Supporting Information

Cooperativity Effect of the π···π Interaction between Drug and DNA on Intercalative Binding Induced by H-bonds: A QM/QTAIM Investigation of the Curcumin···Adenine···H_2O Model System

Wen-jing Shi [a] , and Fu-de Ren[b]

[a] The Second Hospital of Shanxi Medical University, Taiyuan 030053, China

[b] School of Chemical Engineering and Technology, North University of China, Taiyuan 030051, China

(1) A systematic and comprehensive search for the stable conformations of the curcumin···adenine binary complexes.

(2) A systematic and comprehensive search for the stable conformations of the ternary complexes.

(3) Table S1. Structures, AIM results and intermolecular interaction energies of binary system curcumin···adenine at the M06-2X/6-311++G(2d,p), MP2(full)/6-311++G(2d,p) and B3LYP-D3/6-311++G(2d,p) levels.

(4) Table S2. Structures, AIM results and intermolecular interaction energies of binary system curcumin···H_2O at the M06-2X/6-311++G(2d,p), MP2(full)/6-311++G(2d,p) and B3LYP-D3/6-311++G(2d,p) levels.

(5) Table S3. Structures, AIM results and intermolecular interaction energies of binary system adenine···H_2O at the M06-2X/6-311++G(2d,p), MP2(full)/6-311++G(2d,p) and B3LYP-D3/6-311++G(2d,p) levels.

(6) Fig. S1. AIM results of the binary complexes.

(7) Fig. S2. AIM results of the ternary complexes.

(8) Fig. S3. Plots of the RDG versus the electron density multiplied by the sign of the second Hessian eigenvalue (λ_2) for binary complexes and Low-gradient (s=0.5 a.u.) isosurfaces.

(9) Cartesian orientation of eight optimized ternary systems at the M06-2X/6-311++G(2d,p) level.

(1)

A systematic and comprehensive search for the stable conformations of the curcumin···adenine binary complexes

When the aromatic or heteroaromatic rings of drug slide between the base pairs of DNA, besides the π···π stacking interactions between the drug and DNA, the hydrogen bonds have also been found in experimental and theoretical investigations.[40, 42−45] Therefore, in the simulation of the intercalative binding mode of curcumin with the DNA base pairs, both the π···π stacking and H-bonding interactions were considered. Furthermore, adenine interacts with curcumin by atomic groups that are actually involved in binding to the complementary Thymine. In other words, when the aromatic ring or the C=C bond of curcumin slides between the A-T (adenine-thymine) base pairs, two kinds of stacking, i.e., interaction between the π-electronic moieties of curcumin and adenine as well as that between curcumin and thymine, are in essence both the π···π stacking. Therefore, in the modeling of the intercalative binding mode of curcumin with the A-T base pairs, only the π···π stacking interaction between the ring or C=C bond of curcumin and adenine was considered. Thus, the structures of the curcumin···adenine (marked as "cur···ad") binary complexes were designed according to the possible π···π stacking interactions between the benzene ring or C=C bond of curcumin and two N-containing heterocyclic rings of adenine, as well as the H-bonding interactions between the O=C–, –OH, –O–, –CH groups of curcumin and the $–NH_2$ (or –NH–), nitrogen atom with lone pair electrons of adenine. More than 50 predicted structures were optimized at the HF/6-311G** level. Most of the cur···ad binary complexes, in which the π···π or H-bonded distances are too large, were deleted. Then, the selected HF/6-311G** structures were re-optimized at the M06-

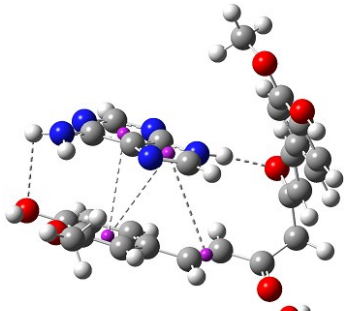
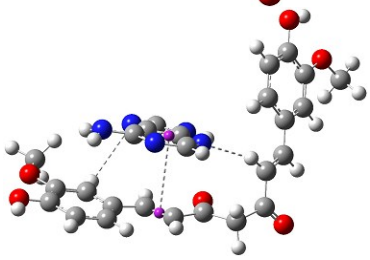
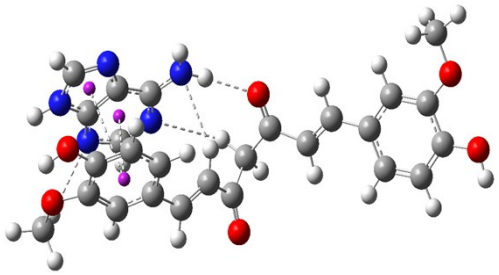
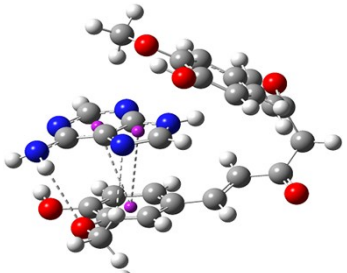
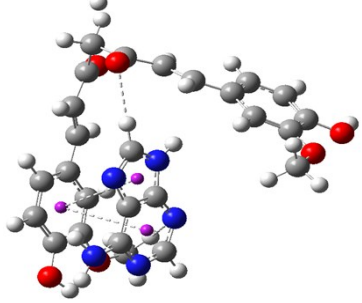
2X/6-311++G(2d,p) level. Finally, seven stable conformations (Nimag=0), i.e., A~G (see Table S1), were confirmed to depict the stronger π···π and H-bonding intermolecular interactions at the M06-2X/6-311++G(2d,p) level. It is worth mentioning that, although many of the cur···ad binary complexes were formed by the strong N–H···O=C, C–H···O=C, C–H···N, and T-shape N–H···π, O–H···π or C–H···π H-bonds with the intermolecular interactions of more than 30.0 kJ/mol, due to none of the π···π interactions or very weak π···π interactions, they were not considered in this work. As mentioned above, one of the aims in this work is to investigate the cooperativity effect involving the π···π stacking interaction in the intercalative mode.

(2)

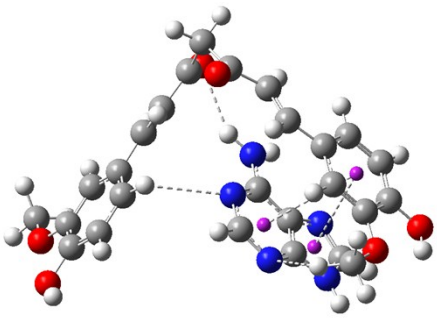
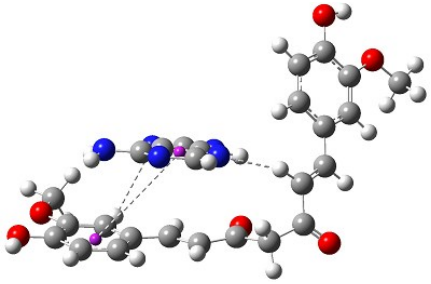
A systematic and comprehensive search for the stable conformations of the ternary complexes

In the conformational search, the cur···ad···H_2O ternary complex was regarded as the initial formation of the cur···ad complex followed by addition of H_2O, and the H and O atoms of H_2O pointed towards the electron-rich and electron-deficient atoms or groups of the cur···ad complex, respectively. Thus, except for the intermolecular links mentioned above in the cur···ad complex, the intermolecular H···π and conventional H-bonding interactions involving the –OH group of H_2O, such as O–H···O–H, O–H···O=C, N–H···O–H, C–H···O–H, O–H···N, etc., were also considered. More than 100 designed ternary conformations were optimized at HF/6-31G** level, then at the M06-2X/6-311++G(2d,p) level, some selected HF/6-31G** conformations were optimized and finally eight stable cur···ad···H_2O complexes (NImag=0) with the strong π···π stacking interactions were confirmed and discussed in the following section.

Table S1. Structures (Å), AIM results (a.u.) and intermolecular interaction energies ($E_{int.}$, kJ/mol) of binary system curcumin···adenine at the M06-2X/6-311++G(2d,p) (in plain), MP2(full)/6-311++G(2d,p) (in bold) and B3LYP-D3/6-311++G(2d,p) (in italic) levels.

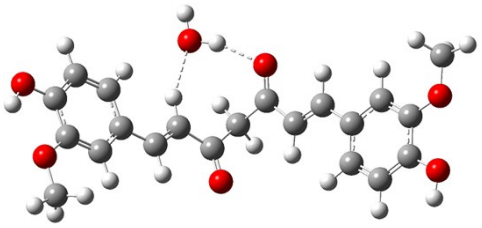
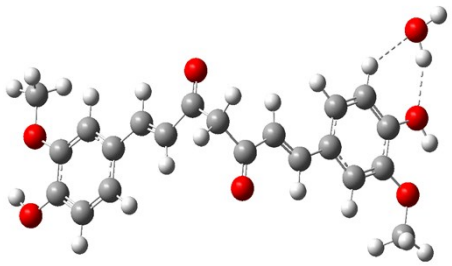
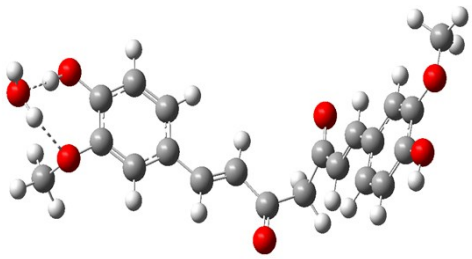
	Structures	Geometric parameters and AIM results	$E_{int.}$[a]
A		$R_{N–H···O=C}$=2.005Å, $R_{N–H···O-H}$= 2.844Å, R_{2-5}=3.808Å, R_{6-5}=3.486Å, R_{6-6}=3.435Å $\rho_{N–H···O=C}$=0.0196 a.u., $\rho_{N–H···O-H}$= 0.0069 a.u., ρ_{2-5}= 0.0048 a.u., ρ_{6-5}= 0.0049 a.u., ρ_{6-6}= 0.0047 a.u. $\nabla^2\rho_{N–H···O=C}$= 0.0793 a.u., $\nabla^2\rho_{N–H···O-H}$= 0.0229 a.u., $\nabla^2\rho_{2-5}$= 0.0192 a.u., $\nabla^2\rho_{6-5}$= 0.0183 a.u., $\nabla^2\rho_{6-6}$= 0.0179 a.u.	–64.5 (–55.3) **–72.7** **(–65.6)** *–62.3*
B		$R_{C–H···N}$= 2.870Å, $R_{C=C–H···N}$= 2.351Å, R_{2-6}=3.813 Å $\rho_{C–H···N}$= 0.0063a.u., $\rho_{C=C–H···N}$=0.0137a.u., ρ_{2-6}=0.0018a.u. $\nabla^2\rho_{C–H···N}$= 0.0187 a.u., $\nabla^2\rho_{C=C–H···N}$=0.0429 a.u., $\nabla^2\rho_{2-6}$=0.0076 a.u.	–64.0 (–56.2) **–69.8** **(–58.0)**
C		$R_{N–H···O=C}$=2.034 Å, $R_{C–H···N}$=2.812 Å, $R_{C=C–H···N}$=2.645 Å, $R_{O-C–H···N}$=2.766 Å R_{6-5}=3.360 Å, R_{6-6}=3.467 Å $\rho_{N–H···O=C}$=0.0192a.u., $\rho_{C–H···N}$=0.0064a.u., $\rho_{C=C–H···N}$=0.0081 a.u., $\rho_{O-C–H···N}$=0.0065 a.u. ρ_{6-5}=0.0045 a.u., ρ_{6-6}=0.0039 a.u. $\nabla^2\rho_{N–H···O=C}$=0.0766 a.u., $\nabla^2\rho_{C–H···N}$=0.0162 a.u., $\nabla^2\rho_{C=C–H···N}$=0.0244 a.u., $\nabla^2\rho_{O-C–H···N}$=0.0170 a.u. $\nabla^2\rho_{6-5}$=0.0159a.u., $\nabla^2\rho_{6-6}$=0.0147 a.u.	–57.1 (–48.6) **–56.0** **(–49.0)** *–54.0*
D		$R_{C–H···N}$=2.757 Å, $R_{N–H···O}$=2.693 Å, R_{6-5}=3.407Å, R_{6-6}=3.335Å $\rho_{C–H···N}$=0.0067 a.u., $\rho_{N–H···O}$=0.0071 a.u., ρ_{6-5}=0.0050 a.u., ρ_{6-6}=0.0046 a.u. $\nabla^2\rho_{C–H···N}$=0.0179 a.u., $\nabla^2\rho_{N–H···O}$=0.0234 a.u., $\nabla^2\rho_{6-5}$=0.0199 a.u., $\nabla^2\rho_{6-6}$=0.0166 a.u.	–70.5 (–58.3) **–79.2** **(–67.5)**
E		$R_{C–H···O=C}$= 2.356Å, R_{6-5}=3.502Å, R_{6-6}=3.341Å $\rho_{C–H···O=C}$=0.0107 a.u., ρ_{6-5}=0.0043 a.u., ρ_{6-6}=0.0047 a.u. $\nabla^2\rho_{C–H···O=C}$=0.0365 a.u., $\nabla^2\rho_{6-5}$=0.0169a.u., $\nabla^2\rho_{6-6}$=0.0170a.u.	–69.9 (–51.8) **–78.0** **(–63.6)** *–75.2*

