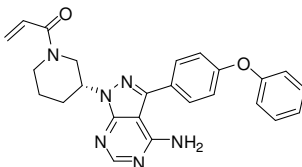




## Certificate of Analysis

**Axon Catalogue ID:** 1858 **Batch Number:** 1  
**Product Name:** PCI 32765  
**Alternative Name(s):** Ibrutinib  
**IUPAC 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

**Structure:**



**Amount:**

**CAS number(s):** 936563-96-1  
**Molecular Formula:** C<sub>25</sub>H<sub>24</sub>N<sub>6</sub>O<sub>2</sub> **Molecular Weight:** 440.50  
**Batch Molecular Formula:** C<sub>25</sub>H<sub>24</sub>N<sub>6</sub>O<sub>2</sub>·0.33H<sub>2</sub>O **Batch Molecular Weight:** 446.44  
**Appearance:** White solid **Observed mp:** 155 - 155.3 °C  
**TLC (R<sub>f</sub>):** 0.45 DCM/MeOH (9:1)  
**Chemical Purity:** 99.7%  
**Optical Rotation (Det.):** [α]<sub>D</sub> = -129.3° with c = 0.567 in MeOH  
**<sup>1</sup>H-NMR:** Analytical data confirm chemical structure  
**Mass Spec:** Analytical data confirm chemical structure  
**Microanalysis:** Calculated: C 67.25, H 5.57, N 18.82; Found: C 67.21, H 5.35, N 18.83  
**Storage Conditions:** Desiccate at +4 °C

Solubility Data:	Solvent	Solubility (mg/ml)	Solubility (mM)	Remarks
	Water			Not Tested
	0.1N NaOH (aq)			Not Tested
	0.1N HCl (aq)			Not Tested
	DMSO	35.6	79.7	
	EtOH			Not Tested

**Remarks:**

**QC Date:** 8-12-2022

The purity of Axon Ligands is confirmed by HPLC, MS, NMR and/or microanalysis. Analytical data are available upon request. Request can be submitted by e-mail to [info@axonmedchem.com](mailto:info@axonmedchem.com) indicating Catalogue ID and Batch number.

**Caution: Not fully tested. For research purposes only**