

Product Name: MZ 1

Catalog No.: 6154

Batch No.: 3

CAS Number: 1797406-69-9

IUPAC Name: (2*S*,4*R*)-1-((*S*)-2-(*tert*-butyl)-17-((*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)-4,16-dioxo-6,9,12-trioxa-3,15-diazaheptadecanoyl)-4-hydroxy-*N*-(4-(4-methylthiazol-5-yl)benzyl)pyrrolidine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₄₉H₆₀ClN₉O₈S₂.H₂O

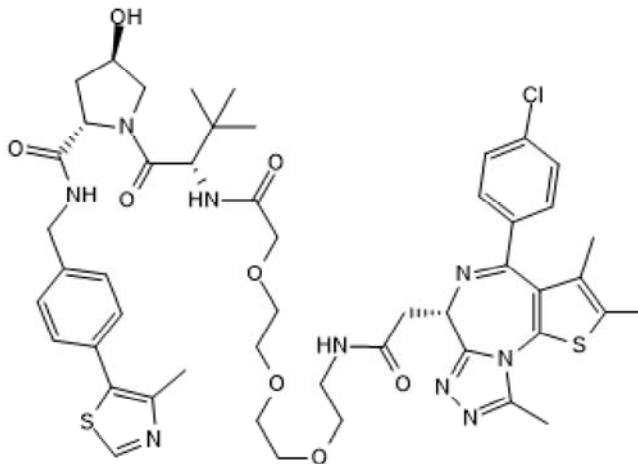
Batch Molecular Weight: 1020.66

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.38 (Dichloromethane:Methanol [95:5])

HPLC: Shows 98.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.66	6.12	12.35
Found	57.33	5.92	12.27

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

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

Product Name: MZ 1

Catalog No.: 6154

Batch No.: 3

CAS Number: 1797406-69-9

IUPAC Name: (2*S*,4*R*)-1-((*S*)-2-(tert-butyl)-17-((*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)-4,16-dioxo-6,9,12-trioxa-3,15-diazaheptadecanoyl)-4-hydroxy-*N*-(4-(4-methylthiazol-5-yl)benzyl)pyrrolidine-2-carboxamide

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 ($K_d = 13-60$ 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. PROTAC[®] is a registered trademark of Arvinas Operations, Inc., and is used under license. Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:

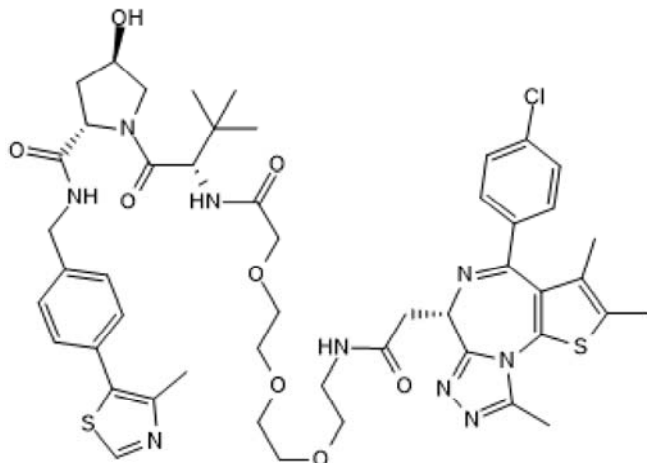
Batch Molecular Formula: C₄₉H₆₀ClN₉O₈S₂.H₂O

Batch Molecular Weight: 1020.66

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

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

Wurz *et al* (2017) A "click chemistry platform" for the rapid synthesis of bispecific molecules for inducing protein degradation. *J.Med.Chem.* PMID: 28378579.

Zengerle *et al* (2015) Selective small molecule induced degradation of the BET bromodomain protein BRD4. *ACS.Chem.Biol.* **10** 1770. PMID: 26035625.

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

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

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