

Supplementary material

The xyz geometries of all compounds optimized at RI-MP2 level with cc-pVDZ basis set are collected in the file ***b707182e.txt***.

Table 1S. The interaction energies (in kcal/mol) obtained by methods mentioned in this article (RI-MP2 in bold, other methods in italics), relative differences between RI-MP2 energies and energies obtained by tested methods and RMSD deviations between RI-MP2 and DFT-based geometries (in Å).

Method	RI-MP2	BH&H	Ediff	RMSD	SCC-DFTB	Ediff	RMSD	TPSS-D	Ediff	RMSD	TPSS	Ediff	RMSD	MO5-2x	Ediff	RMSD	PWB6K	Ediff	RMSD
Structure																			
CCC																			
HB/HB 1	-41.55	-58.44	16.89	0.14	-37.80	-3.75	0.23	-46.39	4.84	0.11	-38.72	-2.84	0.16	-42.09	0.54	0.07	-41.95	0.40	0.07
HB/HB 2	-41.28	-58.54	17.25	0.15	-34.95	-6.33	0.24	-40.57	-0.72	0.09	-38.43	-2.85	0.14	-42.81	1.52	0.11	-41.92	0.64	0.11
HB/HB 3	-39.67	-56.35	16.68	0.12	-32.86	-6.81	0.15	-43.29	3.62	0.04	-35.41	-4.26	0.04	-42.29	2.61	0.15	-41.14	1.47	0.07
HB/HB 4	-38.55	-55.28	16.73	0.11	-36.07	-2.48	0.07	-39.34	0.79	0.07	-37.08	-1.47	0.09	-40.82	2.27	0.22	-40.40	1.85	0.09
HB/HB 5	-36.24	-52.41	16.17	0.11	-31.96	-4.28	0.20	-36.41	0.18	0.10	-33.38	-2.86	0.03	-39.61	3.37	0.08	-38.33	2.09	0.07
HB/HB 6	-29.50	-43.70	14.20	0.47	-29.08	-0.42	0.91	-36.22	6.72	0.45	-28.28	-1.22	0.25	-33.46	3.97	3.00	-31.89	2.39	2.86
HB/S 1	-37.70	-49.37	11.67	0.08	-33.45	-4.25	0.32	-38.12	0.42	0.68	-24.20	-13.50	0.78	-35.04	-2.66	0.11	-31.36	-6.34	0.10

HB/S 2	-36.67	-46.67	10.00	0.22	-34.75	-1.92	0.28	-37.09	0.42	0.54	-28.05	-8.62	2.81	-33.15	-3.52	0.10	-30.37	-6.30	0.10
HB/S 3	-35.58	-48.57	12.99	0.35	-31.95	-3.63	0.28	-36.34	0.76	0.15	-33.25	-2.33	1.57	-32.55	-3.02	0.26	-29.21	-6.37	0.17
HB/S 4	-35.08	-54.84	19.76	2.36	-29.98	-5.10	0.18	-37.01	1.93	0.45	-36.64	1.56	2.41	-33.39	-1.70	0.10	-30.74	-4.34	0.11
HB/T 1	-37.79	-53.07	15.28	0.83	-32.65	-5.14	0.42	-40.72	2.93	0.19	-33.01	-4.78	0.66	-36.75	-1.04	0.34	-36.02	-1.77	0.18
S/S 1	-26.01	-26.20	0.20	0.93	-25.88	-0.12	1.08	-37.00	10.99	2.06	-36.65	10.64	2.66	-22.70	-3.31	0.15	-18.56	-7.45	0.13
S/T 1	-36.05	-47.64	11.59	0.12	-32.89	-3.16	0.27	-36.55	0.50	0.15	-24.08	-11.96	0.40	-33.81	-2.24	0.13	-31.34	-4.71	0.13
T/T 1	-31.72	-41.98	10.26	0.08	-27.97	-3.74	0.55	-32.74	1.03	0.12	-31.57	-0.15	2.03	-31.63	-0.08	0.32	-28.44	-3.27	0.26

CGCplus

HB/HB 1	-73.68	-87.14	13.46	0.12	-62.61	-11.07	0.15	-75.99	2.31	0.02	-73.42	-0.25	0.02	-71.23	-2.44	0.17	-71.09	-2.59	0.05
HB/HB 2	-71.51	-89.81	18.30	0.14	-66.32	-5.19	0.43	-76.05	4.54	0.08	-74.11	2.60	0.10	-71.39	-0.12	0.11	-71.90	0.39	0.13
HB/HB 3	-70.45	-92.89	22.43	0.11	-64.48	-5.97	0.07	-76.57	6.12	0.04	-61.44	-9.02	0.03	-71.89	1.43	0.10	-72.21	1.76	0.05
HB/HB 4	-70.31	-88.54	18.23	0.14	-67.84	-2.47	0.17	-74.83	4.52	0.06	-64.58	-5.73	0.05	-70.16	-0.15	0.08	-70.89	0.58	0.09
HB/HB 5	-69.56	-86.30	16.74	0.13	-64.06	-5.50	0.18	-73.15	3.59	0.07	-66.41	-3.15	0.06	-68.85	-0.71	0.07	-69.37	-0.19	0.08

HB/HB 6	-68.79	-85.71	16.91	0.12	-64.76	-4.04	0.11	-72.27	3.48	0.05	-69.00	0.21	0.05	-68.09	-0.71	0.09	-68.73	-0.07	0.09
HB/HB 7	-68.58	-87.36	18.78	0.15	-61.66	-6.92	0.31	-73.97	5.40	0.04	-68.91	0.33	0.06	-70.06	1.48	0.11	-70.15	1.57	0.09
HB/HB 8	-66.66	-83.62	16.96	0.14	-60.58	-6.08	0.47	-71.14	4.48	0.05	-60.35	-6.31	0.05	-67.04	0.38	0.12	-67.42	0.76	0.08
HB/S 1	-64.92	-76.93	12.01	0.22	-63.63	-1.29	0.28	-65.24	0.32	0.29	-68.25	3.33	2.91	-59.26	-5.67	0.20	-57.84	-7.08	0.12
HB/S 2	-57.08	-75.63	18.55	0.54	-63.91	6.83	0.24	-63.16	6.08	0.13	-53.06	-4.02	2.57	-53.81	-3.28	0.09	-50.86	-6.22	0.15
HB/T 1	-64.75	-79.14	14.40	0.17	-61.51	-3.23	0.34	-68.17	3.42	0.15	-65.57	0.83	0.27	-63.45	-1.30	0.16	-63.71	-1.04	0.11
S/T 1	-64.80	-76.24	11.43	0.28	-63.91	-0.90	0.44	-65.25	0.45	0.20	-60.55	-4.26	2.74	-58.92	-5.88	0.15	-57.58	-7.23	0.25
S/T 2	-60.26	-73.76	13.49	0.52	-61.17	0.91	0.51	-60.93	0.66	0.14	-58.18	-2.09	2.61	-54.67	-5.59	0.77	-53.81	-6.46	0.13
GGG																			
T/T 2	-47.37	-58.64	11.27	1.51	-46.96	-0.41	0.08	-49.68	2.31	0.49	-47.87	0.51	1.18	-49.73	2.36	0.15	-47.72	0.35	0.10
HB/HB 1	-46.27	-72.52	26.25	0.11	-44.85	-1.43	0.06	-49.76	3.49	0.01	-48.08	1.80	0.02	-49.89	3.62	1.72	-47.81	1.54	1.64
HB/HB 2	-35.51	-54.18	18.67	0.19	-32.03	-3.48	0.23	-37.90	2.38	0.13	-34.88	-0.64	0.13	-39.00	3.49	0.27	-38.22	2.71	0.24
HB/T 1	-43.26	-61.59	18.33	0.67	-39.66	-3.60	1.09	-43.76	0.50	0.17	-40.27	-2.99	0.42	-41.72	-1.54	0.52	-40.88	-2.38	0.36

