

Product Name: Ibrutinib

Catalog No.: 6813

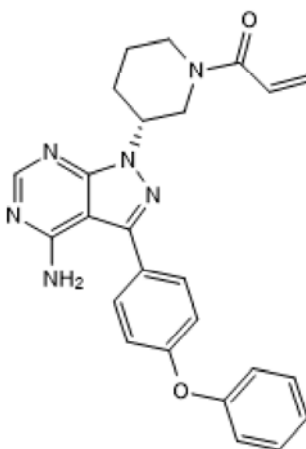
Batch No.: 2

CAS Number: 936563-96-1

IUPAC Name: 1-[(3*R*)-3-[4-Amino-3-(4-phenoxyphenyl)-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl]-1-piperidiny]-2-propen-1-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₄N₆O₂
Batch Molecular Weight: 440.5
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity
Chiral HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 68.17 | 5.49 | 19.08 |
| Found | 68.01 | 5.42 | 19 |

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

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Description:

Ibrutinib is a potent and selective BTK inhibitor (IC₅₀ = 0.5 nM). Selective for BTK against a screening panel of kinase enzymes. Inhibits autophosphorylation of BTK, phosphorylation of PLCγ, and phosphorylation of ERK (IC₅₀ of 11 nM, 29 nM and 13 nM, respectively). Also inhibits ErbB4 (IC₅₀ = 0.25-3.4 nM). Induces cytotoxicity of chronic lymphocytic leukemia (CLL) cells. Reduces clinical arthritis scores in a mouse model.

Physical and Chemical Properties:

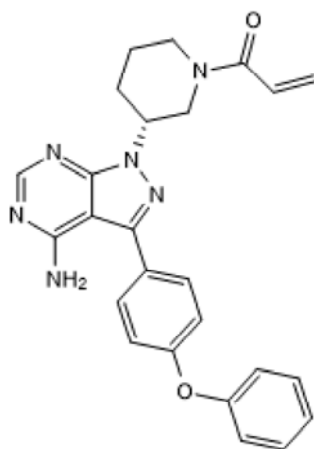
Batch Molecular Formula: C₂₅H₂₄N₆O₂

Batch Molecular Weight: 440.5

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°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.

References:

Estupiñán *et al* (2021) Comparative analysis of BTK inhibitors and mechanisms underlying adverse effects. *Front.Cell Dev.Biol.* **9** 630942. PMID: 33777941.

Honigberg *et al* (2010) The Bruton tyrosine kinase inhibitor PCI-32765 blocks B-cell activation and is efficacious in models of autoimmune disease and B-cell malignancy. *Proc.Natl.Acad.Sci.USA* **107** 13075. PMID: 20615965 .

Pan *et al* (2007) Discovery of selective irreversible inhibitors for Bruton's tyrosine kinase. *Chem.Med.Chem.* **2** 58. PMID: 17154430.

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