

Product Name: ERK5-IN-1

Catalog No.: 5393

Batch No.: 1

CAS Number: 1435488-37-1

IUPAC Name: 11-Cyclopentyl-2-[[2-ethoxy-4-[[4-(4-methyl-1-piperazinyl)-1-piperidinyl]carbonyl]phenyl]amino]-5,11-dihydro-5-methyl-6H-pyrimido[4,5-b][1,4]benzodiazepin-6-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₆H₄₆N₈O₃.H₂O

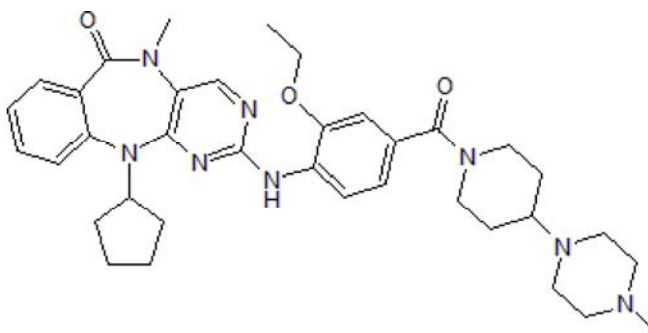
Batch Molecular Weight: 656.82

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.83	7.37	17.06
Found	65.86	7.34	17.05

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

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Description:

ERK5-IN-1 is a potent and selective ERK5 inhibitor; inhibits EGFR-induced ERK5 autophosphorylation (EC₅₀ = 90 nM) and ERK5 enzymatic activity (IC₅₀ = 162 nM). Exhibits at least 30-fold selectivity for ERK5 over LRRK2 in a cell based assay. Also selective for ERK5 over a panel of other kinases. Orally bioavailable.

Physical and Chemical Properties:

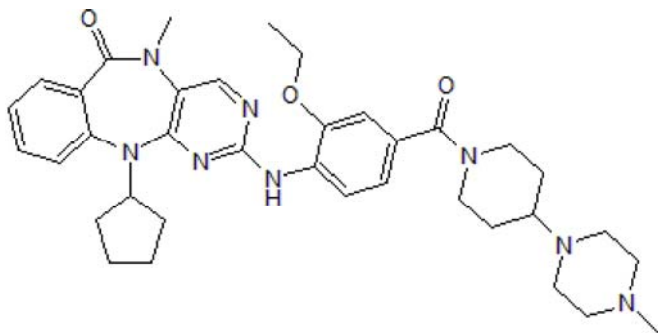
Batch Molecular Formula: C₃₆H₄₆N₈O₃.H₂O

Batch Molecular Weight: 656.82

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Deng et al (2013) Structural determinants for ERK5 (MAPK7) and leucine rich repeat kinase 2 activities of benzo[e]pyrimido-[5,4-b]diazepine-6(11H)-ones. *Eur.J.Med.Chem.* **70** 758. PMID: 24239623.

Elkins et al (2013) X-ray crystal structure of ERK5 (MAPK7) in complex with a specific inhibitor. *J.Med.Chem.* **56** 4413. PMID: 23656407.

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