

## **Certificate of Analysis**

**Axon Catalogue ID:** 2121 **Batch Number:** 

**Product Name: INNO 406** 

Alternative Name(s): Bafetinib; NS 187

(S)-N-(3-(4,5'-Bipyrimidin-2-ylamino)-4-methylphenyl)-4-((3-(dimethylamino)pyrrolidin-1-methylphenyl**IUPAC Name:** 

yl)methyl)-3-(trifluoromethyl)benzamide

Structure:

CAS number(s): 859212-16-1

Molecular Formula: C30H31F3N8O Molecular Weight: 576.62

**Batch Molecular Formula:** C30H31F3N8O.0.33H2O **Batch Molecular Weight:** 

Appearance: Off-white solid Observed mp: 186.9 - 187.3 °C

TLC (R<sub>f</sub>): 0.54 DCM/MeOH/NH3 (9:1:0.1)

**Chemical Purity:** 98.7%

Optical Purity (ee): Optical pure

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

Mass Spec: Analytical data confirm chemical structure

Microanalysis: Calculated: C 61.84, H 5.48, N 19.23; Found: C 61.80, H 5.20, N 19.23

**Storage Conditions:** Store at +4 °C

**Solubility Data:** Solvent Solubility Solubility Remarks (mg/ml) (mM) Water Not Tested 0.1N NaOH (aq) Not Tested 0.1N HCl (aq) 14.1 24.2 DMSO 48.1 28.0 **EtOH** Not Tested

Remarks:

QC Date: 17-12-2018

> 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