TABLE S 2: Comparison of the parameters of the Intramolecular H-bond of Acylphloroglucinols in Vacuo, in Chloroform, in Acetonitrile and in Water. PCM HF/6-31G(d,p) results.

The torsion angles of the atoms involved in the H-bond and the angle of O11 with the plane of the benzene ring are also included, to provide a complete description of the geometry aspects related to the intramolecular H-bond.
The main geometry changes occurring in solution (with respect to *in vacuo*) are indicated with the following symbols:

– to inform of a downwards rotation of the ortho OH not engaged in the H-bond, occurring in the given solvent and turning a conformer from u-type (*in vacuo*) into to the corresponding non-u type (so that the u-type conformer does not exist in that solution).

* to inform of a rotation of the O9H15 group, occurring in the given solvent and turning a r conformer (*in vacuo*) into to the corresponding w conformer (so that the r conformer does not exist in that solution).

Structure, conformer and medium	H-bond parameters			Torsion angles of the atoms involved in the H-bond		∠O11 with the plane
	H···O Å	O···O Å	OĤO	H atom	O atom	
A						
d-r						
in vacuo	1.785	2.625	153.36	0.000	180.000	0.000
in chloroform	1.786	2.628	145.21	0.000	180.000	0.000
in acetonitrile	1.785	2.628	145.43	0.000	180.000	0.000
in water	1.790	2.631	145.03	0.000	180.000	0.000
d-w						
in vacuo	1.792	2.630	153.36	0.000	180.000	0.000
in chloroform	1.791	2.633	145.28	0.000	180.000	0.000
in acetonitrile	1.789	2.632	145.54	0.000	180.000	0.000
in water	1.794	2.635	145.13	0.000	180.000	0.000
s-r						
in vacuo	1.811	2.639	151.42	−180.000	0.000	0.000
in chloroform	1.809	2.640	143.68	180.000	0.000	0.000
in acetonitrile	1.806	2.638	143.90	180.000	0.000	0.000
in water	1.813	2.641	143.23	180.000	0.000	0.000
s-w						
in vacuo	1.808	2.636	151.42	180.000	0.000	0.000
in chloroform	1.815	2.645	143.64	180.000	0.000	0.000
in acetonitrile	1.814	2.645	143.85	180.000	0.000	0.000
in water	1.820	2.647	143.24	180.000	0.000	0.000
d-r-u						
in vacuo	1.780	2.616	153.36	0.000	180.000	0.000
in chloroform	1.771	2.611	144.94	0.000	180.000	0.000
in acetonitrile	1.766	2.608	145.17	0.000	180.000	0.000

in water	1.769	2.610	145.01	0.000	180.000	0.000
d-w-u						
in vacuo	1.788	2.623	153.36	0.000	180.000	0.000
in chloroform	1.777	2.616	145.01	0.000	180.000	0.000
in acetonitrile	1.771	2.612	145.30	0.000	180.000	0.000
in water	1.773	2.614	145.09	0.000	180.000	0.000
s-r-u						
in vacuo	1.811	2.633	151.42	180.000	0.000	0.000
in chloroform	1.797	2.625	143.42	180.000	0.000	0.000
in acetonitrile	1.791	2.621	143.64	180.000	0.000	0.000
in water	1.794	2.622	143.34	180.000	0.000	0.000
s-w-u						
in vacuo	1.804	2.627	151.42	180.000	0.000	0.000
in chloroform	1.791	2.620	143.46	180.000	0.000	0.000
in acetonitrile	1.786	2.617	143.67	180.000	0.000	0.000
in water	1.790	2.620	143.37	180.000	0.000	0.000
AA						
d-r						
in vacuo	1.811	2.641	143.42	–0.011	179.987	0.010
in chloroform	1.810	2.643	143.86	–0.008	–179.972	0.037
in acetonitrile	1.809	2.643	144.07	–0.002	–179.990	0.011
in water	1.818	2.647	143.48	–0.004	–179.980	0.021
d-w						
in vacuo	1.816	2.645	143.45	–0.010	179.988	0.009
in chloroform	1.814	2.646	143.90	–0.002	–179.991	0.008
in acetonitrile	1.810	2.645	144.21	–0.009	179.989	0.009
in water	1.819	2.649	143.54	0.001	–179.979	0.024
d-r-u						
in vacuo	1.805	2.631	143.05	–0.007	179.991	0.006
in chloroform	1.796	2.626	143.56	–0.006	–179.990	0.002
in acetonitrile	1.786	2.619	143.97	–0.011	179.989	0.016
in water	1.796	2.626	143.42	–0.003	179.989	0.020
d-w-u						
in vacuo	1.811	2.636	143.09	0.008	–179.995	0.001
in chloroform	1.800	2.629	143.66	0.014	–179.986	0.012
in acetonitrile	1.792	2.624	144.03	0.008	–179.999	0.001
in water	1.798	2.628	143.56	0.005	–179.984	0.007
B						
d-r						
in vacuo	1.672	2.523	146.69	–0.011	–180.007	0.003
in chloroform	1.667	2.522	146.46	–0.001	–179.994	0.008
in acetonitrile	1.665	2.522	146.70	0.000	–179.996	0.002
in water	1.666	2.522	146.61	–0.001	–179.992	0.018

d-w						
in vacuo	1.689	2.534	146.69	–0.043	–179.952	0.031
in chloroform	1.683	2.533	145.75	0.003	–179.975	0.024
in acetonitrile	1.690	2.535	145.01	0.009	179.995	0.031
in water	1.683	2.534	145.80	0.014	179.996	0.011
s-r						
in vacuo	1.704	2.541	144.92	–179.325	0.623	0.623
in chloroform	1.699	2.540	144.62	179.988	0.036	0.036
in acetonitrile	1.695	2.539	144.94	179.989	0.054	0.054
in water	1.700	2.540	144.47	–179.991	–0.002	0.002
s-w						
in vacuo	1.702	2.540	144.90	–179.994	–0.014	0.014
in chloroform	1.696	2.538	144.66	179.993	0.015	0.015
in acetonitrile	1.693	2.537	144.94	180.000	0.031	0.031
in water	1.697	2.539	144.51	179.998	0.042	0.042
d-r-u						
in vacuo	1.697	2.539	146.51	2.466	171.360	12.684
in chloroform	1.694	2.539	145.33	2.589	170.727	13.653
in acetonitrile	–	–	–	–	–	–
in water	–	–	–	–	–	–
d-w-u						
in vacuo	1.715	2.550	146.55	2.482	171.653	12.200
in chloroform	1.709	2.549	144.66	2.583	170.978	13.382
in acetonitrile	–	–	–	–	–	–
in water	1.710	2.551	144.64	3.043	170.876	12.525
s-r-u						
in vacuo	1.735	2.561	145.54	–178.158	–14.857	14.857
in chloroform	1.728	2.559	143.48	–178.259	–15.379	15.379
in acetonitrile	–	–	–	–	–	–
in water	–	–	–	–	–	–
s-w-u						
in vacuo	1.733	2.560	144.70	–178.384	–13.748	13.748
in chloroform	1.727	2.559	143.50	–178.483	–14.964	14.964
in acetonitrile	–	–	–	–	–	–
in water	–	–	–	–	–	–
BB						
d-r						
in vacuo	1.700	2.540	144.28	–0.017	179.984	0.010
in chloroform	1.693	2.538	144.97	0.014	–179.984	0.012
in acetonitrile	1.690	2.537	145.26	0.013	179.982	0.002
in water	1.696	2.540	144.89	–0.019	–179.937	0.080
d-w						

in vacuo	1.703	2.543	144.31	0.011	179.998	0.005
in chloroform	1.696	2.540	145.02	–0.009	179.962	0.114
in acetonitrile	1.694	2.540	145.27	0.018	179.954	0.063
in water	1.697	2.542	144.94	–0.025	–179.918	0.035
d-r-u						
in vacuo	1.723	2.554	143.33	2.290	172.100	11.960
in chloroform	1.718	2.553	143.93	2.361	171.384	11.178
in acetonitrile	1.715	2.552	144.17	2.368	171.575	12.851
in water	1.719	2.555	143.84	2.571	172.123	13.226
d-w-u						
in vacuo	1.729	2.558	143.31	2.563	171.697	12.132
in chloroform	1.721	2.556	143.95	2.583	170.954	13.587
in acetonitrile	1.719	2.556	144.17	2.592	171.036	13.481
in water	1.723	2.558	143.83	2.896	171.385	12.086
B-ET2						
s-w						
in vacuo	1.733	2.561	142.90	–177.003	–13.764	13.764
in chloroform	1.723	2.556	143.61	–177.158	–13.133	13.133
in acetonitrile	1.719	2.554	143.84	–177.207	–12.844	12.844
in water	1.732	2.562	143.11	–176.668	–13.965	13.965
s-r						
in vacuo	1.743	2.568	142.79	–176.503	–15.214	15.214
in chloroform	1.729	2.561	143.53	–176.719	–14.146	14.146
in acetonitrile	1.724	2.558	143.79	–176.817	–13.581	13.581
in water	1.738	2.566	142.98	–176.220	–14.634	14.634
B-ET24						
s-w						
in vacuo	1.733	2.561	142.96	–177.092	–13.936	13.936
in chloroform	1.724	2.557	143.58	–177.223	–13.376	13.376
in acetonitrile	1.720	2.554	143.79	–177.262	–13.036	13.036
in water	1.734	2.563	142.99	–176.675	–14.338	14.338
B-ET4						
s-w						
in vacuo	1.703	2.541	144.03	–179.989	–0.020	0.020
in chloroform	1.697	2.539	144.64	180.000	–0.021	0.021
in acetonitrile	1.693	2.537	144.90	–179.985	–0.024	0.024
in water	1.698	2.539	144.40	–179.991	0.062	0.062
d-w						
in vacuo	1.694	2.538	145.03	–0.001	179.994	0.007
in chloroform	1.687	2.536	145.76	–0.013	–179.982	0.039
in acetonitrile	1.683	2.534	146.08	0.008	179.999	0.004
in water	1.686	2.536	145.78	–0.003	179.993	0.004
d-r						

