Supporting Information

Serinol in the Solid State: Structural Diversity and Packing Motifs in Free Base and Salt Forms

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Table S1. List of the structures currently present in the Cambridge Structural Database (CSD) containing the serinol molecule.

CSD Refcode	Role of the serinol molecule
AGIHAD	Ligand in the preparation of a Ni substituted Krebs-type sandwich-tungstobismuthates, $\{(serinol)_2Ni_4(BiW_9)_2\}$, with antibacterial activiy.
EXIFOJ	Two protonated serinol molecules are part of the complex organic counter-cation $[Na_5(H_2O)_{18}\{(HOCH_2)_2CHNH_3\}_2]^{7+}$ which crystallizes with the Anderson–Evans type tungstoantimonate anion $[Sb^{V}W^{VI}_6O_{24}]^{7-}$. Serinol acts also as a mild buffering agent during the crystallization process.
MAQWOU	Four protonated serinol molecules coordinate six sodium ions to form the complex organic counter-cation $[Na_6((CH_2OH)_2CHNH_3)_4]^{10+}$ which counterbalance the paradodecatungstate B anion $[W12O40(OH)2]^{10-}$ in the $[Na_6(C_3H_{10}NO_2)_4][W_{12}O_{40}(OH)_2]\cdot 10H_2O$ compound.
ORABUH	Co-crystallization agent of the nonsteroidal-anti-inflammatory-drug flufenamic acid. The crystallization process leads to the formation of a simple organic salt which can form both hydro- and organo-gels.
YAWLIU	Co-crystallization agent of the nonsteroidal-anti-inflammatory-drug tolfenamic acid. The two compounds form a gelator salt which can form gels with chlorobenzene and bromobenzene.

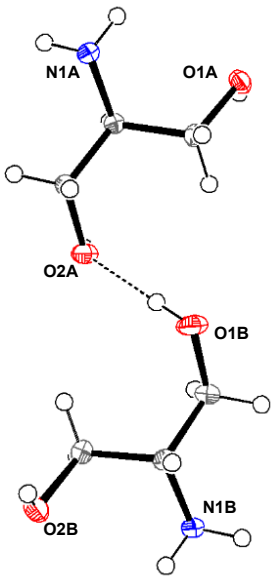

Figure S1. Ortep representations of **SFB** asymmetric units with labels on the heteroatoms. Color code: C, grey; N, blue; O, red; Cl, green; H, white. Ellipsoids are drawn at 50% probability.

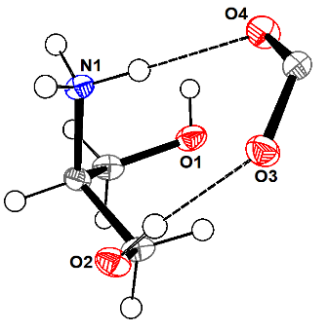

Figure S2. Ortep representations of **SOx** asymmetric units with labels on the heteroatoms. Color code: C, grey; N, blue; O, red; Cl, green; H, white. Ellipsoids are drawn at 50% probability.

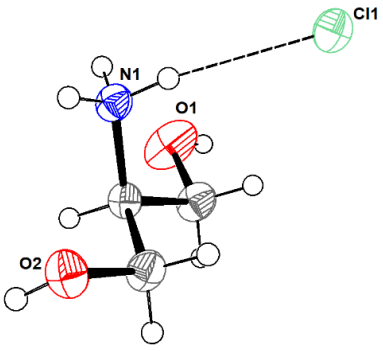

Figure S3. Ortep representations of **SHCl** asymmetric units with labels on the heteroatoms. Color code: C, grey; N, blue; O, red; Cl, green; H, white. Ellipsoids are drawn at 50% probability.

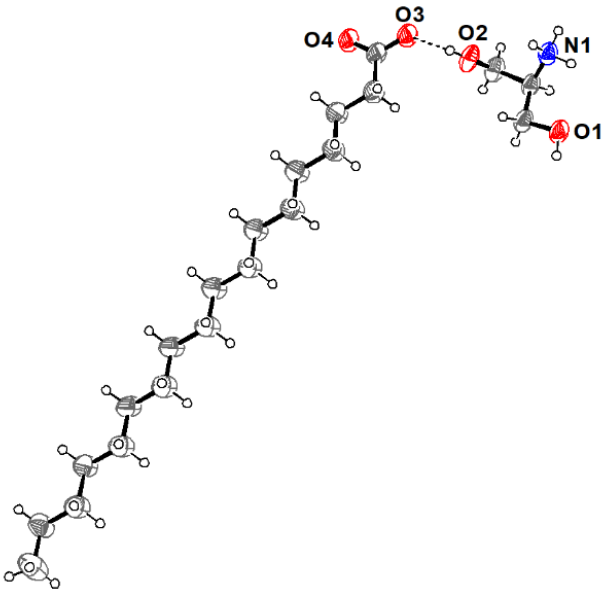

Figure S4. Ortep representations of **SSt** asymmetric units with labels on the heteroatoms. Color code: C, grey; N, blue; O, red; Cl, green; H, white. Ellipsoids are drawn at 50% probability.

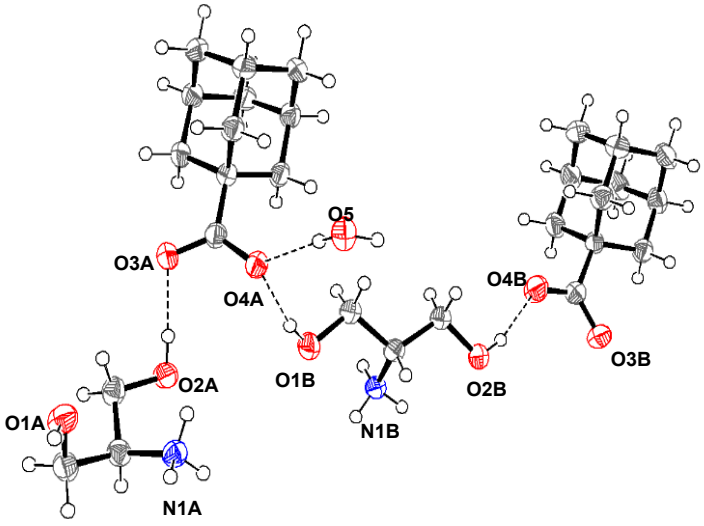

Figure S5. Ortep representations of **SAd** asymmetric units with labels on the heteroatoms. Color code: C, grey; N, blue; O, red; Cl, green; H, white. Ellipsoids are drawn at 50% probability.

