_{2}\text{O} \)

Batch Molecular Weight: 398

Physical Appearance: White solid

Solubility:
- DMSO to 12 mM
- 1eq. HCl to 25 mM
- Ethanol to 50 mM

Storage: Store at RT

Batch Molecular Structure:

![Batch Molecular Structure](image)

2. ANALYTICAL DATA

TLC: \( R_f = 0.4 \) (Chloroform:Methanol [9:1])

HPLC: Shows 98.3% 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>57.34</td>
<td>57.35</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.96</td>
<td>6.85</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>10.56</td>
<td>10.57</td>
</tr>
</tbody>
</table>
Product Information

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Description:
Potent, selective 5-HT₄ receptor antagonist (pKᵦ = 9.43 in human colonic muscle, and Kᵦ = 0.15 nM for binding to cloned human 5-HT₄ receptors). Displays > 300-fold selectivity over 5-HT₁A, 5-HT₁B, 5-HT₂A, 5-HT₂C and 5-HT₃ receptors.

Physical and Chemical Properties:
Batch Molecular Formula: C_{19}H_{27}N_{2}O_{4}S·½H₂O
Batch Molecular Weight: 398
Physical Appearance: White solid

Minimum Purity: >98%

Storage: Store at RT

Solubility & Usage Info:
- DMSO to 12 mM
- 1eq. HCl to 25 mM
- Ethanol to 50 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:

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