

Supporting information:**Water adsorbing silver-adenine interpenetrated framework****Jitendra Kumar,^a Prakash Kanoo,^b Tapas Kumar Maji^{b*} and Sandeep Verma^{a*}**^aDepartment of Chemistry, Indian Institute of Technology Kanpur, Kanpur-208016 (UP), India. E-mail: sverma@iitk.ac.in; Tel: +91 512 259 7643^bChemistry and Physics of Materials Unit (CPMU), Jawaharlal Nehru Center for Advanced Scientific Research (JNCASR); Bangalore 560064; India. E-mail: tmaji@jncasr.ac.in; Fax: +91 80 2208 2766; Tel: +91 80 2208 2826

Crystal structure refinement details for 1: Crystal was coated with light hydrocarbon oil and mounted in the 100 K dinitrogen stream of a Bruker SMART APEX CCD diffractometer equipped with CRYO Industries low-temperature apparatus, and intensity data were collected using graphite-monochromated Mo KR radiation. The data integration and reduction were processed with the *SAINT* software. An absorption correction was applied. Structures were solved by the direct method using SHELXS-97 and refined on F^2 by a full-matrix least-squares technique using the *SHELXL-97* program package. Non-hydrogen atoms were refined anisotropically except for the disordered water molecule. In the refinement, hydrogens were treated as riding atoms using the *SHELXL* default parameters. Crystal refinement parameters are given in Table S2.

In the crystal lattice, two water molecules are present and the hydrogens were not located on Fourier map for both the water molecules but has been added in the empirical formula while creating the .cif file. Consequently in the check-cif report, there are few 'A' and 'B' level alerts are present, quoting "isolated oxygen atoms" and "short contact between atoms" whereas few 'C' and 'G' level alerts are due to difference between given and expected empirical formula.

Table S1: Mass spectral (HRMS) characterization for 1.[#]

ESI (+) mode		
Fragment	Calculated	Found
[L+Ag] ⁺	349.9477; 351.9474	349.9535; 351.9517
[2L+Ag] ⁺	592.9903; 594.9900	594.9963
[2L+2Ag-H] ⁺	698.8876; 700.8872;	698.8989; 700.8954;
	702.8869	702.8862
[3L+2Ag-H] ⁺	941.9302; 943.9299	941.9304; 943.9346
ESI (-) mode		
[2L+Ag-2H] ⁻	592.9743	592.9785
[3L+2Ag-3H] ⁻	941.9142	941.9209

[#]where L denotes neutral 9-SA molecule.

Table S2: Crystal structural refinement parameters for complex 1.

Empirical formula	C ₇ H ₁₂ AgN ₅ O ₅ S
Formula weight	386.15
Temperature	100(2) K
40 Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	C2/c
Unit cell dimensions	$a = 11.115(5) \text{ \AA}$ $\alpha = 90.00^\circ$ $b = 14.361(6) \text{ \AA}$ $\beta = 92.75(5)^\circ$ $c = 14.281(5) \text{ \AA}$ $\gamma = 90.00^\circ$
45 Volume	2276.9(16) Å ³
Z	8
Density (calculated)	2.253 mg/m ³
Absorption coefficient	1.982 mm ⁻¹
50 $F(000)$	1536
Crystal size	0.27 x 0.22 x 0.20 mm ³
θ range for data collection	2.32 to 25.0°
Index ranges	$-13 \leq h \leq 6$, $-17 \leq k \leq 16$, $-16 \leq l \leq 16$
Reflections collected	5500
55 Independent reflections	1989 [$R(\text{int}) = 0.0654$]
Completeness to $\theta = 25.00^\circ$	99.4 %
Absorption correction	multi-scan
Max. and min. transmission	0.6926 and 0.6167
Refinement method	Full-matrix least-squares on F^2
60 Data / restraints / parameters	1989 / 0 / 166
Goodness-of-fit on F^2	1.083
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0660$, $wR2 = 0.1500$
R indices (all data)	$R1 = 0.0840$, $wR2 = 0.1606$
Largest diff. peak and hole	1.405 and -1.028 e.Å ⁻³

