

Certificate of Analysis

Product Name: GR 55562 dihydrochloride

Catalog No.: 1054

Batch No.: 7

CAS Number: 159533-25-2

IUPAC Name: 3-[3-(Dimethylamino)propyl]-4-hydroxy-*N*-[4-(4-pyridinyl)phenyl]benzamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{25}N_3O_2 \cdot 2HCl \cdot \frac{1}{2}H_2O$

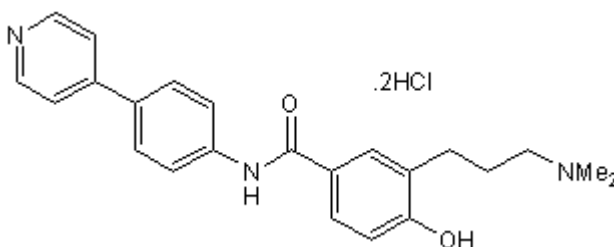
Batch Molecular Weight: 457.4

Physical Appearance: Pale yellow solid

Solubility: water to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.42$ (Chloroform:Methanol:Ammonia soln. [85:13.5:1.5])

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.4	6.17	9.19
Found	60.25	6.29	9.14

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

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IUPAC Name: 3-[3-(Dimethylamino)propyl]-4-hydroxy-N-[4-(4-pyridinyl)phenyl]benzamide dihydrochloride

Description:

A selective competitive 5-HT_{1B} (5-HT_{1Dβ}) silent antagonist with pK_B values of 7.3 and 6.3 for human cloned 5-HT_{1B} and 5-HT_{1D} receptors respectively and only weak binding at a number of other 5-HT subtypes.

Physical and Chemical Properties:

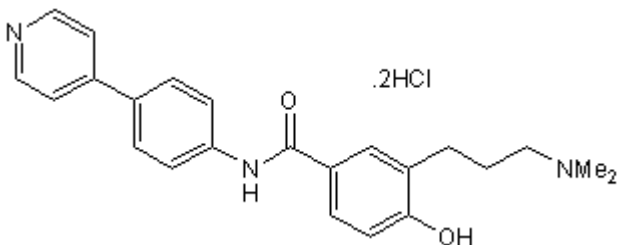
Batch Molecular Formula: C₂₃H₂₅N₃O₂.2HCl.½H₂O

Batch Molecular Weight: 457.4

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Walsh et al (1995) The activity of 5-HT_{1D} receptor ligands at cloned human 5-HT_{1Dα} and 5-HT_{1Dβ} receptors. *Eur.J.Pharmacol.* **287** 79. PMID: 8666030.

Connor et al (1995) Use of GR55562, a selective 5-HT_{1D} antagonist, to investigate 5-HT_{1D} receptor subtypes mediating cerebral vasoconstriction. *Cephalalgia* **15** (suppl. 14) 99.

MacLean et al (1996) Evidence for 5-HT₁-like receptor-mediated vasoconstriction in human pulmonary artery. *Br.J.Pharmacol.* **119** 277. PMID: 8886409.

Storage: Desiccate at +4°C

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.

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