Product Name: RS 100329 hydrochloride
Catalog No.: 1325
Batch No.: 3

CAS Number: 121565-26-4
IUPAC Name: 5-Methyl-3-[3-[4-[2-(2,2,2-trifluoroethoxy)phenyl]-1-piperazinyl]propyl]-2,4-(1H,3H)-pyrimidinedione hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \(\text{C}_{20}\text{H}_{25}\text{F}_3\text{N}_4\text{O}_3\cdot\text{HCl} \cdot 1\frac{1}{4}\text{H}_2\text{O}\)

Batch Molecular Weight: 485.41

Physical Appearance: White solid

Solubility:
- ethanol to 100 mM
- water to 100 mM

Storage: Store at RT

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

\(^1\text{H NMR:}\) Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
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<td>Theoretical</td>
<td>49.45</td>
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<td>Found</td>
<td>49.48</td>
<td>5.82</td>
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</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: RS 100329 hydrochloride  
Catalog No.: 1325  
Batch No.: 3

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

**Physical and Chemical Properties:**
Batch Molecular Formula: $C_{20}H_{25}F_2N_4O_3\cdot HCl\cdot 1\frac{1}{4}H_2O$
Batch Molecular Weight: 485.41
Physical Appearance: White solid

Minimum Purity: >99%

**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.

**References:**