Table S2. Distances [Å], angles [°] and type for hydrogen bond intermolecular interactions observed in SFB and in the salts discussed in this work.

Chemical compound	N°	Interaction type D-H⋯A	Distance / Å D(-H) ⋯ A	Angle / ° D-H-A
SFB	1	O1 -H7⋯ N1[1]	2.7697(17)	179(3)
	2	O2 -H8⋯ N2[2]	2.7321(17)	175(2)
	3	O3- H9 ⋯ O2	2.6601(17)	174(2)
	4	O4- H10⋯ O3[3]	2.7146(16)	170(2)
	5	N1- H11⋯ O1[4]	3.1446(19)	173(2)
	6	N1- H12⋯ O4[5]	3.1288(15)	158(2)
	7	N2- H13⋯ O4[6]	3.153(2)	174(2)
	8	N2- H14⋯ O1[7]	3.1239(15)	157(2)
[1]1/2-X,1/2+Y,1/2+Z; [2]1-X,2-Y,-1/2+Z; [3]1-X,1-Y,-1/2+Z; [4]+X,+Y,-1+Z; [5]-1/2+X,3/2-Y,+Z; [6]+X,+Y,1+Z; [7]1/2+X,3/2-Y,+Z				
SOx	1	O1- H1⋯ O2[3]	2.6867(7)	177.1
	2	O2- H2⋯ O3	2.6264(7)	172.2
	3	N1- H4⋯ O3[4]	2.8371(7)	166.5(10)
	4	N1- H4⋯ O4[5]	3.1025(8)	118.7(8)
	5	N1- H5⋯ O4	2.8006(8)	166.8(11)
	6	N1- H6⋯ O3[6]	3.0490(8)	153.0(10)
	7	N1- H6⋯ O4[1]	3.0107(8)	134.0(9)
[1]+X,-1+Y,+Z; [2]1/2-X,-1/2+Y,1/2-Z; [3]-1/2+X,1/2+Y,+Z; [4]-1/2+X,-1/2+Y,+Z; [5]1/2-X,3/2-Y,1-Z; [6]1-X,1-Y,1-Z				
SHCl	1	N1- H5⋯ Cl1	3.2935(9)	169.9(16)
	2	O2- H3⋯ Cl1[1]	3.2106(8)	163.3(18)
	3	N1- H4⋯ Cl1[2]	3.2634(8)	155.3(13)
	4	N1- H6⋯ O2[3]	2.9353(11)	148.2(17)
	5	O1- H1⋯ Cl1[4]	3.2204(9)	165.4(18)
[1]1/2+X,1/2-Y,1/2+Z; [2]+X,-1+Y,+Z; [3]1/2-X,-1/2+Y,5/2-Z; [4]1/2-X,-1/2+Y,3/2-Z				
SSt	1	O2- H4B⋯ O3	2.602(4)	177(6)
	2	N1- H4C⋯ O2[1]	2.791(5)	154(4)
	3	N1- H4D⋯ O1[2]	2.741(5)	143(4)
	4	N1- H4E⋯ O3[3]	2.701(5)	149(4)
	5	O1- H4A⋯ O4[4]	2.646(5)	166(4)
[1]-X,-Y,-Z; [2]-X,-1-Y,-Z; [3]-1-X,-Y,-Z; [4]1+X,-1+Y,+Z				
SAd	1	O1- H1 ⋯ O8[1]	2.725(3)	165.0
	2	O3- H3 ⋯ O8	2.754(3)	168.4
	3	O4- H4 ⋯ O6	2.615(3)	164.2
	4	N1- H2A⋯ O9[1]	2.822(3)	175(4)
	5	N1- H2B⋯ O1[2]	2.887(3)	173(4)
	6	N1- H2C⋯ O5[3]	2.739(3)	175(4)
	7	N2- H5A⋯ O3[4]	2.848(3)	149(3)
	8	N2- H5B⋯ O5[5]	2.726(3)	164(4)
	9	N2- H5C⋯ O2[4]	2.817(3)	157(4)
	10	O2- H6 ⋯ O7	2.675(3)	176(4)
	11	O9- H7 ⋯ O8	2.745(3)	168(4)
	12	O9- H8 O7[6]	2.762(3)	167(3)
[1]1-X,-1/2+Y,1/2-Z; [2]1-X,1/2+Y,1/2-Z; [3]1-X,1-Y,1-Z; [4]1-X,-Y,1-Z; [5]+X,-1+Y,+Z; [6]+X,1+Y,+Z				

Table S3. Torsional angles of SFB and its salts.

Chemical compound	Atoms A B C D	Angle / °
SFB	C1 C2 C3 O2	-61.88(16)
	C4 C5 C6 O4	-172.42(11)
	N1 C2 C3 O2	177.80(12)
	N2 C5 C6 O4	68.48(15)
	O1 C1 C2 C3	176.21(11)
	O1 C1 C2 N1	-64.39(14)
	O3 C4 C5 C6	69.31(15)
	O3 C4 C5 N2	-170.96(12)
SOx	O1 C1 C2 N1	60.71(7)
	O1 C1 C2 C3	-59.82(7)
	N1 C2 C3 O2	53.69(7)
	C1 C2 C3 O2	175.19(5)
SHCl	O1 C1 C2 N1	-58.01(12)
	O1 C1 C2 C3	179.79(9)
	N1 C2 C3 O2	58.62(10)
	C1 C2 C3 O2	-179.39(8)
SSt	C1 C2 C3 O2	63.7(6)
	O1 C1 C2 C3	-173.5(4)
	O1 C1 C2 N1	-52.9(5)
	O3 C4 C5 C6	-176.9(4)
	O4 C4 C5 C6	3.7(7)
	N1 C2 C3 O2	-57.5(5)
SAd	C1 C2 C3 O2	168.4(2)
	C4 C5 C6 O4	179.5(2)
	N1 C2 C3 O2	46.9(3)
	N2 C5 C6 O4	-57.4(3)
	O1 C1 C2 C3	-63.9(3)
	O1 C1 C2 N1	57.8(3)
	O3 C4 C5 N2	-172.8(2)
	O3 C4 C5 N2	65.2(3)

