

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]pyrrolidine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₄₈H₅₈ClN₉O₅S₃·½H₂O

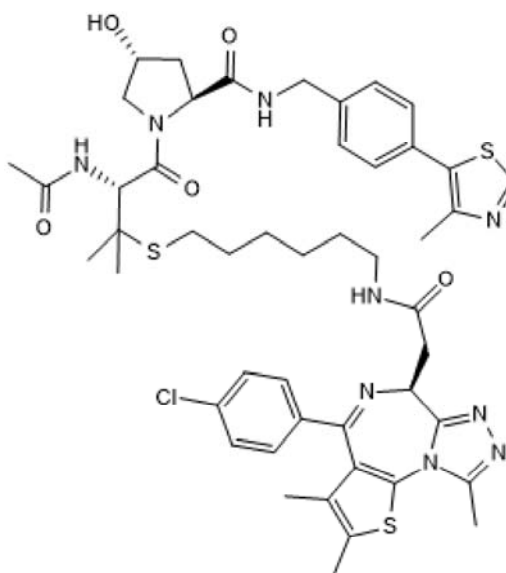
Batch Molecular Weight: 977.18

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

¹H 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

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

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Description:

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. PROTACs are bi-functional small molecules that harness the ubiquitin/proteasome system (UPS) to selectively and catalytically remove target proteins from cells.

Physical and Chemical Properties:

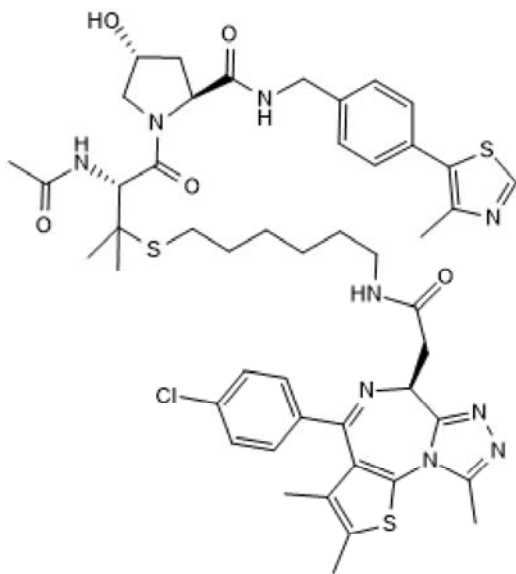
Batch Molecular Formula: C₄₈H₅₈ClN₉O₅S₃·½H₂O

Batch Molecular Weight: 977.18

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

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

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:

Sold under licence from the University of Dundee

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