in vacuo	1.693	2.535	144.66	–0.350	–179.672	0.022
in chloroform	1.686	2.533	145.29	–0.302	–179.529	0.258
in acetonitrile	*	*	*	*	*	*
in water	*	*	*	*	*	*
d-w-u						
in vacuo	1.720	2.555	144.05	–2.719	–171.267	12.549
in chloroform	1.714	2.554	144.67	–2.723	–170.717	13.552
in acetonitrile	–	–	–	–	–	–
in water	–	–	–	–	–	–
s-w-u						
in vacuo	1.704	2.537	143.52	–179.999	–0.035	0.035
in chloroform	1.702	2.535	143.49	–179.992	–0.053	0.053
in acetonitrile	–	–	–	–	–	–
in water	–	–	–	–	–	–
B-ET46						
d-w						
in vacuo	1.683	2.528	145.08	0.019	179.946	0.058
in chloroform	1.676	2.527	145.84	0.016	179.956	0.046
in acetonitrile	1.673	2.525	146.07	0.010	179.975	0.024
in water	1.676	2.576	145.76	0.021	179.888	0.148
d-r						
in vacuo	1.682	2.525	144.70	–0.434	–179.393	0.315
in chloroform	1.676	2.523	145.32	–0.396	–179.312	0.493
in acetonitrile	1.673	2.522	145.56	–0.428	–179.057	0.847
B-ET6						
d-r						
in vacuo	1.660	2.513	145.91	0.000	180.000	0.000
in chloroform	1.656	2.513	146.55	–0.012	–179.968	0.031
in acetonitrile	1.654	2.512	146.80	–0.012	–179.958	0.039
in water	1.656	2.514	146.60	–0.132	–179.654	0.415
d-w						
in vacuo	1.678	2.524	145.11	0.001	179.998	0.001
in chloroform	1.673	2.523	145.83	–0.008	–179.989	0.011
in acetonitrile	1.670	2.523	146.12	–0.006	–179.984	0.017
in water	1.673	2.524	145.83	–0.103	–179.687	
BB-ET24						
d-r						
in vacuo	1.689	2.530	144.40	–0.059	–179.877	0.134
in chloroform	1.684	2.529	145.01	–0.031	–179.929	0.075
in acetonitrile	1.682	2.528	145.20	–0.035	–179.917	0.091
in water	1.687	2.531	144.67	–0.076	–179.847	0.184
d-w						
in vacuo	1.699	2.538	144.23	0.001	–179.999	0.014

in chloroform	1.689	2.533	145.03	–0.009	179.993	–0.004
in acetonitrile	1.685	2.532	145.28	–0.008	–179.980	0.024
in water	1.692	2.535	144.77	–0.049	–179.915	0.184
BB-ET4						
d-r						
in vacuo	1.700	2.540	144.34	0.010	179.956	0.041
in chloroform	1.693	2.538	144.98	0.004	179.972	0.024
in acetonitrile	1.692	2.538	145.16	0.004	179.990	0.007
in water	1.696	2.540	144.77	–0.019	–179.984	0.024
d-w						
in vacuo	1.708	2.547	144.27	0.012	179.993	0.009
in chloroform	1.701	2.544	144.97	0.012	179.979	0.028
in acetonitrile	1.696	2.542	145.28	–0.003	179.967	0.042
in water	1.701	2.545	144.84	0.017	–179.980	0.051
d-r-u						
in vacuo	1.700	2.535	143.91	0.003	179.977	0.017
in chloroform	1.690	2.530	144.54	0.012	179.988	0.019
in acetonitrile	1.685	2.528	144.77	0.028	179.908	0.116
in water	1.695	2.539	144.78	0.006	179.972	0.029
d-w-u						
in vacuo	1.711	2.544	143.80	0.004	179.995	0.009
in chloroform	1.697	2.537	144.55	–0.014	–179.969	0.023
in acetonitrile	1.723	2.559	144.13	2.730	170.834	13.611
in water	1.731	2.564	143.60	3.256	170.505	13.111
B-B35						
d-r						
in vacuo	1.673	2.523	145.61	–0.019	–179.962	0.043
in chloroform	1.668	2.522	146.22	–0.005	–179.993	0.008
in acetonitrile	1.666	2.521	146.45	–0.002	–179.983	0.022
in water	1.665	2.520	146.32	–0.231	–179.448	0.647
B-B35-ET4						
d-r						
in vacuo	1.694	2.534	144.46	0.622	178.961	0.719
in chloroform	1.687	2.532	145.11	0.686	178.740	1.074
in acetonitrile	1.684	2.530	145.32	0.742	178.434	1.516
in water	1.692	2.534	144.78	1.995	175.568	4.965
B-P3						
d-r						
in vacuo	1.667	2.521	146.11	–0.176	179.789	0.049
in chloroform	1.663	2.520	146.68	–0.256	179.757	0.003
in acetonitrile	1.660	2.519	146.93	0.254	179.702	0.092
in water	1.663	2.520	146.69	–0.153	179.705	0.129
d-w						

in vacuo	1.683	2.531	145.36	0.469	–179.849	0.013
in chloroform	1.676	2.529	146.13	0.364	–179.887	0.044
in acetonitrile	1.673	2.527	146.45	0.367	–179.987	0.129
in water	1.674	2.528	146.28	0.467	179.976	0.214
s-r						
in vacuo	1.699	2.537	144.02	–179.335	1.132	1.132
in chloroform	1.689	2.532	144.75	–179.619	1.754	1.754
in acetonitrile	1.685	2.530	145.00	–179.748	2.098	2.098
in water	1.690	2.532	144.51	179.954	3.057	3.057
s-w						
in vacuo	1.699	2.537	144.03	–179.874	–0.142	0.142
in chloroform	1.691	2.534	144.77	–179.990	–0.244	0.244
in acetonitrile	1.688	2.533	145.01	–179.942	–0.796	0.796
in water	1.692	2.535	144.57	–179.790	–1.807	1.807
B-P3-ET2						
s-w						
in vacuo	1.745	2.570	142.59	–176.683	–16.840	16.840
in chloroform	1.735	2.565	143.29	–176.899	–16.276	16.276
in acetonitrile	1.732	2.563	143.51	–176.947	–15.969	15.969
in water	1.743	2.570	142.80	–176.410	–16.962	16.962
s-r						
in vacuo	1.754	2.578	142.52	–176.239	–17.930	17.930
in chloroform	1.742	2.571	143.20	–176.389	–17.045	17.045
in acetonitrile	1.737	2.567	143.43	–176.334	–16.503	16.503
in water	1.749	2.574	142.63	–175.684	–17.619	17.619
B-P3-ET6						
d-r						
in vacuo	1.656	2.511	146.17	–0.104	179.674	0.095
in chloroform	1.651	2.510	146.78	–0.195	179.595	0.199
in acetonitrile	1.649	2.509	147.00	–0.185	179.511	0.310
in water	1.653	2.511	146.71	–0.103	179.612	0.270
d-w						
in vacuo	1.672	2.520	145.41	0.412	–179.818	0.029
in chloroform	1.665	2.519	146.18	0.337	–179.895	0.033
in acetonitrile	1.662	2.518	146.48	0.295	–179.848	0.031
in water	1.664	2.519	146.30	0.434	–179.988	0.126
D						
d-r						
in vacuo	1.666	2.517	145.76	–0.028	–179.970	0.035
in chloroform	1.660	2.515	146.46	–0.013	–179.989	0.010
in acetonitrile	1.658	2.515	146.70	–0.008	–179.991	0.013
in water	1.657	2.514	146.67	0.000	179.945	0.062
d-w						