(Continued)

F		$R_{N–H···O=C}$=2.297Å, $R_{O-C–H···N}$=2.655Å, $R_{C–H···N}$=2.90948Å R_{6-5}=3.340Å, R_{6-6}=3.407Å $\rho_{N–H···O=C}$=0.0116 a.u., $\rho_{O-C–H···N}$ =0.0079 a.u., $\rho_{C–H···N}$=0.0058 a.u. ρ_{6-5}=0.0050 a.u., ρ_{6-6}=0.0050 a.u. $\nabla^2\rho_{N–H···O=C}$=0.0433 a.u., $\nabla^2\rho_{O-C–H···N}$ =0.0215 a.u., $\nabla^2\rho_{C–H···N}$=0.0175 a.u. $\nabla^2\rho_{6-5}$=0.0185 a.u., $\nabla^2\rho_{6-6}$=0.0191 a.u.	–63.1 (–54.9) **–72.3** **(–61.8)** *–62.6*
G		$R_{C–H···N}$= 2.869Å, $R_{C=C–H···N}$= 2.352Å, R_{6-6}=3.623 Å $\rho_{C–H···N}$=0.0064 a.u., $\rho_{C=C–H···N}$= 0.0136 a.u., ρ_{6-6}=0.0052 a.u. $\nabla^2\rho_{C–H···N}$= 0.0187 a.u., $\nabla^2\rho_{C=C–H···N}$= 0.0428 a.u., $\nabla^2\rho_{6-6}$=0.0103 a.u.	–64.0 (–53.2) **–65.1** **(–50.2)** *–63.7*

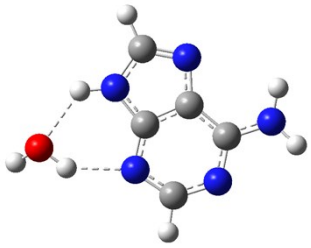
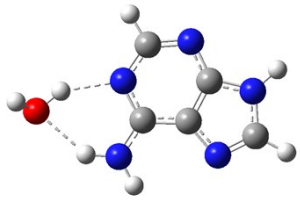
[a] The values in parenthesis are corrected for BSSE.

Table S2. Structures (Å), AIM results (a.u.) and intermolecular interaction energies ($E_{int.}$, kJ/mol) of binary system curcumin···H_2O at the M06-2X/6-311++G(2d,p) (in plain), MP2(full)/6-311++G(2d,p) (in bold) and B3LYP-D3/6-311++G(2d,p) (in italic) levels.

	Structures	Geometric parameters and AIM results	$E_{int.}$[a]
Ⅰ		$R_{C-H\cdots O}$=2.279Å, $R_{O-H\cdots O}$=1.88Å $\rho_{C-H\cdots O}$=0.0124 a.u., $\rho_{O-H\cdots O}$=0.0271 a.u. $\nabla^2\rho_{C-H\cdots O}$=0.0441 a.u., $\nabla^2\rho_{O-H\cdots O}$=0.1071 a.u.	–41.5 (–36.2) **–48.3** **(–36.7)** *–43.7*
Ⅱ		$R_{O-H\cdots O}$=2.008Å, $R_{C-H\cdots O}$=2.420Å $\rho_{O-H\cdots O}$=0.0191 a.u., $\rho_{C-H\cdots O}$=0.0102 a.u. $\nabla^2\rho_{O-H\cdots O}$=0.0817 a.u., $\nabla^2\rho_{C-H\cdots O}$=0.0346 a.u.	–40.5 (–37.0) **–45.2** **(–40.6)** *–40.8*
Ⅲ		$R_{O-H\cdots O(H2O)}$= 1.821 Å, $R_{(H2O)O-H\cdots O}$=2.016 Å $\rho_{O-H\cdots O(H2O)}$= 0.0312 a.u., $\rho_{(H2O)O-H\cdots O}$=0.0224 a.u. $\nabla^2\rho_{O-H\cdots O(H2O)}$= 0.1166 a.u., $\nabla^2\rho_{(H2O)O-H\cdots O}$=0.0917 a.u.	–30.6 (–28.5) **–33.1** **(–28.7)** *–30.0*

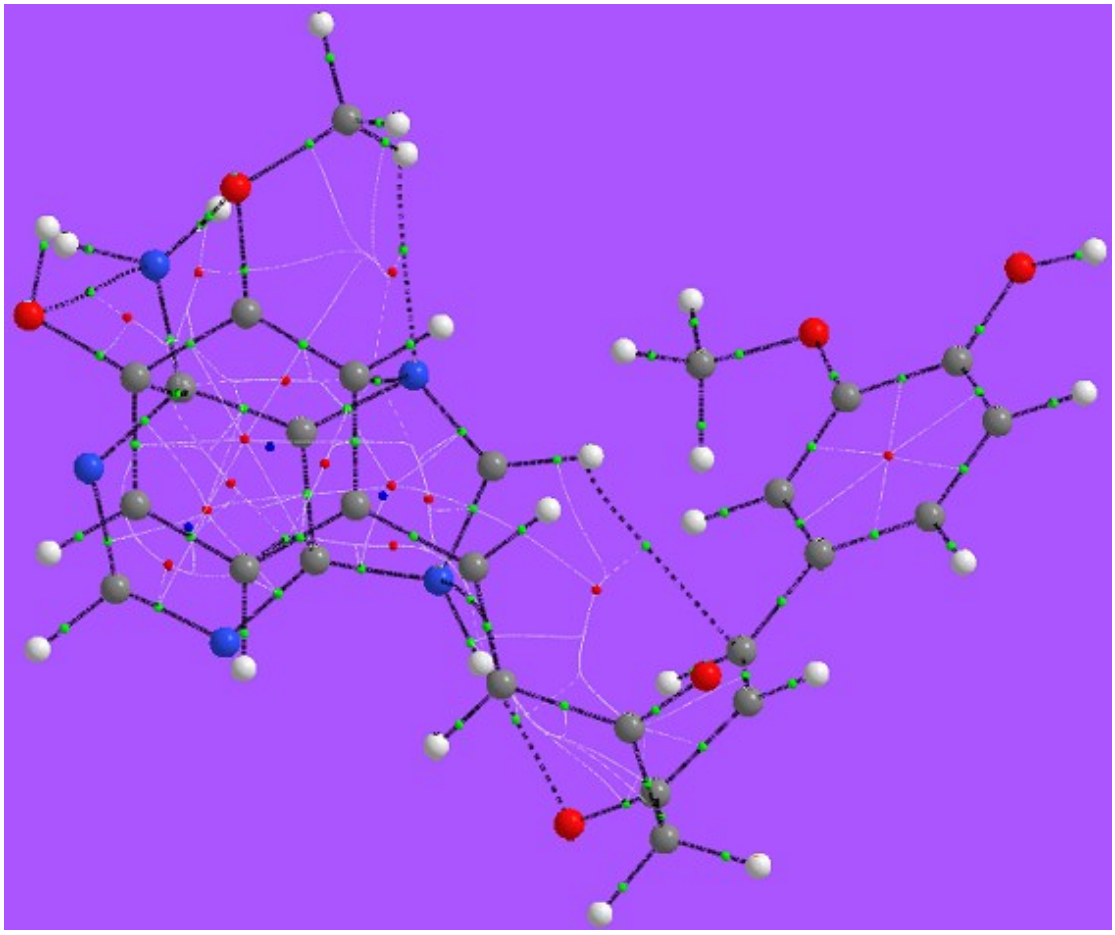
[a] The values in parenthesis are corrected for BSSE.

Table S3. Structures (Å), AIM results (a.u.) and intermolecular interaction energies ($E_{int.}$, kJ/mol) of binary system adenine···H_2O at the M06-2X/6-311++G(2d,p) (in plain), MP2(full)/6-311++G(2d,p) (in bold) and B3LYP-D3/6-311++G(2d,p) (in italic) levels.

