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分子间相互作用研究的 APF-D 密度泛函 SAM 色散校正方法改进

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An Improvement of the SAM Dispersion Correction in the APF-D Density Functional Method for Studying Intermolecular Interactions

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Table S1 Binding energies (kJ mol^{-1}) for the S66 Data Set

		APF-D					APF-D*					ωB97X-D	B3LYP-D3
	Ref	**BS1**	**BS2**	**BS3**	**BS4**	**BS5**	**BS1**	**BS2**	**BS3**	**BS4**	**BS5**	**BS6**	**BS4**
01 Water-Water	**-20.562**	-22.912	-21.616	-21.699	-21.950	-22.159	-22.502	-21.206	-21.290	-21.541	-21.750	-20.612	-21.574
02 Water-MeOH	**-23.380**	-25.713	-24.919	-24.877	-24.961	-24.835	-24.981	-24.187	-24.145	-24.229	-24.103	-23.246	-24.166
03 Water-MeNH2	**-28.882**	-32.695	-32.110	-32.110	-31.901	-31.483	-32.064	-31.479	-31.479	-31.270	-30.852	-30.647	-30.981
04 Water-Peptide	**-33.879**	-37.211	-36.291	-36.500	-36.584	-36.249	-36.115	-35.196	-35.405	-35.488	-35.154	-33.992	-34.870
05 MeOH-MeOH	**-24.070**	-26.215	-25.880	-25.880	-26.089	-26.089	-25.270	-24.935	-24.935	-25.145	-25.145	-23.790	-24.835
06 MeOH-MeNH2	**-31.583**	-35.539	-35.329	-35.371	-35.329	-35.288	-34.397	-34.188	-34.230	-34.188	-34.146	-33.406	-33.615
07 MeOH-Peptide	**-34.410**	-37.922	-37.671	-37.922	-38.047	-38.005	-36.496	-36.245	-36.496	-36.621	-36.580	-35.079	-35.915
08 MeOH-Water	**-20.943**	-22.828	-22.076	-22.201	-22.494	-22.870	-22.272	-21.520	-21.645	-21.938	-22.314	-20.654	-21.783
09 MeNH2-MeOH	**-12.790**	-14.257	-13.714	-13.630	-13.714	-13.797	-13.304	-12.760	-12.677	-12.760	-12.844	-12.752	-13.212
10 MeNH2-MeNH2	**-17.393**	-18.522	-17.978	-18.020	-18.104	-18.271	-17.389	-16.845	-16.887	-16.971	-17.138	-18.229	-17.518
11 MeNH2-Peptide	**-22.657**	-24.375	-23.874	-23.915	-23.957	-24.041	-22.623	-22.122	-22.163	-22.205	-22.289	-23.163	-22.703
12 MeNH2-Water	**-30.379**	-34.159	-33.406	-33.448	-33.323	-33.114	-33.318	-32.566	-32.608	-32.482	-32.273	-31.441	-31.776
13 Peptide-MeOH	**-25.868**	-27.469	-26.717	-26.842	-27.051	-27.302	-26.081	-25.328	-25.454	-25.663	-25.914	-25.630	-25.839
14 Peptide-MeNH2	**-31.165**	-34.159	-33.699	-33.657	-33.741	-33.992	-32.654	-32.194	-32.152	-32.236	-32.486	-33.072	-32.319
15 Peptide-Peptide	**-36.082**	-38.967	-38.758	-38.800	-38.883	-38.758	-36.964	-36.755	-36.797	-36.881	-36.755	-37.378	-37.127
16 Peptide-Water	**-21.423**	-22.494	-21.407	-21.616	-21.992	-22.745	-21.791	-20.704	-20.913	-21.290	-22.042	-20.403	-21.365
17 Uracil-Uracil BP	**-71.838**	-76.930	-77.934	-78.185	-78.477	-78.143	-74.886	-75.889	-76.140	-76.433	-76.098	-72.164	-75.927
18 Water-Pyridine	**-28.669**	-31.316	-31.358	-31.399	-31.148	-30.479	-30.571	-30.613	-30.655	-30.404	-29.735	-29.518	-31.065
19 MeOH-Pyridine	**-30.981**	-33.782	-34.033	-34.159	-34.075	-33.615	-32.670	-32.921	-33.047	-32.963	-32.503	-31.650	-33.448
20 AcOH-AcOH	**-79.828**	-89.055	-90.142	-90.979	-91.355	-91.229	-87.149	-88.236	-89.072	-89.448	-89.323	-82.951	-85.585
21 AcNH2-AcNH2	**-68.004**	-72.206	-72.833	-72.833	-73.251	-73.126	-70.617	-71.244	-71.244	-71.662	-71.537	-69.028	-71.161

