Supplementary File 6. Hydrogen bond acceptor properties of the fluorinated ethane derivatives.

TABLE 1: Hydrogen bond energies

	donor	water		amideD		imidazole		hydroxyl		indole		CH_3SH	
[a]method	acceptor	[b]ΔE	[c]ΔE_{BSSE}	[b]ΔE	[c]ΔE_{BSSE}	[b]ΔE	[c]ΔE_{BSSE}	[b]ΔE	[c]ΔE_{BSSE}	[b]ΔE	[c]ΔE_{BSSE}	[b]ΔE	[c]ΔE_{BSSE}
HF	CH_3CH_2F	-3.43	-3.22	-2.71	-2.66	-3.87	-3.66	-3.15	-2.90	-3.26	-3.04	-1.35	-1.09
	CH_3CHF_2	-3.19	-2.92	-2.12	-1.95	-3.22	-2.92	-2.59	-2.20	-2.88	-2.49	-1.32	-0.97
	$CH_3CF_2CH_3$	-3.32	-3.01	-2.05	-1.93	-3.22	-2.94	-2.70	-2.29	-3.18	-2.73	-1.17	-0.85
	CH_3CF_3	-2.65	-2.32	-1.49	-1.26	-2.07	-1.75	-2.64	-2.19	-1.88	-1.38	-0.87	-0.52
MP2	CH_3CH_2F	-4.73	-3.67	-4.41	-3.37	-4.88	-4.17	-4.93	-3.74	-4.59	-3.74	-2.55	-1.43
	CH_3CHF_2	-4.43	-3.41	-3.60	-2.68	-4.58	-3.59	-4.38	-3.05	-5.02	-3.52	-3.73	-1.79
	$CH_3CF_2CH_3$	-4.95	-3.75	-3.58	-2.72	-4.62	-3.72	-4.66	-3.23	-5.26	-3.81	-3.93	-1.81
	CH_3CF_3	-3.95	-2.78	-2.80	-1.74	-3.12	-2.29	-4.20	-3.00	-3.48	-2.24	-2.44	-0.89
BLYP	CH_3CH_2F	-3.83	-3.41	-2.71	-2.60	-3.74	-3.45	-3.40	-2.93	-3.04	-2.97	-1.46	-0.99
	CH_3CHF_2	-3.07	-2.69	-1.93	-1.74	-2.93	-2.64	-2.69	-2.21	-2.80	-2.55	-1.11	-0.72
	$CH_3CF_2CH_3$	-3.55	-3.01	-1.94	-1.73	-3.44	-2.99	-2.82	-2.19	-3.25	-2.68	-1.12	-0.68
	CH_3CF_3	-2.65	-2.19	-1.34	-1.01	-1.86	-1.65	-2.50	-2.00	-1.54	-1.31	-0.72	-0.32
B3LYP	CH_3CH_2F	-4.16	-3.77	-3.00	-2.93	-4.26	-3.82	-3.81	-3.34	-3.78	-3.29	-1.68	-1.25
	CH_3CHF_2	-3.58	-3.20	-2.31	-2.12	-3.14	-2.82	-3.09	-2.63	-3.14	-2.64	-1.42	-1.03
	$CH_3CF_2CH_3$	-4.07	-3.52	-2.33	-2.06	-3.73	-3.23	-3.30	-2.65	-3.63	-3.14	-1.42	-0.96
	CH_3CF_3	-3.10	-2.65	-1.54	-1.31	-2.14	-1.86	-2.96	-2.49	-2.08	-1.50	-0.95	-0.52

[a] All the methods were applied with the same basis set (6-311G**++). [b] Hydrogen bond energy without BSSE correction. [c] Hydrogen bond energy with BSSE correction. Energies are in kcal/mol.