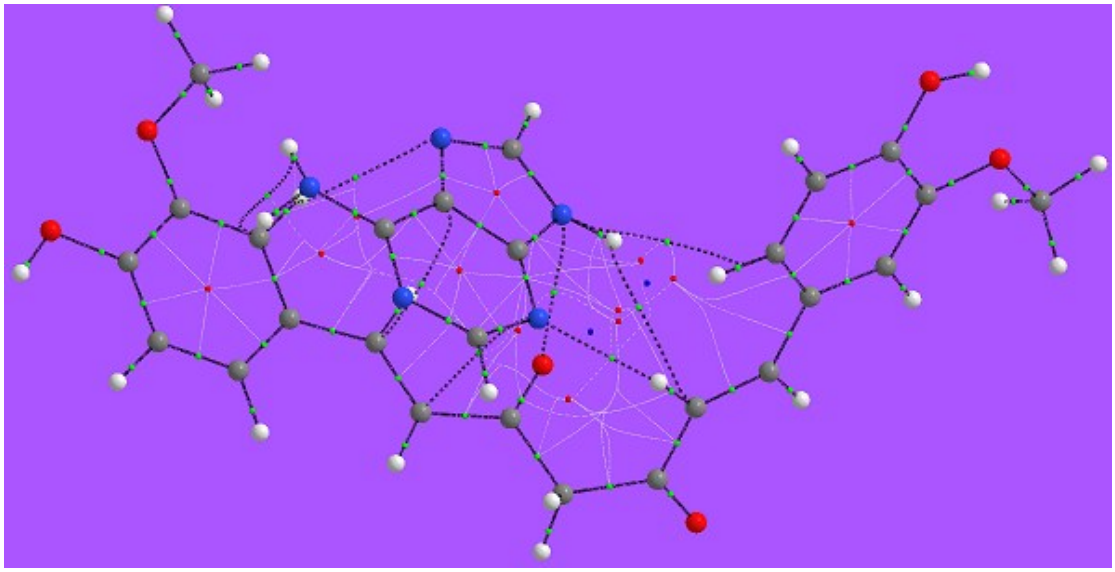
	Structures	Geometric parameters and AIM results	$E_{int.}$[a]
a		$R_{N-H\cdots O}$=2.025Å, $R_{O-H\cdots N}$=1.977Å $\rho_{N-H\cdots O}$=0.0210 a.u., $\rho_{O-H\cdots N}$=0.0260 a.u. $\nabla^2\rho_{N-H\cdots O}$=0.0869 a.u., $\nabla^2\rho_{O-H\cdots N}$=0.0907 a.u.	–50.9 (–46.2) **–54.7 (–48.6)** *–51.6*
b		$R_{N-H\cdots O}$=2.027Å, $R_{O-H\cdots N}$=1.944Å $\rho_{N-H\cdots O}$=0.0205 a.u., $\rho_{O-H\cdots N}$=0.0290 a.u. $\nabla^2\rho_{N-H\cdots O}$=0.0835 a.u., $\nabla^2\rho_{O-H\cdots N}$=0.0936 a.u.	–44.5 (–39.5) **–47.3 (–40.2)** *–46.8*

[a] The values in parenthesis are corrected for BSSE.

(6)

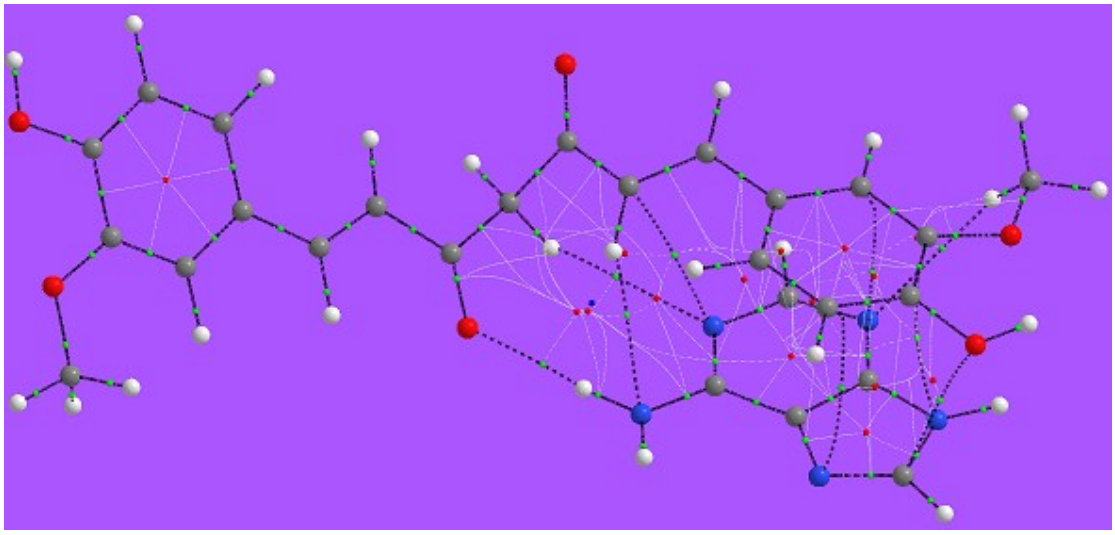


A

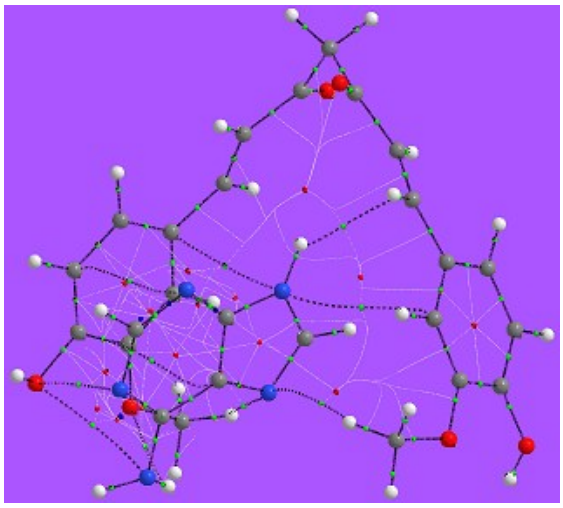


B

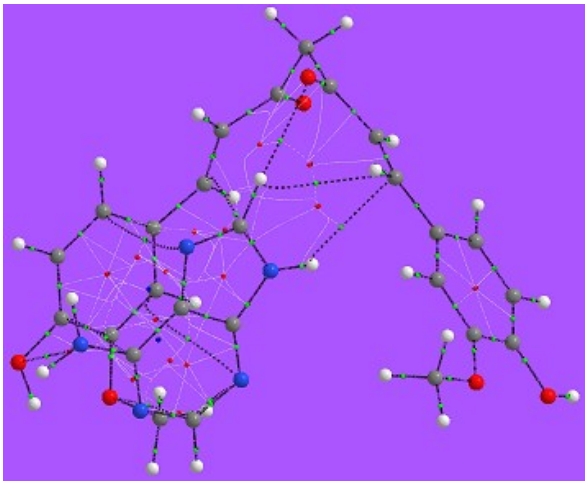
(Continued)



C

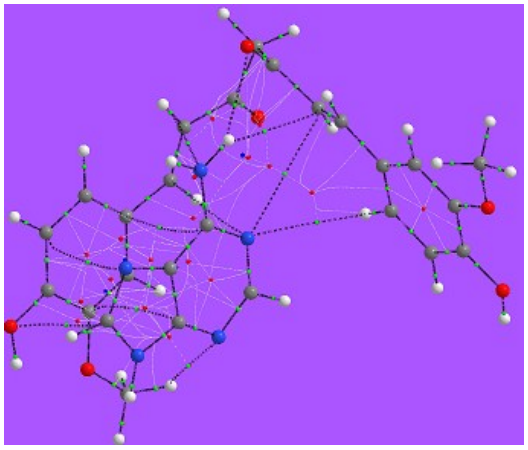


D

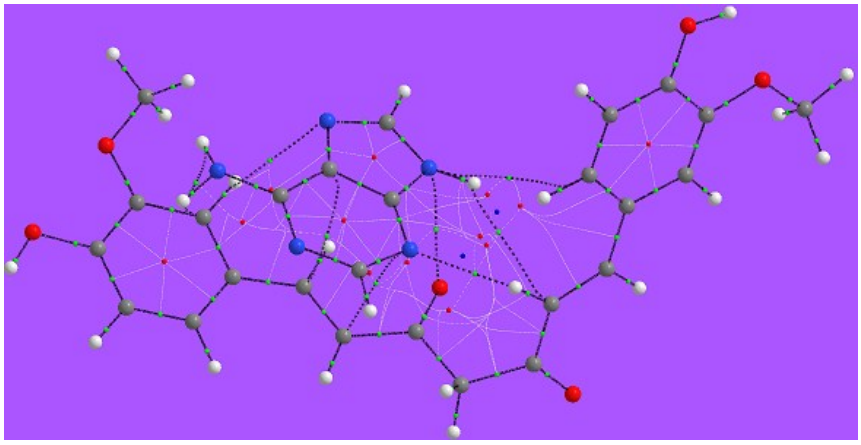


E

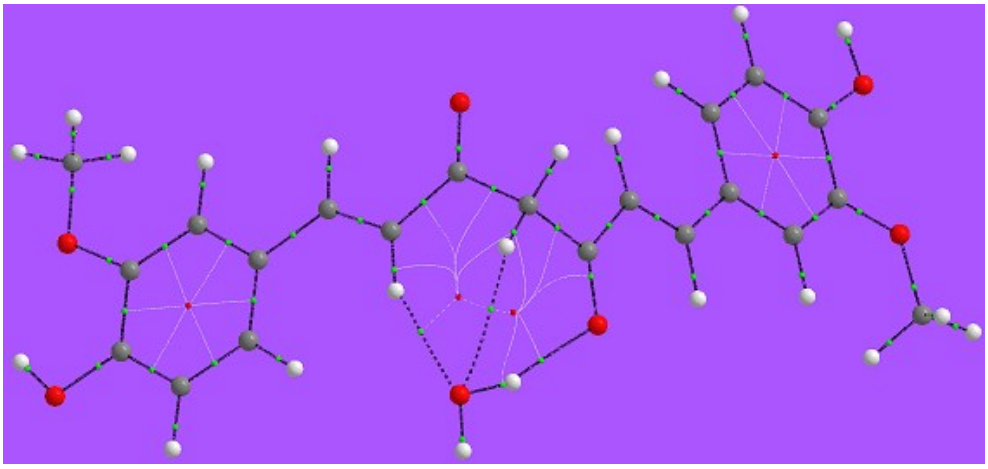
(Continued)



