

Certificate of Analysis

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Product Name: SR 1001

Catalog No.: 4868

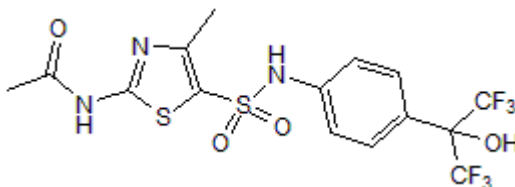
Batch No.: 1

CAS Number: 1335106-03-0

IUPAC Name: *N*-[4-Methyl-5-[[[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]amino]sulfonyl]-2-thiazolyl]acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₃F₆N₃O₄S₂
Batch Molecular Weight: 477.4
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 = 0.7 (Ethyl acetate:Petroleum ether [1:1])
HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	37.74	2.74	8.8
Found	37.92	2.81	8.83

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

Product Information

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Description:

Retinoic acid receptor-related orphan receptor (ROR) α and γ inverse agonist (K_i values are 172 and 111 nM for ROR α and ROR γ respectively). Demonstrates no activity at ROR β or LXR. Suppresses T_H17 cell differentiation and cytokine expression and reduces the severity of disease in an animal model of multiple sclerosis.

Physical and Chemical Properties:

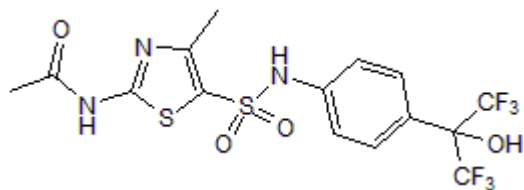
Batch Molecular Formula: C₁₅H₁₃F₆N₃O₄S₂

Batch Molecular Weight: 477.4

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:

Solt et al (2011) Suppression of T_H17 differentiation and autoimmunity by a synthetic ROR ligand. *Nature* **472** 491. PMID: 21499262.

Crumbley et al (2012) Regulation of expression of citrate synthase by the retinoic acid receptor-related orphan receptor α (ROR α). *PLoS ONE* **7** 33804. PMID: 22485150.

Beurel et al (2013) Inflammatory T helper 17 cells promote depression-like behavior in mice. *Biol. Psychiatry* **73** 622. PMID: 23174342.

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