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Interaction of 5-S-cysteinyl-dopamine with graphene oxide: An experimental and theoretical study for the detection of a Parkinson´s disease biomarker

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Supplementary Information

Table of Content:

Figure S-1. UV-Vis absorption spectrum of synthesized CysDA after HPLC purification

Figure S-2. UV-vis absorption spectrum of grapheme oxide (GO) solution.

Figure S-3. XPS spectrum of GO.

Figure S-4. Normal Raman spectrum of GO.

Figure S-5. Normal Raman spectrum of lyophilized CysDA deposited on Al.

Figure S-6. Classification of hydrogen bonds according to geometrical criteria.

Table S-1. Geometrical and topological parameters of the non-covalent interactions.

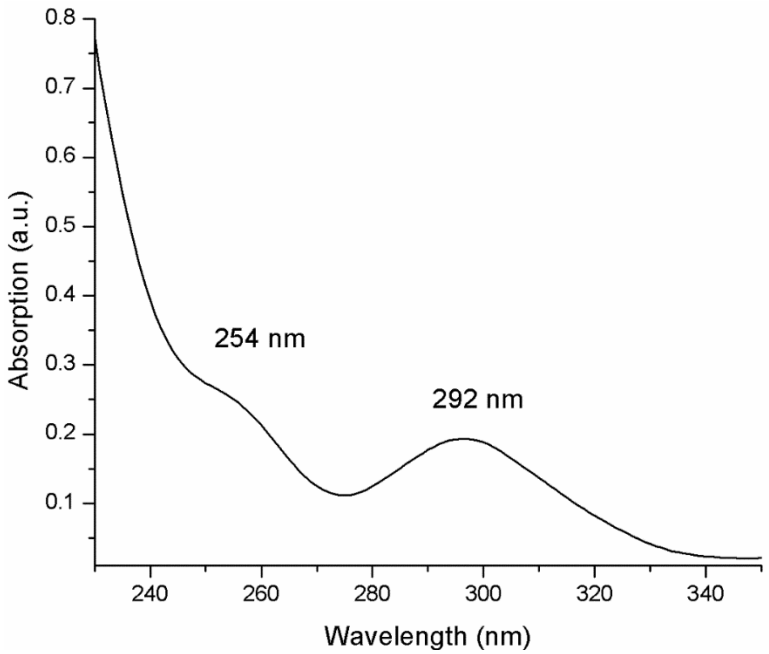

Figure S-1. UV-Vis absorption spectrum of synthesized CysDA after HPLC purification

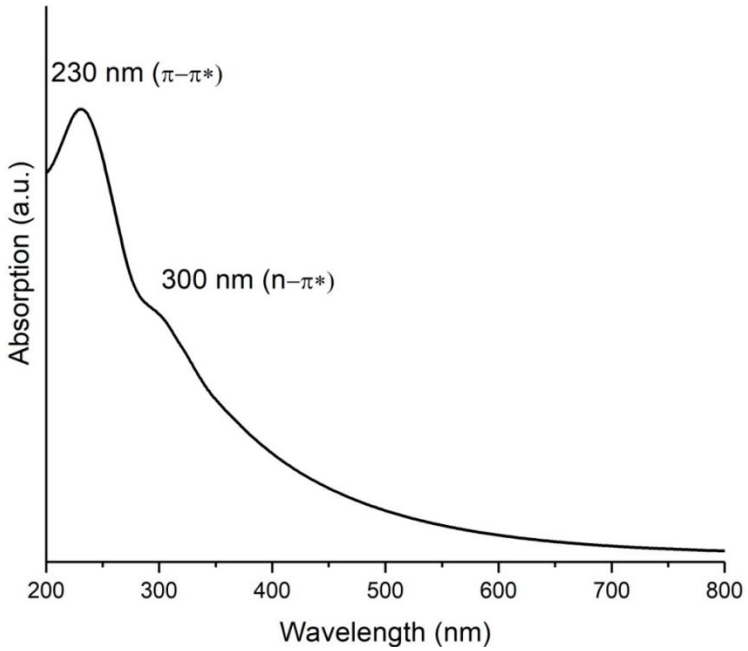

Figure S-2. UV-visabsorption spectrumof grapheme oxide (GO) solution.

