TOCRIS
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Print Date: Feb 23rd 2023

Certificate of Analysis

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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: $C_{23}H_{26}N_6O_4S_2$

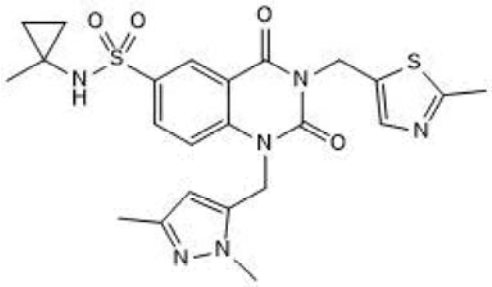
Batch Molecular Weight: 514.62

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.15 (Ethyl acetate)

HPLC: Shows 99.0% purity

^{1}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

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Description:

PDD 00017273 is a potent and selective poly (ADP ribose) glycohydrolase (PARG) inhibitor (IC_{50} = 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:

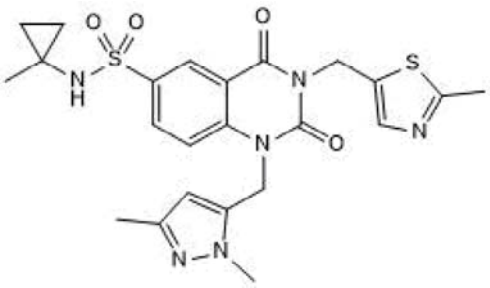
Batch Molecular Formula: $C_{23}H_{26}N_6O_4S_2$

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

When purchased as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Kliza (2021) Reading ADP-ribosylation signaling using chemical biology and interaction proteomics. Mol. Cell ***81*** 4552. PMID: 34551281.

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.