SUPPORTING INFORMATION FOR

Cathinone – carbon nanotube complex: A new way for cancer treatment?

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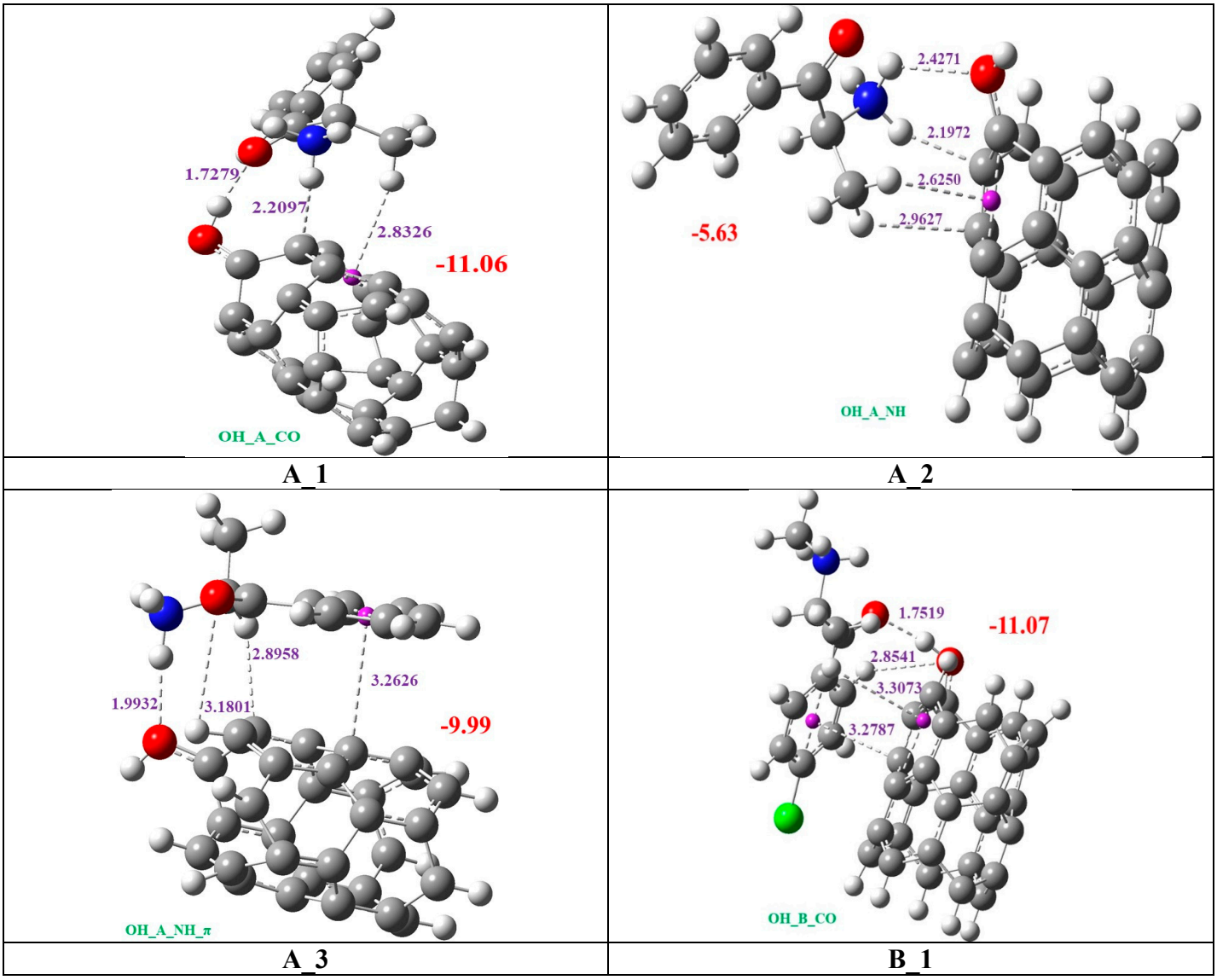


Figure S1. Structures of SWCNT-OH model with cathinones A-D (labelling from Figure 1 in manuscript) complexes. Dash lines indicate intermolecular interactions and their lengths (in Å) are shown in purple. The BSSE-corrected total interaction energies (in kcal/mol) are shown in red.

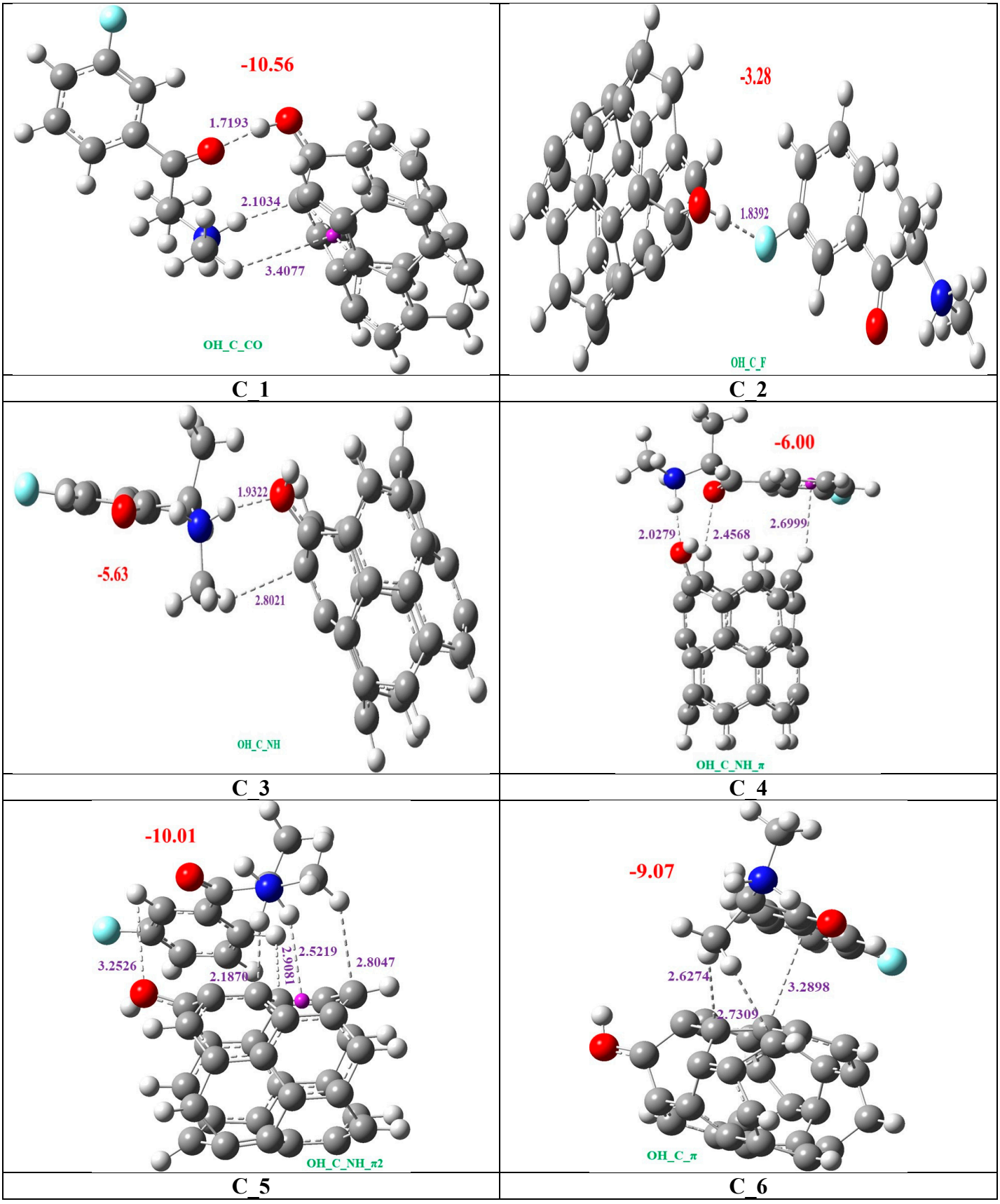


Figure S1. Cont.

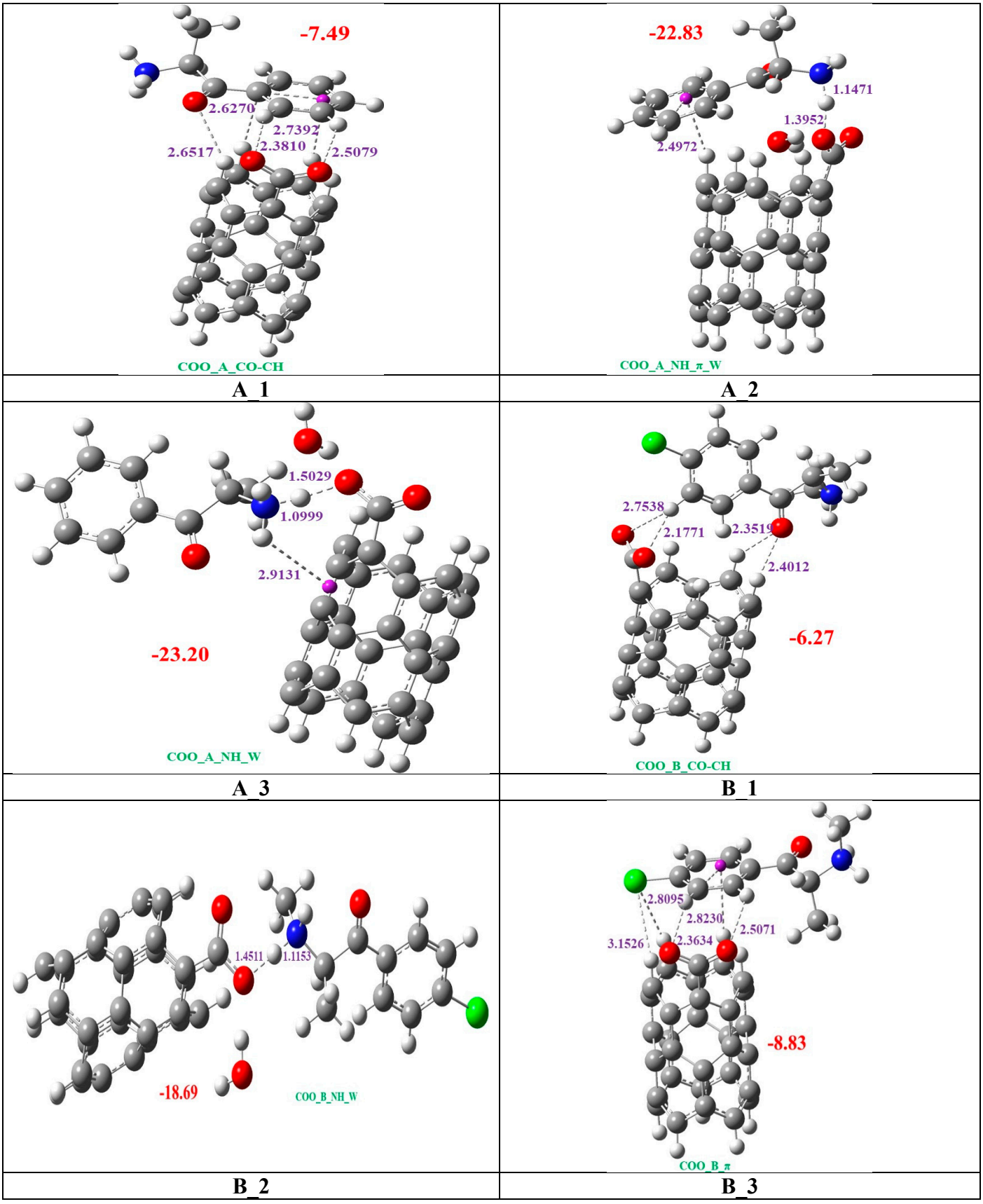


Figure S2. Structures of SWCNT-COO^- model with cathinones A-D (labelling from Figure 1 in manuscript) complexes. Dash lines indicate intermolecular interactions and their lengths (in Å) are shown in purple. The BSSE-corrected total interaction energies (in kcal/mol) are shown in red.

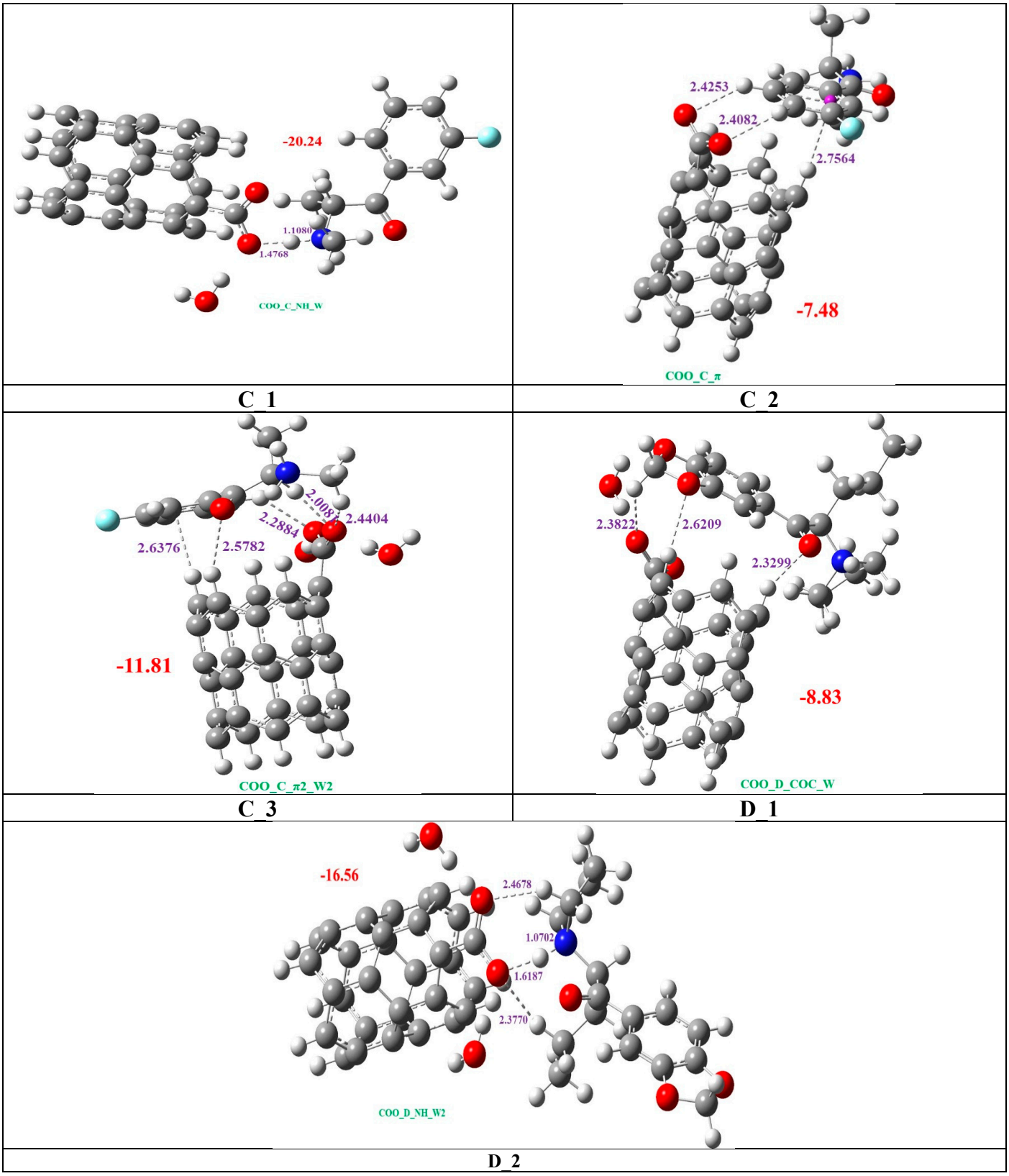


Figure S2. Cont.

