

Product Name: (+)-JQ1 bump, acid functionalized

Catalog No.: 7689

Batch No.: 5

CAS Number: 2421153-77-5

IUPAC Name: (R)-2-((S)-4-(4-Chlorophenyl)-2,3,9-trimethyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepin-6-yl)butanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₁ClN₄O₂S·½H₂O

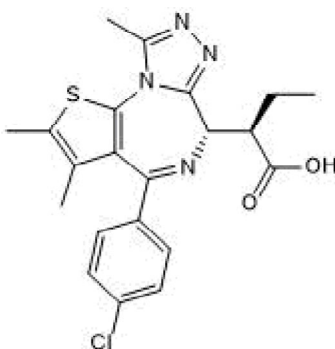
Batch Molecular Weight: 437.95

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.59	5.06	12.79
Found	56.95	5.02	12.7

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Description:

(+)-JQ1 bump, acid functionalized is a BET bromodomain binding analog of (+)-JQ1 (Cat. No. 4499) that selectively binds single point mutant form of Brd4 (Brd4^{BD2 L387A}). Functionalized with a carboxylic acid group to enable onward chemistry. The position of the carboxylic acid group represents an 'exit vector' allowing modification without interfering with compound binding ability.

Physical and Chemical Properties:

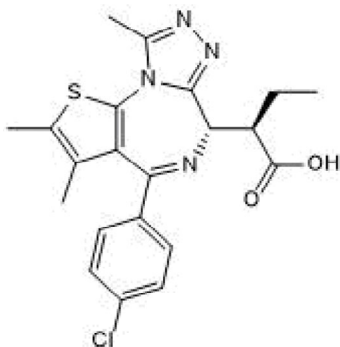
Batch Molecular Formula: C₂₁H₂₁ClN₄O₂S·½H₂O

Batch Molecular Weight: 437.95

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Bond et al (2021) Development of BromoTag: a 'Bump-and-Hole'-PROTAC system to induce potent, rapid, and selective degradation of tagged target proteins. *J.Med.Chem* **64** 15477. PMID: 34652918.

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