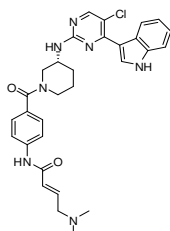


Certificate of Analysis

Axon Catalogue ID: 3402 **Batch Number:** 2
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.H₂O **Batch Molecular Weight:** 576.09
Appearance: White solid **Observed mp:** 139.5 - 142.0 °C
TLC (R_f): 0.4 DCM/MeOH/NH₃ (9:1:0.1)
Chemical Purity: 98.3%
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 62.68, H 5.79, N 16.87
Storage Conditions: Store at -20 °C

| Solubility Data: | Solvent | Solubility (mg/ml) | Solubility (mM) | Remarks |
|------------------|----------------|--------------------|-----------------|------------|
| | Water | 0.0 | 0.0 | Insoluble |
| | 0.1N NaOH (aq) | | | Not Tested |
| | 0.1N HCl (aq) | 34.0 | 59.0 | |
| | DMSO | 57.6 | >100 mM | |
| | EtOH | 57.6 | >100 mM | |

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: 18-8-2022

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