



Certificate of Analysis

Axon Catalogue ID:	3109	Batch Number:	1	
Product Name:	ML-792			
Alternative Name(s):	N.A.			
IUPAC Name:	((1R,2S,4R)-4-(5-(1-(3-Bromobenzyl)-1H-pyrazole-3-carbonyl)pyrimidin-4-ylamino)-2-hydroxycyclopentyl)methyl sulfamate			
Structure:			Amount:	
CAS number(s):	1644342-14-2			
Molecular Formula:	C ₂₁ H ₂₃ BrN ₆ O ₅ S	Molecular Weight:	551.41	
Batch Molecular Formula:	C ₂₁ H ₂₃ BrN ₆ O ₅ S	Batch Molecular Weight:	551.41	
Appearance:	Off-white solid	Observed mp:	121 °C (decomp)	
TLC (R_f):	0.51	DCM/MeOH (9:1)		
Chemical Purity:	99.5%			
Optical Purity (ee):	Optically pure			
¹H-NMR (300 MHz):	Analytical data confirm chemical structure			
Optical Rotation (Det.):	[α] _D = +1.6° with c = 0.5 in MeOH			
Mass Spec:	Analytical data confirm chemical structure			
Microanalysis:	Calculated: C 45.74, H 4.20, N 15.24; Found: C 46.04, H 4.25, N 15.19			
Storage Conditions:	Store at -20 °C			
Solubility Data:	Solvent	Solubility (mg/ml)	Solubility (mM)	Remarks
	Water	0.0	0.0	Insoluble
	0.1N NaOH (aq)	13.7	24.9	
	0.1N HCl (aq)	5.2	9.4	* Warming (40°C) and sonication
	DMSO	55.1	>100 mM	
	EtOH			Not Tested
Remarks:	* Warming (40°C) and sonication enhanced solubility.			
QC Date:	17-4-2020			

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