

Product Name: AX 15836

Catalog No.: 5843

Batch No.: 1

CAS Number: 2035509-96-5

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₂H₄₀N₈O₅S.2H₂O

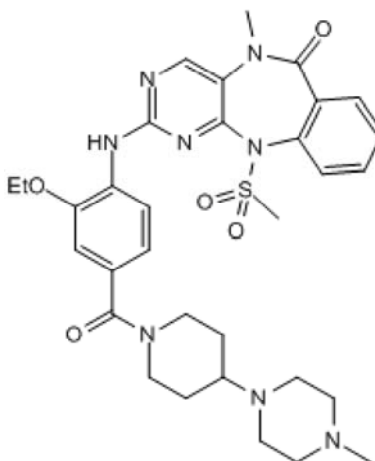
Batch Molecular Weight: 684.81

Physical Appearance: Off White solid

Solubility: 1eq. HCl to 100 mM
DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.11 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.12	6.48	16.36
Found	55.88	6.11	16.22

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Description:

Potent and selective ERK5 inhibitor ($IC_{50} = 8 \text{ nM}$). Exhibits >1,000-fold selectivity for ERK5 over a panel of over 200 kinases. Also exhibits selectivity over bromodomain BRD4 ($K_d = 3,600 \text{ nM}$). Increases vomocytosis in human macrophages in vitro, as well as in an in vivo zebrafish model of cryptococcal disease, reducing spread of infection.

Physical and Chemical Properties:

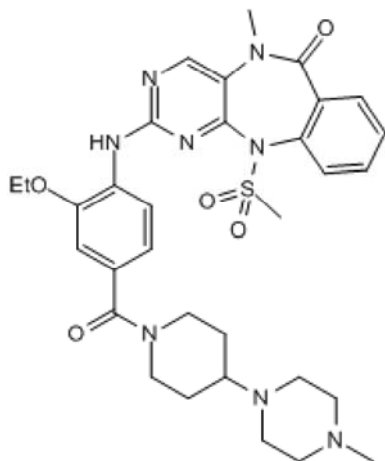
Batch Molecular Formula: $C_{32}H_{40}N_8O_5S \cdot 2H_2O$

Batch Molecular Weight: 684.81

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

1eq. HCl to 100 mM
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 $45\text{-}60^{\circ}\text{C}$ 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:

Gilbert *et al* (2017) Vomocytosis of live pathogens from macrophages is regulated by the atypical MAP kinase ERK5. *Science Advances* **3** e1700898.

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.

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