

Product Name: GR 159897

Catalog No.: 1274

Batch No.: 3

CAS Number: 158848-32-9

IUPAC Name: 5-Fluoro-3-[2-[4-methoxy-4-[(*R*)-phenylsulphonyl]methyl]-1-piperidinyl]ethyl]-1*H*-indole

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₇FN₂O₂S·½H₂O

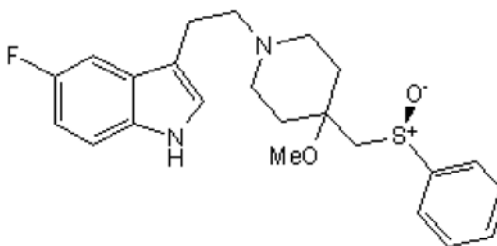
Batch Molecular Weight: 423.55

Physical Appearance: Light buff solid

Solubility: DMSO to 50 mM
ethanol to 10 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.25 (Chloroform:Methanol [9:1])

HPLC: Shows 98.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +91.6 (Concentration = 1.22, Solvent = Chloroform)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.22	6.66	6.61
Found	65.24	6.59	6.46

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Description:

A potent, selective, non-peptide, orally active neurokinin NK₂ receptor antagonist. Competes for binding of [³H]GR100679 to hNK₂-transfected CHO cells with a pK_i of 9.5. Inhibits NK₂ receptor-mediated contraction of guinea pig trachea with a pA₂ of 8.7. Anxiolytic in vivo.

Physical and Chemical Properties:

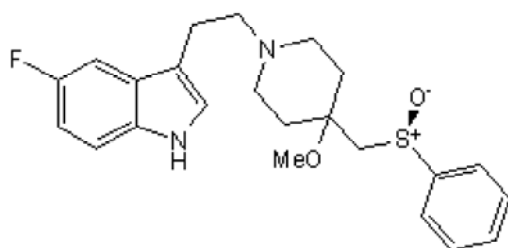
Batch Molecular Formula: C₂₃H₂₇FN₂O₂S.½H₂O

Batch Molecular Weight: 423.55

Physical Appearance: Light buff solid

Minimum Purity: ≥97%

Batch Molecular Structure:



Storage: Desiccate at -20°C

Solubility & Usage Info:

DMSO to 50 mM

ethanol 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.

Other Information:

INFORMATION FOR CUSTOMERS IN THE UK ONLY

This product is a Schedule 1 Home Office controlled substance and customers in the UK are required to hold the relevant licence or be exempt from restrictions in order to purchase and possess this material.

Licensing Information:

Sold with the permission of GlaxoSmithKline

References:

Beresford et al (1995) GR 159897, a potent non-peptide antagonist at tachykinin NK₂ receptors. *Eur.J.Pharmacol.* **272** 241. PMID: 7713168.

Walsh et al (1995) The anxiolytic-like activity of GR 159897, a non-peptide NK₂ receptor antagonist, in rodent and primate models of anxiety. *Psychopharmacology* **121** 186. PMID: 8545524.

Cooper et al (1994) GR 159897 and related analogues as highly potent, orally active non-peptide neurokinin NK₂ receptor antagonists. *Bioorg.Med.Chem.Lett.* **4** 1951.

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