F

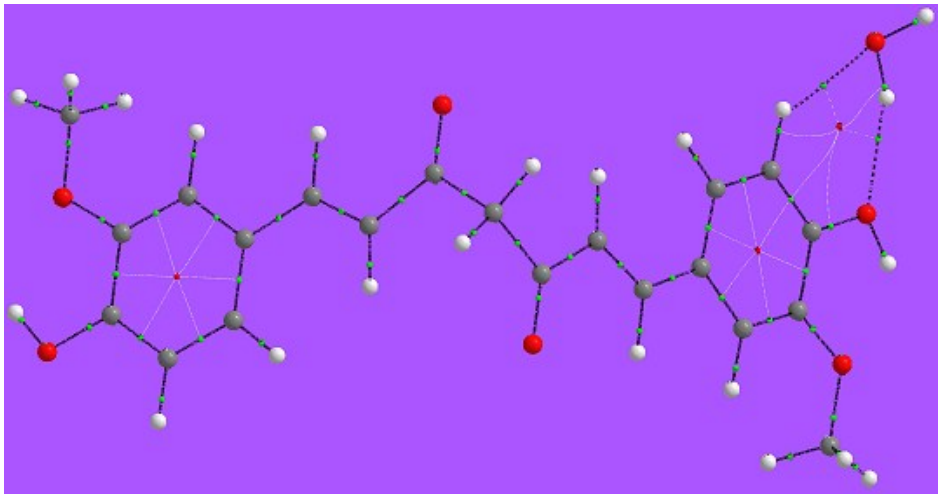


G

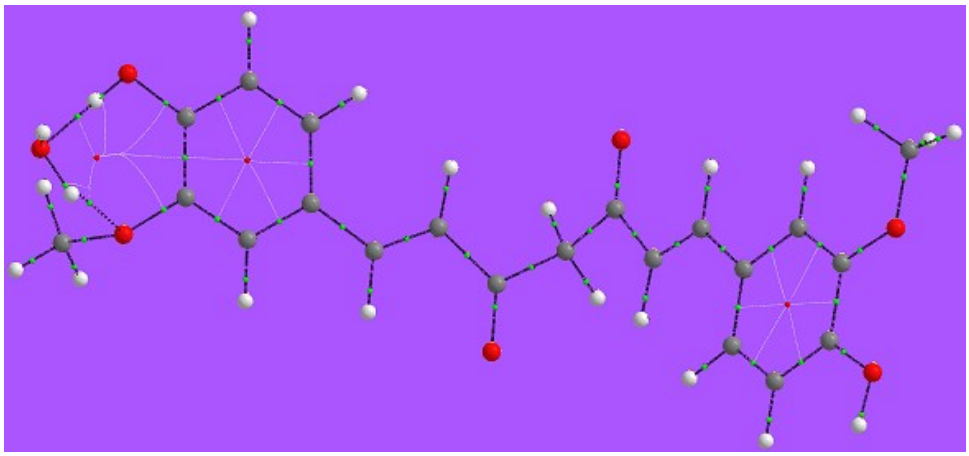


I

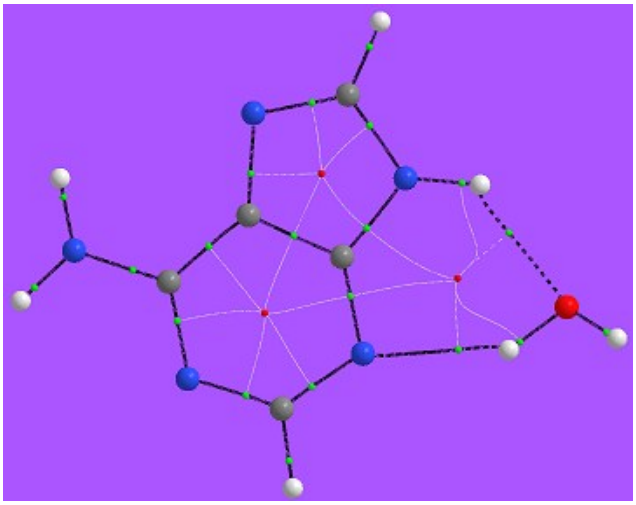
(Continued)



Ⅱ

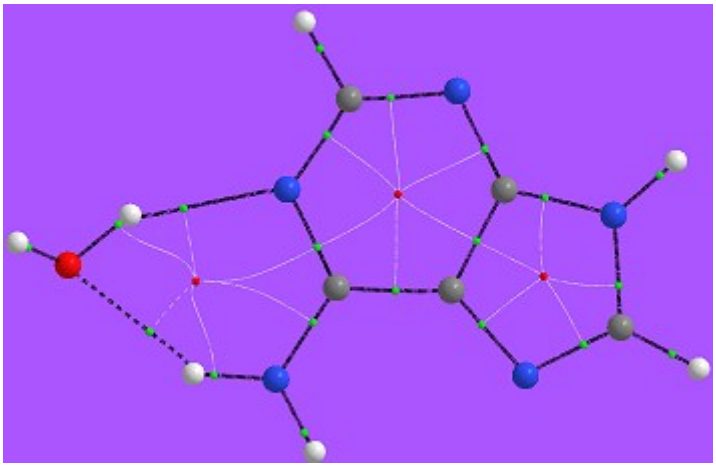


Ⅲ



a

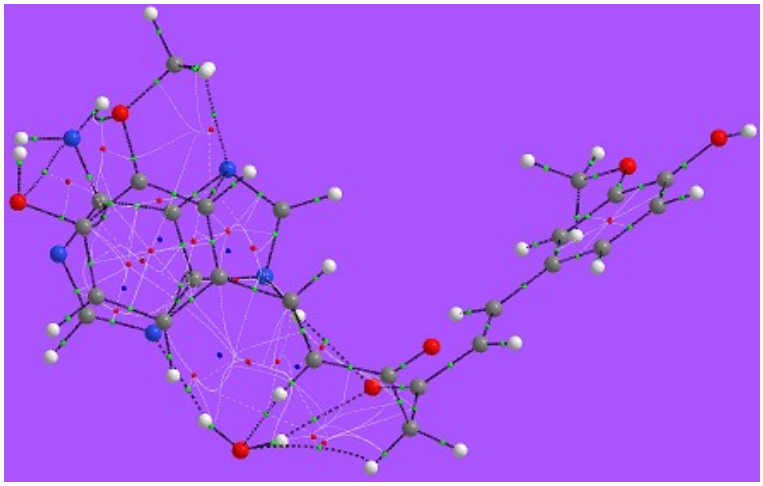
(Continued)



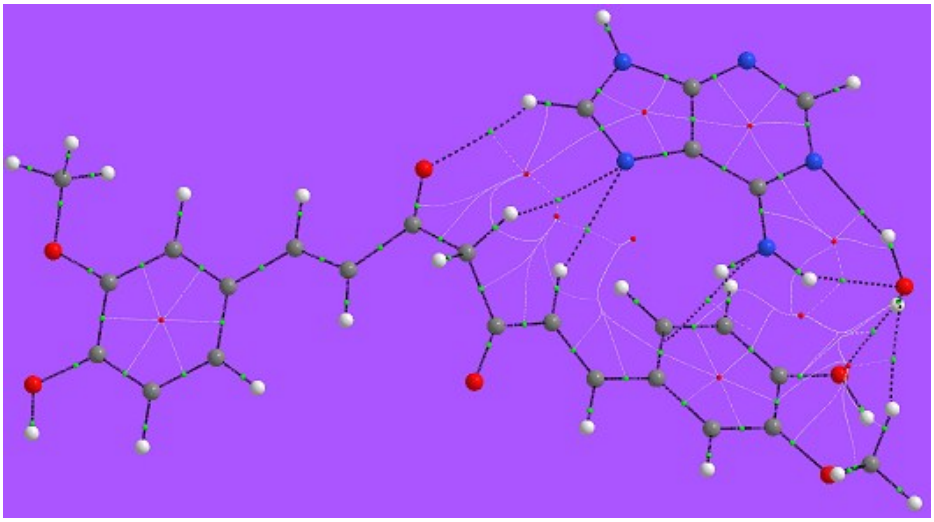
b

Fig. S1. AIM results of the binary complexes.

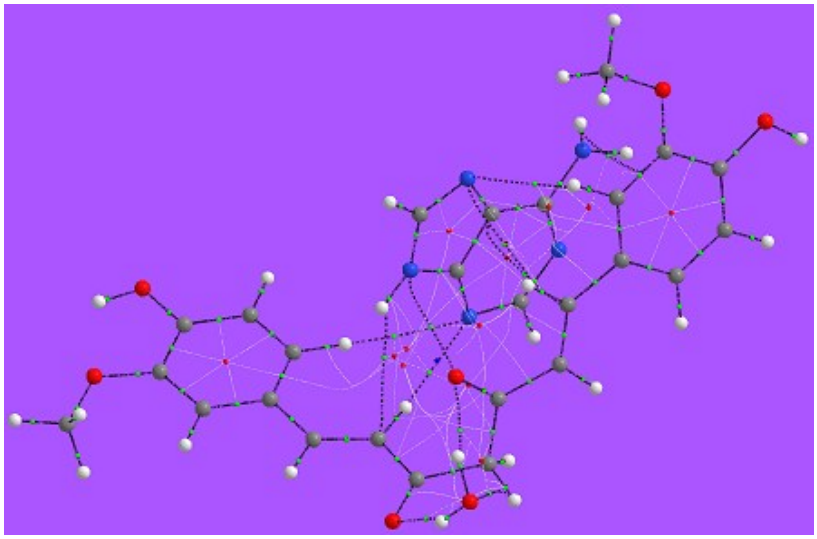
(7)



A-1

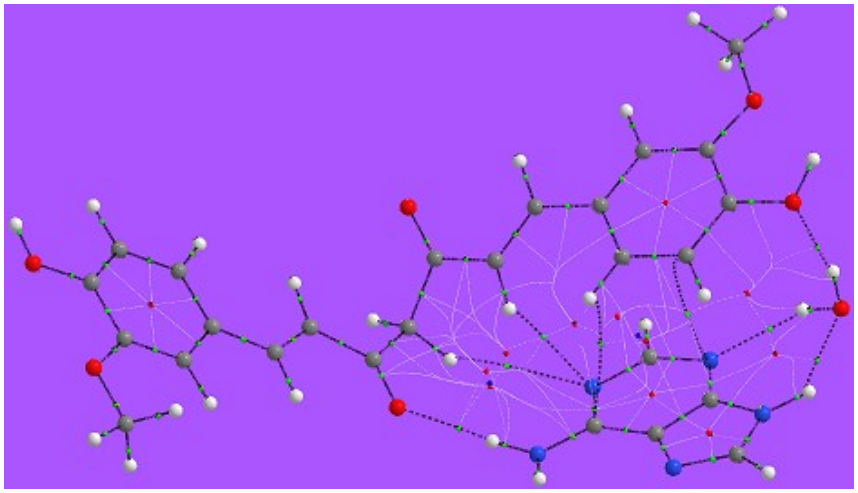


A-2

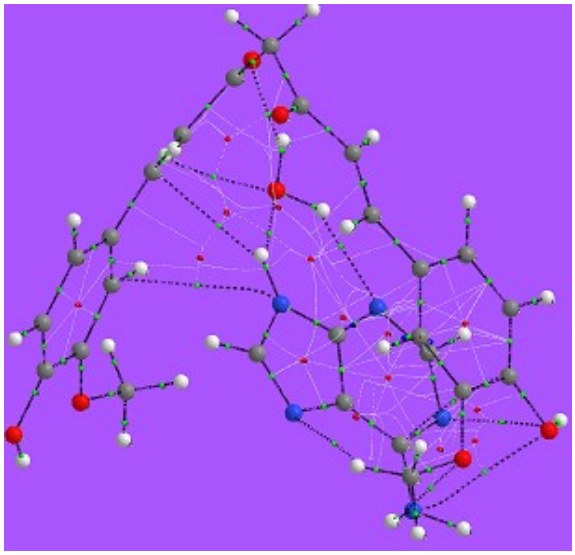


B-1

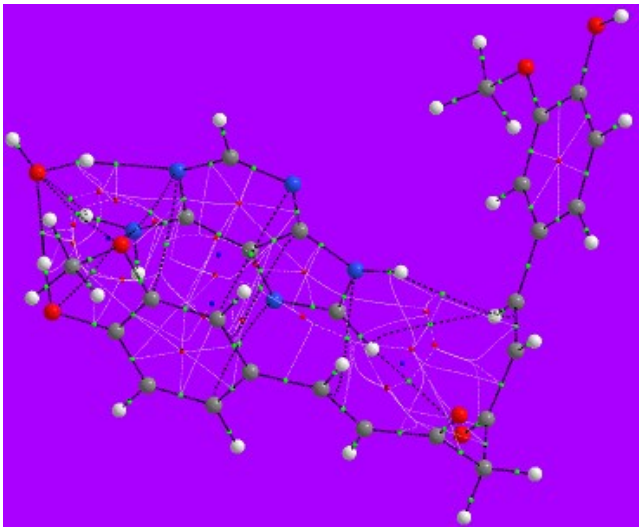
(continued)



