

Electronic Supplementary Information

Multiply Protonated Betaine Clusters are Stable in the Gas Phase.

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Complete citation for reference 9: Gaussian 03, Revision B.04, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

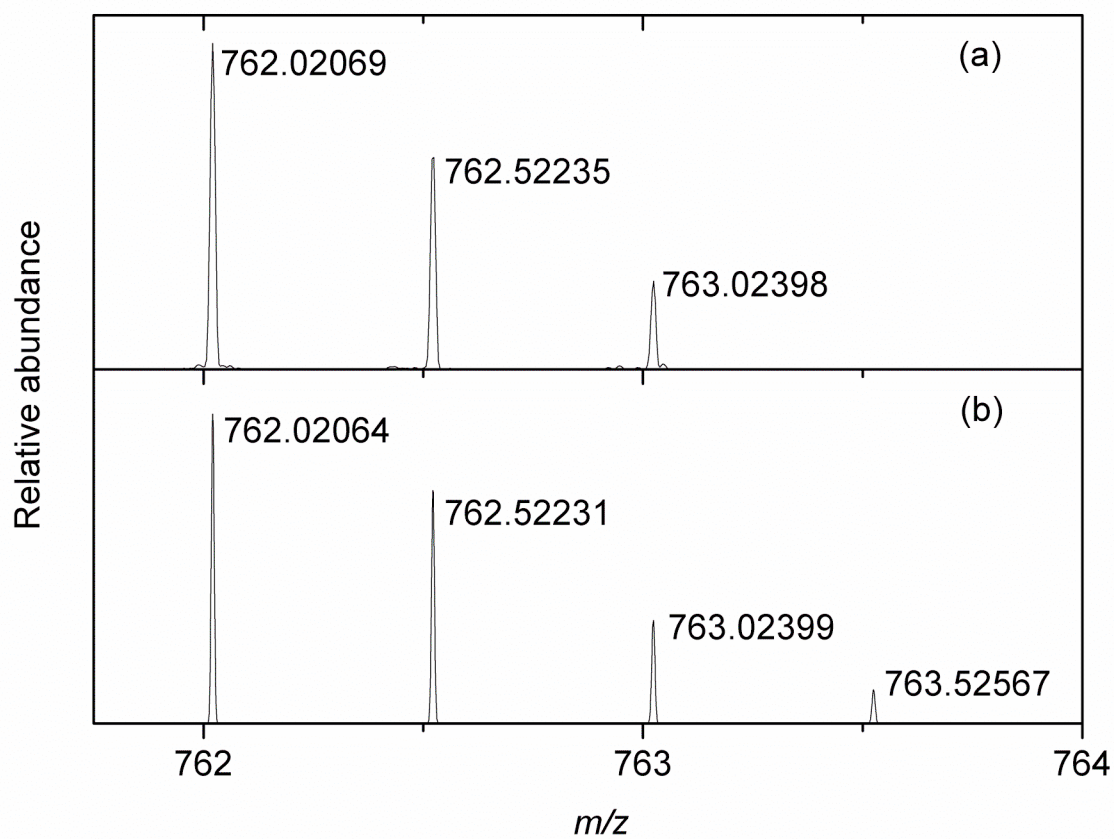
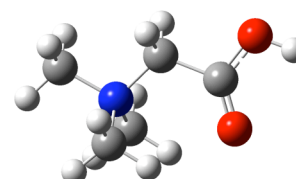
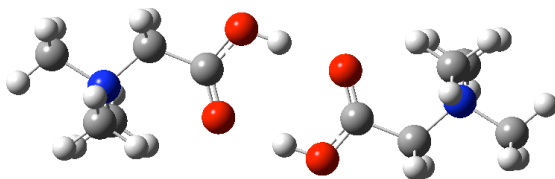


Figure S1: High resolution mass measurement of the $[M_{13} + 2H]^{2+}$ of betaine generated via ESI: (a) experimental data; (b) theoretical data