TABLE 2: Hydrogen bond geometric characteristics

	donor	water			amideD			imidazole			hydroxyl			indole			CH_3SH		
[a]method	acceptor	[b]d, Å	[c]angle, °	[d]Δr, mÅ	[b]d, Å	[c]angle, °	[d]Δr, mÅ	[b]d, Å	[c]angle, °	[d]Δr, mÅ	[b]d, Å	[c]angle, °	[d]Δr, mÅ	[b]d, Å	[c]angle, °	[d]Δr, mÅ	[b]d, Å	[c]angle, °	[d]Δr, mÅ
HF	CH_3CH_2F	2.084	154.831	2.5	2.222	172.571	3.0	2.103	178.140	2.3	2.119	155.562	1.9	2.153	176.423	2.4	2.482	175.159	0.0
	CH_3CHF_2	2.211	123.177	1.5	2.370	170.829	1.6	2.234	174.468	1.5	2.266	149.053	1.1	2.271	171.641	1.2	2.646	159.513	0.4
	$CH_3CF_2CH_3$	2.572	139.011	1.8	2.291	174.321	1.4	2.172	172.270	2.0	2.220	155.213	1.2	2.250	172.265	1.6	2.584	155.533	-0.5
	CH_3CF_3	2.509	125.460	1.1	2.451	169.959	0.5	2.311	170.529	0.9	2.472	126.931	0.9	2.236	169.709	0.6	2.762	162.810	-0.5
MP2	CH_3CH_2F	2.010	148.567	3.7	2.026	175.387	3.2	2.026	177.697	2.9	2.026	175.387	3.2	2.026	177.697	2.9	2.369	148.934	-2.3
	CH_3CHF_2	2.247	122.209	2.1	2.152	163.025	1.5	2.125	176.170	1.9	2.152	163.025	1.5	2.125	176.170	1.9	2.477	149.535	-0.1
	$CH_3CF_2CH_3$	2.129	137.015	2.8	2.047	171.537	1.9	2.089	170.470	2.0	2.047	171.537	1.9	2.089	170.470	2.0	2.427	134.670	1.6
	CH_3CF_3	2.352	124.691	1.6	2.233	166.900	1.8	2.200	169.361	0.6	2.233	166.900	1.8	2.200	169.361	0.6	2.528	160.231	0.4
BLYP	CH_3CH_2F	1.989	160.366	5.0	2.144	165.543	2.5	2.049	178.083	6.4	2.052	157.902	2.9	2.249	177.162	3.1	2.363	171.397	0.4
	CH_3CHF_2	2.204	130.982	2.3	2.365	155.522	1.6	2.205	172.500	5.0	2.168	151.905	1.5	2.254	173.347	0.6	2.506	165.807	-0.2
	$CH_3CF_2CH_3$	2.090	144.344	3.3	2.255	176.468	2.9	2.127	169.894	2.3	2.185	152.022	2.0	2.187	172.005	3.3	2.487	155.774	-0.1
	CH_3CF_3	2.314	132.532	1.6	2.457	165.471	1.2	2.261	169.937	0.4	2.592	122.560	0.3	2.234	173.871	1.6	2.831	154.534	-0.2
B3LYP	CH_3CH_2F	1.961	158.266	5.1	2.079	174.026	3.2	2.030	174.546	4.4	2.013	155.452	2.8	2.013	155.452	2.8	2.303	170.430	1.2
	CH_3CHF_2	2.174	129.169	2.7	2.312	155.892	1.8	2.184	171.791	2.8	2.139	150.998	1.6	2.139	150.998	1.6	2.475	158.554	0.2
	$CH_3CF_2CH_3$	2.080	142.302	3.0	2.189	176.309	1.2	2.100	171.442	3.3	2.128	152.521	2.1	2.128	152.521	2.1	2.420	154.250	-0.1
	CH_3CF_3	2.277	131.102	1.6	2.329	162.255	2.4	2.247	169.811	2.4	2.460	123.314	0.7	2.460	123.314	0.7	2.671	152.755	-0.5

[a]All the methods were applied with the same basis set (6-311G**++). [b]Hydrogen bond length. [c]Hydrogen bond angle. [d]D-H bond shift.