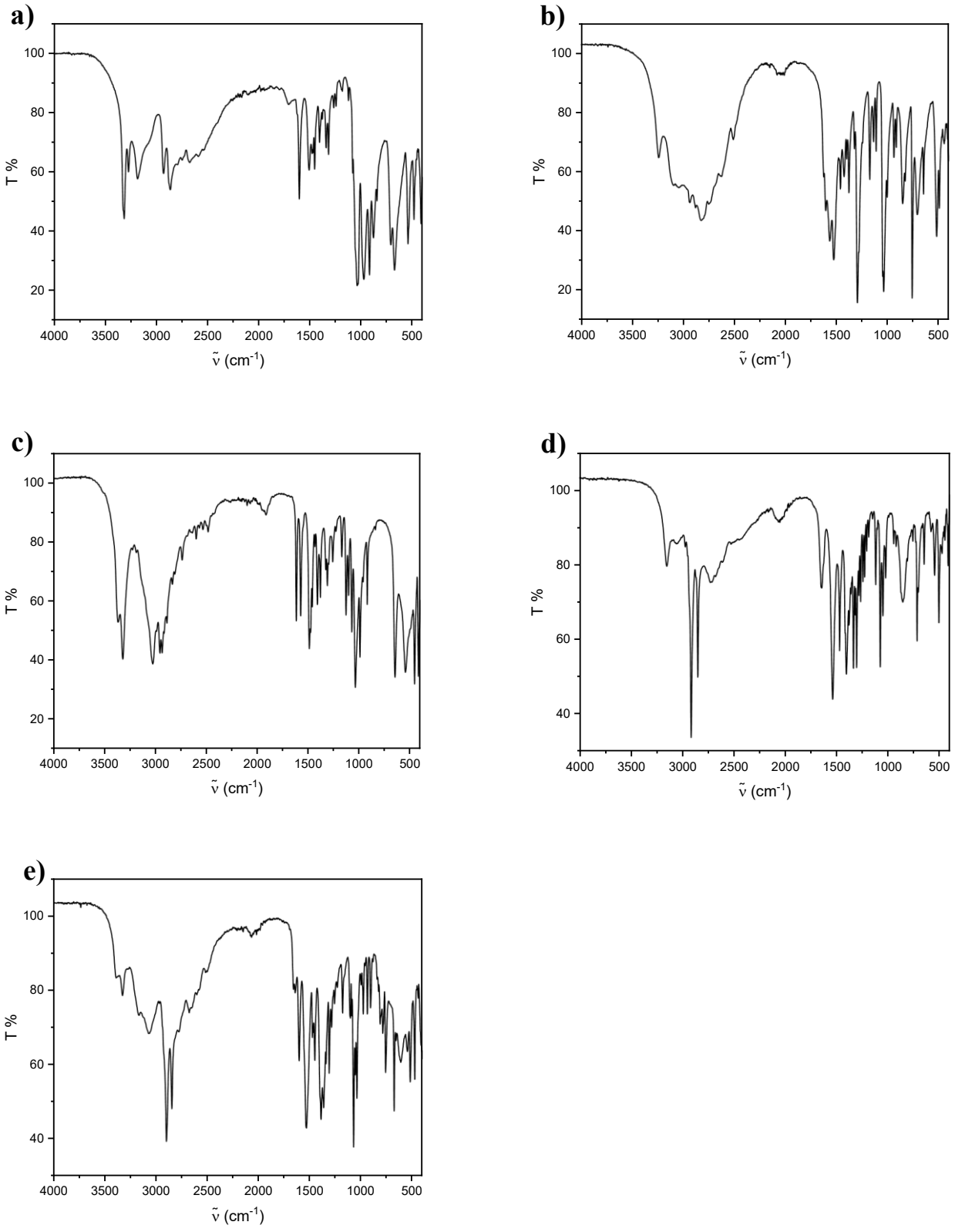

Figure S6. FT-IR spectra of (a) **SFB,** (b) **SOx**, (c) **SHCl**, (d) **SSt** and (e) **SAd**.

