**Product Data Sheet**

**Chemical Properties**

- **Product Name:** (-)-JQ1
- **Cas No.:** 1268524-71-5
- **M.Wt:** 456.99
- **Formula:** C23H25ClN4O2S
- **Synonyms:** (-)-JQ1

- **Chemical Name:** (R)-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:** $\geq 22.8 \text{mg/mL in DMSO}$
- **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.
- **Shopping Condition:** Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request

**Biological Activity**

- **Targets:** Chromatin/Epigenetics
- **Pathways:** Bromodomain

**Description:**

(-)-JQ1 is the stereoisomer of JQ1, a cell-permeable small-molecule inhibitor of BET bromodomain that competitively binds to acetyl-lysine recognition motifs. JQ1 is a novel thieno-triazolo-1,4-diazepine with an appended and bulky t-butyl ester functional group at C6 position in its chemical structure, which allows for additional pendant group diversity and
mitigates binding to the central benzodiazepine receptor. JQ1 competitively binds to the bromodomain displacing the BRD4 fusion oncoprotein from chromatin, which induces squamous differentiation and specific anti-proliferative effect in BRD4-dependent cell lines and patient-derived xenograft models. However, study results have shown that (-)-JQ1 fails to significantly interact with any bromodomain tested and exhibits inhibition against BRD4(1) with 50% inhibition concentration IC50 value of 10,000 nM.

Reference:

Protocol

Cell experiment:

Cell lines BRD4-dependent NMC 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.
Reacting conditions 250 nM, 72 hours for proliferation inhibition 250 nM, 48 hours for cell-cycle arrest induction
Applications In BRD4-dependent NMC cells, differentiation is expectedly accompanied by growth arrest, as demonstrated by reduced Ki67 staining, sustained inhibition of proliferation and G1 cell-cycle arrest. The quantitative RT-PCR for RAD21 and RAN was performed. (-)-JQ1 enantiomer was an inactive control of (+)-JQ1. (+)-JQ1 potently decreased expression of both BRD4 target genes, whereas (-)-JQ1 had no effect.

Animal experiment [3]:

Animal models Female NCr nude mice bearing NMC 797 xenografts
Dosage form Intraperitoneal injection, 50 mg/kg, daily
Applications After 4 days of therapy, mice were evaluated by FDG-PET imaging. A marked reduction in FDG uptake was observed with JQ1 ((+)/(-)) treatment, whereas vehicle-treated mice demonstrated progressive
disease. Tumour-volume measurements confirmed a reduction in tumour growth with JQ1 treatment. JQ1 was well tolerated at this dose and schedule without overt signs of toxicity or weight loss.

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


Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.