

# Ibrutinib

SYN-1171

(R)-1-(3-(4-amino-3-(4-phenoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl)piperidin-1-yl)prop-2-en-1-one

CAS Registry No.: 936563-96-1

**Smiles String:**

C=CC(=O)N1CCC[C@H](C1)N2C3=NC=N(C=C3C(=N2)C4=CC=C(C=C4)OC5=CC=CC=C5)N

Molecular Weight: 440.5

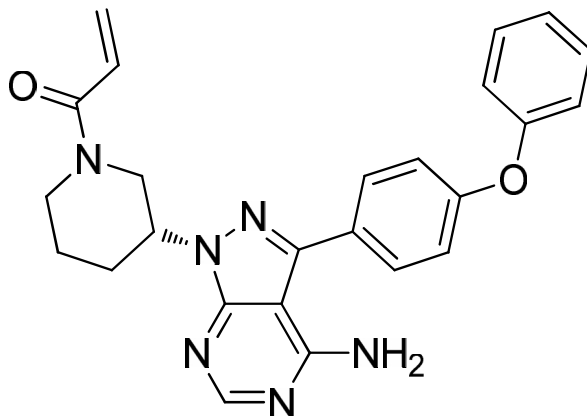
Molecular Formula: C<sub>25</sub>H<sub>24</sub>N<sub>6</sub>O<sub>2</sub>

Lot Number: Refer to vial

<sup>1</sup>H-NMR: Available on request

HPLC (Purity): > 95.0% @ 254 nm

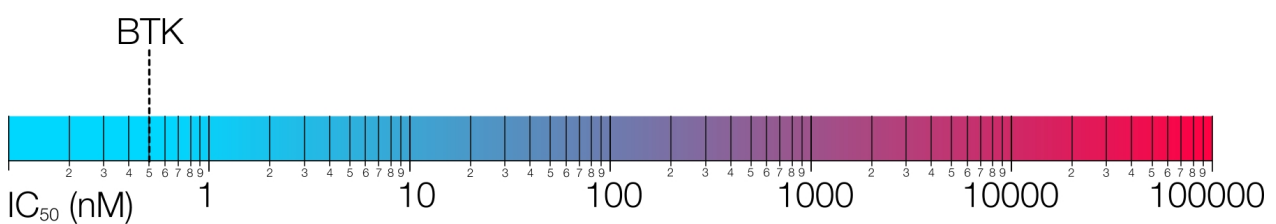
ES-MS: Available on request



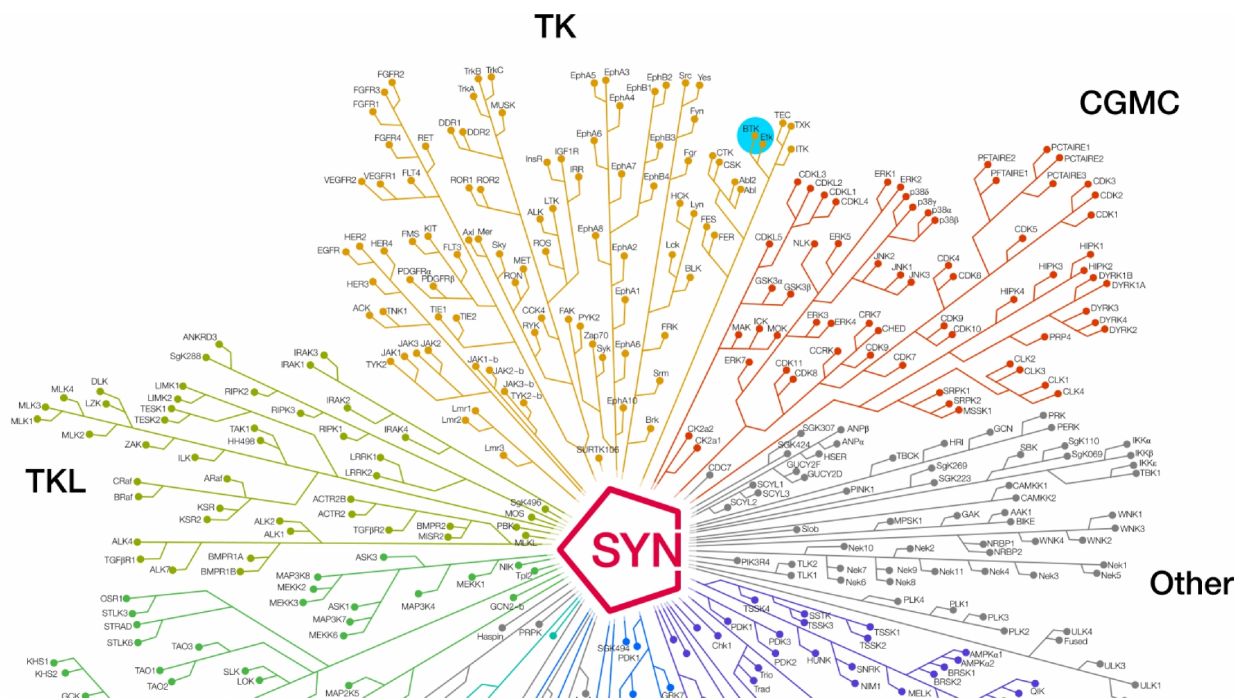
## Description:

PCI-32765 (Ibrutinib) is a potent and highly selective Btk inhibitor with an IC<sub>50</sub> of 0.5 nM.

## Biological Activity



# Kinome Mapping



## Shipping and Storage Temperature

**Shipping:**  
Ambient

**Storage:**  
2 years -20C, Powder 1 month, -4C in DMSO, More than one month -80C in DMSO

## Solubility

DMSO 88mg/mL, Ethanol 1mg/mL

## Preparing Stock Solutions

Stock Solution (1ml DMSO)	1mM	10mM	20mM	50mM
Mass(mg)	0.4405	4.4050	8.8100	22.0250

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## References

1. Honigberg LA, Smith AM, Sirisawad M, Verner E, Louny D, Chang B, Li S, Pan Z, Thamm DH, Miller RA, Buggy JJ. 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 U S A. 2010 Jul 20;107(29):13075-80. doi: 10.1073/pnas.1004594107. Epub 2010 Jul 6.

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## Ordering Information

To order more of this or any other SYNkinase compound, go to [synkinase.com](http://synkinase.com), Call us Toll Free (US Only) at 1- 877-854-6273 or email [orders@synkinase.com](mailto:orders@synkinase.com).

Product Datasheet (Rev. 1.1)