

Product Name: MPD 2

Catalog No.: 8802

Batch No.: 1

IUPAC Name: 3-((6-((2-(2,6-Dioxopiperidin-3-yl)-1,3-dioxoisindolin-4-yl)oxy)hexyl)oxy)benzyl ((2S,3R)-3-(*tert*-butoxy)-1-(((S)-3-cyclohexyl-1-oxo-1-(((S)-1-oxo-3-((S)-2-oxopyrrolidin-3-yl)propan-2-yl)amino)propan-2-yl)amino)-1-oxobutan-2-yl) carbamate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₅₁H₆₈N₆O₁₃·¼H₂O

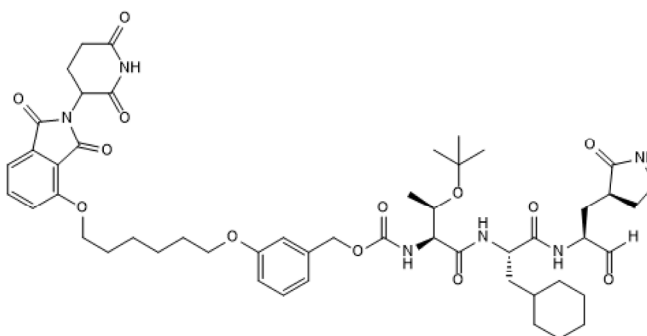
Batch Molecular Weight: 977.63

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	62.66	7.06	8.6
Found	61.73	7.1	8.48

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Description:

MPD 2 is a SARS-CoV-2 M^{pro} Degradator (PROTAC®) (DC₅₀ = 296 nM in 293T cells). M^{pro} degradation is time-dependent and CRBN-mediated. Antiviral in A549-ACE2 cells infected with several SARS-CoV-2 strains (EC₅₀ = 492 nM at delta variant) and against a nirmatrelvir-resistant mutant of SARS-CoV-2, NSP5 E166A (EC₅₀ = 460 nM).

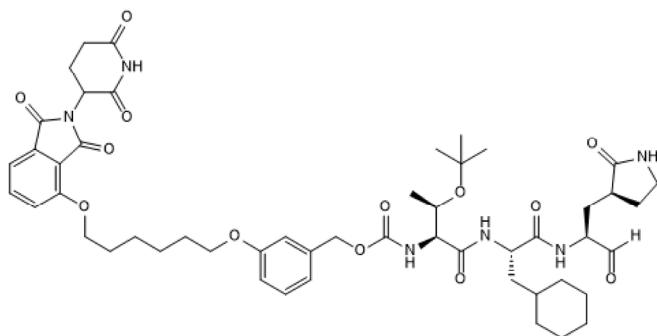
Physical and Chemical Properties:

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References:

Alugubelli *et al* (2024) Discovery of first-in-class PROTAC Degradators of SARS-CoV-2 main protease. *J.Med.Chem.* **67** 6495. PMID: 38608245.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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. *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.

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