Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Examination of the Hydrogen-Bonding Networks in Small Water Clusters (n=2-5,13,17) using Absolutely Localized Molecular Orbital Energy Decomposition Analysis

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Figure S1: Extended Version of Figure 4. Three key types of rings, and their associated ALMO-EDA terms, that are found in the 13-mer and 17-mer. a) Type A tetramer (each water is both a single proton-acceptor and a single proton donor, as indicated by the "AD" labels) located within the 13-mer (see Figure 2b for relative location). b) Type A pentamer located within the 17-mer (see Figure 2d for relative location). c) Type B pentamer (containing AD waters as well as some waters that are double proton acceptors; "AA", and some that are double proton-donors; "DD") located within the 17-mer (see Figure 2d for relative location). d) Type C tetramer (no AD waters) located within the 13 mer (see Figure 2b for relative location).

Figure S2: Additional rings (not covered in Fig. S1) within the 13-mer, and their associated ALMO-EDA terms. See Figure 2b for relative location. a) Type A Tetramer: 7, 8, 10, 12; b) Type C Tetramer: 1, 2, 7, 12; c) Type A Tetramer: 1, 3, 5, 7; d) Type A Tetramer: 1, 2, 6, 11; e) Type B Pentamer: 1, 5, 6, 9, 13; f) Type C Tetramer: 6, 8, 10, 11; g) Type A Pentamer: 4, 6, 8, 9, 13; h) Type A Tetramer: 2, 10, 11, 12; i) Type A Tetramer: 1, 6, 7, 8.

Figure S3: Additional rings (not covered in Fig. S1) within the 17-mer, and their associated ALMO-EDA terms. See Figure 2d for relative location. a) Type A Pentamer: 2, 6, 9, 12, 15; b) Type C Tetramer: 3, 7, 8, 11; c) Type A Pentamer: 4, 7, 11, 14, 17; d) Type C Tetramer: 1, 2, 3, 15; e) Type B Hexamer: 1, 3, 5, 9, 12, 15; f) Type C Tetramer: 1, 4, 5, 14; g) Type B Tetramer: 4, 13, 16, 17; h) Type B Hexamer: 4, 5, 6, 12, 14, 16; i) Type B Hexamer: 2, 3, 7, 13, 15, 17; j) Type B Tetramer: 2, 6, 13, 16; k) Type A Pentamer: 5, 8, 10, 11, 14.

Table S3: Comparison of ALMO-EDA calculations using the B3LYP and ωB97X-D density functionals for the water 13-mer, organized by the 2- and 3-body interactions of each water (energies in kcal/mol; details as for Table S1).

Table S4: Cartesian coordinates for the optimized water dimer-pentamer (MP2/aug-cc-pVTZ), 13-mer (B3LYP/6-311+G(d,p), and 17-mer (MP2/aug-cc-pVTZ) structures used throughout this work.

Table S1: Extended Version of Table 3. Comparison of ALMO-EDA calculations using the B3LYP and ωB97X-D density functionals for the water tetramer shown in Fig. 1 The aug-cc-pVQZ basis is used; ΔE = total interaction energy; "FRZ" = ΔE_{FRZ} = frozen density interaction energy; "POL" = ΔE_{POL} = polarization energy; "CT" = ΔE_{CT} = intermolecular charge transfer energy. Energies are in kcal/mol.

Tetramer: B3LYP						
	Two-Body					
	1,2	1,3	1,4	2,3	2,4	3,4
DE	-4.0	-4.0	-1.3	-1.3	-4.0	-4.0
FRZ	1.6	1.6	-1.2	-1.2	1.6	1.6
POL	-2.8	-2.8	-0.1	-0.1	-2.8	-2.8
CT	-2.8	-2.8	0.0	0.0	-2.8	-2.8
	Three-Body					
	1,2,3	1,2,4	1,3,4	2,3,4		
DE	-1.7	-1.7	-1.7	-1.7		
FRZ	-0.1	-0.1	-0.1	-0.1		
POL	-1.2	-1.2	-1.2	-1.2		
CT	-0.4	-0.4	-0.4	-0.4		
	Sum 2-body	Sum 3-body	Sum 2/3-body	Tetramer Total	% Total Recovered by 2/3-body terms	
DE	-18.7	-6.8	-25.5	-26.1	97.8	
FRZ	3.9	-0.4	3.5	3.6	98.0	
POL	-11.2	-4.8	-16.0	-16.4	97.7	
CT	-11.4	-1.6	-13.0	-13.3	98.2	

Tetramer: ωB97X-D						
	Two-Body					
	1,2	1,3	1,4	2,3	2,4	3,4
DE	-4.2	-4.2	-1.6	-1.6	-4.2	-4.2
FRZ	0.9	0.9	-1.5	-1.5	0.9	0.9
POL	-2.8	-2.8	-0.1	-0.1	-2.8	-2.8
CT	-2.3	-2.3	0.0	0.0	-2.3	-2.3
	Three-Body					
	1,2,3	1,2,4	1,3,4	2,3,4		
DE	-1.7	-1.6	-1.6	-1.6		
FRZ	-0.1	-0.1	-0.1	-0.1		
POL	-1.2	-1.2	-1.2	-1.2		
CT	-0.3	-0.3	-0.3	-0.3		
	Sum 2-body	Sum 3-body	Sum 2/3-body	Tetramer Total	% Total Recovered by 2/3-body terms	
DE	-20.2	-6.6	-26.8	-27.3	98.1	
FRZ	0.7	-0.4	0.2	0.3	82.9	
POL	-11.4	-4.9	-16.3	-16.6	97.9	
CT	-9.4	-1.3	-10.7	-10.9	98.2	

Table S2: Extended Version of Table 4. Comparison of ALMO-EDA calculations using the B3LYP and ωB97X-D density functionals for the water pentamer shown in Fig. 1 (energies in kcal/mol; details as for Table S1).

Pentamer: B3LYP										
	Two-Body									
	1,2	1,3	1,4	1,5	2,3	2,4	2,5	3,4	3,5	4,5
DE	-3.9	-0.9	-1.0	-3.4	-3.8	-0.9	-0.9	-3.9	-0.8	-3.9
FRZ	2.3	-0.8	-0.9	2.3	2.3	-0.8	-0.9	2.3	-0.8	2.3
POL	-3.1	0.0	0.0	-2.9	-3.1	0.0	0.0	-3.1	0.0	-3.1
CT	-3.1	0.0	0.0	-2.8	-3.0	0.0	0.0	-3.1	0.0	-3.1
	Three-Body									
	1,2,3	1,2,4	1,2,5	1,3,4	1,3,5	1,4,5	2,3,4	2,3,5	2,4,5	3,4,5
DE	-1.7	-0.4	-1.6	-0.4	-0.4	-1.6	-1.7	-0.4	-0.4	-1.6
FRZ	-0.1	0.0	-0.1	0.0	0.0	-0.1	-0.1	0.0	0.0	-0.1
POL	-1.2	-0.3	-1.1	-0.3	-0.3	-1.1	-1.1	-0.3	-0.3	-1.1
CT	-0.4	-0.1	-0.4	-0.1	-0.1	-0.4	-0.4	-0.1	-0.1	-0.4

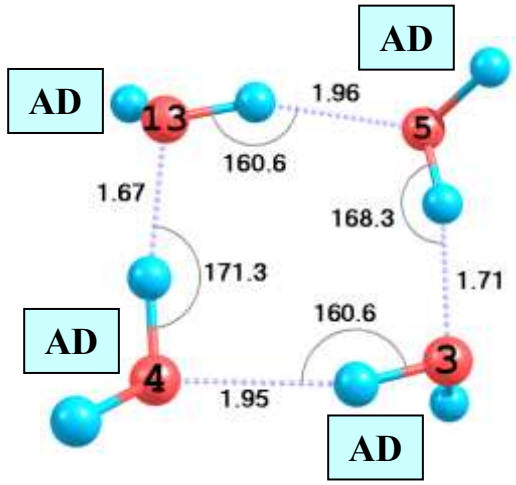
	Sum 2-body	Sum 3-body	Sum 2/3-body	Pentamer Total	% Total Recovered by 2/3-body terms
ΔE	-23.3	-10.1	-33.4	-34.7	96.2
FRZ	7.2	-0.8	6.4	6.5	98.7
POL	-15.4	-7.1	-22.4	-23.3	96.3
CT	-15.1	-2.2	-17.4	-17.9	97.0