22 AcOH-Uracil	**-81.492**	-88.428	-89.432	-90.059	-90.393	-90.184	-86.480	-87.483	-88.110	-88.445	-88.236	-83.076	-86.338
23 AcNH2-Uracil	**-80.229**	-85.543	-86.170	-86.338	-86.714	-86.630	-83.708	-84.335	-84.502	-84.878	-84.795	-81.279	-84.205
24 Benzene-Benzene pi-pi	**-11.799**	-14.634	-14.843	-14.508	-14.466	-14.257	-11.443	-11.652	-11.318	-11.276	-11.067	-13.630	-12.752
25 Pyridine-Pyridine pi-pi	**-16.285**	-19.442	-19.567	-19.191	-19.149	-18.940	-16.051	-16.176	-15.800	-15.758	-15.549	-18.062	-17.435
26 Uracil-Uracil pi-pi	**-41.095**	-49.503	-49.210	-49.252	-49.210	-48.960	-43.650	-43.357	-43.399	-43.357	-43.106	-40.807	-42.688
27 Benzene-Pyridine pi-pi	**-14.378**	-17.393	-17.560	-17.142	-17.100	-16.933	-14.077	-14.245	-13.827	-13.785	-13.618	-16.139	-15.428
28 Benzene-Uracil pi-pi	**-23.886**	-28.473	-28.514	-28.305	-28.222	-27.929	-23.844	-23.886	-23.677	-23.593	-23.301	-24.208	-24.083
29 Pyridine-Uracil pi-pi	**-28.510**	-32.654	-32.863	-32.695	-32.570	-32.236	-28.088	-28.297	-28.130	-28.004	-27.670	-28.473	-28.974
30 Benzene-Ethene	**-5.987**	-6.690	-6.940	-6.690	-6.648	-6.481	-4.934	-5.184	-4.934	-4.892	-4.725	-7.150	-6.188
31 Uracil-Ethene	**-14.132**	-15.386	-15.553	-15.470	-15.428	-15.302	-13.082	-13.250	-13.166	-13.124	-12.999	-14.843	-14.341
32 Uracil-Ethyne	**-15.629**	-16.640	-16.682	-16.640	-16.557	-16.390	-14.629	-14.671	-14.629	-14.546	-14.378	-15.595	-15.846
33 Pyridine-Ethene	**-7.827**	-8.487	-8.738	-8.487	-8.446	-8.278	-6.660	-6.911	-6.660	-6.619	-6.451	-8.822	-8.069
34 Pentane-Pentane	**-15.787**	-19.191	-19.442	-19.233	-19.274	-19.065	-15.549	-15.800	-15.591	-15.633	-15.424	-22.243	-16.724
35 Neopentane-Pentane	**-10.925**	-12.877	-12.919	-13.087	-13.128	-13.003	-10.432	-10.473	-10.641	-10.682	-10.557	-14.968	-11.372
36 Neopentane-Neopentane	**-7.430**	-8.655	-8.738	-8.780	-8.822	-8.738	-6.945	-7.028	-7.070	-7.112	-7.028	-9.951	-7.777
37 Cyclopentane-Neopentane	**-10.051**	-12.167	-12.250	-12.292	-12.334	-12.250	-9.821	-9.905	-9.947	-9.988	-9.905	-14.132	-10.745
38 Cyclopentane-Cyclopentane	**-12.530**	-15.177	-15.428	-15.386	-15.428	-15.302	-12.363	-12.614	-12.572	-12.614	-12.489	-17.184	-13.546
39 Benzene-Cyclopentane	**-14.947**	-18.647	-18.564	-18.313	-18.355	-18.271	-15.453	-15.369	-15.118	-15.160	-15.077	-18.313	-15.679
40 Benzene-Neopentane	**-12.104**	-14.550	-14.174	-14.257	-14.257	-14.257	-12.117	-11.740	-11.824	-11.824	-11.824	-14.675	-12.376
41 Uracil-Pentane	**-20.269**	-24.417	-24.542	-24.542	-24.542	-24.375	-20.094	-20.219	-20.219	-20.219	-20.052	-23.539	-20.529
42 Uracil-Cyclopentane	**-17.301**	-20.947	-21.114	-21.114	-21.114	-20.947	-17.113	-17.280	-17.280	-17.280	-17.113	-19.609	-17.518
43 Uracil-Neopentane	**-15.520**	-18.062	-18.187	-18.146	-18.146	-17.978	-15.027	-15.152	-15.110	-15.110	-14.943	-17.644	-15.762
44 Ethene-Pentane	**-8.383**	-9.324	-9.533	-9.407	-9.449	-9.324	-7.547	-7.756	-7.630	-7.672	-7.547	-10.829	-8.822
45 Ethyne-Pentane	**-7.308**	-8.237	-8.362	-8.111	-8.111	-8.028	-6.769	-6.894	-6.644	-6.644	-6.560	-8.571	-7.693
46 Peptide-Pentane	**-17.828**	-21.114	-21.198	-21.198	-21.198	-21.072	-17.497	-17.581	-17.581	-17.581	-17.456	-21.407	-17.853

