



Certificate of Analysis

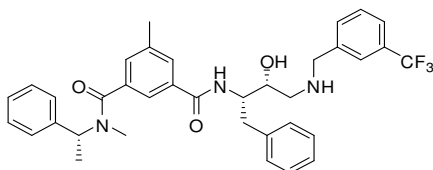
Axon Catalogue ID: 2957 **Batch Number:** 1

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: 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 (mg/ml)	Solubility (mM)	Remarks
	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:

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