HB/T 2	-43.14	-61.42	18.28	0.96	-40.32	-2.82	0.26	-43.48	0.34	0.31	-39.08	-4.06	0.52	-42.93	-0.21	0.24	-40.54	-2.60	0.38
HB/T 3	-41.75	-60.83	19.08	0.44	-38.99	-2.76	0.72	-43.21	1.46	0.29	-38.94	-2.82	0.93	-42.47	0.72	0.12	-41.02	-0.74	0.10
HB/T 4	-39.30	-56.65	17.36	0.25	-37.60	-1.70	0.53	-40.92	1.63	0.23	-36.56	-2.74	0.25	-40.07	0.77	0.16	-38.91	-0.38	0.13
HB/T 5	-36.01	-51.32	15.31	0.91	-33.75	-2.26	0.81	-36.18	0.18	1.00	-34.34	-1.66	0.90	-35.85	-0.16	0.29	-35.11	-0.90	0.23
S/S 1	-28.68	-52.41	23.73	2.84	-38.12	9.44	2.20	-24.34	-4.34	0.80	-34.89	6.21	3.94	-26.94	-1.74	0.81	-21.10	-7.58	0.61
S/T 1	-44.81	-55.16	10.35	0.13	-42.70	-2.11	0.20	-29.15	-15.66	0.26	-28.99	-15.82	2.07	-37.70	-7.11	0.12	-33.51	-11.30	0.12
S/T 2	-44.42	-58.36	13.94	0.14	-43.62	-0.80	0.25	-41.58	-2.84	0.15	-33.36	-11.06	0.61	-41.99	-2.43	0.24	-38.76	-5.66	0.38
T/T 1	-47.39	-57.56	10.17	0.28	-44.47	-2.92	0.30	-42.26	-5.13	0.62	-30.85	-16.55	0.75	-41.64	-5.75	0.22	-34.82	-12.57	0.37
mAmUmU																			
HB/HB 1	-27.82	-41.09	13.28	0.15	-22.57	-5.24	0.47	-30.09	2.27	0.10	-24.23	-3.59	0.09	-27.79	-0.02	0.18	-26.43	-1.39	0.18
HB/HB 2	-27.50	-41.09	13.60	0.15	-22.57	-4.92	0.47	-30.09	2.59	0.10	-24.23	-3.27	0.09	-28.26	0.76	0.14	-26.97	-0.53	0.13
HB/S 1	-27.06	-34.13	7.07	0.23	-25.38	-1.68	0.81	-26.55	-0.51	0.15	-15.61	-11.46	0.69	-23.67	-3.39	0.22	-21.28	-5.78	0.23
S/S 1	-27.53	-25.99	-1.55	0.14	-25.19	-2.34	0.43	-21.82	-5.71	0.18	-5.56	-21.97	0.84	-18.28	-9.25	0.17	-13.89	-13.65	0.16

S/S 2	-24.70	-25.09	0.39	0.24	-23.39	-1.31	0.36	-20.55	-4.15	0.24	-16.23	-8.46	2.52	-17.83	-6.87	0.20	-12.98	-11.72	0.22
S/T 1	-33.08	-41.36	8.29	0.10	-32.82	-0.25	0.41	-32.56	-0.52	0.12	-21.97	-11.11	2.62	-28.09	-4.99	0.13	-24.28	-8.79	0.13
S/T 2	-32.36	-41.49	9.13	0.15	-33.24	0.88	0.28	-30.37	-1.99	0.15	-21.81	-10.55	2.24	-28.32	-4.04	0.23	-25.28	-7.08	0.17
S/T 3	-32.11	-40.29	8.18	0.10	-31.92	-0.19	0.39	-29.95	-2.16	0.24	-21.69	-10.52	3.11	-27.33	-4.78	0.09	-23.98	-8.13	0.14
S/T 4	-31.95	-31.07	-0.88	0.25	-32.38	0.42	0.32	-29.82	-2.13	0.21	-21.35	-10.60	2.77	-27.98	-3.97	0.16	-24.08	-7.88	0.23
S/T 5	-31.93	-39.79	7.86	0.08	-33.25	1.32	0.45	-29.15	-2.78	0.15	-15.40	-16.53	0.63	-26.66	-5.28	0.12	-22.16	-9.77	0.13
S/T 6	-28.72	-40.58	11.85	0.19	-25.93	-2.79	0.42	-27.40	-1.33	0.13	-15.59	-13.13	0.54	-24.36	-4.36	0.17	-20.89	-7.83	0.15
S/T 7	-27.31	-35.70	8.39	0.35	-26.80	-0.51	1.08	-27.06	-0.25	0.18	-16.50	-10.81	0.70	-24.31	-3.00	0.18	-21.22	-6.09	0.20
mCmCmC																			
HB/HB 1	-23.80	-40.84	17.03	1.07	-26.23	2.43	1.00	-28.72	4.92	0.23	-21.69	-2.11	0.30	-24.53	0.73	3.90	-23.61	-0.20	3.30
HB/S 1	-38.61	-50.75	12.14	2.75	-36.25	-2.36	0.51	-38.17	-0.44	0.60	-23.86	-14.75	0.70	-30.29	-8.32	0.65	-28.66	-9.95	0.26
HB/S 2	-36.09	-48.23	12.14	0.21	-36.25	0.17	0.62	-38.22	2.13	0.21	-19.22	-16.87	0.30	-30.31	-5.78	0.37	-23.40	-12.69	0.37
HB/T 1	-17.34	-34.26	16.92	0.24	-21.81	4.48	1.56	-23.33	5.99	1.82	-18.53	1.19	0.92	-17.93	0.60	0.25	-16.11	-1.22	0.25

S/S 1	-28.12	-35.07	6.95	0.31	-26.47	-1.64	1.07	-24.43	-3.69	0.70	-9.80	-18.32	1.52	-19.27	-8.84	0.21	-16.31	-11.81	0.14
S/T 1	-39.57	-52.30	12.73	0.20	-36.42	-3.15	0.84	-39.56	-0.01	0.25	-26.23	-13.34	4.09	-31.86	-7.71	0.33	-29.43	-10.14	0.26
S/T 2	-38.60	-48.26	9.66	0.19	-33.85	-4.75	0.68	-37.04	-1.56	0.15	-29.35	-9.25	1.56	-29.27	-9.33	0.16	-26.28	-12.33	0.15
S/T 3	-34.15	-47.15	12.99	2.99	-34.95	0.80	0.84	-33.98	-0.18	0.21	-20.24	-13.91	1.46	-31.29	-2.87	0.20	-27.45	-6.70	0.27
S/T 4	-32.95	-44.17	11.22	0.17	-33.72	0.77	0.51	-32.00	-0.95	0.17	-11.00	-21.96	0.69	-26.84	-6.11	0.20	-26.81	-6.14	0.14
S/T 5	-28.46	-45.04	16.58	1.12	-32.61	4.15	0.99	-35.90	7.44	1.10	-30.22	1.76	1.94	-28.53	0.07	1.20	-19.36	-9.10	0.13
S/T 6	-25.97	-37.49	11.52	0.47	-28.63	2.66	0.98	-28.10	2.13	1.07	-18.66	-7.31	1.03	-9.89	-16.08	0.23	-19.60	-6.37	0.63
T/T 1	-35.77	-47.03	11.26	0.70	-31.90	-3.87	0.58	-35.55	-0.22	0.14	-22.69	-13.08	0.64	-31.87	-3.90	0.22	-27.08	-8.69	0.21
mTmUmU																			
HB/HB 1	-20.13	-35.02	14.89	0.11	-21.63	1.51	0.48	-20.47	0.34	0.04	-18.26	-1.87	0.12	-19.99	-0.14	0.17	-19.35	-0.78	0.13
HB/HB 2	-19.61	-30.55	10.94	0.11	-20.99	1.39	0.21	-19.70	0.09	0.12	-15.85	-3.76	0.10	-19.26	-0.35	0.16	-18.77	-0.84	0.14
HB/S 1	-24.07	-31.08	7.02	0.14	-24.88	0.81	0.58	-22.78	-1.29	0.16	-12.14	-11.93	1.17	-20.01	-4.06	0.13	-17.89	-6.17	0.14
HB/T 1	-22.09	-32.63	10.54	0.14	-22.57	0.47	0.43	-22.26	0.17	0.12	-15.22	-6.87	0.44	-22.01	-0.08	0.15	-21.00	-1.10	0.19

S/S 1	-22.10	-25.25	3.15	0.23	-21.53	-0.57	0.32	-19.35	-2.75	0.25	-12.41	-9.69	2.48	-16.96	-5.14	0.33	-12.92	-9.18	0.32
S/S 2	-21.07	-30.26	9.19	1.56	-21.31	0.24	0.57	-18.23	-2.84	0.24	-5.16	-15.91	0.76	-15.02	-6.05	0.51	-11.16	-9.91	0.58
S/T 1	-28.45	-38.67	10.22	3.72	-30.73	2.28	0.42	-26.69	-1.77	0.11	-16.02	-12.43	1.95	-24.38	-4.07	0.19	-21.98	-6.47	0.11
S/T 2	-28.37	-38.20	9.83	0.15	-30.57	2.20	0.37	-26.57	-1.79	0.13	-16.12	-12.25	1.99	-24.41	-3.95	0.20	-21.59	-6.78	0.15
S/T 3	-26.89	-36.25	9.36	0.26	-27.08	0.19	0.50	-25.80	-1.09	0.15	-14.51	-12.38	0.72	-23.56	-3.34	0.19	-20.29	-6.60	0.12
S/T 4	-25.00	-35.99	10.99	0.18	-25.13	0.13	0.36	-24.16	-0.84	0.23	-14.02	-10.98	2.04	-20.37	-4.63	0.32	-17.74	-7.26	0.27
S/T 5	-22.28	-29.27	6.99	0.21	-22.33	0.06	0.41	-20.93	-1.34	0.37	-11.39	-10.88	0.56	-19.80	-2.47	0.33	-17.57	-4.71	0.35
T/T 1	-27.56	-36.96	9.40	0.15	-29.97	2.41	0.44	-25.41	-2.15	0.17	-14.33	-13.23	1.67	-23.56	-4.00	0.19	-21.18	-6.38	0.11
mUmUmU																			
HB/HB 1	-20.77	-32.80	12.03	0.14	-20.62	-0.15	0.11	-21.77	1.01	0.13	-16.13	-4.64	0.12	-9.20	-11.57	0.13	-20.93	0.16	0.13
HB/HB 2	-19.99	-31.28	11.28	0.13	-20.21	0.22	0.18	-19.96	-0.04	0.13	-16.69	-3.40	0.02	-7.23	-12.76	0.11	-19.47	-0.52	0.11
HB/HB 3	-15.35	-25.46	10.11	1.19	-17.86	2.51	0.75	-15.92	0.57	0.04	-12.03	-3.32	0.07	-16.59	1.24	1.06	-15.45	0.10	0.24
HB/S 1	-26.15	-36.69	10.53	0.69	-28.10	1.95	0.44	-24.45	-1.70	0.06	-14.34	-11.82	0.44	-24.73	-1.42	0.75	-21.22	-4.94	0.18

HB/S 2	-25.01	-35.41	10.40	0.13	-26.96	1.95	0.62	-23.60	-1.41	0.14	-13.23	-11.78	0.54	-23.88	-1.13	0.17	-20.46	-4.55	0.18
HB/S 3	-24.07	-32.99	8.92	0.12	-25.08	1.01	0.50	-23.13	-0.94	0.07	-13.77	-10.30	0.48	-22.55	-1.52	0.14	-11.50	-12.57	0.13
HB/S 4	-23.14	-31.41	8.27	0.14	-24.14	0.99	0.46	-21.65	-1.49	0.18	-12.32	-10.83	0.46	-21.31	-1.83	0.13	-17.98	-5.16	0.13
S/S 1	-17.35	-20.46	3.10	1.58	-17.08	-0.27	0.68	-14.42	-2.94	0.12	-5.98	-11.38	2.45	-11.93	-5.42	0.67	-8.41	-8.94	0.29
S/T 1	-27.25	-37.21	9.95	0.13	-29.61	2.36	0.41	-25.77	-1.49	0.16	-14.33	-12.93	1.39	-24.36	-2.89	0.17	-21.32	-5.94	0.10
S/T 2	-23.98	-32.31	8.33	0.13	-24.72	0.74	0.47	-25.21	1.24	0.42	-14.35	-9.62	0.52	-22.29	-1.89	0.41	-19.60	-4.38	0.33
T/T 1	-28.16	-38.85	10.88	0.29	-30.38	2.22	0.40	-26.24	-1.92	0.12	-16.14	-12.02	1.78	-25.34	-2.82	0.17	-22.38	-5.78	0.12
T/T 2	-25.33	-34.68	9.35	0.24	-25.88	0.54	0.36	-25.27	-0.06	0.15	-15.13	-10.20	0.59	-23.88	-1.45	0.17	-21.04	-4.29	0.18
TAT																			
HB/HB 1	-34.19	-47.75	13.56	0.12	-30.47	-3.71	0.15	-33.65	-0.53	0.05	-30.78	-3.41	0.06	-32.21	-1.97	0.13	-32.20	-1.99	0.08
HB/HB 2	-31.85	-44.99	13.13	0.17	-27.83	-4.02	0.42	-32.09	0.24	0.10	-26.90	-4.95	0.15	-29.21	-2.65	0.48	-28.86	-3.00	0.41
HB/HB 3	-31.56	-45.01	13.45	0.28	-27.04	-4.52	0.26	-31.85	0.29	0.25	-30.05	-1.52	0.25	-30.71	-0.85	0.36	-30.83	-0.74	0.28
HB/HB 4	-27.63	-40.83	13.21	0.21	-22.41	-5.21	0.27	-28.01	0.39	0.10	-24.00	-3.63	0.11	-26.94	-0.89	0.08	-26.17	-1.46	0.10

HB/S 1	-29.53	-39.74	10.21	2.83	-31.79	2.26	0.85	-29.43	-0.10	0.28	-30.75	1.22	3.01	-25.88	-3.66	0.42	-23.77	-5.76	0.34
S/S 1	-23.89	-22.12	-1.77	0.09	-22.65	-1.25	0.21	-17.26	-6.64	0.24	-29.15	5.26	3.34	-13.97	-9.92	0.16	-9.98	-13.91	0.16
S/S 2	-21.13	-20.50	-0.63	0.21	-20.41	-0.72	0.68	-15.50	-5.63	0.27	-21.59	0.46	3.63	-12.77	-8.37	0.20	-8.27	-12.86	0.19
S/T 1	-33.10	-42.16	9.06	0.46	-33.34	0.24	0.15	-30.55	-2.56	0.13	-23.23	-9.87	0.69	-27.01	-6.09	0.14	-24.26	-8.84	0.12
S/T 2	-32.81	-41.55	8.74	0.50	-33.15	0.34	0.19	-30.17	-2.64	0.13	-19.97	-12.84	1.68	-26.86	-5.95	0.13	-24.59	-8.22	0.13
S/T 3	-31.74	-39.52	7.78	0.27	-31.88	0.13	0.64	-29.29	-2.46	0.16	-22.02	-9.72	2.41	-26.20	-5.54	0.20	-23.47	-8.28	0.12
S/T 4	-30.41	-37.22	6.81	0.21	-28.33	-2.08	0.26	-28.85	-3.56	0.22	-15.85	-14.56	0.63	-22.82	-7.59	0.21	-20.32	-10.09	0.18
T/T 1	-29.79	-39.72	9.93	0.50	-30.23	0.45	0.33	-28.05	-1.74	0.52	-30.74	0.96	3.08	-24.60	-5.18	0.16	-23.18	-6.61	0.11
UUA																			
HB/HB 1	-34.04	-47.94	13.90	0.12	-30.61	-3.43	0.17	-33.71	-0.33	0.05	-30.91	-3.13	0.07	-32.50	-1.54	0.10	-32.46	-1.59	0.09
HB/HB 2	-33.36	-46.64	13.28	0.12	-29.54	-3.82	0.06	-33.13	-0.24	0.07	-30.48	-2.88	0.06	-31.54	-1.82	0.10	-31.71	-1.65	0.09
HB/HB 3	-32.97	-46.23	13.26	0.12	-26.43	-6.54	0.15	-28.48	-4.49	0.04	-29.81	-3.16	0.05	-31.56	-1.41	0.09	-31.34	-1.64	0.08
HB/HB 4	-32.77	-45.06	12.29	0.12	-27.03	-5.74	0.07	-32.12	-0.65	0.03	-30.08	-2.69	0.02	-30.85	-1.93	0.08	-30.94	-1.83	0.08

