

Product Name: GR 127935 hydrochloride

Catalog No.: 1477

Batch No.: 5

CAS Number: 148642-42-6

IUPAC Name: *N*-[4-Methoxy-3-(4-methyl-1-piperazinyl)phenyl]-2'-methyl-4'-(5-methyl-1,2,4-oxadiazol-3-yl)-1,1'-biphenyl-4-carboxamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₉H₃₁N₅O₃·HCl·H₂O

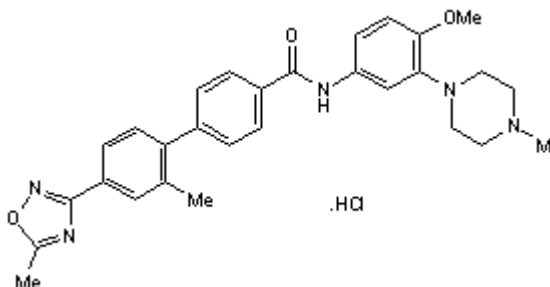
Batch Molecular Weight: 552.08

Physical Appearance: Off-white solid

Solubility: water to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.59 (Dichloromethane:Methanol:Ammonia soln. [9:1:2])

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.09	6.21	12.69
Found	63.09	6.07	12.51

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

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Description:

Potent and selective 5-HT_{1B/1D} receptor antagonist (pK_i values are 8.5 for both guinea pig 5-HT_{1D} and rat 5-HT_{1B} receptors). Displays > 100-fold selectivity over 5HT_{1A}, 5-HT_{2A}, 5-HT_{2C} receptors and other receptor types. Centrally active following oral administration.

Physical and Chemical Properties:

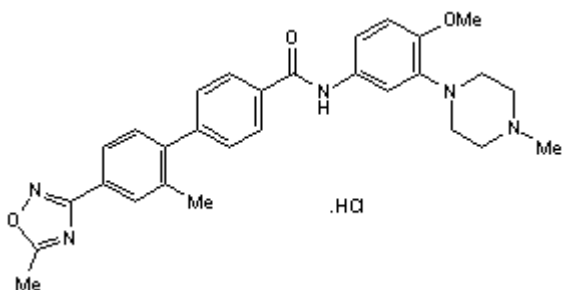
Batch Molecular Formula: C₂₉H₃₁N₅O₃.HCl.H₂O

Batch Molecular Weight: 552.08

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water 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:

Clitherow et al (1994) Evolution of a novel series of [(*N,N*-dimethylamino)propyl]- and piperazinylbenzalides as the first selective 5-HT_{1D} antagonists. *J.Med.Chem.* **37** 2253. PMID: 8057272.

De Vries et al (1996) Blockade of porcine carotid vascular response to sumatriptan by GR 127935, a selective 5-HT_{1D} receptor antagonist. *Br.J.Pharmacol.* **118** 85. PMID: 8733580.

Knobelman et al (2001) Genetic regulation of extracellular serotonin by 5-hydroxytryptamine_{1A} and 5-hydroxytryptamine_{1B} autoreceptors in different brain regions of the mouse. *J.Pharmacol.Exp.Ther.* **298** 1083. PMID: 11504805.

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