

**Product Name:** PDD 00017273

**Catalog No.:** 5952

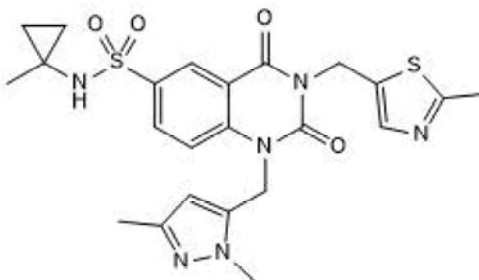
**Batch No.:** 2

CAS Number: 1945950-21-9

IUPAC Name: 1-[(1,3-Dimethyl-1*H*-pyrazol-5-yl)methyl]-1,2,3,4-tetrahydro-*N*-(1-methylcyclopropyl)-3-[(2-methyl-5-thiazolyl)methyl]-2,4-dioxo-6-quinazolinesulfonamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>23</sub>H<sub>26</sub>N<sub>6</sub>O<sub>4</sub>S<sub>2</sub>  
**Batch Molecular Weight:** 514.62  
**Physical Appearance:** Off White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.15 (Ethyl acetate)  
**HPLC:** Shows 99% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	53.68	5.09	16.33
Found	53.39	5.16	16.1

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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**Description:**

Potent and selective poly (ADP ribose) glycohydrolase (PARG) inhibitor (IC<sub>50</sub> = 26 nM). Exhibits >350-fold selectivity for PARG over a panel of ion channels, enzymes and receptors, including PARP1 and ARH3. Maintains PAR chains and induces DNA double-stranded breaks in cells following DNA damage. Decreases colony formation of ZR-75-1 BRCA1 WT cells and inhibits cancer cell survival. Cell permeable.

**Physical and Chemical Properties:**

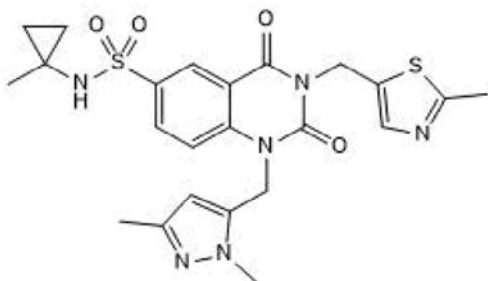
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Batch Molecular Weight: 514.62

Physical Appearance: Off White solid

**Minimum Purity:** ≥98%

**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:**

**Houl et al** (2019) Selective small molecule PARG inhibitor causes replication fork stalling and cancer cell death. *Nat.Commun.* **10** 5654. PMID: 31827085.

**Gravells et al** (2017) Specific killing of DNA damage-response deficient cells with inhibitor of poly(ADP-ribose) glycohydrolase. *DNA Repair* **52** 81. PMID: 28254358.

**James et al** (2016) First-in-class chemical probes against poly(ADP-ribose) glycohydrolase (PARG) inhibit DNA repair with differential pharmacology to Olaparib. *ACS Chem.Biol.* **11** 3179. PMID: 27689388.

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