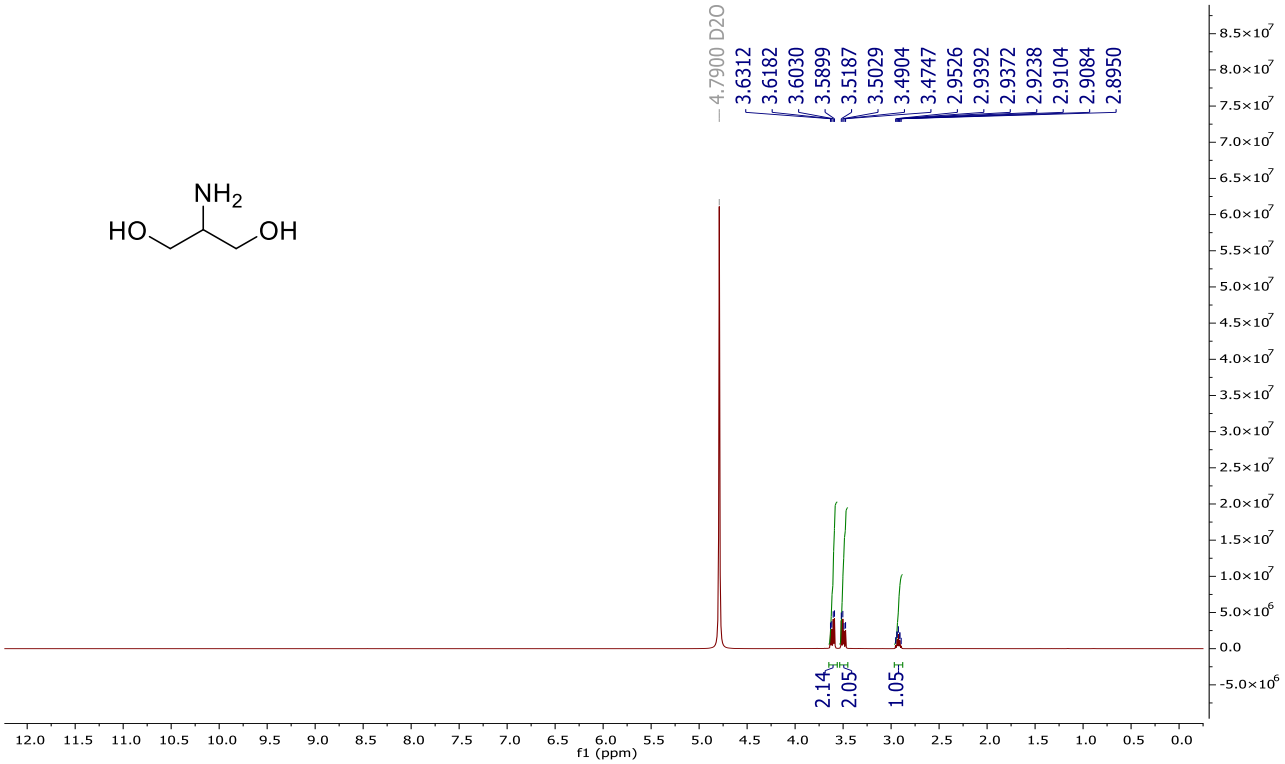

Figure S7. [1]H NMR s pectrum of ***SFB***.

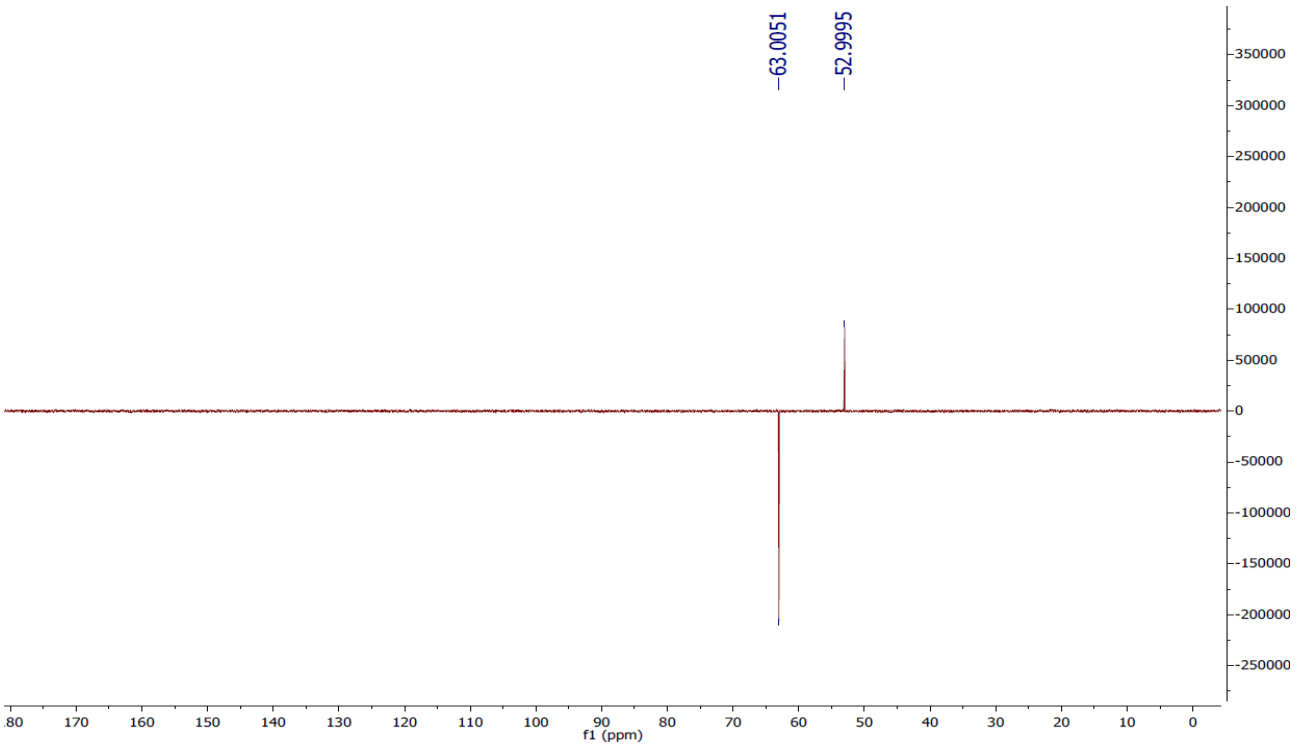

Figure S8. [13]C APT NMR spectrum of ***SFB***.

