

Certificate of Analysis

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Product Name: RS 102895 hydrochloride

Catalog No.: 2089

Batch No.: 3

CAS Number: 1173022-16-6

IUPAC Name: 1'-[2-[4-(Trifluoromethyl)phenyl]ethyl]-spiro[4H-3,1-benzoxazine-4,4'-piperidin]-2(1H)-one hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₁F₃N₂O₂.HCl

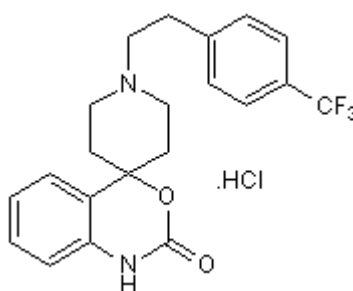
Batch Molecular Weight: 426.86

Physical Appearance: Off White solid

Solubility: DMSO to 75 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.9 (Chloroform:Methanol:Et3N [90:10:1])

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.09	5.19	6.56
Found	59.05	5.17	6.37

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

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Description:

CCR2-selective chemokine receptor antagonist (IC₅₀ values are 0.36 and 17.8 μM for inhibition of human recombinant CCR2b and CCR1 receptors respectively). Blocks MCP-1-stimulated calcium influx and chemotaxis with IC₅₀ values of 32 nM and 1.7 μM respectively. Also inhibits α_{1A}, α_{1D} and 5-HT_{1A} receptors.

Physical and Chemical Properties:

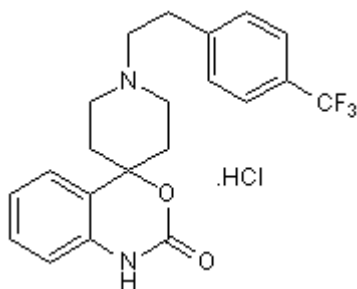
Batch Molecular Formula: C₂₁H₂₁F₃N₂O₂.HCl

Batch Molecular Weight: 426.86

Physical Appearance: Off White solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Clark et al (1983) Synthesis and antihypertensive activity of 4'-substituted spiro[4*H*-3,1-benzoxazine-4,4'-piperidin]-2(1*H*)-ones. *J.Med.Chem.* **26** 657. PMID: 6842505.

Mirzadegan et al (2000) Identification of the binding site for a novel class of CCR2b chemokine receptor antagonists. *J.Biol.Chem.* **275** 25562. PMID: 10770925.

Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 75 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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