

Product Name:

Certificate of Analysis

Print Date: Oct 23rd 2019

Batch No.: 2

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Catalog No.: 6482

CAS Number: 2061980-01-4

IUPAC Name: 4-[(6,10-Dihydro-5,10-dimethyl-6-oxo-5*H*-pyrimido[5,4-*b*]thieno[3,2-*e*][1,4]diazepin-2-yl)amino]benzenesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

XMU MP 1

Batch Molecular Formula: $C_{17}H_{16}N_6O_3S_2.^3/4H_2O$

Batch Molecular Weight: 429.99
Physical Appearance: Brown solid

Solubility: DMSO to 100 mM Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 47.49 4.1 19.54 Found 47.52 3.95 19.57

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Product Information

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Description:

Potent and selective ATP-competitive mammalian sterile 20-like kinase (MST) 1/2 inhibitor (IC $_{50}$ values are 38.1 and 71.1 nM for MST2 and MST1, respectively). Enhances activity of downstream YAP in vitro. Augments mouse intestinal repair and promotes liver repair and regeneration in a mouse model of acute and chronic liver injury. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₁₆N₆O₃S₂.³/₄H₂O

Batch Molecular Weight: 429.99 Physical Appearance: Brown solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°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.

Licensing Information:

Sold under license from Dana-Farber Cancer Institute.

References:

Crunkhorn et al (2016) Regenerative medicine: Inhibiting Hippo repairs tissue. Nat.Rev.Drug Discov. 15 678. PMID: 27681796.

Fan et al (2016) Pharmacological targeting of kinases MST1 and MST2 augments tissue repair and regeneration. Sci.Transl.Med. 8 352. PMID: 27535619.

Ray et al (2016) Therapy: Targeting liver tissue repair and regeneration. Nat.Rev.Gastroenterol.Hepatol. 13 559. PMID: 27605063.

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