47 Benzene-Benzene TS	**-12.025**	-14.006	-13.630	-13.546	-13.588	-13.588	-11.928	-11.552	-11.468	-11.510	-11.510	-13.087	-12.292
48 Pyridine-Pyridine TS	**-14.780**	-16.515	-16.097	-15.971	-15.971	-15.930	-14.424	-14.006	-13.881	-13.881	-13.839	-15.553	-15.093
49 Benzene-Pyridine TS	**-13.927**	-16.306	-15.804	-15.721	-15.762	-15.804	-14.190	-13.689	-13.605	-13.647	-13.689	-15.135	-14.383
50 Benzene-Ethyne CH-pi	**-11.987**	-14.132	-13.170	-13.463	-13.546	-13.672	-12.798	-11.836	-12.129	-12.213	-12.338	-12.668	-12.501
51 Ethyne-Ethyne TS	**-6.372**	-7.275	-6.982	-7.191	-7.191	-7.191	-6.811	-6.518	-6.727	-6.727	-6.727	-6.522	-7.108
52 Benzene-AcOH OH-pi	**-19.680**	-24.166	-23.246	-23.790	-23.832	-23.915	-21.996	-21.076	-21.620	-21.662	-21.745	-19.400	-19.400
53 Benzene-AcNH2 NH-pi	**-18.233**	-20.989	-20.445	-20.529	-20.571	-20.529	-19.224	-18.681	-18.764	-18.806	-18.764	-18.856	-18.480
54 Benzene-Water OH-pi	**-13.701**	-16.933	-15.804	-15.971	-16.013	-16.055	-15.645	-14.516	-14.684	-14.725	-14.767	-14.634	-14.048
55 Benzene-MeOH OH-pi	**-17.510**	-21.156	-20.403	-20.654	-20.696	-20.696	-19.028	-18.275	-18.526	-18.568	-18.568	-18.438	-17.811
56 Benzene-MeNH2 NH-pi	**-13.509**	-15.553	-14.926	-15.052	-15.093	-15.093	-13.567	-12.940	-13.066	-13.107	-13.107	-14.968	-13.797
57 Benzene-Peptide NH-pi	**-22.084**	-26.006	-25.170	-25.337	-25.379	-25.462	-23.117	-22.281	-22.448	-22.490	-22.573	-24.166	-22.577
58 Pyridine-Pyridine CH-N	**-17.334**	-16.849	-16.682	-16.557	-16.599	-16.557	-15.721	-15.553	-15.428	-15.470	-15.428	-16.264	-16.724
59 Ethyne-Water CH-O	**-11.916**	-13.128	-12.167	-12.292	-12.585	-13.170	-12.798	-11.836	-11.962	-12.255	-12.840	-11.414	-12.543
60 Ethyne-AcOH OH-pi	**-20.353**	-23.832	-23.372	-23.957	-23.957	-23.832	-23.506	-23.046	-23.631	-23.631	-23.506	-20.821	-21.825
61 Pentane-AcOH	**-12.175**	-15.010	-15.177	-15.135	-15.177	-15.052	-12.334	-12.501	-12.459	-12.501	-12.376	-14.132	-12.418
62 Pentane-AcNH2	**-14.776**	-17.435	-17.518	-17.560	-17.560	-17.435	-14.575	-14.659	-14.700	-14.700	-14.575	-17.309	-15.010
63 Benzene-AcOH	**-15.892**	-19.107	-18.773	-18.647	-18.689	-18.564	-16.465	-16.130	-16.005	-16.047	-15.921	-17.226	-15.971
64 Peptide-Ethene	**-12.539**	-13.965	-13.714	-13.714	-13.755	-13.630	-12.229	-11.979	-11.979	-12.020	-11.895	-13.128	-12.836
65 Pyridine-Ethyne	**-16.686**	-17.978	-18.020	-18.020	-18.020	-17.978	-17.389	-17.431	-17.431	-17.431	-17.389	-17.351	-18.564
66 MeNH2-Pyridine	**-16.590**	-17.268	-17.058	-16.933	-16.933	-16.766	-15.478	-15.269	-15.144	-15.144	-14.976	-17.058	-16.724

BS1:6-311++G(*2d,p*) ; BS2:aug-cc-pVDZ；BS3:aug-cc-pVTZ；BS4:Def2QZVP；BS5:Def2TZVPP；BS6:6311++G(*3df,3pd*)

The reference binding energies (Ref.) are the S66A binding energies from Rezac et al.[14]

Table S2 the correlation of ζ and $\Delta E_{\text{APF-D*}} - \Delta E_{\text{ref}}$ (kJ mol^{-1})

ζ	APF-D* S66 set MAD										$\overline{\text{MAD}}$	（$\overline{\text{MAD}}$+$\overline{\text{RMSD}}$）/2
	6-311g(2d,p)	6-311++g(2d,p)	6-311++G(2d,2p)	cc-pVDZ	aug-cc-pVDZ	cc-pVTZ	aug-cc-pVTZ	Def2QZVP	Def2TZVP	Def2TZVPP		
0.76	1.840	1.756	1.798	2.341	1.798	1.881	1.881	1.923	2.007	1.923	1.923	2.099
0.77	1.756	1.672	1.714	2.216	1.714	1.798	1.798	1.798	1.923	1.840	1.840	2.007
0.78	1.672	1.589	1.631	2.132	1.631	1.672	1.714	1.714	1.840	1.756	1.714	1.919
0.79	1.589	1.505	1.547	2.007	1.547	1.589	1.631	1.631	1.756	1.672	1.631	1.840
0.8	1.505	1.463	1.463	1.923	1.463	1.505	1.547	1.547	1.672	1.589	1.547	1.769
0.81	1.422	1.380	1.380	1.798	1.380	1.422	1.463	1.463	1.589	1.505	1.463	1.706
0.82	1.380	1.338	1.338	1.714	1.296	1.338	1.380	1.422	1.547	1.422	1.422	1.656
0.83	1.296	1.296	1.254	1.631	1.212	1.296	1.338	1.338	1.463	1.380	1.338	1.614
0.84	1.254	1.254	1.212	1.505	1.171	1.212	1.254	1.296	1.422	1.338	1.296	1.580
0.85	1.254	1.212	1.171	1.422	1.129	1.171	1.212	1.254	1.380	1.254	1.254	1.560
0.86	1.212	1.212	1.129	1.380	1.087	1.129	1.171	1.212	1.338	1.254	1.212	1.551
0.87	1.254	1.212	1.129	1.296	1.087	1.087	1.171	1.212	1.338	1.212	1.212	1.568
0.88	1.296	1.296	1.212	1.254	1.171	1.129	1.212	1.254	1.338	1.254	1.254	1.606
0.89	1.380	1.380	1.296	1.254	1.254	1.171	1.296	1.338	1.380	1.296	1.296	1.668
0.9	1.463	1.505	1.422	1.254	1.338	1.254	1.380	1.422	1.463	1.380	1.380	1.748
0.91	1.547	1.589	1.505	1.296	1.422	1.380	1.505	1.547	1.589	1.505	1.505	1.835
0.92	1.672	1.714	1.631	1.338	1.547	1.463	1.589	1.631	1.672	1.589	1.589	1.936
0.93	1.798	1.840	1.756	1.422	1.672	1.589	1.714	1.756	1.798	1.714	1.714	2.040
0.94	1.923	1.965	1.881	1.505	1.798	1.714	1.840	1.881	1.923	1.840	1.840	2.153
0.95	2.007	2.091	2.007	1.631	1.923	1.840	1.965	2.007	2.049	1.965	1.965	2.274
0.96	2.132	2.258	2.132	1.714	2.091	1.965	2.091	2.174	2.174	2.091	2.091	2.396
0.97	2.258	2.383	2.300	1.840	2.216	2.091	2.258	2.300	2.300	2.216	2.216	2.521
0.98	2.383	2.509	2.425	1.965	2.341	2.216	2.383	2.425	2.425	2.383	2.341	2.651

0.99	2.509	2.676	2.592	2.049	2.467	2.383	2.509	2.592	2.592	2.509	2.467	2.785
1	2.634	2.801	2.718	2.174	2.634	2.509	2.676	2.718	2.718	2.634	2.634	2.918

ζ	APF-D* S66 set RMSD										$\overline{RMSD}$	（$\overline{MAD}$+$\overline{RMSD}$）/2
	6-311g(2d,p)	6-311++g(2d,p)	6-311++G(2d,2p)	cc-pVDZ	aug-cc-pVDZ	cc-pVTZ	aug-cc-pVTZ	Def2QZVP	Def2TZVP	Def3TZVPP		
0.76	2.216	2.049	2.132	2.676	2.132	2.341	2.258	2.341	2.300	2.341	2.300	2.099
0.77	2.132	1.965	2.049	2.550	2.049	2.258	2.174	2.258	2.216	2.258	2.174	2.007
0.78	2.049	1.881	1.965	2.467	1.965	2.132	2.132	2.174	2.132	2.174	2.091	1.919
0.79	1.965	1.840	1.881	2.341	1.881	2.091	2.049	2.091	2.091	2.132	2.049	1.840
0.8	1.923	1.756	1.840	2.258	1.840	2.007	2.007	2.049	2.007	2.049	1.965	1.769
0.81	1.881	1.714	1.798	2.174	1.798	1.965	1.965	2.007	1.965	2.007	1.923	1.706
0.82	1.840	1.714	1.756	2.091	1.756	1.923	1.923	2.007	1.923	1.965	1.881	1.656
0.83	1.798	1.714	1.756	2.049	1.756	1.881	1.923	1.965	1.923	1.965	1.881	1.614
0.84	1.798	1.714	1.756	1.965	1.756	1.881	1.923	2.007	1.881	1.965	1.881	1.580
0.85	1.798	1.714	1.756	1.923	1.756	1.881	1.923	2.007	1.923	1.965	1.881	1.560
0.86	1.840	1.756	1.798	1.923	1.798	1.881	1.965	2.049	1.923	2.007	1.881	1.551
0.87	1.881	1.840	1.840	1.881	1.840	1.923	2.007	2.091	1.965	2.007	1.923	1.568
0.88	1.923	1.881	1.923	1.881	1.923	1.965	2.049	2.132	2.007	2.091	1.965	1.606
0.89	2.007	1.965	1.965	1.881	1.965	2.049	2.132	2.174	2.049	2.132	2.049	1.668
0.9	2.049	2.049	2.049	1.923	2.049	2.091	2.174	2.258	2.132	2.216	2.091	1.748
0.91	2.174	2.132	2.174	1.965	2.132	2.174	2.258	2.341	2.216	2.258	2.174	1.835
0.92	2.258	2.258	2.258	2.007	2.258	2.258	2.383	2.425	2.300	2.383	2.258	1.936
0.93	2.341	2.341	2.383	2.091	2.341	2.341	2.467	2.550	2.383	2.467	2.383	2.040
0.94	2.467	2.467	2.467	2.174	2.467	2.467	2.592	2.634	2.509	2.550	2.467	2.153
0.95	2.592	2.592	2.592	2.258	2.592	2.550	2.676	2.759	2.634	2.676	2.592	2.274
0.96	2.676	2.718	2.718	2.341	2.718	2.676	2.801	2.885	2.718	2.801	2.718	2.396
0.97	2.801	2.843	2.843	2.425	2.843	2.801	2.927	3.010	2.843	2.927	2.843	2.521

0.98	2.927	3.010	2.969	2.550	2.969	2.927	3.052	3.136	2.969	3.052	2.969	2.651
0.99	3.094	3.136	3.136	2.676	3.094	3.052	3.178	3.261	3.094	3.178	3.094	2.785
1	3.219	3.261	3.261	2.801	3.219	3.178	3.303	3.387	3.219	3.303	3.219	2.918

