

**Product Name:** ME 0328

**Catalog No.:** 5054

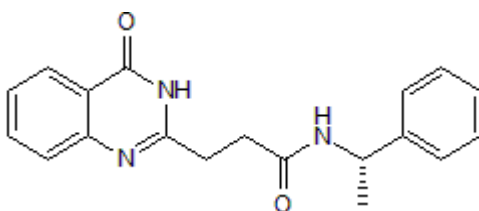
**Batch No.:** 1

CAS Number: 1445251-22-8

IUPAC Name: 3,4-Dihydro-4-oxo-3,4-Dihydro-4-oxo-N-[(1S)-1-phenylethyl]-2-quinazolinepropanamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>19</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub>  
**Batch Molecular Weight:** 321.37  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.6 (Chloroform:Methanol [9:1])  
**HPLC:** Shows 99.6% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = -37.8 (Concentration = 0.65, Solvent = DMSO)  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	71.01	5.96	13.08
Found	70.83	5.94	13.03

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

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**Description:**

Inhibitor of PARP-3 ( $IC_{50} = 0.89 \mu M$ ). Displays selectivity for PARP-3 over PARP-1, PARP-2 and other ARDT enzymes ( $IC_{50}$  values are 6.3, 10.8 and  $>30 \mu M$  respectively). Enhances CRISPR-Cas9-mediated HER2 mutation frequency, resulting in increased reduction in proliferation of HER2-positive breast cancer cells. Cell permeable.

**Physical and Chemical Properties:**

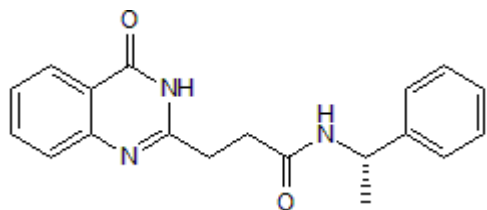
Batch Molecular Formula:  $C_{19}H_{19}N_3O_2$

Batch Molecular Weight: 321.37

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Wang and Sun** (2016) CRISPR-mediated targeting of HER2 inhibits cell proliferation through a dominant negative mutation. *Cancer Lett.* PMID: 27815036.

**Lindgren et al** (2013) PARP inhibitor with selectivity toward ADP-ribosyltransferase ARTD3/PARP3. *ACS Chem.Biol.* **8** 1698. PMID: 23742272.

**Storage:** Store at +4°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.

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