Certificate of Analysis

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-phthalazinyl)methyl]benzoyl]-1-piperazinyl]-3-pyridinyl]-3*H*-diazirine-3-propanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{34}H_{31}N_9O_3.¼H_2O$

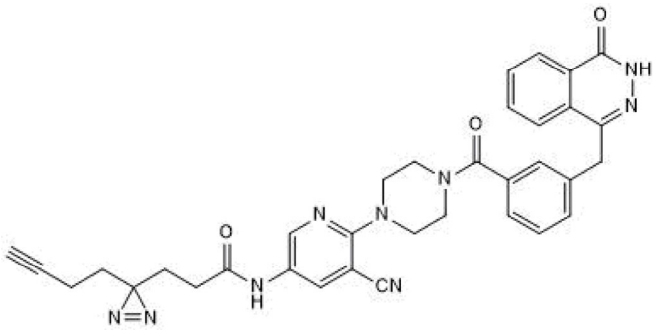
Batch Molecular Weight: 618.18

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

^{1}H 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 (AfBP) for poly(ADP-ribose) polymerase (PARP) (IC_{50} values for PARP2, PARP1 and PARP6 are 6, 38 and 230 nM, respectively). Can be used to fluorescently label PARP1 and PARP2 in cells when an azide functionalized probe is attached via copper catalysed click-chemistry. PARPYnD enriches recombinant PARP6 spiked into cellular lysates and inhibits PARP6 in cell-free assays; does not label PARP6 in intact cells. Photocrosslinking can be performed by irradiating at 365 nm.

Physical and Chemical Properties:

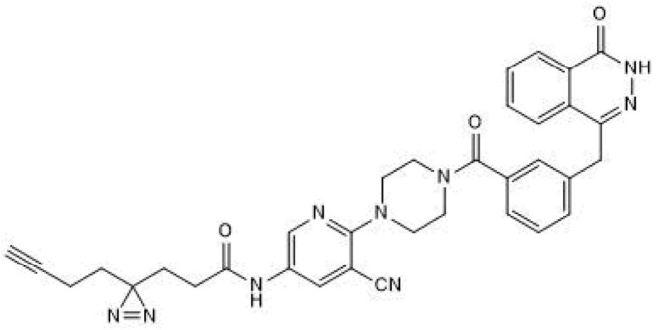
Batch Molecular Formula: $C_{34}H_{31}N_9O_3.¼H_2O$

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. *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.

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.