

Product Name: (-)-JQ1

Catalog No.: 5603

Batch No.: 1

CAS Number: 1268524-71-5

IUPAC Name: (6*R*)-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: C₂₃H₂₅ClN₄O₂S · ½H₂O

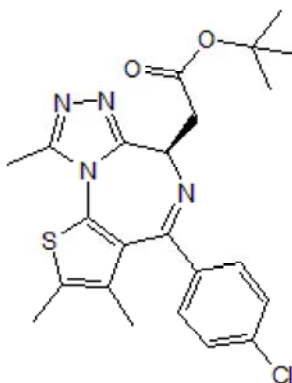
Batch Molecular Weight: 466

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.0% purity

Chiral HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.28	5.62	12.02
Found	59.25	5.5	11.75

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Description:

(-)-JQ1 is an inactive control for (+)-JQ1. Exhibits no significant interaction with BRD1-4 or a panel of other bromodomains. Active Enantiomer also available.

Physical and Chemical Properties:

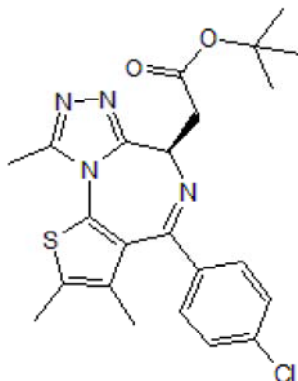
Batch Molecular Formula: C₂₃H₂₅ClN₄O₂S·½H₂O

Batch Molecular Weight: 466

Physical Appearance: Pale yellow 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 compound is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the (+)-JQ1 probe summary on the SGC website.

References:

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

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