1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{36}H_{46}N_{8}O_{3}.H_{2}O

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:

![Molecular Structure Image]

2. ANALYTICAL DATA

- **HPLC:** Shows 98.2% purity

- **\textsuperscript{1}H NMR:** Consistent with structure

- **Mass Spectrum:** Consistent with structure

- **Microanalysis:**
  - Carbon: Theoretical 65.83, Found 65.86
  - Hydrogen: Theoretical 7.37, Found 7.34
  - Nitrogen: Theoretical 17.06, Found 17.05

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Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: ERK5-IN-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

Description:
Potent and selective ERK5 inhibitor; inhibits EGFR-induced ERK5 autophosphorylation (EC_{50} = 90 nM) and ERK5 enzymatic activity (IC_{50} = 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: C_{38}H_{46}N_{11}O_{10}.H_{2}O
Batch Molecular Weight: 656.82
Physical Appearance: White solid
Minimum Purity: >98%

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.

References: