

Product Name: XMD 8-92

Catalog No.: 4132

Batch No.: 2

CAS Number: 1234480-50-2

IUPAC Name: 2-[[2-Ethoxy-4-(4-hydroxy-1-piperidyl)phenyl]amino]-5,11-dihydro-5,11-dimethyl-6H-pyrimido[4,5-b][1,4]benzodiazepin-6-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₃₀N₆O₃·¼H₂O

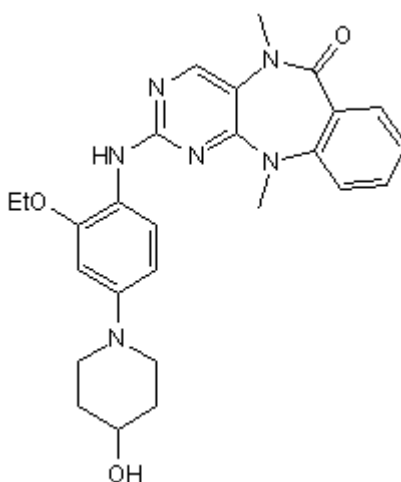
Batch Molecular Weight: 479.05

Physical Appearance: Light beige solid

Solubility: DMSO to 40 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.22 (Chloroform:Methanol [95:5])

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 65.19 | 6.42 | 17.54 |
| Found | 65.19 | 6.45 | 17.23 |

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Description:

Highly selective ERK5/BMK1 inhibitor (K_D values are 80, 190, 600 and 890 nM for BMK1, DCAMKL2, PLK4 and TNK1 respectively). Displays selectivity over 402 diverse kinases. Blocks growth factor-induced activation of cellular BMK1 and reduces BMK1 activity in in vitro kinase assays. Also reduces BMK1-dependent transactivating activity of MEF2C. Inhibits proliferation in a variety of cancer cell lines; blocks tumor cell proliferation and tumor-associated angiogenesis.

Physical and Chemical Properties:

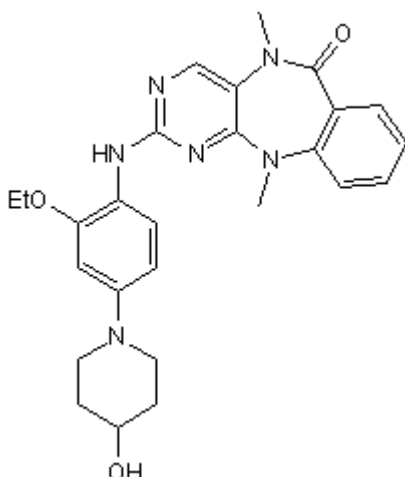
Batch Molecular Formula: $C_{26}H_{30}N_6O_3 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 479.05

Physical Appearance: Light beige solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 40 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:

Yang et al (2010) Pharmacological inhibition of BMK1 suppresses tumor growth through promyelocytic leukemia protein. *Cancer Cell* **18** 258. PMID: 20832753.

Yang and Lee (2011) Targeting the BMK1 MAP kinase pathway in cancer therapy. *Clin.Cancer Res.* **17** 3527. PMID: 21385929.

Deng et al (2011) Discovery of a benzo[e]pyrimido-[5,4-b][1,4]diazepin-6(11H)-one as a potent and selective inhibitor of big MAP kinase 1. *ACS Med.Chem.Lett.* **2** 195. PMID: 21412406.

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