Supplementary Table 1a Observed and optimized parameter values of title compounds. [Bond length in (Å).]

HMTSA			3MASSA			4MAHS			2AAHM			4EAHM		
Atoms	**XRD**	**DFT**	**Atoms**	**XRD**	**DFT**	**Atoms**	**XRD**	**DFT**	**Atoms**	**XRD**	**DFT**	**Atoms**	**XRD**	**DFT**
O(1)-C(1)	1.270(5)	1.333	**O1A- C1A**	1.297(3)	1.351	**O1-C1**	1.286(3)	1.330	**O1-C1**	1.253(3)	1.342	**O1- C1**	1.223(6)	1.216
O(2)-C(1)	1.188(5)	1.225	**O2A- C1A**	1.211(3)	1.212	**O2-C1**	1.229(3)	1.227	**O2-C1**	1.249(3)	1.208	**O2-C1**	1.256(6)	1.325
C(1)-C(2)	1.509(4)	1.516	**C1A- C2A**	1.497(3)	1.514	**C1-C2**	1.495(3)	1.517	**C1-C2**	1.509(3)	1.536	**C1-C2**	1.519(6)	1.539
C(2)-C(3)	1.405(5)	1.476	**C2A- C3A**	1.509(3)	1.537	**C2-C3**	1.508(3)	1.537	**C2-C3**	1.482(4)	1.546	**C2-C3**	1.512(2)	1.558
C(3)-C(4)	1.500(4)	1.509	**C3A- C4A**	1.502(3)	1.517	**C3-C4**	1.511(3)	1.529	**C3-C4**	1.513(4)	1.526	**C3-C4**	1.519(4)	1.507
O(3)-C(4)	1.170(4)	1.214	**O3A- C4A**	1.286(3)	1.220	**O3-C4**	1.257(3)	1.267	**O3-C4**	1.200(3)	1.213	**O3 -C4**	1.310(4)	1.341
O(4)-C(4)	1.301(4)	1.358	**O4A- C4A**	1.221(2)	1.305	**O4-C4**	1.253(3)	1.25	**O4-C4**	1.304(3)	1.347	**O4- C4**	1.195(4)	1.221
N(1)-C(6)	1.474(3)	1.468	**O1B- C1B**	1.272(2)	1.270	**O5-C5**	1.300(3)	1.343	**O5 -C3**	1.425(3)	1.412	**O5-C2**	1.392(5)	1.400
N(1)-C(7)	1.473(3)	1.476	**O2B- C1B**	1.240(2)	1.268	**O6-C5**	1.217(3)	1.220	**N1-C5**	1.462(3)	1.429	**N1-C5**	1.459(1)	1.434
N(1)-C(10)	1.479(3)	1.477	**C1B- C2B**	1.495(3)	1.522	**C5-C6**	1.497(3)	1.510	**C5-C6**	1.371(4)	1.401	**C5-C6**	1.395(1)	1.394
N(2)-C(7)	1.448(3)	1.479	**C2B- C3B**	1.496(3)	1.542	**C6-C7**	1.514(3)	1.540	**C6-C7**	1.401(4)	1.399	**C6-C7**	1.397(8)	1.398
N(2)-C(5)	1.451(3)	1.469	**C3B- C4B**	1.507(3)	1.529	**C7-C8**	1.502(3)	1.527	**C7-C8**	1.360(5)	1.394	**C7-C8**	1.348(8)	1.398
N(2)-C(8)	1.462(3)	1.478	**O3B- C4B**	1.240(2)	1.346	**O7-C8**	1.227(3)	1.255	**C8-C9**	1.359(5)	1.394	**C8-C9**	1.375(8)	1.403
N(3)-C(5)	1.473(3)	1.488	**O4B- C4B**	1.269(3)	1.211	**O8-C8**	1.281(3)	1.275	**C9-C10**	1.374(5)	1.394	**C9-C10**	1.381(8)	1.387
N(3)-C(6)	1.472(3)	1.476	**N1A- C5A**	1.463(3)	1.467	**N1-C9**	1.461(3)	1.485	**C5-C10**	1.380(4)	1.396	**C10-C5**	1.337(6)	1.401
N(3)-C(9)	1.473(3)	1.477	**C5A- C6A**	1.373(3)	1.392	**C9-C10**	1.365(3)	1.393	**N2-C6**	1.379(4)	1.420	**C8-O6**	1.371(8)	1.366
N(4)-C(8)	1.461(3)	1.469	**C5A- C10A**	1.361(3)	1.393	**C10-C11**	1.387(4)	1.395				**O6 –C11**	1.417(8)	1.426
N(4)-C(9)	1.456(3)	1.477	**C6A- C7A**	1.387(3)	1.401	**C11-C12**	1.372(4)	1.404				**C11-C12**	1.513(7)	1.518
N(4)-C(10)	1.454(3)	1.478	**C7A- C8A**	1.368(4)	1.410	**C12-C13**	1.379(4)	1.408						

