



Certificate of Analysis

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|---------------------------------|--|--------------------------------|------------------------|----------------|
| Axon Catalogue ID: | 1839 | Batch Number: | 6 | |
| Product Name: | Zosuquidar trihydrochloride | | | |
| Alternative Name(s): | LY335979 | | | |
| IUPAC Name: | (αR)-4-[(1α,6α,10β)-1,1-Difluoro-1,1a,6,10b-tetrahydrobenzo[a,e]cyclopropa[c]cyclohepten-6-yl]-α-[(5-quinolinyl)oxy)methyl]-1-piperazineethanol trihydrochloride | | | |
| Structure: | HCl HCl HCl | | Amount: | |
| CAS number(s): | 167354-41-8 (parent), 167465-36-3 (HCl (1:3)) | | | |
| Molecular Formula: | C32H31F2N3O2.3HCl | Molecular Weight: | 636.99 | |
| Batch Molecular Formula: | C32H31F2N3O2.3HCl.2H2O | Batch Molecular Weight: | 673.02 | |
| Appearance: | Yellow solid | Observed mp: | 197.0 - 198.5 °C | |
| TLC (R_f): | 0.5 | DCM/MeOH (9:1) | | |
| Chemical Purity: | 99.9% | | | |
| Optical Purity (ee): | Optically pure | | | |
| Optical Rotation (Det.): | [α] _D = +11.2° with c = 0.5 in MeOH | | | |
| ¹H-NMR: | Analytical data confirm chemical structure | | | |
| Mass Spec: | Analytical data confirm chemical structure | | | |
| Microanalysis: | Calculated: C 57.11, H 5.69, N 6.24; Found: C 57.04, H 5.99, N 6.19 | | | |
| Storage Conditions: | Desiccate at -20 °C | | | |
| Solubility Data: | Solvent | Solubility (mg/ml) | Solubility (mM) | Remarks |
| | Water | 29.3 | 43.6 | |
| | 0.1N NaOH (aq) | | | Not Tested |
| | 0.1N HCl (aq) | | | Not Tested |
| | DMSO | 67.3 | >100 mM | |
| | EtOH | 0.0 | 0.0 | Insoluble |
| Remarks: | | | | |
| QC Date: | 25-11-2022 | | | |

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