

Product Name: YKL 5-124

Catalog No.: 7157

Batch No.: 1

CAS Number: 1957203-01-8

IUPAC Name: *N*-[(1*S*)-2-(Dimethylamino)-1-phenylethyl]-4,6-dihydro-6,6-dimethyl-3-[[4-[(1-oxo-2-propen-1-yl)amino]benzoyl]amino]pyrrolo[3,4-*c*]pyrazole-5(1*H*)-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₃₃N₇O₃.H₂O

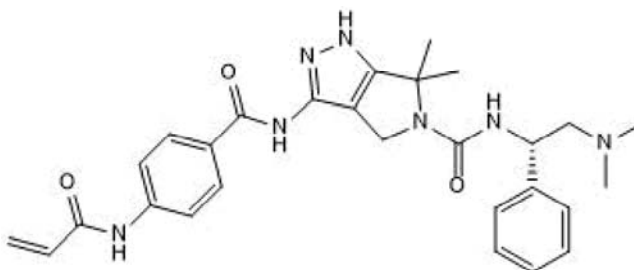
Batch Molecular Weight: 533.64

Physical Appearance: White solid

Solubility: DMSO to 20 mM
ethanol to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 95.5% purity

Chiral HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.02	6.61	18.37
Found	62.7	6.54	18.2

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Description:

YKL-5-124 is a potent and selective CDK7/Mat1/CycH and cyclin dependent kinase (CDK7) inhibitor (IC₅₀ values = 9.7 nM and 53.5 nM, respectively). YKL-5-124 shows 100-fold selectivity over CDK9 and CDK2. YKL-5-124 induces cell cycle arrest at the G₁/S transition, inhibits E2F-driven gene expression and inhibits CDK1 and CDK3 T-loop phosphorylation.

Physical and Chemical Properties:

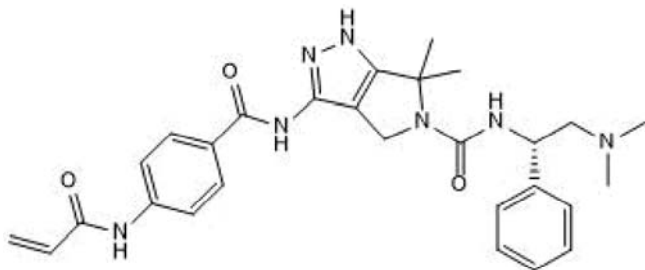
Batch Molecular Formula: C₂₈H₃₃N₇O₃·H₂O

Batch Molecular Weight: 533.64

Physical Appearance: White solid

Minimum Purity: ≥95%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 mM

ethanol to 20 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:

Olson *et al* (2019) Development of a selective CDK7 covalent inhibitor reveals predominant cell-cycle phenotype. *Cell Chem.Biol.* **26** 792. PMID: 30905681.

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