

Product Name: LDC 000067

Catalog No.: 6752

Batch No.: 1

CAS Number: 1073485-20-7

IUPAC Name: 3-[[6-(2-Methoxyphenyl)-4-pyrimidinyl]amino]benzenesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₈N₄O₃S·¼H₂O

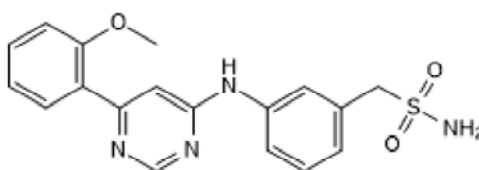
Batch Molecular Weight: 374.93

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.66	4.97	14.94
Found	57.95	4.84	14.51

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

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Description:

Potent and selective CDK9 inhibitor (IC₅₀ = 44 nM at CDK9-cyclin T1). Inhibits other CDKs in the micromolar range (IC₅₀ values are 2.4, 5.5, 9.2, >10 and >10 μM for CDK2-cyclin A, CDK1-cyclin B1, CDK4-cyclin D1, CDK6-cyclin D3 and CDK7-cyclin H-MAT1, respectively). Inhibits P-TEFb-dependent in vitro transcription. Induces apoptosis in vitro and in vivo in combination with BI 894999.

Physical and Chemical Properties:

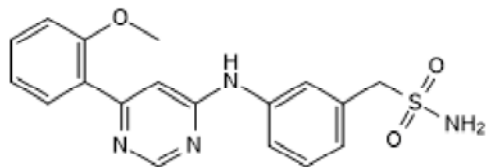
Batch Molecular Formula: C₁₈H₁₈N₄O₃S.¼H₂O

Batch Molecular Weight: 374.93

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO 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:

Gerlach et al (2018) The novel BET bromodomain inhibitor BI 894999 represses super-enhancer-associated transcription and synergizes with CDK9 inhibition in AML. *Oncogene* **37** 2687. PMID: 29491412.

Jorda et al (2018) How selective are pharmacological inhibitors of cell-cycle-regulating cyclin-dependent kinases? *J.Med.Chem.* **61** 9105. PMID: 30234987.

Brägelmann et al (2017) Systematic kinase inhibitor profiling identifies CDK9 as a synthetic lethal target in NUT midline carcinoma. *Cell Rep.* **20** 2833. PMID: 28930680.

Albert et al (2014) Characterization of molecular and cellular functions of the cyclin-dependent kinase CDK9 using a novel specific inhibitor. *Br.J.Pharmacol.* **171** 55. PMID: 24102143.

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