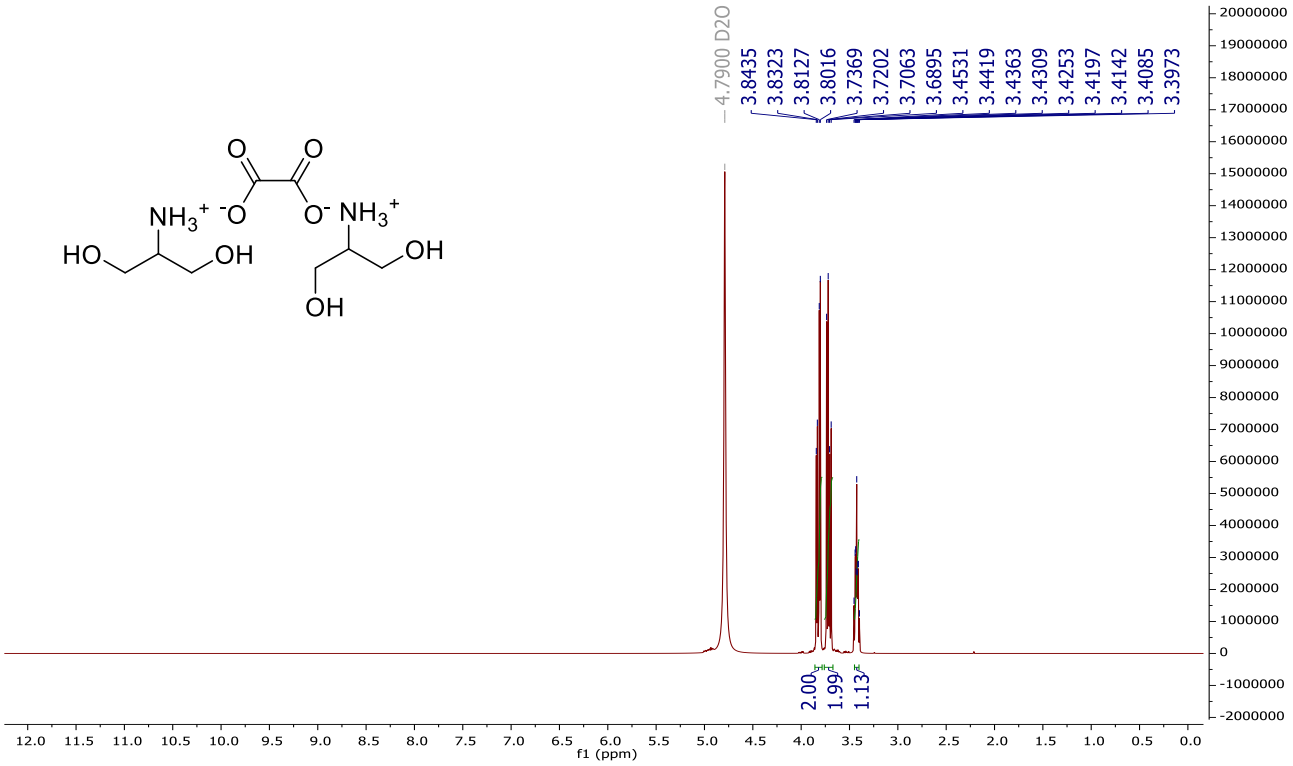

Figure S9. ^{1}H NMR spectrum of ***SOx***.

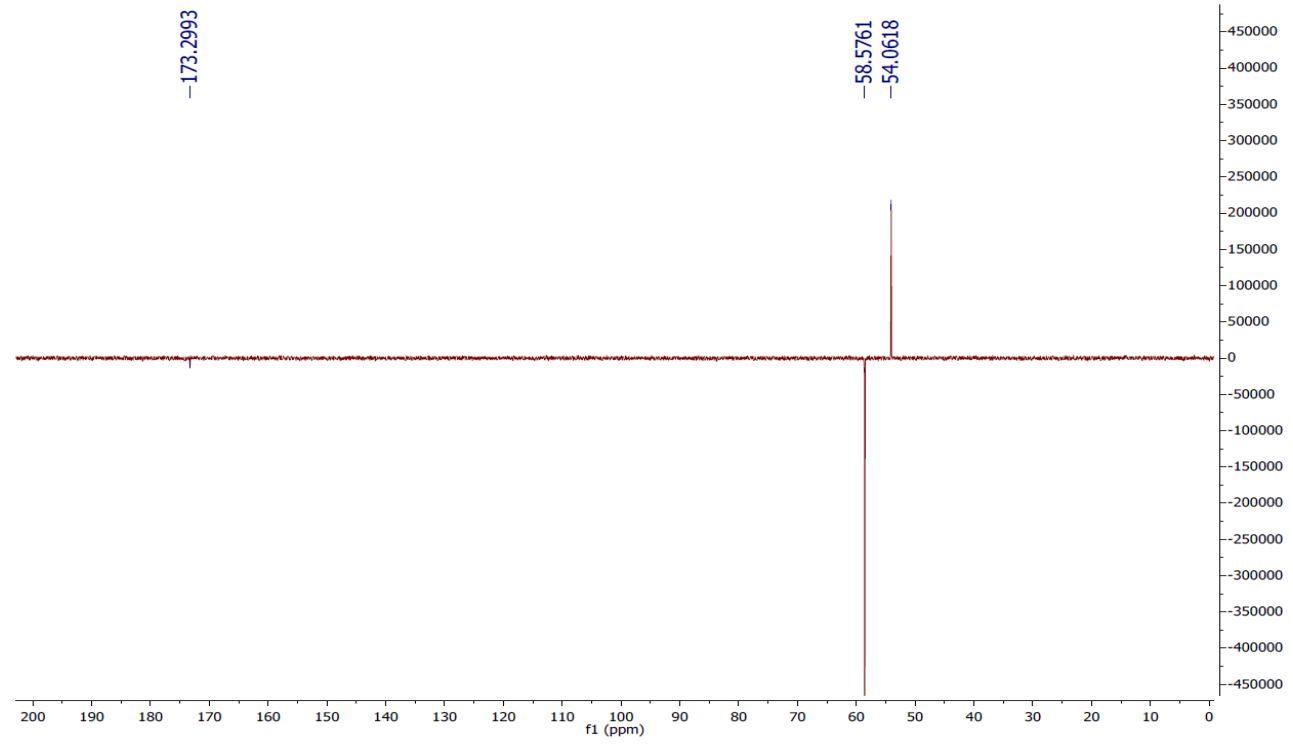

Figure S10. ^{13}C APT NMR spectrum of ***SOx***.