HB/HB 5	-31.71	-46.19	14.48	0.13	-29.67	-2.04	0.21	-32.65	0.94	0.07	-29.29	-2.42	0.10	-31.67	-0.04	0.12	-31.24	-0.47	0.07
HB/HB 6	-31.29	-45.73	14.44	0.13	-28.43	-2.86	0.13	-33.77	2.48	0.13	-27.23	-4.06	0.17	-29.86	-1.43	0.41	-29.32	-1.97	0.38
HB/HB 7	-27.56	-40.86	13.30	0.44	-22.39	-5.17	0.26	-30.88	3.32	0.08	-24.22	-3.34	0.09	-27.22	-0.34	0.08	-26.38	-1.17	0.08
HB/HB 8	-27.42	-40.80	13.38	0.13	-22.39	-5.03	0.24	-26.36	-1.06	0.10	-24.00	-3.42	0.04	-27.15	-0.27	0.09	-26.36	-1.06	0.08
HB/HB 9	-25.92	-39.88	13.96	0.10	-22.66	-3.27	0.17	-26.13	0.20	0.19	-21.95	-3.97	0.05	-26.42	0.50	0.08	-25.41	-0.52	0.08
HB/HB 10	-24.34	-37.44	13.10	0.12	-24.05	-0.29	0.31	-24.00	-0.34	0.04	-20.85	-3.49	0.07	-24.02	-0.32	0.45	-23.81	-0.53	0.09
HB/S 1	-27.24	-35.71	8.47	0.22	-25.74	-1.50	0.51	-27.27	0.03	0.32	-19.77	-7.47	1.19	-22.72	-4.52	0.33	-20.20	-7.04	0.32
S/S 1	-21.44	-20.80	-0.64	0.60	-21.31	-0.13	0.45	-17.28	-4.16	0.51	-16.89	-4.55	3.23	-13.61	-7.83	0.27	-10.24	-11.21	0.20
S/S 2	-19.22	-20.22	1.00	0.18	-20.49	1.27	0.44	-16.29	-2.93	0.43	-26.90	7.68	3.14	-13.84	-5.37	0.20	-10.10	-9.12	0.21
S/T 1	-32.51	-42.43	9.92	0.43	-32.97	0.46	0.14	-31.48	-1.03	0.03	-30.45	-2.06	4.19	-27.20	-5.31	0.18	-25.30	-7.21	0.12
S/T 2	-32.13	-41.28	9.15	0.39	-32.66	0.53	0.17	-28.96	-3.17	0.12	-19.72	-12.40	1.44	-26.89	-5.24	0.12	-24.64	-7.49	0.11
S/T 3	-30.73	-36.55	5.82	0.14	-25.73	-5.00	0.19	-27.39	-3.34	0.07	-17.82	-12.91	0.56	-24.15	-6.68	0.19	-21.35	-9.38	0.10

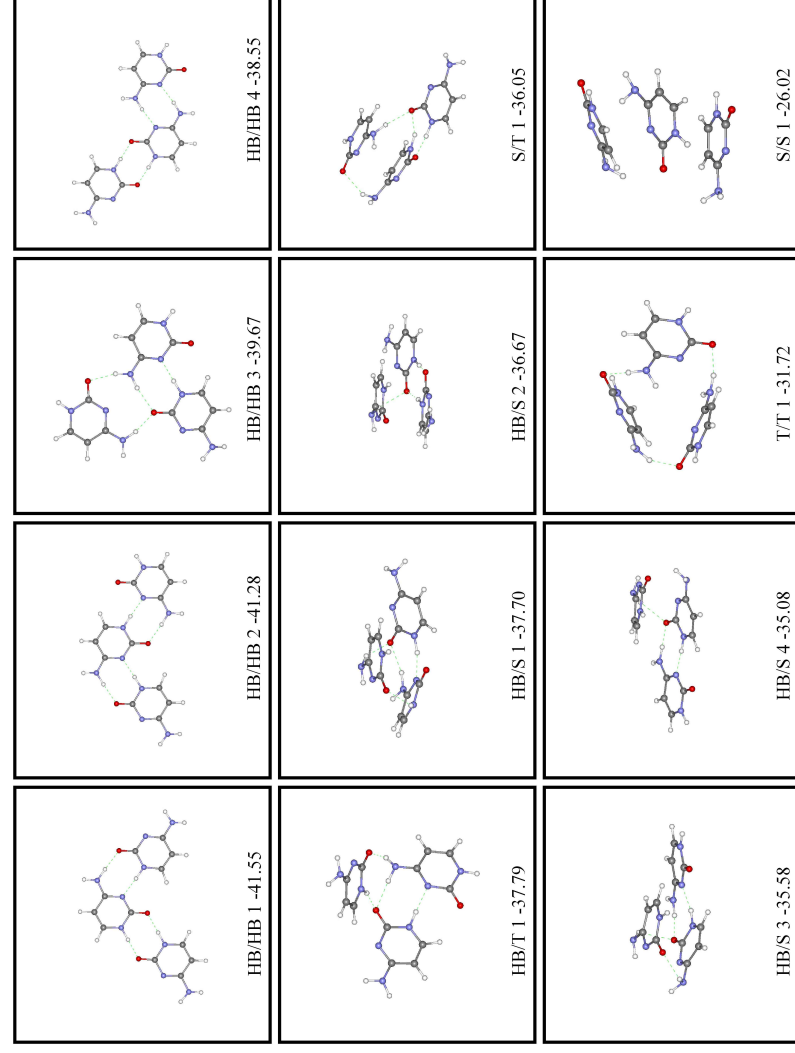
UUT

HB/HB 1	-32.77	-45.64	12.87	0.16	-32.81	0.03	0.05	-32.56	-0.21	0.04	-30.65	-2.12	0.04	-32.30	-0.48	0.13	-32.54	-0.24	0.10
HB/HB 2	-32.72	-44.10	11.38	2.59	-32.68	-0.04	0.05	-32.65	-0.07	0.04	-30.41	-2.31	0.03	-32.02	-0.70	0.11	-32.09	-0.63	0.09
HB/HB 3	-31.84	-44.62	12.78	0.49	-32.01	0.17	0.05	-32.93	1.08	0.03	-27.80	-4.04	0.03	-31.44	-0.40	0.22	-31.28	-0.56	0.08
HB/HB 4	-31.82	-45.00	13.18	0.16	-32.13	0.31	0.05	-32.90	1.08	0.03	-27.78	-4.04	0.04	-30.98	-0.84	0.30	-31.31	-0.51	0.07
HB/HB 5	-28.99	-42.05	13.06	0.14	-29.86	0.87	0.20	-29.37	0.38	0.04	-26.58	-2.40	0.02	-28.99	0.01	0.14	-28.75	-0.24	0.13
S/S 1	-15.78	-17.76	1.99	0.32	-18.00	2.22	0.66	-13.36	-2.42	0.36	-15.26	-0.52	3.38	-10.47	-5.31	0.40	-7.82	-7.96	0.32
S/S 2	-15.22	-26.15	10.93	2.57	-17.45	2.24	0.60	-13.03	-2.19	0.34	-11.52	-3.70	2.78	-10.00	-5.22	0.45	-7.27	-7.95	0.27
S/T 1	-28.87	-42.15	13.28	1.78	-30.43	1.56	0.27	-28.00	-0.87	0.45	-30.47	1.60	3.86	-25.74	-3.13	0.42	-23.79	-5.08	0.45
S/T 2	-27.65	-40.47	12.82	0.15	-29.71	2.06	0.43	-26.82	-0.83	0.31	-20.93	-6.71	1.38	-24.76	-2.89	0.42	-22.70	-4.95	0.30
S/T 3	-19.76	-38.09	18.33	1.79	-24.67	4.91	1.19	-20.83	1.07	1.40	-19.08	-0.68	1.90	-16.67	-3.09	0.18	-14.53	-5.23	0.16
T/T 1	-28.87	-40.41	11.53	0.15	-30.00	1.12	0.07	-28.41	-0.46	0.03	-19.14	-9.74	0.10	-25.22	-3.66	0.11	-22.11	-6.76	0.09
T/T 2	-25.10	-37.95	12.85	0.18	-28.20	3.10	0.36	-25.32	0.22	0.07	-17.26	-7.84	0.12	-23.81	-1.29	0.14	-22.28	-2.82	0.12

