Electronic Supplementary Information to the paper entitled "The Molecular Self-association of Carboxylic Acids in Solution: Testing the Validity of the Link Hypothesis using a Quantum Mechanical Continuum Solvation Approach" by Devis Di Tommaso.

Table SI.1. Trimerization of TTA. Gas phase interaction energies ($\Delta E_{e,gas}$), standard state (1 atm) gas-phase free energies of association (ΔG°_{ass}) at 298 K computed at the M06-2X/aug-cc-pVDZ//M06-2X/6-31++G(d,p) level of theory. Standard state (1M) free energies of association in chloroform (ΔG^{*}_{ass}) computed the using the SMD solvation model at the M06-2X/aug-cc-pVDZ level of theory with gas-phase geometries. Values in kcal mol^{-1}.

	$\Delta E_{e,gas}$	ΔG°_{ass}	ΔG^{*}_{ass}
c1_$(TTA)_3$	-7.10	5.82	5.47
c2_$(TTA)_3$	-10.84	3.05	2.47
c3_$(TTA)_3$	-11.53	1.69	2.25
c7_$(TTA)_3$	-11.15	2.38	2.07
c9_$(TTA)_3$	-11.46	1.07	2.17
c10_$(TTA)_3$	**-11.21**	**0.65**	**0.08**
c11_$(TTA)_3$	-7.10	5.82	5.47
c12_$(TTA)_3$	-10.54	3.53	3.36
c13_$(TTA)_3$	-11.53	1.72	2.28
c14_$(TTA)_3$	-7.11	5.41	5.14
c16_$(TTA)_3$	-7.10	5.82	5.47
c18_$(TTA)_3$	-11.92	0.84	2.89
c19_$(TTA)_3$	-11.67	2.18	3.27
c21_$(TTA)_3$	-7.23	6.54	6.39
c22_$(TTA)_3$	-7.22	6.47	6.34
c25_$(TTA)_3$	-8.41	2.55	1.82
c30_$(TTA)_3$	-12.32	0.54	1.08
c31_$(TTA)_3$	-11.58	1.60	1.88
c32_$(TTA)_3$	-12.32	0.64	1.12
c34_$(TTA)_3$	-12.30	0.84	1.36
c36_$(TTA)_3$	-11.52	1.47	2.54
c37_$(TTA)_3$	**-12.33**	**-1.48**	**-0.94**
c38_$(TTA)_3$	-12.05	1.34	2.08
c39_$(TTA)_3$	**-12.43**	**-0.85**	**-0.20**
c41_$(TTA)_3$	-11.37	1.14	1.69
c42_$(TTA)_3$	-13.28	0.12	2.35
c44_$(TTA)_3$	-12.35	1.85	2.41
c45_$(TTA)_3$	-11.55	1.66	2.21
c46_$(TTA)_3$	-11.67	1.39	2.52
c47_$(TTA)_3$	-10.50	3.60	3.08
c48_$(TTA)_3$	-9.99	1.97	2.05
c49_$(TTA)_3$	-9.26	4.57	4.95
c50_$(TTA)_3$	-10.61	2.47	2.03

c51_$(TTA)_3$	-10.74	2.91	2.56
c52_$(TTA)_3$	-10.53	2.48	2.03
c53_$(TTA)_3$	-11.95	0.71	2.73
c54_$(TTA)_3$	-11.36	2.71	4.52
c55_$(TTA)_3$	-11.94	1.35	3.39
c56_$(TTA)_3$	-11.31	0.41	2.22
c58_$(TTA)_3$	-10.52	3.68	3.24
c59_$(TTA)_3$	-10.28	3.19	4.46
c60_$(TTA)_3$	**-11.54**	**-2.59**	**-3.08**

Table SI.2. Formation of TTA tetramers modelled according to the reaction $(TTA)_2 + (TTA)_2 \rightarrow (TTA)_4$. Gas phase interaction energies ($\Delta E_{e,gas}$), standard state (1 atm) gas-phase free energies of association (ΔG°_{ass}) at 298 K computed at the M06-2X/aug-cc-pVDZ//M06-2X/6-31++G(d,p) level of theory. Standard state (1M) free energies of association in chloroform (ΔG^{*}_{ass}) computed the using the SMD solvation model at the M06-2X/aug-cc-pVDZ level of theory with gas-phase geometries. Values in kcal mol^{-1}.

	$\Delta E_{e,gas}$	ΔG°_{ass}	ΔG^{*}_{ass}
c1_$(TTA)_4$	-20.73	-2.05	4.12
c2_$(TTA)_4$	-18.61	-0.86	5.78
c3_$(TTA)_4$	-19.88	-0.26	5.67
c4_$(TTA)_4$	-11.78	5.08	9.35
c5_$(TTA)_4$	-19.42	-0.90	5.13
c6_$(TTA)_4$	-13.54	0.94	6.43
c8_$(TTA)_4$	-14.12	-0.37	4.96
c10_$(TTA)_4$	-19.86	0.05	6.09
c11_$(TTA)_4$	-20.02	-0.36	5.83
c12_$(TTA)_4$	-19.89	0.72	6.43
c13_$(TTA)_4$	-18.52	-2.07	4.66
c15_$(TTA)_4$	-13.29	1.19	6.59
c16_$(TTA)_4$	-11.60	6.33	10.72
c17_$(TTA)_4$	-19.92	-1.23	4.94
c18_$(TTA)_4$	-19.87	-3.43	2.78
c19_$(TTA)_4$	-13.54	0.94	6.43
c20_$(TTA)_4$	-14.95	3.58	8.77
c23_$(TTA)_4$	-13.31	4.47	9.86
c24_$(TTA)_4$	-11.78	7.35	11.55
c25_$(TTA)_4$	-19.43	1.02	6.97
c26_$(TTA)_4$	-17.35	3.08	8.44
c27_$(TTA)_4$	-18.60	-1.49	5.14
c29_$(TTA)_4$	-14.46	2.49	8.11
c30_$(TTA)_4$	-11.70	4.35	8.61
c31_$(TTA)_4$	-19.83	1.09	5.53
c32_$(TTA)_4$	-19.92	-1.57	4.65
c33_$(TTA)_4$	-16.86	-1.83	5.21
c34_$(TTA)_4$	-19.64	0.97	5.61
c35_$(TTA)_4$	-19.90	-2.16	4.01
c36_$(TTA)_4$	-19.53	0.98	6.99
c37_$(TTA)_4$	-19.53	0.98	6.99
c38_$(TTA)_4$	-19.24	-0.34	5.70
c39_$(TTA)_4$	-18.46	-1.33	5.02
c40_$(TTA)_4$	-19.53	0.98	6.99
c41_$(TTA)_4$	-19.69	-0.59	5.76
c44_$(TTA)_4$	-19.23	-1.06	5.35
c45_$(TTA)_4$	-19.72	-0.52	5.45
c46_$(TTA)_4$	-18.37	0.02	6.84

c49_$(TTA)_4$	-20.01	0.04	6.20
c50_$(TTA)_4$	-18.52	-2.22	5.58

Table SI.3. Formation of TTA tetramers modelled according to the reaction $(TTA)_2 + (TTA)_2 \rightarrow (TTA)_4$. Gas phase interaction energies ($\Delta E_{e,gas}$), standard state (1 atm) gas-phase free energies of association (ΔG°_{ass}) at 298 K computed at the M06-2X/aug-cc-pVDZ//M06-2X/6-31++G(d,p) level of theory. Standard state (1M) free energies of association in chloroform (ΔG^{*}_{ass}) computed the using the SMD solvation model at the M06-2X/aug-cc-pVDZ level of theory with gas-phase geometries. Values in kcal mol^{-1}.

	$\Delta E_{e,gas}$	ΔG°_{ass}	ΔG^{*}_{ass}
c1_$(TTA)_4$	-15.63	-0.12	-0.21
c2_$(TTA)_4$	-13.51	1.07	1.44
c3_$(TTA)_4$	-14.78	1.67	1.34
c4_$(TTA)_4$	-6.69	7.01	5.02
c5_$(TTA)_4$	-14.33	1.03	0.79
c6_$(TTA)_4$	-8.44	2.87	2.09
c8_$(TTA)_4$	-9.02	1.56	0.63
c10_$(TTA)_4$	-14.76	1.98	1.75
c11_$(TTA)_4$	-14.92	1.57	1.50
c12_$(TTA)_4$	-14.79	2.65	2.09
c13_$(TTA)_4$	-13.43	-0.13	0.32
c15_$(TTA)_4$	-8.19	3.12	2.26
c16_$(TTA)_4$	-6.51	8.26	6.38
c17_$(TTA)_4$	-14.83	0.70	0.61
c18_$(TTA)_4$	**-14.77**	**-1.50**	**-1.55**
c19_$(TTA)_4$	-8.44	2.87	2.09
c20_$(TTA)_4$	-9.85	5.51	4.43
c23_$(TTA)_4$	-8.22	6.40	5.52
c24_$(TTA)_4$	-6.69	9.28	7.21
c25_$(TTA)_4$	-14.34	2.95	2.64
c26_$(TTA)_4$	-12.25	5.02	4.11
c27_$(TTA)_4$	-13.51	0.44	0.80
c29_$(TTA)_4$	-9.36	4.42	3.78
c30_$(TTA)_4$	-6.61	6.28	4.27
c31_$(TTA)_4$	-14.73	3.02	1.19
c32_$(TTA)_4$	-14.83	0.36	0.32
c33_$(TTA)_4$	-11.77	0.10	0.87
c34_$(TTA)_4$	-14.55	2.90	1.27
c35_$(TTA)_4$	**-14.80**	**-0.23**	**-0.33**
c36_$(TTA)_4$	-14.43	2.91	2.65
c37_$(TTA)_4$	-14.43	2.91	2.65
c38_$(TTA)_4$	-14.15	1.59	1.37
c39_$(TTA)_4$	-13.37	0.60	0.69
c40_$(TTA)_4$	-14.43	2.91	2.65
c41_$(TTA)_4$	-14.60	1.34	1.43
c44_$(TTA)_4$	-14.13	0.87	1.01
c45_$(TTA)_4$	-14.63	1.41	1.11
c46_$(TTA)_4$	-13.27	1.95	2.50

c49_$(TTA)_4$	-14.91	1.97	1.86
c50_$(TTA)_4$	-13.43	-0.29	1.24

Table SI.4. Dimerization of the non-zwitterionic form of *m*-aminobenzoic acid. Gas phase interaction energies ($\Delta E_{e,gas}$), standard state (1 atm) gas-phase free energies of association (ΔG°_{ass}) at 298 K computed at the M06-2X/aug-cc-pVDZ//M06-2X/6-31++G(d,p) level of theory. Standard state (1M) free energies of association in chloroform (ΔG^{*}_{ass}) computed the using the SMD solvation model at the M06-2X/aug-cc-pVDZ level of theory with gas-phase geometries. Values in kcal mol^{-1}.