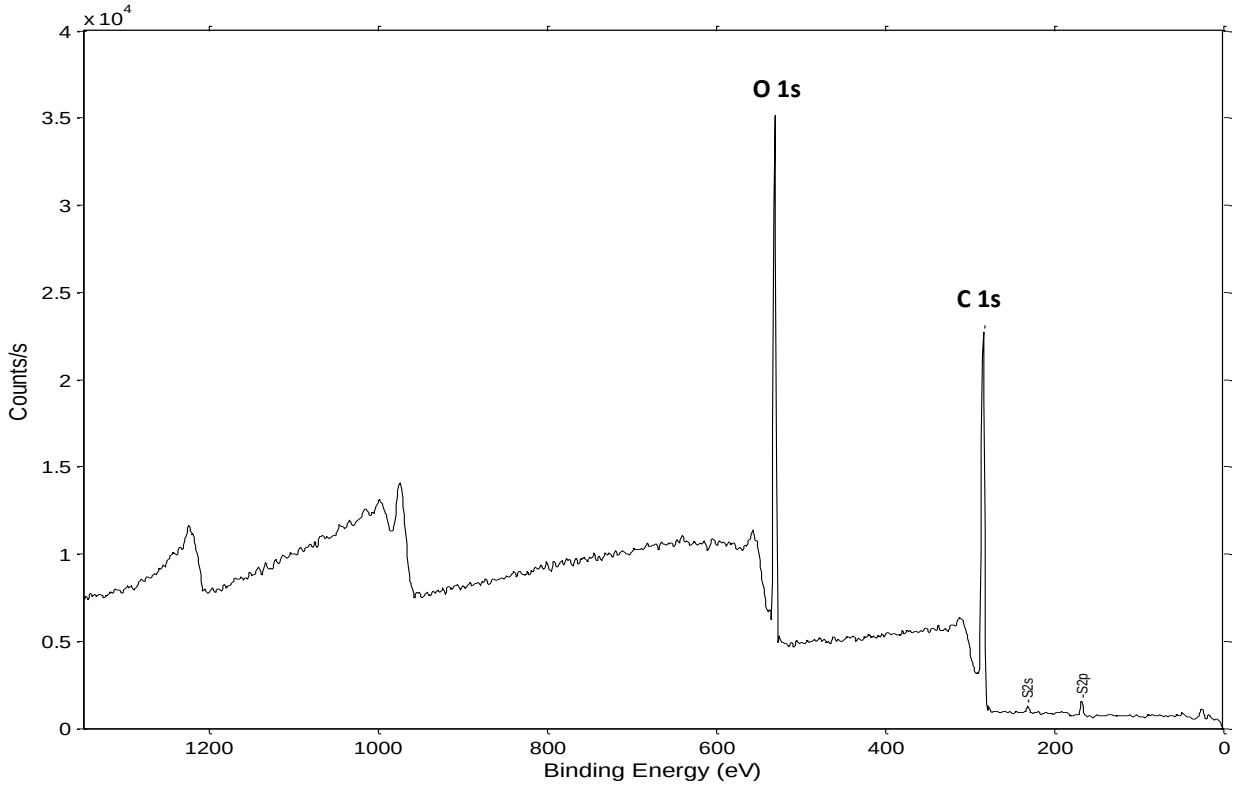

Figure S-3. XPS spectrum of GO.

