

Product Name: GR 89696 fumarate

Catalog No.: 1483

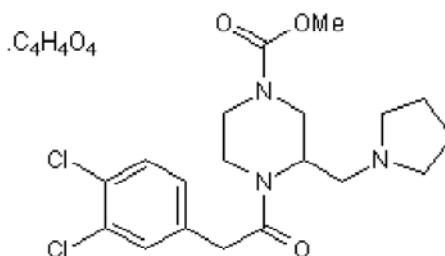
Batch No.: 2

CAS Number: 126766-32-3

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₂₅Cl₂N₃O₃·C₄H₄O₄
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
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.08	5.51	7.92
Found	52.18	5.51	7.89

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

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Description:

Highly potent and selective κ -opioid agonist ($IC_{50} = 0.04$ nM) that may be selective for the putative κ_2 receptor. Anti-nociceptive and neuroprotective in vivo.

Physical and Chemical Properties:

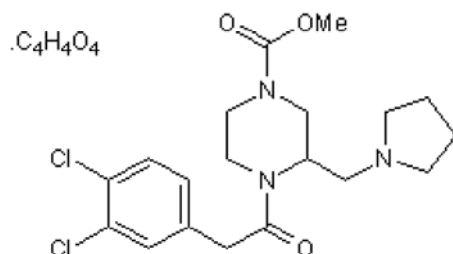
Batch Molecular Formula: $C_{19}H_{25}Cl_2N_3O_3 \cdot C_4H_4O_4$

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:

Butelman et al (2001) GR89,696: a potent κ -opioid agonist with subtype selectivity in rhesus monkeys. *J.Pharmacol.Exp.Ther.* **298** 1049. PMID: 11504802.

Naylor et al (1993) A potent new class of κ -receptor agonist: 4-substituted 1-(arylacetyl)-2-[(dialkylamino)methyl]piperazines. *J.Med.Chem.* **36** 2075. PMID: 8393489.

Birch et al (1991) Neuroprotective actions of GR89696, a highly potent and selective κ -opioid receptor agonist. *Br.J.Pharmacol.* **103** 1819. PMID: 1657267.

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