[M₂+2H]²⁺

C	1.91470600	0.42380000	0.00000000
C	3.42450900	0.66135600	0.00000000
O	1.05971600	1.30245900	0.00000000
O	1.67971200	-0.87043700	0.00000000
N	3.89325700	2.09898600	0.00000000
H	3.84755900	0.16976000	0.88128000
H	3.84755900	0.16976100	-0.88128200
H	0.69975300	-1.06103700	0.00000000
C	-1.91470600	-0.42380000	0.00000000
C	-3.42450900	-0.66135600	0.00000000
O	-1.05971600	-1.30245900	0.00000000
O	-1.67971200	0.87043700	0.00000000
N	-3.89325700	-2.09898600	0.00000000
H	-3.84755900	-0.16976000	0.88128000
H	-3.84755900	-0.16976100	-0.88128200
H	-0.69975300	1.06103700	0.00000000
C	3.42450900	2.83251100	-1.24130000
C	5.41076300	2.07420300	0.00000000
C	3.42450900	2.83251000	1.24130100
H	2.33824800	2.89396600	-1.22861500
H	3.77312900	2.28786000	-2.12082500
H	3.86100200	3.83209300	-1.22912400
H	5.77094200	3.10372200	0.00000100
H	5.75998500	1.55781400	-0.89567500
H	5.75998500	1.55781300	0.89567500
H	3.86100200	3.83209200	1.22912600
H	3.77312900	2.28785800	2.12082500
H	2.33824800	2.89396400	1.22861600
C	-3.42450900	-2.83251100	-1.24130000
C	-5.41076300	-2.07420300	0.00000000
C	-3.42450900	-2.83251000	1.24130100
H	-2.33824800	-2.89396600	-1.22861500
H	-3.77312900	-2.28786000	-2.12082500
H	-3.86100200	-3.83209300	-1.22912400
H	-5.77094200	-3.10372200	0.00000100
H	-5.75998500	-1.55781400	-0.89567500
H	-5.75998500	-1.55781300	0.89567500
H	-3.86100200	-3.83209200	1.22912600
H	-3.77312900	-2.28785800	2.12082500
H	-2.33824800	-2.89396400	1.22861600

Filename: betaine_dimerSYM

Sum of electronic and zero-point energies = -805.074 Hartrees

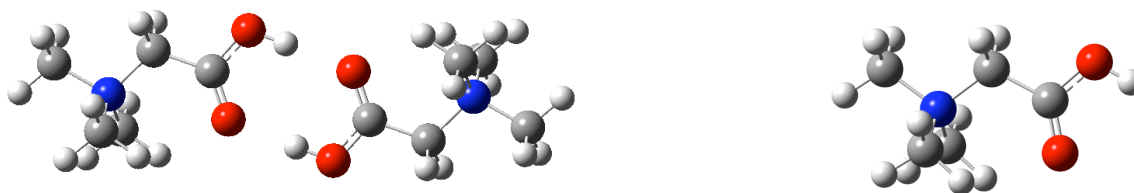
[M+H]⁺

C	-1.54210100	0.00529600	0.00000000
C	-0.26634800	-0.83895700	0.00000000
O	-1.59526900	1.21318900	0.00000000
O	-2.59010300	-0.82144400	-0.00000100
N	1.02846700	-0.05507500	0.00000000
H	-0.26782700	-1.48440600	0.88309400
H	-0.26782600	-1.48440500	-0.88309500
H	-3.41903600	-0.30058400	-0.00000100
C	1.14603900	0.80906700	-1.24016400
C	2.16199400	-1.05732600	0.00000000
C	1.14603900	0.80906700	1.24016500
H	0.35541800	1.55647400	-1.22484400
H	1.05635900	0.16859600	-2.11964300
H	2.12637200	1.28732600	-1.22719300
H	3.10625200	-0.51122700	0.00000000
H	2.09105400	-1.67774100	-0.89497900
H	2.09105400	-1.67774100	0.89497800
H	2.12637200	1.28732500	1.22719500
H	1.05635900	0.16859500	2.11964300
H	0.35541700	1.55647400	1.22484500

Filename: betaineH+

Sum of electronic and zero-point energies = -402.558 Hartrees

Figure S2: B3LYP/6-31+G(d) calculated cartesian coordinates and energies (Hartrees) for species relevant to the $[M_2 + 2H]^{2+}$



