

Product Name: LLY 507

Catalog No.: 5365

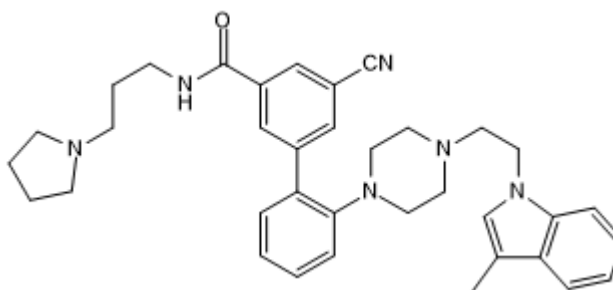
Batch No.: 1

CAS Number: 1793053-37-8

IUPAC Name: 3-Cyano-5-[2-[4-[2-(3-methyl-1*H*-indol-1-yl)ethyl]piperazin-1-yl]phenyl]-*N*-[3-(pyrrolidin-1-yl)propyl]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₆H₄₂N₆O.½H₂O
Batch Molecular Weight: 583.77
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 99% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	74.07	7.42	14.4
Found	74.26	7.41	14.38

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

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Description:

Potent SMYD2 inhibitor (IC₅₀ = 15 nM). Exhibits >100-fold selectivity for SMYD2 over 25 other methyltransferases including SMYD3, SUV420H1 and SUV420H2. Inhibits SMYD2-mediated p53 methylation in vitro. Also inhibits proliferation of a range of esophageal, liver and breast cancer cell lines.

Physical and Chemical Properties:

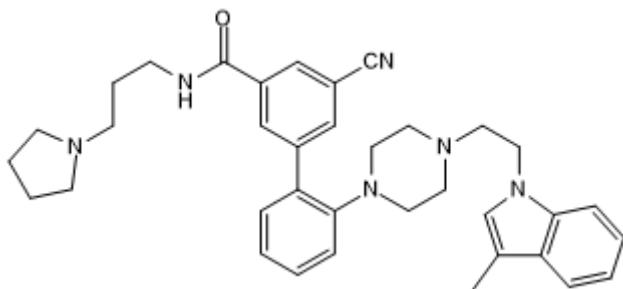
Batch Molecular Formula: C₃₆H₄₂N₆O.½H₂O

Batch Molecular Weight: 583.77

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Nguyen et al (2015) LLY-507, a cell-active, potent, and selective inhibitor of protein-lysine methyltransferase SMYD2. *J.Biol.Chem.* **290** 13641. PMID: 25825497.

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 45-60°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:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the LLY 507 probe summary on the SGC website.

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