TABLE 3: Hydrogen bond charge transfer characteristics: hydrogen and acceptor charge transfer

	donor	water		amideD		imidazole		hydroxyl		indole		CH_3SH	
[a]method	acceptor	[b]Δq(H)	[c]Δq(A)	[b]Δq(H)	[c]Δq(A)	[b]Δq(H)	[c]Δq(A)	[b]Δq(H)	[c]Δq(A)	[b]Δq(H)	[c]Δq(A)	[b]Δq(H)	[c]Δq(A)
HF	CH_3CH_2F	0.023	0.007	0.115	0.006	0.199	-0.015	0.089	0.020	0.166	-0.006	-0.014	0.028
	CH_3CHF_2	0.016	-0.008	0.109	0.022	0.291	0.010	0.026	0.008	0.115	0.020	0.014	0.029
	$CH_3CF_2CH_3$	0.010	-0.012	0.163	-0.004	0.178	0.031	0.076	0.030	0.143	0.044	0.010	0.014
	CH_3CF_3	0.008	-0.009	0.111	0.014	0.235	0.006	0.014	0.004	0.107	0.013	0.001	0.020
MP2	CH_3CH_2F	0.009	0.005	0.088	0.016	0.185	-0.014	0.056	0.022	0.169	-0.004	-0.018	0.019
	CH_3CHF_2	0.012	-0.014	0.078	0.024	0.116	0.006	0.018	0.008	0.094	0.025	0.020	0.027
	$CH_3CF_2CH_3$	-0.003	-0.016	0.136	0.000	0.170	0.021	0.054	0.031	0.150	0.042	0.011	0.010
	CH_3CF_3	0.016	-0.011	0.120	0.012	0.163	-0.001	0.007	0.000	0.118	0.013	0.006	0.017
BLYP	CH_3CH_2F	-0.006	0.007	0.103	-0.001	0.190	-0.012	-0.030	0.020	0.044	0.016	0.141	0.000
	CH_3CHF_2	0.003	-0.010	0.051	0.022	0.102	0.007	0.002	0.025	0.008	0.006	0.116	0.020
	$CH_3CF_2CH_3$	-0.011	-0.011	0.116	0.006	0.171	0.029	0.002	0.014	0.036	0.027	0.155	0.043
	CH_3CF_3	0.001	-0.015	0.063	0.001	0.156	0.002	-0.001	0.019	0.005	0.008	0.125	0.015
B3LYP	CH_3CH_2F	-0.002	0.008	0.113	0.001	0.188	-0.012	0.052	0.017	0.178	-0.009	-0.025	0.022
	CH_3CHF_2	0.006	-0.012	0.056	0.023	0.103	0.011	0.015	0.010	0.114	0.018	0.008	0.027
	$CH_3CF_2CH_3$	-0.007	-0.012	0.133	-0.001	0.177	0.029	0.042	0.029	0.153	0.044	0.002	0.007
	CH_3CF_3	0.003	-0.015	0.087	0.011	0.157	0.002	0.007	0.011	0.112	0.013	-0.001	0.019

[a]All the methods were applied with the same basis set (6-311G**++). [b]Hydrogen charge transfer.

[c]Acceptor charge transfer.

TABLE 4: Hydrogen bond energies

	donor	water		amided		imidazole		hydroxyl		indole		CH_3SH	
[a]method	acceptor	[b]ΔE	[c]ΔE_{BSSE}	[b]ΔE	[c]ΔE_{BSSE}	[b]ΔE	[c]ΔE_{BSSE}	[b]ΔE	[c]ΔE_{BSSE}	[b]ΔE	[c]ΔE_{BSSE}	[b]ΔE	[c]ΔE_{BSSE}
HF	amideA	-6.26	-6.06	-5.31	-5.36*	-7.31	-7.16	-5.68	-5.47	-6.20	-6.04	-2.48	-2.25
	imidazole	-6.02	-5.73	-5.14	-5.17*	-6.89	-6.73	-5.49	-5.24	-5.80	-5.60	-2.48	-2.18
	ketone	-5.30	-5.05	-4.37	-4.33*	-5.92	-5.68	-4.93	-4.65	-5.15	-4.89	-2.09	-1.78
	furan	-2.77	-2.42	-1.89	-1.70	-3.31	-2.98	-2.55	-2.21	-2.20	-1.91	-0.96	-0.61
MP2	amideA	-7.54	-6.25	-6.31	-5.46	-8.70	-7.73	-7.99	-6.94	-8.27	-7.33	-4.01	-2.68
	imidazole	-7.80	-6.82	-8.42	-7.52	-10.05	-9.16	-8.27	-6.98	-9.58	-8.49	-5.19	-3.64
	ketone	-6.55	-5.34	-5.72	-4.89	-6.89	-6.07	-6.89	-5.51	-6.92	-5.81	-3.33	-2.29
	furan	-3.78	-2.88	-4.73	-3.36	-5.30	-4.34	-4.26	-3.14	-4.54	-3.34	-3.91	-1.89
B3LYP	amideA	-6.91	-6.38	-5.05	-5.14	-7.05	-6.75	-6.20	-5.96	-6.46	-5.97	-2.62	-2.20
	imidazole	-7.20	-6.88	-5.74	-5.89	-7.97	-7.59	-6.02	-5.95	-7.12	-6.48	-2.92	-2.56
	ketone	-5.87	-5.37	-3.78	-3.96	-5.43	-5.14	-5.10	-4.85	-5.06	-4.73	-2.08	-1.68
	furan	-2.86	-2.42	-1.47	-1.71	-3.05	-2.94	-2.30	-2.04	-2.71	-1.97	-0.51	-0.27
B3PLYP	amideA	-7.41	-7.00	-5.61	-5.73	-7.79	-7.57	-6.81	-6.76	-6.94	-6.68	-2.94	-2.60
	imidazole	-7.50	-7.25	-6.31	-6.44	-8.43	-8.07	-6.54	-6.48	-7.50	-6.90	-3.25	-2.89
	ketone	-6.56	-5.92	-4.61	-4.55	-5.70	-5.24	-5.91	-5.45	-5.66	-5.06	-2.62	-2.05
	furan	-3.30	-3.00	-1.97	-2.16	-3.46	-3.33	-2.75	-2.48	-2.99	-2.28	-0.88	-0.62