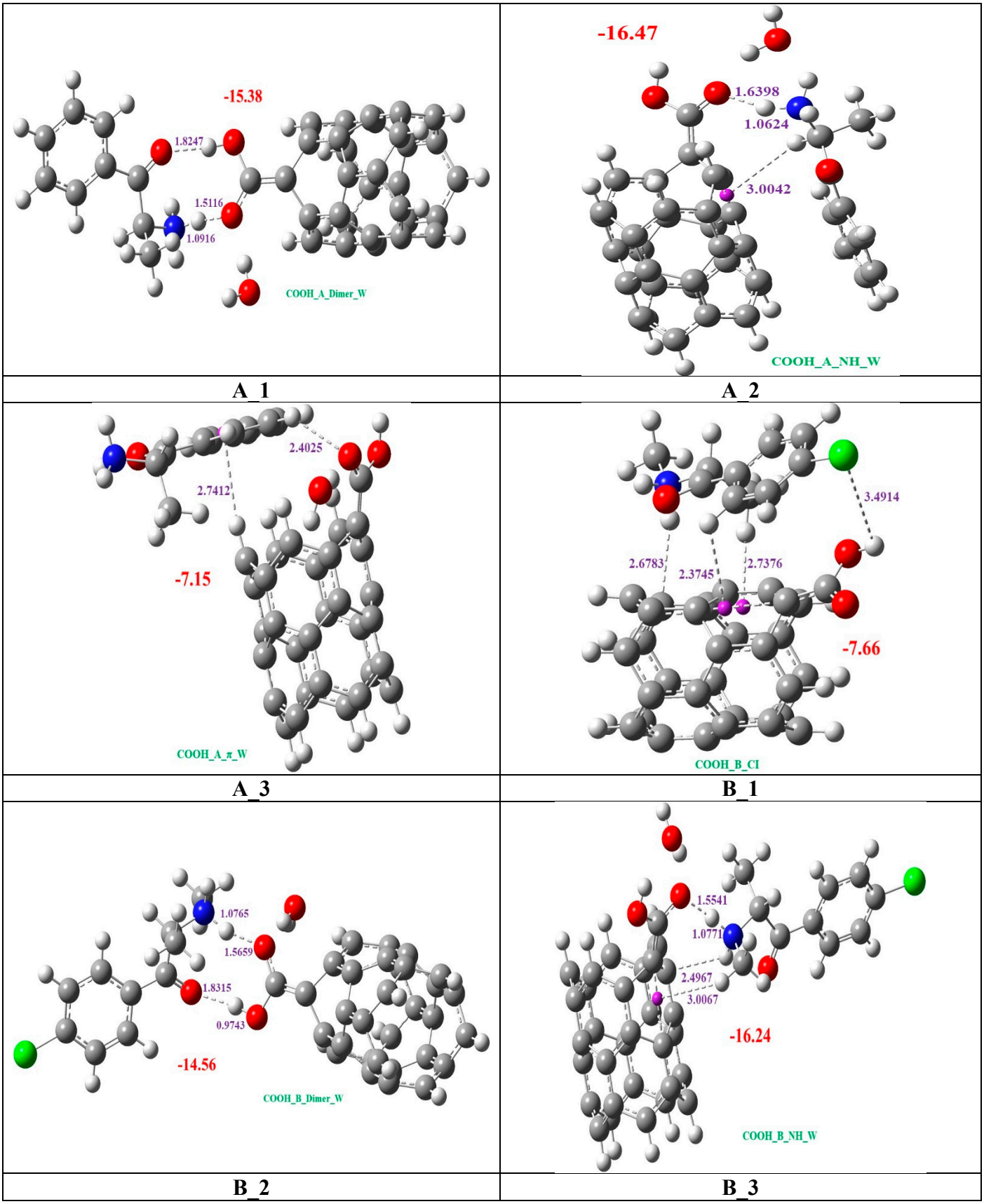


Figure S3. Structures of SWCNT-COOH model with cathinones A-D (labelling from Figure 1 in manuscript) complexes. Dash lines indicate intermolecular interactions and their lengths (in