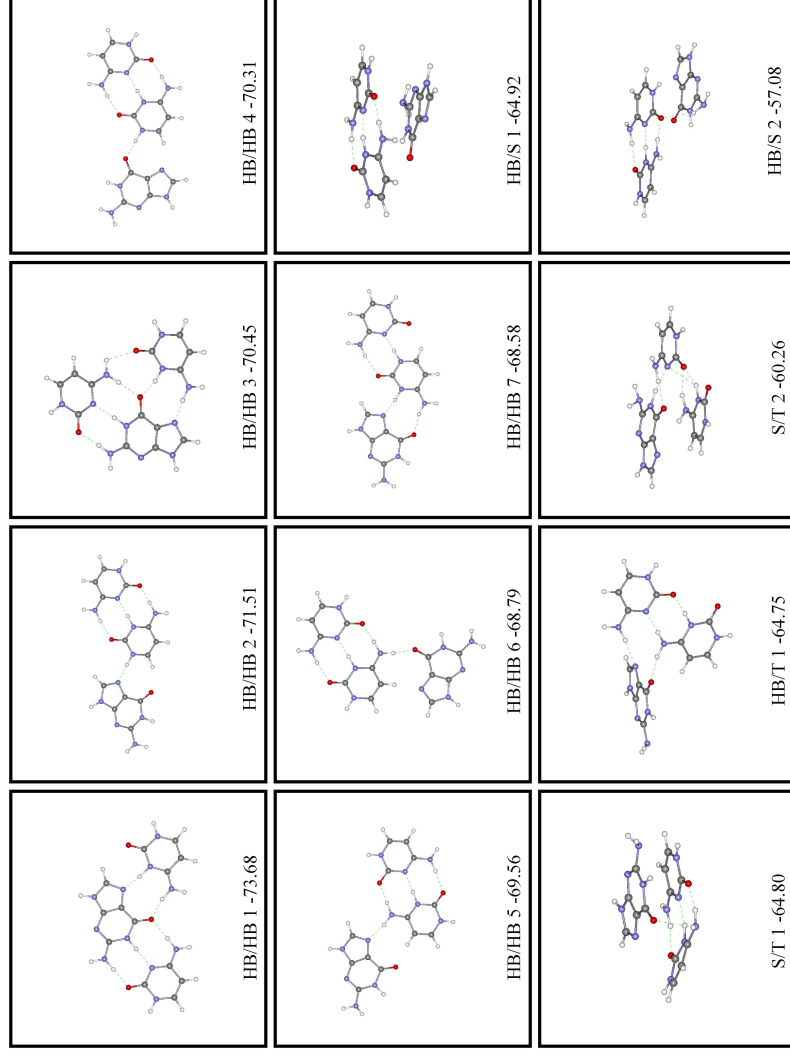
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HB/HB 1	-32.67	-47.40	14.73	0.12	-32.84	0.17	0.63	-33.23	0.56	0.04	-32.44	-0.23	0.04	-32.25	-0.42	0.10	-32.28	-0.39	0.09
HB/HB 2	-31.63	-47.13	15.50	0.13	-31.97	0.34	1.15	-32.58	0.95	0.02	-27.67	-3.96	0.03	-31.11	-0.52	0.23	-31.25	-0.38	0.09
HB/HB 3	-28.83	-41.97	13.14	0.13	-29.85	1.02	0.38	-28.32	-0.51	0.04	-26.45	-2.38	0.01	-28.81	-0.02	0.17	-28.65	-0.18	0.14
HB/HB 4	-25.63	-38.09	12.46	0.14	-26.94	1.31	0.20	-26.33	0.70	0.04	-21.60	-4.03	0.02	-25.44	-0.20	0.15	-25.13	-0.50	0.14
HB/HB 5	-26.93	-39.92	12.99	0.14	-28.25	1.32	0.19	-26.54	-0.39	0.04	-24.69	-2.24	0.04	-26.78	-0.15	0.12	-26.55	-0.39	0.11
HB/S 1	-26.57	-36.72	10.14	0.21	-28.36	1.78	0.44	-25.76	-0.81	0.28	-27.92	1.35	2.45	-23.93	-2.65	0.23	-21.60	-4.97	0.22
HB/T 1	-20.44	-32.72	12.28	0.38	-23.39	2.95	0.20	-20.35	-0.09	0.08	-14.73	-5.71	0.45	-19.24	-1.20	0.45	-18.39	-2.05	0.59
HB/T 2	-19.81	-32.72	12.91	0.77	-21.90	2.09	0.50	-20.82	1.01	0.05	-13.73	-6.08	0.45	-18.17	-1.64	0.20	-18.49	-1.32	0.08
S/S 1	-15.89	-18.83	2.94	0.41	-17.79	1.91	0.04	-12.86	-3.02	0.24	-15.41	-0.48	2.36	-11.82	-4.06	0.19	-9.48	-6.41	0.14
S/T 1	-27.56	-38.44	10.88	0.53	-30.16	2.60	0.06	-27.16	-0.40	0.62	-30.55	3.00	3.54	-25.15	-2.41	0.42	-21.43	-6.13	0.15
S/T 2	-26.96	-36.71	9.76	0.14	-27.65	0.70	0.96	-26.40	-0.56	0.11	-28.96	2.01	1.87	-23.48	-3.48	0.16	-22.27	-4.69	0.11
S/T 3	-25.62	-35.12	9.50	0.75	-27.93	2.31	0.84	-24.46	-1.16	0.24	-19.02	-6.60	1.95	-21.86	-3.76	0.21	-19.02	-6.60	0.10
S/T 4	-26.24	-35.93	9.69	0.12	-27.58	1.34	0.20	-25.84	-0.40	0.50	-27.69	1.45	2.31	-23.63	-2.61	0.23	-22.39	-3.85	0.14
T/T 1	-28.92	-42.07	13.15	0.11	-30.12	1.20	0.06	-28.46	-0.46	0.13	-22.07	-6.85	0.09	-25.62	-3.30	0.08	-22.03	-6.89	0.12

