

Product Name: XMD 8-87

Catalog No.: 6061

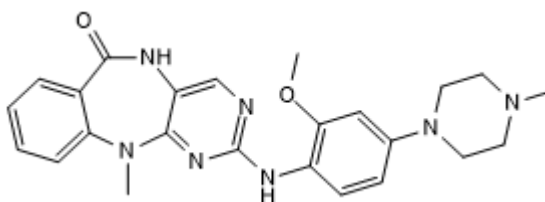
Batch No.: 1

CAS Number: 1234480-46-6

IUPAC Name: 5,11-Dihydro-2-[[2-methoxy-4-(4-methyl-1-piperazinyl)phenyl]amino]-11-methyl-6*H*-pyrimido[4,5-*b*][1,4]benzodiazepin-6-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₇N₇O₂
Batch Molecular Weight: 445.52
Physical Appearance: Off White solid
Solubility: 1eq. HCl to 100 mM
 DMSO to 50 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.23 (Dichloromethane:Methanol [7:3])
HPLC: Shows >98.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	64.7	6.11	22.01
Found	64.47	6.18	22.3

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

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Description:

Potent Ack1/TNK2 inhibitor (IC₅₀ = 38 and 113 nM in Ba/F3 cell lines containing leukemia-associated D163E and R806Q mutations respectively). Blocks phosphorylation of TNK2 receptors containing solid-tumor type truncation mutations.

Physical and Chemical Properties:

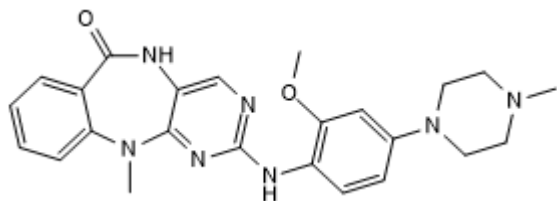
Batch Molecular Formula: C₂₄H₂₇N₇O₂

Batch Molecular Weight: 445.52

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

1eq. HCl to 100 mM
DMSO 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.

Licensing Information:

Sold under license from Dana-Farber Cancer Institute.

References:

Maxson et al (2015) Identification and characterization of tyrosine kinase nonreceptor 2 mutations in leukemia through integration of kinase inhibitor screening and genomic analysis. *Cancer.Res.* **76** 127. PMID: 26677978.

Maxson et al (2014) Development and repurposing of small-molecule kinase inhibitors to target novel leukemogenic TNK2 mutations *Blood* **124** 435.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956