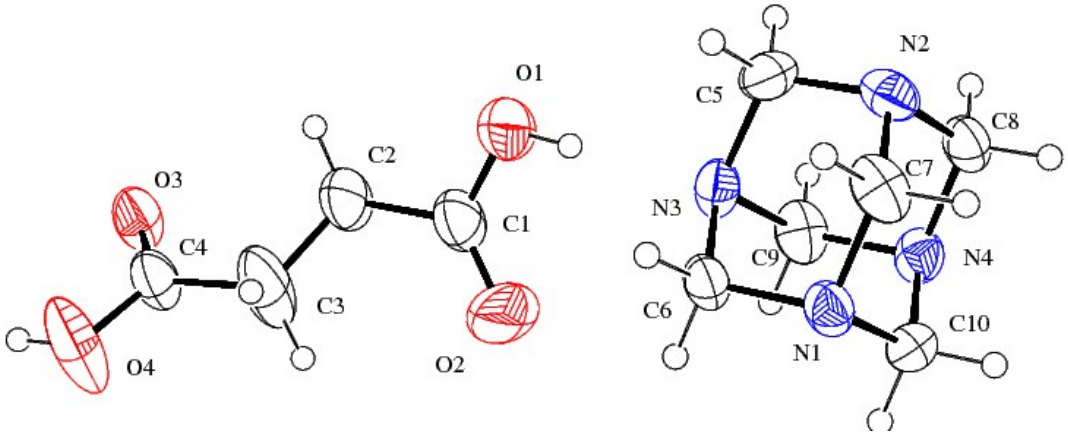
			C7A- C11A	1.487(4)	1.510	**C13-C14**	1.369(4)	1.392						
			C8A- C9A	1.366(4)	1.394	**C14-C9**	1.368(4)	1.410						
			C9A- C10A	1.384(4)	1.396	**C12-O9**	1.365(3)	1.346						
			N1B- C5B	1.465(3)	1.424	**O9-C15**	1.416(4)	1.435						
			C5B- C6B	1.371(3)	1.401	**N2-C16**	1.459(3)	1.479						
			C6B- C7B	1.388(3)	1.392	**C16-C17**	1.368(4)	1.394						
			C7B- C8B	1.375(4)	1.395	**C17-C18**	1.386(4)	1.399						
			C8B- C9B	1.362(4)	1.401	**C18-C19**	1.374(4)	1.409						
			C9B- C10B	1.377(4)	1.394	**C19-C20**	1.377(4)	1.410						
			C5B- C10B	1.372(3)	1.399	**C20-C21**	1.372(4)	1.385						
			C7B- C11B	1.501(4)	1.510	**C21-C16**	1.370(4)	1.399						
						C19-O10	1.361(3)	1.345						
						O10-C22	1.417(4)	1.439						

Supplementary Table 1b Observed and optimized parameter values of title compounds. [Bond angles in (º).]