in vacuo	1.682	2.527	144.99	0.003	−179.986	0.013
in chloroform	1.676	2.526	145.74	0.005	179.964	0.055
in acetonitrile	1.673	2.525	146.01	−0.005	−179.975	0.033
in water	1.674	2.525	145.87	−0.148	−179.627	0.428
s-r						
in vacuo	1.698	2.534	143.87	−179.350	0.708	0.708
in chloroform	1.689	2.530	144.65	−179.399	0.900	0.900
in acetonitrile	1.685	2.529	144.90	−179.501	1.385	1.385
in water	1.692	2.532	144.36	179.770	4.517	4.517
s-w						
in vacuo	1.696	2.533	143.93	179.999	0.001	0.001
in chloroform	1.688	2.530	144.68	−179.987	0.006	0.006
in acetonitrile	1.686	2.530	144.89	−179.999	0.021	0.021
in water	1.689	2.530	144.54	−179.992	−0.007	0.007
d-r-u						
in vacuo	1.667	2.514	145.41	−0.009	179.960	0.000
in chloroform	1.657	2.509	146.01	−0.022	−179.955	0.054
in acetonitrile	1.652	2.506	146.37	−0.011	179.997	0.002
in water	1.696	2.541	145.12	−4.018	−168.412	15.698
d-w-u						
in vacuo	1.687	2.555	144.52	0.005	−179.996	0.004
in chloroform	1.701	2.542	144.68	−2.539	−170.968	13.345
in acetonitrile	1.669	2.517	145.66	0.001	−179.989	0.008
in water	1.711	2.550	144.41	−3.776	−168.708	15.419
s-r-u						
in vacuo	1.729	2.554	142.76	−177.910	−15.070	15.070
in chloroform	1.724	2.554	143.36	−177.922	−16.206	16.206
in acetonitrile	1.685	2.529	144.91	−179.500	1.410	1.410
in water	1.729	2.558	143.06	−177.007	−15.968	15.968
s-w-u						
in vacuo	1.725	2.526	142.84	−178.192	−13.535	13.535
in chloroform	1.721	2.552	143.44	−178.274	−15.157	15.157
in acetonitrile	1.718	2.551	143.69	−178.237	−15.040	15.040
in water						
DD						
d-r						
in vacuo	1.694	2.533	144.23	0.001	−179.996	0.002
in chloroform	1.688	2.532	144.88	0.001	179.992	0.004
in acetonitrile	1.682	2.529	145.25	0.013	−179.984	0.018
in water	1.688	2.532	144.89	0.025	179.975	0.031
d-w						
in vacuo	1.694	2.534	144.31	0.001	−179.991	0.010
in chloroform	1.689	2.533	144.98	−0.004	−179.996	0.005
in acetonitrile	1.684	2.531	145.33	−0.002	179.932	0.098

in water	1.687	2.532	144.98	–0.002	179.995	0.002
d-r-u						
in vacuo	1.696	2.530	143.78	–0.001	179.970	0.033
in chloroform	1.685	2.524	144.44	0.002	179.998	0.001
in acetonitrile	1.679	2.522	144.81	–0.005	179.999	0.011
in water	1.680	2.522	144.58	–0.001	179.993	0.009
d-w-u						
in vacuo	1.701	2.534	143.76	0.001	179.998	0.002
in chloroform	1.687	2.527	144.57	–0.006	–179.960	0.061
in acetonitrile	1.681	2.524	144.86	–0.002	–179.981	0.025
in water	1.680	2.522	144.62	–0.019	–179.971	0.046
E1						
d-r						
in vacuo	1.664	2.516	145.83	0.006	–179.996	0.008
in chloroform	1.659	2.515	146.44	–0.008	–179.955	0.054
in acetonitrile	1.657	2.514	146.72	–0.008	–179.981	0.028
in water	1.656	2.514	146.67	–0.038	–179.857	0.182
d-w						
in vacuo	1.683	2.527	144.98	0.002	–179.992	0.017
in chloroform	1.676	2.526	145.73	–0.012	–179.973	0.030
in acetonitrile	1.672	2.524	146.04	–0.011	–179.973	0.035
in water	1.675	2.526	145.85	0.046	179.907	0.112
s-r						
in vacuo	1.697	2.533	143.88	–179.358	0.732	0.732
in chloroform	1.688	2.529	144.63	–179.419	0.973	0.973
in acetonitrile	1.684	2.528	144.90	–179.467	1.332	1.332
in water	1.693	2.532	144.33	179.579	5.071	5.071
s-w						
in vacuo	1.695	2.533	143.93	–179.993	0.025	0.025
in chloroform	1.687	2.530	144.68	180.000	0.043	0.043
in acetonitrile	1.683	2.528	144.96	–179.993	0.050	0.050
in water	1.687	2.529	144.59	179.997	–0.020	0.020
d-r-u						
in vacuo	1.666	2.512	145.42	–0.002	–179.998	0.000
in chloroform	1.690	2.535	145.22	–3.232	–169.313	15.039
in acetonitrile	1.688	2.534	145.46	–3.258	–169.312	14.984
in water	1.694	2.539	145.19	4.009	168.426	15.489
d-w-u						
in vacuo	1.686	2.530	144.54	0.001	179.978	0.000
in chloroform	1.674	2.519	145.31	–0.015	–179.976	0.030
in acetonitrile	1.668	2.516	145.63	–0.009	–179.962	0.058
in water	1.711	2.550	144.40	3.935	168.417	15.629

s-r-u						
in vacuo	1.731	2.556	142.71	177.557	15.770	15.770
in chloroform	1.726	2.556	143.28	177.633	17.066	17.066
in acetonitrile	1.719	2.552	143.63	177.606	15.769	15.769
in water	1.738	2.565	142.78	176.579	18.251	18.251
EE1						
d-r						
in vacuo	1.692	2.532	144.23	0.001	180.000	0.001
in chloroform	1.685	2.529	144.97	–0.006	179.994	0.004
in acetonitrile	1.681	2.528	145.26	0.002	–179.980	0.021
in water	1.686	2.531	144.92	–0.009	–179.987	0.018
d-w						
in vacuo	1.695	2.534	144.22	–0.003	–179.995	0.003
in chloroform	1.687	2.532	145.00	–0.003	179.989	0.012
in acetonitrile	1.686	2.532	145.27	–0.012	–179.996	0.002
in water	1.687	2.532	144.97	–0.009	–179.984	0.022
d-r-u						
in vacuo	1.695	2.529	143.80	–0.006	–179.990	0.018
in chloroform	1.683	2.523	144.48	–0.003	–179.981	0.010
in acetonitrile	1.679	2.521	144.76	–0.019	–179.960	0.053
in water	1.679	2.521	144.57	0.006	179.974	0.047
d-w-u						
in vacuo	1.699	2.533	143.84	0.004	179.982	0.025
in chloroform	1.687	2.527	144.49	0.006	–179.981	0.009
in acetonitrile	–	–	–	–	–	–
in water	1.730	2.561	143.38	–4.179	–167.695	16.936
E1-ET4						
s-w						
in vacuo	1.696	2.534	143.97	179.985	–0.001	0.001
in chloroform	1.688	2.530	144.65	–179.998	0.003	0.003
in acetonitrile	1.684	2.528	144.90	179.991	0.026	0.026
in water	1.687	2.529	144.47	–179.962	–0.204	0.204
d-w						
in vacuo	1.687	2.531	145.00	–0.002	179.997	0.002
in chloroform	1.678	2.528	145.78	–0.004	–179.999	0.010
in acetonitrile	1.674	2.526	146.09	–0.016	179.988	0.021
in water	1.676	2.527	145.84	0.004	–179.989	0.010
d-r						
in vacuo	1.685	2.527	144.64	0.072	179.770	0.072
in chloroform	1.678	2.525	145.29	–0.344	–179.460	0.329
in acetonitrile	*	*	*	*	*	*
in water	*	*	*	*	*	*
s-w-u						

in vacuo	1.698	2.530	143.49	–179.998	0.000	0.000
in chloroform	1.686	2.524	144.19	179.989	0.079	0.079
in acetonitrile	–	–	–	–	–	–
in water	1.670	2.517	144.46	–179.910	–0.322	0.322
d-w-u						
in vacuo	1.689	2.529	144.59	–0.009	–179.996	0.009
in chloroform	1.677	2.522	145.31	0.003	179.981	0.040
in acetonitrile	1.672	2.519	145.62	–0.017	–179.993	0.006
in water	1.670	2.517	145.51	0.005	179.992	0.018
EE1-ET4						
d-r						
in vacuo	1.693	2.533	144.27	–0.011	–179.963	0.035
in chloroform	1.686	2.530	144.95	–0.004	179.995	0.016
in acetonitrile	1.682	2.529	145.20	–0.011	–179.977	0.019
in water	1.686	2.531	144.82	0.005	179.994	0.000
d-w						
in vacuo	1.701	2.539	144.15	–0.006	179.969	0.026
in chloroform	1.691	2.535	144.98	–0.009	–179.942	0.072
in acetonitrile	1.687	2.533	145.27	0.015	179.993	0.001
in water	1.691	2.535	144.88	0.072	179.818	0.213
d-r-u						
in vacuo	1.693	2.529	143.87	–0.010	–179.971	0.042
in chloroform	1.712	2.547	143.84	–2.771	–170.550	13.986
in acetonitrile	–	–	–	–	–	–
in water	1.680	2.521	144.45	0.003	179.996	0.020
d-w-u						
in vacuo	1.704	2.537	143.76	–0.010	–179.977	0.033
in chloroform	1.691	2.530	144.50	–0.009	–179.969	0.055
in acetonitrile	–	–	–	–	–	–
in water	1.730	2.561	143.40	–3.977	–168.703	15.308
E2						
d-r						
in vacuo	1.661	2.512	146.17	3.796	171.058	9.722
in chloroform	1.657	2.511	146.30	–3.971	–170.476	10.384
in acetonitrile	1.659	2.614	146.43	–4.351	–169.492	11.462
in water	1.677	2.527	145.85	–5.818	–166.200	14.948
d-w						
in vacuo	1.679	2.523	146.06	3.738	171.130	9.663
in chloroform	1.672	2.521	145.58	3.784	170.827	10.062
in acetonitrile	1.668	2.520	145.91	3.590	171.200	9.713
in water	1.682	2.530	145.38	4.789	168.386	12.725
s-r						
in vacuo	1.724	2.553	144.96	–175.053	–17.123	17.123