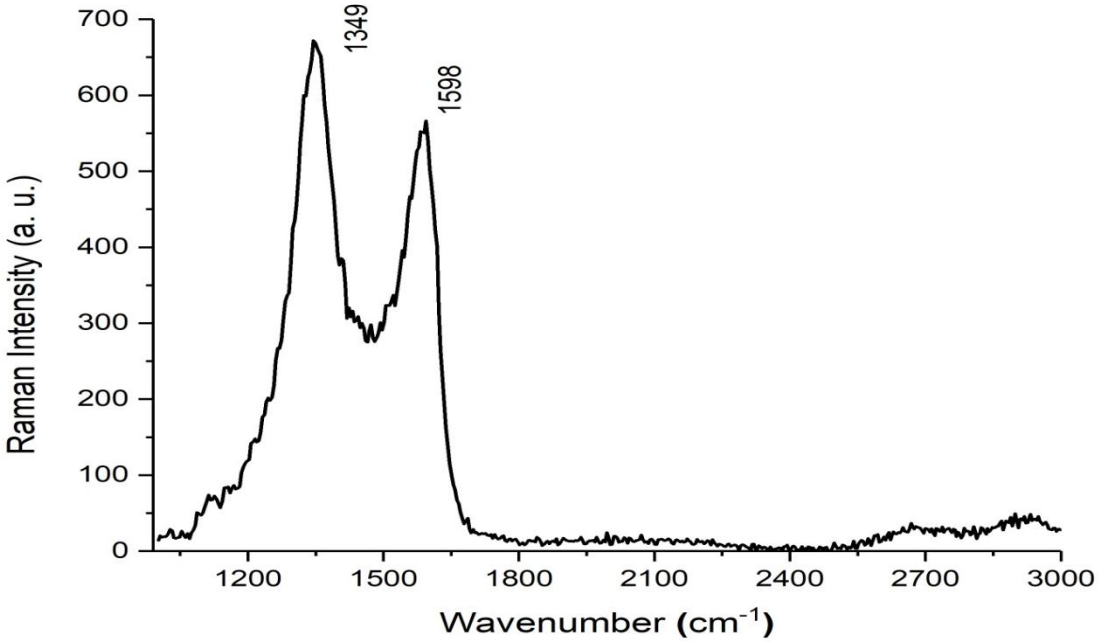

Figure S-4. Normal Raman spectrum of GO.

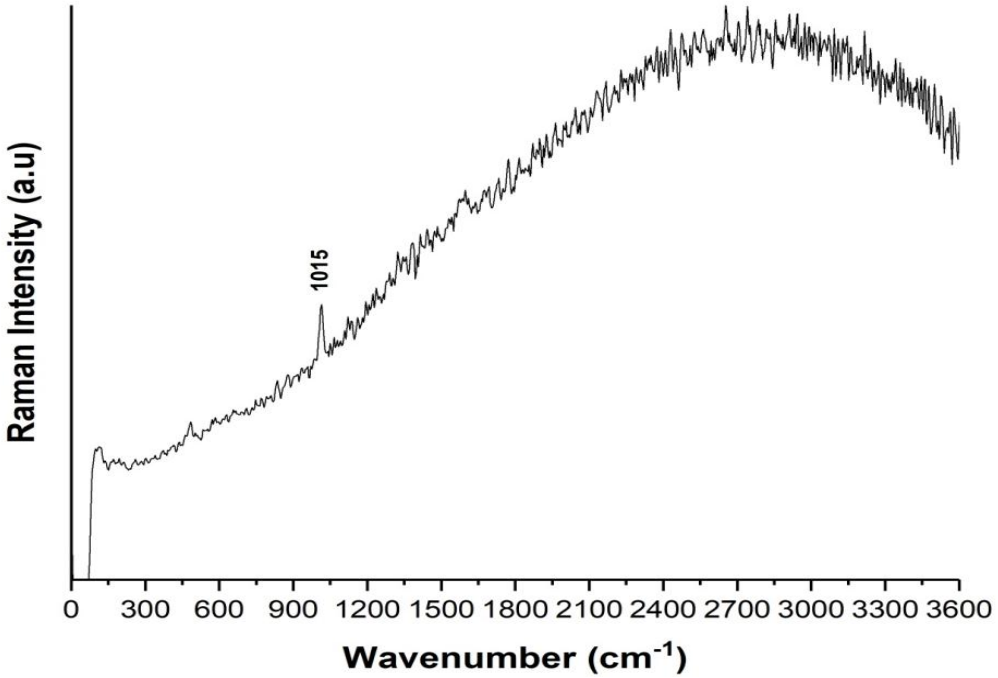

Figure S-5. Normal Raman spectrum of lyophilized CysDA deposited on Al.

