

Certificate of Analysis

Print Date: Dec 3rd 2020

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Product Name: SET 2 Catalog No.: 6990 Batch No.: 1

CAS Number: 2313525-20-9

IUPAC Name: N-(2-Furanylmethyl)-3-[[4-(methylpropylamino)-6-(trifluoromethyl)-2-pyrimidinyl]thio]propanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{21}F_3N_4O_2S$

Batch Molecular Weight: 402.44

Physical Appearance: White solid

Solubility: DMSO to 100 mM

ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 50.74 5.26 13.92 Found 50.71 5.28 13.89



Product Information

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IUPAC Name: N-(2-Furanylmethyl)-3-[[4-(methylpropylamino)-6-(trifluoromethyl)-2-pyrimidinyl]thio]propanamide

Description:

TRPV2 (transient receptor potential vanilloid type 2) antagonist (IC $_{50}$ = 0.46 μ M). Selective for TRPV2 over TRPV1, TRPV3 and TRPV4 expressed in HEK293 cells. Inhibits lyosphosphatidic acid (LPA)-induced prostate cancer cell migration in vitro.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₂₁F₃N₄O₂S

Batch Molecular Weight: 402.44 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM ethanol to 50 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:

Chai et al (2019) Structure-based discovery of a subtype-selective inhibitor targeting a transient receptor potential vanilloid channel. J.Med.Chem. 62 1373. PMID: 30620187.

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