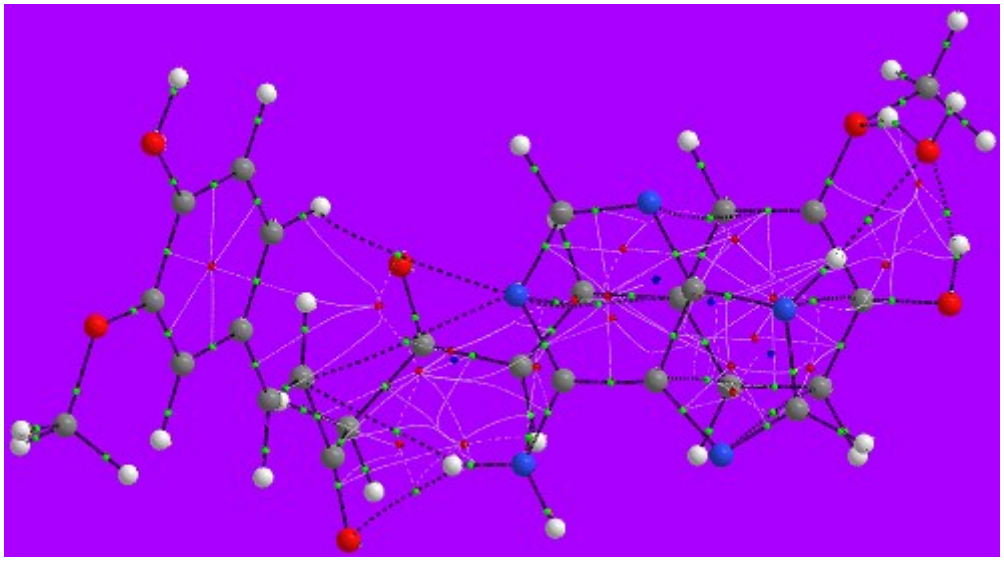
C-1



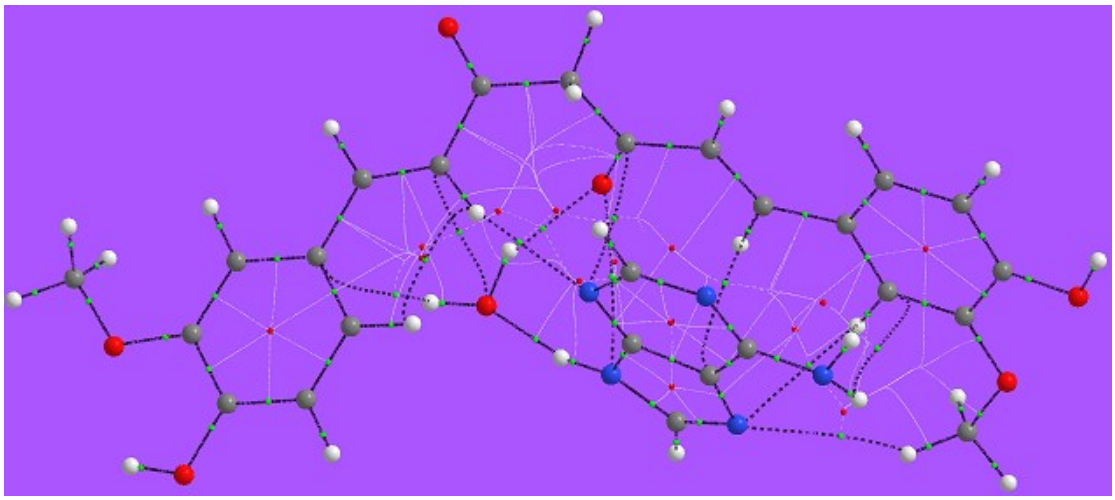
D-1



E-1
(continued)



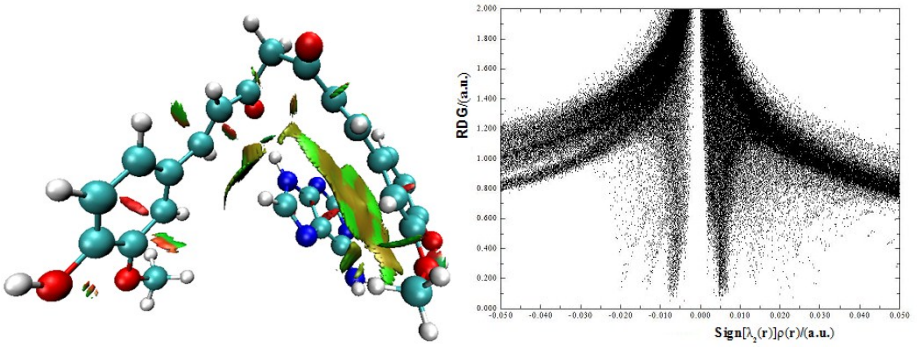
F-1



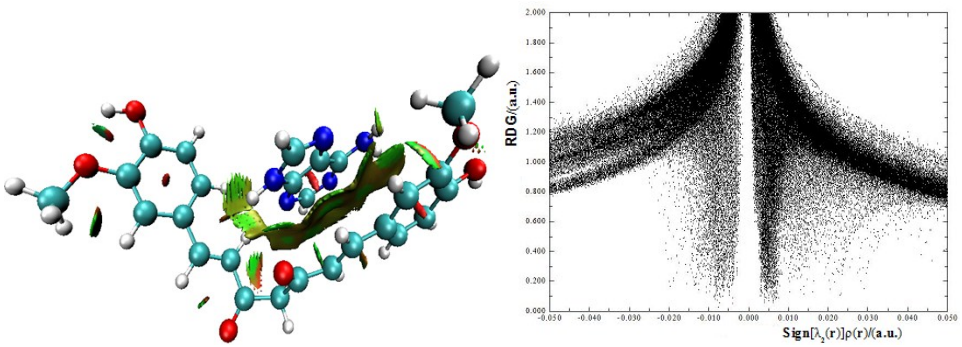
G-1

Fig. S2. AIM results of the ternary complexes

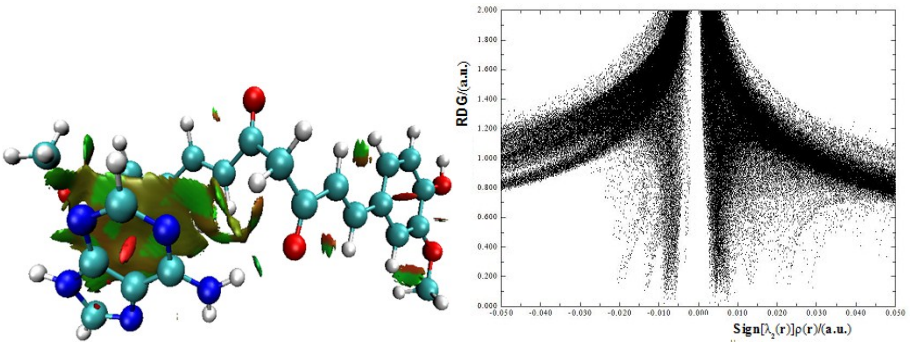
(8)



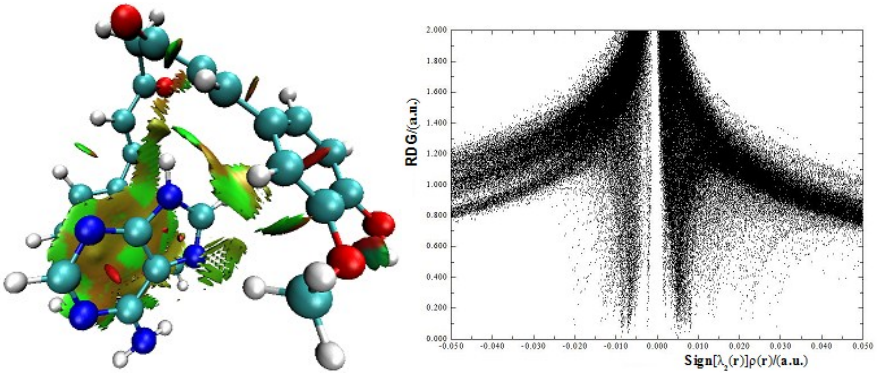
A



B

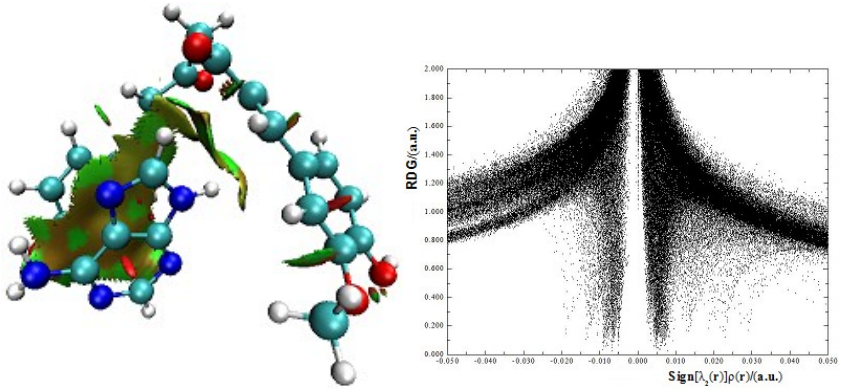


C

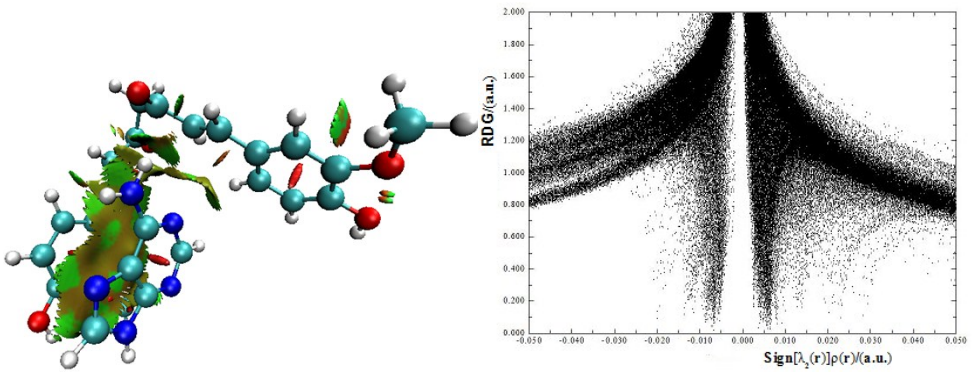


D

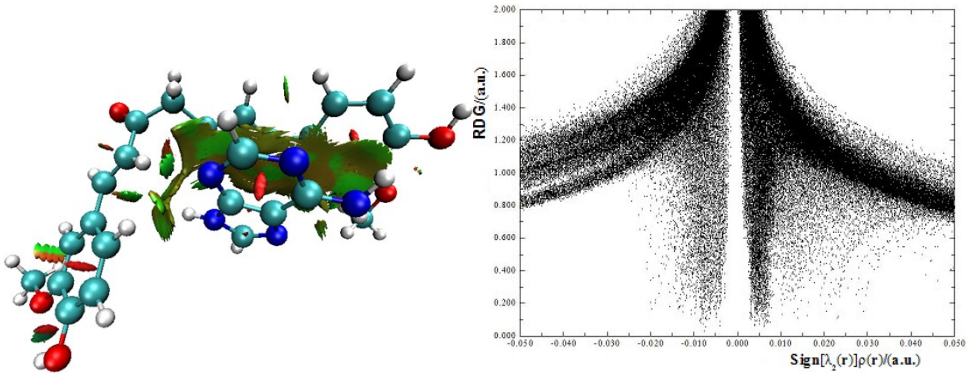
(Continued)