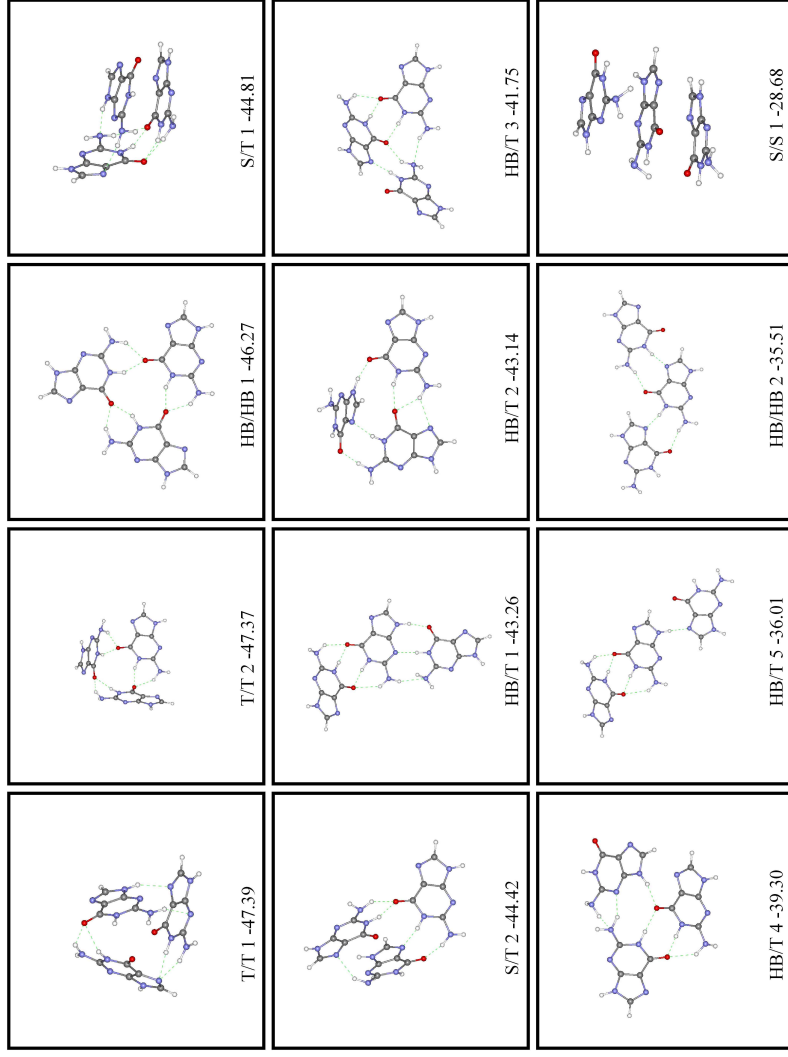
Figure 1S. Twelve optimized structures for each of eleven different trimers combinations which were used in this database. Below each structure the structural motif and RI-MP2 interaction energy (in kcal/mol) calculated employing the TZVPP basis set is depicted. If more than twelve structures for a given trimer were taken into account, their geometries can be found at the Supplementary material *all_structures_xyz.txt*.



