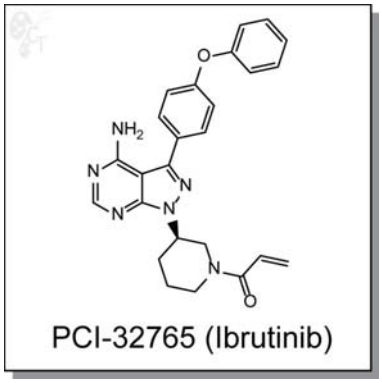
# Product Specification Sheet

**Product Name:** PCI-32765 (Ibrutinib)

**Catalog Number:** C7327




**Technical information:**

| | |
|---|---|
| Chemical Formula: | $C_{25}H_{24}N_6O_2$ |
| CAS #: | 936563-96-1 |
| Molecular Weight: | 440.5 |
| Purity: | > 99% |
| Appearance: | White solid |
| Solubility: | Soluble in DMSO up to 100 mM |
| Chemical Name: | (R)-1-(3-(4-amino-3-(4-phenoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl)piperidin-1-yl)prop-2-en-1-one |
| Storage: | Store solid powder at 4°C desiccated; Store DMSO solution at -20°C. |
| Shelf Life: | In the unopened package, powder is stable for 1 year and DMSO solution is stable for 6 months under proper storage condition. |

**Handling:**

- To make 10 mM stock solution, add 0.227mL of DMSO for each mg of PCI-32765 (Ibrutinib)
- For DMSO solution, briefly spin the vial at 500 rpm in a 50 mL conical tube to ensure maximum sample recovery.

**Biological Activity:**

PCI-32765 (Ibrutinib) is a selective and irreversible pyrrolopyrimidine-based inhibitor of BTK with IC50 of 0.5 nM. [1] PCI-32765 binds irreversibly to Cys-481 in BTK and thus is only active with other kinases with such a modifiable cysteine residue. In DOHH2 cells, in which the BCR pathway can be activated by anti-IgG, PCI-32765 inhibits autophosphorylation of BTK (IC50, 11 nM), BTK's physiological substrate, PLCg (IC50, 29 nm), and downstream ERK (IC50, 13 nm). [1]

Additionally, PCI-32765 has been shown in CD40- or BCR-activated chronic lymphocytic leukemia cells to inhibit ERK1/2, PI3K, and NFkB. [2] PCI-32765 is efficacious in collagen-induced arthritis models in a dose dependent manner, reversing inflammation at an ED50 of 2.6 mg/kg/day. [3]. PCI-32765 also inhibits BCR-activated primary B-cell proliferation at an IC50 of 8 nM. [3]

**Reference:**

1. Honigberg et al., 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. 2010, 107(29), 13075-13080. Pubmed ID: 20615965
2. Herman et al., Bruton tyrosine kinase represents a promising therapeutic target for treatment of chronic lymphocytic leukemia and is effectively targeted by PCI-32765. Blood, 2011, 117, 6287-6296. Pubmed ID: 21422473
3. Chang et al., The Bruton tyrosine kinase inhibitor PCI-32765 ameliorates autoimmune arthritis by inhibition of multiple effector cells. Arthritis Res. Ther. 2011. 13(4). R115. Pubmed ID: 21752263

To reorder: http://www.cellagentech.com/PCI-32765-Ibrutinib/

For Technical Support: technical@cellagentech.com

*Chemicals are sold for research use only, not for clinical or diagnostic use.*