

Product Name: DCLK1-IN-1

Catalog No.: 7285

Batch No.: 1

CAS Number: 2222635-15-4

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₂₈F₃N₇O₂ · ½H₂O

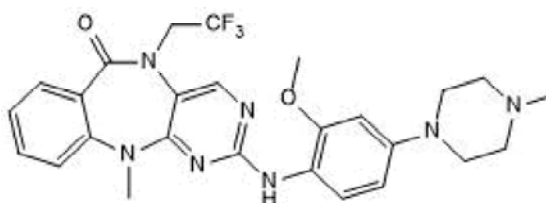
Batch Molecular Weight: 536.56

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.2	5.45	18.27
Found	58.21	5.32	18.14

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

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Description:

Potent and selective doublecortin like kinase 1/2 (DCLK1/2) inhibitor (IC₅₀ values are DCLK1 =9.5 and 57.2 nM and DCLK2 = 31 and 103 nM in binding and kinase assay, respectively). Exhibits no significant activity against ERK5, ACK, BRD4 and LRRK2. Exhibits DCLK inhibition in pancreatic ductal adenocarcinoma (PDAC) organoid models. Orally bioavailable.

Physical and Chemical Properties:

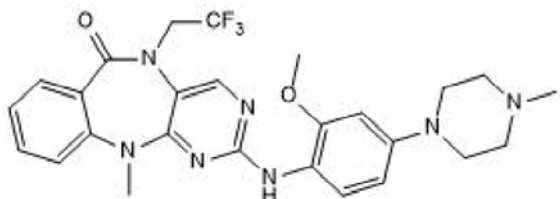
Batch Molecular Formula: C₂₆H₂₈F₃N₇O₂·½H₂O

Batch Molecular Weight: 536.56

Physical Appearance: Pale yellow 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:

Ferguson *et al* (2020) Discovery of a selective inhibitor of doublecortin like kinase 1. *Nat.Chem.Biol.* **16** 635. PMID: 32251410.

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