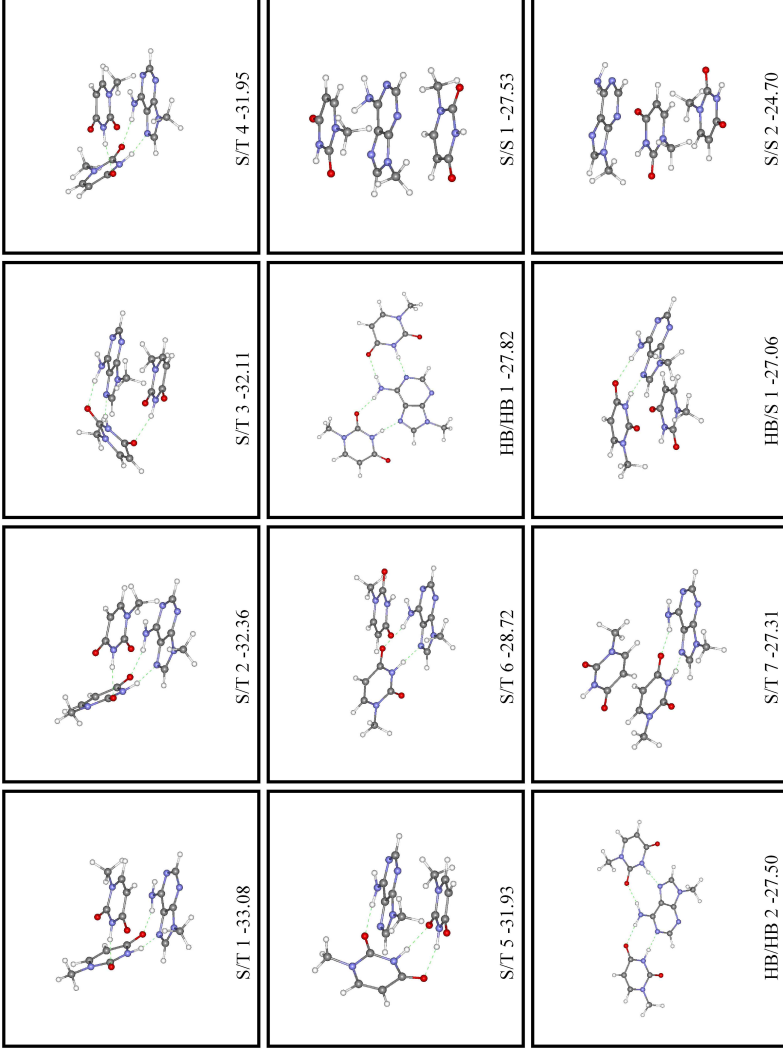
CCC trimers



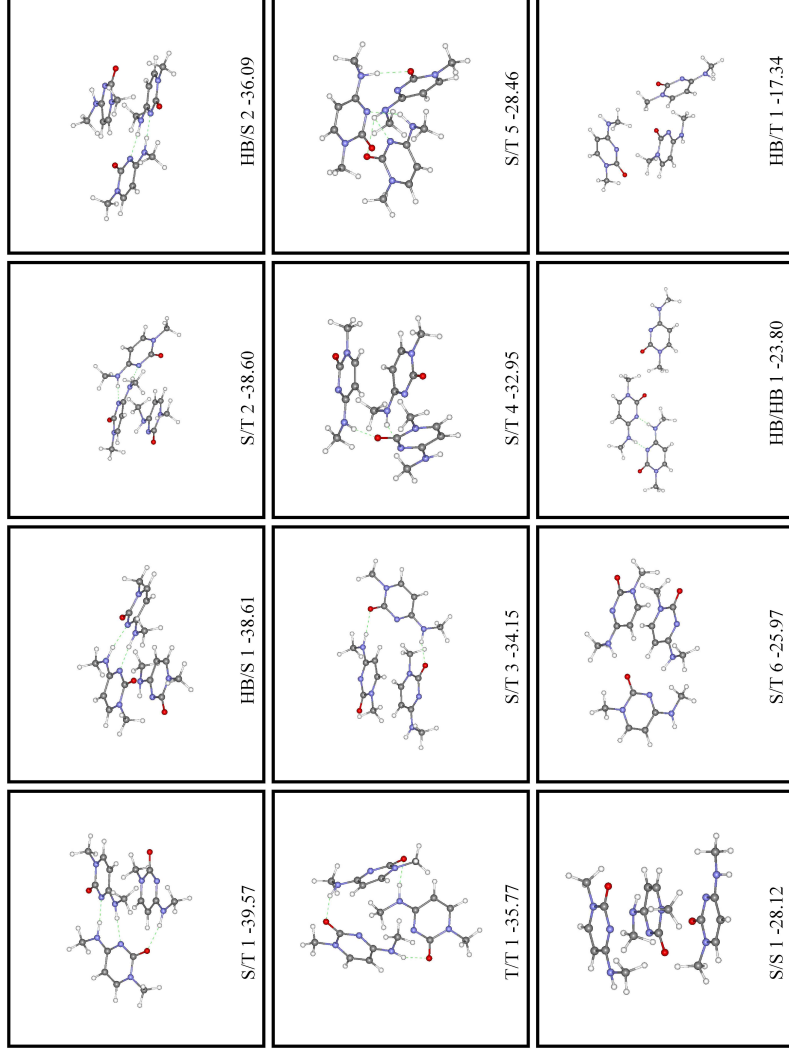
CGCplus trimers



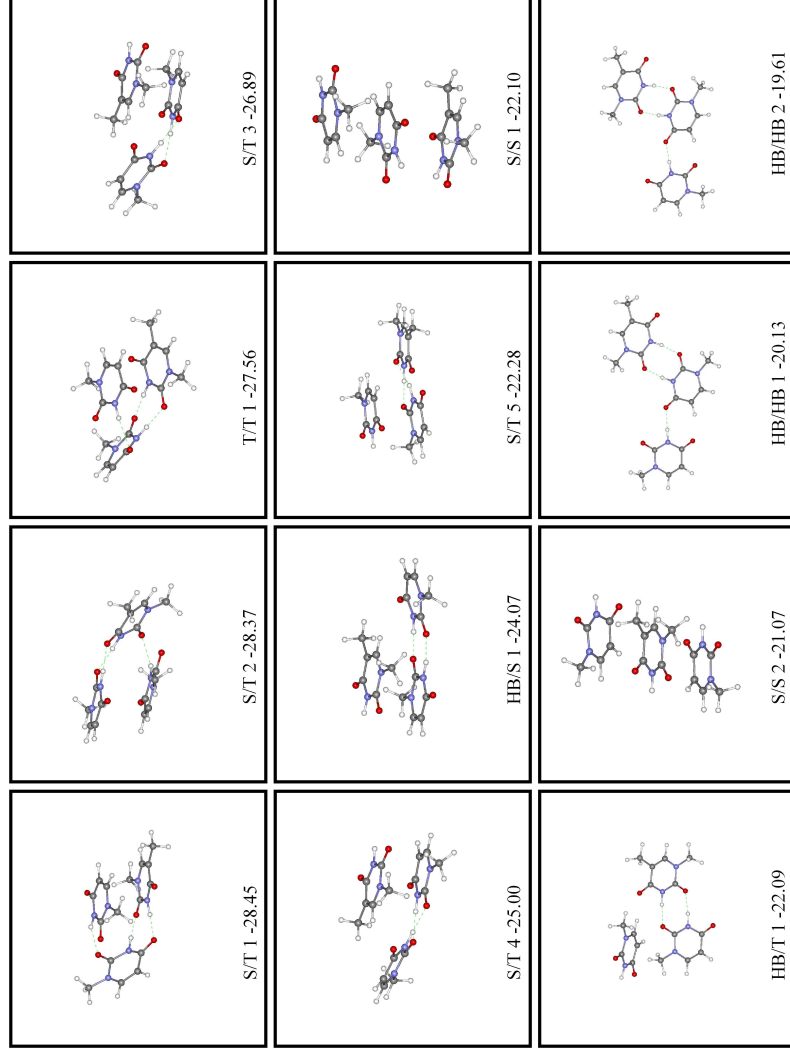
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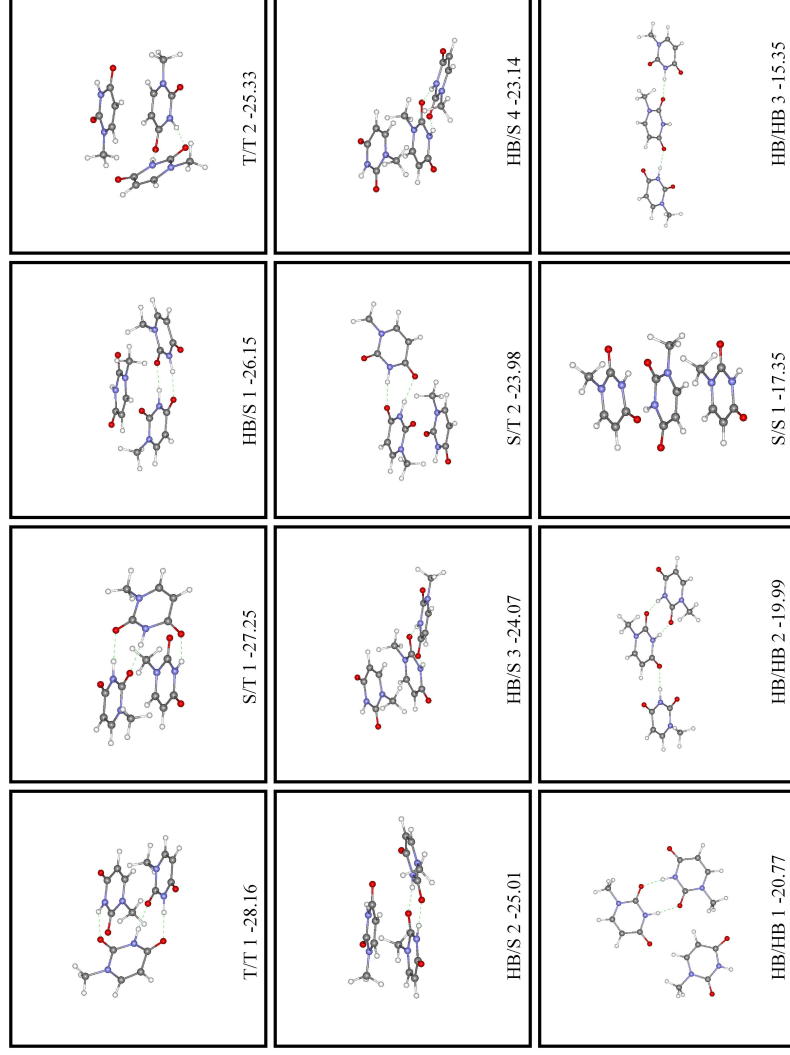
mAmUmU trimers



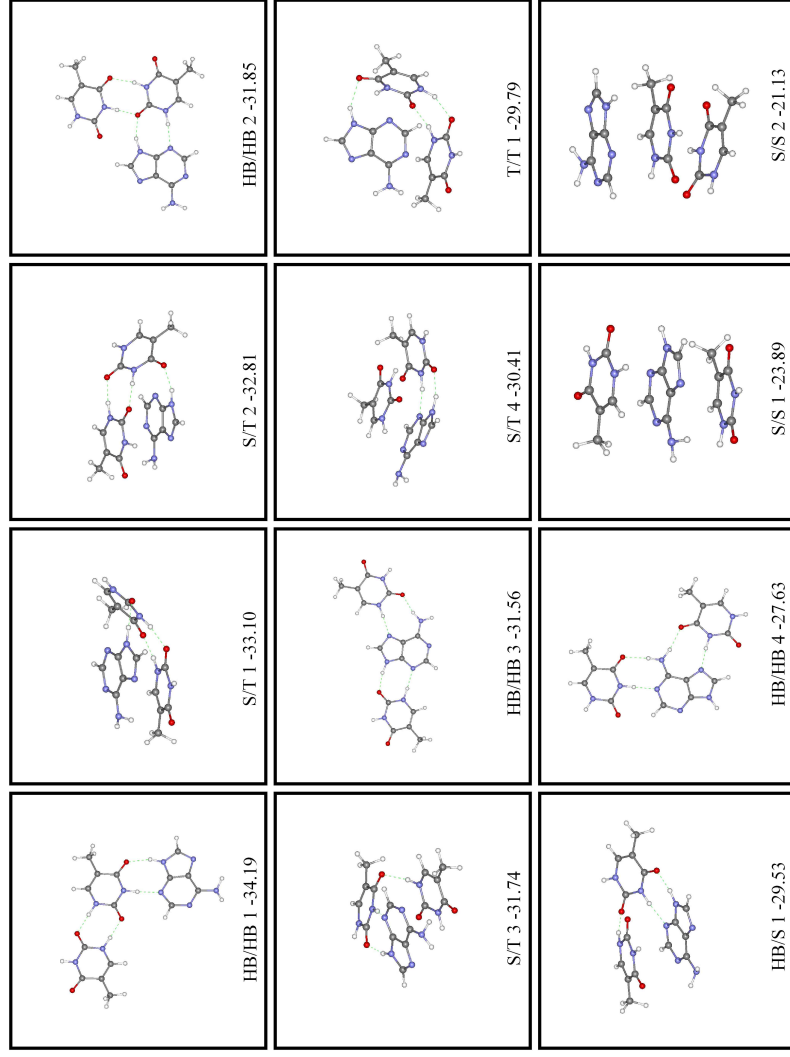
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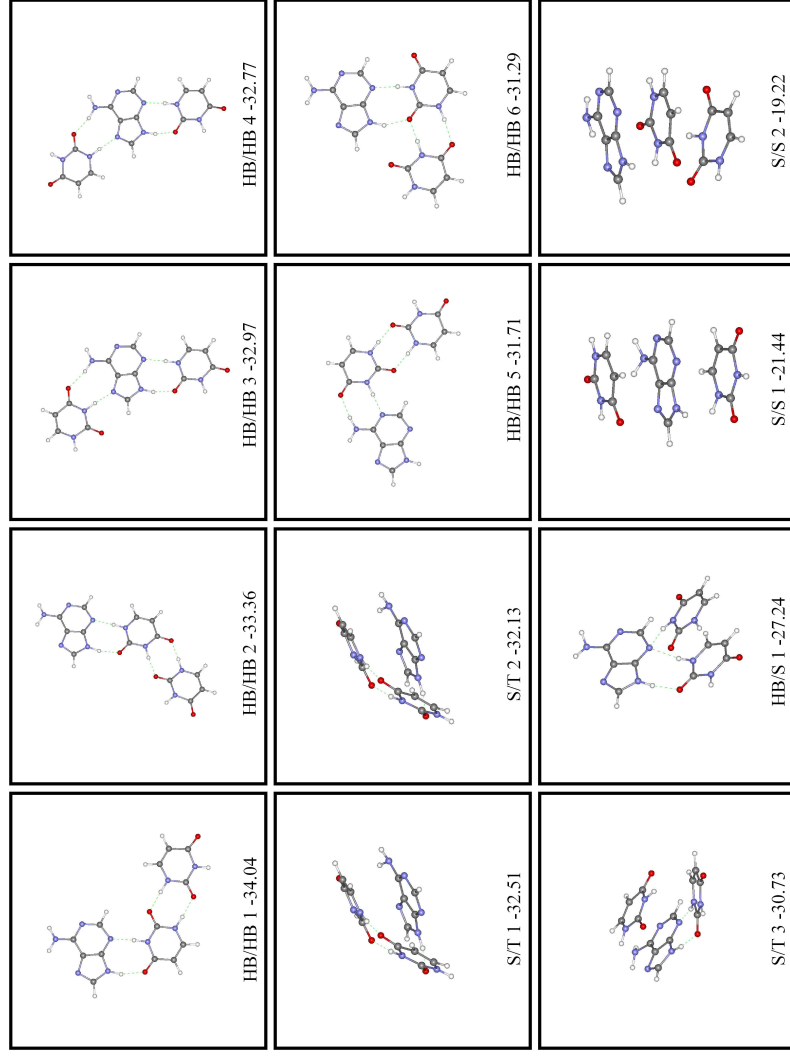
mTmUmU trimers



