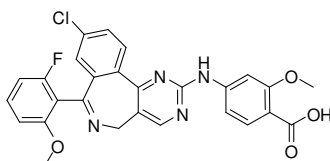




Certificate of Analysis

Axon Catalogue ID: 2003 **Batch Number:** 1
Product Name: MLN8237
Alternative Name(s): Alisertib
IUPAC Name: 4-(9-Chloro-7-(2-fluoro-6-methoxyphenyl)-5H-benzo[e]pyrimido[5,4-c]azepin-2-ylamino)-2-methoxybenzoic acid

Structure:



Amount:

CAS number(s): 1028486-01-2
Molecular Formula: C₂₇H₂₀ClFN₄O₄ **Molecular Weight:** 518.92
Batch Molecular Formula: C₂₇H₂₀ClFN₄O₄.0.25H₂O **Batch Molecular Weight:** 523.43
Appearance: Yellow solid **Observed mp:** 249 - 250 °C
TLC (R_f): 0.5 DCM/MeOH (9:1)
Chemical Purity: 99.6%
Optical Purity (ee): N.A.
¹H-NMR (300 MHz): Analytical data confirm chemical structure
Mass Spec: Analytical data confirm chemical structure
Microanalysis: Calculated: C 61.95, H 3.95, N 10.70; Found: C 61.90, H 3.62, N 10.69
Storage Conditions: Store at +4 °C

Solubility Data:	Solvent	Solubility (mg/ml)	Solubility (mM)	Remarks
	Water	0.0	0.0	Insoluble
	0.1N NaOH (aq)	10.0	19.1	* Warming (40°C) enhances solubility
	0.1N HCl (aq)	0.0	0.0	Insoluble
	DMSO	36.0	68.8	
	EtOH			Not Tested

Remarks:

QC Date: 25-5-2018

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