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Table S3: Selected bond distances [Å] and bond angles [°] for 1.^a

Bond distances			Bond angles		
70 Ag1—N1	2.2052(63)	N1—Ag1—N7	162.376(229)	N7—Ag1—O2	98.734(214)
Ag1—N7	2.1947(65)	N1—Ag1—O1	79.931(220)	N7—Ag1—O1W	87.986(335)
Ag1—O1	2.7528(70)	N1—Ag1—O2	94.662(205)	O1—Ag1—O1W	73.954(401)
Ag1—O1W	2.7241(167)	N1—Ag1—O1W	94.819(334)	O1—Ag1—O2	51.209(182)
Ag1—O2	2.8236(59)	N7—Ag1—O1	117.471(226)	O2—Ag1—O1W	121.279(315)

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^aSymmetry transformation for N1; $x, -y, \frac{1}{2}+z$ and for O1 & O2; $\frac{1}{2}+x, \frac{1}{2}+y, z$.

Table S4: Hydrogen bonding distances [\AA] and bond angles [$^\circ$] for **1**.^b

D—H...A	Symmetry of A	D—H	H...A	D...A	$\angle\text{D—H...A}$
N6—H6A...O3	-x, -y, -z	0.86	2.25	2.989(9)	144
N6—H6B...O2	1/2+x, 1/2+y, z	0.86	2.00	2.818(9)	158
C8—H8...O3	-x, y, 1/2-z	0.93	2.24	3.139(10)	162
C10—H10A...O1	-x, y, 1/2-z	0.97	2.40	3.335(12)	163
C10—H10B...O2W	-1/2+x, -1/2-y, -1/2+z	0.97	2.51	3.213(17)	129

^bWhere D is donor and A is acceptor

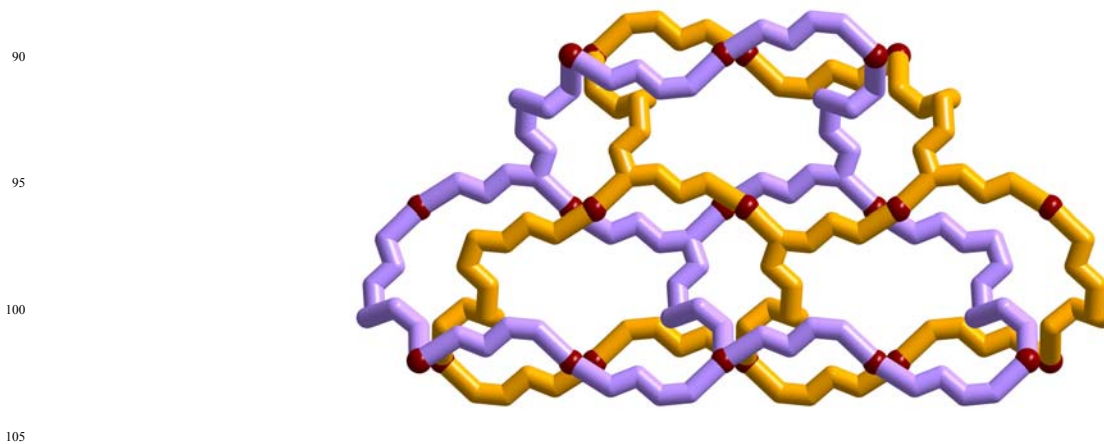


Figure S1. Polycatenated structure in case of **1** as represented with different color codes (silver ions are highlighted and part of the lattice is omitted for clarity).

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Figure S2. HRMS of silver complex 1 of 2-(N9-adeninyl) sulfonic acid in ES (+) mode.