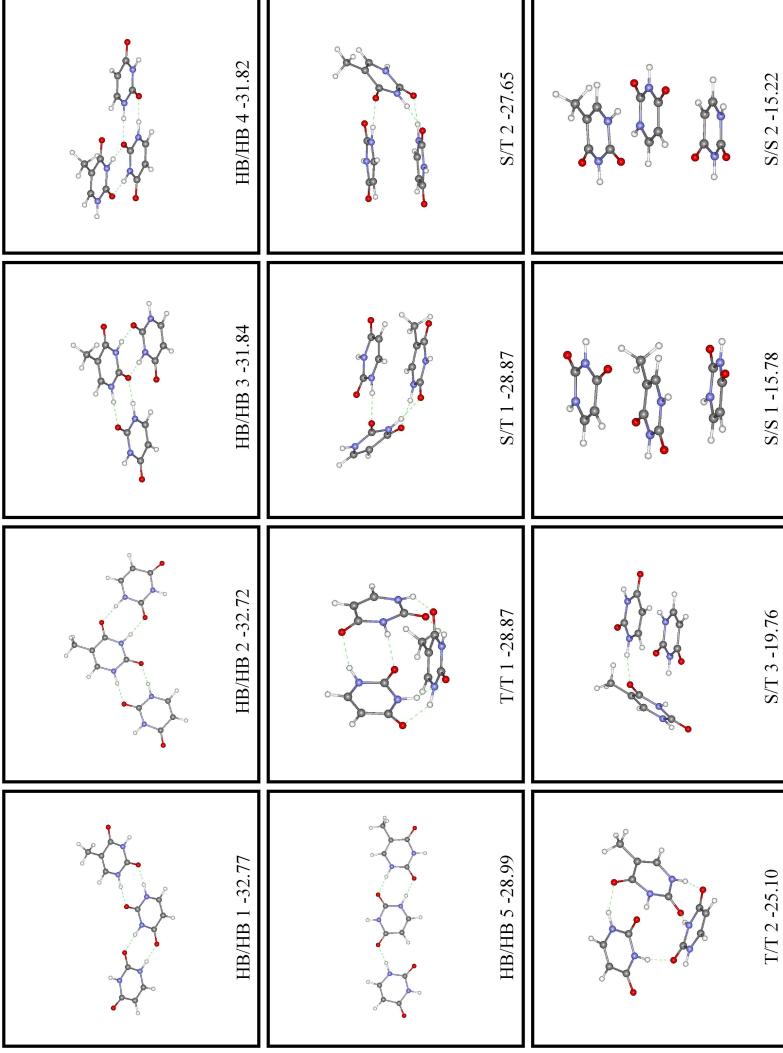
mUmUmU trimers



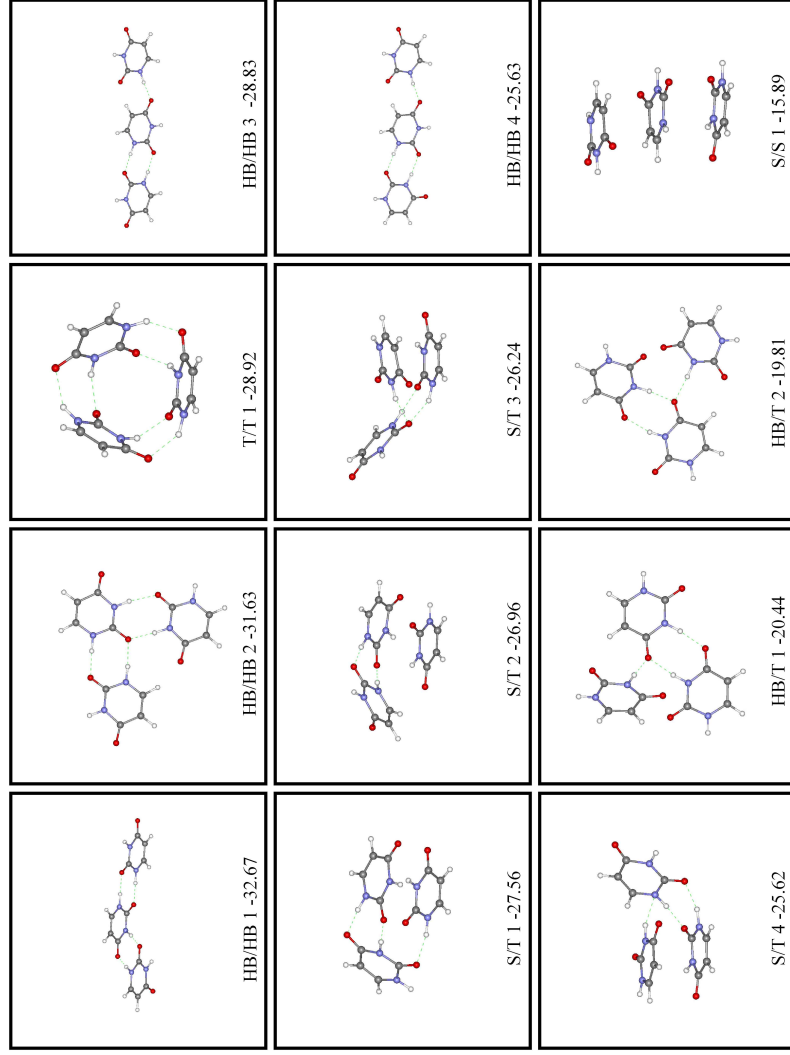
TAT trimers



UUA trimers



UUT trimers



UUU trimers