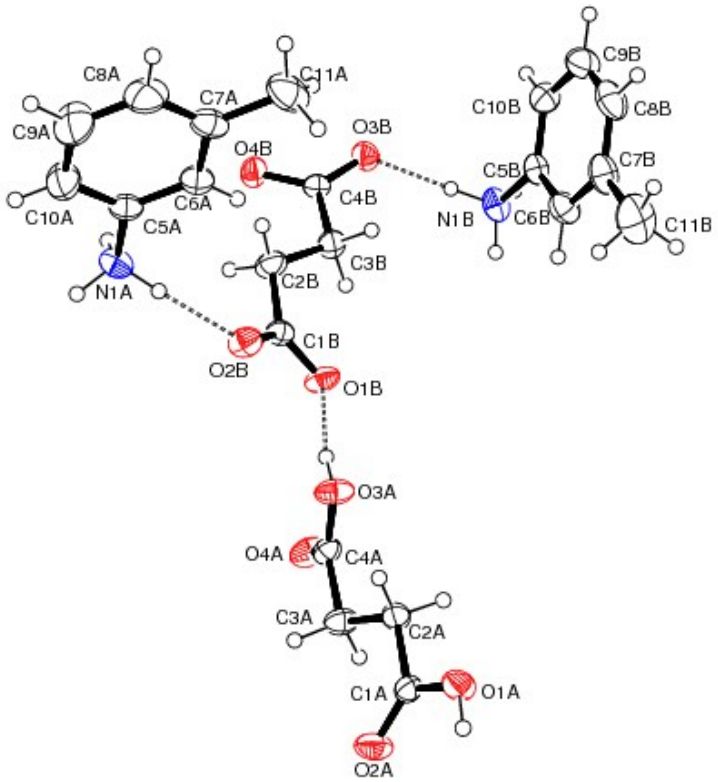
HMTSA			3MASSA			4MAHS			2AAHM			4EAHM		
Atoms	**XRD**	**DFT**	**Atoms**	**XRD**	**DFT**	**Atoms**	**XRD**	**DFT**	**Atoms**	**XRD**	**DFT**	**Atoms**	**XRD**	**DFT**
O(2)-C(1)-O(1)	122.6(3)	123.54	**O1A- C1A- O2A**	123.1(19)	122.71	**O1-C1-O2**	122.4(2)	124.21	**O1-C1-O2**	124.8(2)	122.11	**O1-C1-O2**	122.2(7)	123.21
O(2)-C(1)-C(2)	123.5(4)	124.0	**O1A- C1A- C2A**	114.1(18)	112.13	**C1-C2-C3**	115.9(2)	115.95	**O1-C1-C2**	118.6(2)	116.18	**O1-C1-C2**	119.6(5)	119.48
O(1)-C(1)-C(2)	113.9(3)	112.45	**O2A- C1A- C2A**	122.7(19)	125.13	**C2-C3-C4**	114.1(2)	112.62	**O2-C1-C2**	116.6(2)	121.67	**O2-C1-C2**	118.2(5)	117.27
C(3)-C(2)-C(1)	111.7(3)	112.57	**C1A- C2A- C3A**	114.4(18)	111.43	**O3-C4-O4**	124.0(2)	122.50	**C1-C2-C3**	116.2(2)	114.38	**C1-C2-C3**	112.3(3)	109.44
C(2)-C(3)-C(4)	117.9(3)	112.79	**C2A- C3A- C4A**	114.6(18)	112.81	**O1-C1-C2**	116.1(2)	115.15	**C2-C3-C4**	111.9(2)	109.68	**C2-C3-C4**	110.5(2)	111.26
O(3)-C(4)-O(4)	123.1(4)	122.10	**O3A- C4A- O4A**	123.7(19)	123.86	**O2-C1-C2**	121.4(2)	120.59	**O3-C4-O4**	124.0(2)	122.76	**C3-C4-O4**	124.0(5)	123.98
O(3)-C(4)-C(3)	125.1(4)	126.36	**O3A- C4A- C3A**	115.7(17)	112.94	**C3-C4-O3**	117.0(2)	118.75	**O3-C4-C3**	123.2(2)	126.03	**C3-C4-O3**	112.2(4)	113.79
O(4)-C(4)-C(3)	111.6(3)	111.53	**O4A- C4A- C3A**	120.4(19)	123.18	**C3-C4-O4**	118.9(2)	118.70	**O4-C4-C3**	112.8(2)	111.17	**O5-C2-C1**	111.5(4)	109.69
C(6)-N(1)-C(7)	108.1(18)	108.39	**O1B- C1B- O2B**	122.8(18)	125.47	**O5-C5-O6**	123.8(2)	122.09	**O5-C3-C2**	112.2(2)	112.13	**O5-C2-C3**	108.5(3)	111.01
C(6)-N(1)-C(10)	107.8(17)	108.25	**O1B- C1B- C2B**	117.2(17)	117.62	**C6-C5-O5**	114.0(2)	113.99	**O5-C3-C4**	106.4(2)	112.01	**C7-C8-O6**	126.9(8)	124.99
C(7)-N(1)-C(10)	107.7(17)	108.24	**O2B- C1B- C2B**	119.9(19)	116.82	**O6-C5-C6**	122.2(2)	123.87	**C6-C5-C10**	121.6(3)	119.84	**O6-C8-C9**	115.6(9)	115.77
C(7)-N(2)-C(5)	108.3(19)	108.26	**C1B- C2B- C3B**	116.4(19)	114.35	**C7-C8-O7**	120.5(2)	118.60	**N1-C5-C6**	119.5(2)	120.19	**O4-C4-O3**	123.8(5)	122.22
C(7)-N(2)-C(8)	108.8(18)	107.97	**C2B- C3B- C4B**	115.8(18)	111.64	**C7-C8-O8**	115.9(2)	114.95	**C5-C6-C7**	117.4(3)	118.95	**N1-C5-C6**	116.5(3)	120.76
C(5)-N(2)-C(8)	107.9(18)	108.26	**O3B- C4B- O4B**	122.9(18)	121.10	**C5-C6-C7**	114.0(2)	114.31	**C6-C7-C8**	120.8(3)	120.88	**N1-C5-C10**	121.6(5)	120.17
C(5)-N(3)-C(9)	107.9(18)	108.12	**O3B- C4B- C3B**	119.7(19)	123.20	**C6-C7-C8**	113.8(2)	112.65	**C7-C8-C9**	120.9(3)	119.89	**C5-C6-C7**	116.8(6)	120.80
C(5)-N(3)-C(6)	108.4(18)	108.12	**O4B- C4B- C3B**	117.2(18)	115.66	**O7-C8-O8**	123.6(2)	126.43	**C9-C10-C5**	119.6(3)	120.59	**C6-C7-C8**	122.6(8)	119.97
C(9)-N(3)-C(6)	107.8(18)	107.70	**N1A- C5A- C6A**	119.2(19)	119.70	**N1-C9-C10**	120.2(2)	118.59	**C8-C9-C10**	119.7(3)	119.77	**C7-C8-C9**	117.4(9)	119.23

