

**Product Name:** GR 203040

**Catalog No.:** 4647

**Batch No.:** 1

CAS Number: 168398-02-5

IUPAC Name: (2S,3S)-N-[[2-Methoxy-5-(1H-tetrazol-1-yl)phenyl]methyl]-2-phenyl-3-piperidinamine dihydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>20</sub>H<sub>24</sub>N<sub>6</sub>O.2HCl.½H<sub>2</sub>O

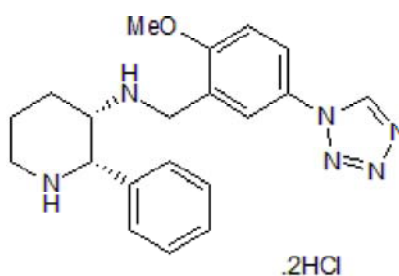
**Batch Molecular Weight:** 446.38

**Physical Appearance:** White solid

**Solubility:** water to 20 mM  
DMSO to 20 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.32 (DCM / MeOH / NH<sub>4</sub>OH (90:9:1))

**HPLC:** Shows 99.2% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	53.82	6.1	18.83
Found	53.79	5.94	18.72

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**Description:**

Potent and selective NK<sub>1</sub> receptor antagonist. Potently inhibits substance P binding to NK<sub>1</sub> receptors (pK<sub>i</sub> = 10.1 to 10.5). Displays antiemetic activity in vivo.

**Physical and Chemical Properties:**

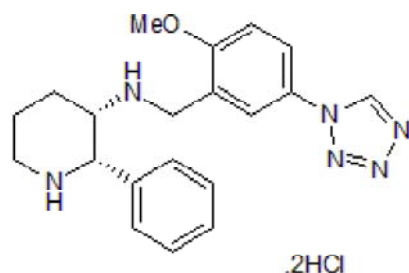
Batch Molecular Formula: C<sub>20</sub>H<sub>24</sub>N<sub>6</sub>O.2HCl.½H<sub>2</sub>O

Batch Molecular Weight: 446.38

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

water to 20 mM

DMSO to 20 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.

**Licensing Information:**

Sold for research purposes under agreement from GlaxoSmithKline

**References:**

**Beattie et al** (1995) The pharmacology of GR203040, a novel, potent and selective non-peptide tachykinin NK<sub>1</sub> receptor antagonist. Br.J.Pharmacol. **116** 3149. PMID: 8719789.

**Gardner et al** (1995) The broad-spectrum anti-emetic activity of the novel non-peptide tachykinin NK<sub>1</sub> receptor antagonist GR203040. Br.J.Pharmacol. **116** 3158. PMID: 8719790.

**Ward et al** (1995) Discovery of an orally bioavailable NK<sub>1</sub> receptor antagonist, (2S,3S)-(2-methoxy-5-tetrazol-1-ylbenzyl) (2-phenylpiperidin-3-yl)amine (GR203040), with potent antiemetic activity. J.Med.Chem. **38** 4985. PMID: 8544174.

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