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Print Date: Sep 12th 2017

Certificate of Analysis

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Product Name: **(+)-JQ1** **Catalog No.: 4499** **Batch No.: 8**

CAS Number: 1268524-70-4

IUPAC Name: (6*S*)-4-(4-Chlorophenyl)-2,3,9-trimethyl-6*H*-thieno[3,2-*f*][1,2,4]triazolo[4,3-*a*][1,4]diazepine-6-acetic acid 1,1-dimethylethyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{25}ClN_4O_2S.¼H_2O$

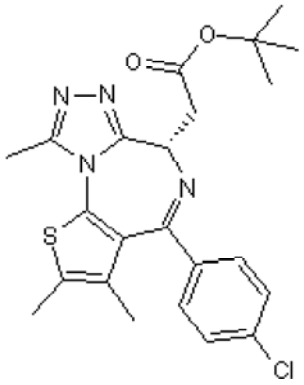
Batch Molecular Weight: 461.49

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.5% purity

Chiral HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +44.2 (Concentration = 0.5, Solvent = Chloroform)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.86	5.57	12.14
Found	59.56	5.64	12.11

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Product Information

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CAS Number: 1268524-70-4

IUPAC Name: (6*S*)-4-(4-Chlorophenyl)-2,3,9-trimethyl-6*H*-thieno[3,2-*f*][1,2,4]triazolo[4,3-*a*][1,4]diazepine-6-acetic acid 1,1-dimethylethyl ester

Description:

Potent, high affinity, selective BET bromodomain inhibitor (IC_{50} values are 17.7, 32.6, 76.9 and 12942 nM for BRD2 (N-terminal (N)), BRD4 (C-terminal (C)), BRD4 (N) and CREBBP respectively; K_d values are 49, 59.5, 82, 90.1, 128 and 190 nM for BRD4 (N), BRD3 (N), BRD3 (C), BRD4 (C), BRD2 (N) and BRDT (N) respectively). Induces squamous differentiation in NUT midline carcinoma (NMC) cell lines; inhibits tumor growth in NMC xenograft models in vivo. Exhibits reversible contraceptive effects in germ cells from male mice. Inactive analog (-)-JQ1 available.

Physical and Chemical Properties:

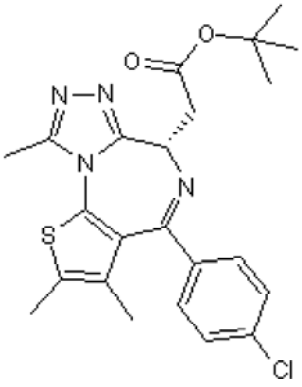
Batch Molecular Formula: $C_{23}H_{25}ClN_4O_2S.¼H_2O$

Batch Molecular Weight: 461.49

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the (+)-JQ1 probe summary on the SGC website.

References:

Herrmann *et al* (2012) Small-molecule inhibition of BRD4 as a new potent approach to eliminate leukemic stem- and progenitor cells in acute myeloid leukemia AML. Oncotarget. [Epub ahead of print] ***3*** 1588. PMID: 23249862.

Matzuk *et al* (2012) Small-molecule inhibition of BRDT for male contraception. Cell ***150*** 673. PMID: 22901802.

Filippakopoulos *et al* (2010) Selective inhibition of BET bromodomains. Nature ***468*** 1067. PMID: 20871596.

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