

## **Certificate of Analysis**

Axon Catalogue ID: 1144 Batch Number: 1

Product Name: Thio-aripiprazole

Alternative Name(s): N.A.

IUPAC Name: 7-(4-(4-(2,3-Dichlorophenyl)piperazin-1-yl)butoxy)-3,4-dihydroquinoline-2(1H)-thione

Structure: Amount:

CINN

**CAS number(s):** 573691-04-0

Molecular Formula: C23H27Cl2N3OS Molecular Weight: 464.45

Batch Molecular Formula: C23H27CI2N3OS Batch Molecular Weight: 464.45

Appearance: White solid Observed mp: 139.7 - 141.5 °C

TLC ( $R_f$ ): 0.7 DCM/MeOH (9:1)

Chemical Purity: 99.5%

**1H-NMR:** Analytical data confirm chemical structure

Mass Spec: Analytical data confirm chemical structure

Microanalysis: Calculated: C 59.48, H 5.86, N 9.05; Found: C 59.39, H 5.85, N 8.97

Storage Conditions: Store at +4 °C

Solubility Data: Solubility Solubility Solvent Remarks (mg/ml) (mM) Water 0.0 Insoluble 0.1N NaOH (aq) Not Tested 0.1N HCI (aq) 0.0 0.0 Insoluble

DMSO 46.4 >100 mM EtOH 4.4 9.5 \*Warming (40°C)

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

QC Date: 27-9-2023

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