in chloroform	1.718	2.551	143.67	175.130	17.593	17.593
in acetonitrile	1.719	2.553	143.80	175.077	18.316	18.316
in water	1.763	2.585	142.28	173.723	23.121	23.121
s-w						
in vacuo	1.701	2.536	143.26	–175.950	–12.247	12.247
in chloroform	1.698	2.536	144.19	–175.805	–13.207	13.207
in acetonitrile	1.697	2.537	144.38	–175.729	–13.840	13.840
in water	1.723	2.555	143.31	–174.293	–17.999	17.999
d-r-u						
in vacuo	1.728	2.560	145.33	–6.076	–162.904	22.499
in chloroform	1.729	2.565	144.17	7.101	160.338	24.191
in acetonitrile	1.737	2.572	144.15	7.638	158.953	25.599
in water	1.772	2.598	142.91	9.937	155.047	29.324
d-w-u						
in vacuo	1.742	2.570	145.40	–6.798	–161.769	22.311
in chloroform	1.742	2.573	143.60	6.899	160.756	23.748
in acetonitrile	1.747	2.579	143.66	7.383	159.546	24.964
in water	1.782	2.603	142.33	9.514	155.379	29.352
s-r-u						
in vacuo	1.768	2.586	144.16	174.555	24.458	24.458
in chloroform	1.736	2.561	142.76	–174.448	–20.618	20.618
in acetonitrile	–	–	–	–	–	–
in water	1.750	2.570	142.06	–174.059	–22.592	22.592
s-w-u						
in vacuo	1.750	2.568	152.71	–174.959	–22.514	22.514
in chloroform	–	–	–	–	–	–
in acetonitrile	–	–	–	–	–	–
in water	1.739	2.562	142.32	–174.418	–21.261	21.261
EE2						
d-r						
in vacuo	1.692	2.530	145.56	2.581	173.694	7.091
in chloroform	1.676	2.521	144.987	2.712	173.305	7.546
in acetonitrile	1.673	2.520	145.25	2.665	173.382	7.476
in water	1.685	2.529	144.71	3.666	171.026	9.997
d-w						
in vacuo	1.684	2.524	145.66	3.569	171.631	9.137
in chloroform	1.685	2.528	144.83	3.535	171.531	9.335
in acetonitrile	1.678	2.524	145.240	3.163	172.319	8.554
in water	1.688	2.531	144.71	4.014	170.399	10.605
d-r-u						
in vacuo	1.748	2.572	144.94	6.313	162.693	21.760
in chloroform	1.747	2.574	142.98	6.394	161.804	23.003
in acetonitrile	1.754	2.581	142.96	6.855	160.479	24.509
in water	1.788	2.605	141.66	8.802	156.827	27.924

d-w-u						
in vacuo	1.756	2.578	144.83	6.886	161.848	22.328
in chloroform	1.752	2.578	142.98	6.795	161.183	23.421
in acetonitrile	1.760	2.586	142.94	7.251	159.750	25.153
in water	1.792	2.608	141.63	9.211	156.255	28.390
E2-B35						
d-r						
in vacuo	1.684	2.528	144.878	6.250	165.804	15.103
in chloroform	1.685	2.532	145.33	6.617	164.738	16.298
in acetonitrile	1.686	2.533	145.49	6.766	164.130	17.029
in water	1.724	2.561	144.24	8.707	159.392	22.332
d-w						
in vacuo	1.709	2.546	144.265	8.240	162.178	16.338
in chloroform	1.703	2.542	145.00	6.907	164.173	16.603
in acetonitrile	1.698	2.540	144.8	6.798	164.396	16.389
in water	1.727	2.560	143.71	8.645	160.922	19.681
E2-D3						
d-r						
in vacuo	1.662	2.512	145.55	2.781	171.731	8.955
in chloroform	1.661	2.514	146.05	3.354	170.540	10.230
in acetonitrile	1.660	2.514	146.26	3.509	170.108	10.722
in water	1.668	2.520	145.94	4.142	168.656	12.217
d-w						
in vacuo	1.677	2.523	145.13	3.994	169.517	11.173
in chloroform	1.671	2.521	145.87	4.109	169.250	11.522
in acetonitrile	1.668	2.521	146.18	4.078	169.169	11.686
in water	1.673	2.524	145.91	4.361	168.578	12.311
s-r						
in vacuo	1.722	2.551	143.05	–174.670	–17.043	17.043
in chloroform	1.716	2.549	143.68	–174.555	–17.312	17.312
in acetonitrile	1.714	2.549	143.91	–174.494	17.508	17.508
in water	1.744	2.570	142.73	–172.761	–21.008	21.008
s-w						
in vacuo	1.703	2.537	143.44	–175.648	–13.828	13.828
in chloroform	1.701	2.538	144.03	–175.452	–14.835	14.835
in acetonitrile	1.701	2.540	144.25	–175.568	–15.257	15.257
in water	1.733	2.562	143.03	–173.673	–19.842	19.842
d-r-u						
in vacuo	1.724	2.559	143.89	5.807	162.095	22.116
in chloroform	1.730	2.566	144.09	6.277	160.556	23.963
in acetonitrile	1.738	2.573	144.03	6.901	159.185	25.314
in water	1.772	2.598	142.81	9.005	155.227	29.213
d-w-u						

in vacuo	1.738	2.569	143.57	6.609	161.163	22.801
in chloroform	1.738	2.572	143.97	6.763	160.136	24.228
in acetonitrile	1.745	2.579	144.0	7.271	158.822	25.639
in water	1.778	2.602	142.77	9.391	154.900	29.579
s-r-u						
in vacuo	1.770	2.587	141.89	–174.584	–24.536	24.536
in chloroform	1.771	2.592	142.26	–174.476	–26.067	26.067
in acetonitrile	1.777	2.597	142.26	–173.921	–27.437	27.437
in water	1.818	2.626	140.73	–171.812	–30.503	30.503
s-w-u						
in vacuo	1.762	2.581	141.96	–174.994	–23.844	23.844
in chloroform	1.764	2.586	142.34	–174.879	–25.441	25.441
in acetonitrile	1.771	2.592	142.37	–174.286	–26.433	26.433
in water	1.810	2.620	140.91	–172.538	–29.906	29.906
E2X'						
d-r						
in vacuo	1.657	2.509	145.853	3.811	171.057	9.472
in chloroform	1.655	2.510	146.348	4.081	170.029	10.625
in acetonitrile	1.654	2.511	146.546	4.198	169.550	11.192
in water	1.666	2.518	145.857	5.030	169.728	11.608
d-w						
in vacuo	1.673	2.519	145.103	4.439	171.170	9.743
in chloroform	1.667	2.518	145.802	4.326	170.915	10.058
in acetonitrile	1.664	2.517	146.106	4.218	170.946	10.054
in water	1.672	2.523	145.787	5.112	169.126	11.939
s-r						
in vacuo	1.721	2.550	143.075	–173.298	–16.805	16.805
in chloroform	1.716	2.549	143.618	–173.441	–17.567	17.567
in acetonitrile	1.713	2.548	143.835	–173.523	–18.040	18.040
in water	1.758	2.581	142.432	–173.533	–22.297	22.297
s-w						
in vacuo	1.706	2.539	143.387	–175.343	–14.160	14.160
in chloroform	1.705	2.542	143.916	–175.168	–15.608	15.608
in acetonitrile	1.707	2.544	144.058	–175.066	–16.602	16.602
in water	1.745	2.572	142.795	–173.892	–21.290	21.290
EE2-ET4						
d-r						
in vacuo	1.681	2.522	144.35	2.430	174.050	6.747
in chloroform	1.675	2.521	145.00	2.533	173.665	7.216
in acetonitrile	1.672	2.520	145.25	2.552	173.487	7.446
in water	1.688	2.530	144.54	3.872	170.488	10.637
d-w						
in vacuo	1.699	2.536	144.02	4.023	170.893	9.842
in chloroform	1.690	2.532	144.77	3.974	170.819	9.989

