

Product Name: RN 9893 hydrochloride

Catalog No.: 5678

Batch No.: 1

CAS Number: 2109450-40-8

IUPAC Name: *N*-[4-[[4-(1-Methylethyl)-1-piperazinyl]sulfonyl]phenyl]-2-nitro-4-(trifluoromethyl)benzamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₃F₃N₄O₅S.HCl

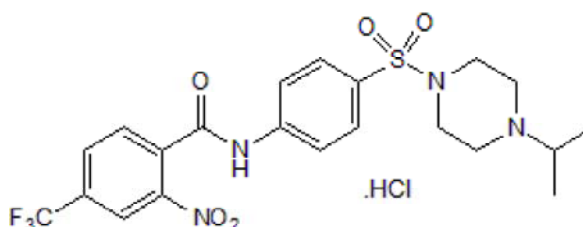
Batch Molecular Weight: 536.95

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.36 (Chloroform:Methanol [9:1])

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	46.97	4.51	10.43	6.6
Found	46.85	4.17	10.29	6.33

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

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IUPAC Name: N-[4-[[4-(1-Methylethyl)-1-piperazinyl]sulfonyl]phenyl]-2-nitro-4-(trifluoromethyl)benzamide hydrochloride

Description:

Potent and selective TRPV4 antagonist (IC₅₀ values are 320, 420 and 660 nM for mouse, human and rat channels, respectively). Exhibits >15-fold selectivity for TRPV4 over TRPV1, TRPV3 and TRPM8, and a panel of 54 other common biological targets. Orally bioavailable.

Physical and Chemical Properties:

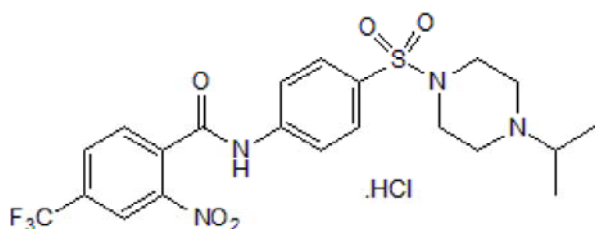
Batch Molecular Formula: C₂₁H₂₃F₃N₄O₅S.HCl

Batch Molecular Weight: 536.95

Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:



References:

Wei *et al* (2015) Identification of orally-bioavailable antagonists of the TRPV4 ion-channel. *Bioorg.Med.Chem.Lett.* **25** 4011. PMID: 26235950.

Storage: Desiccate at RT

Solubility & Usage Info:

DMSO 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.

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