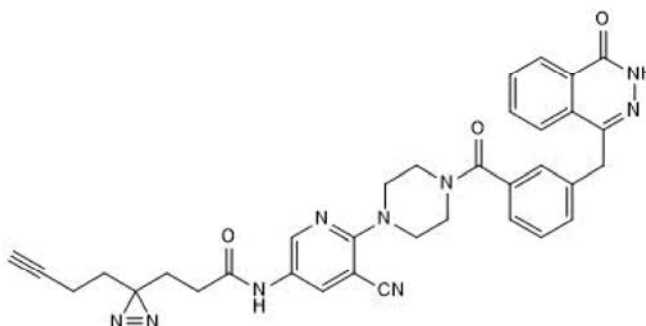


Product Name: PARPYnD **Catalog No.:** 7410 **Batch No.:** 1
CAS Number: 2561483-27-8
IUPAC Name: 3-(3-Butyn-1-yl)-N-[5-cyano-6-[4-[3-[(3,4-dihydro-4-oxo-1-phthalaziny)methyl]benzoyl]-1-piperaziny]-3-pyridiny]-3H-diazirine-3-propanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₄H₃₁N₉O₃·1/4H₂O
Batch Molecular Weight: 618.18
Physical Appearance: Beige solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 96.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.06	5.14	20.39
Found	66.01	5.2	20.39

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Description:

PARPYnD is a potent photoaffinity probe for poly(ADP-ribose) polymerase (PARP) (IC₅₀ values for PARP2, PARP1 and PARP6 are 6, 38 and 230 nM, respectively). PARPYnD labels PARP1 and PARP2 in the cell when an N3 functionalized fluorescent probe is attached and can inhibit isolated PARP6.

Physical and Chemical Properties:

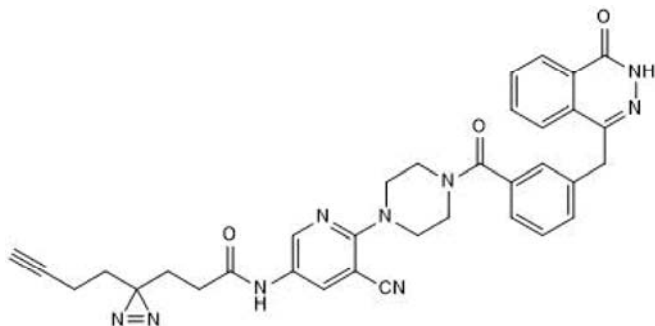
Batch Molecular Formula: C₃₄H₃₁N₉O₃·1/4H₂O

Batch Molecular Weight: 618.18

Physical Appearance: Beige solid

Minimum Purity: ≥95%

Batch Molecular Structure:



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.

References:

Howard *et al* (2020) Structure-guided design and in-cell target profiling of a cell-active target engagement probe for PARP inhibitors. ACS Chem.Biol. **15** 325. PMID: 32017532.

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