C(10)-N(4)-C(9)	108.8(18)	108.25	**N1A- C5A- C10A**	119.4(2)	120.78	**C9-C10-C11**	120.0(2)	119.72	**C5-C6-N2**	120.7(2)	118.57	**C8-C9-C10**	122.4(8)	120.50
C(10)-N(4)-C(8)	108.2(17)	108.25	**C6A- C5A- C10A**	121.3(2)	119.45	**C10-C11-C12**	119.9(3)	119.43	**N2-C6-C7**	121.8(3)	122.42	**C9-C10-C5**	118.6(8)	120.49
C(9)-N(4)-C(8)	108.0(18)	108.32	**C5A- C6A- C7A**	120.7(2)	121.25	**C11-C12-C13**	119.5(3)	120.17	**N1-C5-C10**	118.8(3)	119.90	**C10-C5-C6**	122.0(5)	118.98
N(2)-C(5)-N(3)	112.0(18)	111.89	**C6A- C7A- C8A**	117.8(2)	118.74	**C12-C13-C14**	120.3(3)	120.84				**C8-O6-C11**	116.8(8)	118.58
			C6A- C7A- C11A	120.8(2)	119.99	**C13-C14-C9**	120.2(3)	118.02				**O6-C11-C12**	106.0(8)	107.57
			C8A- C7A- C11A	121.3(2)	121.22	**C14-C9-C10**	120.1(2)	121.77						
			C7A- C8A- C9A	121.2(2)	120.22	**C14-C9-N1**	119.6(2)	119.61						
			C8A- C9A- C10A	121.1(3)	120.86	**C12-O9-C15**	117.6(2)	118.55						
			C5A- C10A- C9A	117.9(3)	119.48	**N2-C16-C17**	120.6(2)	120.11						
			N1B- C5B- C6B	119.3(2)	119.68	**C16-C17-C18**	120.0(3)	119.32						
			N1B- C5B- C10B	119.4(2)	118.54	**C17-C18-C19**	120.0(3)	119.46						
			C6B- C5B- C10B	121.2(2)	121.76	**C18-C19-C20**	119.4(3)	120.12						
			C5B- C6B- C7B	120.1(2)	120.12	**C19-C20-C21**	120.4(3)	120.35						
			C6B- C7B- C8B	118.1(2)	118.20	**C20-C21-C16**	120.1(3)	118.95						
			C6B- C7B- C11B	119.2(3)	120.58	**C21-C16-N2**	119.4(2)	118.00						
			C8B- C7B- C11B	122.7(2)	121.20	**C19-O10-C22**	118.2(3)	118.11						
			C7B- C8B- C9B	121.6(2)	121.19	**C21-C16-C17**	120.0(2)	121.78						
			C8B- C9B- C10B	120.3(3)	120.51									
			C5B- C10B- C9B	118.7(2)	118.18									

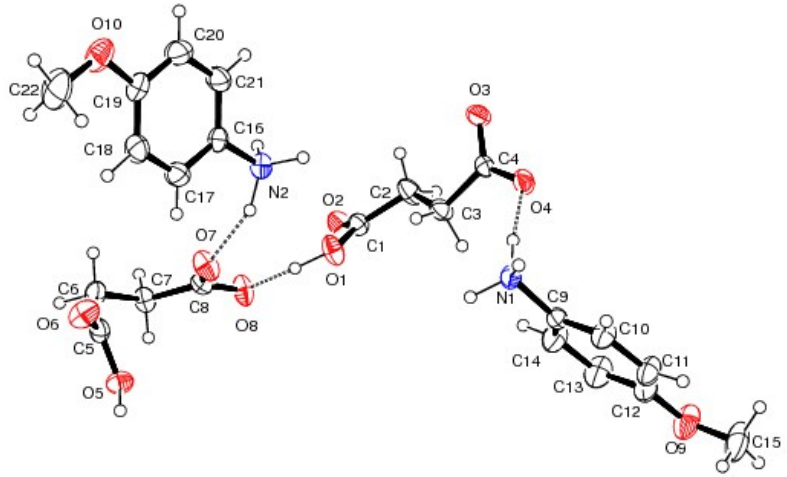
Figure 1-5 ORTEP diagram of compound 1-5



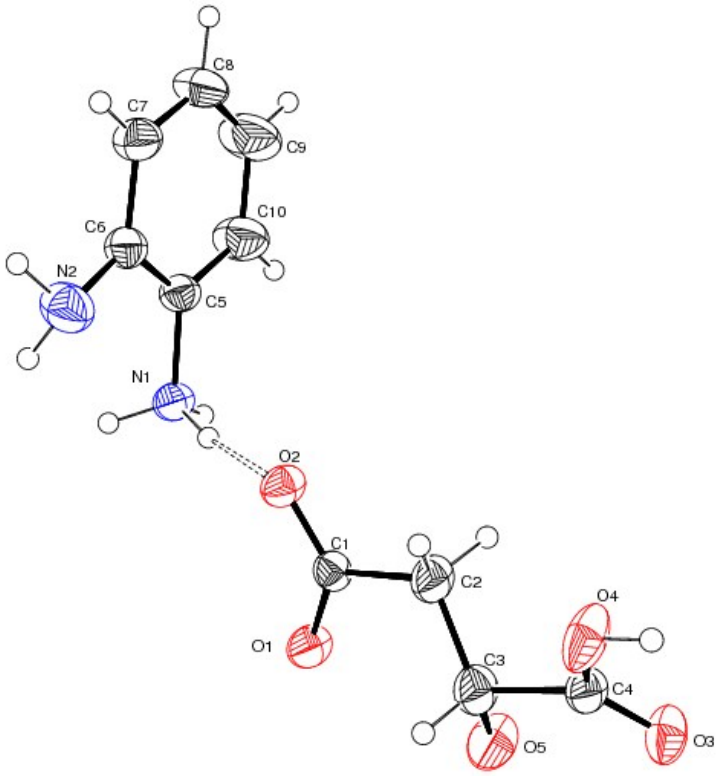
(1) ORTEP of Hexamethylenetetramine succinic acid



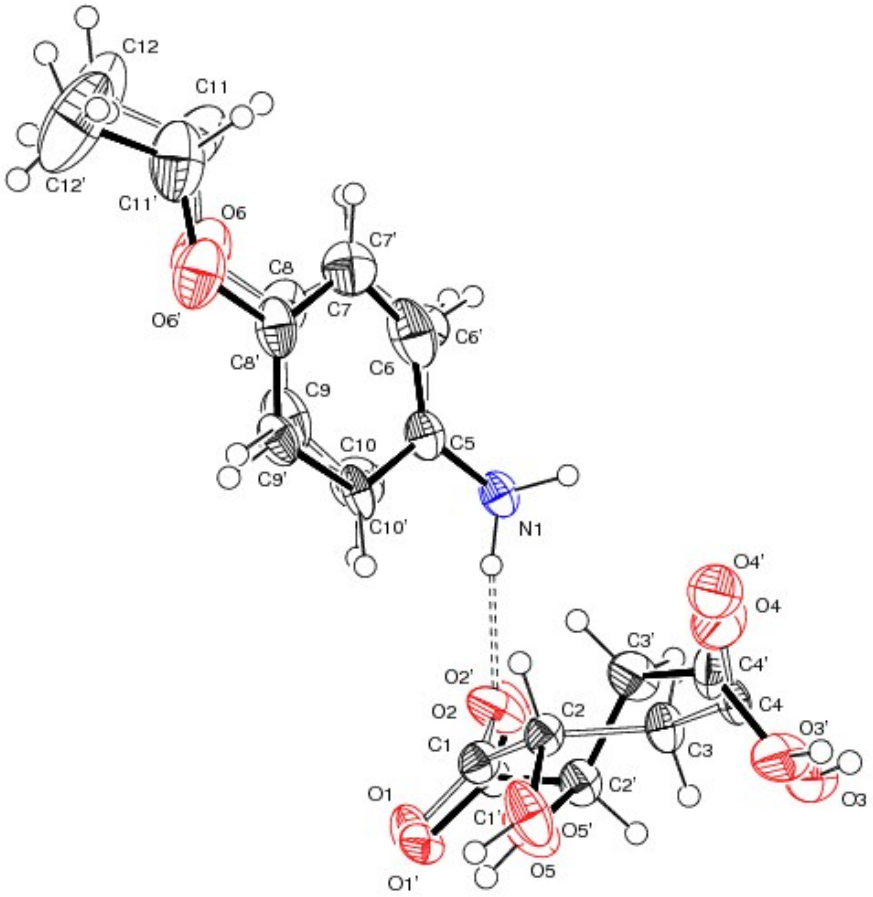
(2) ORTEP of Bis-(3-methylanilinium) succinate succinic acid



(3) ORTEP of 4-Methoxyanilinium hydrogen succinate



(4) ORTEP of 2-aminoanilinium hydrogen malate



(5) ORTEP of 4-Ethoxyanilinium hydrogen malate