in acetonitrile	1.686	2.531	145.06	3.895	170.840	10.037
in water	1.702	2.542	144.34	5.115	167.989	13.048
d-r-u						
in vacuo	1.745	2.570	142.67	6.080	163.098	21.463
in chloroform	1.727	2.574	142.98	6.305	161.905	22.984
in acetonitrile	1.754	2.580	142.95	6.794	160.586	24.356
in water	1.790	2.606	141.53	8.855	156.730	27.951
d-w-u						
in vacuo	1.762	2.584	142.43	7.287	161.418	22.634
in chloroform	1.757	2.583	142.93	7.100	160.824	23.616
in acetonitrile	1.766	2.591	142.83	7.631	159.262	25.465
in water	1.806	2.619	141.30	9.901	155.117	29.409
E2-P3						
in vacuo						
in chloroform	1.658	2.510	145.93	3.661	170.676	8.598
in acetonitrile	1.655	2.511	146.46	4.043	169.404	11.252
in water	1.656	2.513	146.59	4.179	168.950	11.773
in water	1.675	2.526	145.92	5.713	165.664	13.653
d-w						
in vacuo	1.675	2.521	145.11	4.605	170.545	10.966
in chloroform	1.669	2.520	145.84	4.580	170.142	10.875
in acetonitrile	1.665	2.518	146.16	4.464	170.277	10.749
in water	1.676	2.526	145.77	5.559	168.000	14.364
s-r						
in vacuo	1.720	2.550	143.14	−173.349	−16.536	16.536
in chloroform	1.713	2.547	143.72	−173.497	−17.186	17.186
in acetonitrile	1.712	2.547	143.90	−173.574	−17.694	17.694
in water	1.744	2.569	142.66	−172.455	−21.484	21.484
s-w						
in vacuo	1.707	2.539	143.42	−175.317	−14.089	14.089
in chloroform	1.707	2.543	143.92	−175.101	−15.763	15.763
in acetonitrile	1.707	2.544	144.11	−175.127	−16.421	16.421
in water	1.740	2.567	142.91	−173.929	−20.639	20.639
F1						
d-r						
in vacuo	1.663	2.515	145.85	−0.001	−179.982	0.008
in chloroform	1.659	2.514	146.47	−0.012	−179.977	0.031
in acetonitrile	1.654	2.512	146.78	0.003	179.962	0.067
in water	1.656	2.513	146.68	0.002	−179.993	0.009
d-w						
in vacuo	1.682	2.527	145.02	0.001	180.000	0.001
in chloroform	1.675	2.524	145.74	0.000	−179.977	0.028
in acetonitrile	1.670	2.523	146.09	−0.014	−179.991	0.011
in water	1.672	2.524	145.88	0.005	179.995	0.006

s-r						
in vacuo	1.697	2.533	143.86	179.273	–0.552	0.552
in chloroform	1.688	2.529	144.64	179.485	–1.210	1.210
in acetonitrile	1.684	2.528	144.91	179.482	–1.329	1.329
in water	1.693	2.533	144.32	–179.335	–5.916	5.916
s-w						
in vacuo	1.695	2.532	143.97	–179.993	–0.002	0.002
in chloroform	1.688	2.530	144.63	179.995	0.013	0.013
in acetonitrile	1.683	2.528	144.97	–179.980	0.060	0.060
in water	1.686	2.529	144.58	–179.825	–0.767	0.767
d-r-u						
in vacuo	1.665	2.512	145.44	–0.001	179.998	0.001
in chloroform	1.656	2.508	146.08	–0.001	179.998	0.006
in acetonitrile	1.686	2.533	145.50	–3.192	–169.476	14.784
d-w-u						
in vacuo	1.685	2.530	144.57	0.004	179.999	0.001
in chloroform	1.673	2.518	145.32	–0.001	–179.993	0.006
in acetonitrile	1.667	2.515	145.63	–0.006	–179.991	0.011
s-r-u						
in vacuo	1.731	2.556	142.73	–177.493	–15.849	15.849
in chloroform	1.726	2.556	143.30	–177.641	–16.960	16.960
in acetonitrile	1.720	2.553	143.61	–177.571	–16.159	16.159
s-w-u						
in vacuo	1.698	2.525	143.44	–179.997	–0.006	0.006
in chloroform	1.686	2.523	144.20	179.990	–0.002	0.002
in acetonitrile	1.721	2.554	143.59	177.890	16.197	16.197
FF1						
d-r						
in vacuo	1.692	2.532	144.24	0.000	179.996	0.004
in chloroform	1.686	2.530	144.94	–0.008	–179.986	0.010
in acetonitrile	1.681	2.528	145.28	–0.015	179.974	0.054
in water	1.686	2.531	144.93	–0.008	–179.998	0.001
d-w						
in vacuo	1.696	2.535	144.24	0.006	–179.995	0.003
in chloroform	1.687	2.531	145.02	–0.004	–179.973	0.026
in acetonitrile	1.683	2.530	145.33	–0.014	179.993	0.002
in water	1.686	2.532	145.01	–0.025	–179.975	0.016
d-r-u						
in vacuo	1.694	2.529	143.81	–0.004	179.988	0.010
in chloroform	1.683	2.523	144.51	0.059	–179.954	0.027
in acetonitrile	1.687	2.520	144.78	–0.019	–179.952	0.063
in water	1.679	2.521	144.58	–0.029	–179.956	0.047

d-w-u						
in vacuo	1.699	2.533	143.85	0.002	179.992	0.010
in acetonitrile	1.680	2.523	144.87	–0.017	–179.965	0.041
in water	1.680	2.522	144.65	–0.020	–179.950	0.066
F2						
d-r						
in vacuo	1.667	2.517	145.65	0.003	–179.998	6.387
in chloroform	1.663	2.517	146.24	3.210	172.588	7.669
in acetonitrile	1.661	2.517	146.48	3.287	172.320	7.983
in water	1.669	2.522	146.18	4.092	170.460	10.035
d-w						
in vacuo	1.664	2.529	144.79	2.710	173.863	6.310
in chloroform	1.679	2.527	145.55	2.985	173.032	9.211
in acetonitrile	1.677	2.527	145.81	3.088	172.649	7.654
in water	1.683	2.531	145.46	3.697	171.240	7.205
s-r						
in vacuo	1.708	2.541	143.52	–177.376	–9.644	9.644
in chloroform	1.702	2.540	144.14	–177.086	–11.018	11.018
in acetonitrile	1.702	2.540	144.32	–176.977	–11.857	11.857
in water	1.731	2.560	143.13	–175.675	–16.664	16.664
s-w						
in vacuo	1.700	2.536	143.73	–177.382	–7.152	7.152
in chloroform	1.694	2.534	144.41	–177.143	–8.298	8.298
in acetonitrile	1.694	2.535	144.57	–176.941	–9.128	9.128
in water	1.724	2.554	143.02	–175.567	–13.754	13.754
d-r-u						
in vacuo	1.699	2.539	144.52	4.407	167.727	16.023
in chloroform	1.701	2.543	144.87	4.603	166.371	17.908
in acetonitrile	1.699	2.543	145.10	4.658	166.203	18.085
in water	1.713	2.553	144.56	5.783	164.431	19.669
d-w-u						
in vacuo	1.717	2.559	143.77	4.367	168.059	15.515
in chloroform	1.716	2.553	144.24	4.461	166.810	17.419
in acetonitrile	1.712	2.551	144.51	4.473	166.708	17.561
in water	1.726	2.561	143.89	5.520	164.898	19.246
s-r-u						
in vacuo	1.739	2.562	142.51	–176.497	–18.140	18.140
in chloroform	1.738	2.565	142.95	–176.535	–19.626	19.626
in acetonitrile	1.734	2.565	143.20	–176.496	–19.500	19.500
in water	1.757	2.579	142.20	–175.246	–21.863	21.863
s-w-u						
in vacuo	1.735	2.550	142.59	–176.730	–16.886	16.886
in chloroform	1.735	2.653	143.04	–176.810	–18.761	18.761