	$\Delta E_{e,gas}{}^{a}$	ΔG°_{ass}	ΔG^{*}_{ass}		
			water	**methanol**	**acetonitrile**
c1_(*m*ABA)$_2$	-0.52	11.45	11.85	13.08	13.89
c2_(*m*ABA)$_2$	-10.59	4.38	4.47	6.04	6.83
c3_(*m*ABA)$_2$	-11.35	-0.43	3.85	4.15	3.16
c4_(*m*ABA)$_2$	-10.59	3.96	3.97	5.51	6.32
c5_(*m*ABA)$_2$	-6.87	4.97	7.54	8.18	8.03
c6_(*m*ABA)$_2$	-6.80	4.83	4.93	6.20	6.77
c7_(*m*ABA)$_2$	-6.87	3.55	6.07	6.73	6.58
c8_(*m*ABA)$_2$	-8.89	4.14	3.37	4.65	6.30
c10_(*m*ABA)$_2$	-6.71	4.75	7.29	7.96	7.72
c11_(*m*ABA)$_2$	-10.72	2.70	3.11	4.35	5.18
c12_(*m*ABA)$_2$	-10.71	3.20	3.66	4.91	5.71
c13_(*m*ABA)$_2$	-0.69	12.05	10.32	10.73	10.94
c14_(*m*ABA)$_2$	-0.68	8.80	7.02	7.46	7.65
c15_(*m*ABA)$_2$	-6.89	6.32	9.03	9.64	9.36
c16_(*m*ABA)$_2$	**-17.73**	**-5.79**	**0.43**	**0.78**	**-2.00**
c17_(*m*ABA)$_2$	-8.55	3.91	4.53	6.30	6.65
c18_(*m*ABA)$_2$	-7.79	4.98	6.42	7.30	7.27
c19_(*m*ABA)$_2$	-7.00	5.98	3.43	5.21	6.30
c20_(*m*ABA)$_2$	-4.92	7.69	9.18	9.97	10.32
c21_(*m*ABA)$_2$	-3.68	8.12	7.72	8.88	9.31
c22_(*m*ABA)$_2$	-8.54	3.72	4.31	6.04	6.41
c23_(*m*ABA)$_2$	-7.87	5.98	2.50	3.63	4.64
c24_(*m*ABA)$_2$	-6.54	4.81	4.80	5.87	5.00
c25_(*m*ABA)$_2$	-6.45	4.77	3.69	5.05	5.21
c26_(*m*ABA)$_2$	-8.47	2.20	5.38	5.62	4.47
c27_(*m*ABA)$_2$	-8.66	5.32	5.62	5.60	7.25
c28_(*m*ABA)$_2$	-11.10	1.29	3.07	4.12	4.63
c29_(*m*ABA)$_2$	-11.10	1.23	3.14	4.17	4.63
c30_(*m*ABA)$_2$	-10.89	0.97	3.92	4.71	4.86
c31_(*m*ABA)$_2$	-4.90	5.59	5.74	6.46	7.22
c32_(*m*ABA)$_2$	-11.10	0.94	3.03	4.04	4.36
c33_(*m*ABA)$_2$	-11.10	1.01	3.08	4.07	4.42
c34_(*m*ABA)$_2$	-10.89	2.03	4.85	5.69	5.98
c35_(*m*ABA)$_2$	-8.57	4.58	7.07	7.47	8.02
c36_(*m*ABA)$_2$	-11.27	2.10	6.40	6.73	5.69
c37_(*m*ABA)$_2$	-11.10	1.47	3.32	4.38	4.88
c38_(*m*ABA)$_2$	-10.89	1.51	4.35	5.15	5.41

c39_(*m*ABA)$_2$	-11.65	2.06	20.70	24.21	23.68
c40_(*m*ABA)$_2$	-11.10	1.27	3.18	4.25	4.68
c41_(*m*ABA)$_2$	-11.14	0.70	2.27	3.16	3.59
c42_(*m*ABA)$_2$	**-17.73**	**-6.44**	**-0.19**	**0.11**	**-2.64**
c43_(*m*ABA)$_2$	-8.34	4.04	7.26	7.52	6.32
c44_(*m*ABA)$_2$	-8.65	3.43	6.82	7.03	5.90
c45_(*m*ABA)$_2$	**-17.79**	**-5.85**	**0.46**	**0.78**	**-1.98**
c46_(*m*ABA)$_2$	**-17.79**	**-5.84**	**0.43**	**0.73**	**-2.05**
c47_(*m*ABA)$_2$	**-17.79**	**-6.22**	**0.12**	**0.40**	**-2.39**
c48_(*m*ABA)$_2$	-6.59	3.82	4.14	5.19	4.30
c49_(*m*ABA)$_2$	-5.47	6.82	7.31	7.67	7.22
c50_(*m*ABA)$_2$	-7.64	6.87	4.17	5.49	6.86
c51_(*m*ABA)$_2$	-8.61	3.57	6.94	7.20	6.02
c52_(*m*ABA)$_2$	-5.10	7.98	4.54	6.06	7.78
c53_(*m*ABA)$_2$	-2.12	8.88	5.83	6.69	7.58
c54_(*m*ABA)$_2$	-8.75	4.80	4.72	5.76	6.33
c55_(*m*ABA)$_2$	-6.34	6.23	3.71	5.55	6.86
c56_(*m*ABA)$_2$	-8.75	4.97	4.80	5.81	6.47
c57_(*m*ABA)$_2$	-8.89	5.21	4.69	5.98	6.77
c58_(*m*ABA)$_2$	-6.52	4.49	7.34	7.82	6.87
c59_(*m*ABA)$_2$	-6.46	4.66	7.42	7.93	6.97
c60_(*m*ABA)$_2$	**-17.79**	**-6.68**	**-0.35**	**-0.06**	**-2.92**
c61_(*m*ABA)$_2$	**-17.73**	**-5.31**	**1.07**	**1.29**	**-1.55**
c62_(*m*ABA)$_2$	-0.41	9.01	7.44	7.77	7.53
c63_(*m*ABA)$_2$	-0.31	9.78	7.95	8.25	8.28
c64_(*m*ABA)$_2$	-8.50	2.88	4.33	4.79	5.30
c65_(*m*ABA)$_2$	-10.50	0.85	5.17	5.34	4.87
c66_(*m*ABA)$_2$	-8.75	4.71	4.60	5.63	2.41
c67_(*m*ABA)$_2$	-9.57	3.24	8.28	8.21	8.03
c68_(*m*ABA)$_2$	-9.96	4.23	4.09	4.39	6.72
c69_(*m*ABA)$_2$	-9.35	3.45	2.71	2.67	4.98
c70_(*m*ABA)$_2$	-10.88	2.24	1.28	1.85	4.16
c71_(*m*ABA)$_2$	-10.80	1.99	2.08	2.68	3.98
c72_(*m*ABA)$_2$	-10.81	1.29	4.54	5.36	5.87
c73_(*m*ABA)$_2$	-8.43	4.13	2.77	2.82	5.62
c74_(*m*ABA)$_2$	-10.67	3.19	2.53	3.34	5.48
c75_(*m*ABA)$_2$	-12.15	1.07	3.21	4.12	4.63
c76_(*m*ABA)$_2$	-11.09	2.15	4.01	5.03	5.51
c77_(*m*ABA)$_2$	-11.05	1.57	3.67	4.66	5.01
c78_(*m*ABA)$_2$	-10.89	2.21	5.05	5.86	6.11

Table SI.5. Association of the non-zwitterionic, *m*ABA, and zwitterionic, *m*ABA$^{\pm}$, forms of *m*-aminobenzoic acid. Gas phase interaction energies ($\Delta E_{e,gas}$), standard state (1 atm) gas-phase free energies of association (ΔG°_{ass}) at 298 K computed at the M06-2X/aug-cc-pVDZ//M06-2X/6-31++G(d,p) level of theory. Standard state (1M) free energies of association in chloroform (ΔG^{*}_{ass}) computed the using the SMD solvation model at the M06-2X/aug-cc-pVDZ level of theory with gas-phase geometries. Values in kcal mol^{-1}.

	$\Delta E_{e,gas}$ [a]	ΔG°_{ass} [a]	ΔG^{*}_{ass} [b]		
			water	**methanol**	**acetonitrile**
c1_(*m*ABA)(mABA$^{\pm}$)	-27.43	-13.94	7.35	8.07	8.63
c2_(*m*ABA)(mABA$^{\pm}$)	-29.51	-14.13	6.36	7.36	8.44
c3_(*m*ABA)(mABA$^{\pm}$)	-32.77	-18.94	6.82	6.95	3.63
c4_(*m*ABA)(mABA$^{\pm}$)	-31.96	-18.46	5.22	5.05	4.12
c5_(*m*ABA)(mABA$^{\pm}$)	-31.98	-19.12	4.27	4.21	3.45
c6_(*m*ABA)(mABA$^{\pm}$)	-27.45	-14.43	7.45	8.24	8.15
c7_(*m*ABA)(mABA$^{\pm}$)	-27.98	-13.70	7.64	8.33	8.87
c8_(*m*ABA)(mABA$^{\pm}$)	-31.91	-18.28	5.71	5.55	4.29
c9_(*m*ABA)(mABA$^{\pm}$)	-25.07	-10.27	8.90	10.00	12.31
c10_(*m*ABA)(mABA$^{\pm}$)	-29.52	-15.70	5.33	5.46	6.88
c11_(*m*ABA)(mABA$^{\pm}$)	-31.94	-19.18	4.14	4.11	3.39
c12_(*m*ABA)(mABA$^{\pm}$)	-31.97	-19.47	3.93	3.88	3.11
c13_(*m*ABA)(mABA$^{\pm}$)	-25.05	-10.25	8.58	9.69	12.33
c14_(*m*ABA)(mABA$^{\pm}$)	-29.52	-16.86	4.00	4.17	5.71
c15_(*m*ABA)(mABA$^{\pm}$)	-33.19	-19.42	6.29	6.40	3.15
c16_(*m*ABA)(mABA$^{\pm}$)	-29.52	-16.23	4.78	4.95	6.34
c17_(*m*ABA)(mABA$^{\pm}$)	-31.97	-17.46	5.80	5.77	5.12
c18_(*m*ABA)(mABA$^{\pm}$)	-15.58	-3.85	5.53	5.66	18.73
c19_(*m*ABA)(mABA$^{\pm}$)	-32.11	-17.65	6.30	6.89	4.92
c20_(*m*ABA)(mABA$^{\pm}$)	-15.56	-2.52	6.94	7.09	20.06
c21_(*m*ABA)(mABA$^{\pm}$)	-29.52	-16.24	4.73	4.88	6.34
c22_(*m*ABA)(mABA$^{\pm}$)	-31.96	-19.31	4.25	4.19	3.27
c23_(*m*ABA)(mABA$^{\pm}$)	-29.53	-16.41	4.65	4.76	6.17
c24_(*m*ABA)(mABA$^{\pm}$)	-33.18	-19.04	6.66	6.76	3.54
c25_(*m*ABA)(mABA$^{\pm}$)	-31.95	-17.79	5.64	5.65	4.78
c26_(*m*ABA)(mABA$^{\pm}$)	-31.96	-19.11	4.18	4.17	3.47
c27_(*m*ABA)(mABA$^{\pm}$)	-13.13	-0.26	8.01	7.82	22.32
c28_(*m*ABA)(mABA$^{\pm}$)	-15.60	-2.20	18.35	19.32	20.37
c29_(*m*ABA)(mABA$^{\pm}$)	-29.51	-14.34	6.36	7.38	8.23
c30_(*m*ABA)(mABA$^{\pm}$)	-31.94	-19.61	3.88	3.85	2.97
c31_(*m*ABA)(mABA$^{\pm}$)	-14.83	-2.64	6.03	6.02	19.94
c32_(*m*ABA)(mABA$^{\pm}$)	-31.15	-17.79	6.16	6.50	4.79
c33_(*m*ABA)(mABA$^{\pm}$)	-33.19	-19.57	6.10	6.19	3.01
c34_(*m*ABA)(mABA$^{\pm}$)	-27.96	-13.15	5.80	6.86	9.42
c35_(*m*ABA)(mABA$^{\pm}$)	-27.98	-13.65	7.61	8.34	8.92
c36_(*m*ABA)(mABA$^{\pm}$)	-31.64	-17.17	4.27	5.04	5.41
c37_(*m*ABA)(mABA$^{\pm}$)	**-36.35**	**-21.15**	**-3.17**	**-2.41**	**1.43**

c38_(*m*ABA)(mABA$^{\pm}$)	**-36.19**	**-21.82**	**2.15**	**3.18**	**0.75**
c39_(*m*ABA)(mABA$^{\pm}$)	-27.96	-13.40	5.44	6.48	9.18
c40_(*m*ABA)(mABA$^{\pm}$)	-25.05	-10.51	8.69	9.78	12.06
c41_(*m*ABA)(mABA$^{\pm}$)	-25.06	-10.46	8.70	9.80	12.12
c42_(*m*ABA)(mABA$^{\pm}$)	-29.50	-16.28	4.92	5.00	4.98
c43_(*m*ABA)(mABA$^{\pm}$)	-29.52	-16.43	4.51	4.65	4.82
c44_(*m*ABA)(mABA$^{\pm}$)	-29.52	-16.09	5.09	5.20	5.16
c45_(*m*ABA)(mABA$^{\pm}$)	-29.52	-16.86	4.21	4.30	4.40
c46_(*m*ABA)(mABA$^{\pm}$)	-31.98	-19.19	4.21	4.19	2.07
c47_(*m*ABA)(mABA$^{\pm}$)	-32.01	-18.50	5.49	5.32	2.76
c48_(*m*ABA)(mABA$^{\pm}$)	-29.52	-16.81	4.20	4.32	4.45
c49_(*m*ABA)(mABA$^{\pm}$)	-29.47	-15.91	5.18	5.32	5.34
c50_(*m*ABA)(mABA$^{\pm}$)	-32.11	-17.51	6.47	7.04	3.75
c51_(*m*ABA)(mABA$^{\pm}$)	-32.11	-17.96	6.26	6.86	3.29
c52_(*m*ABA)(mABA$^{\pm}$)	-31.63	-18.69	2.67	3.48	2.57
c53_(*m*ABA)(mABA$^{\pm}$)	-32.11	-17.61	6.58	7.14	3.64
c54_(*m*ABA)(mABA$^{\pm}$)	-31.92	-19.79	3.57	3.56	1.46
c55_(*m*ABA)(mABA$^{\pm}$)	-32.01	-20.22	3.14	3.08	1.03
c56_(*m*ABA)(mABA$^{\pm}$)	-31.96	-18.91	4.71	4.65	2.35
c57_(*m*ABA)(mABA$^{\pm}$)	-29.02	-14.97	7.57	8.25	6.28

Table SI-6. Dimerization of the zwitterionic form of *m*ABA. Standard state (1M) free energies of association in water. Free energies obtained at the SMD/M06-2X/aug-cc-pVDZ//B97-D/6-31++G(d,p) level of theory with liquid-phase geometries. Values in kcal mol^{-1}.

	ΔG^*_{ass} (water)
c1_$(mABA^{\pm})_2$	3.74
c2_$(mABA^{\pm})_2$	3.24
c3_$(mABA^{\pm})_2$	4.91
c4_$(mABA^{\pm})_2$	3.25
c5_$(mABA^{\pm})_2$	4.59
c6_$(mABA^{\pm})_2$	-8.42
c7_$(mABA^{\pm})_2$	-6.37
c8_$(mABA^{\pm})_2$	-2.61
c9_$(mABA^{\pm})_2$	-7.48
c10_$(mABA^{\pm})_2$	-2.95
c11_$(mABA^{\pm})_2$	-3.81
c12_$(mABA^{\pm})_2$	-6.81
c13_$(mABA^{\pm})_2$	-3.82
c14_$(mABA^{\pm})_2$	-10.04
c15_$(mABA^{\pm})_2$	-10.11
c16_$(mABA^{\pm})_2$	-3.59
c17_$(mABA^{\pm})_2$	-2.68
c18_$(mABA^{\pm})_2$	-6.80
c19_$(mABA^{\pm})_2$	-9.78
c20_$(mABA^{\pm})_2$	-4.03
c21_$(mABA^{\pm})_2$	-9.88
c22_$(mABA^{\pm})_2$	-8.19
c23_$(mABA^{\pm})_2$	-9.06
c24_$(mABA^{\pm})_2$	-2.23
c25_$(mABA^{\pm})_2$	-9.12
c26_$(mABA^{\pm})_2$	-1.34
c27_$(mABA^{\pm})_2$	-6.23
c28_$(mABA^{\pm})_2$	-3.56
c29_$(mABA^{\pm})_2$	-6.45
c30_$(mABA^{\pm})_2$	-10.11
c31_$(mABA^{\pm})_2$	-1.80
c32_$(mABA^{\pm})_2$	-0.42
c33_$(mABA^{\pm})_2$	3.81
c34_$(mABA^{\pm})_2$	-4.12
c35_$(mABA^{\pm})_2$	7.96
c36_$(mABA^{\pm})_2$	-9.05
c37_$(mABA^{\pm})_2$	7.96
c39_$(mABA^{\pm})_2$	-6.57
c40_$(mABA^{\pm})_2$	-3.20
c41_$(mABA^{\pm})_2$	-8.80

c43_$(mABA^{\pm})_2$	5.03
c44_$(mABA^{\pm})_2$	-3.24
c45_$(mABA^{\pm})_2$	5.10
c46_$(mABA^{\pm})_2$	7.40
c47_$(mABA^{\pm})_2$	3.79
c48_$(mABA^{\pm})_2$	3.30
c49_$(mABA^{\pm})_2$	2.93
c50_$(mABA^{\pm})_2$	-6.67
c51_$(mABA^{\pm})_2$	-6.96
c52_$(mABA^{\pm})_2$	-6.97
c53_$(mABA^{\pm})_2$	5.36
c54_$(mABA^{\pm})_2$	-5.85
c55_$(mABA^{\pm})_2$	-7.27
c56_$(mABA^{\pm})_2$	-3.63
c57_$(mABA^{\pm})_2$	2.09
c58_$(mABA^{\pm})_2$	2.52

Table SI.7. Dimerization of the zwitterionic form of *m*ABA. Standard state (1M) free energies of association in methanol. Free energies obtained at the SMD/M06-2X/aug-cc-pVDZ//B97-D/6-31++G(d,p) level of theory with liquid-phase geometries. Values in kcal mol^{-1}.

	ΔG^*_{ass} (methanol)
c1_$(mABA^{\pm})_2$	-9.53
c2_$(mABA^{\pm})_2$	-2.87
c3_$(mABA^{\pm})_2$	9.28
c4_$(mABA^{\pm})_2$	-2.82
c5_$(mABA^{\pm})_2$	0.35
c6_$(mABA^{\pm})_2$	-7.36
c7_$(mABA^{\pm})_2$	-14.60
c8_$(mABA^{\pm})_2$	-2.66
c9_$(mABA^{\pm})_2$	-7.17
c10_$(mABA^{\pm})_2$	-3.26
c11_$(mABA^{\pm})_2$	-4.00
c12_$(mABA^{\pm})_2$	-7.56
c13_$(mABA^{\pm})_2$	-7.08
c14_$(mABA^{\pm})_2$	-10.51
c15_$(mABA^{\pm})_2$	-3.05
c16_$(mABA^{\pm})_2$	-6.15
c17_$(mABA^{\pm})_2$	-3.11
c18_$(mABA^{\pm})_2$	-8.26
c19_$(mABA^{\pm})_2$	-10.31
c20_$(mABA^{\pm})_2$	-3.98
c21_$(mABA^{\pm})_2$	-3.29
c22_$(mABA^{\pm})_2$	-9.17
c23_$(mABA^{\pm})_2$	-10.33
c24_$(mABA^{\pm})_2$	-7.04
c25_$(mABA^{\pm})_2$	-2.64
c26_$(mABA^{\pm})_2$	-0.88
c27_$(mABA^{\pm})_2$	-7.06
c28_$(mABA^{\pm})_2$	-9.58
c29_$(mABA^{\pm})_2$	-7.42
c30_$(mABA^{\pm})_2$	-10.22
c32_$(mABA^{\pm})_2$	-0.29
c33_$(mABA^{\pm})_2$	-10.48
c34_$(mABA^{\pm})_2$	-2.63
c35_$(mABA^{\pm})_2$	7.33
c36_$(mABA^{\pm})_2$	-2.98
c37_$(mABA^{\pm})_2$	6.51
c38_$(mABA^{\pm})_2$	-9.92
c39_$(mABA^{\pm})_2$	-6.75
c40_$(mABA^{\pm})_2$	-8.10
c41_$(mABA^{\pm})_2$	-9.62

c42_$(mABA^{\pm})_2$	0.57
c43_$(mABA^{\pm})_2$	8.02
c44_$(mABA^{\pm})_2$	-9.38
c45_$(mABA^{\pm})_2$	8.45
c46_$(mABA^{\pm})_2$	7.49
c47_$(mABA^{\pm})_2$	6.69
c48_$(mABA^{\pm})_2$	6.09
c49_$(mABA^{\pm})_2$	6.09
c50_$(mABA^{\pm})_2$	-7.16
c51_$(mABA^{\pm})_2$	-7.57
c52_$(mABA^{\pm})_2$	-7.57
c53_$(mABA^{\pm})_2$	-9.00
c54_$(mABA^{\pm})_2$	-7.10
c55_$(mABA^{\pm})_2$	-6.80
c56_$(mABA^{\pm})_2$	-3.04
c57_$(mABA^{\pm})_2$	6.08
c58_$(mABA^{\pm})_2$	-9.91
c59_$(mABA^{\pm})_2$	-9.27
c60_$(mABA^{\pm})_2$	-7.39

Table SI.8. Dimerization of *m*HBA. Gas phase interaction energies ($\Delta E_{e,gas}$), standard state (1 atm) gas-phase free energies of association (ΔG°_{ass}) at 298 K computed at the M06-2X/aug-cc-pVDZ//M06-2X/6-31++G(d,p) level of theory. Standard state (1M) free energies of association in chloroform (ΔG^{*}_{ass}) computed the using the SMD solvation model at the M06-2X/aug-cc-pVDZ level of theory with gas-phase geometries. Values in kcal mol^{-1}.

	$\Delta E_{e,gas}$ [a]	ΔG°_{ass} [a]	ΔG^{*}_{ass} [b]			
			water	**ethanol**	**acetonitrile**	**ethyl acetate**
c1_(*m*HBA)$_2$	-5.76	4.73	4.56	5.38	5.44	5.02
c2_(*m*HBA)$_2$	-5.32	6.37	5.36	6.30	6.60	6.34
c3_(*m*HBA)$_2$	-10.02	0.88	4.80	5.39	4.45	2.95
c4_(*m*HBA)$_2$	-9.48	1.02	3.16	3.58	2.78	1.92
c5_(*m*HBA)$_2$	-7.09	5.25	5.71	6.04	5.83	5.33
c6_(*m*HBA)$_2$	-7.09	4.46	4.89	5.34	5.02	4.59
c7_(*m*HBA)$_2$	-6.71	4.05	4.26	5.51	5.71	5.11
c8_(*m*HBA)$_2$	-7.09	5.51	6.05	6.47	6.17	5.70
c9_(*m*HBA)$_2$	-5.33	6.85	6.56	7.36	7.28	6.90
c10_(*m*HBA)$_2$	-7.97	5.18	6.30	7.43	7.63	6.96
c11_(*m*HBA)$_2$	-5.33	6.85	6.73	7.59	7.42	6.89
c12_(*m*HBA)$_2$	-5.33	6.85	6.73	7.54	7.41	6.92
c13_(*m*HBA)$_2$	-10.18	1.79	3.70	4.69	5.32	4.28
c14_(*m*HBA)$_2$	-6.26	5.52	2.52	3.49	5.28	5.60
c15_(*m*HBA)$_2$	-13.43	1.44	5.30	6.39	6.10	4.59
c16_(*m*HBA)$_2$	-5.75	4.57	4.42	5.25	5.33	4.90
c17_(*m*HBA)$_2$	-6.26	4.63	1.75	2.66	4.36	4.71
c18_(*m*HBA)$_2$	-8.07	4.99	6.20	7.50	7.64	6.87
c19_(*m*HBA)$_2$	-7.09	3.59	4.06	4.51	4.19	3.74
c20_(*m*HBA)$_2$	-4.77	6.13	5.67	6.18	6.22	6.04
c21_(*m*HBA)$_2$	-7.79	4.33	3.31	4.41	5.44	5.12
c22_(*m*HBA)$_2$	-8.45	5.34	6.14	7.07	7.80	7.19
c23_(*m*HBA)$_2$	-11.75	2.01	5.29	6.23	6.67	5.78
c24_(*m*HBA)$_2$	-4.53	6.01	6.42	7.06	6.87	6.32
c25_(*m*HBA)$_2$	-13.43	0.76	4.59	5.75	5.42	3.90
c26_(*m*HBA)$_2$	-13.44	0.98	4.88	5.98	5.62	4.11
c27_(*m*HBA)$_2$	-4.21	7.32	7.75	8.69	9.05	8.49
c28_(*m*HBA)$_2$	-9.70	3.29	5.44	5.87	5.06	4.21
c29_(*m*HBA)$_2$	-7.79	3.70	2.69	3.79	4.87	4.53
c30_(*m*HBA)$_2$	-9.64	3.18	5.34	5.73	4.98	4.12
c31_(*m*HBA)$_2$	-8.39	3.77	0.88	2.01	3.76	4.03
c32_(*m*HBA)$_2$	-7.12	4.98	5.39	5.86	5.58	5.16
c33_(*m*HBA)$_2$	-6.83	3.58	4.08	5.04	5.26	4.63
c34_(*m*HBA)$_2$	-10.03	0.89	4.92	5.50	4.54	3.02
c35_(*m*HBA)$_2$	-9.64	3.42	5.57	6.00	5.19	4.33
c36_(*m*HBA)$_2$	-9.64	1.15	3.30	3.65	2.92	2.05
c37_(*m*HBA)$_2$	-6.83	5.81	6.21	7.13	7.34	6.70
c38_(*m*HBA)$_2$	-8.39	3.53	0.71	1.83	3.62	3.86

c39_(*m*HBA)$_2$	-13.44	0.94	4.88	6.05	5.56	4.03
c40_(*m*HBA)$_2$	-10.20	3.98	3.46	4.51	5.28	5.35
c41_(*m*HBA)$_2$	-7.10	4.87	5.33	5.75	5.41	5.00
c42_(*m*HBA)$_2$	-9.63	0.59	2.70	3.15	2.41	1.55
c43_(*m*HBA)$_2$	-9.64	2.23	4.35	4.79	4.01	3.16
c44_(*m*HBA)$_2$	-9.64	1.62	3.78	4.18	3.38	2.54
c45_(*m*HBA)$_2$	-9.64	0.63	2.79	3.21	2.43	1.59
c46_(*m*HBA)$_2$	-13.44	0.83	4.67	5.82	5.49	3.97
c47_(*m*HBA)$_2$	-8.39	3.77	0.88	2.00	3.75	4.03
c48_(*m*HBA)$_2$	-8.87	5.47	5.47	6.58	6.92	6.65
c49_(*m*HBA)$_2$	-7.76	4.73	3.65	4.70	5.87	5.55
c50_(*m*HBA)$_2$	-9.64	2.23	4.35	4.79	4.01	3.17
c51_(*m*HBA)$_2$	**-17.32**	**-5.90**	**0.14**	**0.24**	**-2.23**	**-3.78**
c52_(*m*HBA)$_2$	**-17.32**	**-6.07**	**-0.01**	**0.08**	**-2.40**	**-3.95**
c53_(*m*HBA)$_2$	**-17.42**	**-5.57**	**0.44**	**0.66**	**-1.92**	**-3.43**
c54_(*m*HBA)$_2$	**-17.42**	**-5.56**	**0.40**	**0.65**	**-1.91**	**-3.43**
c55_(*m*HBA)$_2$	**-17.42**	**-5.38**	**0.56**	**0.82**	**-1.73**	**-3.26**
c56_(*m*HBA)$_2$	**-18.18**	**-6.29**	**0.31**	**0.48**	**-2.09**	**-3.76**
c57_(*m*HBA)$_2$	**-18.01**	**-6.10**	**0.45**	**0.52**	**-1.88**	**-3.57**
c58_(*m*HBA)$_2$	-8.79	2.44	5.87	6.14	5.07	3.78
c59_(*m*HBA)$_2$	-11.76	-0.66	4.67	4.91	3.95	2.21
c60_(*m*HBA)$_2$	**-18.03**	**-6.71**	**0.01**	**0.17**	**-2.20**	**-4.12**
c61_(*m*HBA)$_2$	-9.01	2.94	4.49	4.77	4.45	3.79
c62_(*m*HBA)$_2$	-8.77	3.29	2.13	2.86	4.37	4.24
c63_(*m*HBA)$_2$	-5.03	5.85	5.26	5.94	6.26	5.75
c64_(*m*HBA)$_2$	-9.81	2.85	4.61	5.14	4.66	3.81
c65_(*m*HBA)$_2$	-8.77	2.89	1.71	2.42	3.97	3.83
c66_(*m*HBA)$_2$	-9.63	3.49	3.94	4.91	5.66	5.17
c67_(*m*HBA)$_2$	-5.40	3.95	2.86	3.76	4.66	4.30
c68_(*m*HBA)$_2$	-8.84	4.65	6.15	7.25	7.42	6.44
c69_(*m*HBA)$_2$	-9.63	3.76	4.22	5.22	5.90	5.45
c70_(*m*HBA)$_2$	-9.01	2.30	3.92	7.39	4.07	3.16
c71_(*m*HBA)$_2$	-10.10	3.55	3.30	4.33	5.73	5.36
c72_(*m*HBA)$_2$	-8.56	5.53	6.47	7.58	7.44	4.39
c73_(*m*HBA)$_2$	-8.84	4.47	5.90	6.96	7.18	6.22
c74_(*m*HBA)$_2$	-8.84	4.25	25.25	6.82	6.95	6.03
c75_(*m*HBA)$_2$	-8.02	2.36	3.79	4.90	5.00	4.04
c77_(*m*HBA)$_2$	-11.46	2.67	23.67	27.14	23.82	5.69
c78_(*m*HBA)$_2$	-8.91	3.43	1.61	2.64	-0.68	4.12
c79_(*m*HBA)$_2$	-8.56	3.87	4.87	5.95	5.82	5.20
c80_(*m*HBA)$_2$	-11.53	1.32	2.86	3.77	4.30	3.47
c81_(*m*HBA)$_2$	-9.37	3.32	5.98	6.76	7.16	6.09
c83_(*m*HBA)$_2$	-10.11	3.63	3.41	4.42	5.75	5.42
c84_(*m*HBA)$_2$	-8.77	2.95	1.73	2.46	4.12	3.88
c85_(*m*HBA)$_2$	-10.05	2.79	2.88	3.85	5.09	4.62
c87_(*m*HBA)$_2$	-6.93	5.25	4.60	5.75	6.26	6.03