Pentamer: ωB97X-D										
	Two-Body									
	1,2	1,3	1,4	1,5	2,3	2,4	2,5	3,4	3,5	4,5
DE	-4.1	-1.1	-1.1	-3.6	-4.0	-1.1	-1.1	-4.1	-1.0	-4.1
FRZ	1.6	-1.0	-1.1	1.7	1.6	-1.0	-1.1	1.6	-1.0	1.6
POL	-3.1	0.0	0.0	-2.9	-3.1	0.0	0.0	-3.1	0.0	-3.1
CT	-2.5	0.0	0.0	-2.3	-2.5	0.0	0.0	-2.6	0.0	-2.5
	Three-Body									
	1,2,3	1,2,4	1,2,5	1,3,4	1,3,5	1,4,5	2,3,4	2,3,5	2,4,5	3,4,5
DE	-1.6	-0.4	-1.5	-0.4	-0.4	-1.4	-1.5	-0.3	-0.4	-1.5
FRZ	-0.1	0.0	-0.1	0.0	0.0	-0.1	-0.1	0.0	0.0	-0.1
POL	-1.2	-0.3	-1.1	-0.3	-0.3	-1.1	-1.2	-0.3	-0.3	-1.1
CT	-0.3	0.0	-0.3	0.0	0.0	-0.3	-0.3	0.0	0.0	-0.3

	Sum 2-body	Sum 3-body	Sum 2/3-body	Pentamer Total	% Total Recovered by 2/3-body terms
DE	-25.2	-9.4	-34.6	-35.8	96.6
FRZ	2.9	-0.4	2.4	2.5	98.9
POL	-15.6	-7.1	-22.7	-23.5	96.5
CT	-12.5	-1.8	-14.3	-14.8	97.1

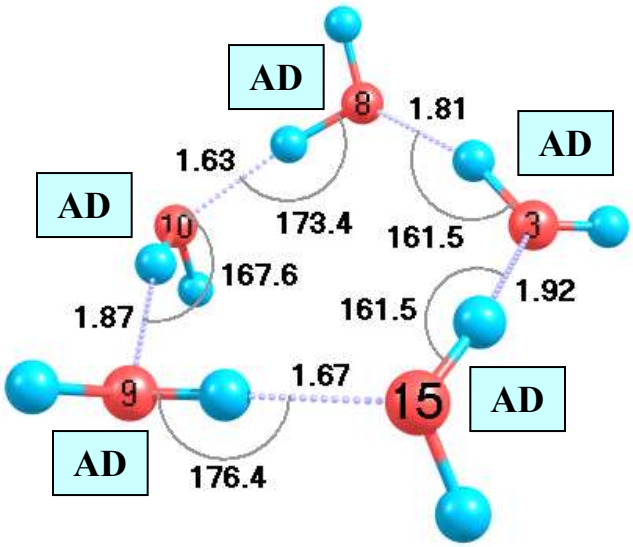
Figure S1: Extended Version of Figure 4. Three key types of rings, and their associated ALMO-EDA terms (kcal/mol, ωB97X-D/aug-cc-pVQZ), that are found in the 13-mer and 17-mer. a) Type A tetramer (each water is both a single proton-acceptor and a single proton donor, as indicated by the "AD" labels) located within the 13-mer (see Figure 2b for relative location). b) Type A pentamer located within the 17-mer (see Figure 2d for relative location). c) Type B pentamer (containing AD waters as well as some waters that are double proton acceptors; "AA", and some that are double proton-donors; "DD") located within the 17-mer (see Figure 2d for relative location). d) Type C tetramer (no AD waters) located within the 13 mer (see Figure 2b for relative location).

a) Type A Tetramer



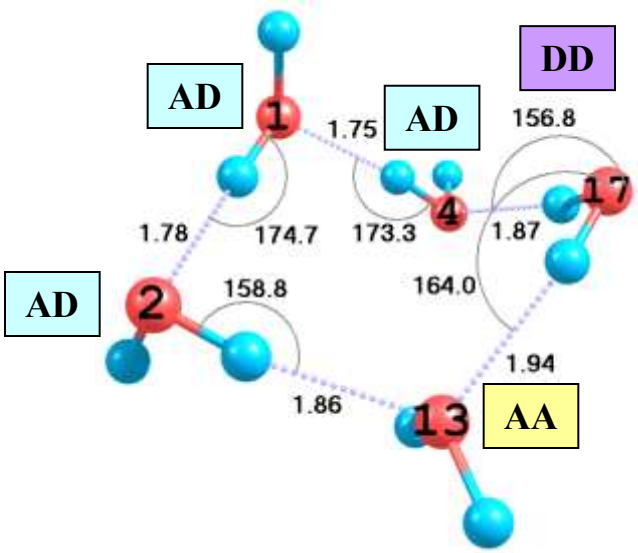
Type A Tetramer (3, 4, 5, 13) within the 13-Mer Water Cluster						
	Two-Body					
	3,4	3,5	3,13	4,5	4,13	5,13
DE	**-4.5**	**-4.1**	**-1.6**	**-1.3**	**-3.8**	**-4.6**
FRZ	-1.5	2.3	-1.5	-1.3	3.4	-1.7
POL	-1.6	-3.5	-0.1	0.0	-4.0	-1.6
CT	-1.3	-3.0	0.0	0.0	-3.2	-1.3
	Three-Body					
	3,4,5	3,4,13	3,5,13	4,5,13		
DE	**-1.3**	**-1.6**	**-1.4**	**-1.4**		
FRZ	0.0	-0.1	-0.1	0.0		
POL	-1.0	-1.1	-1.0	-1.1		
CT	-0.3	-0.3	-0.3	-0.3		

b) Type A Pentamer



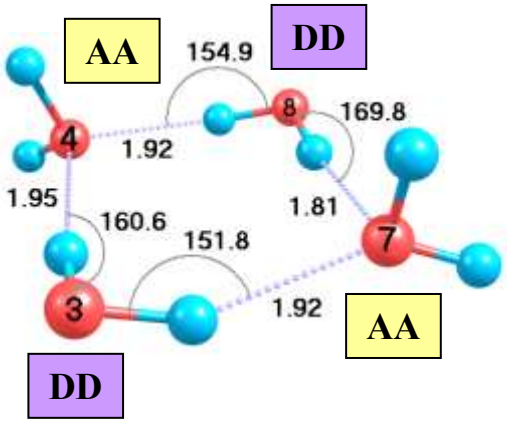
Type A Pentamer (3, 8, 9, 10, 15) within the 17-mer Water Cluster					
	Two-Body				
	3,8	3,9	3,10	3,15	8,9
DE	**-4.0**	**-1.0**	**-1.3**	**-3.7**	**-0.9**
FRZ	0.3	-1.0	-1.2	-0.9	-0.9
POL	-2.4	0.0	0.0	-1.7	0.0
CT	-1.9	0.0	0.0	-1.1	0.0
	Two-Body, Continued				
	8,10	8,15	9,10	9,15	10,15
DE	**-3.1**	**-0.8**	**-4.4**	**-3.6**	**-0.9**
FRZ	5.3	-0.8	-0.7	3.6	-0.9
POL	-4.6	0.0	-2.0	-3.9	0.0
CT	-3.7	0.0	-1.6	-3.3	0.0
	Three-Body (three-adjacent-water terms only)				
	3,8,10	3,8,15	3,9,15	8,9,10	9,10,15
DE	**-1.8**	**-1.1**	**-1.3**	**-1.5**	**-1.4**
FRZ	-0.1	-0.1	-0.1	0.0	0.0
POL	-1.3	-0.9	-1.0	-1.1	-1.0

c) Type B Pentamer



Type B Pentamer (1, 2, 4, 13, 17) within the 17-Mer Water Cluster					
	Two-Body				
	1,2	1,4	1,13	1,17	2,4
DE	-3.7	-3.9	-0.9	-0.8	-1.0
FRZ	1.5	1.4	-0.8	-0.7	-1.0
POL	-2.7	-2.9	-0.1	-0.1	0.0
CT	-2.5	-2.4	0.0	0.0	0.0
	Two-Body, Continued				
	2,13	2,17	4,13	4,17	13,17
DE	-2.8	0.7	-0.9	-3.5	-3.4
FRZ	1.1	0.7	-0.9	0.2	-0.3
POL	-2.1	0.0	-0.1	-2.1	-1.7
CT	-1.7	0.0	0.0	-1.7	-1.4
	Three-Body (three-adjacent-water terms only)				
	1,2,4	1,2,13	1,4,17	2,13,17	4,13,17
DE	-1.4	-0.9	-1.3	0.8	0.7
FRZ	0.0	-0.1	-0.2	-0.1	0.1
POL	-1.1	-0.7	-0.9	0.8	0.5

d) Type C Tetramer

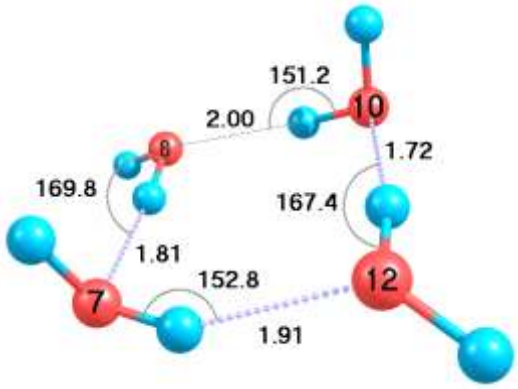


Type C Tetramer (3, 4, 7, 8) within the 13-Mer Water Cluster						
	Two-Body					
	3,4	3,7	3,8	4,7	4,8	7,8
DE	-4.5	-4.0	1.2	1.1	-4.1	-4.3
FRZ	-1.5	-1.1	1.4	1.1	-1.0	0.4
POL	-1.6	-1.7	-0.1	0.0	-1.8	-2.5
CT	-1.3	-1.2	-0.1	0.0	-1.3	-2.2
	Three-Body					
	3,4,7	3,7,8	3,4,8	4,7,8		
DE	0.4	0.4	0.4	0.6		
FRZ	0.0	0.0	0.0	0.1		
POL	0.3	0.3	0.3	0.4		
CT	0.1	0.1	0.1	0.1		

Figure S2: Additional rings (not covered in Fig. S1) within the 13-mer, and their associated ALMO-EDA terms (kcal/mol, ωB97X-D/aug-cc-pVQZ). See Figure 2b for relative location. a) Type A Tetramer: 7, 8, 10, 12; b) Type C Tetramer: 1, 2, 7, 12; c) Type A Tetramer: 1, 3, 5, 7; d) Type A Tetramer: 1, 2, 6, 11; e) Type B Pentamer: 1, 5, 6, 9, 13; f) Type C Tetramer: 6, 8, 10, 11; g) Type A Pentamer: 4, 6, 8, 9, 13; h) Type A Tetramer: 2, 10, 11, 12; i) Type A Tetramer: 1, 6, 7, 8.

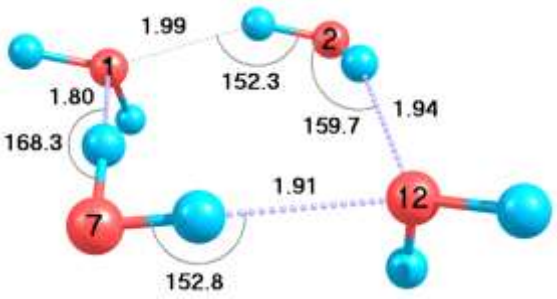
a) Type A Tetramer: 7, 8, 10, 12

Type A Tetramer: 7,8,10,12						
	Two-Body					
	7,8	7,10	7,12	8,10	8,12	10,12
ΔE	-4.33	-1.21	-4.06	-3.90	-1.33	-4.19
FRZ	0.42	-1.13	-0.92	-1.71	-1.28	2.00
POL	-2.50	-0.06	-1.77	-1.31	-0.04	-3.33
CT	-2.25	-0.02	-1.37	-0.88	-0.01	-2.86
	Three-Body					
	7,8,10	7,8,12	7,10,12	8,10,12		
ΔE	-1.13	-1.18	-1.43	-1.17		
FRZ	-0.16	0.02	-0.16	0.02		
POL	-0.80	-0.95	-1.01	-0.97		
CT	-0.17	-0.24	-0.26	-0.22		



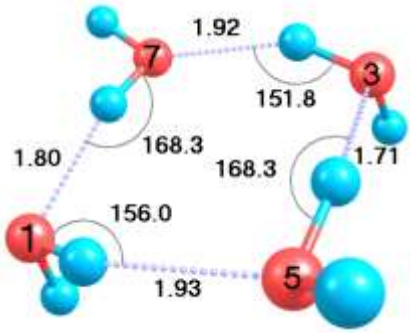
b) Type C Tetramer: 1, 2, 7, 12

Type C Tetramer: 1,2,7,12						
	Two-Body					
	1,2	1,7	1,12	2,7	2,12	7,12
ΔE	-3.93	-4.36	0.94	1.34	-4.54	-4.06
FRZ	-1.71	0.43	0.97	1.59	-1.62	-0.92
POL	-1.34	-2.52	-0.03	-0.17	-1.64	-1.77
CT	-0.88	-2.27	0.00	-0.08	-1.27	-1.37
	Three-Body					
	1,2,7	1,2,12	1,7,12	2,7,12		
ΔE	0.28	0.45	0.64	0.29		
FRZ	-0.02	0.04	0.09	-0.02		
POL	0.20	0.35	0.42	0.23		
CT	0.10	0.07	0.13	0.08		



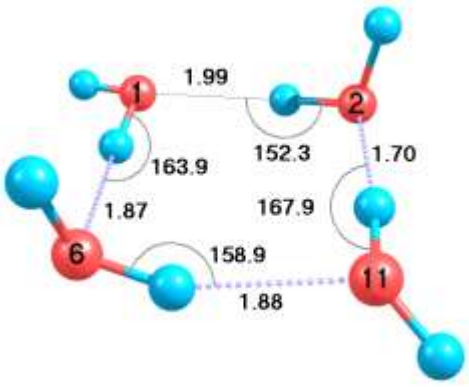
c) Type A Tetramer: 1, 3, 5, 7

Type A Tetramer: 1,3,5,7						
	Two-Body					
	1,3	1,5	1,7	3,5	3,7	5,7
ΔE	-1.18	-4.33	-4.36	-4.11	-3.96	-1.61
FRZ	-1.12	-1.24	0.43	2.34	-1.12	-1.53
POL	-0.05	-1.73	-2.52	-3.45	-1.68	-0.06
CT	-0.02	-1.35	-2.27	-2.99	-1.16	-0.02
	Three-Body					
	1,3,5	1,3,7	1,5,7	3,5,7		
ΔE	-1.43	-1.24	-1.23	-1.41		
FRZ	-0.13	-0.13	-0.02	-0.03		
POL	-1.03	-0.91	-0.96	-1.11		
CT	-0.27	-0.21	-0.25	-0.27		



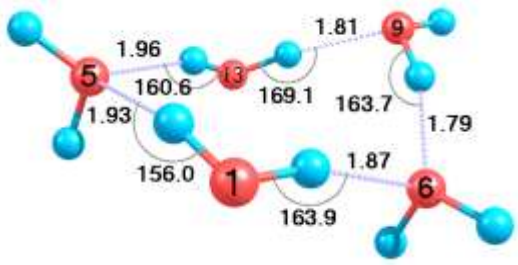
d) Type A Tetramer: 1, 2, 6, 11

Type A Tetramer: 1,2,6,11						
	Two-Body					
	1,2	1,6	1,11	2,6	2,11	6,11
ΔE	-3.93	-4.49	-1.38	-1.23	-4.06	-4.21
FRZ	-1.71	-0.53	-1.32	-1.15	2.53	-0.63
POL	-1.34	-2.07	-0.04	-0.06	-3.55	-2.00
CT	-0.88	-1.88	-0.01	-0.02	-3.04	-1.58
	Three-Body					
	1,2,6	1,2,11	1,6,11	2,6,11		
ΔE	-1.04	-1.23	-1.16	-1.49		
FRZ	-0.12	0.00	0.00	-0.14		
POL	-0.76	-1.00	-0.92	-1.06		
CT	-0.16	-0.23	-0.24	-0.29		



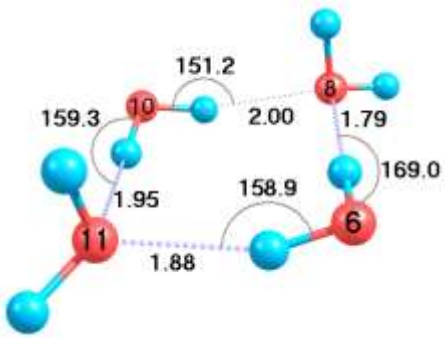
e) Type B Pentamer: 1, 5, 6, 9, 13

Type B Pentamer: 1,5,6,9,13					
	Two-Body				
	1,5	1,6	1,9	1,13	5,6
ΔE	-4.33	-4.49	0.26	0.73	0.75
FRZ	-1.24	-0.53	0.31	0.79	0.77
POL	-1.73	-2.07	-0.05	-0.05	-0.02
CT	-1.35	-1.88	-0.01	-0.02	0.00
	Two-Body				
	5,9	5,13	6,9	6,13	9,13
ΔE	0.44	-4.56	-3.77	-1.43	-4.04
FRZ	0.46	-1.68	0.73	-1.38	0.35
POL	-0.02	-1.58	-2.53	-0.05	-2.45
CT	0.00	-1.30	-1.97	-0.01	-1.94
	Three-Body				
	1,5,6	1,5,13	1,6,9	5,9,13	6,9,13
ΔE	0.62	0.45	0.67	0.67	-1.11
FRZ	0.11	0.00	-0.05	0.11	-0.10
POL	0.39	0.37	0.57	0.43	-0.80
CT	0.12	0.08	0.15	0.12	-0.22



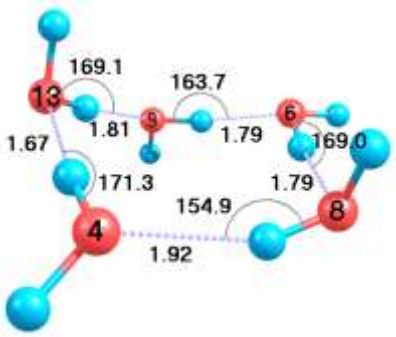
f) Type C Tetramer: 6, 8, 10, 11

Type C Tetramer: 6,8,10,11						
	Two-Body					
	6,8	6,10	6,11	8,10	8,11	10,11
ΔE	-4.22	1.28	-4.21	-3.90	0.98	-4.53
FRZ	0.67	1.49	-0.63	-1.71	1.01	-1.62
POL	-2.60	-0.15	-2.00	-1.31	-0.03	-1.64
CT	-2.29	-0.06	-1.58	-0.88	0.00	-1.27
	Three-Body					
	6,8,10	6,8,11	6,10,11	8,10,11		
ΔE	0.30	0.74	0.33	0.41		
FRZ	-0.01	0.11	-0.01	0.03		
POL	0.22	0.49	0.25	0.32		
CT	0.09	0.15	0.08	0.06		



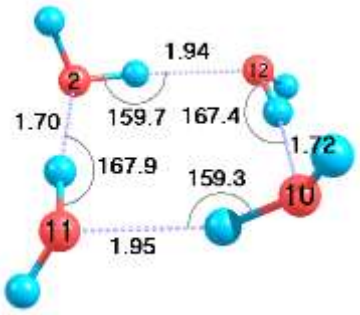
g) Type A Pentamer: 4, 6, 8, 9, 13

Type A Pentamer: 4,6,8,9,13					
	Two-Body				
	4,6	4,8	4,9	4,13	6,8
ΔE	-1.12	-4.09	-0.99	-3.76	-4.22
FRZ	-1.09	-0.97	-0.96	3.45	0.67
POL	-0.03	-1.77	-0.03	-3.97	-2.60
CT	-0.01	-1.34	-0.01	-3.24	-2.29
	Two-Body				
	6,9	6,13	8,9	8,13	9,13
ΔE	-3.77	-1.43	-0.89	-0.89	-4.04
FRZ	0.73	-1.38	-0.87	-0.85	0.35
POL	-2.53	-0.05	-0.02	-0.03	-2.45
CT	-1.97	-0.01	0.00	-0.01	-1.94
	Three-Body				
	4,6,8	4,8,13	4,9,13	6,8,9	6,9,13
ΔE	-1.15	-1.41	-1.40	-1.19	-1.11
FRZ	0.00	-0.10	-0.01	-0.07	-0.10
POL	-0.92	-1.04	-1.09	-0.87	-0.80
CT	-0.23	-0.27	-0.31	-0.25	-0.22



h) Type A Tetramer: 2, 10, 11, 12

Type A Tetramer: 2,10,11,12						
	Two-Body					
	2,10	2,11	2,12	10,11	10,12	11,12
ΔE	-1.38	-4.06	-4.54	-4.53	-4.19	-1.52
FRZ	-1.30	2.53	-1.62	-1.62	2.00	-1.45
POL	-0.06	-3.55	-1.64	-1.64	-3.33	-0.05
CT	-0.02	-3.04	-1.27	-1.27	-2.86	-0.02
	Three-Body					
	2,10,11	2,10,12	2,11,12	10,11,12		
ΔE	-1.46	-1.42	-1.38	-1.36		
FRZ	-0.13	-0.12	-0.05	-0.05		
POL	-1.05	-1.03	-1.06	-1.04		
CT	-0.28	-0.27	-0.28	-0.27		



i) Type A Tetramer: 1, 6, 7, 8

Type A Tetramer: 1,6,7,8						
	Two-Body					
	1,6	1,7	1,8	6,7	6,8	7,8
ΔE	-4.49	-4.36	-1.45	-1.22	-4.22	-4.33
FRZ	-0.53	0.43	-1.34	-1.15	0.67	0.42
POL	-2.07	-2.52	-0.07	-0.05	-2.60	-2.50
CT	-1.88	-2.27	-0.03	-0.02	-2.29	-2.25
	Three-Body					
	1,6,7	1,6,8	1,7,8	6,7,8		
ΔE	-1.24	-1.38	-1.44	-1.41		
FRZ	-0.02	-0.09	-0.10	-0.05		
POL	-0.94	-0.99	-1.03	-1.05		
CT	-0.28	-0.29	-0.31	-0.31		

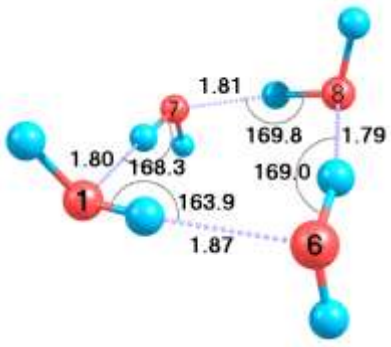
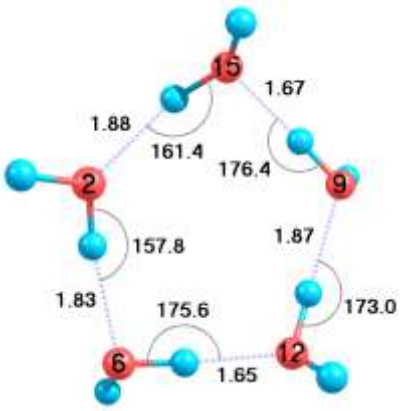


Figure S3: Additional rings (not covered in Fig. S1) within the 17-mer, and their associated ALMO-EDA terms (kcal/mol, ωB97X-D/aug-cc-pVQZ). See Figure 2d for relative location. a) Type A Pentamer: 2, 6, 9, 12, 15; b) Type C Tetramer: 3, 7, 8, 11; c) Type A Pentamer: 4, 7, 11, 14, 17; d) Type C Tetramer: 1, 2, 3, 15; e) Type B Hexamer: 1, 3, 5, 9, 12, 15; f) Type C Tetramer: 1, 4, 5, 14; g) Type B Tetramer: 4, 13, 16, 17; h) Type B Hexamer: 4, 5, 6, 12, 14, 16; i) Type B Hexamer: 2, 3, 7, 13, 15, 17; j) Type B Tetramer: 2, 6, 13, 16; k) Type A Pentamer: 5, 8, 10, 11, 14.

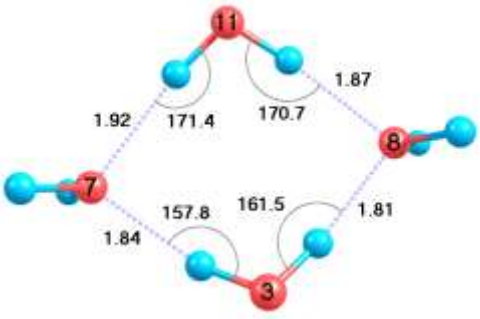
a) Type A Pentamer: 2, 6, 9, 12, 15

Type A Pentamer: 2,6,9,12,15					
	Two-Body				
	2,6	2,9	2,12	2,15	6,9
ΔE	-3.87	-1.09	-1.27	-3.62	-0.91
FRZ	0.14	-1.05	-1.22	-0.45	-0.88
POL	-2.23	-0.04	-0.04	-1.87	-0.03
CT	-1.78	-0.01	-0.01	-1.30	0.00
	Two-Body				
	6,12	6,15	9,12	9,15	12,15
ΔE	-3.39	-0.77	-4.54	-3.60	-0.86
FRZ	4.23	-0.75	-0.93	3.60	-0.83
POL	-4.21	-0.01	-2.01	-3.90	-0.03
CT	-3.41	0.00	-1.60	-3.30	-0.01
	Three-Body				
	2,6,12	2,6,15	2,9,15	6,9,12	9,12,15
ΔE	-1.69	-1.14	-1.31	-1.43	-1.38
FRZ	-0.14	-0.05	-0.11	-0.04	-0.03
POL	-1.22	-0.91	-0.95	-1.10	-1.05
CT	-0.33	-0.19	-0.25	-0.30	-0.30



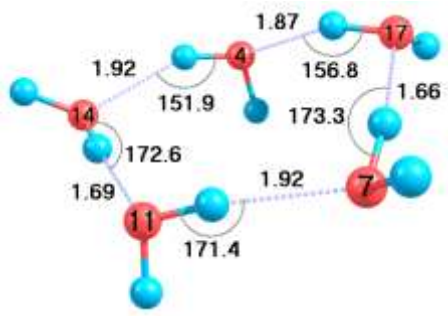
b) Type C Tetramer: 3, 7, 8, 11

Type C Tetramer: 3,7,8,11						
	Two-Body					
	3,7	3,8	3,11	7,8	7,11	8,11
ΔE	-3.75	-3.96	1.55	1.08	-4.55	-4.50
FRZ	0.10	0.35	1.89	1.11	-1.33	-0.88
POL	-2.16	-2.40	-0.23	-0.04	-1.79	-2.02
CT	-1.69	-1.91	-0.11	0.00	-1.43	-1.59
	Three-Body					
	3,7,8	3,7,11	3,8,11	7,8,11		
ΔE	0.74	0.42	0.48	0.62		
FRZ	0.09	-0.08	-0.06	0.05		
POL	0.51	0.36	0.40	0.46		
CT	0.13	0.13	0.14	0.11		



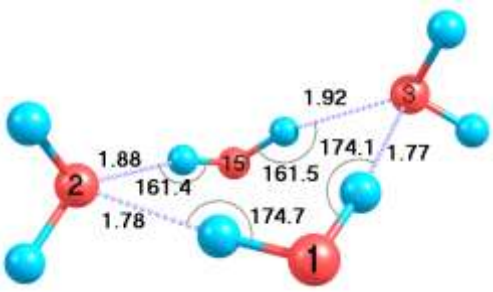
c) Type A Pentamer: 4, 7, 11, 14, 17

Type A Pentamer: 4,7,11,14,17					
	Two-Body				
	4,7	4,11	4,14	4,17	7,11
ΔE	-1.23	-1.30	-3.14	-3.52	-4.55
FRZ	-1.17	-1.19	-0.10	0.20	-1.33
POL	-0.04	-0.08	-1.72	-2.07	-1.79
CT	-0.02	-0.03	-1.32	-1.65	-1.43
	Two-Body				
	7,14	7,17	11,14	11,17	14,17
ΔE	-0.71	-3.33	-3.70	-1.03	-0.71
FRZ	-0.69	4.08	2.70	-1.00	-0.70
POL	-0.02	-4.10	-3.60	-0.03	-0.01
CT	0.00	-3.32	-2.80	-0.01	0.00
	Three-Body				
	4,7,17	4,11,14	4,14,17	7,11,14	7,11,17
ΔE	-1.45	-1.14	-0.95	-1.27	-1.40
FRZ	-0.07	-0.12	0.00	-0.03	-0.03
POL	-1.11	-0.81	-0.78	-0.99	-1.07
CT	-0.27	-0.20	-0.17	-0.25	-0.29



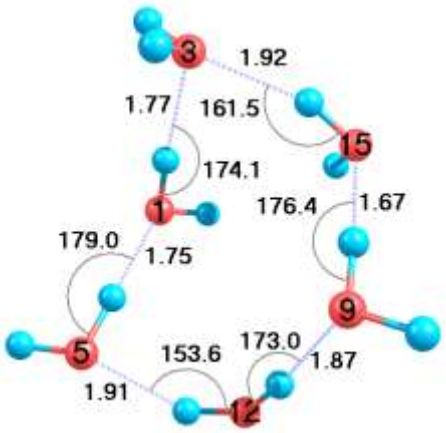
d) Type C Tetramer: 1, 2, 3, 15

Type C Tetramer: 1,2,3,15						
	Two-Body					
	1,2	1,3	1,15	2,3	2,15	3,15
ΔE	-3.69	-3.51	2.07	1.04	-3.62	-3.73
FRZ	1.46	1.89	2.58	1.08	-0.45	-0.89
POL	-2.68	-2.82	-0.35	-0.04	-1.87	-1.70
CT	-2.47	-2.58	-0.16	0.00	-1.30	-1.15
	Three-Body					
	1,2,3	1,2,15	1,3,15	2,3,15		
ΔE	0.63	0.48	0.46	0.72		
FRZ	0.08	-0.11	-0.12	0.06		
POL	0.38	0.39	0.40	0.57		
CT	0.17	0.19	0.18	0.10		



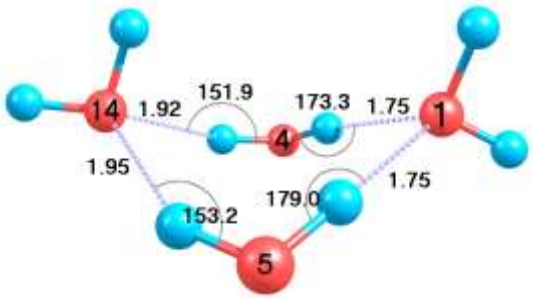
e) Type B Hexamer: 1, 3, 5, 9, 12, 15

Type B Hexamer: 1,3,5,9,12,15					
	Two-Body				
	1,3	1,5	1,9	1,12	1,15
ΔE	-3.51	-3.95	0.95	-1.16	2.07
FRZ	1.89	1.29	1.03	-1.04	2.58
POL	-2.82	-2.94	-0.06	-0.09	-0.35
CT	-2.58	-2.30	-0.02	-0.03	-0.16
	Two-Body				
	3,5	3,9	3,12	3,15	5,9
ΔE	-0.60	-1.01	-0.12	-3.73	0.75
FRZ	-0.57	-0.97	-0.11	-0.89	0.79
POL	-0.02	-0.04	-0.01	-1.70	-0.04
CT	-0.01	0.00	0.00	-1.15	0.00
	Two-Body				
	5,12	5,15	9,12	9,15	12,15
ΔE	-3.17	0.33	-4.54	-3.60	-0.86
FRZ	-0.12	0.33	-0.93	3.60	-0.83
POL	-1.78	-0.01	-2.01	-3.90	-0.03
CT	-1.27	0.00	-1.60	-3.30	-0.01
	Three-Body				
	1,3,5	1,3,15	1,5,12	3,9,15	5,9,12
ΔE	-1.28	0.46	-1.15	-1.27	0.65
FRZ	-0.04	-0.12	-0.25	-0.07	0.08
POL	-0.96	0.40	-0.75	-0.96	0.48
CT	-0.28	0.18	-0.16	-0.24	0.09
	9,12,15				
ΔE	-1.38				
FRZ	-0.03				
POL	-1.05				
CT	-0.30				



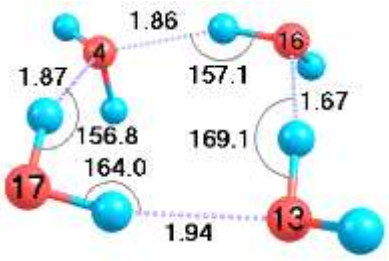
f) Type C Tetramer: 1, 4, 5, 14

Type C Tetramer: 1,4,5,14						
	Two-Body					
	1,4	1,5	1,14	4,5	4,14	5,14
ΔE	-3.90	-3.95	0.84	1.77	-3.14	-3.46
FRZ	1.38	1.29	0.90	2.15	-0.10	-0.64
POL	-2.93	-2.94	-0.05	-0.26	-1.72	-1.61
CT	-2.35	-2.30	0.00	-0.11	-1.32	-1.21
	Three-Body					
	1,4,5	1,4,14	1,5,14	4,5,14		
ΔE	0.62	0.83	0.85	0.26		
FRZ	0.03	0.10	0.10	-0.02		
POL	0.42	0.59	0.61	0.20		
CT	0.17	0.14	0.14	0.09		



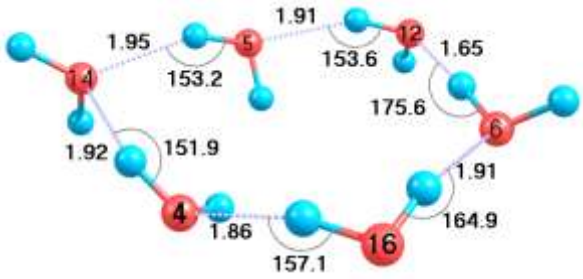
g) Type B Tetramer: 4, 13, 16, 17

Type B Tetramer: 4,13,16,17						
	Two-Body					
	4,13	4,16	4,17	13,16	13,17	16,17
ΔE	-0.92	-3.02	-3.52	-3.62	-3.38	-0.25
FRZ	-0.86	0.64	0.20	3.67	-0.33	-0.14
POL	-0.05	-2.03	-2.07	-3.96	-1.68	-0.08
CT	-0.01	-1.63	-1.65	-3.34	-1.38	-0.03
	Three-Body					
	4,13,16	4,13,17	4,16,17	13,16,17		
ΔE	-1.14	0.75	0.64	-1.02		
FRZ	-0.10	0.12	-0.05	-0.01		
POL	-0.81	0.50	0.58	-0.78		
CT	-0.24	0.13	0.11	-0.24		



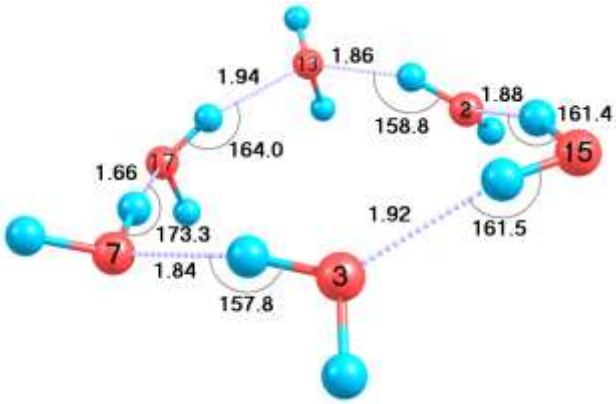
h) Type B Hexamer: 4, 5, 6, 12, 14, 16

Type B Hexamer: 4,5,6,12,14,16					
	Two-Body				
	4,5	4,6	4,14	4,16	5,6
ΔE	1.77	0.33	-3.14	-3.02	-0.92
FRZ	2.15	0.34	-0.10	0.64	-0.89
POL	-0.26	-0.02	-1.72	-2.03	-0.03
CT	-0.11	0.00	-1.32	-1.63	-0.01
	Two-Body				
	5,12	5,14	6,12	6,14	6,16
ΔE	-3.17	-3.46	-3.39	0.04	-3.73
FRZ	-0.12	-0.64	4.23	0.04	-0.60
POL	-1.78	-1.61	-4.21	0.00	-1.75
CT	-1.27	-1.21	-3.41	0.00	-1.38
	Two-Body				
	12,14	12,16	14,16		
ΔE	-0.35	-0.57	-0.70		
FRZ	-0.34	-0.54	-0.68		
POL	-0.01	-0.03	-0.01		
CT	0.00	0.00	0.00		
	Three-Body				
	4,5,14	4,6,16	4,14,16	5,6,12	5,12,14
ΔE	0.26	1.01	-0.63	-1.17	-0.79
FRZ	-0.02	0.21	-0.03	-0.01	-0.05
POL	0.20	0.66	-0.46	-0.94	-0.61
CT	0.09	0.14	-0.14	-0.22	-0.13
	6,12,16				
ΔE	-1.08				
FRZ	0.02				
POL	-0.84				
CT	-0.26				



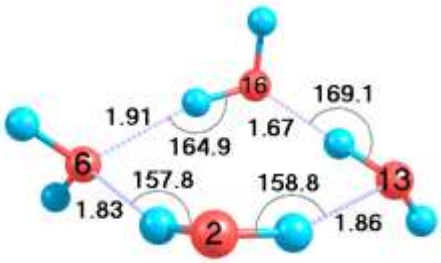
i) Type B Hexamer: 2, 3, 7, 13, 15, 17

Type B Hexamer: 2,3,7,13,15,17				
	Two-Body			
	2,3	2,13	2,15	2,17
ΔE	1.04	-2.76	-3.62	0.66
FRZ	1.08	1.08	-0.45	0.70
POL	-0.04	-2.10	-1.87	-0.03
CT	0.00	-1.74	-1.30	-0.01
	Two-Body			
	3,7	3,15	3,17	7,13
ΔE	-3.75	-3.73	-0.92	-0.50
FRZ	0.10	-0.89	-0.88	-0.48
POL	-2.16	-1.70	-0.02	-0.02
CT	-1.69	-1.15	-0.01	0.00
	Two-Body			
	7,15	7,17	13,15	13,17
ΔE	-0.45	-3.33	-0.72	-3.38
FRZ	-0.44	4.08	-0.70	-0.33
POL	-0.01	-4.10	-0.02	-1.68
CT	0.00	-3.32	0.00	-1.38
	Three-Body			
	2,3,15	2,13,15	2,13,17	3,7,15
ΔE	0.72	-0.62	0.80	-0.95
FRZ	0.06	-0.07	-0.08	-0.02
POL	0.57	-0.41	0.75	-0.77
CT	0.10	-0.14	0.13	-0.17
	3,7,17	7,13,17		
ΔE	-1.54	-0.95		
FRZ	-0.10	-0.08		
POL	-1.13	-0.66		
CT	-0.31	-0.21		



j) Type B Tetramer: 2, 6, 13, 16

Type B Tetramer: 2,6,13,16						
	Two-Body					
	2,6	2,13	2,16	6,13	6,16	13,16
ΔE	-3.87	-2.76	-0.53	-0.48	-3.73	-3.62
FRZ	0.14	1.08	-0.30	-0.43	-0.60	3.67
POL	-2.23	-2.10	-0.17	-0.04	-1.75	-3.96
CT	-1.78	-1.74	-0.07	0.00	-1.38	-3.34
	Three-Body					
	2,6,13	2,6,16	2,13,16	6,13,16		
ΔE	0.94	0.61	-1.41	-1.04		
FRZ	0.17	-0.12	-0.18	-0.12		
POL	0.62	0.56	-0.97	-0.71		
CT	0.15	0.17	-0.27	-0.21		



k) Type A Pentamer: 5, 8, 10, 11, 14

Type A Pentamer: 5,8,10,11,14					
	Two-Body				
	5,8	5,10	5,11	5,14	8,10
ΔE	-1.27	-3.46	-1.20	-3.46	-3.10
FRZ	-1.22	0.76	-1.12	-0.64	5.26
POL	-0.04	-2.29	-0.06	-1.61	-4.61
CT	-0.01	-1.94	-0.02	-1.21	-3.75
	Two-Body				
	8,11	8,14	10,11	10,14	11,14
ΔE	-4.50	-0.83	-1.06	-0.84	-3.70
FRZ	-0.88	-0.80	-1.02	-0.82	2.70
POL	-2.02	-0.02	-0.03	-0.02	-3.60
CT	-1.59	0.00	-0.01	0.00	-2.80
	Three-Body				
	5,8,10	5,10,14	5,11,14	8,10,11	8,11,14
ΔE	-1.57	-1.00	-1.13	-1.53	-1.32
FRZ	-0.06	0.01	-0.10	-0.06	-0.03
POL	-1.17	-0.82	-0.82	-1.14	-1.03
CT	-0.34	-0.19	-0.21	-0.33	-0.26

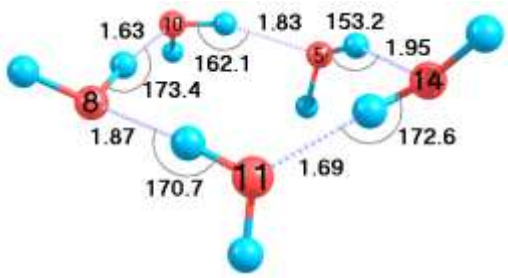


Table S3: Comparison of ALMO-EDA calculations using the B3LYP and ωB97X-D density functionals for the water 13-mer, organized by the two- and three-body interactions of each water (energies in kcal/mol; details as for Table S1); four-coordinate waters are listed first, followed by three- and two-coordinate waters, respectively.

Four-coordinate waters:

Water #1: B3LYP, Correct Parameters				
Two-Body	FRZ	POL	CT	ΔE
1,2	-1.35	-1.21	-1.11	-3.68
1,5	-0.71	-1.64	-1.68	-4.03
1,6	0.15	-2.00	-2.32	-4.17
1,7	1.15	-2.47	-2.77	-4.08
Three-Body	FRZ	POL	CT	ΔE
1,2,5	-0.03	-0.59	-0.14	-0.76
1,2,6	-0.10	-0.74	-0.21	-1.05
1,2,7	0.09	0.20	0.13	0.42
1,5,6	0.08	0.40	0.16	0.64
1,5,7	-0.03	-0.95	-0.31	-1.29
1,6,7	-0.02	-0.94	-0.35	-1.31

Water #1: ωB97X-d, Correct Parameters				
Two-Body	FRZ	POL	CT	ΔE
1,2	-1.71	-1.34	-0.88	-3.93
1,5	-1.24	-1.73	-1.35	-4.33
1,6	-0.53	-2.07	-1.88	-4.49
1,7	0.43	-2.52	-2.27	-4.36
Three-Body	FRZ	POL	CT	ΔE
1,2,5	-0.02	-0.59	-0.13	-0.74
1,2,6	-0.12	-0.76	-0.16	-1.04
1,2,7	-0.02	0.20	0.10	0.28
1,5,6	0.11	0.39	0.12	0.62
1,5,7	-0.02	-0.96	-0.25	-1.23
1,6,7	-0.02	-0.94	-0.28	-1.24

Water #6: B3LYP, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,6	0.15	-2.00	-2.32	-4.17
6,8	1.41	-2.55	-2.79	-3.93
6,9	1.22	-2.45	-2.38	-3.60
6,11	-0.04	-1.91	-1.94	-3.90
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,6,8	-0.06	-0.98	-0.37	-1.41
1,6,9	-0.08	0.54	0.19	0.65
1,6,11	-0.04	-0.92	-0.30	-1.25
6,8,9	-0.12	-0.86	-0.31	-1.29
6,8,11	0.08	0.49	0.18	0.75
6,9,11	-0.05	-0.70	-0.23	-0.99

Water #6: ωB97X-d, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,6	-0.53	-2.07	-1.88	-4.49
6,8	0.67	-2.60	-2.29	-4.22
6,9	0.73	-2.53	-1.97	-3.77
6,11	-0.63	-2.00	-1.58	-4.21
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,6,8	-0.09	-0.99	-0.29	-1.38
1,6,9	-0.05	0.57	0.15	0.67
1,6,11	0.00	-0.92	-0.24	-1.16
6,8,9	-0.07	-0.87	-0.25	-1.19
6,8,11	0.11	0.49	0.15	0.74
6,9,11	-0.03	-0.71	-0.19	-0.93

Water #7: B3LYP, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,7	1.15	-2.47	-2.77	-4.08
3,7	-0.67	-1.56	-1.45	-3.68
7,8	1.16	-2.44	-2.75	-4.03
7,12	-0.35	-1.68	-1.70	-3.73
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,3,7	-0.13	-0.89	-0.26	-1.28
1,7,8	-0.06	-1.03	-0.39	-1.48
1,7,12	0.05	0.42	0.17	0.64
3,7,8	0.07	0.28	0.14	0.49
3,7,12	-0.03	-0.63	-0.16	-0.82
7,8,12	-0.02	-0.94	-0.30	-1.26

Water #7: ωB97X-d, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,7	0.43	-2.52	-2.27	-4.36
3,7	-1.12	-1.68	-1.16	-3.96
7,8	0.42	-2.50	-2.25	-4.33
7,12	-0.92	-1.77	-1.37	-4.06
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,3,7	-0.13	-0.91	-0.21	-1.24
1,7,8	-0.10	-1.03	-0.31	-1.44
1,7,12	0.09	0.42	0.13	0.64
3,7,8	0.00	0.29	0.10	0.39
3,7,12	-0.02	-0.63	-0.14	-0.79
7,8,12	0.02	-0.95	-0.24	-1.18

Water #8: B3LYP, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
4,8	-0.43	-1.67	-1.67	-3.77
6,8	1.41	-2.55	-2.79	-3.93
7,8	1.16	-2.44	-2.75	-4.03
8,10	-1.33	-1.18	-1.11	-3.62
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
4,6,8	-0.05	-0.92	-0.29	-1.25
4,7,8	0.02	0.43	0.17	0.62
4,8,10	-0.05	-0.62	-0.14	-0.81
6,7,8	-0.04	-1.04	-0.39	-1.48
6,8,10	0.07	0.22	0.12	0.41
7,8,10	-0.13	-0.78	-0.22	-1.14

Water #8: ωB97X-d, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
4,8	-0.97	-1.77	-1.34	-4.09
6,8	0.67	-2.60	-2.29	-4.22
7,8	0.42	-2.50	-2.25	-4.33
8,10	-1.71	-1.31	-0.88	-3.90
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
4,6,8	0.00	-0.92	-0.23	-1.15
4,7,8	0.06	0.43	0.13	0.62
4,8,10	-0.04	-0.63	-0.13	-0.79
6,7,8	-0.05	-1.05	-0.31	-1.41
6,8,10	-0.01	0.22	0.09	0.30
7,8,10	-0.16	-0.80	-0.17	-1.13

Three-coordinate waters:

Water #2: B3LYP, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,2	-1.35	-1.21	-1.11	-3.68
2,11	3.33	-3.54	-3.66	-3.87
2,12	-1.14	-1.54	-1.58	-4.27
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,2,11	-0.04	-1.00	-0.29	-1.32
1,2,12	0.01	0.35	0.08	0.43
2,11,12	-0.06	-1.06	-0.34	-1.46

Water #2: ωB97X-d, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,2	-1.71	-1.34	-0.88	-3.93
2,11	2.53	-3.55	-3.04	-4.06
2,12	-1.62	-1.64	-1.27	-4.54
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,2,11	0.00	-1.00	-0.23	-1.23
1,2,12	0.04	0.35	0.07	0.45
2,11,12	-0.05	-1.06	-0.28	-1.38

Water #3: B3LYP, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
3,4	-1.00	-1.54	-1.66	-4.20
3,5	3.14	-3.44	-3.61	-3.91
3,7	-0.67	-1.56	-1.45	-3.68
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
3,4,5	-0.05	-1.03	-0.35	-1.43
3,4,7	-0.01	0.34	0.10	0.43
3,5,7	-0.04	-1.10	-0.33	-1.48

Water #3: ωB97X-d, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
3,4	-1.54	-1.64	-1.33	-4.51
3,5	2.34	-3.45	-2.99	-4.11
3,7	-1.12	-1.68	-1.16	-3.96
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
3,4,5	-0.02	-1.03	-0.28	-1.33
3,4,7	0.02	0.34	0.08	0.44
3,5,7	-0.03	-1.11	-0.27	-1.41

Water #4: B3LYP, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
3,4	-1.00	-1.54	-1.66	-4.20
4,8	-0.43	-1.67	-1.67	-3.77
4,13	4.26	-3.98	-3.88	-3.60
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
3,4,8	0.04	0.32	0.11	0.47
3,4,13	-0.12	-1.09	-0.37	-1.59
4,8,13	-0.13	-1.02	-0.33	-1.49

Water #4: ωB97X-d, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
3,4	-1.54	-1.64	-1.33	-4.51
4,8	-0.97	-1.77	-1.34	-4.09
4,13	3.45	-3.97	-3.24	-3.76
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
3,4,8	-0.02	0.32	0.09	0.39
3,4,13	-0.14	-1.11	-0.30	-1.55
4,8,13	-0.10	-1.04	-0.27	-1.41

Water #5: B3LYP, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,5	-0.71	-1.64	-1.68	-4.03
3,5	3.14	-3.44	-3.61	-3.91
5,13	-1.19	-1.48	-1.61	-4.29
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,3,5	-0.12	-1.02	-0.34	-1.49
1,5,13	-0.02	0.37	0.10	0.45
3,5,13	-0.11	-1.01	-0.36	-1.47

Water #5: ωB97X-d, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,5	-1.24	-1.73	-1.35	-4.33
3,5	2.34	-3.45	-2.99	-4.11
5,13	-1.68	-1.58	-1.30	-4.56
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
1,3,5	-0.13	-1.03	-0.27	-1.43
1,5,13	0.00	0.37	0.08	0.45
3,5,13	-0.13	-1.02	-0.28	-1.43

Water #10: B3LYP, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
8,10	-1.33	-1.18	-1.11	-3.62
10,11	-1.14	-1.54	-1.57	-4.25
10,12	2.76	-3.31	-3.45	-3.99
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
8,10,11	0.00	0.32	0.07	0.39
8,10,12	-0.02	-0.96	-0.27	-1.25
10,11,12	-0.06	-1.04	-0.34	-1.43

Water #10: ωB97X-d, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
8,10	-1.71	-1.31	-0.88	-3.90
10,11	-1.62	-1.64	-1.27	-4.53
10,12	2.00	-3.33	-2.86	-4.19
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
8,10,11	0.03	0.32	0.06	0.41
8,10,12	0.02	-0.97	-0.22	-1.17
10,11,12	-0.05	-1.04	-0.27	-1.36

Water #11: B3LYP, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
2,11	3.33	-3.54	-3.66	-3.87
6,11	-0.04	-1.91	-1.94	-3.90
10,11	-1.14	-1.54	-1.57	-4.25
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
2,6,11	-0.12	-1.04	-0.36	-1.52
2,10,11	-0.11	-1.04	-0.35	-1.49
6,10,11	0.07	0.25	0.11	0.44

Water #11: ωB97X-d, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
2,11	2.53	-3.55	-3.04	-4.06
6,11	-0.63	-2.00	-1.58	-4.21
10,11	-1.62	-1.64	-1.27	-4.53
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
2,6,11	-0.14	-1.06	-0.29	-1.49
2,10,11	-0.13	-1.05	-0.28	-1.46
6,10,11	-0.01	0.25	0.08	0.33

Water #12: B3LYP, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
2,12	-1.14	-1.54	-1.58	-4.27
7,12	-0.35	-1.68	-1.70	-3.73
10,12	2.76	-3.31	-3.45	-3.99
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
2,7,12	0.07	0.23	0.10	0.40
2,10,12	-0.10	-1.01	-0.33	-1.45
7,10,12	-0.13	-1.00	-0.32	-1.45

Water #12: ωB97X-d, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
2,12	-1.62	-1.64	-1.27	-4.54
7,12	-0.92	-1.77	-1.37	-4.06
10,12	2.00	-3.33	-2.86	-4.19
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
2,7,12	-0.02	0.23	0.08	0.29
2,10,12	-0.12	-1.03	-0.27	-1.42
7,10,12	-0.16	-1.01	-0.26	-1.43

Water #13: B3LYP, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
4,13	4.26	-3.98	-3.88	-3.60
5,13	-1.19	-1.48	-1.61	-4.29
9,13	0.97	-2.38	-2.37	-3.78
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
4,5,13	-0.05	-1.06	-0.35	-1.46
4,9,13	-0.06	-1.08	-0.37	-1.51
5,9,13	0.09	0.45	0.16	0.69

Water #13: ωB97X-d, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
4,13	3.45	-3.97	-3.24	-3.76
5,13	-1.68	-1.58	-1.30	-4.56
9,13	0.35	-2.45	-1.94	-4.04
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
4,5,13	-0.02	-1.06	-0.28	-1.36
4,9,13	-0.01	-1.09	-0.31	-1.40
5,9,13	0.11	0.43	0.12	0.67

Two-coordinate waters:

Water #9: B3LYP, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
6,9	1.22	-2.45	-2.38	-3.60
9,13	0.97	-2.38	-2.37	-3.78
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
6,9,13	-0.11	-0.79	-0.27	-1.17

Water #9: ωB97X-d, Correct Parameters				
Two-Body	**FRZ**	**POL**	**CT**	**ΔE**
6,9	0.73	-2.53	-1.97	-3.77
9,13	0.35	-2.45	-1.94	-4.04
Three-Body	**FRZ**	**POL**	**CT**	**ΔE**
6,9,13	-0.10	-0.80	-0.22	-1.11

Table S4: Cartesian coordinates for the optimized water dimer-pentamer (MP2/aug-cc-pVTZ), 13-mer[i] (B3LYP/6-311+G(d,p), and 17-mer[ii] (MP2/aug-cc-pVTZ) structures used throughout this work.

Dimer:

H	-1.941434	-0.022736	0.737432
H	-0.577666	0.003649	0.054296
O	-1.528686	-0.000341	-0.129479
H	1.728828	0.769074	-0.341876
H	1.707555	-0.751721	-0.397710
O	1.368710	-0.003814	0.104189

Trimer:

O	0.178452	-1.587978	0.100697
H	-0.625886	-1.040418	0.042458
H	0.098269	-2.231822	-0.608269
O	-1.478583	0.642263	-0.087562
H	-2.030834	1.068201	0.573258
H	-0.612949	1.085095	-0.028468
O	1.295138	0.958871	-0.088399
H	1.953427	1.210575	0.564558
H	1.218720	-0.010581	-0.019327

Tetramer:

O	1.903404	-0.329047	-0.012821
H	1.455011	0.544333	0.004897
H	2.503335	-0.291520	-0.762447
H	0.544669	-1.455303	-0.006491
O	-0.328695	-1.903617	0.012272
H	-0.294846	-2.493340	0.770157
O	0.329305	1.902945	0.012701
H	0.292014	2.498854	0.765550
H	-0.544082	1.454724	-0.006847
O	-1.902527	0.328755	-0.012943
H	-2.510191	0.296574	-0.756556
H	-1.457802	-0.546605	-0.001937

Pentamer:

O	2.093229	0.967267	0.059558
O	-0.281993	2.284909	0.074803
O	-2.260665	0.443954	-0.173978
O	-1.127259	-1.999047	0.154680
O	1.564247	-1.705081	-0.054450
H	2.666339	1.445307	-0.545158
H	-0.503517	2.793252	0.859657
H	-2.784561	0.397008	-0.977935
H	-1.281374	-2.470856	0.977449
H	2.001932	-2.086076	-0.819984
H	1.251107	1.475636	0.071457
H	-1.026293	1.651366	-0.035650

H	-1.891802	-0.459839	-0.052151
H	-0.149216	-1.929641	0.077939
H	1.821371	-0.756700	-0.051286

13-mer:

O	-0.094000000	-0.018000000	-1.916000000
H	-0.013000000	0.752000000	-1.316000000
H	0.813000000	-0.227000000	-2.209000000
O	-2.976000000	0.206000000	-1.929000000
H	-3.208000000	-0.596000000	-1.428000000
H	-2.061000000	0.073000000	-2.231000000
O	2.183000000	-2.680000000	-0.078000000
H	2.414000000	-2.207000000	0.743000000
H	1.216000000	-2.783000000	-0.040000000
O	2.665000000	-0.758000000	2.02100000
H	3.058000000	-0.110000000	1.370000000
H	3.299000000	-0.849000000	2.738000000
O	2.618000000	-0.870000000	-2.022000000
H	2.516000000	-1.623000000	-1.380000000
H	3.158000000	-1.195000000	-2.749000000
O	-0.175000000	1.930000000	0.124000000
H	-1.105000000	2.225000000	0.099000000
H	-0.127000000	1.256000000	0.840000000
O	-0.568000000	-2.069000000	-0.110000000
H	-1.516000000	-2.291000000	-0.083000000
H	-0.466000000	-1.414000000	-0.836000000
O	-0.106000000	-0.197000000	1.893000000
H	-0.253000000	-0.938000000	1.265000000
H	0.808000000	-0.328000000	2.210000000
O	2.229000000	3.231000000	-0.115000000
H	2.332000000	4.030000000	0.408000000
H	1.303000000	2.931000000	-0.002000000
O	-2.988000000	0.053000000	1.957000000
H	-3.070000000	0.882000000	1.452000000
H	-2.064000000	0.023000000	2.257000000
O	-2.972000000	2.117000000	-0.048000000
H	-3.576000000	2.847000000	-0.211000000
H	-3.053000000	1.489000000	-0.815000000
O	-3.369000000	-1.831000000	0.065000000
H	-4.111000000	-2.423000000	0.220000000
H	-3.323000000	-1.207000000	0.836000000
O	3.604000000	0.829000000	0.104000000
H	3.396000000	0.388000000	-0.738000000
H	3.226000000	1.730000000	0.039000000

17-mer:

O	-0.014931030	-0.115973990	0.085047940
H	-0.548308270	-0.796720510	0.549240040
H	0.261422490	0.500394370	0.797999140
O	-1.406000790	-2.024866370	1.514491180

H	-1.977442780	-2.382359750	0.807837240
H	-0.702707400	-2.690312040	1.636192750
O	0.699955020	1.485235120	2.197780760
H	0.726680550	2.390898500	1.831965090
H	1.629723170	1.189832240	2.226976110
O	1.718826950	-1.366747400	-1.609382630
H	1.925597610	-0.711000800	-2.296990130
H	1.147421760	-0.867782480	-0.985747380
O	-0.828921330	1.175976340	-2.178154710
H	-0.537541940	0.702306680	-1.369633060
H	-0.025868490	1.207906980	-2.724990020
O	-2.624919520	-2.630280760	-0.890405530
H	-3.366596240	-3.182884460	-1.153686480
H	-2.875520440	-1.703116410	-1.155895150
O	3.225684860	0.515808340	1.601846900
H	3.158873630	-0.446556640	1.354681370
H	4.071477910	0.604622480	2.051022550
O	0.700245530	3.770120310	0.658756770
H	-0.179459860	3.669700440	0.193789590
H	0.794325270	4.706547860	0.854641470
O	-3.278999020	1.544716350	0.807884800
H	-2.786241260	1.148711810	1.575401520
H	-4.122746600	1.835211500	1.167188280
O	-1.567769610	3.324269080	-0.577588590
H	-2.208889870	2.824839430	-0.039763890
H	-1.333736690	2.697140160	-1.290066380
O	2.635195850	2.180686930	-0.673868120
H	2.920505460	1.600931170	0.053537620
H	2.010633010	2.807369550	-0.267245300
O	-3.225227390	-0.127276750	-1.493395300
H	-3.319818270	0.428982920	-0.698133080
H	-2.516432550	0.303320520	-2.000998140
O	0.796098480	-3.714392380	1.251173930
H	0.544773560	-3.776854170	0.289888420
H	0.936250800	-4.618831810	1.547055050
O	1.898272840	1.081630470	-2.997573870
H	2.222109900	1.534601650	-2.178749040
H	2.422643080	1.438103020	-3.720027880
O	-1.890005940	0.441963410	2.798253660
H	-0.989122970	0.807742960	2.801110400
H	-1.772195910	-0.489172140	2.541688170
O	0.049095210	-3.573728940	-1.290363790
H	0.604521840	-2.856909080	-1.649837400
H	-0.863685320	-3.238475120	-1.323308540
O	3.055595970	-1.989163610	0.759282440
H	2.366535040	-2.591444630	1.088985340
H	2.808469630	-1.856977480	-0.174997730

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