YKL-5-124 TFA

Cat. No.: HY-101257B

CAS No.: 2748220-93-9

Molecular Formula: $C_{30}H_{34}F_3N_7O_5$

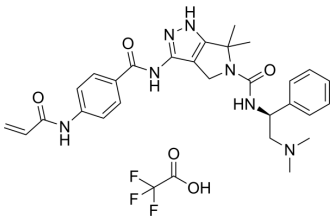
Molecular Weight: 629.63

Target: CDK

Pathway: Cell Cycle/DNA Damage

Storage: 4°C, sealed storage, away from moisture

* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (158.82 mM)

H_2O : 50 mg/mL (79.41 mM; Need ultrasonic)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.5882 mL	7.9412 mL	15.8823 mL
5 mM	0.3176 mL	1.5882 mL	3.1765 mL
10 mM	0.1588 mL	0.7941 mL	1.5882 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: PBS
   Solubility: 50 mg/mL (79.41 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (3.97 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (3.97 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (3.97 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

YKL-5-124 TFA is a potent, selective, irreversible and covalent CDK7 inhibitor with IC_{50}s of 53.5 nM and 9.7 nM for CDK7 and CDK7/Mat1/CycH, respectively. YKL-5-124 TFA is >100-fold greater selective for CDK7 than CDK9 and CDK2, and inactive against CDK12 and CDK13. YKL-5-124 TFA induces a strong cell-cycle arrest, inhibits E2F-driven gene expression, and exhibits little effect on RNA polymerase II phosphorylation status[1].

IC_{50} & Target	CDK7 53.5 nM (IC_{50})	CDK7/Mat1/CycH 9.7 nM (IC_{50})	CDK2 1300 nM (IC_{50})	CDK9 3020 nM (IC_{50})

In Vitro

YKL-5-124 (0-2000 nM; 72 hours; HAP1 cells) treatment causes a dose-dependent increase in G1- and G2/M-phase cells and a corresponding loss of S-phase cells[1].

?YKL-5-124 (0-2000 nM; 24 hours; HAP1 WT cells) treatment inhibits CDK1 T-loop phosphorylation, and to a lesser extent CDK2 T-loop phosphorylation in a concentration-dependent fashion[1].

?Treatment of cells with YKL-5-124 as a competitor at a concentration of about 30 nM blocks pull-down of CDK7-cyclin H but has no effect on the pull-down of cyclin K-CDK12/13 in HAP1 cells. Treatment with 100 nM YKL-5-124 reduces CDK7-cyclin H binding to bioTHZ1 by >50% at 30 min[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Cycle Analysis[1]

Cell Line:	HAP1 cells
Concentration:	0 nM, 0.2 nM, 0.7 nM, 2 nM, 6.3 nM, 20 nM, 60 nM, 200 nM, 633.3 nM, 2000 nM
Incubation Time:	72 hours
Result:	Caused a dose-dependent increase in G1- and G2/M-phase cells and a corresponding loss of S-phase cells.

Western Blot Analysis[1]

Cell Line:	HAP1 WT cells
Concentration:	0 nM, 125 nM, 250 nM, 500 nM, 1000 nM, 2000 nM
Incubation Time:	24 hours
Result:	Inhibited CDK1 T-loop phosphorylation, and to a lesser extent CDK2 T-loop phosphorylation in a concentration-dependent fashion.

CUSTOMER VALIDATION

- Cell Discov. 2022 Oct 6;8(1):102.
- J Biomed Sci. 2022 Feb 14;29(1):13.
- Int J Mol Sci. 2023 Apr 10, 24(8), 7009.
- J Cancer Res Clin Oncol. 2022 Nov 18.
- bioRxiv. 2023 Apr 23.

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REFERENCES

[1]. Olson CM, et al. Development of a Selective CDK7 Covalent Inhibitor Reveals Predominant Cell-Cycle Phenotype. Cell Chem Biol. 2019 Jun 20;26(6):792-803.e10.

Caution: Product has not been fully validated for medical applications. For research use only.

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