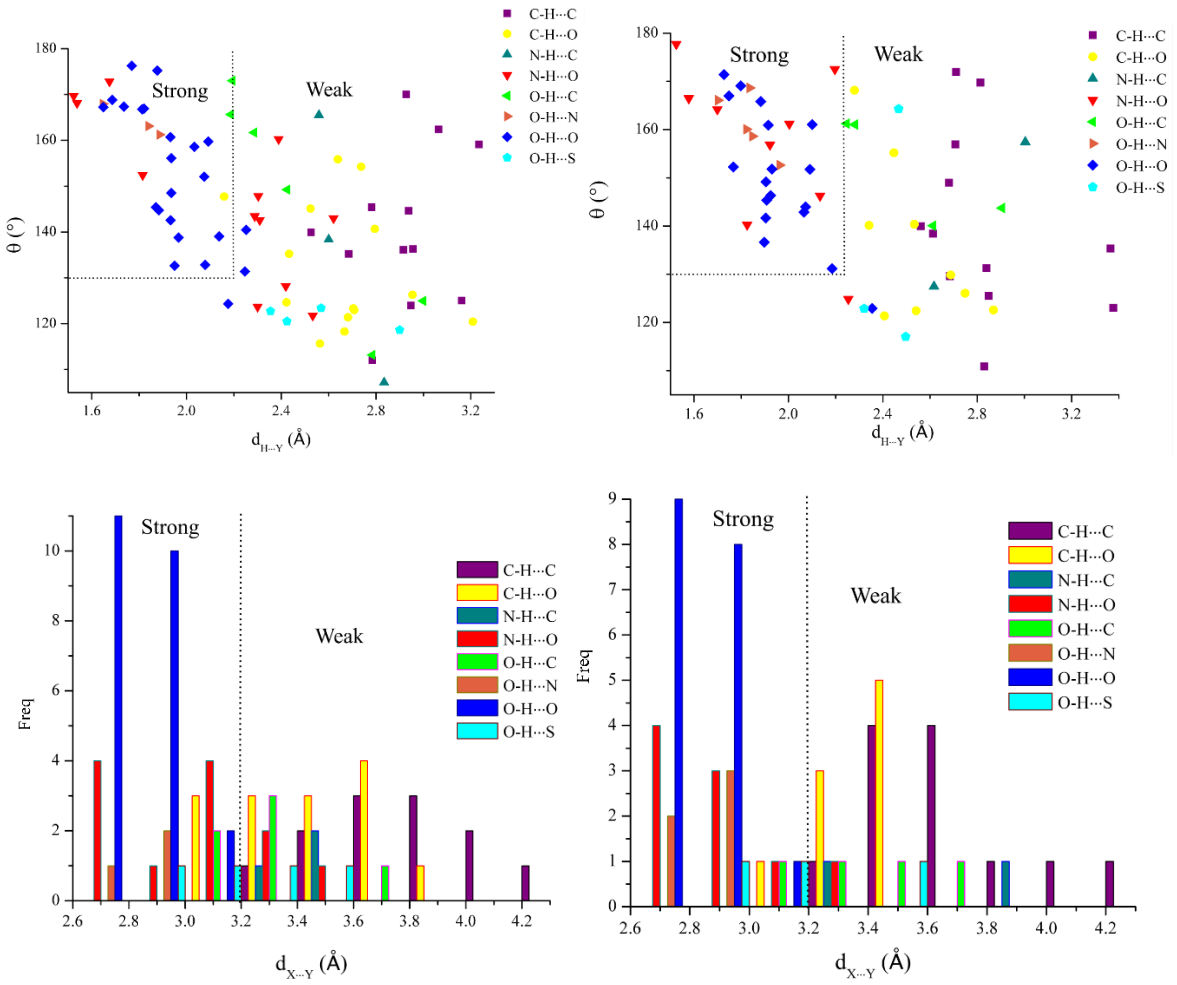

Figure S-6. Classification of hydrogen bonds according to geometrical criteria: H···Y and X ··· Y distances ($d_{H\cdots Y}$ and $d_{X\cdots Y}$, respectively, where X is the atom to which H is covalently bonded and Y is the atom forming the HB), as well as the X-H···Y angles (θ). Hydrated and solvent-free complexes in right and left columns, respectively.

Table S-1. Geometrical and topological parameters of the non-covalent interactions found in the studied structures of **1**, **2**, **3** and **4**. The laplacian of *ρ* evaluated at the BCP is positive in all cases.

1a

HB	$d_{H\cdots Y}$ (Å)	d_{X-Y} (Å)	Angle (θ)	ρ_{BCP}(a.u.)	EML (kcal/mol)	Freq.
C-H···C	2.526	3.432	139.90	0.0111	-1.9	
C-H···C	2.785	3.348	112.02	0.0081	-1.4	

C-H···C	3.235	4.269	159.09	0.0025	-0.3	
C-H···C	2.916	3.777	136.10	0.0057	-0.9	4
C-H···O	3.209	3.871	120.45	0.0022	-0.3	
C-H···O	2.954	3.701	126.32	0.0039	-0.5	
C-H···O	2.708	3.429	122.96	0.0069	-1.2	
C-H···O	2.704	3.426	123.33	0.0064	-1.1	
C-H···O	2.639	3.658	155.85	0.0054	-1.0	
C-H···O	2.667	3.319	118.30	0.0070	-1.2	6
N-H···O	1.675	2.728	172.82	0.0501	-15.3	
N-H···O	2.300	2.990	123.67	0.0126	-2.7	
N-H···O	1.815	2.776	152.41	0.0351	-9.5	
N-H···O	2.389	3.360	160.22	0.0096	-1.7	4
O-H···C	2.425	3.297	149.25	0.0124	-2.0	
O-H···C	2.999	3.642	124.98	0.0041	-0.6	2
O-H···O	2.092	3.023	159.74	0.0164	-3.5	
O-H···O	1.932	2.868	160.69	0.0247	-6.1	
O-H···O	1.883	2.745	144.74	0.0289	-7.5	
O-H···O	1.736	2.707	167.33	0.0406	-12.0	
O-H···O	2.079	2.833	132.83	0.0198	-4.7	
O-H···O	2.138	2.949	139.04	0.0168	-3.5	6
NHB						
C···O				0.0082	-1.4	1
C···C				0.0048	-0.7	1

1b

HB	$d_{H\cdots Y}$ (Å)	d_{X-Y} (Å)	Angle (θ)	ρ_{BCP}(a.u.)	EML (kcal/mol)	Freq.

C-H···C	3.162	3.886	125.04	0.0031	-0.4	
C-H···C	2.947	3.668	123.95	0.0061	-0.9	
C-H···C	2.956	3.820	136.27	0.0052	-0.8	3
C-H···O	2.524	3.474	145.11	0.0093	-1.7	
C-H···O	2.737	3.746	154.23	0.0058	-0.9	
C-H···O	2.433	3.295	135.25	0.0112	-2.2	3
N-H···O	2.533	3.190	121.76	0.0075	-1.5	
N-H···O	2.309	3.178	142.58	0.0121	-2.4	2
O-H···C	2.194	3.164	173.01	0.0174	-2.9	1
O-H···N	1.647	2.656	167.94	0.0634	-18.5	1
O-H···O	2.247	2.980	131.39	0.0117	-2.6	
O-H···O	2.176	2.843	124.34	0.0159	-3.7	2
O-H···S	2.424	3.038	120.51	0.0198	-4.0	1
NHB						
C···O				0.0107	-2.2	
C···O				0.0059	-1.0	2
O···O				0.0092	-1.7	1

1c

HB	$d_{H\cdots Y}$ (Å)	d_{X-Y} (Å)	Angle (θ)	ρ_{BCP}(a.u.)	EML (kcal/mol)	Freq.
C-H···C	2.928	4.007	170.01	0.0046	-0.7	1
C-H···O	2.682	3.379	121.39	0.0073	-1.3	
C-H···O	2.563	3.19	115.66	0.0090	-1.8	2
N-H···O	2.288	3.161	143.42	0.0117	-2.4	
N-H···O	2.419	3.149	128.19	0.0091	-1.9	2
O-H···C	2.187	3.144	165.64	0.0191	-3.2	

O-H···C	2.285	3.225	161.7	0.0143	-2.3	2
O-H···O	1.933	2.776	142.58	0.0252	-6.3	
O-H···O	1.95	2.708	132.65	0.0258	-6.6	
O-H···O	1.813	2.776	166.77	0.0341	-9.3	3
NHB						
C···C				0.0041	-0.5	1
C···S				0.0046	-0.7	
C···S				0.0041	-0.5	
C···S				0.0063	-0.9	
C···S				0.0051	-0.6	4
C···O				0.0090	-1.7	1
C···N				0.0061	-1.0	1

2a

HB	$d_{H\cdots Y}$ (Å)	d_{X-Y} (Å)	Angle (θ)	ρ_{BCP}(a.u.)	EML (kcal/mol)	Freq.
C-H···C	2.685	3.547	135.23	0.0079	-1.3	
C-H···C	2.782	3.731	145.38	0.0068	-1.0	
C-H···C	2.938	3.887	144.60	0.0057	-0.8	
C-H···C	3.064	4.126	162.37	0.0043	-0.6	4
C-H···O	2.422	3.169	124.65	0.0112	-2.4	1
N-H···O	1.524	2.602	169.66	0.0727	-25.4	
N-H···O	2.621	3.487	142.99	0.0065	-1.1	2
O-H···N	1.840	2.803	163.09	0.0396	-9.8	1
O-H···O	1.967	2.776	138.78	0.0217	-5.4	
O-H···O	1.936	2.818	148.52	0.0261	-6.4	
O-H···O	2.075	2.966	152.06	0.0182	-4.0	

O-H···O	2.252	3.071	140.47	0.0127	-2.4	4
O-H···S	2.900	3.472	118.64	0.0066	-1.0	1
NHB						
C···C				0.0038	-0.5	
C···C				0.0052	-0.8	
C···C				0.0043	-0.6	3
C···O				0.0049	-0.7	
C···O				0.0093	-1.8	2
C···S				0.0080	-1.3	1
S···O				0.0040	-0.6	1

2b

HB	$d_{H\cdots Y}$ (Å)	d_{X-Y} (Å)	Angle (θ)	ρ_{BCP}(a.u.)	EML (kcal/mol)	Freq.
C-H···O	2.795	3.703	140.67	0.0041	-0.7	1
N-H···C	2.834	3.282	107.20	0.0077	-1.4	
N-H···C	2.559	3.552	165.50	0.0096	-1.5	2
N-H···O	1.538	2.604	168.09	0.0694	-24.0	1
O-H···N	1.887	2.849	161.22	0.0359	-8.3	1
O-H···O	1.871	2.731	145.38	0.0299	-8.1	
O-H···O	1.769	2.753	176.25	0.0393	-11.2	
O-H···O	1.821	2.785	166.91	0.0314	-8.5	
O-H···O	1.649	2.641	167.23	0.0510	-16.2	4
O-H···S	2.355	2.999	122.73	0.0224	-4.5	1
NHB						
C···N				0.0076	-1.5	1
C···O				0.0081	-1.5	

