

**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:** C<sub>48</sub>H<sub>58</sub>ClN<sub>9</sub>O<sub>5</sub>S<sub>3</sub>·½H<sub>2</sub>O

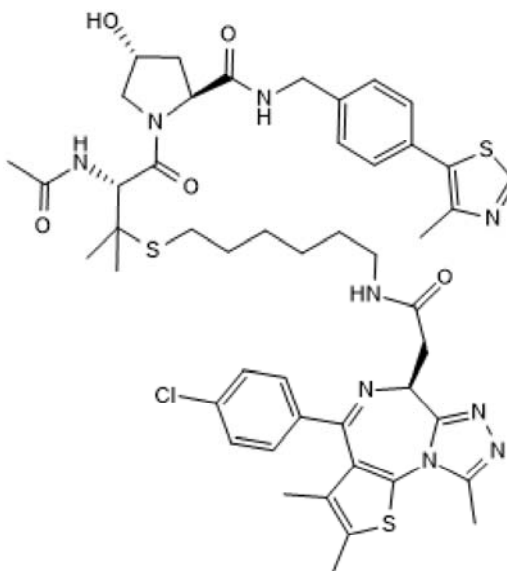
**Batch Molecular Weight:** 977.18

**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<sub>f</sub> = 0.41 (Dichloromethane:Methanol [9:1])

**HPLC:** Shows 98.5% purity

**<sup>1</sup>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

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**Description:**

AT 1 is a cell penetrant Proteolysis Targeting Chimera (PROTAC<sup>®</sup>) 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<sup>®</sup> is a registered trademark of Arvinas Operations, Inc., and is used under license

**Physical and Chemical Properties:**

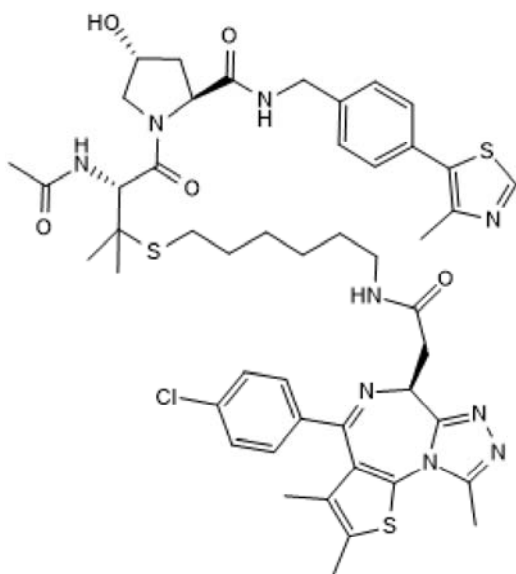
Batch Molecular Formula: C<sub>48</sub>H<sub>58</sub>ClN<sub>9</sub>O<sub>5</sub>S<sub>3</sub>·¼H<sub>2</sub>O

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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