Product Name: Bromodomain Inhibitor, (+)-JQ1

Chemical Properties

**Product Name:** Bromodomain Inhibitor, (+)-JQ1

**Cas No.:** 1268524-70-4  
**M.Wt:** 456.99  
**Formula:** C23H25ClN4O2S

**Chemical Name:** (S)-tert-butyl 2-(4-(4-chlorophenyl)-2,3,9-trimethyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepin-6-yl)acetate

**Canonical SMILES:** CC1=C(C)SC2=C1C(C3=CC=C(Cl)C=C3)=N[C@@H](CC(OC(C)(C)C)=O)C4=NN=C(C)N24

**Solubility:** >22.8mg/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.

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

Biological Activity

**Targets:** Bromodomain

**Pathways:** Chromatin/Epigenetics >> Bromodomain

**Description:**
Bromodomain Inhibitor, (+)-JQ1 is a potent and highly specific inhibitor for the BET (bromodomain and extra-terminal) family of bromodomains. (+)-JQ1 binds to BRD4 bromodomains 1 and 2 with Kd values of ~ 50 and 90 nM, respectively. The binding is competitive with acetyl lysine. (+)-JQ1 can be a useful chemical probe to investigate the role of BET
bromodomains in the transcriptional regulation of oncogenesis. JQ1 exhibited strong dose-and time-dependent inhibition of BRDT and could significantly diminish the activity of a close structural relative of BRDT. A close look at JQ1 bound BRDT confirmed that the acetyl-lysine recognition site of BRDT was blocked. [1] JQ1 does not produce sedative or anxiolytic effects and is instead a potent and selective inhibitor of the bromodomain testis-specific protein BRDT [2], which is essential for chromatin remodeling during spermatogenesis. By blocking BRDT, JQ1 effectively blocks the production of sperm in the testes and consequently produces effective contraception, without the negative side effects associated with previously researched hormonal contraceptives for men.

Reference:

Protocol

Cell experiment:

Cell lines
Human Leukemia OCI-AML3 (AML-M4 subtype, DNMT3A-R882, NPM1c-mutated, p53-wildtype) cell lines

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.

Reacting conditions
0.25 μM JQ1 for 24 h incubation

Applications
BRD4 bromodomain inhibitor JQ1 is highly active against human leukemia OCI-AML3 mutation lines such as nucleophosmin (NPM1) and DNA methyltransferase 3 (DNMT3A). JQ1 causes caspase 3/7-mediated apoptosis and DNA damage response in these cells. JQ1 prevented BRD4-mediated recruitment of p53 to chromatin targets following its activation in OCI-AML3 cells resulting in cell cycle arrest and apoptosis in a c-MYC-independent manner.

Animal experiment [3]:

Animal models
Male C57BL/6J (The Jackson Laboratory) and BALB/cJ (Charles River) mice, 6–8 wk of age

Dosage form
10% (w:v) JQ1 solution in 2-hydroxypropyl-β-cyclodextrin solvent (Sigma-Aldrich);
injected into the contralateral side of the abdomen

Applications

JQ1 ablated cytokine production and blunted the “cytokine storm” in endotoxemic mice by reducing levels of IL-6 and TNF-α while rescuing mice from LPS-induced death. JQ1 benefited hyper-inflammatory conditions associated with high levels of cytokine production.

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.

Reference:


Product Citations


Product Validation
ES cells were kept in 15% FBS media throughout the time course. Drug treatments were applied continuously at the designated concentrations for the entire duration of the time course, with daily media change. The effect of JQ1 is: a later suppression of MyoG expression.

(+)-JQ1 shows potent inhibition of H4Kac4 binding. The IC50 value of 10nM for murine BRDT(1) and 11 nM for human BRDT(1). On the other hand, the (-)-JQ1 enantiomer was inactive for either ortholog.