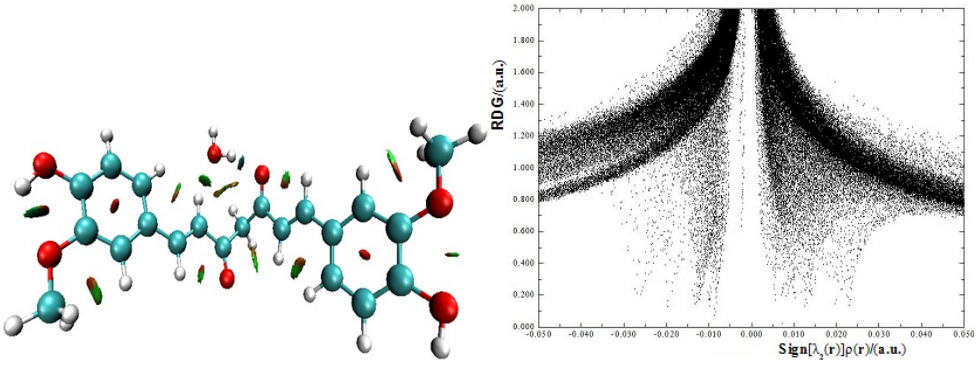
E



F

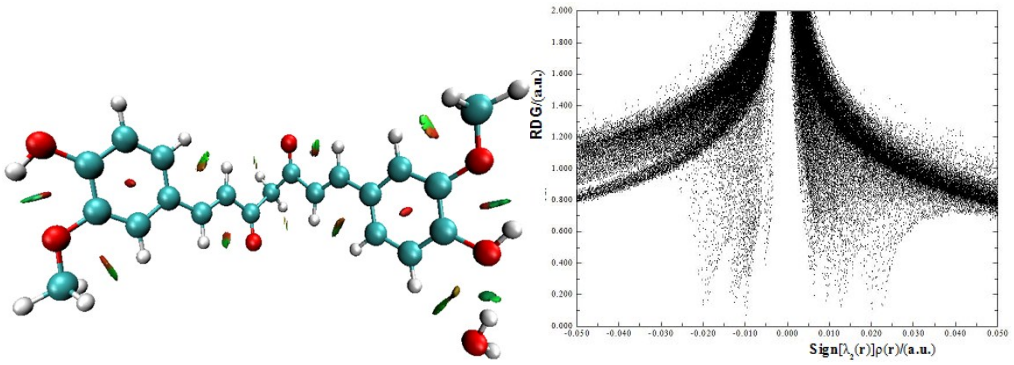


G

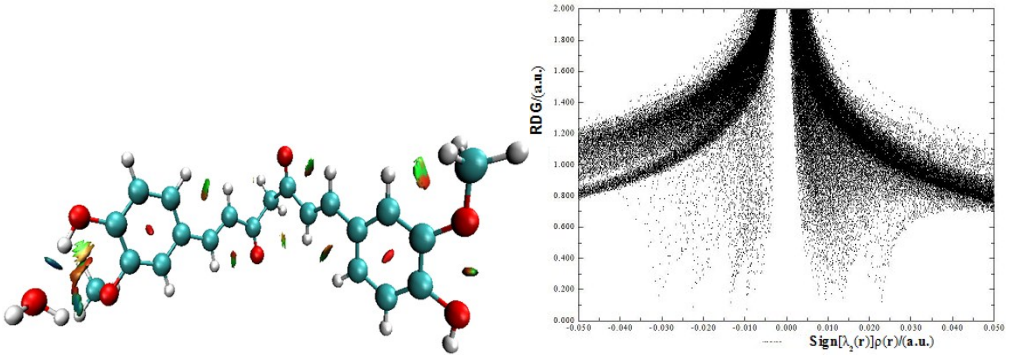


I

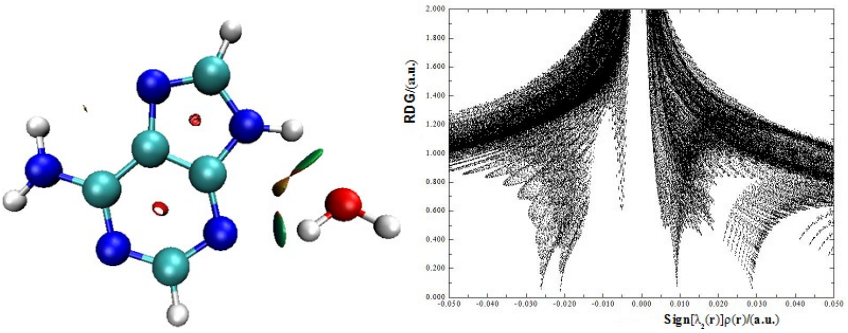
(Continued)



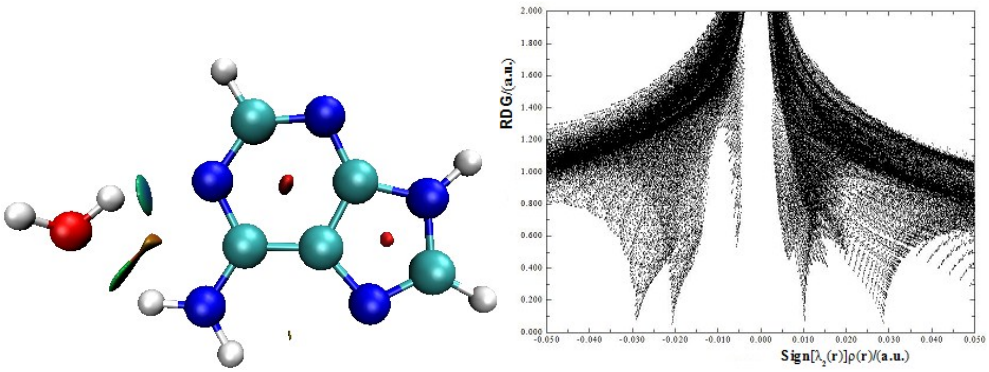
Ⅱ



Ⅲ



a



c

Fig. S3. Plots of the RDG versus the electron density multiplied by the sign of the second Hessian eigenvalue (λ_2) for binary complexes and Low-gradient (s=0.5 a.u.) isosurfaces. The surfaces are colored on a green-brown-red scale according to values of sign(λ_2)ρ. Green indicates

strong attractive interaction, brown indicates weak attractive interaction or vdW interaction, and red indicates steric effect.

Cartesian orientation of eight optimized ternary systems at the M06-2X/6-311++G(2d,p) level.

(A-1)

6	0	2.468303	-1.514156	-0.988034
6	0	1.975655	-0.413420	-1.677387
6	0	3.773906	-0.302212	-2.953949
6	0	3.732050	-1.975423	-1.384228
6	0	0.588640	-1.086537	-0.122244
1	0	4.334902	0.174063	-3.751110
1	0	-0.301395	-1.092752	0.489529
7	0	1.583818	-1.924128	-0.011043
7	0	0.757230	-0.158031	-1.114830
1	0	0.120341	0.594975	-1.355949
7	0	2.595091	0.236003	-2.670043
7	0	4.363704	-1.356084	-2.382858
7	0	4.323517	-3.047914	-0.800150
1	0	5.315713	-3.133083	-0.961399
1	0	3.978893	-3.320628	0.107551
8	0	1.395534	2.906771	-2.485446
1	0	1.874400	2.110524	-2.769364
1	0	0.460463	2.680060	-2.564668
6	0	-6.553019	-1.362714	-0.191621
6	0	-5.429707	-0.718105	-0.677616
6	0	-4.770113	0.266685	0.075543
6	0	-5.256196	0.583460	1.340444
6	0	-6.378338	-0.060122	1.835735
6	0	-7.033766	-1.023973	1.085657
1	0	-5.044921	-0.963913	-1.658270
1	0	-4.760285	1.326122	1.950824
1	0	-6.755937	0.184942	2.822559
8	0	-8.133583	-1.681108	1.518339
1	0	-8.370988	-1.367426	2.396387
8	0	-7.252563	-2.316085	-0.844958
6	0	-6.797219	-2.687226	-2.129726
1	0	-5.786253	-3.101197	-2.083665
1	0	-7.485787	-3.449704	-2.483213
1	0	-6.814188	-1.835175	-2.814662
6	0	-3.603865	0.918314	-0.503855
6	0	-2.915581	1.950096	0.005420
1	0	-3.261111	0.534331	-1.462427
1	0	-3.175892	2.427279	0.942041
6	0	-1.755400	2.494600	-0.712188
8	0	-1.291121	1.970372	-1.714965
6	0	-1.097308	3.709743	-0.091302
1	0	-0.443293	4.177936	-0.825625
1	0	-1.847499	4.402815	0.286768
6	0	-0.290000	3.173821	1.099343
8	0	-0.783084	3.134599	2.204063
6	0	1.032768	2.631423	0.749212
6	0	1.649891	1.770572	1.568571

1	0	1.420585	2.867078	-0.236672
1	0	1.150693	1.521729	2.503041
6	0	2.911131	1.092143	1.291883
6	0	3.224976	-0.058954	2.025719
6	0	3.795961	1.528595	0.303854
6	0	4.378547	-0.765313	1.753896
1	0	2.525180	-0.412276	2.771436
6	0	4.976602	0.846158	0.062999
1	0	3.565094	2.413271	-0.277083
6	0	5.274827	-0.297945	0.784825
1	0	5.676010	1.175317	-0.694471
8	0	6.418100	-0.978760	0.536465
1	0	6.466700	-1.713738	1.161270
8	0	4.751291	-1.940217	2.348405
6	0	3.803169	-2.546040	3.210833
1	0	2.861438	-2.716524	2.681188
1	0	4.235604	-3.493984	3.520834
1	0	3.625938	-1.924362	4.091691

(A-2)

