

**Product Name:** AZ 20

**Catalog No.:** 5198

**Batch No.:** 1

CAS Number: 1233339-22-4

IUPAC Name: 4-[4-[(3*R*)-3-Methyl-4-morpholinyl]-6-[1-(methylsulfonyl)cyclopropyl]-2-pyrimidinyl]-1*H*-indole

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>21</sub>H<sub>24</sub>N<sub>4</sub>O<sub>3</sub>S.¼H<sub>2</sub>O

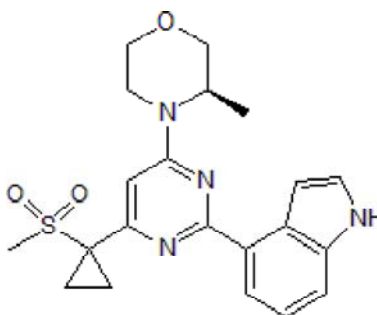
**Batch Molecular Weight:** 417.01

**Physical Appearance:** Off White solid

**Solubility:** DMSO to 50 mM  
ethanol to 10 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.2% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	60.49	5.92	13.44
Found	60.21	5.81	13.26

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

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**Description:**

Potent and selective ATR kinase inhibitor ( $IC_{50} = 5$  nM). Exhibits 7.6-fold selectivity over mTOR and selectivity over a panel of 442 kinases, including ATM kinase, PI3-K isoforms, and DNA-PK. Inhibits cell growth in cell lines with high baseline levels of replication stress. Displays antitumor effects in vivo.

**Physical and Chemical Properties:**

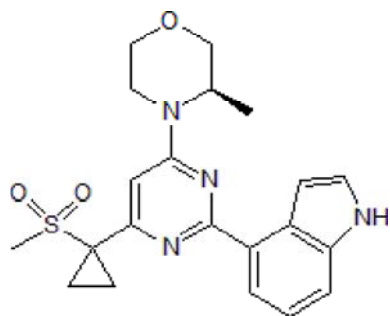
Batch Molecular Formula:  $C_{21}H_{24}N_4O_3S \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 417.01

Physical Appearance: Off White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 50 mM  
ethanol to 10 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.

**Licensing Information:**

Sold for research purposes under agreement from AstraZeneca

**References:**

Foot et al (2013) Discovery of 4-[4-[(3R)-3-Methylmorpholin-4-yl]-6-[1-(methylsulfonyl)cyclopropyl]pyrimidin-2-yl]-1H-indole (AZ20): a potent and selective inhibitor of ATR protein kinase with monotherapy in vivo antitumor activity. *J. Med. Chem.* **56** 2125. PMID: 23394205.

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