in acetonitrile	1.733	2.563	143.24	−176.793	−19.076	19.076
in water	1.752	2.575	142.33	−175.589	−21.409	21.409
FF2						
d-r						
in vacuo	1.694	2.533	144.10	2.394	174.524	5.639
in chloroform	1.688	2.532	144.78	2.692	173.674	6.552
in acetonitrile	1.685	2.531	145.06	2.702	173.530	6.725
in water	1.696	2.537	144.52	3.556	171.524	8.996
d-w						
in vacuo	1.699	2.537	144.11	2.683	174.012	6.154
in chloroform	1.691	2.534	144.81	2.886	173.337	6.867
in acetonitrile	1.688	2.533	145.11	2.868	173.278	6.949
in water	1.697	2.539	144.60	3.644	171.448	9.032
d-r-u						
in vacuo	1.723	2.552	143.08	4.054	168.694	15.112
in chloroform	1.724	2.556	143.51	4.238	167.249	17.267
in acetonitrile	1.723	2.556	143.69	4.363	166.869	17.767
in water	1.740	2.567	142.94	5.296	165.289	19.245
d-w-u						
in vacuo	1.729	2.557	143.07	4.471	168.158	15.386
in chloroform	1.729	2.560	143.50	4.591	166.671	17.719
in acetonitrile	1.725	2.559	143.76	4.523	166.626	17.910
in water	1.742	2.570	142.99	5.417	164.992	19.561
F3						
d-r						
in vacuo	1.695	2.538	144.74	−8.075	−161.403	19.121
in chloroform	1.694	2.539	145.25	−8.114	−160.959	19.737
in acetonitrile	1.693	2.540	145.46	−8.075	−160.803	19.977
in water	1.716	2.556	144.59	−9.175	−158.767	22.127
d-w						
in vacuo	1.713	2.551	144.38	−9.131	−159.487	20.898
in chloroform	1.708	2.549	144.61	−7.868	−161.301	19.379
in acetonitrile	1.702	2.547	145.38	−8.822	−160.014	20.688
in water	1.725	2.561	144.06	−8.555	−159.662	21.253
s-r						
in vacuo	1.726	2.553	142.95	−174.667	−17.721	17.721
in chloroform	1.722	2.554	143.52	−174.641	−18.680	18.680
in acetonitrile	1.727	2.559	143.57	−174.531	−19.646	19.646
in water	1.772	2.590	141.91	−172.922	−24.211	24.211
s-w						
in vacuo	1.706	2.539	143.45	−175.316	−13.715	13.715
in chloroform	1.706	2.542	143.95	−175.021	−15.261	15.261
in acetonitrile	1.707	2.544	144.11	−174.894	−16.033	16.033

in water	1.739	2.567	142.89	–173.598	–20.254	20.254
d-r-u						
in vacuo	1.748	2.577	143.34	–8.517	–157.727	26.810
in chloroform	1.745	2.577	143.71	–8.515	–157.395	27.197
in acetonitrile	1.745	2.578	143.80	–8.483	–157.260	27.473
s-w-u						
in vacuo	1.755	2.575	142.12	–174.852	–22.710	22.710
in chloroform	1.752	2.576	142.60	–175.176	–23.633	23.633
in acetonitrile	–	–	–	–	–	–
in water	–	–	–	–	–	–
FF3						
d-r						
in vacuo	1.683	2.523	144.26	–2.699	–173.443	7.382
in chloroform	1.676	2.522	145.00	–2.848	–172.942	7.978
in acetonitrile	1.675	2.522	145.21	–2.990	–172.481	8.497
in water	1.687	2.530	144.68	–4.005	–170.280	10.814
d-w						
in vacuo	1.690	2.529	144.19	–3.480	–171.798	9.028
in chloroform	1.683	2.527	144.90	–3.478	–171.678	9.226
in acetonitrile	1.679	2.525	145.22	–3.309	–171.904	9.044
in water	1.692	2.534	144.65	–4.400	–169.494	11.589
d-r-u						
in vacuo	1.742	2.568	142.72	–6.058	–163.221	21.347
in chloroform	1.748	2.575	142.94	–6.408	–161.740	23.225
in acetonitrile	1.757	2.583	142.91	–6.905	–160.258	24.872
in water	1.792	2.608	141.59	–8.806	–156.696	28.132
d-w-u						
in vacuo	1.752	2.575	142.61	–6.669	–162.249	22.042
in chloroform	1.753	2.579	142.96	–6.784	–161.135	23.637
in acetonitrile	1.762	2.588	142.91	–7.308	–159.652	25.326
in water	1.795	2.611	141.62	–9.103	–156.333	28.340
G1						
d-r						
in vacuo	1.663	2.515	145.85	–0.003	179.997	0.003
in chloroform	1.658	2.514	146.48	–0.007	179.993	0.010
in acetonitrile	1.656	2.514	146.79	–0.004	–179.983	0.009
in water	1.656	2.513	146.69	0.086	179.764	0.285
d-w						
in vacuo	1.682	2.527	144.98	–0.007	179.977	0.022
in chloroform	1.675	2.525	145.75	–0.015	179.983	0.009
in acetonitrile	1.671	2.523	146.10	0.007	179.924	0.117
in water	1.672	2.524	145.88	–0.033	–179.900	0.139

s-r						
in vacuo	1.697	2.533	143.88	179.359	–0.784	0.784
in chloroform	1.687	2.529	144.64	179.402	–0.927	0.927
in acetonitrile	1.684	2.528	144.91	179.573	–1.631	1.631
in water	1.694	2.534	144.28	–179.201	–6.348	6.348
s-w						
in vacuo	1.695	2.532	143.96	179.997	0.002	0.002
in chloroform	1.687	2.529	144.69	–179.998	–0.011	0.011
in acetonitrile	1.683	2.528	144.95	179.966	0.042	0.042
in water	1.686	2.528	144.59	–179.999	0.006	0.006
d-r-u						
in vacuo	1.666	2.512	145.41	–0.002	–179.998	0.003
in acetonitrile	1.651	2.505	146.36	0.017	179.953	0.062
in water	1.696	2.540	145.13	–4.103	–167.958	16.088
d-w-u						
in vacuo	1.685	2.530	144.60	–0.004	180.000	0.002
in chloroform	1.672	2.519	145.32	0.010	179.992	0.002
in acetonitrile	1.668	2.516	145.64	0.009	179.965	0.038
in water	1.666	2.514	145.57	0.014	179.955	0.042
s-r-u						
in vacuo	1.731	2.556	142.73	–177.498	–15.808	15.808
in chloroform	1.726	2.556	143.30	–177.643	–17.041	17.041
in acetonitrile	1.720	2.552	143.62	–177.582	–16.038	16.038
in water	1.733	2.561	142.94	–176.744	–17.202	17.202
GG1						
d-r						
in vacuo	1.692	2.532	144.25	0.001	179.997	0.003
in chloroform	1.684	2.529	145.00	–0.001	–179.996	0.003
in acetonitrile	1.681	2.528	145.28	0.018	179.968	0.047
in water	1.685	2.530	144.95	–0.148	–179.559	0.536
d-w						
in vacuo	1.694	2.534	144.29	0.001	179.994	0.007
in chloroform	1.687	2.532	144.99	0.010	179.964	0.042
in acetonitrile	1.682	2.530	145.34	0.008	179.974	0.041
in water	1.686	2.531	145.00	–0.006	–179.979	0.032
d-r-u						
in vacuo	1.693	2.528	143.85	–0.001	179.995	0.004
in chloroform	1.683	2.523	144.50	–0.013	–179.972	0.029
in acetonitrile	1.678	2.521	144.78	–0.010	–179.987	0.007
in water	1.724	2.556	143.46	3.838	168.597	15.798
d-w-u						
in vacuo	1.699	2.533	143.81	0.000	179.999	0.001
in chloroform	1.686	2.526	144.55	0.002	179.995	0.020

in acetonitrile	1.713	2.549	144.12	3.079	169.812	14.753
in water	1.680	2.522	144.67	0.002	–179.997	0.000
G2						
d-r						
in vacuo	1.663	2.515	145.83	0.245	179.469	0.553
in chloroform	1.656	2.513	146.52	0.300	179.312	0.719
in acetonitrile	1.654	2.512	146.80	0.330	179.206	0.836
in water	1.655	2.512	146.68	0.373	179.173	0.851
d-w						
in vacuo	1.682	2.526	144.98	0.224	179.496	0.527
in chloroform	1.674	2.524	145.75	0.268	179.350	0.680
in acetonitrile	1.670	2.522	146.09	0.321	179.247	0.792
in water	1.672	2.523	145.88	0.357	179.138	0.920
s-r						
in vacuo	1.696	2.532	143.88	179.614	–1.441	1.441
in chloroform	1.687	2.529	144.63	179.769	–1.976	1.976
in acetonitrile	1.684	2.528	144.89	179.881	–2.509	2.509
in water	1.699	2.537	144.10	–178.341	–8.918	8.918
s-w						
in vacuo	1.694	2.532	143.96	–179.811	–0.533	0.533
in chloroform	1.686	2.528	144.68	–179.762	–0.663	0.663
in acetonitrile	1.684	2.527	144.96	–179.760	–0.811	0.811
in water	1.686	2.528	144.58	–179.532	–1.177	1.177
GG2						
d-r						
in vacuo	1.691	2.531	144.24	0.190	179.564	0.458
in chloroform	1.684	2.529	144.97	0.209	179.485	0.541
in acetonitrile	1.680	2.527	145.27	0.245	179.397	0.630
in water	1.685	2.529	144.91	0.218	179.535	0.448
d-w						
in vacuo	1.694	2.533	144.23	0.220	179.525	0.501
in chloroform	1.686	2.531	145.03	0.216	179.498	0.508
in acetonitrile	1.682	2.529	145.33	0.224	179.462	0.538
in water	1.686	2.531	144.99	0.193	179.646	0.313
d-r-u						
in vacuo	1.715	2.546	143.31	2.841	171.237	12.500
in chloroform	1.718	2.551	143.68	15.612	169.077	3.364
in acetonitrile	1.716	2.552	143.91	3.431	168.831	15.930
in water	1.726	2.558	143.39	4.019	168.086	16.327
d-w-u						
in vacuo	1.698	2.532	143.80	0.238	179.523	0.496
in chloroform	1.719	2.552	143.77	–3.392	–169.238	15.223
in acetonitrile	1.715	2.551	144.03	–3.292	–169.371	15.219
in water	1.727	2.559	143.42	–4.134	–167.899	16.593

