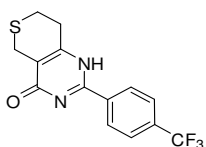




## Certificate of Analysis

**Axon Catalogue ID:** 1527 **Batch Number:** 2  
**Product Name:** XAV939  
**Alternative Name(s):** N.A.  
**IUPAC Name:** 2-(4-(Trifluoromethyl)phenyl)-7,8-dihydro-1H-thiopyrano[4,3-d]pyrimidin-4(5H)-one

**Structure:**



**Amount:**

**CAS number(s):** 284028-89-3  
**Molecular Formula:** C<sub>14</sub>H<sub>11</sub>F<sub>3</sub>N<sub>2</sub>O<sub>2</sub> **Molecular Weight:** 312.31  
**Batch Molecular Formula:** C<sub>14</sub>H<sub>11</sub>F<sub>3</sub>N<sub>2</sub>O<sub>2</sub>.0.25H<sub>2</sub>O **Batch Molecular Weight:** 316.81  
**Appearance:** White solid **Observed mp:** >265 °C (decomp)  
**TLC (R<sub>f</sub>):** 0.3 Hex/EtOAc (4:1)  
**Chemical Purity:** 99.1%  
**Optical Purity (ee):** N.A.  
**<sup>1</sup>H-NMR (300 MHz):** Analytical data confirm chemical structure  
**Mass Spec:** Analytical data confirm chemical structure  
**Microanalysis:** Calculated: C 53.08, H 3.66, N 8.84; Found: C 53.38, H 3.54, N 8.79  
**Storage Conditions:** Store at +4 °C

<b>Solubility Data:</b>	<b>Solvent</b>	<b>Solubility (mg/ml)</b>	<b>Solubility (mM)</b>	<b>Remarks</b>
	Water	0.0	0.0	Insoluble
	0.1N NaOH (aq)			Not Tested
	0.1N HCl (aq)			Not Tested
	DMSO	8.8	27.8	
	EtOH			Not Tested

**Remarks:**

**QC Date:** 17-9-2020

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**