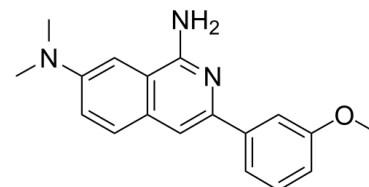


Data Sheet

Product Name:	3-arylisoquinolinamine derivative
Cat. No.:	CS-B0390
CAS No.:	1029008-71-6
Molecular Formula:	C ₁₈ H ₁₉ N ₃ O
Molecular Weight:	293.36
Target:	Others
Pathway:	Others
Solubility:	DMSO : ≥ 50 mg/mL (170.44 mM); H ₂ O : < 0.1 mg/mL (insoluble)



BIOLOGICAL ACTIVITY:

3-arylisoquinolinamine derivative is a 3-arylisoquinolinamine derivative with antitumor activity. IC₅₀ & Target: IC₅₀: 21 nM (breast MDA-MB-231), 19 nM (pancreas PANC-1), 17 nM (colon HCT 116), 19 nM (prostate PC3), 14 nM (ovary OVCAR-3), 32 nM (melanoma SK-MEL-28), 22 nM (kidney Caki-1), 32 nM (glioblastoma SNB19)^[1] **In Vitro:** 3-arylisoquinolinamine derivative is a 3-arylisoquinolinamine derivative, extracted from the reference[1], compound 7b. 3-arylisoquinolinamine derivative (7b) shows more effective activity against Paclitaxel-resistant HCT-15 human colorectal cancer cell lines when compared to the original cytotoxic cancer drug, Paclitaxel. The cell cycle dynamics is analyzed by flow cytometry. Treatment of human HCT-15 cells with 3-arylisoquinolinamine derivative (7b) blocks or delays the progression of cells from G₀/G₁ phase into S phase, and induces cell death. Treatment with 3-arylisoquinolinamine derivative (7b) also significantly inhibits the growth of tumors and enhances tumor regression in a Paclitaxel-resistant HCT-15 xenograft model. 3-arylisoquinolinamine derivative (7b) inhibits the cell growth at IC₅₀ value ranges from 14 nM to 32 nM in the human cancer cells tested. In cell cycle analysis using HCT-15 cells, treatment of 1 nM of 3-arylisoquinolinamine derivative (7b) displays a significant increase in G₀/G₁ phase at 24 h with a decrease in G₂/M phase, but the increase of G₀/G₁ phase at 48 h is not significant. At higher concentration of 3-arylisoquinolinamine derivative (7b) (10 nM), there are a significant increase in G₀/G₁ phase and decrease in G₂/M phase, and an emergence of sub-G₁ phase, at both 24 h and 48 h. 3-arylisoquinolinamine derivative (7b) blocks or delays the progression of cells from G₀/G₁ phase into S phase, and induces cell death^[1]. 3-arylisoquinolinamine derivative is a 3-arylisoquinolinamine derivative, extracted from the reference[1], compound 13. 3-arylisoquinolinamine derivative (compound 13) is tested in colon cancer cells and its antitumor activity is compared with Paclitaxel. 3-arylisoquinolinamine derivative (IC₅₀: 15 nM in HCT-15 cells, 17 nM in HCT116 cells) shows potent antiproliferative activities with IC₅₀ value in the low nanomolar range in both cells and higher antitumor activities than that of Paclitaxel against Paclitaxel-resistant HCT-15 colorectal cancer cells^[2]. **In Vivo:** 3-arylisoquinolinamine derivative (Compound 13) has higher antitumor efficacy (69.2 % inhibition) than that of the control drug, Paclitaxel (48.8 % inhibition) in the inhibition of growth of tumor in an animal model^[2].

PROTOCOL (Extracted from published papers and Only for reference)

Animal Administration: 3-arylisoquinolinamine derivative (Compound 13) is dissolved in 5 % Cremophor and 5 % ethanol in PBS and solvent alone served as vehicle control^[2]. Mice^[2]

The six-week-old female athymic mice (BALB/c nu/nu) are used. All study medications (vehicle control, Paclitaxel: 10 mg/kg/day, 3-arylisoquinolinamine derivative: 10 mg/kg/day) are given by intraperitoneal injections three times per week starting from day 10 and ending on day 29 after inoculation of HCT 15 cells. To quantify tumor growth, three perpendicular diameters of the tumors are measured with calipers every 3-5 days, and the body weight of the mice was monitored for toxicity. The tumor volume is calculated^[2].

References:

[1]. Yang SH, et al. Synthesis, in vitro and in vivo evaluation of 3-arylisquinolinamines as potent antitumor agents. Bioorg Med Chem Lett. 2010 Sep 1;20(17):5277-81.

[2]. Young Bok Lee, et al. 5, 6, or 7-substituted-s- (hetero)arylisquinolinamine derivatives as antitumor agents. WO 2008063548 A2.

CAIndexNames:

1,7-Isoquinolinediamine, 3-(3-methoxyphenyl)-N7,N7-dimethyl-

SMILES:

NC1=NC(C2=CC=CC(OC)=C2)=CC(C=C3)=C1C=C3N(C)C

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

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