

**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<sub>23</sub>H<sub>25</sub>F<sub>3</sub>N<sub>4</sub>O<sub>5</sub>·2HCl·1½H<sub>2</sub>O

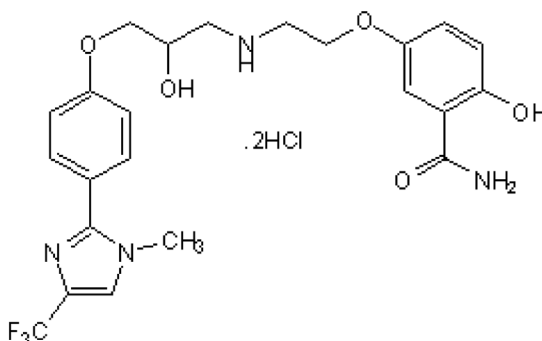
**Batch Molecular Weight:** 594.41

**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<sub>f</sub> = 0.64 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

**HPLC:** Shows 98.3% purity

**<sup>1</sup>H 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:**

CGP 20712 dihydrochloride is a highly selective and potent  $\beta_1$ -adrenoceptor antagonist ( $IC_{50}$  = 0.7 nM). Displays 10,000-fold selectivity over  $\beta_2$ -adrenoceptors.

**Physical and Chemical Properties:**

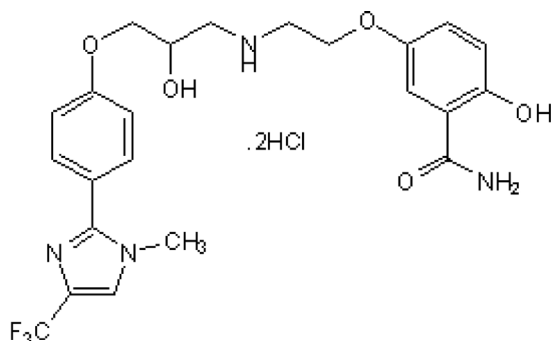
Batch Molecular Formula:  $C_{23}H_{25}F_3N_4O_5 \cdot 2HCl \cdot 1\frac{1}{2}H_2O$

Batch Molecular Weight: 594.41

Physical Appearance: Off-white solid

**Minimum Purity:**  $\geq 96\%$

**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. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

**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:**

**Hieble et al** (1995)  $\alpha$ - and  $\beta$ -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  $\beta$ -adrenoceptor subtype on rat isolated ventricular myocytes by use of highly selective  $\beta$ -antagonists. *Br.J.Pharmacol.* **116** 1635. PMID: 8564230.

**Dooley et al** (1986) CGP 20712A: a useful tool for quantitating  $\beta_1$ - and  $\beta_2$ -adrenoceptors. *Eur.J.Pharmacol.* **130** 137. PMID: 2877892.

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**bio-techne.com**

info@bio-techne.com  
techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com  
Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors  
Tel: +1 612 379 2956