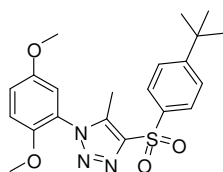




Certificate of Analysis

Axon Catalogue ID: 2807 **Batch Number:** 1
Product Name: SPA70
Alternative Name(s): LC-1; Specific PXR antagonist #70
IUPAC Name: 4-(4-tert-Butylphenylsulfonyl)-1-(2,5-dimethoxyphenyl)-5-methyl-1H-1,2,3-triazole

Structure:



Amount:

CAS number(s): 931314-31-7
Molecular Formula: C₂₁H₂₅N₃O₄S **Molecular Weight:** 415.51
Batch Molecular Formula: C₂₁H₂₅N₃O₄S **Batch Molecular Weight:** 415.51
Appearance: Light-orange solid **Observed mp:** 195.5 - 197.5 °C
TLC (R_f): 0.35 Hex/EtOAc (2:1)
Chemical Purity: 99.5%
Optical Purity (ee): N.A.
¹H-NMR (300 MHz): Analytical data confirm chemical structure
Mass Spec: Analytical data confirm chemical structure
Microanalysis: Calculated: C 60.70, H 6.06, N 10.11; Found: C 60.31, H 6.05, N 10.14
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)			Not Tested
	DMSO	41.6	>100 mM	
	EtOH			Not Tested

Remarks:

QC Date: 14-12-2018

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