

**Product Name:** PDD 00031705

**Catalog No.:** 7009

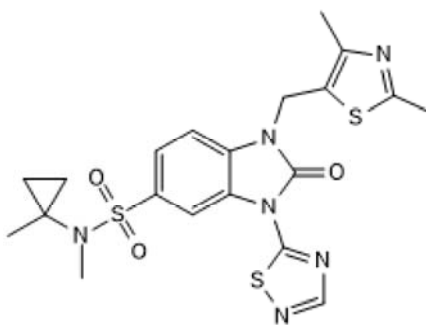
**Batch No.:** 1

CAS Number: 2032096-45-8

IUPAC Name: 1-[(2,4-Dimethyl-5-thiazolyl)methyl]-2,3-dihydro-*N*-methyl-*N*-(1-methylcyclopropyl)-2-oxo-3-(1,2,4-thiadiazol-5-yl)-1*H*-benzimidazole-5-sulfonamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>20</sub>H<sub>22</sub>N<sub>6</sub>O<sub>3</sub>S<sub>3</sub>  
**Batch Molecular Weight:** 490.62  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 10 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 97.9% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	48.96	4.52	17.13
Found	49.08	4.53	17.05

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

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IUPAC Name:	1-[(2,4-Dimethyl-5-thiazolyl)methyl]-2,3-dihydro- <i>N</i> -methyl- <i>N</i> -(1-methylcyclopropyl)-2-oxo-3-(1,2,4-thiadiazol-5-yl)-1 <i>H</i> -benzimidazole-5-sulfonamide			

**Description:**

PDD 00031705 is a negative control for PDD 00017238 (Cat. No. 7007).

**Physical and Chemical Properties:**

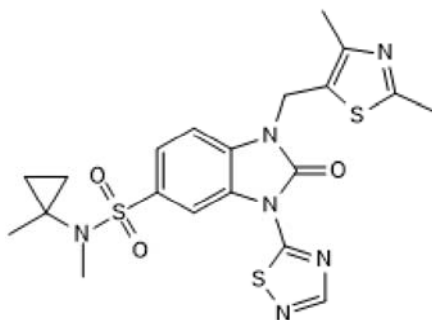
Batch Molecular Formula: C<sub>20</sub>H<sub>22</sub>N<sub>6</sub>O<sub>3</sub>S<sub>3</sub>

Batch Molecular Weight: 490.62

Physical Appearance: White solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 10 mM

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:**

**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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