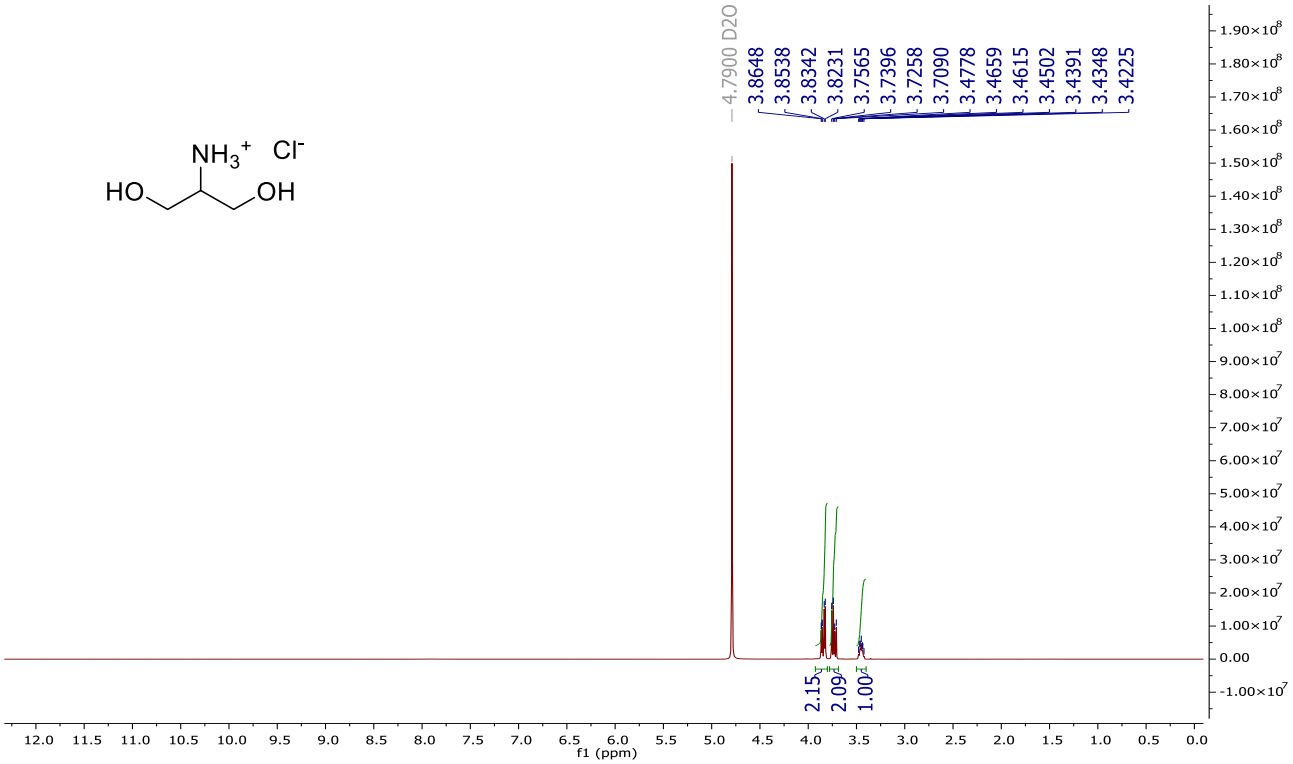

Figure S11. ^{1}H NMR spectrum of ***SHCl***.

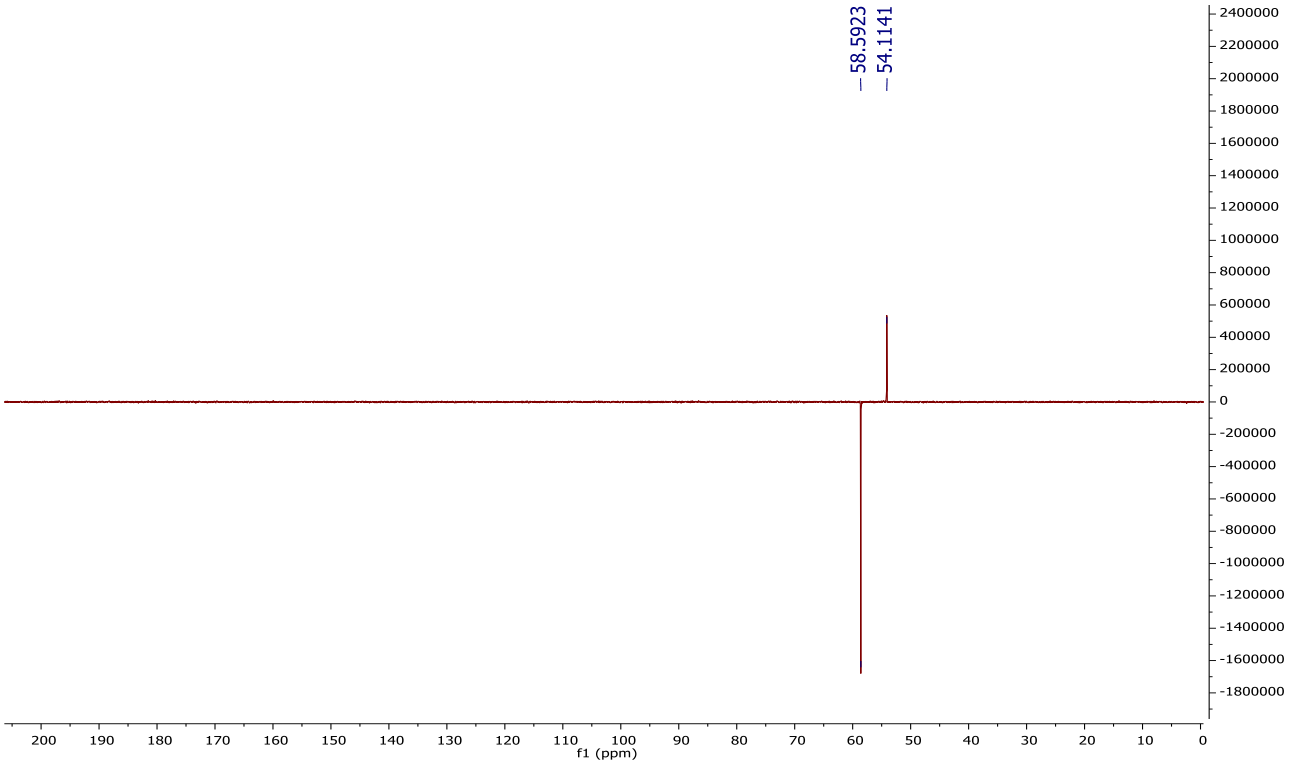

Figure S12. ^{13}C APT NMR spectrum of ***SHCl***.