Table S3 ΔE - ΔE_{ref} (kJ mol^{-1}) for the S66 Data Set

		APF-D					APF-D*					ωB97X-D	B3LYP-D3
	Ref	BS1	BS2	BS3	BS4	BS5	BS1	BS2	BS3	BS4	BS5	BS6	BS4
01 Water-Water	**-20.562**	-2.350	-1.054	-1.304	-1.137	-1.388	-1.940	-0.644	-0.895	-0.727	-0.978	-0.050	-1.012
02 Water-MeOH	**-23.380**	-2.333	-1.539	-0.786	-1.497	-1.580	-1.601	-0.807	-0.054	-0.765	-0.849	0.134	-0.786
03 Water-MeNH2	**-28.882**	-3.813	-3.228	-1.555	-3.228	-3.019	-3.182	-2.596	-0.924	-2.596	-2.387	-1.764	-2.099
04 Water-Peptide	**-33.879**	-3.332	-2.412	-1.451	-2.621	-2.705	-2.237	-1.317	-0.355	-1.526	-1.610	-0.113	-0.991
05 MeOH-MeOH	**-24.070**	-2.145	-1.810	-1.727	-1.810	-2.019	-1.200	-0.865	-0.782	-0.865	-1.075	0.280	-0.765
06 MeOH-MeNH2	**-31.583**	-3.955	-3.746	-3.286	-3.788	-3.746	-2.814	-2.605	-2.145	-2.647	-2.605	-1.823	-2.032
07 MeOH-Peptide	**-34.410**	-3.512	-3.261	-3.303	-3.512	-3.637	-2.086	-1.835	-1.877	-2.086	-2.212	-0.669	-1.505
08 MeOH-Water	**-20.943**	-1.886	-1.133	-2.053	-1.258	-1.551	-1.330	-0.577	-1.497	-0.702	-0.995	0.288	-0.840
09 MeNH2-MeOH	**-12.790**	-1.468	-0.924	-0.840	-0.840	-0.924	-0.514	0.029	0.113	0.113	0.029	0.038	-0.422
10 MeNH2-MeNH2	**-17.393**	-1.129	-0.585	-0.627	-0.627	-0.711	0.004	0.548	0.506	0.506	0.422	-0.836	-0.125
11 MeNH2-Peptide	**-22.657**	-1.718	-1.217	-1.258	-1.258	-1.300	0.033	0.535	0.493	0.493	0.452	-0.506	-0.046
12 MeNH2-Water	**-30.379**	-3.780	-3.027	-1.773	-3.069	-2.943	-2.939	-2.187	-0.932	-2.228	-2.103	-1.062	-1.396
13 Peptide-MeOH	**-25.868**	-1.601	-0.849	-1.350	-0.974	-1.183	-0.213	0.539	0.038	0.414	0.205	0.238	0.029
14 Peptide-MeNH2	**-31.165**	-2.994	-2.534	-2.785	-2.492	-2.575	-1.488	-1.029	-1.279	-0.987	-1.070	-1.907	-1.154
15 Peptide-Peptide	**-36.082**	-2.885	-2.676	-2.509	-2.718	-2.801	-0.882	-0.673	-0.506	-0.715	-0.799	-1.296	-1.045
16 Peptide-Water	**-21.423**	-1.070	0.017	-1.447	-0.192	-0.569	-0.368	0.719	-0.744	0.510	0.134	1.020	0.059
17 Uracil-Uracil BP	**-71.838**	-5.092	-6.096	-5.970	-6.347	-6.639	-3.048	-4.051	-3.926	-4.302	-4.595	-0.326	-4.089