6	0	-2.991165	2.357586	-0.485805
6	0	-2.987867	3.534600	0.248972
6	0	-5.101916	3.314444	0.801314
6	0	-4.203399	1.647397	-0.526028
6	0	-1.008945	3.104746	-0.621767
1	0	-5.989226	3.671488	1.313255
1	0	0.044801	3.217247	-0.837323
7	0	-1.744962	2.106328	-1.025324
7	0	-1.704152	4.004007	0.148181
1	0	-1.347767	4.847101	0.568431
7	0	-4.019363	4.065708	0.910896
7	0	-5.249436	2.157167	0.140112
7	0	-4.351609	0.502390	-1.223290
1	0	-5.145752	-0.080752	-0.978669
1	0	-3.505315	0.040277	-1.521389
8	0	-6.926198	-0.149409	0.222993
1	0	-6.618860	0.776526	0.234148
1	0	-6.799447	-0.449221	1.130732
6	0	7.803693	-0.043157	0.896371
6	0	6.601965	0.548900	0.550394
6	0	5.604503	-0.166963	-0.129712
6	0	5.831957	-1.503461	-0.441444
6	0	7.029836	-2.106000	-0.090491
6	0	8.017709	-1.393035	0.569457
1	0	6.417258	1.586145	0.795957
1	0	5.072443	-2.086727	-0.944826
1	0	7.204394	-3.150253	-0.326899
8	0	9.205079	-1.931762	0.935151
1	0	9.239617	-2.850737	0.652235
8	0	8.821703	0.570636	1.541000
6	0	8.646873	1.929629	1.880870
1	0	7.804053	2.059541	2.565423
1	0	9.565012	2.235624	2.375011
1	0	8.491297	2.541918	0.988152
6	0	4.368987	0.524767	-0.480094
6	0	3.397644	0.080327	-1.285977

1	0	4.226889	1.513103	-0.048282
1	0	3.450251	-0.877286	-1.791307
6	0	2.201740	0.905103	-1.543582
8	0	1.988927	1.965747	-0.992258
6	0	1.222451	0.334167	-2.558865
1	0	0.412094	1.051495	-2.694146
1	0	1.747112	0.145487	-3.496730
6	0	0.671943	-0.996203	-2.058241
8	0	1.077023	-2.051366	-2.491059
6	0	-0.376804	-0.878796	-1.024742
6	0	-1.185764	-1.904432	-0.745164
1	0	-0.534811	0.104145	-0.598575
1	0	-1.021491	-2.836877	-1.280722
6	0	-2.332096	-1.851818	0.162187
6	0	-3.351532	-2.796269	0.009051
6	0	-2.479154	-0.857917	1.136540
6	0	-4.496355	-2.722344	0.777928
1	0	-3.257615	-3.587333	-0.726793
6	0	-3.612403	-0.797077	1.928373
1	0	-1.695807	-0.122856	1.276881
6	0	-4.626213	-1.728026	1.746726
1	0	-3.732700	-0.032373	2.685423
8	0	-5.754321	-1.670804	2.501300
1	0	-6.255694	-2.479229	2.316135
8	0	-5.533135	-3.616601	0.671529
6	0	-6.289424	-3.477471	-0.536643
1	0	-5.666124	-3.706615	-1.403234
1	0	-7.100391	-4.199459	-0.474658
1	0	-6.687773	-2.463281	-0.619262

(B-1)

6	0	-1.380798	-1.569485	-0.051420
6	0	-0.228946	-0.865069	-0.376039
6	0	-0.751749	-0.824453	-2.517185
6	0	-2.242513	-1.871324	-1.118503
6	0	-0.412696	-1.173488	1.787698
1	0	-0.522279	-0.539090	-3.538890
1	0	-0.153336	-1.108319	2.833299
7	0	-1.480844	-1.754442	1.313816
7	0	0.394858	-0.634558	0.820081
1	0	1.176801	-0.008817	0.966565
7	0	0.141625	-0.473869	-1.599744
7	0	-1.902433	-1.480998	-2.350295
7	0	-3.395769	-2.554851	-0.942982
1	0	-4.062512	-2.504994	-1.697793
1	0	-3.766142	-2.605249	-0.006409
8	0	0.499085	5.329208	1.337383
1	0	0.350785	4.480291	1.766954
1	0	1.338326	5.202191	0.874790
6	0	-5.554709	-0.613292	0.874862
6	0	-4.338951	0.020265	1.064273
6	0	-3.777526	0.834934	0.069985
6	0	-4.465496	1.007544	-1.125923
6	0	-5.690303	0.386546	-1.318809
6	0	-6.243436	-0.417831	-0.333988
1	0	-3.779892	-0.135734	1.976902
1	0	-4.049451	1.616741	-1.917285

1	0	-6.227598	0.520586	-2.251708
8	0	-7.428580	-1.059833	-0.476780
1	0	-7.817009	-0.828032	-1.325936
8	0	-6.141820	-1.450178	1.761433
6	0	-5.451080	-1.687074	2.973769
1	0	-5.342192	-0.763001	3.547880
1	0	-6.060918	-2.391876	3.532195
1	0	-4.462837	-2.118631	2.788157
6	0	-2.464348	1.411900	0.329763
6	0	-1.705084	2.149528	-0.488493
1	0	-2.031984	1.180308	1.301445
1	0	-2.015444	2.428697	-1.488283
6	0	-0.348044	2.532322	-0.055415
8	0	0.075928	2.295540	1.060817
6	0	0.534632	3.237357	-1.072871
1	0	0.373224	2.793944	-2.059316
1	0	0.242101	4.290277	-1.094059
6	0	1.989146	3.104037	-0.663219
8	0	2.614302	4.041320	-0.212860
6	0	2.553266	1.748141	-0.810260
6	0	3.731603	1.431424	-0.260647
1	0	1.946239	1.020515	-1.338365
1	0	4.264573	2.227462	0.255005
6	0	4.364011	0.115442	-0.271346
6	0	5.638259	-0.020282	0.300587
6	0	3.745343	-1.009791	-0.818223
6	0	6.272929	-1.246447	0.312551
1	0	6.116085	0.851717	0.727659
6	0	4.380040	-2.240954	-0.801703
1	0	2.760345	-0.929916	-1.263877
6	0	5.640688	-2.367474	-0.242983
1	0	3.912637	-3.122134	-1.221592
8	0	6.256380	-3.570211	-0.231356
1	0	7.119728	-3.464615	0.188753
8	0	7.507555	-1.503331	0.833212
6	0	8.219674	-0.411020	1.381489
1	0	7.676742	0.022638	2.224904
1	0	9.169971	-0.808871	1.726842
1	0	8.395719	0.356075	0.623533

(C-1)

6	0	-3.016823	2.892573	-0.090910
6	0	-4.235248	2.273611	-0.322225
6	0	-3.392559	1.016740	-1.926458
6	0	-1.938522	2.473288	-0.891315
6	0	-4.354662	3.713956	1.324659
1	0	-3.507392	0.244181	-2.679916
1	0	-4.797012	4.284817	2.126823
7	0	-3.106916	3.793555	0.950089
7	0	-5.091895	2.821046	0.593117
1	0	-6.043103	2.488713	0.734000
7	0	-4.480437	1.317959	-1.230390
7	0	-2.162099	1.533499	-1.819837
7	0	-0.702422	2.973088	-0.733001
1	0	0.093598	2.547879	-1.196249
1	0	-0.541677	3.610106	0.029644
8	0	-6.983807	0.790415	0.244926

1	0	-6.314947	0.622777	-0.439752
1	0	-6.789808	0.165239	0.954664
6	0	7.606000	0.189538	1.101787
6	0	6.386114	0.650588	0.639714
6	0	5.594199	-0.118717	-0.227267
6	0	6.056299	-1.369626	-0.624481
6	0	7.278263	-1.837524	-0.168276
6	0	8.056940	-1.075402	0.688250
1	0	6.022888	1.622320	0.946207
1	0	5.468383	-1.987900	-1.289621
1	0	7.638574	-2.812415	-0.478926
8	0	9.255943	-1.484341	1.165046
1	0	9.457849	-2.358066	0.816620
8	0	8.429981	0.860224	1.937772
6	0	8.003821	2.129953	2.385218
1	0	7.063405	2.057122	2.938414
1	0	8.786093	2.493017	3.046091
1	0	7.882812	2.822992	1.548092
6	0	4.320184	0.432525	-0.670927
6	0	3.420913	-0.141467	-1.479817
1	0	4.069987	1.424873	-0.302292
1	0	3.556716	-1.130045	-1.903043
6	0	2.173255	0.563304	-1.822103
8	0	1.881113	1.655051	-1.371533
6	0	1.233408	-0.177080	-2.755150
1	0	0.426995	0.498424	-3.045366
1	0	1.780757	-0.543326	-3.623873
6	0	0.652826	-1.384382	-2.022242
8	0	1.021062	-2.509794	-2.268832
6	0	-0.384748	-1.050193	-1.027042
6	0	-1.245013	-1.977595	-0.598825
1	0	-0.492529	-0.004094	-0.769603
1	0	-1.106924	-2.990642	-0.969902
6	0	-2.409258	-1.738017	0.251915
6	0	-3.395773	-2.732860	0.319596
6	0	-2.604567	-0.543264	0.941829
6	0	-4.560892	-2.513450	1.027703
1	0	-3.239782	-3.664220	-0.208673
6	0	-3.771495	-0.323038	1.657825
1	0	-1.848186	0.231591	0.917815
6	0	-4.753146	-1.294956	1.688817
1	0	-3.939132	0.608352	2.185649
8	0	-5.924152	-1.065279	2.348727
1	0	-6.435083	-1.886555	2.341810
8	0	-5.597705	-3.389292	1.158733
6	0	-5.488741	-4.629850	0.486210
1	0	-4.628788	-5.195414	0.852965
1	0	-6.403573	-5.174399	0.702796
1	0	-5.397862	-4.477169	-0.591829

(D-1)

6	0	1.468462	-1.617798	-0.334673
6	0	0.793088	-0.783145	-1.215247
6	0	2.296913	-1.097893	-2.799627
6	0	2.667172	-2.177186	-0.801742
6	0	-0.225376	-0.915326	0.719375
1	0	2.660706	-0.915642	-3.805866

1	0	-0.990239	-0.733899	1.462289
7	0	0.818930	-1.687014	0.879535
7	0	-0.293024	-0.338501	-0.518700
1	0	-1.011600	0.264646	-0.910547
7	0	1.159290	-0.502117	-2.474841
7	0	3.069181	-1.892889	-2.046190
7	0	3.417476	-2.998317	-0.027984
1	0	4.391347	-3.061278	-0.286392
1	0	3.245032	-2.933293	0.964917
8	0	-1.427164	0.780854	-2.807306
1	0	-1.645204	1.713520	-2.937207
1	0	-0.526389	0.623651	-3.129615
6	0	3.766335	0.201096	1.226773
6	0	2.716114	1.035819	1.569157
6	0	2.159417	1.923499	0.638018
6	0	2.704669	1.987168	-0.641450
6	0	3.773451	1.176039	-0.980862
6	0	4.299642	0.272799	-0.069522
1	0	2.279072	0.981033	2.556888
1	0	2.305354	2.675765	-1.374731
1	0	4.202030	1.221758	-1.975829
8	0	5.306719	-0.580522	-0.387083
1	0	5.296739	-0.721519	-1.342093
8	0	4.312102	-0.731613	2.045995
6	0	3.683540	-0.926641	3.299658
1	0	2.633927	-1.205486	3.164694
1	0	4.223790	-1.736772	3.783183
1	0	3.752844	-0.029324	3.920160
6	0	1.021852	2.735930	1.051620
6	0	0.184156	3.419438	0.261772
1	0	0.816618	2.775993	2.119382
1	0	0.264127	3.402635	-0.820398
6	0	-0.948535	4.163430	0.854048
8	0	-1.074285	4.347000	2.043341
6	0	-2.014630	4.629744	-0.131870
1	0	-2.804686	5.122606	0.436751
1	0	-1.591692	5.315515	-0.866958
6	0	-2.572908	3.424899	-0.870444
8	0	-2.556299	3.367904	-2.084531
6	0	-3.027693	2.315455	-0.009647
6	0	-3.414384	1.152309	-0.548335
1	0	-2.921340	2.444414	1.062544
1	0	-3.455383	1.095805	-1.631882
6	0	-3.649938	-0.094579	0.169495
6	0	-3.448636	-1.287185	-0.542125
6	0	-3.946255	-0.153373	1.530358
6	0	-3.500628	-2.502711	0.109270
1	0	-3.198427	-1.229246	-1.594705
6	0	-4.033803	-1.376258	2.177640
1	0	-4.123475	0.759287	2.085360
6	0	-3.804158	-2.550526	1.478701
1	0	-4.273708	-1.442837	3.230891
8	0	-3.871995	-3.737239	2.116371
1	0	-3.648852	-4.433497	1.484512
8	0	-3.273100	-3.718543	-0.457363
6	0	-2.724461	-3.724487	-1.765355
1	0	-1.803937	-3.135645	-1.796224

