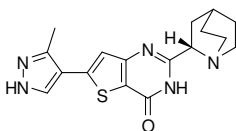




Certificate of Analysis

Axon Catalogue ID: 3605 **Batch Number:** 1
Product Name: TAK-931
Alternative Name(s): Simurosertib
IUPAC Name: (S)-6-(3-Methyl-1H-pyrazol-4-yl)-2-(quinuclidin-2-yl)thieno[3,2-d]pyrimidin-4(3H)-one

Structure:



Amount:

CAS number(s): 1330782-76-7
Molecular Formula: C₁₇H₁₉N₅O₅ **Molecular Weight:** 341.43
Batch Molecular Formula: C₁₇H₁₉N₅O₅.0.75H₂O **Batch Molecular Weight:** 354.94
Appearance: White solid **Observed mp:** >220 °C (decomp)
TLC (R_f): 0.75 DCM/MeOH/NH₃ (4:1:0.1)
Chemical Purity: 99.9%
Optical Purity (ee): 100%
Optical Rotation (Det.): [α]_D = -20.1° with c = 1 in DMSO
¹H-NMR: Analytical data confirm chemical structure
Mass Spec: Analytical data confirm chemical structure
Microanalysis: Calculated: C 57.53, H 5.82, N 19.73; Found: C 57.54, H 5.57, N 19.58
Storage Conditions: Store at +4 °C

Solvent	Solubility (mg/ml)	Solubility (mM)	Remarks
Water	0.0	0.0	Insoluble
0.1N NaOH (aq)			Not Tested
0.1N HCl (aq)	11.2	31.6	
DMSO	35.5	>100 mM	
EtOH	5.0	14.1	* Warming (40°C)

Remarks: * Warming (40°C) enhanced solubility.

QC Date: 28-3-2022

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 indicating Catalogue ID and Batch number.

Caution: Not fully tested. For research purposes only