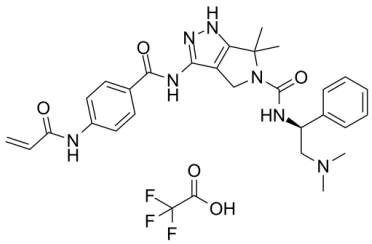
Data Sheet

Product Name:	YKL-5-124 (TFA)
Cat. No.:	CS-7542
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
Solubility:	DMSO : ≥ 100 mg/mL (158.82 mM); H2O : 50 mg/mL (79.41 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

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]. **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].

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.

CAIndexNames:

Pyrrolo[3,4-c]pyrazole-5(1H)-carboxamide, N-[(1S)-2-(dimethylamino)-1-phenylethyl]-4,6-dihydro-6,6-dimethyl-3-[[4-[(1-oxo-2-propen-1-yl)amino]benzoyl]amino]-, 2,2,2-trifluoroacetate (1:1)

SMILES:

CC1(C)N(C(N[C@@H](C2=CC=CC=C2)CN(C)C)=O)CC3=C1NN=C3NC(C4=CC=C(NC(C=C)=O)C=C4)=O.FC(F)(C(O)=O)F

Tel: 610-426-3128 Fax: 888-484-5008 E-mail: sales@ChemScene.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA