

Supporting information for Molecular properties affecting the hydration of acid–base clusters

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Binding enthalpies and entropies for hydrated base monomers are given in Table S1 and for sulfuric acid–base heterodimers in Table S2.

Table S1: Calculated binding enthalpies (ΔH in kcal/mol) and entropies (ΔS in cal/(mol·K)) for hydrated base monomer 1BASE n W.

1BASE n W n	AMM		DMA		TMAO		GUA	
	ΔH	ΔS	ΔH	ΔS	ΔH	ΔS	ΔH	ΔS
1	-4.7	-21.1	-6.2	-24.5	-11.7	-27.8	-9.0	-30.6
2	-12.1	-55.2	-13.6	-54.1	-21.8	-56.4	-17.9	-62.2
3	-20.8	-87.4	-22.2	-87.6	-30.7	-86.8	-26.1	-93.1
4	-27.4	-113.1	-29.9	-117.6	-38.6	-120.2	-35.3	-123.4
5	-35.9	-147.8	-38.5	-158.8	-48.2	-156.3	-43.5	-155.8
6	-44.9	-183.5	-48.8	-192.6	-59.4	-197.1	-54.9	-198.9
7	-58.8	-229.9	-59.7	-230.5	-69.1	-232.1	-65.3	-237.7
8	-66.6	-256.4	-68.5	-256.8	-79.3	-266.6	-74.5	-270.1
9	-74.4	-285.8	-77.7	-292.8	-89.1	-301.9	-87.1	-302.4
10	-84.6	-323.2	-86.4	-329.1	-96.8	-328.6	-96.2	-336.4
11	-96.8	-371.4	-96.9	-365.5	-108.9	-368.6	-102.6	-358.3
12	-104.0	-396.6	-107.6	-404.8	-117.3	-402.7	-114.3	-404.7
13	-115.2	-438.1	-115.2	-433.2	-127.2	-438.7	-124.0	-442.3
14	-123.3	-462.7	-126.8	-473.7	-137.4	-470.6	-132.9	-480.3
15	-134.9	-507.8	-135.3	-507.4	-147.4	-508.2	-143.6	-517.3
16	-143.8	-542.3	-145.3	-540.0	-156.1	-541.8	-151.7	-544.0
17	-153.3	-574.5	-154.7	-574.7	-167.7	-580.1	-163.4	-586.0
18	-161.3	-602.8	-164.1	-610.5	-176.7	-615.5	-176.5	-619.5
19	-172.0	-640.3	-174.6	-642.0	-186.3	-649.9	-182.6	-648.8
20	-178.4	-664.3	-184.9	-681.7	-198.0	-689.6	-196.8	-691.7

Table S2: Calculated binding enthalpies (ΔH in kcal/mol) and entropies (ΔS in cal/(mol·K)) for hydrated sulfuric acid–base heterodimer 1SA1BASE n W.

1SA1BASE n W	SA-AMM		SA-DMA		SA-TMAO		SA-GUA	
n	ΔH	ΔS	ΔH	ΔS	ΔH	ΔS	ΔH	ΔS
0	-15.1	-29.2	-22.2	-30.3	-32.2	-34.9	-29.4	-30.4
1	-25.1	-62.5	-35.3	-66.1	-41.4	-62.9	-41.2	-68.6
2	-39.1	-95.1	-47.2	-100.2	-53.1	-98.4	-57.1	-102.3
3	-49.8	-124.5	-58.0	-131.3	-64.7	-133.8	-70.8	-137.1
4	-59.7	-160.3	-66.8	-161.2	-74.6	-165.2	-80.1	-166.7
5	-71.6	-195.7	-78.8	-199.7	-84.7	-195.8	-89.7	-199.9
6	-81.0	-227.4	-87.2	-225.3	-96.4	-235.9	-103.2	-240.1
7	-95.8	-273.9	-100.2	-271.4	-105.9	-262.7	-113.1	-272.3
8	-105.0	-301.2	-109.3	-302.0	-115.9	-297.3	-123.9	-309.3
9	-114.3	-333.5	-118.8	-337.1	-125.5	-332.4	-132.8	-337.7
10	-124.2	-365.6	-128.8	-369.5	-137.8	-375.6	-144.5	-379.1
11	-134.1	-395.8	-140.3	-411.8	-144.8	-401.5	-154.4	-414.8
12	-146.4	-444.1	-147.8	-439.4	-155.7	-431.5	-164.1	-446.7
13	-155.0	-473.4	-159.6	-479.0	-166.6	-472.4	-176.3	-489.5
14	-167.6	-512.5	-172.1	-520.3	-176.5	-507.4	-183.0	-512.8
15	-179.3	-551.3	-178.2	-544.1	-188.2	-545.2	-195.8	-557.2
16	-184.4	-575.3	-190.6	-587.2	-195.5	-578.5	-206.1	-589.5
17	-196.9	-613.3	-199.7	-618.5	-207.3	-616.2	-213.6	-620.2
18	-207.1	-652.9	-206.8	-651.2	-216.3	-648.3	-224.2	-655.0
19	-215.6	-683.1	-217.0	-685.7	-227.7	-688.8	-234.4	-687.8
20	-227.4	-725.3	-227.1	-722.6	-238.0	-725.0	-245.4	-732.1