[M₂+2H]²⁺

C	-0.53360600	1.94595500	0.00007700
C	-0.99478600	3.39507300	-0.00045800
O	0.61689600	1.52091000	0.00003000
O	-1.54176200	1.07675000	0.00059100
N	0.09097100	4.47731700	-0.00013300
H	-1.65437900	3.54816600	-0.88965400
H	-1.65531800	3.54858900	0.88797100
H	-1.24072700	0.15657600	0.00079200
C	0.53360600	-1.94595500	0.00007700
C	0.99478600	-3.39507300	-0.00045800
O	-0.61689600	-1.52091000	0.00003000
O	1.54176200	-1.07675000	0.00059100
N	-0.09097100	-4.47731700	-0.00013300
H	1.65437900	-3.54816600	-0.88965400
H	1.65531800	-3.54858900	0.88797100
H	1.24072700	-0.15657600	0.00079200
C	0.95516600	4.38770800	1.24248600
C	-0.61689600	5.82775500	-0.00037300
C	0.95591400	4.38765100	-1.24223300
H	1.55005900	3.45841300	1.26137300
H	0.34196300	4.42015100	2.15824500
H	1.66607900	5.23123100	1.28643800
H	0.11310700	6.65614100	-0.00029700
H	-1.25444700	5.94997400	0.89172000
H	-1.25410600	5.94983300	-0.89272800
H	1.66694800	5.23109500	-1.28572800
H	0.34326900	4.42019500	-2.15836200
H	1.55070600	3.45828500	-1.26079700
C	-0.95516600	-4.38770800	1.24248600
C	0.61689600	-5.82775500	-0.00037300
C	-0.95591400	-4.38765100	-1.24223300
H	-1.55005900	-3.45841300	1.26137300
H	-0.34196300	-4.42015100	2.15824500
H	-1.66607900	-5.23123100	1.28643800
H	-0.11310700	-6.65614100	-0.00029700
H	1.25444700	-5.94997400	0.89172000
H	1.25410600	-5.94983300	-0.89272800
H	-1.66694800	-5.23109500	-1.28572800
H	-0.34326900	-4.42019500	-2.15836200
H	-1.55070600	-3.45828500	-1.26079700

Filename: betaine_dimerSYM_PM3
Total energy = 0.265 Hartrees

[M+H]⁺

C	-1.54329700	-0.02529400	0.00000100
C	-0.25952600	-0.84342800	0.00000300
O	-1.66121600	1.18461900	0.00001000
O	-2.64041700	-0.80016800	-0.00001400
N	1.04895300	-0.04693300	0.00000100
H	-0.27274500	-1.51763000	0.88968800
H	-0.27274300	-1.51763600	-0.88967600
H	-3.43574500	-0.27339800	-0.00001400
C	1.16752400	0.81486100	-1.24208700
C	2.19255100	-1.05357600	-0.00000100
C	1.16752900	0.81486100	1.24208900
H	0.40679300	1.61591400	-1.25950900
H	1.04570900	0.21274600	-2.15731600
H	2.15606600	1.30222700	-1.28721500
H	3.16988700	-0.54143100	-0.00000200
H	2.15795100	-1.70164800	-0.89173500
H	2.15795300	-1.70165200	0.89173000
H	2.15607100	1.30222700	1.28721300
H	1.04571800	0.21274700	2.15732000
H	0.40679700	1.61591400	1.25951300

Filename: betaineH+PM3
Total energy = 0.109 Hartrees

Figure S3: PM3 calculated Cartesian coordinates and energies (Hartrees) for species relevant to the $[M_2 + 2H]^{2+}$

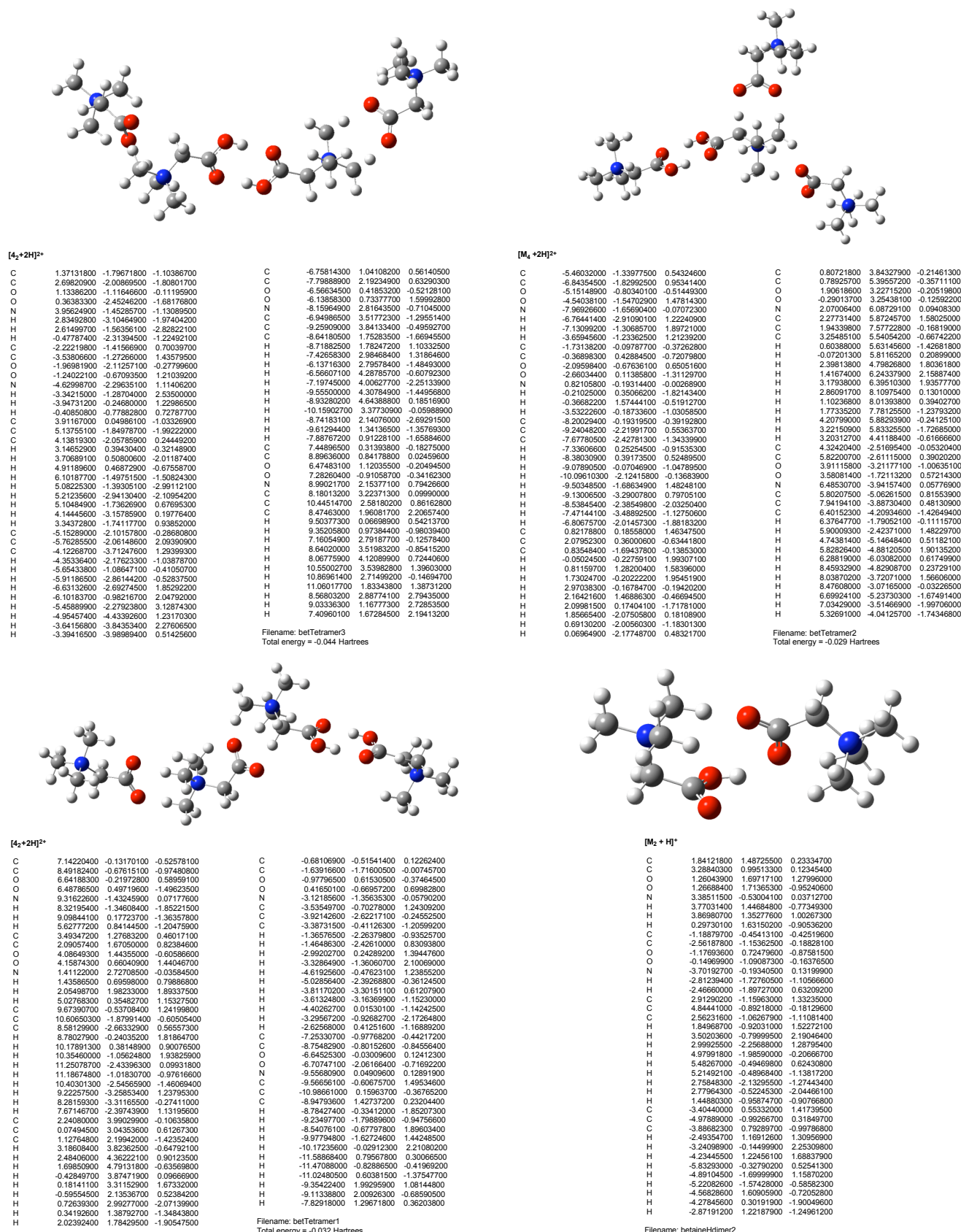
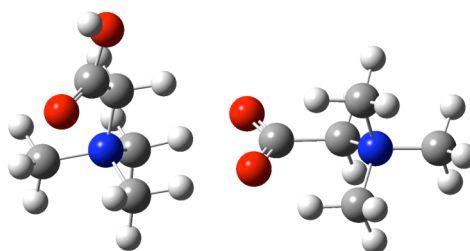


Figure S4: PM3 calculated Cartesian coordinates and energies (Hartrees) for species relevant to the $[M_4 + 2H]^{2+}$

Figure S4 (continued): PM3 calculated Cartesian coordinates and energies (Hartrees) for species relevant to the $[M_4 + 2H]^{2+}$



[M ₂ + H] ⁺			
C	-2.99912700	1.54686000	-0.12079600
C	-2.45400600	0.27734200	-0.74175300
O	-3.60515100	1.69592700	0.92374000
O	-2.76051200	2.63891500	-0.87323600
N	-2.57991900	-0.99757600	0.09480000
H	-2.95554000	0.12023600	-1.72504800
H	-1.36854400	0.43107900	-0.98142300
H	-3.12796300	3.41674100	-0.46257900
C	-1.79967600	-0.87142900	1.37903500
C	-1.98792700	-2.12789000	-0.72360100
C	-4.03048600	-1.32007500	0.38894500
H	-2.19874700	-0.07472400	2.02566200
H	-0.70890800	-0.63536300	1.17091700
H	-1.82986300	-1.81182800	1.94936900
H	-1.98209800	-3.06937500	-0.15453600
H	-0.91735100	-1.89187100	-1.00655100
H	-2.55312600	-2.29449600	-1.65268500
H	-4.11794500	-2.30747300	0.87089900
H	-4.62990600	-1.34347700	-0.53482700
H	-4.48667800	-0.58239500	1.07138300
C	1.37231400	-0.66587900	-0.43252500
C	2.90354200	-0.72893200	-0.70502200
O	0.94857500	-0.26295600	0.68837100
O	0.59521000	-1.02932200	-1.33486100
N	3.73051800	0.25571400	0.11270900
C	3.35066000	1.67698100	-0.25264200
C	5.19992000	0.04806500	-0.20673400
C	3.49841900	0.03180200	1.58878300
H	3.24171900	-1.76382900	-0.48351000
H	3.09592800	-0.56228700	-1.78743600
H	2.29235500	1.87059500	-0.00655300
H	3.48554100	1.85958600	-1.33047600
H	3.96473300	2.40702600	0.29789700
H	5.83201300	0.73072800	0.38363700
H	5.40887300	0.23195600	-1.27296000
H	5.51656800	-0.98219900	0.02374200
H	3.92552600	0.84084100	2.19740000
H	3.93126200	-0.92202400	1.92353800
H	2.38117600	-0.01599900	1.75733100

Filename: betaineHdimer2x
Total energy = -0.037 Hartrees

Table S1: Predicted m/z values for $[M_n + xH]^{x+}$ clusters of betaine

Size of cluster / n	$[M+H]^+$	$[M_2+2H]^{2+}$	$[M_3+3H]^{3+}$	$[M_4+4H]^{4+}$
1	118.09	59.55	40.03	30.28
2	235.16	118.09	79.06	59.55
3	352.24	176.62	118.09	88.82
4	469.32	235.16	157.11	118.09
5	586.40	293.70	196.14	147.36
6	703.48	352.24	235.16	176.62
7	820.56	410.78	274.19	205.89
8	937.63	469.32	313.22	235.16
9	1054.71	527.86	352.24	264.43
10	1171.79	586.40	391.27	293.70
11	1288.87	644.94	430.29	322.97
12	1405.95	703.48	469.32	352.24
13	1523.03	762.02	508.35	381.51
14	1640.11	820.56	547.37	410.78
15	1757.18	879.10	586.40	440.05
16	1874.26	937.63	625.43	469.32
17	1991.34	996.17	664.45	498.59
18	2108.42	1054.71	703.48	527.86
19	2225.50	1113.25	742.50	557.13
20	2342.58	1171.79	781.53	586.40
21	2459.65	1230.33	820.56	615.67
22	2576.73	1288.87	859.58	644.94
23	2693.81	1347.41	898.61	674.21
24	2810.89	1405.95	937.63	703.48
25	2927.97	1464.49	976.66	732.75
26	3045.05	1523.03	1015.69	762.02
27	3162.12	1581.57	1054.71	791.29
28	3279.20	1640.11	1093.74	820.56
29	3396.28	1698.64	1132.77	849.83
30	3513.36	1757.18	1171.79	879.10
31	3630.44	1815.72	1210.82	908.37
32	3747.52	1874.26	1249.84	937.63
33	3864.60	1932.80	1288.87	966.90
34	3981.67	1991.34	1327.90	996.17
35	4098.75	2049.88	1366.92	1025.44
36	4215.83	2108.42	1405.95	1054.71
37	4332.91	2166.96	1444.97	1083.98
38	4449.99	2225.50	1484.00	1113.25
39	4567.07	2284.04	1523.03	1142.52
40	4684.14	2342.58	1562.05	1171.79
41	4801.22	2401.12	1601.08	1201.06
42	4918.30	2459.65	1640.11	1230.33
43	5035.38	2518.19	1679.13	1259.60
44			1718.16	1288.87
45			1757.18	1318.14
46			1796.21	1347.41
47			1835.24	1376.68
48			1874.26	1405.95

Table S1 (continued): Predicted m/z values for $[M_n + xH]^{x+}$ clusters of betaine

Size of cluster / n	$[M+H]^+$	$[M_2+2H]^{2+}$	$[M_3+3H]^{3+}$	$[M_4+4H]^{4+}$
49			1913.29	1435.22
50			1952.31	1464.49
51			1991.34	1493.76
52			2030.37	1523.03
53			2069.39	1552.30
54			2108.42	1581.57
55			2147.45	1610.84
56			2186.47	1640.11
57			2225.50	1669.37
58			2264.52	1698.64
59			2303.55	1727.91
60			2342.58	1757.18
61				1786.45
62				1815.72
63				1844.99
64				1874.26
65				1903.53
66				1932.80
67				1962.07
68				1991.34
69				2020.61
70				2049.88
71				2079.15
72				2108.42
73				2137.69
74				2166.96