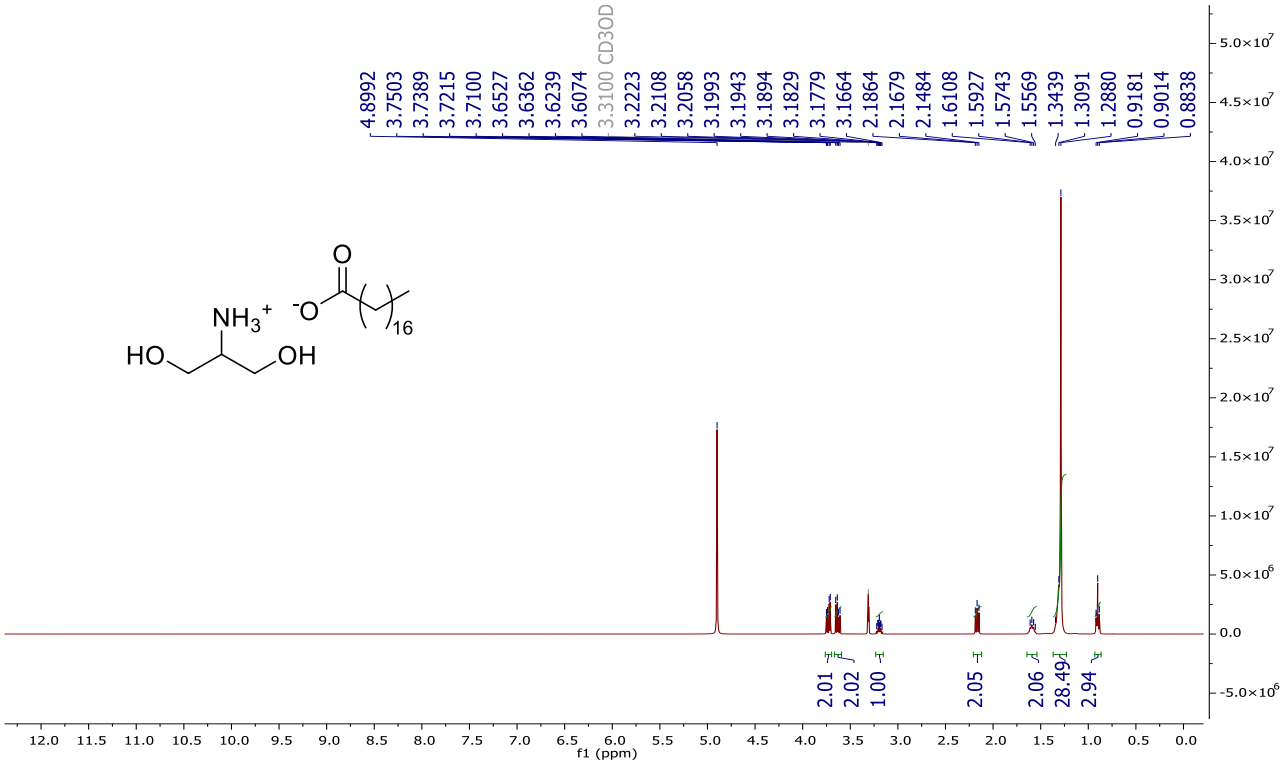

Figure S13. ^{1}H NMR spectrum of ***SSt***.

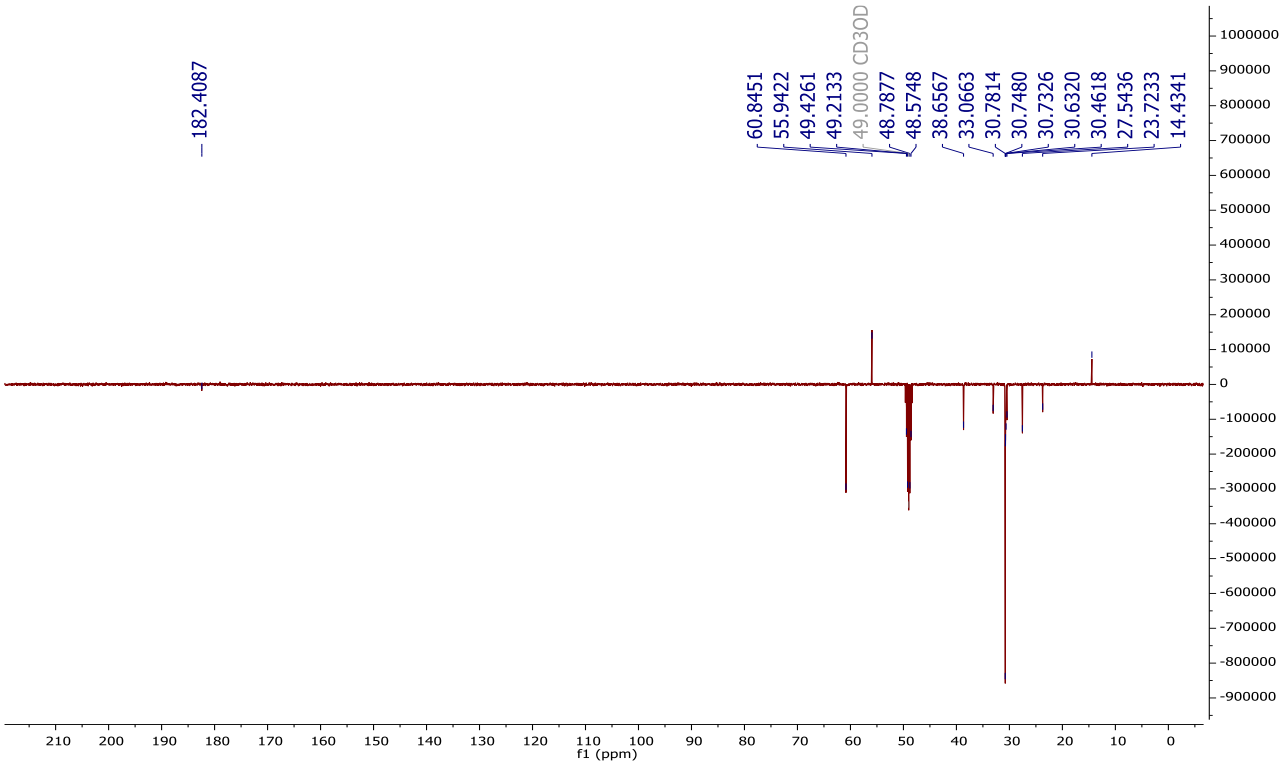

Figure S14. ^{13}C APT NMR spectrum of ***SSt***.