[a]All the methods were applied with the same basis set (6-311G**++). [b] Hydrogen bond energy without BSSE correction. [c] Hydrogen bond energy with BSSE correction. Energies are in kcal/mol.

TABLE 5: Hydrogen bond geometric characteristics

	donor	water			amideD			imidazole			hydroxyl			indole			CH_3SH		
[a]method	acceptor	[b]d, Å	[c]angle, °	[d]Δr, mÅ	[b]d, Å	[c]angle, °	[d]Δr, mÅ	[b]d, Å	[c]angle, °	[d]Δr, mÅ	[b]d, Å	[c]angle, °	[d]Δr, mÅ	[b]d, Å	[c]angle, °	[d]Δr, mÅ	[b]d, Å	[c]angle, °	[d]Δr, mÅ
HF	amideA	1.991	166.690	7.1	2.120	179.218	4.6	2.005	148.822	7.2	2.016	176.060	4.8	2.040	178.079	6.4	2.383	171.632	1.1
	imidazole	2.094	171.049	7.9	2.117	178.906	8.5	2.131	178.955	9.8	2.116	170.668	6.8	2.181	178.774	8.6	2.497	163.719	1.7
	ketone	2.038	166.113	5.5	2.177	178.557	3.9	2.072	178.678	4.6	2.063	166.899	4.5	2.100	174.664	4.3	2.451	170.328	0.4
	furan	2.176	171.110	2.2	2.125	179.030	2.1	2.188	173.057	3.0	2.241	149.812	1.6	2.291	178.279	2.7	2.787	155.855	-0.3
MP2	amideA	1.885	165.762	10.6	1.993	171.629	2.1	1.918	177.472	4.8	1.993	171.629	2.1	1.918	177.472	4.8	2.162	167.383	4.0
	imidazole	1.978	170.993	11.7	2.027	178.668	10.0	1.940	178.841	17.8	2.027	178.668	10.0	1.940	178.841	17.8	2.236	160.720	7.6
	ketone	1.936	164.360	8.7	2.022	170.927	3.3	1.990	179.276	4.8	2.022	170.927	3.3	1.990	179.276	4.8	2.245	162.617	2.3
	furan	2.081	167.152	3.3	2.100	174.819	2.4	2.056	174.273	3.2	2.100	174.819	2.4	2.056	174.273	3.2	2.320	161.790	-1.8
B3LYP	amideA	1.883	168.714	12.8	2.036	172.967	6.2	1.954	176.193	9.8	1.898	175.393	10.5	1.967	175.176	13.0	2.204	176.352	4.2
	imidazole	1.953	174.639	16.7	2.090	179.119	13.7	2.000	175.822	18.4	1.996	167.467	12.3	2.033	179.547	16.7	2.292	166.024	7.1
	ketone	1.924	166.400	9.4	2.117	171.709	5.1	2.043	171.394	5.0	1.966	166.053	8.9	2.048	176.941	5.3	2.334	168.417	3.3
	furan	2.086	177.038	5.1	2.187	157.041	4.4	2.110	172.145	3.3	2.184	149.892	1.4	2.189	176.266	4.2	2.655	159.184	-0.9
B3PLYP	amideA	1.860	168.728	12.7	1.994	173.872	6.1	1.937	176.201	11.5	1.860	174.925	10.7	1.860	174.925	10.7	2.202	177.625	5.0
	imidazole	1.941	175.673	17.5	2.087	179.440	12.4	1.990	175.808	17.4	1.966	168.974	12.7	1.966	168.974	12.7	2.332	165.157	6.8
	ketone	1.910	166.766	10.2	2.074	171.644	5.3	2.041	169.845	8.4	1.951	165.255	8.6	1.951	165.255	8.6	2.283	169.111	2.9
	furan	2.048	176.820	4.5	2.167	176.929	3.8	2.121	172.220	5.9	2.177	149.612	2.5	2.177	149.612	2.5	2.612	110.817	1.2

