

**Product Name:** XMD 8-92

**Catalog No.:** 4132

**Batch No.:** 3

CAS Number: 1234480-50-2

IUPAC Name: 2-[[2-Ethoxy-4-(4-hydroxy-1-piperidinyl)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:** C<sub>26</sub>H<sub>30</sub>N<sub>6</sub>O<sub>3</sub>·1/4H<sub>2</sub>O

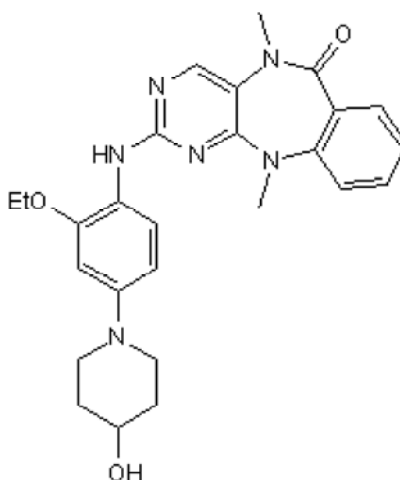
**Batch Molecular Weight:** 479.05

**Physical Appearance:** Yellow solid

**Solubility:** DMSO to 40 mM

**Storage:** Store at RT

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.0% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	65.19	6.42	17.54
Found	65	6.21	17.55

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**Description:**

XMD 8-92 is an ERK5 (BMK1) and BRD4 inhibitor ( $K_d$  values are 80 and 190 nM, respectively). Also inhibits DCAMKL2, PLK4 and TNK1 ( $K_d$  values are 190, 600 and 890 nM). 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:**

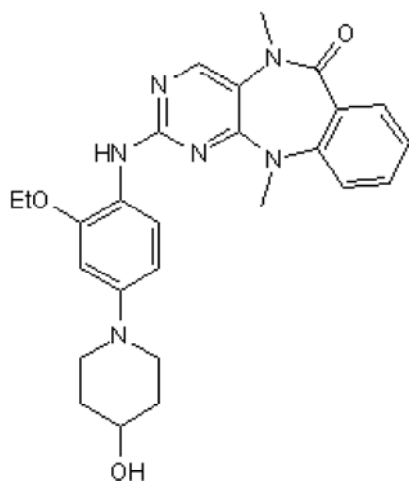
Batch Molecular Formula:  $C_{26}H_{30}N_6O_3 \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 479.05

Physical Appearance: Yellow solid

**Minimum Purity:**  $\geq 98\%$

**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.

**Licensing Information:**

Sold under license from the Dana-Farber Cancer Institute.

**References:**

Lin *et al* (2016) ERK5 kinase activity is dispensable for cellular immune response and proliferation. *Proc.Natl.Acad.Sci.U.S.A.* **113** 11865. PMID: 27679845.

Erazo *et al* (2013) Canonical and kinase activity-independent mechanisms for extracellular signal-regulated kinase 5 (ERK5) nuclear translocation require dissociation of Hsp90 from the ERK5-Cdc37 complex. *Mol.Cell Biol.* **33** 1671. PMID: 23428871.

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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