bio-techne
TOCRIS

Print Date: Oct 11th 2024

Certificate of Analysis

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Product Name: **AT 1** **Catalog No.: 6356** **Batch No.: 1**

CAS Number: 2098836-45-2

IUPAC Name: (2*S*,4*R*)-1-(2*R*)-2-Acetamido-3-[[6-[2-[(6*S*)-4-(4-chlorophenyl)-2,3,9-trimethyl-6*H*-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepin-6-yl]acetamido]hexyl]thio]-3-methylbutanoyl]-4-hydroxy-*N*-[4-(4-methylthiazol-5-yl)benzyl)pyrrolidinine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{48}H_{58}ClN_9O_5S_3.¼H_2O$

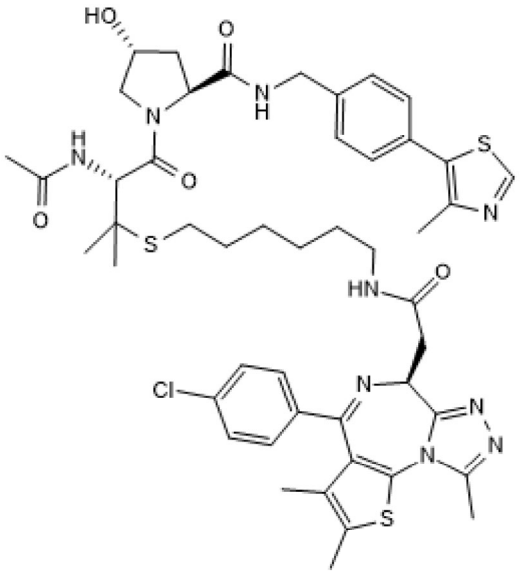
Batch Molecular Weight: 977.18

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 = 0.41 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59	6.03	12.9
Found	58.81	6.04	12.82

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:

AT 1 is a cell penetrant Proteolysis Targeting Chimera (PROTAC®) compound based on (+)-JQ1 (Cat. No. 4499) conjugated to a von Hippel-Lindau (VHL) ligand. Rationally designed based on a ternary complex crystal structure to improve selectivity for BRD4 degradation compared to MZ1 (Cat. No. 6154). Demonstrates profound and selective degradation of BRD4 in cells at 1-3 µM, with negligible loss of BRD2 and BRD3. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license

Physical and Chemical Properties:

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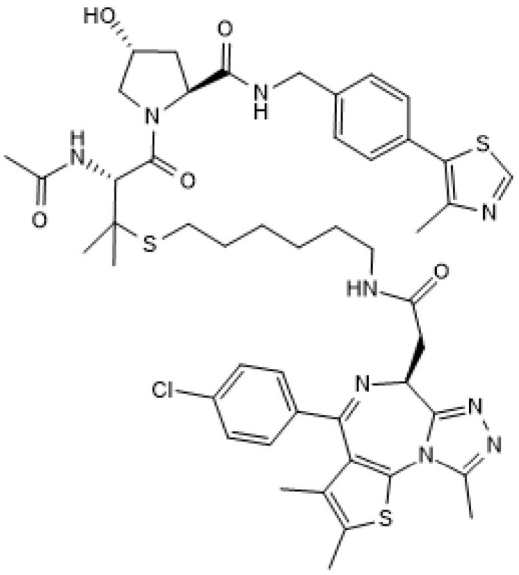
Minimum Purity: ≥98%

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. *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.

Licensing Information:

Sold under licence from the University of Dundee

References:

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