Å) are shown in purple. The BSSE-corrected total interaction energies (in kcal/mol) are shown in red.

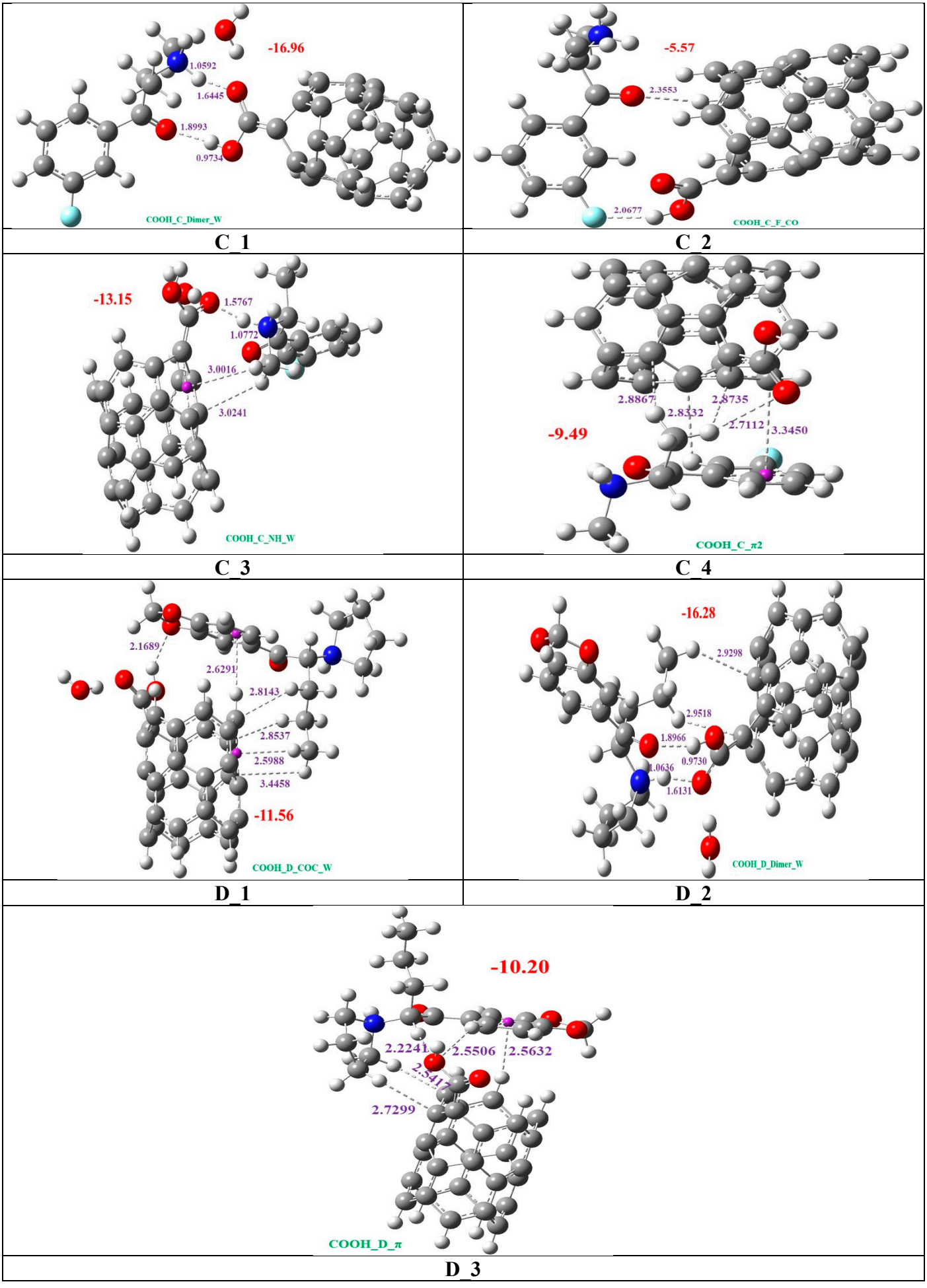
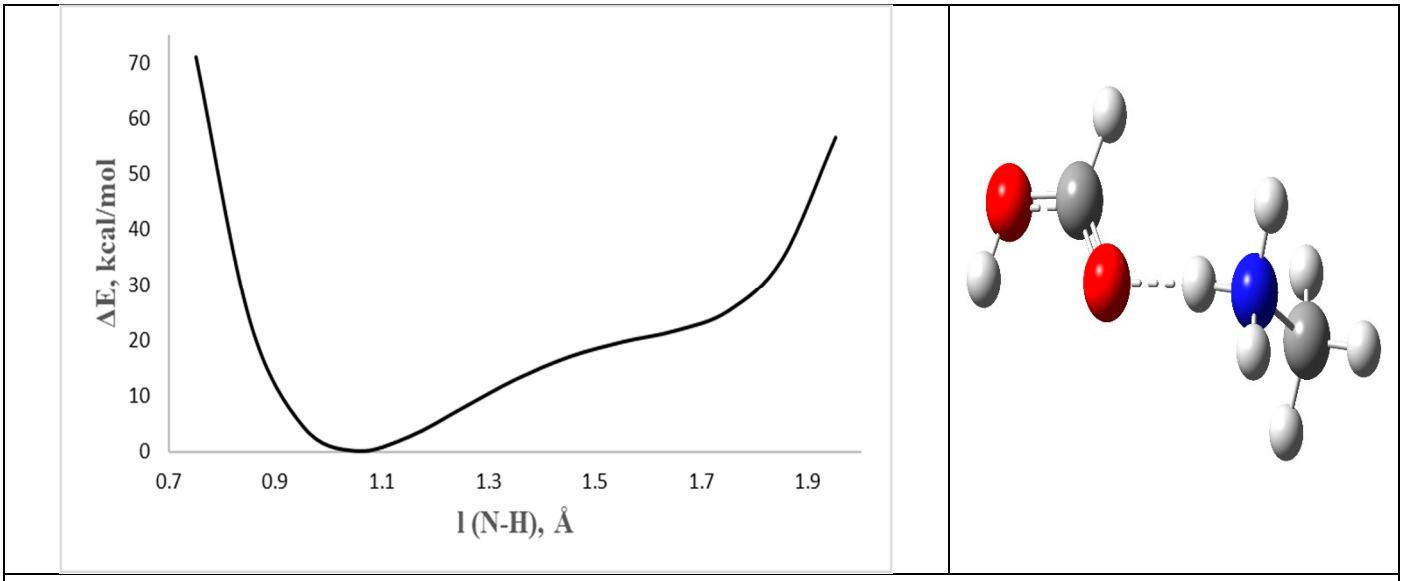
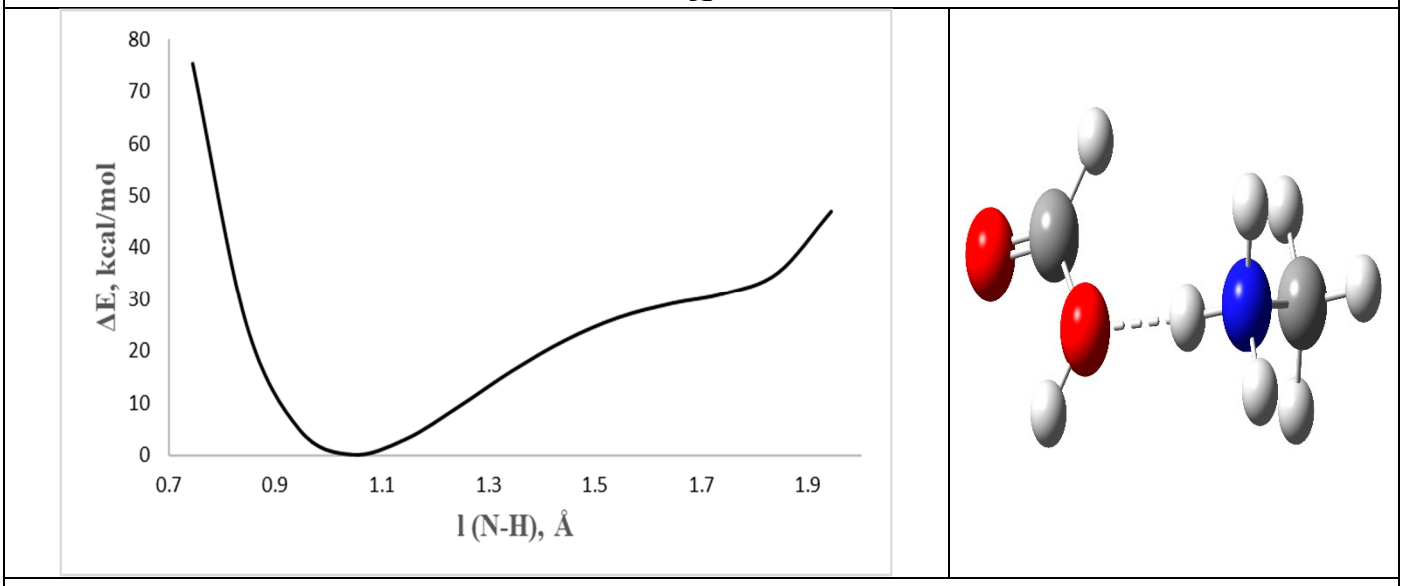


