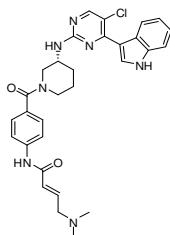




Certificate of Analysis

Axon Catalogue ID: 3402 **Batch Number:** 1
Product Name: THZ531
Alternative Name(s): N.A.
IUPAC Name: (R,E)-N-(4-(3-(5-Chloro-4-(1H-indol-3-yl)pyrimidin-2-ylamino)piperidine-1-carbonyl)phenyl)-4-(dimethylamino)but-2-enamide

Structure:



Amount:

CAS number(s): 1702809-17-3
Molecular Formula: C₃₀H₃₂ClN₇O₂ **Molecular Weight:** 558.07
Batch Molecular Formula: C₃₀H₃₂ClN₇O₂.1H₂O **Batch Molecular Weight:** 576.09
Appearance: White solid **Observed mp:** 144 - 147 °C
TLC (R_f): 0.4 DCM/MeOH/NH₃ (9:1:0.1)
Chemical Purity: 99.4%
Optical Purity (ee): 100%
¹H-NMR: Analytical data confirm chemical structure
Mass Spec: Analytical data confirm chemical structure
Microanalysis: Calculated: C 62.55, H 5.95, N 17.02; Found: C 62.45, H 5.83, N 16.97
Storage Conditions: Store at -20 °C

Solubility Data:	Solvent	Solubility		Remarks
		(mg/ml)	(mM)	
	Water	0.0	0.0	Insoluble
	0.1N NaOH (aq)			Not Tested
	0.1N HCl (aq)	12.7	22.0	
	DMSO	57.6	>100 mM	
	EtOH			Not Tested

Remarks: Suspected to be thermally unstable; store both solid material and stock solutions as cold as possible. It is recommended to use freshly prepared stock solutions for your experiments.

QC Date: 09-06-2021

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