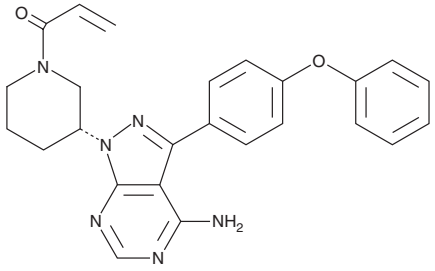
PRODUCT INFORMATION

Ibrutinib

Item No. 16274

CAS Registry No.:	936563-96-1
Formal Name:	1-[(3R)-3-[4-amino-3-(4-phenoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-1-piperidinyl]-2-propen-1-one
Synonyms:	Imbruvica, PCI 32765
MF:	$C_{25}H_{24}N_6O_2$
FW:	440.5
Purity:	≥98%
UV/Vis.:	λ_{max}: 260 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Ibrutinib is supplied as a crystalline solid. A stock solution may be made by dissolving the ibrutinib in the solvent of choice. Ibrutinib is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of ibrutinib in DMSO and DMF is approximately 30 mg/ml and approximately 0.25 mg/ml in ethanol.

Ibrutinib is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, Ibrutinib should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Ibrutinib has a solubility of approximately 0.25 mg/ml in a 1:3 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Bruton's tyrosine kinase (BTK) is a member of the BTK/Tec family of protein tyrosine kinases involved in signal transduction pathways regulating proliferation, survival, migration, and tissue homing of B-cells.[1] Ibrutinib is an irreversible inhibitor of BTK (IC_{50} = 0.5 nM) that selectively blocks B cell activation, promoting apoptosis and preventing homing to the protective tumor microenvironment, at concentrations that do not affect T cell receptor signaling (1,000-fold more potent).[2,3] It has been reported to inhibit autophosphorylation of BTK (IC_{50} = 11 nM), phosphorylation of PLCγ (IC_{50} = 29 nM), a substrate of BTK, and phosphorylation of ERK (IC_{50} = 13 nM), a further downstream kinase.[2] Its use has been examined clinically for the treatment of diseases associated with B cell antigen receptor signaling, including mantle cell lymphoma, chronic lymphocytic leukemia, and non-Hodgkin lymphoma.[1,2,4]

References

1. Leslie, L.A. and Younes, A. *Leuk. Lymphoma* **54(11)**, 2365-2376 (2013).
2. Honigberg, L.A., Smith, A.M., Sirisawad, M., *et al. Proc. Natl. Acad. Sci. USA* **107(29)**, 13075-13080 (2010).
3. Herman, S.E.M., Gordon, A.L., Hertlein, E., *et al. Blood* **117(23)**, 6287-6296 (2011).
4. Wu, M., Akinleye, A., and Zhu, X. *J. Hematol. Oncol.* **6**, 36 (2013).

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