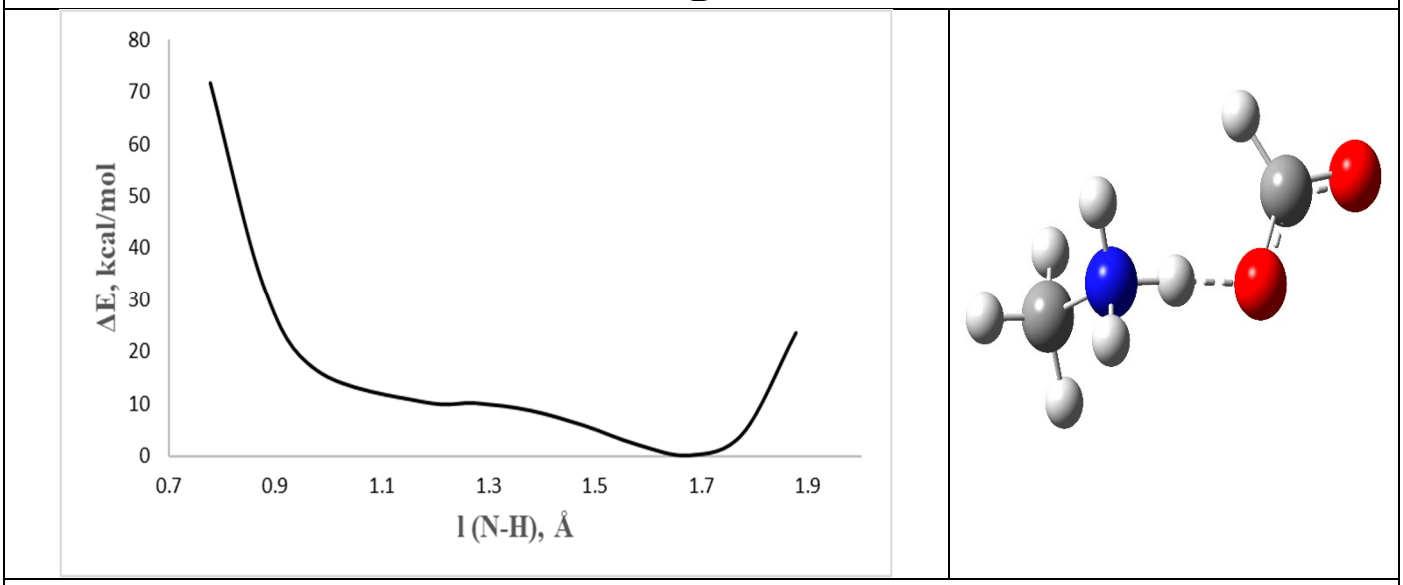
Figure S3. Cont.



