



Certificate of Analysis

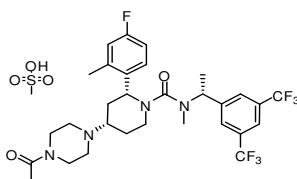
Axon Catalogue ID: 1901 **Batch Number:** 1

Product Name: Casopitant mesylate

Alternative Name(s): GW 679769B

IUPAC Name: (2R,4S)-4-(4-Acetylpiperazin-1-yl)-N-((R)-1-(3,5-bis(trifluoromethyl)phenyl)ethyl)-2-(4-fluoro-2-methylphenyl)-N-methylpiperidine-1-carboxamide methanesulfonate

Structure:



Amount:

CAS number(s): 414910-27-3 (parent), 414910-30-8 (mesylate (1:1))

Molecular Formula: C₃₀H₃₅F₇N₄O₂.CH₄O₃S **Molecular Weight:** 712.72

Batch Molecular Formula: C₃₀H₃₅F₇N₄O₂.CH₄O₃S.1.5H₂O **Batch Molecular Weight:** 739.74

Appearance: White solid **Observed mp:** 249 °C

TLC (R_f): 0.62 DCM/MeOH (9:1)

Chemical Purity: 99.0%

Optical Purity (ee): optically pure

¹H-NMR (300 MHz): Analytical data confirm chemical structure

Mass Spec: Analytical data confirm chemical structure

Microanalysis: Calculated: C 50.33, H 5.72, N 7.57; Found: C 50.29, H 5.69, N 7.61

Storage Conditions: Store at -20 °C

Solubility Data:	Solvent	Solubility (mg/ml)	Solubility (mM)	Remarks
	Water	60.0	81.1	
	0.1N NaOH (aq)			Not Tested
	0.1N HCl (aq)			Not Tested
	DMSO	60.0	81.1	
	EtOH			Not Tested

Remarks: The compound is hygroscopic. Keep dry and avoid light.

QC Date: 11-10-2018

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