



## Certificate of Analysis

<b>Axon Catalogue ID:</b>	4377	<b>Batch Number:</b>	1
<b>Product Name:</b>	PSB-0777 ammonium salt		
<b>Alternative Name(s):</b>	N.A.		
<b>IUPAC Name:</b>	4-(2-(9-((3R,4S,5R)-3,4-Dihydroxy-5-(hydroxymethyl)tetrahydro-2-furyl)-2-adenineylthio)ethyl)benzenesulfonate ammonium salt		
<b>Structure:</b>			<b>Amount:</b>
<b>CAS number(s):</b>	1341190-47-3 (parent), 2122196-16-9 (NH3 (1:1))		
<b>Molecular Formula:</b>	C18H21N5O7S2.NH3	<b>Molecular Weight:</b>	500.55
<b>Batch Molecular Formula:</b>	C18H21N5O7S2.NH3.2H2O	<b>Batch Molecular Weight:</b>	536.58
<b>Appearance:</b>	White solid	<b>Observed mp:</b>	165.5 - 167.0 °C
<b>TLC (R<sub>f</sub>):</b>	0.6 n-BuOH/AcOH/H2O (2:1:1)		
<b>Chemical Purity:</b>	99.4%		
<b>Optical Purity (ee):</b>	Optically pure		
<b>Optical Rotation (Det.):</b>	[α] <sub>D</sub> = -24.6° with c = 1 in MeOH		
<b><sup>1</sup>H-NMR:</b>	Analytical data confirm chemical structure		
<b>Mass Spec:</b>	Analytical data confirm chemical structure		
<b>Microanalysis:</b>	Calculated: C 40.29, H 5.26, N 15.66; Found: C 40.52, H 4.86, N 15.52		
<b>Storage Conditions:</b>	Desiccate at -20 °C		
<b>Solubility Data:</b>	<b>Solvent</b>	<b>Solubility (mg/ml)</b>	<b>Solubility (mM)</b>
	Water	53.7	>100 mM
	0.1N NaOH (aq)		Not Tested
	0.1N HCl (aq)		Not Tested
	DMSO	53.7	>100 mM
	EtOH	3.0	5.6
<b>Remarks:</b>			

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](mailto:info@axonmedchem.com) indicating Catalogue ID and Batch number.

**Caution: Not fully tested. For research purposes only**