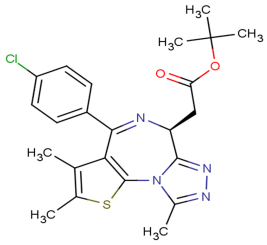
Data Sheet (Cat.No.T2110)

TargetMol
A DRUG SCREENING EXPERT

(+)-JQ-1

Chemical Properties



CAS No. : 1268524-70-4

Formula: C23H25ClN4O2S

Molecular Weight: 456.99

Appearance: no data available

Storage: keep away from direct sunlight
Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	(+)-JQ-1 (JQ1) is a BET bromine domain inhibitor that inhibits BRD4 (1/2) (IC50=77/33 nM) with specificity and reversibility. (+)-JQ-1 induces cell autophagy and inhibits cell proliferation.
Targets(IC50)	Epigenetic Reader Domain,Autophagy,Ligands for Target Protein for PROTAC
In vitro	METHODS: The BRD4-NUT-dependent cell line NMC 797 was treated with (+)-JQ-1 (250 nM) for 48 h. The cell cycle was detected using Flow Cytometry. RESULTS: (+)-JQ-1 induced G1 cell cycle arrest. [1] METHODS: Human multiple myeloma cells KMS11, LR5, OPM1 and INA-6 were treated with (+)-JQ-1 (500 nM) for 24 h, and the expression levels of target proteins were detected by Western Blot. RESULTS: (+)-JQ-1 inhibited c-Myc protein expression in expanded Myc-dependent MM cell lines. [2]
In vivo	METHODS: To detect anti-tumor activity in vivo, (+)-JQ-1 (50 mg/kg, 5% DMSO in 5% dextrose) was administered intraperitoneally to NCr nude mice bearing NMC xenograft tumors once daily for eighteen days. RESULTS: Significant tumor regression and improved overall survival were observed after (+)-JQ-1 treatment. [1] METHODS: To detect anti-tumor activity in vivo, (+)-JQ-1 (50 mg/kg) was intraperitoneally injected into nude mice carrying human gastric cancer tumor HGC27 once daily for two weeks. RESULTS: (+)-JQ-1 prevented the growth of gastric cancer tumors and inhibited tumor metastasis. [3]
Cell Research	Cells were plated at 5,000 cells per well of 96-well plates containing titrations of the compounds as indicated. After incubation, the cells were washed once with PBS and resuspended in 175 µL of ice-cold 70% ethanol and fixed for a minimum of 16 h at 4 °C. The cells were pelleted and washed 1× with PBS and stained for 30 min at room temperature (RT) with 120 µL of staining solution [propidium iodide (20 µg/mL), RNase A (25 µg/mL), 0.1% Triton X-100 in PBS]. Cell number and cell cycle data were obtained by using a flow cytometer using the Express Pro module. DNA content histograms were analyzed by using ModFit LT 3.2 Software. To calculate the number of viable cells in each well, the concentration of events measured using the Guava was multiplied by the volume of cells in the well, then by the fraction of cells in G1+S+G2/M. GI50 values for each cell line were calculated as the concentration of compound giving a 50% reduction

	in cell number relative to the DMSO control [4].
Animal Research	(Harlan) inoculated s.c. with 3 × 10^6 cells per mouse resuspended in 10% Matrigel. Two weeks later (average tumor volume 150 mm3), mice were assigned into two groups: 15 mice were treated with vehicle control (5:95 DMSO:10% 2-Hydroxypropyl-β-cyclodextrin), and 15 mice were treated with 30 mg/kg (+)-JQ1 by i.p. injection twice a day for 28 d. Body weight and tumor volume were measured daily. Tumor volume was calculated from caliper measurements by using the following formula: W × H × L × 0.52. Mice were killed when tumor volume reached 2,000 mm3, when body weight decreased >20% of initial weight, or when the mice were in poor health as established in the IACUC protocol. Survival was plotted and analyzed in GraphPad Prism software, and statistical significance was calculated by using log-rank (Mantel-Cox) and Gehan–Breslow–Wilcoxon tests. MV4-11 xenografts were established in nude mice injected with 10 × 10^6 cells per mouse. JQ1 was dosed i.p. and formulated as described above. Mice were divided into 4 groups of 10 animals: vehicle control once a day; 50 mg/kg (+)-JQ1 once a day; 30 mg/kg (+)-JQ1 twice a day; and cytarabine 100 mg/kg daily (5 d on, 2 d off). Treatment of mice with cytarabine at 100 mg/kg resulted in significant weight loss at day 8 and, therefore, the dose needed to be decreased to 75

Solubility Information

Solubility	Ethanol: 45.7 mg/mL (100 mM), DMSO: 29.41 mg/mL (64.36 mM),Sonification is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.1882 mL	10.9412 mL	21.8823 mL
5 mM	0.4376 mL	2.1882 mL	4.3765 mL
10 mM	0.2188 mL	1.0941 mL	2.1882 mL
50 mM	0.0438 mL	0.2188 mL	0.4376 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.

Reference

Filippakopoulos P, et al. Selective inhibition of BET bromodomains. Nature. 2010 Dec 23;468(7327):1067-73.
Ding L, Chen X, Zhang W, et al.Canagliflozin primes antitumor immunity by triggering PD-L1 degradation in