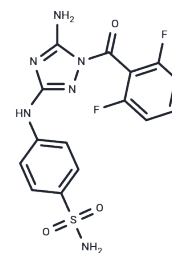


JNJ-7706621

## Chemical Properties

CAS No. : 443797-96-4  
 Formula: C<sub>15</sub>H<sub>12</sub>F<sub>2</sub>N<sub>6</sub>O<sub>3</sub>S  
 Molecular Weight: 394.36  
 Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year  
 Actual storage temperature shall be subject to the COA.



## Biological Description

Description	JNJ-7706621 is a potent aurora kinase inhibitor that also inhibits CDK1 and CDK2.
Targets(IC50)	Apoptosis,CDK,Aurora Kinase
In vitro	JNJ-7706621 (100 or 125 mg/kg) induced tumor regression in mice carrying human melanoma A375 xenografts.
In vivo	JNJ-7706621 demonstrates varied potency across different cell types, exhibiting greater effectiveness in inhibiting the growth of normal cell types, including MRC-5, HASMC, HUVEC, and HMVEC, with IC50 values ranging from 3.67-5.42 μM. It shows high efficacy against CDK1 and 2, with IC50 values of 3-9 nM, and exerts inhibitory effects on a range of human cancer cell types, such as HeLa, HCT-116, SK-OV-3, PC3, DU145, A375, MDA-MB-231, MES-SA, and MES-SA/Dx5, with IC50 values between 112-514 nM, irrespective of p53, retinoblastoma, or P-glycoprotein status. JNJ-7706621 also inhibits CDK3, 4, and 6, with IC50 values of 58-253 nM, and targets Aurora-A and B kinases with IC50 values of 11 and 15 nM, respectively. Furthermore, it inhibits VEGF-R2, FGF-R2, and GSK3β, with IC50 values of 154-254 nM. In HeLa or U937 cells, JNJ-7706621 (0.5-3 μM) delays the exit from the G1 phase, induces cell arrest in the G2-M phase, triggers nuclear replication, activates apoptosis, and reduces colony formation.
Kinase Assay	In vitro kinase assay for CDK1 and Aurora kinases:CDK1 kinase activity is tested by the CDK1/cyclin B complex purified from baculovirus to phosphorylate a biotinylated peptide substrate containing the consensus phosphorylation site for histone H1, which is phosphorylated in vivo by CDK1. Inhibition of CDK1 activity is measured by observing a decreased amount of 33P-γ-ATP incorporation into the immobilized substrate in streptavidin-coated 96-well scintillating microplates. CDK1 enzyme is diluted in 50 mM Tris-HCl (pH 8), 10 mM MgCl <sub>2</sub> , 0.1 mM Na <sub>3</sub> VO <sub>4</sub> , 1 mM DTT, 1% DMSO, 0.25 μM peptide, 0.1 μCi per well 33P-γ-ATP, and 5 μM ATP in the presence or absence of various concentrations of JNJ-7706621 and incubated at 30 °C for 1 hour. The reaction is terminated by washing with PBS containing 100 mM EDTA and plates are counted in a scintillation counter. IC50 is determined by Linear regression analysis of the percent inhibition by JNJ-7706621.The Aurora kinase activity is measured with 10 μM ATP and a peptide containing a dual repeat of the kemptide phosphorylation motif.

Cell Research	Cell lines: HeLa,HCT-116,A375,SK-OV-3,MDA-MB-231 and PC-3 cells. Concentrations: 1 nM - 10 µM,dissolved in DMSO. Method: Measuring incorporation of 14C-labelled thymidine into newly synthesized DNA within the cells to determine the ability of JNJ-7706621 to inhibit the proliferation of cell growth.Cells are trypsinized and counted and 3-8 ×10 <sup>3</sup> cells are added to each well of a 96-well CytoStar tissue culture treated scintillating microplate in 100 µL complete medium in a volume.Cells are incubated for 24 hours at 37 °C in an atmosphere containing 5% CO <sub>2</sub> .Next,1 µL JNJ-7706621 is added to the wells of the plate.Cells are incubated for another 24 hours.Methyl 14C-thymidine 56 mCi/mmol is diluted in complete medium and 0.2 µCi/well is added to each well of the CytoStar plate in a volume of 20 µL.The plate is incubated for 24 hours at 37 °C in JNJ-7706621 with 14C-thymidine.The contents of the plate are discarded and the plate is washed twice with 200 µL PBS.200 µL of PBS is added to each well.The top of the plate is sealed with a transparent plate sealer and a white plate backing sealer is applied to the bottom of the plate.The degree of methyl 14C-thymidine incorporation is quantified on a Packard Top Count.
Animal Research	Animal Models: Mouse xenograft model of A375 cells Formulation & . Dosages: Dissolved in 0.5% methylcellulose containing 0.1% polysorbate 80 in sterile water.100 or 125 mg/kg. Administration: Orally or by intraperitoneal injection

### Solubility Information

Solubility	DMSO: 55 mg/mL (139.47 mM),Sonication is recommended. H <sub>2</sub> O: < 1 mg/mL (insoluble or slightly soluble), Ethanol: < 1 mg/mL (insoluble or slightly soluble), (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (5.07 mM),Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

### Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.5358 mL	12.6788 mL	25.3575 mL
5 mM	0.5072 mL	2.5358 mL	5.0715 mL
10 mM	0.2536 mL	1.2679 mL	2.5358 mL
50 mM	0.0507 mL	0.2536 mL	0.5072 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

### Reference

- Emanuel S, et al. Cancer Res, 2005, 65(19), 9038-9046.
- Seamon JA, et al. Mol Cancer Ther, 2006, 5(10), 2459-2467.
- Lin R, et al. J Med Chem, 2005, 48(13), 4208-4211.

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