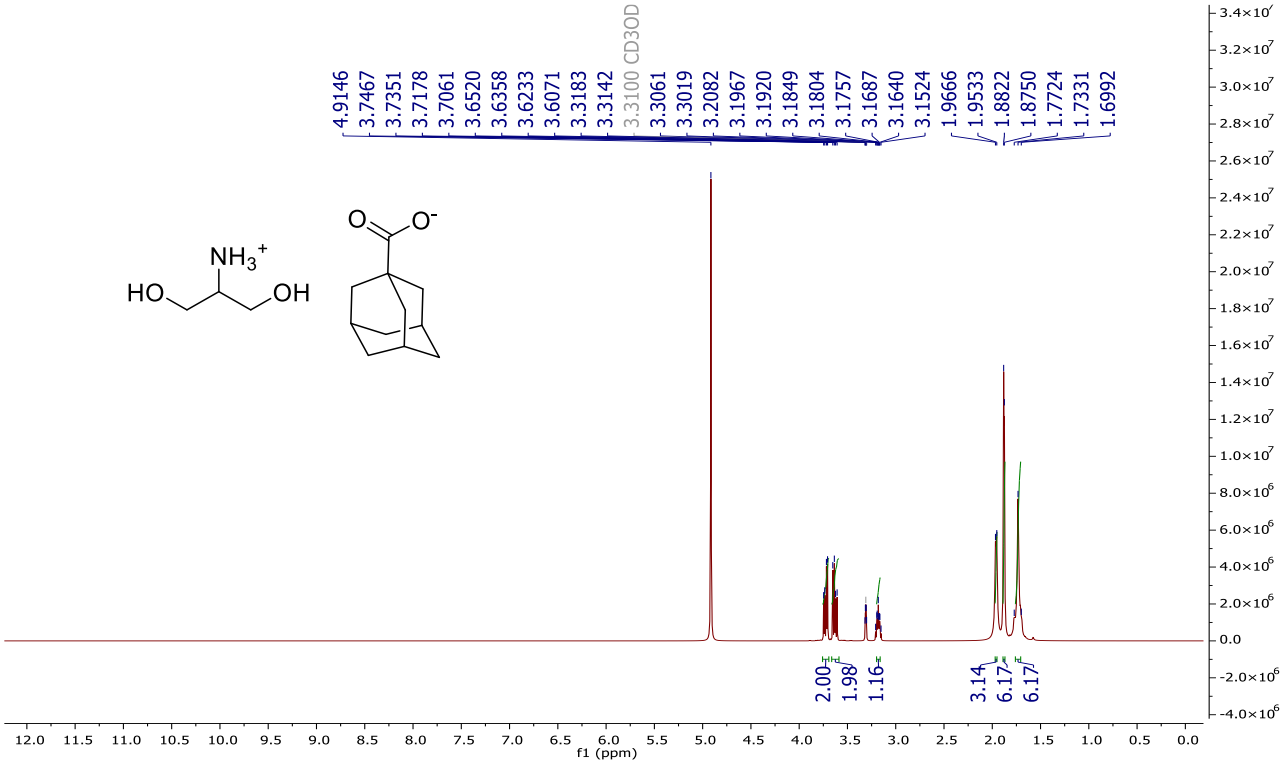

Figure S15. ^{1}H NMR spectrum of ***SAd***.

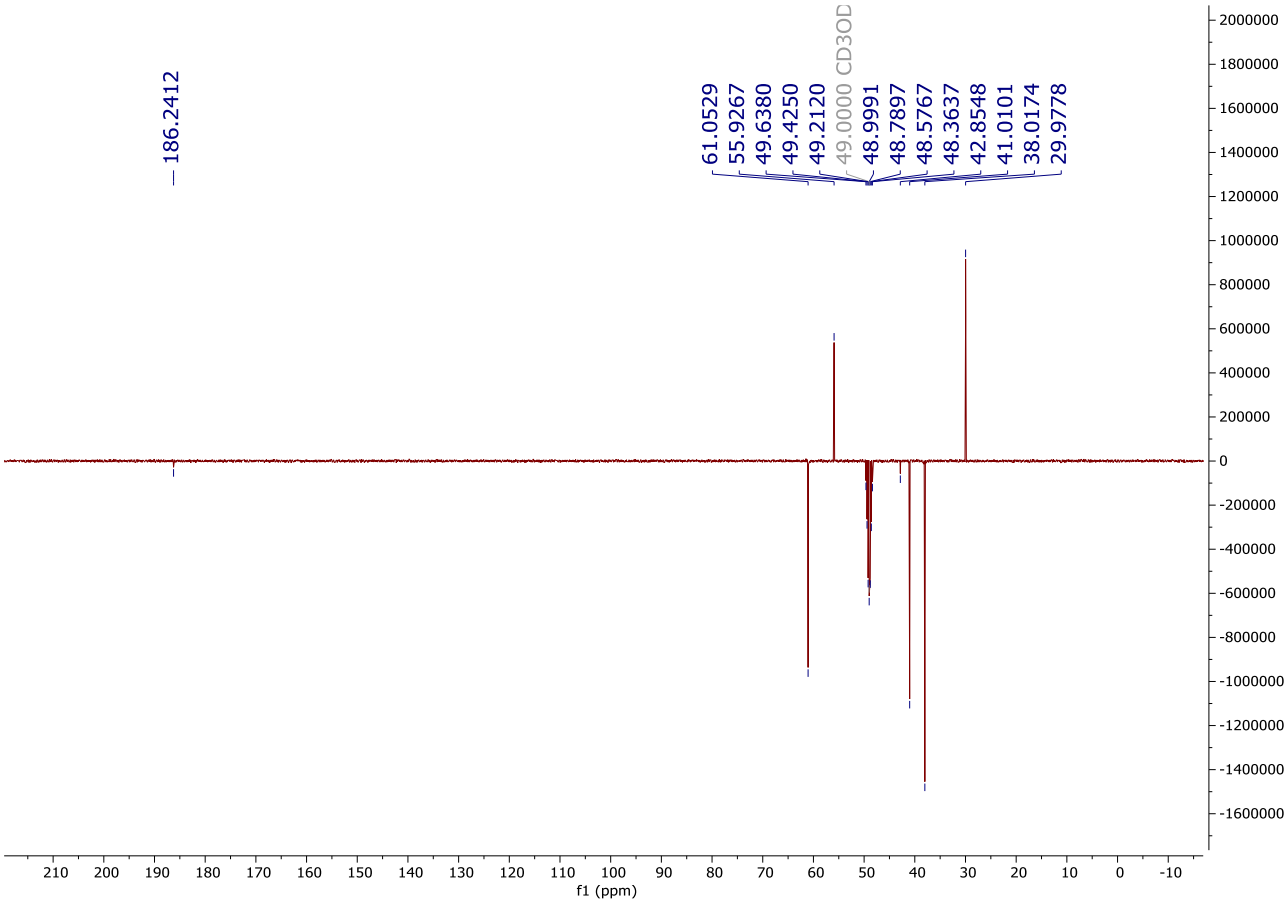

Figure S16. ^{13}C APT NMR spectrum of ***SAd***.