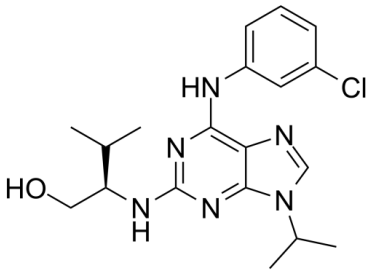
Data Sheet

Product Name:	Purvalanol A
Cat. No.:	CS-4001
CAS No.:	212844-53-6
Molecular Formula:	C19H25ClN6O
Molecular Weight:	388.89
Target:	Apoptosis; Autophagy; CDK
Pathway:	Apoptosis; Autophagy; Cell Cycle/DNA Damage
Solubility:	H2O : < 0.1 mg/mL (insoluble); DMSO : ≥ 50 mg/mL (128.57 mM)



BIOLOGICAL ACTIVITY:

Purvalanol A is a potent **CDK** inhibitor, which inhibits cdc2-cyclin B, cdk2-cyclin A, cdk2-cyclin E, cdk4-cyclin D1, and cdk5-p35 with **IC $_{50}$**s of 4, 70, 35, 850, 75 nM, resepctively. IC50 & Target: IC50: 4 nM (cdc2-cyclin B), 70 nM (cdk2-cyclin A), 35 nM (cdk2-cyclin E), 850 nM (cdk4-cyclin D1), 75 nM (cdk5-p35)[1] **In Vitro:** Purvalanol A inhibits cdc28 (S. cerevisiae) and erk1 with IC_{50}s of 80 and 9000 nM. Purvalanol A shows inhibitory activities against the NCI panel of 60 human tumor cell lines, with average GI50 of 2 μM; two cell lines show an -20-fold increase in sensitivity to purvalanol A: the KM12 colon cancer cell line with a GI_{50} of 76 nM and the NCI-H522 non–small cell lung cancer cell line with a GI_{50} of 347 nM[1]. Purvalanol A is a 2.5-fold more potent inhibitor of CDK2, but also inhibits DYRK1A potently and a number of other protein kinases in the low micromolar range. Purvalanol A inhibits MKK1, MAPK2/ERK2, JNK/SAPK1c with IC_{50}s of 80, 26, 84 μM[2]. Purvalanol A selectively inhibits the phosphorylation of cellular proteins. Purvalanol A prevents the increases of the contents of cyclins D and E during serum-induced G1 phase progression. Purvalanol A does not inhibit transcription under cell-free conditions[3].

PROTOCOL (Extracted from published papers and Only for reference)

Cell assay [4] Cell lines were treated with purvalanol A, PP2, roscovitine or DMSO as a control. After 24 h, cells were collected, fixed in 70% ethanol and stained with propidium iodide. Acquisition was carried out on a FACS can flow cytometer (Becton Dickinson) to identify apoptotic cells with <2N DNA content. In addition, apoptosis was detected by Western blotting with anti-cleaved-caspase 3.

References:

[1]. Gray NS, et al. Exploiting chemical libraries, structure, and genomics in the search for kinase inhibitors. Science. 1998 Jul 24;281(5376):533-8.

[2]. Bain J, et al. The specificities of protein kinase inhibitors: an update. Biochem J. 2003 Apr 1;371(Pt 1):199-204.

[3]. Villerbu N, et al. Cellular effects of purvalanol A: a specific inhibitor of cyclin-dependent kinase activities. Int J Cancer. 2002 Feb 20;97(6):761-9.

CAIndexNames:

1-Butanol, 2-[[6-[(3-chlorophenyl)amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-3-methyl-, (2R)-

SMILES:

CC([C@@H](NC1=NC(NC2=CC=CC(Cl)=C2)=C3N=CN(C(C)C)C3=N1)CO)C

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

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