

Product Name: (+)-JQ1 PA

Catalog No.: 6589

Batch No.: 1

CAS Number: 2115701-93-2

IUPAC Name: (6S)-4-(4-Chlorophenyl)-2,3,9-trimethyl-N-2-propyn-1-yl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepine-6-acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₀ClN₅OS.½H₂O

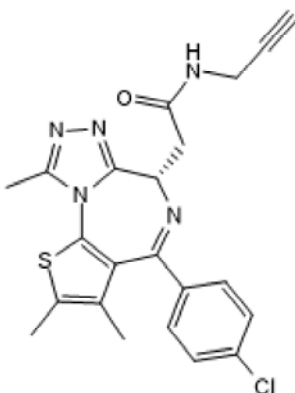
Batch Molecular Weight: 446.96

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 = 0.42 (5% MeOH/DCM)

HPLC: Shows 96.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.12	4.74	15.67
Found	58.94	4.74	15.81

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

(+)-JQ1 PA is a click-activated (alkyne) version of the BET bromodomain inhibitor (+)-JQ1 (Cat. No. 4499). Can be used as a precursor to a PROTAC® targeting BET bromodomains. Supplied with an alkyne functionalized handle for click conjugation to a linker/E3 ligase ligand. Can also be conjugated to fluorescent dyes for imaging applications. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license.

Physical and Chemical Properties:

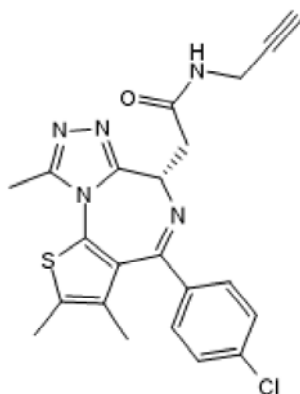
Batch Molecular Formula: C₂₂H₂₀ClN₅OS.½H₂O

Batch Molecular Weight: 446.96

Physical Appearance: White solid

Minimum Purity: ≥95%

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:

Tyler *et al* (2017) Click chemistry enables preclinical evaluation of targeted epigenetic therapies. *Science* **356** 1397. PMID: 28619718.

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