



Certificate of Analysis

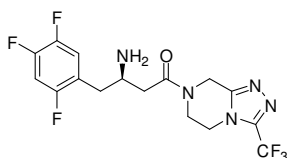
Axon Catalogue ID: 3251 **Batch Number:** 1

Product Name: Sitagliptin

Alternative Name(s): N.A.

IUPAC Name: (R)-3-Amino-1-(3-(trifluoromethyl)-5,6-dihydro-[1,2,4]triazolo[4,3-a]pyrazin-7(8H)-yl)-4-(2,4,5-trifluorophenyl)butan-1-one

Structure:



Amount:

CAS number(s): 486460-32-6

Molecular Formula: C₁₆H₁₅F₆N₅O **Molecular Weight:** 407.31

Batch Molecular Formula: C₁₆H₁₅F₆N₅O.0.2H₂O **Batch Molecular Weight:** 410.92

Appearance: White solid **Observed mp:** 116.4 - 119.3 °C

TLC (R_f): 0.39 DCM/MeOH (9:1)

Chemical Purity: 100%

Optical Purity (ee): Optically pure

Optical Rotation (Det.): [α]_D = -24.1° with c = 0.5 in CHCl₃

¹H-NMR (300 MHz): Analytical data confirm chemical structure

Mass Spec: Analytical data confirm chemical structure

Microanalysis: Calculated: C 46.77, H 3.78, N 17.04; Found: C 47.08, H 4.17, N 17.32

Storage Conditions: Store at +4 °C

Solvent	Solubility (mg/ml)	Solubility (mM)	Remarks
Water	0.0	0.0	Insoluble
0.1N NaOH (aq)			Not Tested
0.1N HCl (aq)	18.4	44.8	
DMSO	41.1	>100 mM	
EtOH			Not Tested

Remarks:

QC Date: 23-10-2020

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