1	0	-2.507195	-4.763103	-1.998471
1	0	-3.440705	-3.329045	-2.488676

(E-1)

6	0	1.184945	1.099731	1.106465
6	0	0.468165	0.858868	-0.057857
6	0	1.691395	2.265586	-1.223895
6	0	2.233887	2.026800	1.011567
6	0	-0.243510	-0.372980	1.619351
1	0	1.945855	2.751848	-2.159322
1	0	-0.836365	-1.117951	2.133822
7	0	0.726834	0.321859	2.147787
7	0	-0.457589	-0.082544	0.294111
1	0	-1.123872	-0.535961	-0.313889
7	0	0.677223	1.422330	-1.253941
7	0	2.468024	2.596451	-0.177860
7	0	2.993761	2.362673	2.076837
1	0	3.874253	2.827822	1.901069
1	0	2.940363	1.754721	2.879355
8	0	5.108268	3.301993	0.052519
1	0	4.177176	3.205082	-0.263339
1	0	5.561664	3.884859	-0.560466
6	0	-4.958801	2.016675	0.009691
6	0	-4.344341	0.950620	0.641598
6	0	-4.160104	-0.277470	-0.013406
6	0	-4.621094	-0.421594	-1.318240
6	0	-5.247256	0.638779	-1.954340
6	0	-5.419090	1.853272	-1.309206
1	0	-3.981440	1.055485	1.655334
1	0	-4.508527	-1.362482	-1.840733
1	0	-5.613223	0.526208	-2.969124
8	0	-6.021102	2.919722	-1.882457
1	0	-6.291670	2.693422	-2.777708
8	0	-5.167194	3.233892	0.555115
6	0	-4.688754	3.444952	1.868016
1	0	-3.605301	3.306996	1.917819
1	0	-4.935820	4.473808	2.114742
1	0	-5.177616	2.771953	2.577698
6	0	-3.466710	-1.341046	0.702199
6	0	-2.978338	-2.480030	0.192833
1	0	-3.298890	-1.175800	1.765030
1	0	-3.069951	-2.734924	-0.857796
6	0	-2.227640	-3.422049	1.054166
8	0	-2.026745	-3.221009	2.232643
6	0	-1.633444	-4.623437	0.338118
1	0	-1.155889	-5.263060	1.080082
1	0	-2.402493	-5.165426	-0.212289
6	0	-0.612647	-4.093274	-0.667330
8	0	-0.809915	-4.178887	-1.858946
6	0	0.543110	-3.399047	-0.070607
6	0	1.351586	-2.650239	-0.833948
1	0	0.651678	-3.453429	1.007370
1	0	1.123723	-2.620721	-1.897717
6	0	2.465939	-1.828234	-0.387420
6	0	3.032176	-0.916418	-1.285843
6	0	2.977079	-1.881411	0.913943
6	0	4.044769	-0.065619	-0.892713

1	0	2.657852	-0.836874	-2.300429
6	0	3.996385	-1.039197	1.310157
1	0	2.565858	-2.581348	1.630325
6	0	4.529524	-0.107125	0.421681
1	0	4.384569	-1.062821	2.320493
8	0	5.495758	0.725271	0.849683
1	0	5.489644	1.563424	0.339586
8	0	4.549645	0.866363	-1.766536
6	0	5.809121	0.489691	-2.315667
1	0	5.703614	-0.413152	-2.922624
1	0	6.136106	1.316955	-2.942371
1	0	6.543106	0.312396	-1.525486

(F-1)

6	0	-1.277462	1.026895	-1.564671
6	0	-1.799078	1.887648	-0.610142
6	0	-0.391423	1.173487	0.921113
6	0	-0.248322	0.171301	-1.140007
6	0	-2.846798	2.058489	-2.530571
1	0	0.007203	1.218033	1.930585
1	0	-3.573969	2.410766	-3.246357
7	0	-1.942702	1.148432	-2.766491
7	0	-2.807648	2.555712	-1.254426
1	0	-3.477649	3.180115	-0.818255
7	0	-1.389067	2.005788	0.657322
7	0	0.194172	0.275894	0.116602
7	0	0.254652	-0.773120	-1.962582
1	0	1.094576	-1.267782	-1.703380
1	0	0.002339	-0.733073	-2.936819
8	0	-4.967858	3.471525	0.473647
1	0	-4.689679	2.896955	1.206982
1	0	-5.236071	4.311711	0.854126
6	0	5.683643	1.589762	0.167886
6	0	5.105405	0.472154	-0.405740
6	0	4.000719	-0.159690	0.185453
6	0	3.461794	0.372190	1.351913
6	0	4.031745	1.497880	1.927213
6	0	5.137069	2.106191	1.355192
1	0	5.508040	0.061694	-1.322188
1	0	2.573710	-0.067769	1.785964
1	0	3.607083	1.923748	2.830283
8	0	5.731047	3.207813	1.874837
1	0	5.270072	3.467915	2.678178
8	0	6.753863	2.257119	-0.323471
6	0	7.315398	1.777110	-1.525796
1	0	6.587126	1.809351	-2.341103
1	0	8.145632	2.439664	-1.755253
1	0	7.686750	0.755301	-1.407656
6	0	3.441039	-1.340412	-0.459508
6	0	2.645271	-2.258123	0.104158
1	0	3.701356	-1.493915	-1.505399
1	0	2.383563	-2.226542	1.155975
6	0	2.099395	-3.364977	-0.707690
8	0	2.117864	-3.354877	-1.922099
6	0	1.455196	-4.506062	0.061902
1	0	1.054813	-5.216808	-0.662185
1	0	2.190647	-4.988526	0.706963

6	0	0.342731	-3.961666	0.948963
8	0	0.394216	-4.074612	2.152884
6	0	-0.740426	-3.241117	0.245234
6	0	-1.583483	-2.479423	0.950145
1	0	-0.758257	-3.282616	-0.838451
1	0	-1.426257	-2.459692	2.026232
6	0	-2.659307	-1.635926	0.444066
6	0	-3.244934	-0.718040	1.316854
6	0	-3.122504	-1.682105	-0.876348
6	0	-4.230798	0.142953	0.880341
1	0	-2.915708	-0.647028	2.347409
6	0	-4.109589	-0.821180	-1.315270
1	0	-2.693467	-2.391537	-1.573159
6	0	-4.661495	0.117697	-0.446890
1	0	-4.448204	-0.832386	-2.343012
8	0	-5.604651	0.970784	-0.914652
1	0	-5.661026	1.756509	-0.348111
8	0	-4.783316	1.064177	1.752084
6	0	-6.014285	0.612687	2.320292
1	0	-5.839560	-0.284191	2.917573
1	0	-6.381902	1.414611	2.957688
1	0	-6.743335	0.394789	1.536020

(G-1)

6	0	1.830636	1.481602	-0.622554
6	0	0.544337	0.968803	-0.490037
6	0	0.730889	-0.192194	-2.356298
6	0	2.561529	1.049251	-1.740421
6	0	1.086373	2.230172	1.207753
1	0	0.310080	-0.872119	-3.091380
1	0	0.974749	2.736190	2.154877
7	0	2.156794	2.277015	0.456646
7	0	0.076857	1.469246	0.691281
1	0	-0.796423	1.195685	1.160674
7	0	-0.062021	0.134624	-1.344268
7	0	1.987393	0.198911	-2.594688
7	0	3.823870	1.476397	-1.984126
1	0	4.358781	0.919019	-2.632460
1	0	4.327548	1.874533	-1.205523
8	0	-2.108210	0.354391	2.042493
1	0	-1.726887	-0.534562	1.959969
1	0	-2.972530	0.307009	1.618943
6	0	5.829158	0.517831	0.766038
6	0	4.539173	0.122029	1.074825
6	0	3.935739	-0.969566	0.434401
6	0	4.663442	-1.674519	-0.518944
6	0	5.963969	-1.298046	-0.819396
6	0	6.554939	-0.212568	-0.190399
1	0	3.957657	0.685175	1.791042
1	0	4.221802	-2.513172	-1.040369
1	0	6.533253	-1.849835	-1.560146
8	0	7.816111	0.206136	-0.456468
1	0	8.215822	-0.375600	-1.110405
8	0	6.462350	1.584733	1.302757
6	0	5.713066	2.389020	2.196755
1	0	5.454536	1.829809	3.100058
1	0	6.358359	3.222713	2.459433

1	0	4.799816	2.758124	1.720928
6	0	2.542510	-1.263157	0.754965
6	0	1.753006	-2.182133	0.186794
1	0	2.085172	-0.637284	1.520076
1	0	2.100983	-2.838700	-0.602106
6	0	0.331885	-2.278523	0.566437
8	0	-0.159793	-1.608328	1.454608
6	0	-0.491011	-3.279488	-0.224839
1	0	-0.321327	-3.081665	-1.289352
1	0	-0.124568	-4.285787	-0.007582
6	0	-1.975170	-3.203870	0.075149
8	0	-2.569209	-4.147348	0.543699
6	0	-2.614638	-1.911111	-0.254320
6	0	-3.907323	-1.695610	0.005516
1	0	-1.970905	-1.146783	-0.677924
1	0	-4.471292	-2.515802	0.444463
6	0	-4.623641	-0.438983	-0.210764
6	0	-5.973530	-0.359986	0.166086
6	0	-4.008301	0.690586	-0.754983
6	0	-6.680105	0.814439	-0.001781
1	0	-6.450301	-1.234326	0.589514
6	0	-4.717023	1.870262	-0.919709
1	0	-2.967661	0.653185	-1.057377
6	0	-6.048357	1.940950	-0.547468
1	0	-4.252479	2.752379	-1.340805
8	0	-6.734923	3.093193	-0.708599
1	0	-7.638761	2.952807	-0.398580
8	0	-7.989675	1.013579	0.322159
6	0	-8.698226	-0.083241	0.866637
1	0	-8.250787	-0.404543	1.810362
1	0	-9.711244	0.267289	1.044092
1	0	-8.716815	-0.919630	0.163801