A

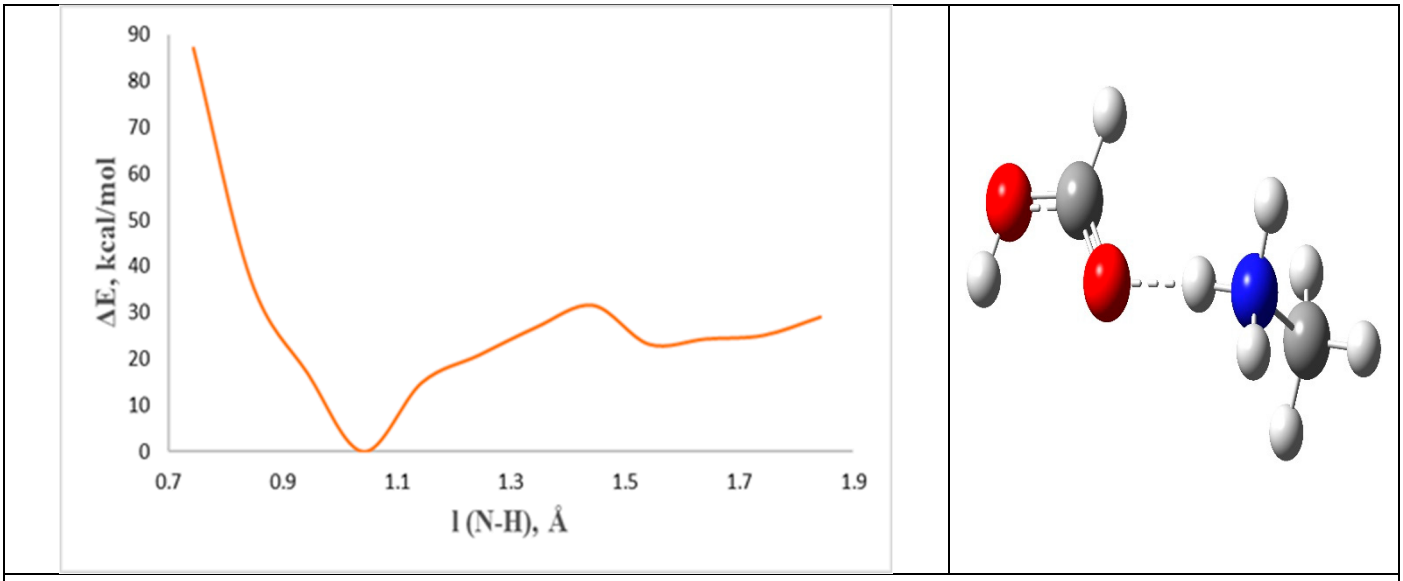


B

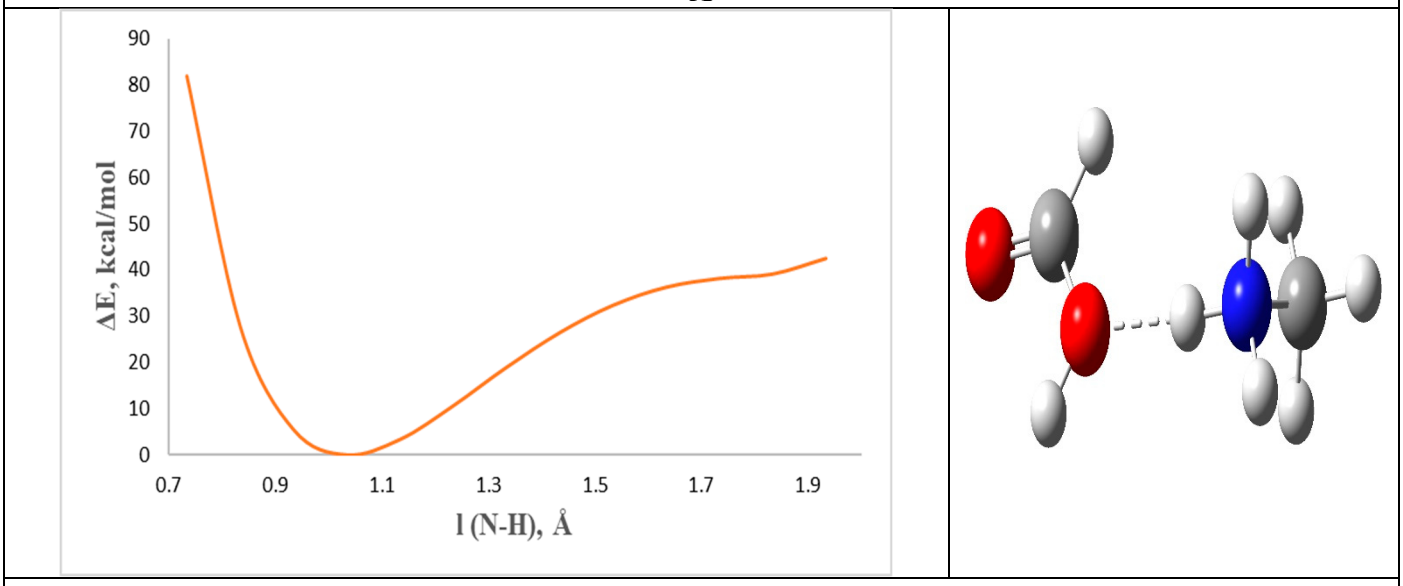


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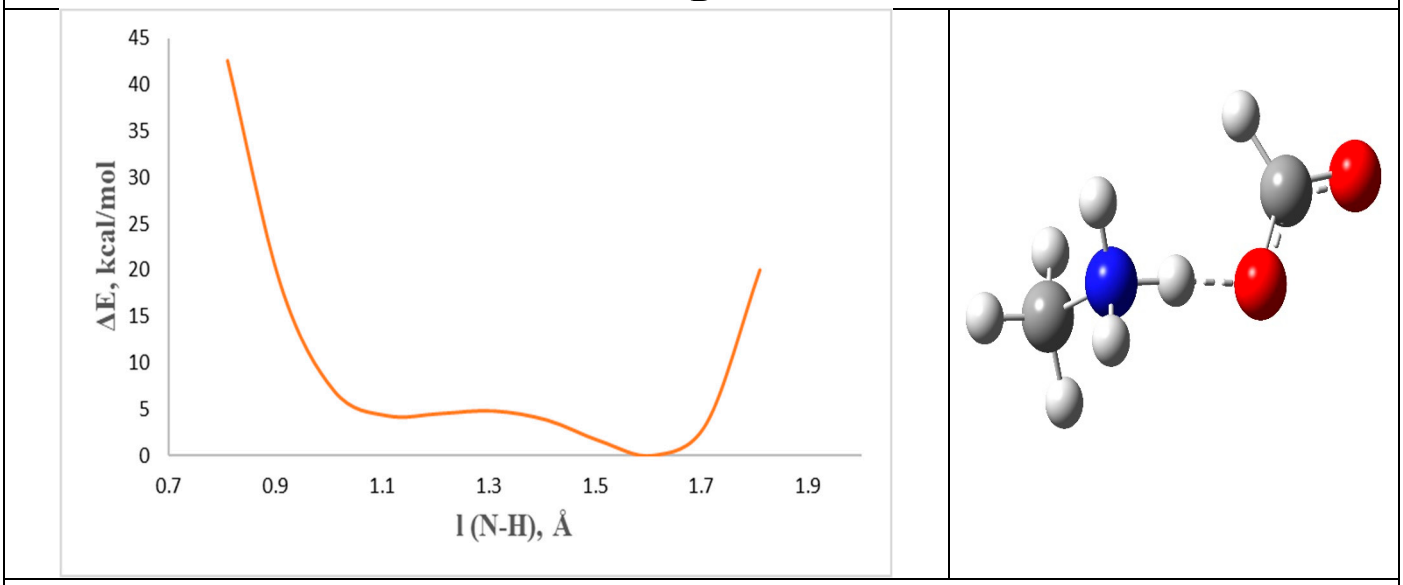
Figure S4. Potential energy curves of model dimers with varying N-H interatomic distance with (A and B) protonated and (C) deprotonated formic acid in the gas phase.



