

Product Name: RQ 00203078

Catalog No.: 5388

Batch No.: 1

CAS Number: 1254205-52-1

IUPAC Name: 4-[[[3-Chloro-5-(trifluoromethyl)-2-pyridinyl]][4-(trifluoromethoxy)phenyl]methyl]amino]sulfonyl]benzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₁₃ClF₆N₂O₅S

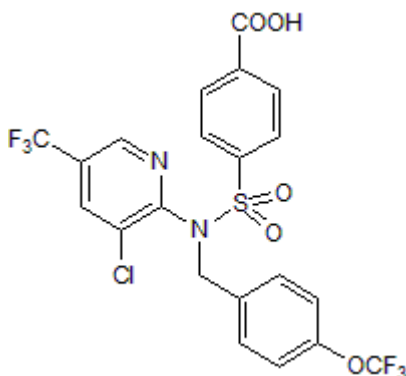
Batch Molecular Weight: 554.85

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.1 (Ethyl acetate:Petroleum ether [1:3])

HPLC: Shows 98% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	45.46	2.36	5.05
Found	45.84	2.32	5.06

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

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Description:

Potent TRPM8 antagonist (IC₅₀ values are 5.3 and 8.3 nM for rat and human channels respectively). Exhibits >350-fold selectivity for TRPM8 over TRPV4, TRPV1 and TRPA1. Reduces HSC3 and HSC4 oral squamous carcinoma cell migration and invasion in vitro. Also attenuates icilin-induced wet dog shakes in rats. Orally active.

Physical and Chemical Properties:

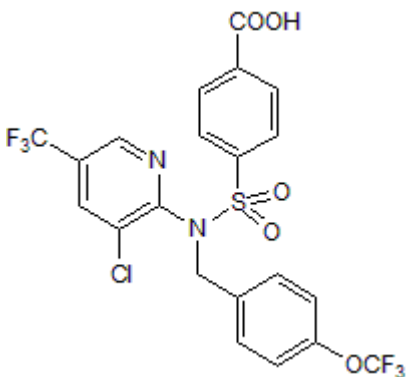
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Batch Molecular Weight: 554.85

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Okamoto et al (2012) Blockade of TRPM8 activity reduces the invasion potential of oral squamous carcinoma cell lines. *Int.J.Oncol.* **40** 1431. PMID: 22267123.

Ohmi et al (2014) Identification of a novel 2-pyridyl-benzensulfonamide derivative, RQ-00203078, as a selective and orally active TRPM8 antagonist. *Bioorg.Med.Chem.Lett.* **24** 5364. PMID: 25455182.

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