[a]All the methods were applied with the same basis set (6-311G**++). [b]Hydrogen bond length. [c]Hydrogen bond angle. [d]D-H bond shift.

TABLE 6: Hydrogen bond charge transfer characteristics: hydrogen and acceptor charge transfer

	donor	water		amideD		imidazole		hydroxyl		indole		CH_3SH	
[a]method	acceptor	[b]Δq(H)	[c]Δq(A)	[b]Δq(H)	[c]Δq(A)	[b]Δq(H)	[c]Δq(A)	[b]Δq(H)	[c]Δq(A)	[b]Δq(H)	[c]Δq(A)	[b]Δq(H)	[c]Δq(A)
HF	amideA	0.060	-0.040	0.207	-0.002	0.538	-0.091	0.198	-0.039	0.208	-0.073	0.020	-0.016
	imidazole	0.145	-0.120	0.276	-0.082	0.607	-0.087	0.247	-0.100	0.198	-0.085	0.024	-0.028
	ketone	0.059	-0.005	0.217	0.031	0.607	0.041	0.178	0.007	0.206	0.038	0.015	0.051
	furan	0.095	-0.046	0.230	0.034	0.641	0.008	0.095	-0.001	0.197	0.016	0.002	0.055
MP2	amideA	0.030	-0.030	0.183	-0.009	0.215	-0.084	0.174	0.014	0.211	-0.061	0.011	-0.001
	imidazole	0.147	-0.121	0.263	-0.072	0.299	-0.062	0.252	-0.092	0.239	-0.053	0.029	-0.038
	ketone	0.029	0.001	0.186	0.004	0.268	0.040	0.163	0.025	0.206	0.031	0.009	0.045
	furan	0.094	-0.063	0.167	0.019	0.302	0.000	0.070	0.004	0.231	0.021	0.003	0.058
B3LYP	amideA	0.016	-0.020	0.191	0.007	0.225	-0.068	-0.041	0.000	0.170	0.005	0.242	-0.055
	imidazole	0.137	-0.112	0.226	-0.035	0.316	-0.034	-0.026	0.007	0.231	-0.060	0.255	-0.014
	ketone	0.018	0.009	0.190	0.024	0.254	0.038	-0.026	0.045	0.098	0.016	0.262	0.046
	furan	0.069	-0.028	0.140	0.021	0.293	0.012	-0.017	0.040	0.062	0.016	0.237	0.036
B3PLYP	amideA	0.028	-0.026	0.207	0.007	0.236	-0.078	0.188	0.000	0.233	-0.059	-0.026	-0.007
	imidazole	0.154	-0.124	0.236	-0.044	0.318	-0.045	0.262	-0.074	0.250	-0.023	-0.012	-0.001
	ketone	0.028	0.006	0.205	0.026	0.251	0.041	0.109	0.017	0.234	0.041	-0.019	0.047
	furan	0.085	-0.036	0.160	0.023	0.295	0.010	0.072	0.012	0.238	0.034	-0.015	0.043

[a]All the methods were applied with the same basis set (6-311G**++). [b]Hydrogen charge transfer. [c]Acceptor charge transfer.