

## **Certificate of Analysis**

| Axon Catalogue ID:       | 2583   |   | Batch Num                         | nber:                               | 2                |
|--------------------------|--|---|-----------------------------------|-------------------------------------|------------------|
| Product Name:            | PXS 4728A  |   |                                   |                                     |                  |
| Alternative Name(s):     | PXS 4728 hydrochloride   |   |                                   |                                     |                  |
| IUPAC Name:              | (E)-4-(2-(Aminomethyl)-3-fluoroallyloxy)-N-tert-butylbenzamide hydrochloride |   |                                   |                                     |                  |
| Structure:               | HN<br>HO<br>HCI<br>Amount:   |   |                                   |                                     |                  |
| CAS number(s):           | 1478364-40-7 (parent), 1478364-68-9 (HCI (1:1))                              |   |                                   |                                     |                  |
| Molecular Formula:       | C15H21FN2O2  | 2.HCI                                       | Molecular Wei                     | ight:                               | 316.80           |
| Batch Molecular Formula: | C15H21FN2O2.HCI  |   | Batch Molecular Weight:           |                                     | 316.80           |
| Appearance:              | White solid  |   | Observed mp:                      |                                     | 183.5 - 184.6 °C |
| TLC (R <sub>f</sub> ):   | 0.2  | DCM/MeOH (9:1)                              |                                   |                                     |                  |
| Chemical Purity:         | 99.8%  |   |                                   |                                     |                  |
| Optical Purity (ee):     | N.A.   |   |                                   |                                     |                  |
| 1H-NMR (300 MHz):        | Analytical data confirm chemical structure                                   |   |                                   |                                     |                  |
| Mass Spec:               | Analytical data confirm chemical structure                                   |   |                                   |                                     |                  |
| Microanalysis:           | Calculated: C 56.87, H 7.00, N 8.84; Found: C 56.54, H 6.74, N 8.72          |   |                                   |                                     |                  |
| Storage Conditions:      | Store at +4 °C   |   |                                   |                                     |                  |
| Solubility Data:         | Solvent<br>Water<br>0.1N NaOH (ac<br>0.1N HCI (aq)<br>DMSO<br>EtOH           | Solubility<br>(mg/ml)<br>31.7<br>a)<br>31.7 | (mM)<br>>100 mM<br>Not<br>>100 mM | narks<br>Tested<br>Tested<br>Tested |                  |

Remarks:

QC Date:

06-02-2018

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

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