

Product Name: RS 100329 hydrochloride

Catalog No.: 1325

Batch No.: 3

CAS Number: 1215654-26-4

IUPAC Name: 5-Methyl-3-[3-[3-[4-[2-(2,2,2-trifluoroethoxy)phenyl]-1-piperazinyl]propyl]-2,4-(1*H*,3*H*)-pyrimidinedione hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₅F₃N₄O₃.HCl.1¼H₂O

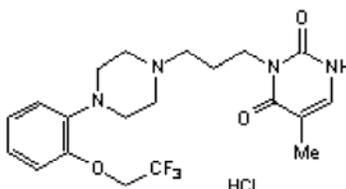
Batch Molecular Weight: 485.41

Physical Appearance: White solid

Solubility: ethanol to 100 mM
water to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.72 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

Melting Point: Between 145 - 147°C

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	
Theoretical	49.45	5.92	11.54	0.00
Found	49.48	5.82	11.42	0.00

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Description:

Subtype-selective α_{1A} -adrenoceptor antagonist ($pK_i = 9.6$ for human cloned α_{1A} receptors). Displays 126- and 50-fold selectivity over human α_{1B} and α_{1D} receptors respectively. Active in vivo.

Physical and Chemical Properties:

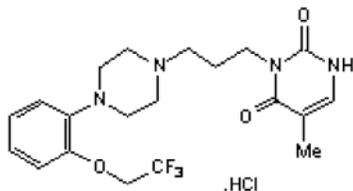
Batch Molecular Formula: $C_{20}H_{25}F_3N_4O_3 \cdot HCl \cdot 1\frac{1}{4}H_2O$

Batch Molecular Weight: 485.41

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

ethanol to 100 mM

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.

Licensing Information:

Sold with the permission of Roche Bioscience

References:

Conley *et al* (2001) The role of α_1 -adrenoceptors and 5-HT_{1A} receptors in the control of the micturition reflex in male anaesthetized rats. *Br.J.Pharmacol.* **133** 61. PMID: 11325795.

Williams *et al* (1999) In vitro α_1 -adrenoceptor pharmacology of Ro 70-0004 and RS-100329, novel α_{1A} -adrenoceptor selective antagonists. *Br.J.Pharmacol.* **127** 252. PMID: 10369480.

Shannon Kava *et al* (1998) α_{1L} -Adrenoceptor mediation of smooth muscle contraction in rabbit bladder neck: a model for lower urinary tract tissues of man. *Br.J.Pharmacol.* **123** 1359. PMID: 9579731.

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