

# PRODUCT INFORMATION

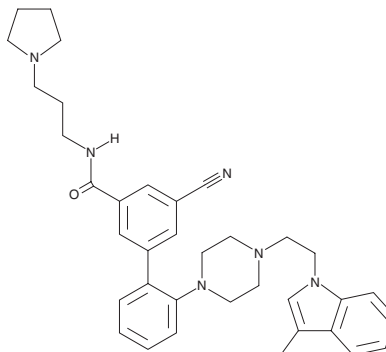


## LLY-507

Item No. 16441

**CAS Registry No.:** 1793053-37-8  
**Formal Name:** 5-cyano-2'-[4-[2-(3-methyl-1H-indol-1-yl)ethyl]-1-piperazinyl]-N-[3-(1-pyrrolidinyl)propyl]-[1,1'-biphenyl]-3-carboxamide

**MF:** C<sub>36</sub>H<sub>42</sub>N<sub>6</sub>O  
**FW:** 574.8  
**Purity:** ≥98%  
**UV/Vis.:** λ<sub>max</sub>: 227 nm  
**Supplied as:** A crystalline solid  
**Storage:** -20°C  
**Stability:** ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

### Laboratory Procedures

LLY-507 is supplied as a crystalline solid. A stock solution may be made by dissolving the LLY-507 in the solvent of choice, which should be purged with an inert gas. LLY-507 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of LLY-507 in these solvents is approximately 25, 30, and 10 mg/ml, respectively.

LLY-507 is sparingly soluble in aqueous solutions. To enhance aqueous solubility, dilute the organic solvent solution into aqueous buffers or isotonic saline. If performing biological experiments, ensure the residual amount of organic solvent is insignificant, since organic solvents may have physiological effects at low concentrations. We do not recommend storing the aqueous solution for more than one day.

### Description

SMYD2 is a lysine N-methyltransferase that methylates both histones and non-histone proteins, including p53 and retinoblastoma-associated protein.<sup>1,2</sup> LLY-507 is a cell-active, small molecule inhibitor of SMYD2 (IC<sub>50</sub> = 15 nM).<sup>3</sup> It has been shown to inhibit p53 lysine<sup>370</sup> monomethylation in KYSE-150 esophageal squamous cell carcinoma cells stably expressing SMYD2 with an IC<sub>50</sub> value of 0.6 μM.<sup>3</sup> LLY-507 is >100-fold selective for SMYD2 over a panel of 27 protein methyltransferases and non-methyltransferase targets.<sup>3</sup> See the Structural Genomics Consortium (SGC) website for more information.

### References

1. Abu-Farha, M., Lambert, J.-P., Al-Madhoun, A.S., *et al.* The tale of two domains: Proteomics and genomics analysis of SMYD2, a new histone methyltransferase. *Mol. Cell Proteomics* **7(3)**, 560-572 (2008).
2. Brown, M.A., Sims, R.J.I., Gottlieb, P.D., *et al.* Identification and characterization of Smyd2: A split SET/MYND domain-containing histone H3 lysine 36-specific methyltransferase that interacts with the Sin3 histone deacetylase complex. *Mol. Cancer* **5**, 26 (2006).
3. Nguyen, H., Allali-Hassani, A., Antonysamy, S., *et al.* LLY-507, a cell-active, potent, and selective inhibitor of protein-lysine methyltransferase SMYD2. *J. Biol. Chem.* **290(22)**, 13641-13653 (2015).

#### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the [complete](#) Safety Data Sheet, which has been sent via email to your institution.

#### WARRANTY AND LIMITATION OF REMEDY

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