Purvalanol A is a cell-permeable, potent, and selective inhibitor of cyclin-dependent kinases (CDKs). CDKs and cyclins form a stoichiometric complex, which is necessary for the CDK subunit to gain its protein kinase activity. It has been shown that these CDK/cyclin complexes play a key role in initiating G2/M transitions of the cell cycle (Jackman & Pines). Purvalanol A acts through competitive inhibition of ATP binding, to inhibit CDK1/cyclin B (IC\textsubscript{50} = 4 nM), CDK2/cyclin A (IC\textsubscript{50} = 70 nM), CDK2/cyclin E (IC\textsubscript{50} = 35 nM), CDK4/cyclin D1 (IC\textsubscript{50} = 850 nM), and CDK5/p35 (IC\textsubscript{50} = 75 nM; Bain et al.; Gray et al.), thereby arresting cells in G1 and G2.

**Molecular Name:** Purvalanol A  
**Alternative Names:** NG 60  
**CAS Number:** 212844-53-6  
**Chemical Formula:** C\textsubscript{19}H\textsubscript{21}ClN\textsubscript{6}O  
**Molecular Weight:** 388.9 g/mol  
**Purity:** ≥ 98%  
**Chemical Name:** (2R)-2-[[6-[[3-chlorophenyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-3-methyl-1-butanol  
**Structure:**

![Structure of Purvalanol A](attachment:structure.png)

**Properties**

**Physical Appearance:** A crystalline solid  
**Storage:** Product stable at -20°C as supplied. Protect product from prolonged exposure to light. For long-term storage store with a desiccant. Stable as supplied for 12 months from date of receipt.  
**Solubility:**  
- DMSO ≤ 75 mM  
- Absolute ethanol ≤ 25 mM  
For example, to prepare a 10 mM stock solution in DMSO, resuspend 1 mg in 257 μL of DMSO. Prepare stock solution fresh before use. Information regarding stability of small molecules in solution has rarely been reported, however, as a general guide we recommend storage in DMSO at -20°C. Aliquot into working volumes to avoid repeated freeze-thaw cycles. The effect of storage of stock solution on compound performance should be tested for each application.  

Compound has low solubility in aqueous media. For use as a cell culture supplement, stock solution should be diluted into culture medium immediately before use. Avoid final DMSO concentration above 0.1% due to potential cell toxicity.
Published Applications

CANCER RESEARCH
- Inhibits proliferation in exponentially growing cancer cell lines and reversibly arrests synchronised cells in G1 and G2 phase of cell cycle (Villerbu et al.).
- Induces apoptosis in MCF-7 estrogen receptor positive breast cancer cells (Obakan et al.).
- Suppresses cancer progression associated with Src up-regulation by the coordinated inhibition of cell cycle progression and tyrosine kinase signaling (Hikita et al.).

References

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