

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: C₂₁H₂₄N₄O₃S·¼H₂O

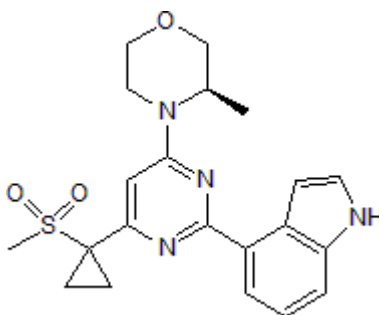
Batch Molecular Weight: 417.01

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 99.8% purity

¹H 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 (IC₅₀ = 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:

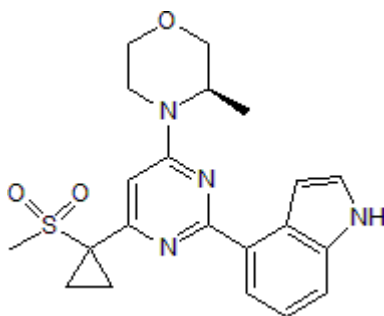
Batch Molecular Formula: C₂₁H₂₄N₄O₃S.¼H₂O

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.

References:

Foote 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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