18 Water-Pyridine	**-28.669**	-2.647	-2.688	-0.723	-2.730	-2.479	-1.902	-1.944	0.021	-1.986	-1.735	-0.849	-2.396
19 MeOH-Pyridine	**-30.981**	-2.801	-3.052	-2.049	-3.178	-3.094	-1.689	-1.940	-0.937	-2.065	-1.982	-0.669	-2.467
20 AcOH-AcOH	**-79.828**	-9.227	-10.315	-11.402	-11.151	-11.527	-7.321	-8.408	-9.495	-9.244	-9.620	-3.123	-5.757
21 AcNH2-AcNH2	**-68.004**	-4.202	-4.829	-4.871	-4.829	-5.247	-2.613	-3.240	-3.282	-3.240	-3.658	-1.024	-3.157
22 AcOH-Uracil	**-81.492**	-6.936	-7.940	-8.567	-8.567	-8.901	-4.988	-5.991	-6.619	-6.619	-6.953	-1.585	-4.846
23 AcNH2-Uracil	**-80.229**	-5.314	-5.941	-6.150	-6.108	-6.485	-3.479	-4.106	-4.315	-4.273	-4.649	-1.049	-3.976
24 Benzene-Benzene pi-pi	**-11.799**	-2.835	-3.044	-2.500	-2.709	-2.667	0.355	0.146	0.690	0.481	0.523	-1.831	-0.953
25 Pyridine-Pyridine pi-pi	**-16.285**	-3.157	-3.282	-2.697	-2.906	-2.864	0.234	0.109	0.694	0.485	0.527	-1.777	-1.150
26 Uracil-Uracil pi-pi	**-41.095**	-8.408	-8.115	-7.864	-8.157	-8.115	-2.555	-2.262	-2.011	-2.304	-2.262	0.288	-1.593
27 Benzene-Pyridine pi-pi	**-14.378**	-3.015	-3.182	-2.555	-2.764	-2.722	0.301	0.134	0.761	0.552	0.594	-1.760	-1.049
28 Benzene-Uracil pi-pi	**-23.886**	-4.587	-4.628	-3.834	-4.419	-4.336	0.042	0.000	0.794	0.209	0.293	-0.322	-0.197
29 Pyridine-Uracil pi-pi	**-28.510**	-4.143	-4.352	-3.474	-4.185	-4.060	0.422	0.213	1.091	0.380	0.506	0.038	-0.464
30 Benzene-Ethene	**-5.987**	-0.702	-0.953	-0.452	-0.702	-0.661	1.054	0.803	1.304	1.054	1.095	-1.162	-0.201
31 Uracil-Ethene	**-14.132**	-1.254	-1.422	-1.045	-1.338	-1.296	1.049	0.882	1.258	0.966	1.008	-0.711	-0.209
32 Uracil-Ethyne	**-15.629**	-1.012	-1.054	-0.636	-1.012	-0.928	0.999	0.957	1.376	0.999	1.083	0.033	-0.217
33 Pyridine-Ethene	**-7.827**	-0.661	-0.911	-0.410	-0.661	-0.619	1.166	0.916	1.417	1.166	1.208	-0.995	-0.242
34 Pentane-Pentane	**-15.787**	-3.403	-3.654	-3.403	-3.445	-3.487	0.238	-0.013	0.238	0.197	0.155	-6.455	-0.937
35 Neopentane-Pentane	**-10.925**	-1.953	-1.994	-2.120	-2.162	-2.203	0.493	0.452	0.326	0.284	0.242	-4.043	-0.447
36 Neopentane-Neopentane	**-7.430**	-1.225	-1.309	-1.392	-1.350	-1.392	0.485	0.401	0.318	0.360	0.318	-2.521	-0.347
37 Cyclopentane-Neopentane	**-10.051**	-2.116	-2.199	-2.199	-2.241	-2.283	0.230	0.146	0.146	0.105	0.063	-4.081	-0.694
38 Cyclopentane-Cyclopentane	**-12.530**	-2.647	-2.897	-2.814	-2.856	-2.897	0.167	-0.084	0.000	-0.042	-0.084	-4.653	-1.016
39 Benzene-Cyclopentane	**-14.947**	-3.700	-3.617	-3.408	-3.366	-3.408	-0.506	-0.422	-0.213	-0.171	-0.213	-3.366	-0.732
40 Benzene-Neopentane	**-12.104**	-2.446	-2.070	-2.195	-2.153	-2.153	-0.013	0.364	0.238	0.280	0.280	-2.571	-0.272
41 Uracil-Pentane	**-20.269**	-4.148	-4.273	-4.189	-4.273	-4.273	0.176	0.050	0.134	0.050	0.050	-3.270	-0.259
42 Uracil-Cyclopentane	**-17.301**	-3.646	-3.813	-3.729	-3.813	-3.813	0.188	0.021	0.105	0.021	0.021	-2.308	-0.217

