

Product Name: APY 29

Catalog No.: 4865

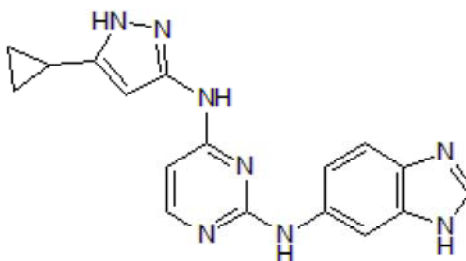
Batch No.: 2

CAS Number: 1216665-49-4

IUPAC Name: *N*²-1*H*-Benzimidazol-6-yl-*N*⁴-(5-cyclopropyl-1*H*-pyrazol-3-yl)-2,4-pyrimidinediamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₆N₈.H₂O
Batch Molecular Weight: 350.38
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 1eq. HCl to 50 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (10%MeOH/DCM+3drops of ammonia)
HPLC: Shows >98% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.28	5.18	31.98
Found	58.54	4.93	31.87

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

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Description:

Allosteric modulator of IRE1α. Inhibits IRE1α autophosphorylation (IC₅₀ = 280 nM) and activates IRE1α ribonuclease activity.

Physical and Chemical Properties:

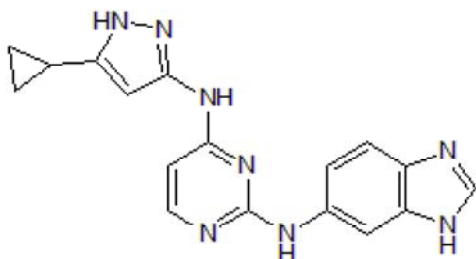
Batch Molecular Formula: C₁₇H₁₆N₈.H₂O

Batch Molecular Weight: 350.38

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Wang *et al* (2012) Divergent allosteric control of the IRE1a endoribonuclease using kinase inhibitors. *Nat.Chem.Biol.* **8** 982. PMID: 23086298.

Korennykh *et al* (2009) The unfolded protein response signals through high-order assembly of Ire1. *Nature* **457** 687. PMID: 19079236.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

1eq. HCl to 50 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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