1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** \( C_{23}H_{27}N_3OS \)

**Batch Molecular Weight:** 393.55

**Physical Appearance:** White crystalline solid

**Solubility:**
- Ethanol to 100 mM
- DMSO to 10 mM

**Storage:** Desiccate at -20°C

**Batch Molecular Structure:**

![Molecular Structure Diagram]

2. ANALYTICAL DATA

**TLC:**
- \( R_f = 0.19 \) (Ethyl acetate:Petroleum ether [1:3])

**Melting Point:**
- At 100°C

**HPLC:**
- Shows >99.4% purity

**\(^1\)H NMR:**
- Consistent with structure

**Microanalysis:**

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
<th>Sulfur</th>
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<tbody>
<tr>
<td>Theoretical</td>
<td>70.2</td>
<td>6.91</td>
<td>10.68</td>
<td>8.15</td>
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<tr>
<td>Found</td>
<td>70.35</td>
<td>6.95</td>
<td>10.71</td>
<td>7.87</td>
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</table>
Product Information

**Product Name:** FIT

**CAS Number:** 85951-63-9

**IUPAC Name:** N-[1-[(4-Isothiocyanatophenyl)ethyl]-4-piperidinyl]-N-phenylpropanamide

**Description:**
Selective and irreversible δ-opioid agonist ($EC_{50} = 8$ nM); acts by alkylating the receptor.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** $C_{22}H_{27}N_{2}O_{3}S$
- **Batch Molecular Weight:** 393.55
- **Physical Appearance:** White crystalline solid
- **Minimum Purity:** >99%

**Storage:** Desiccate at -20°C

**Solubility & Usage Info:**
- ethanol to 100 mM
- DMSO to 10 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:**

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

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