C···O				0.0068	-1.2	
C···O				0.0023	-0.3	3

2c

HB	$d_{H\cdots Y}$ (Å)	d_{X-Y} (Å)	Angle (θ)	ρ_{BCP}(a.u.)	EML (kcal/mol)	Freq.
C-H···O	2.159	3.132	147.73	0.0184	-4.0	1
N-H···C	2.600	3.424	138.38	0.0091	-1.5	1
N-H···O	2.303	3.211	147.81	0.0116	-2.2	1
O-H···C	2.785	3.294	113.19	0.0064	-1.0	1
O-H···O	2.033	2.963	158.59	0.0204	-4.4	
O-H···O	1.687	2.672	168.81	0.0469	-14.5	
O-H···O	1.877	2.856	175.2	0.0285	-7.2	
O-H···O	1.936	2.858	156.1	0.0248	-6.0	4
O-H···S	2.568	3.207	123.4	0.0139	-2.5	1
NHB						
C···O				0.0073	-1.2	
C···O				0.0031	-0.4	2
O···O				0.0116	-2.7	
O···O				0.0027	-0.4	
O···O				0.0062	-1.2	
O···O				0.0027	-0.4	4

3a

HB	$d_{H\cdots Y}$ (Å)	d_{X-Y} (Å)	Angle (θ)	ρ_{BCP}(a.u.)	EML (kcal/mol)	Freq.
C-H···C	2.561	3.469	139.95	0.0101	-1.7	
C-H···C	2.830	3.373	110.86	0.0077	-1.3	

C-H···C	3.365	4.209	135.32	0.0023	-0.2	
C-H···C	2.613	3.502	138.39	0.0098	-1.7	4
C-H···O	2.869	3.570	122.57	0.0042	-0.6	
C-H···O	2.688	3.483	129.82	0.0063	-1.0	
C-H···O	2.447	3.464	155.20	0.0080	-1.6	
C-H···O	2.749	3.496	126.05	0.0055	-0.9	4
N-H···O	2.254	2.960	124.84	0.0139	-3.0	
N-H···O	2.197	3.209	172.52	0.0134	-2.6	
N-H···O	1.525	2.619	177.72	0.0740	-25.7	3
O-H···O	2.091	2.984	151.74	0.0168	-3.7	
O-H···O	1.915	2.853	160.90	0.0257	-6.5	
O-H···O	1.905	2.787	149.16	0.0239	-6.3	
O-H···O	2.185	2.920	131.16	0.0162	-3.5	
O-H···O	2.073	2.923	143.97	0.0192	-4.2	5
O-H···S	2.497	3.067	117.05	0.0172	-3.5	1
NHB						
C···O				0.0090	-1.7	
C···O				0.0081	-1.4	2
C···C				0.0042	-0.6	1

3b

HB	$d_{H\cdots Y}$ (Å)	d_{X-Y} (Å)	Angle (θ)	ρ_{BCP}(a.u.)	EML (kcal/mol)	Freq.
C-H···C	2.814	3.893	169.71	0.0062	-0.9	1
C-H···H	2.664	3.461	129.17	0.0021	-0.3	1
C-H···O	2.534	3.439	140.36	0.0076	-1.4	1
N-H···C	3.004	3.963	157.43	0.0039	-0.5	1

O-H···N	1.822	2.78	160.06	0.0421	-10.5	
O-H···N	1.702	2.698	166.09	0.0558	-15.5	2
O-H···O	1.727	2.711	171.42	0.0417	-12.4	1
NHB						
C···O				0.0112	-2.4	
C···O				0.0084	-1.6	2
O···O				0.0090	-2.0	1

3c

HB	$d_{H\cdots Y}$ (Å)	d_{X-Y} (Å)	Angle (θ)	ρ_{BCP}(a.u.)	EML (kcal/mol)	Freq.
C-H···C	2.711	3.796	171.95	0.0068	-1.1	1
C-H···O	2.407	3.119	121.34	0.0120	-2.5	1
O-H···C	2.247	3.187	161.23	0.0173	-2.9	
O-H···C	2.282	3.219	161.03	0.0143	-2.3	
O-H···C	2.905	3.735	143.73	0.0044	-0.6	3
O-H···O	1.908	2.771	145.34	0.0265	-6.8	
O-H···O	1.767	2.675	152.26	0.0364	-10.6	2
NHB						
C···O				0.0047	-0.7	
C···O				0.0088	-1.7	
C···O				0.0070	-1.3	
C···O				0.0071	-1.2	4
C···S				0.0062	-0.9	
C···S				0.0059	-0.8	
C···S				0.0063	-0.9	3
O···N				0.0024	-0.3	1

