Certificate of Analysis

Product Name: **(+)-JQ1 carboxylic acid** **Catalog No.: 6588** **Batch No.: 1**

CAS Number: 202592-23-2

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. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{17}ClN_4O_2S$

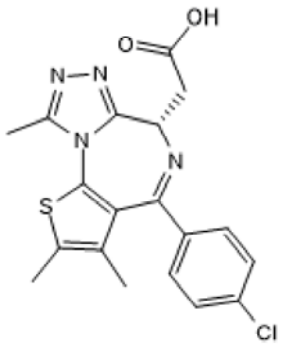
Batch Molecular Weight: 400.88

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.33 (Dichloromethane:Methanol [95:5])

HPLC: Shows 98.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.93	4.27	13.98
Found	56.63	4.36	13.8

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

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Description:

(+)-JQ1 carboxylic acid is a BET bromodomain inhibitor (+)-JQ1 (Cat. No. 4499) with a carboxylic acid functional group for conjugation reactions. Can be used as a precursor to PROTAC® Degraders that targets BET bromodomains after conjugation to a linker and E3 ligase ligand. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license.

Physical and Chemical Properties:

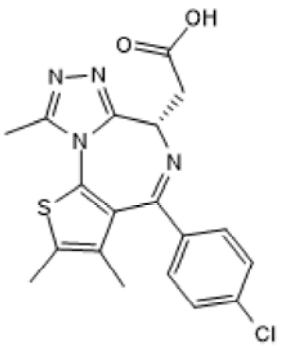
Batch Molecular Formula: $C_{19}H_{17}ClN_4O_2S$

Batch Molecular Weight: 400.88

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.

References:

Gadd *et al* (2017) Structural basis of PROTAC cooperative recognition for selective protein degradation. Nat.Chem.Biol. ***13*** 514. PMID: 28288108.

Winter *et al* (2015) DRUG DEVELOPMENT. Phthalimide conjugation as a strategy for in vivo target protein degradation. Science ***348*** 1376. PMID: 25999370.

Zengerle *et al* (2015) Selective small molecule induced degradation of the BET bromodomain protein BRD4. ACS Chem Biol. ***10*** 1770. PMID: 26035625.