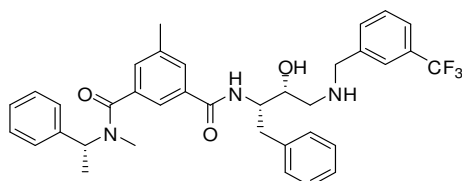




Certificate of Analysis

Axon Catalogue ID: 2957 **Batch Number:** 1
Product Name: BACE-2 Inhibitor
Alternative Name(s): BACE-2 Inhibitor 3I
IUPAC Name: N1-((2S,3R)-3-Hydroxy-1-phenyl-4-(3-(trifluoromethyl)benzylamino)butan-2-yl)-N3,5-dimethyl-N3-((R)-1-phenylethyl)isophthalamide

Structure:



Amount:

CAS number(s): 1676107-08-6
Molecular Formula: C₃₆H₃₈F₃N₃O₃ **Molecular Weight:** 617.70
Batch Molecular Formula: C₃₆H₃₈F₃N₃O₃·0.1H₂O **Batch Molecular Weight:** 619.50
Appearance: White solid **Observed mp:** 67.2 °C
TLC (R_f): 0.8 DCM/MeOH/NH₃ (9:1:0.1)
Chemical Purity: 99.4%
Optical Purity (ee): Optically pure
¹H-NMR (300 MHz): Analytical data confirm chemical structure
Mass Spec: Analytical data confirm chemical structure
Microanalysis: Calculated: C 69.80, H 6.22, N 6.78; Found: C 69.46, H 5.74, N 6.72
Storage Conditions: Store at +4 °C

Solubility Data:	Solvent	Solubility		Remarks
		(mg/ml)	(mM)	
	Water	0.0	0.0	Insoluble
	0.1N NaOH (aq)			Not Tested
	0.1N HCl (aq)	0.0	0.0	Insoluble
	DMSO	62.0	>100 mM	
	EtOH			Not Tested

Remarks:

QC Date: 19-09-2019

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