

**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:** C<sub>51</sub>H<sub>68</sub>N<sub>6</sub>O<sub>13</sub>·¼H<sub>2</sub>O

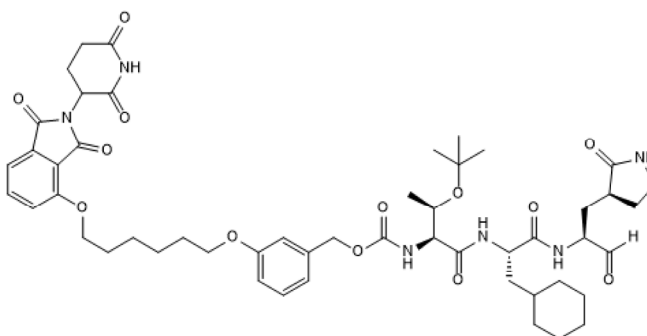
**Batch Molecular Weight:** 977.63

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**<sup>1</sup>H 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<sup>pro</sup> Degradator (PROTAC<sup>®</sup>) (DC<sub>50</sub> = 296 nM in 293T cells). M<sup>pro</sup> degradation is time-dependent and CRBN-mediated. Antiviral in A549-ACE2 cells infected with several SARS-CoV-2 strains (EC<sub>50</sub> = 492 nM at delta variant) and against a nirmatrelvir-resistant mutant of SARS-CoV-2, NSP5 E166A (EC<sub>50</sub> = 460 nM). PROTAC<sup>®</sup> is a registered trademark of Arvinas Operations, Inc., and is used under license.

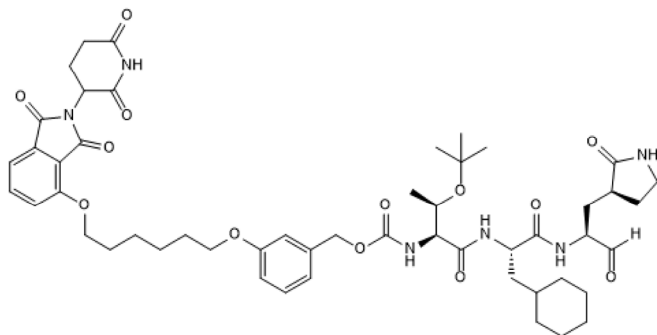
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**References:**

**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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