A

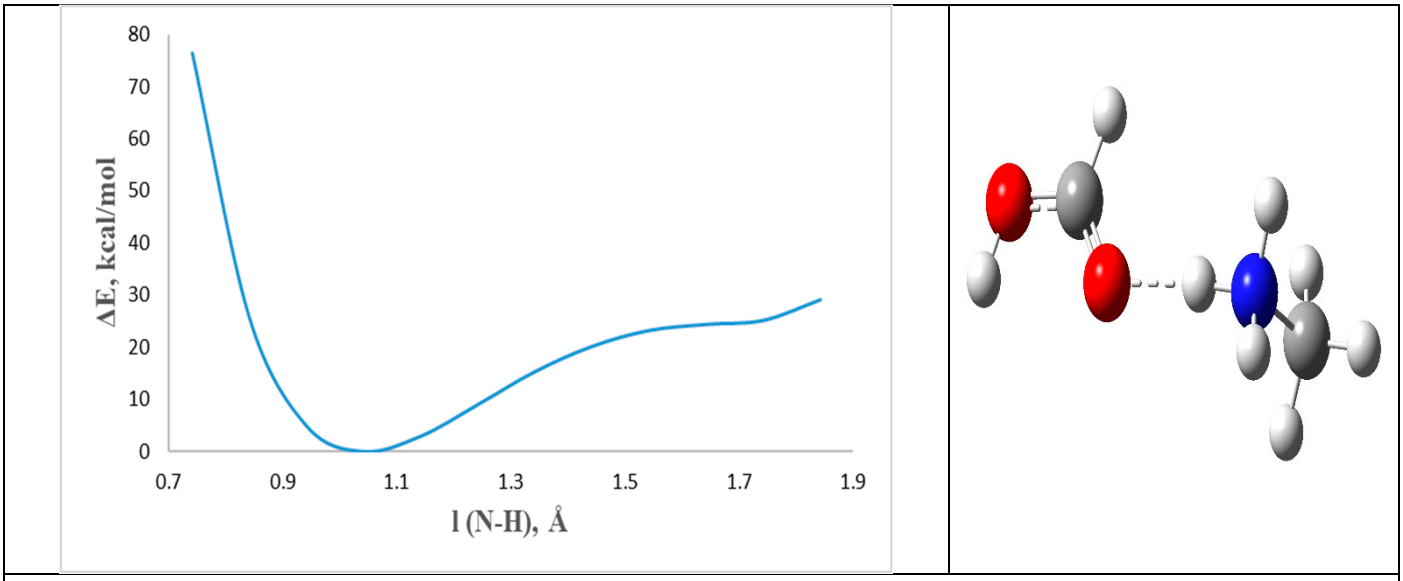


B

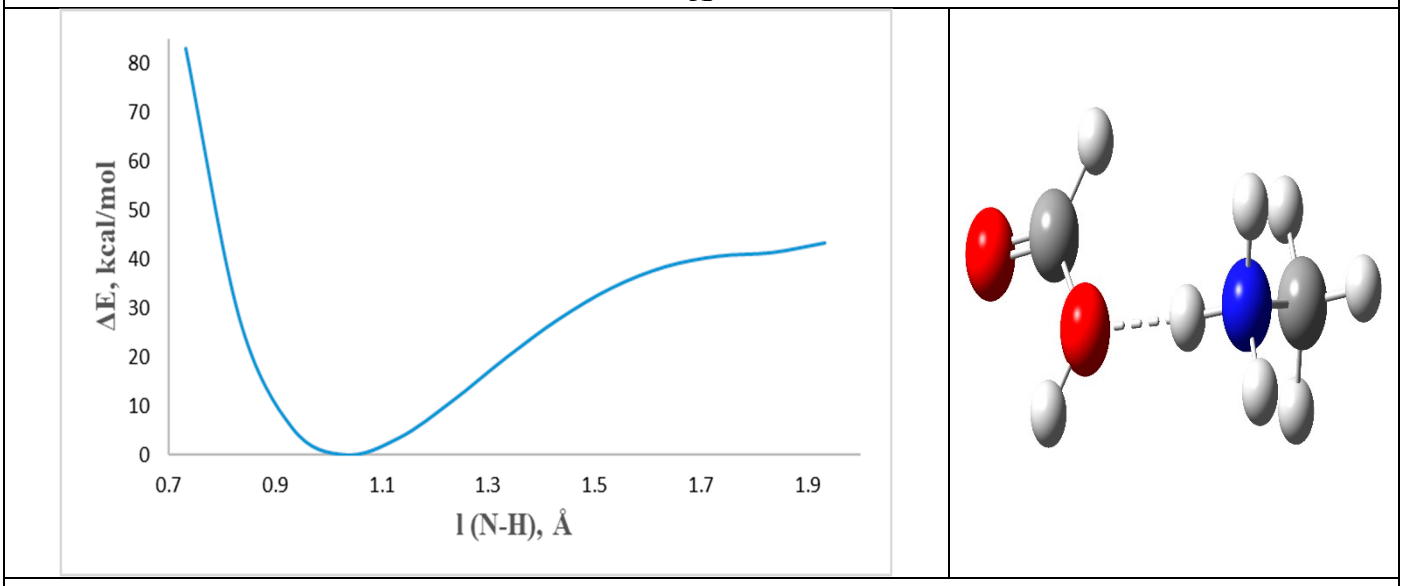


C

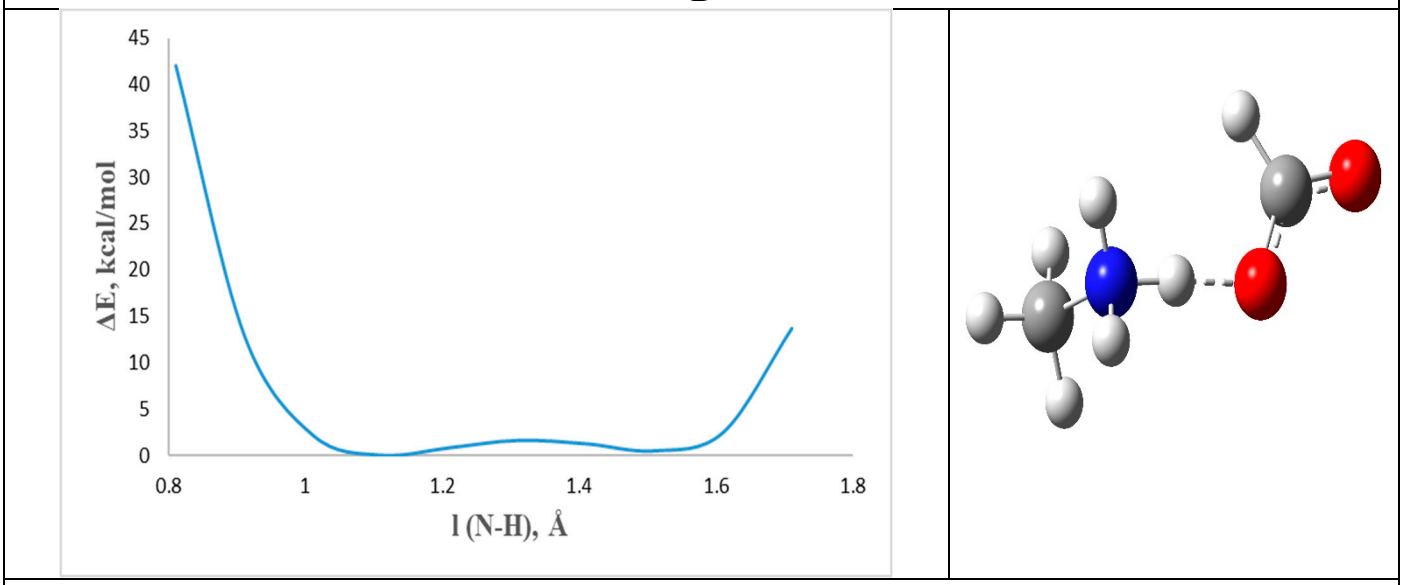
Figure S5. Potential energy curves of model dimers with varying N-H interatomic distance with (A and B) protonated and (C) deprotonated formic acid in chloroform using PCM model.



A



B



C

Figure S6. Potential energy curves of model dimers with varying N-H interatomic distance with (A and B) protonated and (C) deprotonated formic acid in water using PCM model.

Table S1. BSSE-corrected interaction energies (kcal/mol) in complexes of S-cathinone and its derivatives (A-D) with and without discrete water molecule(s) and (5.0) zigzag SWCNT with two "bamboo" units. Label "W" stands for discrete water molecule(s) in the system.

Complex	**E_{BSSE}**	**Complex**	**E_{BSSE}**	**Complex**	**E_{BSSE}**
SWCNT-OH (the same in neutral and acidic pH		**SWCNT-COO^-** (model of neutral healthy tissue pH)		**SWCNT-COOH** (model of acidic cancerous tissue pH)	
A_CO	-11.0556	A_CO-CH	-7.4879	A_Dimer_W	-15.3782
A_NH	-5.6333	A_NH_π_W	-22.8341	A_π_W	-7.1474
A_NH_π	-9.9913	A_NH_W	-23.2044	A_NH_W	-16.4735
B_CO	-11.0684	B_CO-CH	-6.2739	B_CI	-7.6597
C_CO	-10.5607	B_NH_W	-18.6932	B_NH_W	-16.2372
C_F	-3.2792	B_π	-8.8260	B_Dimer_W	-14.5553
C_NH	-5.6249	C_NH_W	-20.2424	C_NH_W	-13.1462
C_NH_π	-6.0032	C_π	-7.4756	C_Dimer_W	-16.9588
C_NH_π2	-10.0124	C_π2_W2	-11.8132	C_π2	-9.4891
C_π	-9.0711			C_F_CO	-5.5671
		D_COC_W	-8.8299	D_COC_W	-11.5632
		D_NH_W2	-16.5568	D_Dimer_W	-16.2812
				D_π	-10.2033