

Product Name: MLN 4924

Catalog No.: 6499

Batch No.: 3

CAS Number: 905579-51-3

IUPAC Name: [(1*S*,2*S*,4*R*)-4-[4-[[[(1*S*)-2,3-Dihydro-1*H*-inden-1-yl]amino]-7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl]-2-hydroxycyclopentyl]methyl sulfamic acid ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₅N₅O₄S.¼H₂O

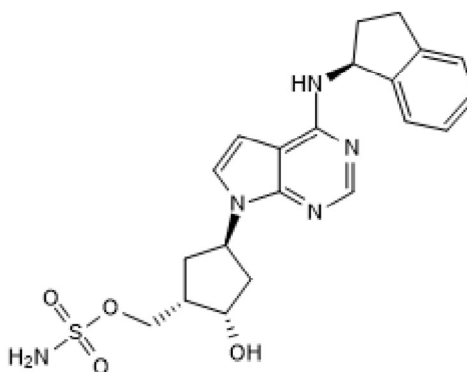
Batch Molecular Weight: 448.02

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.3	5.74	15.63
Found	55.76	5.76	15.42

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Description:

MLN 4924 (TAK 924) is a potent and selective NEDD8 activating enzyme (NAE) inhibitor (IC₅₀ = 4.7 nM). MLN 4924 exhibits selectivity over closely related enzymes UAE, UBA6, SAE, and ATG7 (IC₅₀ = 1.5, 1.8, 8.2, and >10 μM, respectively), and displays minimal activity at adenosine receptors and a panel of 12 cellular kinases. MLN 4924 exhibits cytotoxicity in several human tumor-derived cell lines and causes liver damage in SD rats, when given with TNF-α. It blocks the NEDD8 pathway causing DNA damage in mice bearing HCT-116 xenografts. Cell permeable.

Physical and Chemical Properties:

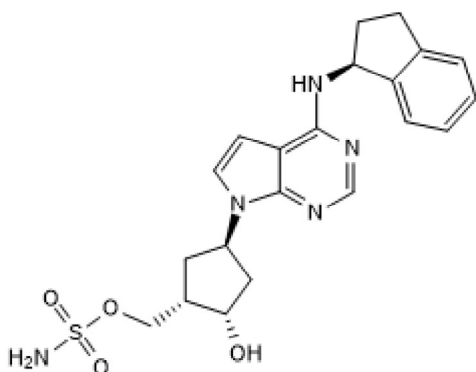
Batch Molecular Formula: C₂₁H₂₅N₅O₄S·¼H₂O

Batch Molecular Weight: 448.02

Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Baek et al (2020) NEDD8 nucleates a multivalent cullin-RING-UBE2D ubiquitin ligation assembly. *Nature* **578** 461. PMID: 32051583.

Hyer et al (2018) A small-molecule inhibitor of the ubiquitin activating enzyme for cancer treatment. *Nat.Med.* **24** 186. PMID: 29334375.

Tong et al (2017) MLN4924 (Pevonedistat), a protein neddylation inhibitor, suppresses proliferation and migration of human clear cell renal cell carcinoma. *Sci.Rep.* **7** 5599. PMID: 28717191.

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

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