c88_(*m*HBA)$_2$	-8.84	2.60	4.12	5.25	5.35	4.41
c89_(*m*HBA)$_2$	**-17.61**	**-4.43**	**1.91**	**2.12**	**-0.31**	**-2.04**
c90_(*m*HBA)$_2$	-12.26	-0.42	5.54	5.85	4.27	2.53
c91_(*m*HBA)$_2$	-7.59	4.46	2.13	3.09	4.26	4.38
c92_(*m*HBA)$_2$	-8.47	2.70	5.87	6.19	5.20	3.93
c93_(*m*HBA)$_2$	-8.90	2.59	2.10	3.11	4.45	4.18
c94_(*m*HBA)$_2$	-8.13	4.52	2.29	3.21	4.88	4.84
c95_(*m*HBA)$_2$	-6.46	4.76	4.22	4.70	5.25	5.05
c96_(*m*HBA)$_2$	-5.02	6.72	6.67	7.24	7.76	7.66
c97_(*m*HBA)$_2$	-12.35	-0.19	5.71	6.02	4.39	2.68
c98_(*m*HBA)$_2$	-12.30	0.06	6.00	6.29	4.66	2.94
c99_(*m*HBA)$_2$	-10.14	3.18	4.62	5.75	5.91	5.17
c100_(*m*HBA)$_2$	-5.21	7.46	7.32	7.89	8.44	8.32
c101_(*m*HBA)$_2$	-14.33	0.08	5.00	5.78	5.35	3.97
c102_(*m*HBA)$_2$	-11.26	2.44	5.44	6.47	5.95	4.88
c103_(*m*HBA)$_2$	-7.57	3.97	1.79	2.75	3.88	3.93
c104_(*m*HBA)$_2$	-15.31	-2.64	5.04	5.26	2.96	1.13
c105_(*m*HBA)$_2$	-10.13	2.07	3.49	4.65	4.83	4.06
c106_(*m*HBA)$_2$	-9.63	3.32	2.29	3.23	5.03	4.79
c107_(*m*HBA)$_2$	-8.65	4.77	4.57	5.61	6.22	5.79
c108_(*m*HBA)$_2$	-3.19	8.57	6.38	6.86	7.73	7.81
c109_(*m*HBA)$_2$	-11.83	1.32	4.00	4.83	4.99	4.03
c110_(*m*HBA)$_2$	-4.09	7.44	5.66	6.34	6.91	6.95
c111_(*m*HBA)$_2$	-15.27	-0.91	6.69	6.94	4.68	2.87
c112_(*m*HBA)$_2$	-7.70	5.42	3.20	4.11	5.25	5.33
c113_(*m*HBA)$_2$	-8.72	5.39	2.87	3.90	5.71	5.82
c114_(*m*HBA)$_2$	-11.84	1.08	3.66	4.55	4.74	3.80
c115_(*m*HBA)$_2$	-10.45	2.25	4.20	5.18	5.01	4.15
c116_(*m*HBA)$_2$	**-17.51**	**-6.36**	**0.32**	**0.47**	**-2.03**	**-3.86**
c117_(*m*HBA)$_2$	-12.31	-1.17	4.65	5.26	3.59	1.83
c118_(*m*HBA)$_2$	-9.50	3.35	2.16	3.66	4.96	4.59
c119_(*m*HBA)$_2$	-8.53	3.85	4.87	6.30	6.33	5.49
c120_(*m*HBA)$_2$	-9.50	3.43	2.23	3.73	5.03	4.66
c121_(*m*HBA)$_2$	-7.70	4.59	4.49	5.74	5.93	5.35
c123_(*m*HBA)$_2$	-8.54	2.98	3.98	5.48	5.48	4.60
c124_(*m*HBA)$_2$	-9.45	3.85	2.50	4.01	5.21	4.91
c125_(*m*HBA)$_2$	-12.47	0.31	6.06	6.71	5.06	3.31
c126_(*m*HBA)$_2$	-10.64	2.30	6.35	7.29	6.62	5.08
c127_(*m*HBA)$_2$	-8.45	3.10	4.07	5.53	5.60	4.76
c128_(*m*HBA)$_2$	-9.24	2.56	1.14	2.39	4.08	3.83
c129_(*m*HBA)$_2$	-10.85	1.15	5.57	6.50	5.64	4.07
c130_(*m*HBA)$_2$	-10.08	2.00	6.33	7.15	5.99	4.38
c131_(*m*HBA)$_2$	-11.67	0.83	1.50	2.83	3.59	3.01
c132_(*m*HBA)$_2$	-12.19	0.68	2.95	4.23	4.39	3.39
c133_(*m*HBA)$_2$	-8.33	4.38	4.81	6.08	6.96	6.42
c134_(*m*HBA)$_2$	-11.57	0.38	3.05	4.43	4.02	2.82

c135_(*m*HBA)$_2$	-11.25	2.79	4.29	5.52	5.84	5.02
c139_(*m*HBA)$_2$	-9.23	2.53	1.13	2.36	4.03	3.81
c140_(*m*HBA)$_2$	**-17.79**	**-6.20**	**0.04**	**0.55**	**-1.93**	**-3.76**