

Product Name: XY-06-007

Catalog No.: 7669

Batch No.: 1

CAS Number: 2757045-94-4

IUPAC Name: (2*R*)-2-((*S*)-6-(4-Chlorophenyl)-8-methoxy-1-methyl-4*H*-benzo[*f*][1,2,4]triazolo[4,3-*a*][1,4]diazepin-4-yl)-*N*-(5-(2-((2-(2,6-dioxopiperidin-3-yl)-1,3-dioxoisindolin-4-yl)oxy)acetamido)pentyl)propanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₄₁H₄₁ClN₈O₈·1¼H₂O

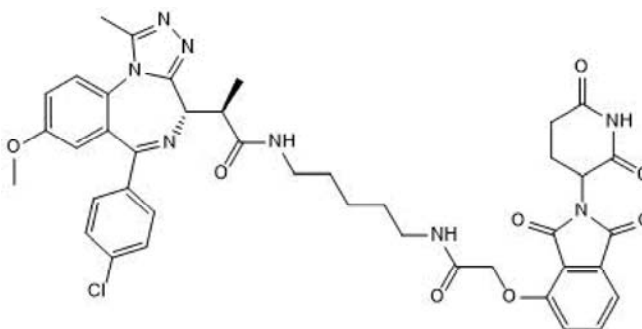
Batch Molecular Weight: 831.8

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.2	5.27	13.47
Found	59.03	5.16	13.37

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Description:

XY-06-007 is a highly selective and potent "Bump & Hole" TAG Degradator ($DC_{50,6h} = 10$ nM, $T_{1/2} < 43.2$ min). XY-06-007 comprises a cereblon (CRBN) E3 ligase ligand joined by a linker to a (+)-JQ1 (Cat. No. 4499) derivative (the "bump" bearer) that selectively binds the Brd4^{BD1 L94V} variant (the "hole"). In cell lines expressing a fusion of the target protein with the tag, Brd4^{BD1 L94V}, XY-06-007 drives formation of a ternary complex between CRBN and the tagged protein, leading to ubiquitination and subsequent proteasomal degradation of the entire protein. XY-06-007 is highly selective for Brd4^{BD1 L94V} over wi... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

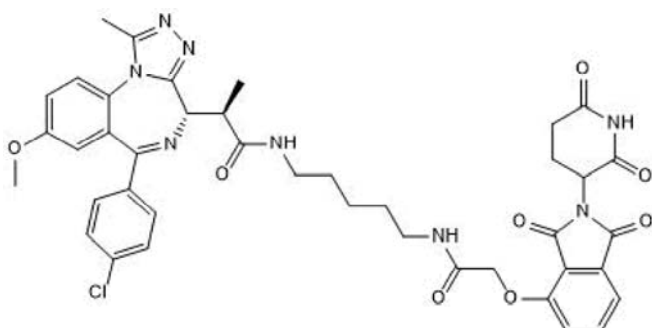
Batch Molecular Formula: C₄₁H₄₁ClN₈O₈·1¼H₂O

Batch Molecular Weight: 831.8

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Nowak et al (2021) Structure-guided design of a "Bump-and-Hole" Bromodomain-based degradation tag. *J.Med.Chem.* **64** 11637. PMID: 34279939.

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. 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 license from Dana-Farber Cancer Institute

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