

Product Data Sheet

Product Name: JNJ-7706621

Cat. No.: GC12612

Chemical Properties

Cas. No. 443797-96-4

Chemical Name 4-[[5-amino-1-(2,6-difluorobenzoyl)-1,2,4-triazol-3-yl]amino]benzenesulfonamide

SMILES C1=CC(=C(C(=C1)F)C(=O)N2C(=NC(=N2)NC3=CC=C(C(=C3)S(=O)(=O)N)N)F

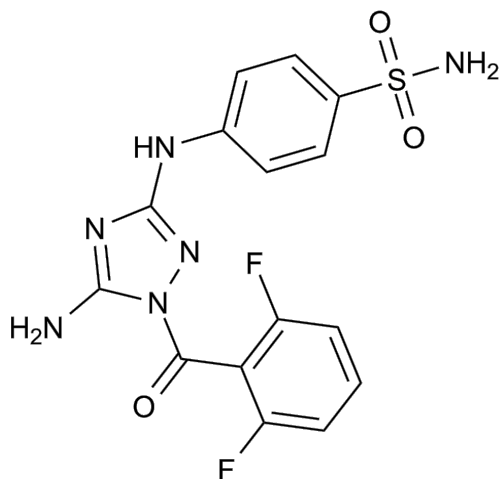
Formula $C_{15}H_{12}F_2N_6O_3S$ M.Wt 394.36

Solubility ≥ 19.7 mg/mL in DMSO Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Protocol

Kinase experiment [1]:

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

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In vitro kinase assay for CDK1 and Aurora kinases

To identify compounds that inhibited CDK1 kinase activity, a screening method was developed using 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 was measured by observing a reduced amount of ³³P-γ-ATP incorporation into the immobilized substrate in streptavidin-coated 96-well scintillating microplates. CDK1 enzyme was diluted in 50 mM Tris-HCl (pH 8), 10 mM MgCl₂, 0.1 mM Na₃VO₄, 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 hr. The reaction was terminated by washing with PBS containing 100 mM EDTA and plates were counted in a scintillation counter. Linear regression analysis of the percent inhibition by JNJ-7706621 was used to determine IC₅₀ values.

Cell experiment [1]:

Cell lines U937 cells

Preparation method

The solubility of this compound in DMSO is >10 mM. General tips for obtaining a higher concentration: Please warm the tube at 37 °C for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below -20 °C for several months.

Reaction Conditions 0, 0.5, 1, 2, 3 or 4 μM; 24 hrs

Applications In U937 cells, JNJ-7706621 time- and dose-dependently induced cell apoptosis.

Animal experiment [1]:

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Animal models	Mouse xenograft model of A375 melanoma human tumor
Dosage form	100 or 125 mg/kg; p.o. or i.p.
Applications	In mouse xenograft model of A375 melanoma human tumor, JNJ-7706621 at the dose of 100 or 125 mg/kg caused tumor regression.
Other notes	Please test the solubility of all compounds indoor, and the actual solubility may slightly differ with the theoretical value. This is caused by an experimental system error and it is normal.

References:

[1]. Stuart Emanuel, Catherine A. Rugg, Robert H. Gruninger, Ronghui Lin, Angel Fuentes-Pesquera, Peter J. Connolly, Steven K. Wetter, Beth Hollister, Walter W. Kruger, Cheryl Napier, Linda Jolliffe, and Steven A. Middleton. The In vitro and In vivo Effects of JNJ-7706621: A Dual Inhibitor of Cyclin-Dependent Kinases and Aurora Kinases. Cancer Res 2005;65:9038-9046.

Background

JNJ-7706621 is a dual inhibitor of cyclin-dependent kinases (CDK) and Aurora kinases that potently inhibits CDK1, CDK2, CDK3, CDK4, CDK6, Aurora-A, and Aurora-B in vitro with 50% inhibition concentration IC₅₀ values of 0.009, 0.004, 0.003, 0.058, 0.253, 0.175, 0.011 and 0.015 µmol/L respectively. JNJ-7706621 selectively inhibits proliferation of both normal human cells and tumor cells of various origins, where the efficacy of JNJ-7706621 is 10-fold greater in tumor cells (IC₅₀ range of 0.112 to 0.514 µmol/L) than normal cells (IC₅₀ range of 3.67 to 5.42 µmol/L). JNJ-7706621 has been found to induce apoptosis, suppress colony formation and inhibit cell growth regardless of p53, retinoblastoma or P-glycoprotein status in human cancer cells.

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[1].Stuart Emanuel, Catherine A. Rugg, Robert H. Gruninger, Ronghui Lin, Angel Fuentes-Pesquera, Peter J. Connolly, Steven K. Wetter, Beth Hollister, Walter W. Kruger, Cheryl Napier, Linda Jolliffe, and Steven A. Middleton. *The In vitro and In vivo Effects of JNJ-7706621: A Dual Inhibitor of Cyclin-Dependent Kinases and Aurora Kinases. Cancer Res 2005;65:9038-9046*

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