



Certificate of Analysis

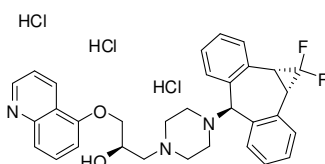
Axon Catalogue ID: 1839 **Batch Number:** 5

Product Name: Zosuquidar trihydrochloride

Alternative Name(s): LY335979

IUPAC Name: (α R)-4-[(1 α ,6 α ,10 β)-1,1-Difluoro-1,1a,6,10b-tetrahydrodibenzo[a,e]cyclopropa[c]cyclohepten-6-yl]- α -[(5-quinolinyl)oxy)methyl]-1-piperazineethanol trihydrochloride

Structure:



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.3H₂O **Batch Molecular Weight:** 691.03

Appearance: Pale-yellow solid **Observed mp:** 130 - 132 °C

TLC (R_f): 0.6 DCM/MeOH (9:1)

Chemical Purity: 99.3%

Optical Purity (ee): Optically pure

Optical Rotation (Det.): $[\alpha]_D = +12.8^\circ$ with c = 0.5 in MeOH

¹H-NMR: Analytical data confirm chemical structure

Mass Spec: Analytical data confirm chemical structure

Microanalysis: Calculated: C 55.62, H 5.83, N 6.08; Found: C 55.51, H 5.69, N 5.99

Storage Conditions: Desiccate at -20 °C

Solubility Data:	Solvent	Solubility (mg/ml)	Solubility (mM)	Remarks
	Water	25.3	36.7	
	0.1N NaOH (aq)			Not Tested
	0.1N HCl (aq)			Not Tested
	DMSO	69.1	>100 mM	
	EtOH	40.0	57.9	

Remarks:

QC Date: 9-11-2022

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