

# Certificate of Analysis

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**Product Name:** JPS016

**Catalog No.:** 8083

**Batch No.:** 1

**CAS Number:** 2669785-77-5

**IUPAC Name:** (2*S*,4*R*)-1-((*S*)-2-(2-((9-(2-((4-((2-Aminophenyl)carbamoyl)phenyl)amino)-2-oxoethoxy)nonyl)oxy)acetamido)-3,3-dimethylbutanoyl)-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>63</sub>N<sub>7</sub>O<sub>8</sub>S.½H<sub>2</sub>O

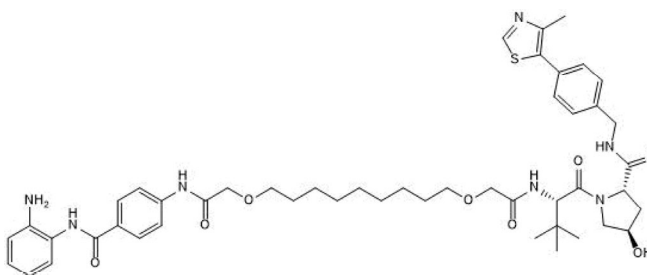
**Batch Molecular Weight:** 907.14

**Physical Appearance:** Off White solid

**Solubility:** DMSO to 10 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 97.8% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	63.55	7.11	10.81
Found	62.8	7.08	10.6

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**Description:**

JSP016 is a selective Degradator (PROTAC®) and inhibitor of class I HDACs (DC<sub>50</sub> values are 530 nM and 550 nM for HDAC3 and HDAC1; D<sub>max</sub> is 77%, 66% and 45% at HDAC1, 3 and 2; IC<sub>50</sub> values are 380 nM, 570 nM and 820 nM at HDAC3, 1 and 2). Comprises a benzamide-based compound joined by a linker to a Von Hippel Lindau (VHL) E3 ligase ligand. JPS016 treatment up- or down-regulates nearly 4000 differentially expressed genes, arrests cells at sub-G<sub>1</sub> phase and promotes apoptosis in HCT116 cells. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license. Please see product specific page on [www.tocris.com](http://www.tocris.com) for full description.

**Physical and Chemical Properties:**

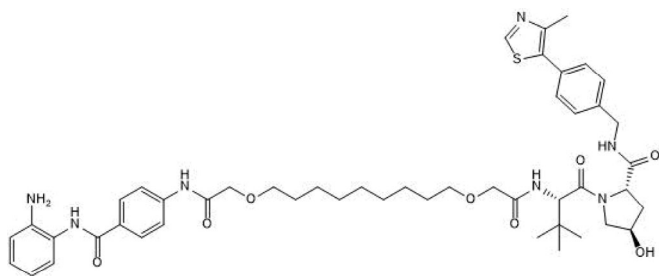
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Batch Molecular Weight: 907.14

Physical Appearance: Off White solid

**Minimum Purity:** ≥97%

**Batch Molecular Structure:**



**References:**

**Smalley et al** (2022) Optimization of class I histone deacetylase PROTACs reveals that HDAC1/2 degradation is critical to induce apoptosis and cell arrest in cancer cells. *J.Med.Chem.* **65** 5642. PMID: 35293758.

**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 10 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 license from the University of Leicester

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