1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** \( \text{C}_{19}\text{H}_{25}\text{Cl}_{2}\text{N}_{3}\text{O}_{3}\cdot \text{C}_{4}\text{H}_{4}\text{O}_{4} \)

**Batch Molecular Weight:** 530.4

**Physical Appearance:** White solid

**Solubility:**
- Water to 25 mM with gentle warming
- DMSO to 100 mM

**Storage:** Store at +4°C

**2. ANALYTICAL DATA**

**HPLC:** Shows 98.5% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

<table>
<thead>
<tr>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
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<tr>
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<tr>
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</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: GR 89696 fumarate  
Catalog No.: 1483  
Batch No.: 2

CAS Number: 126766-32-3  
IUPAC Name: 4-[(3,4-Dichlorophenyl)acetyl]-3-(1-pyrrolidinylmethyl)-1-piperazinecarboxylic acid methyl ester fumarate

Description:
Highly potent and selective κ-opioid agonist (IC₅₀ = 0.04 nM) that may be selective for the putative κ₂ receptor. Anti-nociceptive and neuroprotective in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C₁₉H₂₆Cl₂N₅O₃.C₂H₄O₄
Batch Molecular Weight: 530.4
Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:
- water to 25 mM with gentle warming
- 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: