Product Name: MZ 1
Catalog No.: 6154
Batch No.: 3
CAS Number: 1797406-69-9
IUPAC Name: (2S,4R)-1-((S)-2-(tert-butyl)-17-((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)-4,16-dioxo-6,9,12-trioxo-3,15-diazaheptadecanoyl)- 4-hydroxy-N-(4-(4-methylthiazol-5-yl)benzyl) pyrrolidine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{49}H_{60}ClN_{9}O_{8}S_{2}.H_{2}O
Batch Molecular Weight: 1020.66
Physical Appearance: White solid
Solubility:
- DMSO to 100 mM
- ethanol to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:

![Molecular Structure Image]

2. ANALYTICAL DATA

TLC: R_{f} = 0.38 (Dichloromethane:Methanol [95:5])
HPLC: Shows 98.1% purity
{^{1}H} NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>57.66</td>
<td>57.33</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.12</td>
<td>5.92</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>12.35</td>
<td>12.27</td>
</tr>
</tbody>
</table>

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

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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. Retains high affinity for BRD2, BRD3 and BRD4 bromodomains (Kd = 13-60 nM) but induces preferential degradation of BRD4 over BRD2 and BRD3 (DC50 values for degradation of BRD4 are 8 and 23 nM in H661 and H838 cells, respectively). Exhibits potent cytotoxicity and antiproliferative effects in AML cell lines (pEC50 = 7.6 in Mv4-11 cells). Negative control cis MZ 1 also available.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C54H60ClN9O9S2.H2O
- **Batch Molecular Weight:** 1020.66
- **Physical Appearance:** White solid
- **Minimum Purity:** >98%
- **Batch Molecular Structure:**

```
\[\text{Structure image}\]
```

**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

**References:**