G2-P3

d-r

in vacuo	1.659	2.513	146.19	0.109	179.161	0.616
in chloroform	1.653	2.511	146.73	0.071	178.999	0.809
in acetonitrile	1.650	2.510	146.97	0.071	178.942	0.879
in water	1.653	2.511	146.76	0.481	178.167	1.791

d-w

in vacuo	1.675	2.522	145.34	0.729	179.600	0.581
in chloroform	1.667	2.520	146.12	0.642	179.504	0.655
in acetonitrile	1.663	2.518	146.47	0.635	179.481	0.644
in water	1.663	2.517	146.36	0.794	179.552	0.505

s-r

in vacuo	1.691	2.528	143.96	−179.074	0.405	0.405
in chloroform	1.679	2.522	144.72	−179.239	0.568	0.568
in acetonitrile	1.676	2.521	144.96	−179.536	1.496	1.496
in water	1.678	2.521	144.57	−179.178	0.196	0.196

s-w

in vacuo	1.691	2.528	143.97	−179.611	−0.951	0.951
in chloroform	1.683	2.526	144.71	−179.399	−2.054	2.054
in acetonitrile	1.680	2.524	144.97	−179.467	−2.055	2.055
in water	1.687	2.528	144.46	−178.594	−5.727	5.727

G3

d-r

in vacuo	1.666	2.516	145.68	−2.657	−174.090	6.073
in chloroform	1.662	2.516	146.27	−3.050	−172.962	7.271
in acetonitrile	1.660	2.516	146.51	−3.158	−172.582	7.720
in water	1.667	2.521	146.24	−3.834	−171.193	9.168

d-w

in vacuo	1.685	2.528	144.83	−2.627	−174.096	6.071
in chloroform	1.678	2.526	145.56	−2.853	−173.322	6.897
in acetonitrile	1.675	2.526	145.86	−2.899	−173.094	7.181
in water	1.681	2.529	145.51	−3.677	−171.352	9.072

s-r

in vacuo	1.705	2.538	143.62	176.221	7.859	7.859
in chloroform	1.698	2.536	144.29	175.952	8.985	8.985
in acetonitrile	1.695	2.535	144.53	175.932	9.157	9.157
in water	1.705	2.541	143.93	175.322	10.255	10.255

s-w

in vacuo	1.699	2.535	143.75	177.476	6.894	6.894
in chloroform	1.692	2.533	144.45	177.164	8.181	8.181
in acetonitrile	1.693	2.534	144.61	177.029	8.874	8.874
in water	1.706	2.542	143.90	176.205	11.953	11.953

d-r-u

in vacuo	1.698	2.538	144.55	–4.394	–167.772	15.962
in chloroform	1.701	2.543	144.86	–4.692	–166.237	18.016
in acetonitrile	1.699	2.543	145.08	–4.775	–165.898	18.408
in water	1.711	2.551	144.61	–5.642	–164.698	19.356
s-w-u						
in vacuo	1.734	2.558	142.61	176.740	16.815	16.815
in chloroform	1.734	2.562	143.06	176.823	18.707	18.707
in acetonitrile	1.733	2.562	143.26	176.769	19.164	19.164
in water	1.745	2.569	142.49	175.727	20.264	20.264
GG3						
d-r						
in vacuo	1.694	2.532	144.12	–2.296	–174.783	5.380
in chloroform	1.687	2.531	144.82	–2.669	–173.671	6.583
in acetonitrile	1.684	2.529	145.19	–2.708	–173.510	6.750
in water	1.693	2.535	144.63	–3.428	–171.882	8.565
d-w						
in vacuo	1.699	2.536	144.09	–2.589	–174.250	5.909
in chloroform	1.690	2.533	144.83	–2.878	–173.307	6.921
in acetonitrile	1.688	2.533	145.10	–2.947	–173.067	7.209
in water	1.695	2.537	144.63	–3.587	–171.603	8.845
d-r-u						
in vacuo	1.722	2.551	143.11	–4.031	–168.767	15.008
in chloroform	1.723	2.555	143.52	–4.308	–167.099	17.394
in acetonitrile	1.723	2.556	143.67	–4.452	–166.720	17.872
in water	1.737	2.565	142.99	–5.184	–165.537	18.920
d-w-u						
in vacuo	1.729	2.556	143.07	4.516	168.059	15.449
in chloroform	1.727	2.559	143.53	4.578	166.751	17.561
in acetonitrile	1.725	2.558	143.75	4.587	166.567	17.919
in water	1.742	2.570	142.97	5.545	164.858	19.661
JJ						
d-r						
in vacuo	1.692	2.532	144.25	–0.004	179.998	0.002
in chloroform	1.684	2.529	145.02	0.000	179.991	0.022
in acetonitrile	1.681	2.528	145.28	0.003	179.969	0.040
in water	1.686	2.530	144.95	–0.042	–179.812	0.247
d-w						
in vacuo	1.696	2.535	144.24	–0.001	–179.989	0.005
in chloroform	1.688	2.533	145.00	–0.005	–179.994	0.006
in acetonitrile	1.683	2.530	145.35	–0.050	–179.878	0.143
in water	1.686	2.531	145.02	–0.025	–179.874	0.158
KK						
d-r						

in vacuo	1.692	2.532	144.25	–0.004	179.998	0.000
in chloroform	1.684	2.529	145.01	–0.007	179.989	0.009
in acetonitrile	1.681	2.528	145.28	0.015	179.974	0.027
in water	1.686	2.530	144.93	–0.062	–179.798	0.255
d-w						
in vacuo	1.696	2.535	144.24	–0.001	–179.989	0.009
in chloroform	1.686	2.531	145.05	0.001	–179.000	0.002
in acetonitrile	1.683	2.530	145.35	0.010	179.978	0.026
in water	1.686	2.531	145.02	0.026	179.918	0.098
d-r-u						
in vacuo	1.693	2.528	143.84	0.002	179.992	0.011
in chloroform	1.712	2.547	143.85	–2.912	–170.301	14.133
in acetonitrile	1.710	2.547	144.08	–2.909	–170.178	14.418
in water	1.721	2.554	143.52	–3.653	–169.064	15.249
d-w-u						
in vacuo	1.699	2.533	143.83	–0.002	–179.993	0.010
in chloroform	1.686	2.526	144.56	0.005	179.984	0.026
in acetonitrile	1.713	2.549	144.14	3.068	169.874	14.665
in water	1.729	2.560	143.38	–4.262	–167.561	17.041
L						
d-r						
in vacuo	1.686	2.533	145.23	7.231	163.107	16.975
in chloroform	1.687	2.537	145.74	7.500	162.258	18.040
in acetonitrile	1.689	2.539	145.89	7.531	161.916	18.527
in water	1.716	2.558	144.91	8.703	159.542	21.053
d-w						
in vacuo	1.705	2.545	144.46	–7.174	–162.995	17.089
in chloroform	1.702	2.546	145.08	–7.231	–162.615	17.683
in acetonitrile	1.701	2.547	145.30	–7.177	–162.479	17.997
in water	1.726	2.564	144.32	–8.081	–160.362	20.244
s-r						
in vacuo	1.738	2.566	143.04	171.923	19.413	19.413
in chloroform	1.735	2.567	143.58	171.987	20.112	20.112
in acetonitrile	1.734	2.567	143.75	172.079	20.415	20.415
in water	1.770	2.591	142.29	171.045	23.179	23.179
s-w						
in vacuo	1.725	2.556	143.30	173.369	18.134	18.134
in chloroform	1.726	2.560	143.76	173.256	19.324	19.324
in acetonitrile	1.727	2.562	143.90	173.294	19.887	19.887
in water	1.766	2.590	142.47	172.604	23.211	23.211
d-r-u						
in vacuo	1.746	2.580	144.05	–8.095	–159.486	22.710
in chloroform	1.738	2.576	144.59	–7.977	–159.280	23.215
in acetonitrile	1.734	2.574	144.80	–7.814	–159.367	23.442

