



## Certificate of Analysis

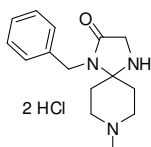
**Axon Catalogue ID:** 3746 **Batch Number:** 1

**Product Name:** PTI-125 dihydrochloride

**Alternative Name(s):** Simufilam

**IUPAC Name:** 1-Benzyl-8-methyl-1,4,8-triazaspiro[4.5]decan-2-one dihydrochloride

**Structure:**



**Amount:**

**CAS number(s):** 1224591-33-6 (parent), 2480226-06-8 (HCl (1:2))

**Molecular Formula:** C<sub>15</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>HCl **Molecular Weight:** 332.27

**Batch Molecular Formula:** C<sub>15</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>HCl<sub>2</sub>·0.5H<sub>2</sub>O **Batch Molecular Weight:** 341.28

**Appearance:** White solid **Observed mp:** 131.5 - 134.0 °C

**TLC (R<sub>f</sub>):** 0.25 DCM/MeOH/NH<sub>3</sub> (20:1:0.1)

**Chemical Purity:** 99.5%

**<sup>1</sup>H-NMR:** Analytical data confirm chemical structure

**Mass Spec:** Analytical data confirm chemical structure

**Microanalysis:** Calculated: C 52.79, H 7.09, N 12.31; Found: C 52.59, H 7.17, N 12.22

**Storage Conditions:** Desiccate at -20 °C

<b>Solubility Data:</b>	<b>Solvent</b>	<b>Solubility (mg/ml)</b>	<b>Solubility (mM)</b>	<b>Remarks</b>
	Water	34.1	>100 mM	
	0.1N NaOH (aq)			Not Tested
	0.1N HCl (aq)			Not Tested
	DMSO	34.1	>100 mM	
	EtOH	0.0	0.0	Insoluble

**Remarks:**

**QC Date:** 15-12-2022

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**