O···O				0.0059	-1.1	1

4a

HB	$d_{H\cdots Y}$ (Å)	d_{X-Y} (Å)	Angle (θ)	ρ_{BCP}(a.u.)	EML (kcal/mol)	Freq.
C-H···O	2.342	3.245	140.13	0.0123	-2.6	1
N-H···O	1.699	2.722	164.18	0.0441	-13.1	
N-H···O	2.134	3.034	146.24	0.0168	-3.7	
N-H···O	1.922	2.903	156.86	0.0248	-6.0	3
O-H···C	2.613	3.421	140.05	0.0087	-1.3	1
O-H···N	1.848	2.800	158.62	0.0394	-9.6	1
O-H···O	2.355	2.997	122.90	0.0106	-2.2	
O-H···O	1.930	2.826	151.80	0.0233	-6.0	
O-H···O	1.925	2.790	146.33	0.0263	-6.6	
O-H···O	2.066	2.898	142.88	0.0188	-4.4	4
NHB						
C···O				0.0102	-2.1	
C···O				0.0069	-1.2	
C···O				0.0005	-0.1	3

4b

HB	$d_{H\cdots Y}$ (Å)	d_{X-Y} (Å)	Angle (θ)	ρ_{BCP}(a.u.)	EML (kcal/mol)	Freq.
C-H···C	2.685	3.487	129.58	0.0076	-1.2	
C-H···C	2.850	3.594	125.51	0.0062	-1.0	
C-H···C	2.840	3.656	131.23	0.0071	-1.2	
C-H···C	2.681	3.665	148.96	0.0086	-1.4	4.0
C-H···O	2.541	3.257	122.41	0.0090	-1.8	1.0
N-H···O	1.578	2.633	166.46	0.0627	-20.9	1.0

O-H···N	1.836	2.817	168.64	0.0398	-9.8	1.0
O-H···O	1.904	2.738	141.65	0.0255	-6.6	
O-H···O	1.883	2.841	165.83	0.0276	-7.0	
O-H···O	2.101	3.035	161.03	0.0164	-3.5	3.0
O-H···S	2.467	3.410	164.29	0.0151	-2.5	1.0
NHB						
C···C				0.0026	-0.3	
C···C				0.0039	-0.5	2.0
C···O				0.0094	-1.7	1.0
C···S				0.0062	-0.9	
C···S				0.0091	-1.6	2.0

4c

HB	$d_{H\cdots Y}$ (Å)	d_{X-Y} (Å)	Angle (θ)	ρ_{BCP}(a.u.)	EML (kcal/mol)	Freq.
C-H···C	3.377	4.070	123.02	0.0025	-0.3	
C-H···C	2.708	3.733	156.91	0.0075	-1.2	2
C-H···O	2.280	3.352	168.16	0.0116	-2.4	1
N-H···C	2.617	3.335	127.46	0.0101	-1.7	1
N-H···O	1.825	2.707	140.26	0.0341	-9.3	
N-H···O	2.004	2.999	161.17	0.0215	-4.8	2
O-H···N	1.963	2.881	152.61	0.0300	-6.5	1
O-H···O	1.898	2.691	136.62	0.0282	-7.6	
O-H···O	1.748	2.715	166.97	0.0411	-12.1	
O-H···O	1.798	2.780	169.06	0.0348	-9.5	3
O-H···S	2.321	2.967	122.86	0.0229	-4.8	1
NHB						
C···O				0.0072	-1.3	

C···O				0.0045	-0.7	
C···O				0.0088	-1.6	3
O···O				0.0059	-1.2	1