



Certificate of Analysis

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Product Name: T 3364366 Catalog No.: 6106 Batch No.: 1

CAS Number: 1356354-09-0

IUPAC Name: N-[2-[[3,4-Dihydro-4-oxo-3-[4-(2,2,2-trifluoroethoxy)phenyl]thieno[3,4-d]pyrimidin-2-yl]thio]ethyl]acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{16}F_3N_3O_3S_2$

Batch Molecular Weight: 443.46 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.35$ (Ethyl acetate:Petroleum ether [7:3])

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 48.75 3.64 9.48 Found 48.79 3.59 9.48

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



Product Information

Print Date: Nov 7th 2018

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Description:

Potent and reversible fatty acid desaturase 1 (FADS1; Δ^5 desaturase) inhibitor (IC₅₀ values are 1.9 nM and 2.1 nM in human and rat hepatocyte cell lines, respectively). Exhibits >300 fold selectivity for FADS1 over FADS2 (Δ^6 desaturase). Inhibits arachidonic acid production in rat and human hepatocyte cell lines. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₁₆F₃N₃O₃S₂

Batch Molecular Weight: 443.46 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

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.

References:

Miyahisa *et al* (2016) T-3364366 targets the desaturase domain of delta-5 desaturase with nanomolar potency and a multihour residence time. ACS Med.Chem.Lett. **7** 868. PMID: 27660693.