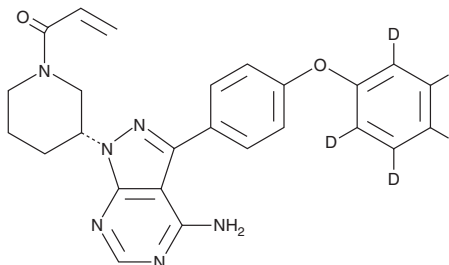


# PRODUCT INFORMATION



## Ibrutinib-d<sub>5</sub> Item No. 22561

**CAS Registry No.:** 1553977-17-5  
**Formal Name:** 1-[(3R)-3-[4-amino-3-[4-(phenoxy-2,3,4,5,6-d<sub>5</sub>)phenyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-1-piperidinyl]-2-propen-1-one  
**MF:** C<sub>25</sub>H<sub>19</sub>D<sub>5</sub>N<sub>6</sub>O<sub>2</sub>  
**FW:** 445.5  
**Chemical Purity:** ≥98% (Ibrutinib)  
**Deuterium Incorporation:** ≥99% deuterated forms (d<sub>1</sub>-d<sub>5</sub>); ≤1% d<sub>0</sub>  
**Supplied as:** A solid  
**Storage:** -20°C  
**Stability:** ≥4 years



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

### Laboratory Procedures

Ibrutinib-d<sub>5</sub> is intended for use as an internal standard for the quantification of ibrutinib (Item No. 16274) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated versus unlabeled).

Ibrutinib-d<sub>5</sub> is supplied as a solid. A stock solution may be made by dissolving the ibrutinib in the solvent of choice, which should be purged with an inert gas. Ibrutinib is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of ibrutinib in ethanol is approximately 0.25 mg/ml and approximately 30 mg/ml in DMSO and DMF.

### Description

Ibrutinib is an irreversible inhibitor of Bruton's tyrosine kinase (BTK; IC<sub>50</sub> = 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).<sup>1,2</sup> It has been reported to inhibit autophosphorylation of BTK (IC<sub>50</sub> = 11 nM), phosphorylation of PLCγ (IC<sub>50</sub> = 29 nM), a substrate of BTK, and phosphorylation of ERK (IC<sub>50</sub> = 13 nM), a further downstream kinase.<sup>1</sup> Formulations containing it have 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.<sup>1,3,4</sup>

### References

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

#### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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