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Certificate of Analysis

www.tocris.com

Product Name: JPS036

Catalog No.: 8085 Batch No.: 1

CAS Number: 2669785-85-5

IUPAC Name:

(2S,4R)-N-[2-[[12-[[4-[(2-Aminophenyl)carbamoyl]phenyl]amino]-12-oxododecyl]oxy]-4-(4-methylthiazol-5-yl)benzyl]-1-[(S)-2-(1-fluorocyclopropan-1-ylcarbonylamino)-3,3-dimethylbutanoyl]-4-hydroxypyrrolidine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: C₅₁H₆₆FN₇O₇S.2H₂O 976.22 White to off-white solid DMSO to 20 mM with gentle warming Store at -20°C

NH

2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

Shows 98.8% purity Consistent with structure Consistent with structure

	Carbon Hydrogen Nitrogen				
Theoretical	62.75	7.23	10.04		
Found	61.91	7.04	9.86		

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

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Description:

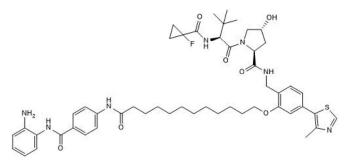
JPS036 is a selective HDAC3 Degrader (PROTAC®) (DC₅₀ = 440 nM; Dmax = 77 %). JPS036 comprises a benzamide-based compound joined by a linker to a Von Hippel Lindau (VHL) E3 ligase ligand. Negative control JPS016NC also available. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{51}H_{66}FN_7O_7S.2H_2O$ Batch Molecular Weight: 976.22 Physical Appearance: White to off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 mM with gentle warming

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a $45-60^{\circ}C$ 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

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.

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