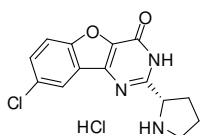




Certificate of Analysis

Axon Catalogue ID: 2268 **Batch Number:** 1
Product Name: XL 413 hydrochloride
Alternative Name(s): BMS 863233 hydrochloride
IUPAC Name: (S)-8-Chloro-2-(pyrrolidin-2-yl)benzofuro[3,2-d]pyrimidin-4(3H)-one hydrochloride

Structure:



Amount:

CAS number(s): 1169558-38-6 (parent), 2062200-97-7 (HCl (1:1))
Molecular Formula: C₁₄H₁₂ClN₃O₂.HCl **Molecular Weight:** 326.18
Batch Molecular Formula: C₁₄H₁₂ClN₃O₂.HCl.1H₂O **Batch Molecular Weight:** 344.19
Appearance: White solid **Observed mp:** 275 °C (decomp)
TLC (R_f): 0.39 DCM/MeOH/NH₃ (1:1:0.1)
Chemical Purity: 99.8%
Optical Purity (ee): Optically pure
¹H-NMR (300 MHz): Analytical data confirm chemical structure
Mass Spec: Analytical data confirm chemical structure
Microanalysis: Calculated: C 48.85, H 4.39, N 12.21; Found: C 49.02, H 4.34, N 12.12
Storage Conditions: Store at +4 °C

Solubility Data:	Solvent	Solubility (mg/ml)	Solubility (mM)	Remarks
	Water	34.4	>100 mM	
	0.1N NaOH (aq)			Not Tested
	0.1N HCl (aq)			Not Tested
	DMSO	3.9	11.3	
	EtOH			Not Tested

Remarks: CAS [1169562-71-3] is for the HCl salt (1:x).

QC Date: 19-11-2019

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