

Product Name: CGP 20712 dihydrochloride

Catalog No.: 1024

Batch No.: 2

CAS Number: 1216905-73-5

IUPAC Name: 1-[2-((3-Carbamoyl-4-hydroxy)phenoxy)ethylamino]-3-[4-(1-methyl-4-trifluoromethyl-2-imidazolyl)phenoxy]-2-propanol dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{25}F_3N_4O_5 \cdot 2HCl \cdot 1\frac{1}{2}H_2O$

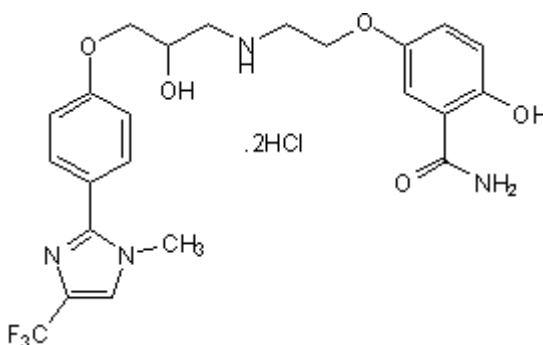
Batch Molecular Weight: 594.41

Physical Appearance: Off-white solid

Solubility: water to 50 mM
ethanol to 100 mM
DMSO to 50 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.64$ (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	46.47	5.09	9.43
Found	46.39	4.94	9.52

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Description:

Highly selective and potent β_1 -adrenoceptor antagonist (IC_{50} = 0.7 nM). Displays 10,000-fold selectivity over β_2 -adrenoceptors. Also available as part of the β -Adrenoceptor Antagonist Tocriset™.

Physical and Chemical Properties:

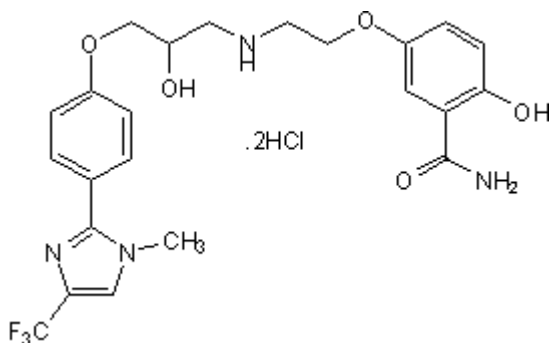
Batch Molecular Formula: $C_{23}H_{25}F_3N_4O_5 \cdot 2HCl \cdot 1 \frac{1}{2}H_2O$

Batch Molecular Weight: 594.41

Physical Appearance: Off-white solid

Minimum Purity: >96%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 50 mM
ethanol to 100 mM
DMSO to 50 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:

Dooley et al (1986) CGP 20712A: a useful tool for quantitating β_1 - and β_2 -adrenoceptors. *Eur.J.Pharmacol.* **130** 137. PMID: 2877892.

Hieble et al (1995) α - and β -adrenoceptors. From the gene to the clinic. 1. Molecular biology and adrenoceptor subclassification. *J.Med.Chem.* **38** 3415. PMID: 7658428.

Kitagawa et al (1995) Determination of β -adrenoceptor subtype on rat isolated ventricular myocytes by use of highly selective β -antagonists. *Br.J.Pharmacol.* **116** 1635. PMID: 8564230.

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