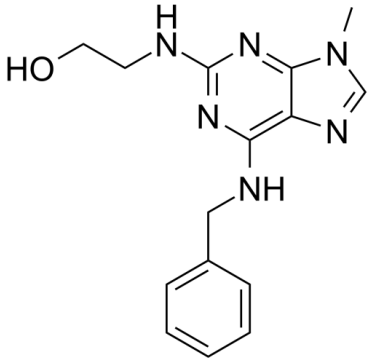
Data Sheet

Product Name:	Olomoucine
Cat. No.:	CS-W012144
CAS No.:	101622-51-9
Molecular Formula:	$C_{15}H_{18}N_6O$
Molecular Weight:	298.34
Target:	CDK
Pathway:	Cell Cycle/DNA Damage
Solubility:	DMSO : 100 mg/mL (335.19 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Olomoucine is an ATP competitive inhibitor of **CDK**s. Olomoucine is a purine (HY-34431) derivative and inhibits CDC2/cyclin B, Cdk2/cyclin A, Cdk2/cyclin E (both **IC_{50}**=7 μM), CDK/p35 kinase (**IC_{50}**=3 μM) and ERK1/p44 MAP kinase (**IC_{50}**=25 μM)[1][2]. Olomoucine regulates cell cycle and shows anti-melanin tumor activity[3][4]. IC50 & Target: Target: CDK (cyclin-dependent kinases)[1]
In Vitro: Olomoucine inhibits CDK2 and CDC2 kinases with IC_{50} of 7 μM (CDC2/cyclin B), 7 μM (CDK2/cyclin A), 7 μM (CDK2/cyclin E), 3 Mm (CDK5/p35), and 25μM (ERK1/p44 MAPK), respectively[1].
Olomoucine (0, 5, 10, 15, and 25 μM) is a competitive inhibitor for ATP and as a non-competitive inhibitor for histone H[1].
Olomoucine (0-1000 μM) inhibits DNA synthesis in interleukin-2-stimulated T lymphocytes (CTLL-2 cells) and triggers a Gl arrest similar to interleukin-2 deprivation[2].
Olomoucine (0-100 μM) inhibits Gl/S transition of non-small cell lung cancer cell line MB65 cells[2].
Olomoucine (0-150 μM) inhibits prophase/metaphase transition of Rdditapes oocytes[2].
Olomoucine inhibits tumor cells survival with IC_{50}s of 32.35 μM (dog melanoma), 42.15 μM (mouse B16 melanoma), 82.30 μM (human melanoma), respectively[3]. **In Vivo:** Olomoucine (8 mg/kg; i.v.; once daily; 7 d) induces apoptosis in tumor cells on the 3rd day after treatment without side effects[3].
Cassette dosing was found to overestimate the AUC while underestimating the Cmax compared with single dosing administration[4].

Cassette dosing pharmacokinetics for olomoucine[4]

Administration	C_{max} (nM)	Cl_{obs} (l/h)	V_{ss}(obs) (l)	MRT_{last} (h)	AUC_{inf}(obs) (nM·h)	$t_{1/2}$ (h)
cassettle	9208 (0.9)	1.10	0.67 (2.8)/td>	0.56	3030	1.03 (0.7)
single	7194 (0.6)	1.18	0.52 (2.1)/td>	0.40	2831	0.98 (0.7)

Note: Single agents dosing=50 mg/kg, cassette dosing=16.66 mg/kg.

References:

[1]. Vesely, J., Havlicek, J., Strnad, M., et al. Inhibition of cyclin-dependent kinases by purine analogues. European Journal of Biochemistry 224, 771-786

(1994).

[2]. Abraham, R.T., Acquarone, M., Andersen, A., et al. Cellular effects of olomoucine, an inhibitor of cyclin-dependent kinases. Biology of the Cell 83(2), 105-120 (1995).

[3]. Hajdúch M, et al. Induction of apoptosis and regression of spontaneous dog melanoma following in vivo application of synthetic cyclin-dependent kinase inhibitor olomoucine. Anticancer Drugs. 1997 Nov. 8(10):1007-13.

[4]. Raynaud FI, et al. Cassette dosing pharmacokinetics of a library of 2,6,9-trisubstituted purine cyclin-dependent kinase 2 inhibitors prepared by parallel synthesis. Mol Cancer Ther. 2004 Mar. 3(3):353-62.

CAIndexNames:

Ethanol, 2-[[9-methyl-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]-

SMILES:

CN1C=NC2=C(NCC3=CC=CC=C3)N=C(NCCO)N=C12

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