43 Uracil-Neopentane	**-15.520**	-2.542	-2.667	-2.500	-2.626	-2.626	0.493	0.368	0.535	0.410	0.410	-2.124	-0.242
44 Ethene-Pentane	**-8.383**	-0.941	-1.150	-0.983	-1.024	-1.066	0.836	0.627	0.794	0.753	0.711	-2.446	-0.439
45 Ethyne-Pentane	**-7.308**	-0.928	-1.054	-0.845	-0.803	-0.803	0.539	0.414	0.623	0.665	0.665	-1.263	-0.385
46 Peptide-Pentane	**-17.828**	-3.286	-3.370	-3.286	-3.370	-3.370	0.330	0.247	0.330	0.247	0.247	-3.579	-0.025
47 Benzene-Benzene TS	**-12.025**	-1.982	-1.606	-1.564	-1.522	-1.564	0.096	0.472	0.514	0.556	0.514	-1.062	-0.268
48 Pyridine-Pyridine TS	**-14.780**	-1.735	-1.317	-1.192	-1.192	-1.192	0.355	0.773	0.899	0.899	0.899	-0.773	-0.314
49 Benzene-Pyridine TS	**-13.927**	-2.379	-1.877	-1.877	-1.794	-1.835	-0.263	0.238	0.238	0.322	0.280	-1.208	-0.456
50 Benzene-Ethyne CH-pi	**-11.987**	-2.145	-1.183	-1.727	-1.476	-1.560	-0.811	0.151	-0.393	-0.142	-0.226	-0.682	-0.514
51 Ethyne-Ethyne TS	**-6.372**	-0.903	-0.610	-0.903	-0.819	-0.819	-0.439	-0.146	-0.439	-0.355	-0.355	-0.151	-0.736
52 Benzene-AcOH OH-pi	**-19.680**	-4.486	-3.566	-4.026	-4.110	-4.152	-2.316	-1.396	-1.856	-1.940	-1.982	0.280	0.280
53 Benzene-AcNH2 NH-pi	**-18.233**	-2.755	-2.212	-2.170	-2.295	-2.337	-0.991	-0.447	-0.406	-0.531	-0.573	-0.623	-0.247
54 Benzene-Water OH-pi	**-13.701**	-3.232	-2.103	-1.978	-2.270	-2.312	-1.944	-0.815	-0.690	-0.983	-1.024	-0.932	-0.347
55 Benzene-MeOH OH-pi	**-17.510**	-3.646	-2.893	-2.977	-3.144	-3.186	-1.518	-0.765	-0.849	-1.016	-1.058	-0.928	-0.301
56 Benzene-MeNH2 NH-pi	**-13.509**	-2.045	-1.417	-1.376	-1.543	-1.585	-0.059	0.569	0.610	0.443	0.401	-1.459	-0.288
57 Benzene-Peptide NH-pi	**-22.084**	-3.922	-3.086	-3.336	-3.253	-3.295	-1.033	-0.197	-0.447	-0.364	-0.406	-2.082	-0.493
58 Pyridine-Pyridine CH-N	**-17.334**	0.485	0.652	0.736	0.778	0.736	1.614	1.781	1.865	1.907	1.865	1.070	0.610
59 Ethyne-Water CH-O	**-11.916**	-1.212	-0.251	-1.296	-0.376	-0.669	-0.882	0.079	-0.966	-0.046	-0.339	0.502	-0.627
60 Ethyne-AcOH OH-pi	**-20.353**	-3.479	-3.019	-3.520	-3.604	-3.604	-3.152	-2.693	-3.194	-3.278	-3.278	-0.468	-1.472
61 Pentane-AcOH	**-12.175**	-2.835	-3.002	-2.918	-2.960	-3.002	-0.159	-0.326	-0.242	-0.284	-0.326	-1.957	-0.242
62 Pentane-AcNH2	**-14.776**	-2.659	-2.743	-2.743	-2.785	-2.785	0.201	0.117	0.117	0.075	0.075	-2.534	-0.234
63 Benzene-AcOH	**-15.892**	-3.215	-2.881	-2.546	-2.755	-2.797	-0.573	-0.238	0.096	-0.113	-0.155	-1.334	-0.079
64 Peptide-Ethene	**-12.539**	-1.426	-1.175	-1.091	-1.175	-1.217	0.309	0.560	0.644	0.560	0.518	-0.590	-0.297
65 Pyridine-Ethyne	**-16.686**	-1.292	-1.334	-1.208	-1.334	-1.334	-0.702	-0.744	-0.619	-0.744	-0.744	-0.665	-1.877
66 MeNH2-Pyridine	**-16.590**	-0.677	-0.468	0.033	-0.343	-0.343	1.112	1.321	1.823	1.447	1.447	-0.468	-0.134
MD		**-2.80**	**-2.60**	**-2.48**	**-2.64**	**-2.70**	**-0.79**	**-0.60**	**-0.48**	**-0.64**	**-0.69**	**-1.27**	**-0.93**

MAD	**2.81**	**2.63**	**2.51**	**2.66**	**2.72**	**1.20**	**1.07**	**1.12**	**1.18**	**1.21**	**1.39**	**0.96**
RMSD	**3.27**	**3.24**	**3.19**	**3.32**	**3.39**	**1.77**	**1.80**	**1.90**	**1.96**	**2.03**	**1.88**	**1.50**

BS1:6-311++G(*2d,p*) ; BS2:aug-cc-pVDZ；BS3:aug-cc-pVTZ；BS4:Def2QZVP；BS5:Def2TZVPP；BS6:6311++G(*3df,3pd*)

The reference binding energies (Ref.) are the S66A binding energies from Rezac et al.[14]

MD、MAD 与 RMAD 统计指标的定义

$$\mathrm{MD} = \frac{1}{\mathrm{n}}\sum_{sys}^{\mathrm{n}}\left(\Delta E - \triangle E_{\mathrm{ref}}\right)$$

$$\mathrm{MAD} = \frac{1}{\mathrm{n}}\sum_{sys}^{\mathrm{n}}\left|\Delta E - \triangle E_{\mathrm{ref}}\right|$$

$$\mathrm{RMSD} = \sqrt{\frac{1}{\mathrm{n}}\sum_{sys}^{\mathrm{n}}\left(\Delta E - \triangle E_{\mathrm{ref}}\right)^2}$$