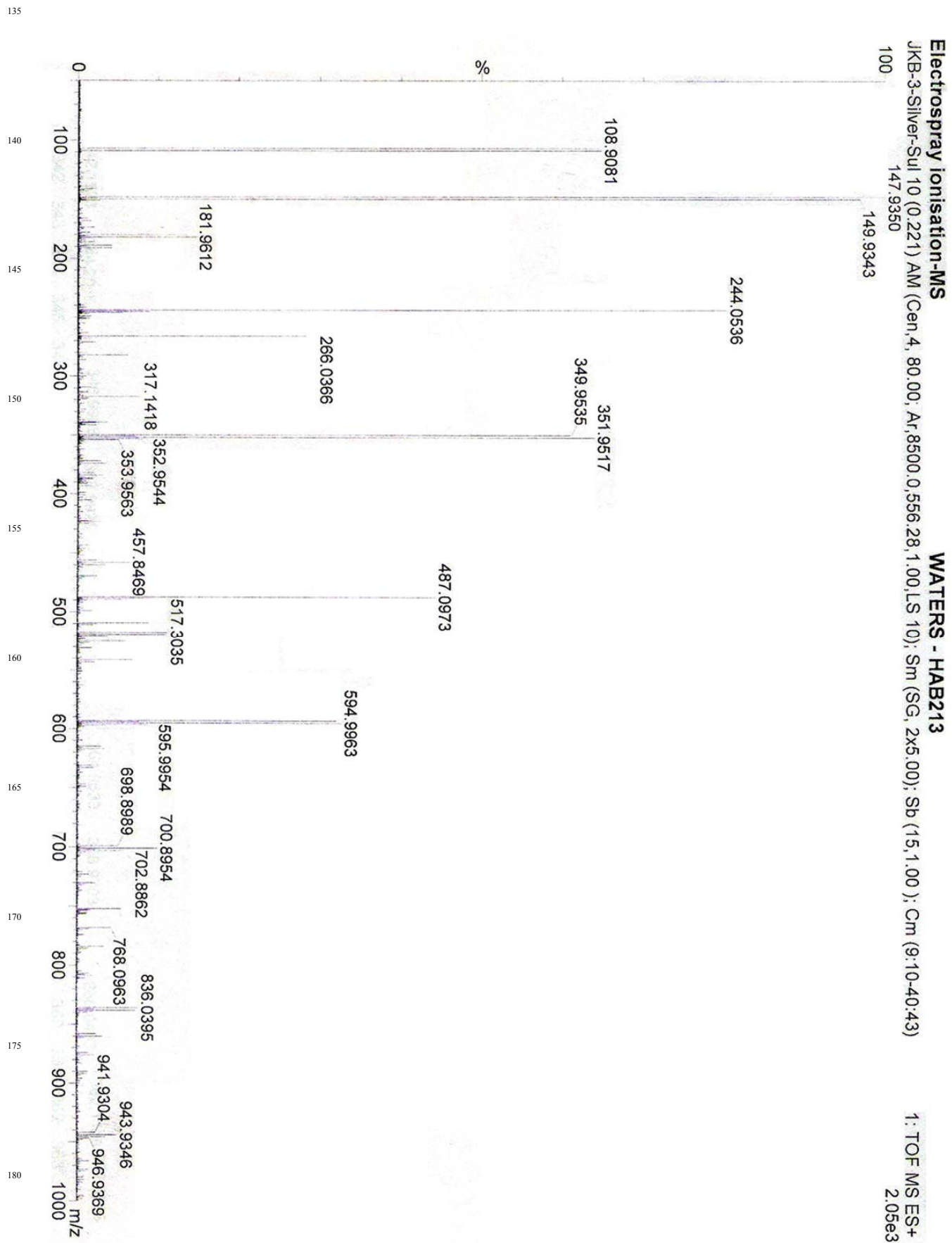
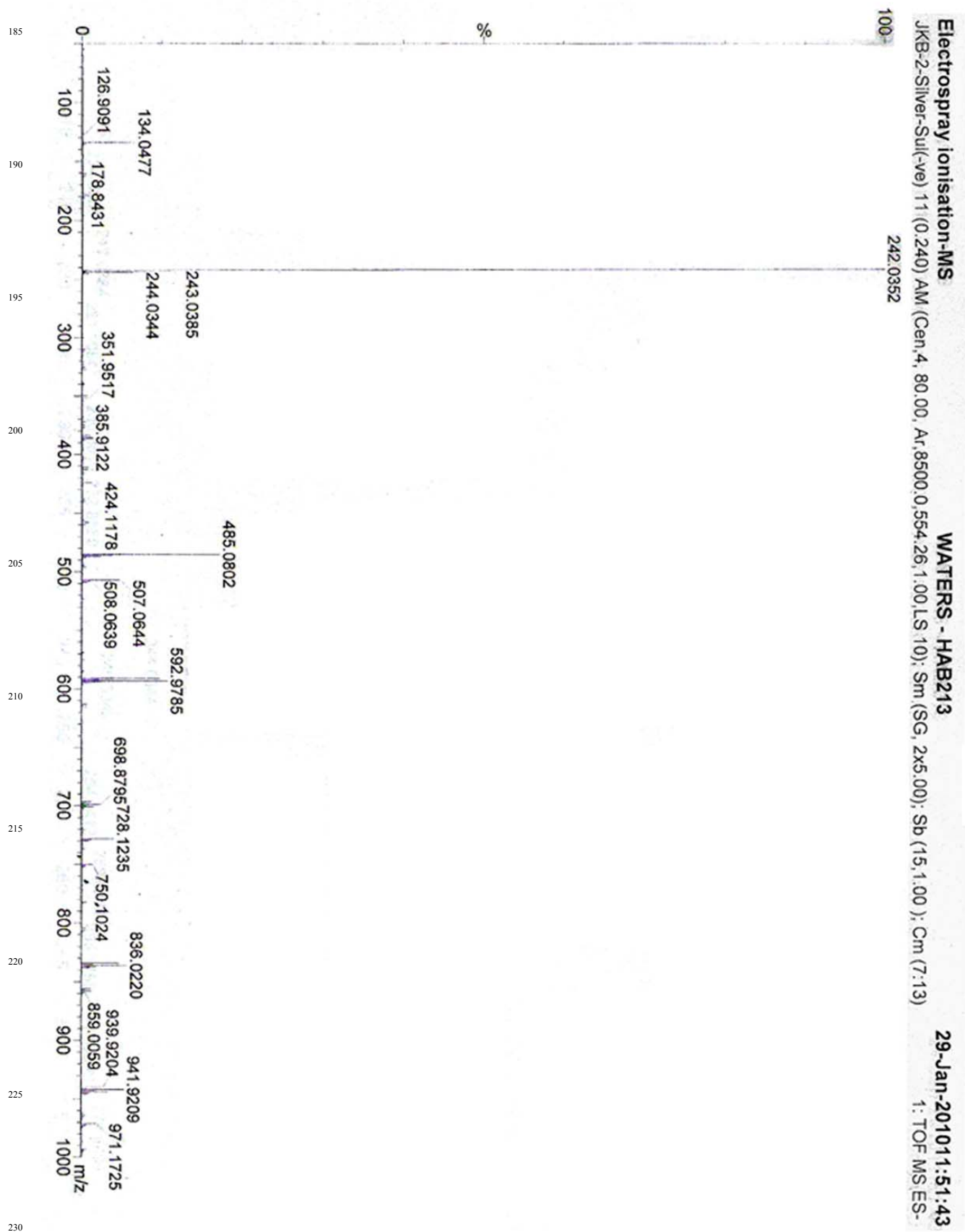


Figure S3. HRMS of silver complex 1 of 2-(N9-adeninyl) sulfonic acid in ES (-) mode.



References:

1. *SAINT+*, 6.02 ed.; Bruker AXS, Madison, WI, 1999.
- 235 2. G. M. Sheldrick, *SADABS 2.0*; University of Göttingen: Göttingen, Germany, 2000.
3. G. M. Sheldrick, *SHELXL-97: Program for Crystal Structure Refinement*; University of Göttingen: Göttingen, Germany, **1997**.