in water	1.749	2.583	143.96	–8.292	–158.222	25.602
d-w-u						
in vacuo	1.765	2.600	143.32	–8.098	–159.359	22.698
in chloroform	1.753	2.586	143.98	–7.825	–159.419	23.008
in acetonitrile	1.747	2.583	144.25	–7.576	–159.665	23.156
in water	1.763	2.592	143.33	–7.887	–158.608	25.223
s-r-u						
in vacuo	1.780	2.600	142.32	173.515	23.587	23.587
in chloroform	1.769	2.590	142.89	173.769	23.967	23.967
in acetonitrile	1.763	2.590	143.11	174.053	24.161	24.161
in water	1.784	2.603	141.93	173.820	26.035	26.035
s-w-u						
in vacuo	1.780	2.593	142.30	173.568	23.111	23.111
in chloroform	1.770	2.596	142.88	173.776	23.532	23.532
in acetonitrile	1.766	2.593	143.09	173.967	23.726	23.726
in water	1.781	2.600	141.98	173.990	25.879	25.879
LL						
d-r						
in vacuo	1.707	2.544	143.90	6.534	164.353	15.788
in chloroform	1.706	2.546	144.47	6.734	163.633	16.746
in acetonitrile	1.707	2.548	144.62	6.803	163.253	17.268
in water	1.737	2.569	143.44	7.802	160.907	19.780
d-w						
in vacuo	1.718	2.552	143.76	–7.172	–163.137	16.895
in chloroform	1.713	2.552	144.39	–7.215	–162.795	17.479
in acetonitrile	1.712	2.552	144.59	–7.197	–162.638	17.792
in water	1.741	2.572	143.46	–8.082	–160.549	20.031
d-r-u						
in vacuo	1.769	2.594	142.73	–7.559	–160.141	22.205
in chloroform	1.760	2.589	143.30	–7.540	–159.923	22.684
in acetonitrile	1.756	2.586	143.51	–7.354	–160.090	22.815
in water	1.775	2.598	142.41	–7.611	–159.148	24.953
d-w-u						
in vacuo	1.777	2.600	142.69	–8.109	–159.406	22.639
in chloroform	1.765	2.594	143.31	–7.905	–159.415	22.985
in acetonitrile	1.759	2.590	143.56	–7.639	–159.688	23.074
in water	1.778	2.600	142.45	–7.853	–158.822	25.170
N						
d-r						
in vacuo	1.794	2.615	142.51	–13.801	–148.465	29.571
in chloroform	1.796	2.618	142.75	–13.735	–148.436	29.985
in acetonitrile	1.797	2.620	142.84	–13.604	–148.461	30.196
in water	1.832	2.644	141.46	–14.285	–147.035	31.865

d-w						
in vacuo	1.813	2.628	141.78	−13.507	−148.236	29.782
in chloroform	1.811	2.628	142.17	−13.285	−148.559	29.842
in acetonitrile	1.810	2.628	142.32	−13.095	−148.714	29.978
in water	1.842	2.650	140.92	−13.393	−147.607	31.288
s-r						
in vacuo	1.851	2.654	140.37	168.128	32.255	32.255
in chloroform	1.849	2.654	140.66	168.452	32.767	32.767
in acetonitrile	1.849	2.654	140.63	168.306	32.527	32.527
in water	1.908	2.694	138.40	168.125	35.112	35.112
s-w						
in vacuo	1.833	2.639	168.89	167.812	30.219	30.219
in chloroform	1.834	2.642	140.94	168.059	30.684	30.684
in acetonitrile	1.835	2.642	141.02	168.238	30.899	30.899
in water	1.888	2.679	138.89	168.243	33.627	33.627
NN						
d-r						
in vacuo	1.814	2.626	141.28	−12.887	−149.390	28.685
in chloroform	1.815	2.629	141.58	−12.759	−149.493	28.951
in acetonitrile	1.814	2.629	141.69	−12.587	−149.644	29.025
in water	1.850	2.652	140.16	−12.914	−148.446	30.419
d-w						
in vacuo	1.823	2.634	141.19	−13.458	−148.509	29.418
in chloroform	1.821	2.634	141.54	−13.218	−148.827	29.462
in acetonitrile	1.817	2.631	141.72	−12.965	−149.232	29.264
in water	1.851	2.653	140.21	−13.246	−148.131	30.548
d-r-u						
in vacuo	1.792	2.607	141.72	−11.638	−153.747	25.062
in chloroform	1.786	2.605	142.24	−11.210	−154.104	25.049
in acetonitrile	1.790	2.608	142.05	−11.467	−153.765	25.252
in water	1.837	2.640	140.20	−11.921	−150.149	31.937
d-w-u						
in vacuo	1.800	2.613	141.67	−12.263	−153.096	25.415
in chloroform	1.793	2.611	142.11	−11.895	−153.387	25.379
in acetonitrile	1.789	2.608	142.30	−11.590	−153.811	25.094
in water	1.839	2.632	140.24	−12.300	−149.808	32.061
Q						
d-r						
in vacuo	1.690	2.535	145.04	6.903	163.958	16.084
in chloroform	1.693	2.540	145.45	7.238	162.934	17.328
in acetonitrile	1.695	2.592	145.60	7.329	162.526	17.877
in water	1.720	2.561	144.67	8.369	160.286	20.252

d-w						
in vacuo	1.709	2.547	144.23	6.850	163.850	16.188
in chloroform	1.707	2.549	144.82	6.947	163.398	16.833
in acetonitrile	1.707	2.550	145.03	6.967	163.066	17.369
in water	1.734	2.569	144.01	7.924	160.734	19.925
s-r						
in vacuo	1.742	2.568	142.81	−172.235	−18.542	18.542
in chloroform	1.739	2.569	143.33	−172.290	−19.212	19.212
in acetonitrile	1.738	2.569	143.50	−172.364	−19.571	19.571
in water	1.772	2.593	142.18	−171.454	−21.558	21.558
s-w						
in vacuo	1.729	2.558	143.07	−173.696	−17.184	17.184
in chloroform	1.731	2.563	143.51	−173.582	−18.362	18.362
in acetonitrile	1.732	2.565	143.65	−173.573	−18.968	18.968
in water	1.767	2.589	142.29	−172.801	−21.977	21.977
W						
d-r						
in vacuo	1.696	2.538	144.82	0.015	179.982	0.008
in chloroform	1.695	2.539	145.20	0.011	179.973	0.034
in acetonitrile	1.694	2.539	145.38	0.009	179.978	0.029
in water	1.693	2.539	145.31	0.012	179.879	0.192
d-w						
in vacuo	1.702	2.543	144.74	0.020	179.988	0.012
in chloroform	1.712	2.551	144.49	−0.001	−179.994	0.012
in acetonitrile	1.710	2.550	144.70	0.006	179.996	0.006
in water	1.710	2.550	144.51	0.029	179.855	0.208
s-r						
in vacuo	1.729	2.556	142.94	−179.415	1.037	1.037
in chloroform	1.725	2.556	143.41	−179.403	1.077	1.077
in acetonitrile	1.722	2.554	143.62	−179.371	1.223	1.223
in water	1.723	2.555	143.53	178.983	7.537	7.537
s-w						
in vacuo	1.728	2.556	142.99	179.985	0.000	0.000
in chloroform	1.725	2.556	143.43	−179.997	−0.022	0.022
in acetonitrile	1.724	2.556	143.58	−179.995	−0.062	0.062
in water	1.725	2.555	143.22	−179.966	0.211	0.211
KT1						
d-w						
in vacuo	1.635	2.493	145.36	−0.014	−179.977	0.004
in chloroform	1.636	2.494	145.46	0.002	−179.980	0.013
in acetonitrile	1.636	2.493	145.40	−0.014	−179.984	0.014
in water	1.642	2.496	144.92	−0.024	−179.950	0.062
d-r						

in vacuo	1.633	2.491	145.31	–0.015	–179.971	0.015
in chloroform	1.635	2.492	145.37	–0.008	–179.985	0.004
in acetonitrile	1.635	2.492	145.31	–0.019	–179.958	0.067
in water	1.642	2.496	144.86	0.017	179.791	0.224
KTT1						
d-w						
in vacuo	1.670	2.512	143.47	0.003	–179.992	0.009
in chloroform	1.669	2.513	143.86	0.002	179.987	–0.010
in acetonitrile	1.669	2.513	143.86	0.000	–179.994	0.011
in water	1.675	2.516	143.36	–0.049	–179.861	0.160
d-r						
in vacuo	1.671	2.512	143.36	0.005	–179.981	0.018
in chloroform	1.670	2.513	143.67	–0.008	179.999	0.001
in acetonitrile	1.670	2.514	143.74	–0.004	–179.988	0.008
in water	1.676	2.516	143.25	–0.034	–179.892	0.128
KT2						
d-w						
in vacuo	1.634	2.491	145.34	0.001	–179.950	0.046
in chloroform	1.635	2.493	145.47	–0.008	–179.986	0.013
in acetonitrile	1.635	2.493	145.49	–0.011	–179.996	0.006
in water	1.641	2.495	144.92	0.008	179.950	0.058
d-r						
in vacuo	1.632	2.490	145.33	–0.010	–179.944	0.048
in chloroform	1.634	2.491	145.34	–0.014	–179.919	0.086
in acetonitrile	1.643	2.491	145.34	0.001	–179.995	0.002
in water	1.643	2.496	144.83	0.248	178.550	1.508
KT3						
d-w						
in vacuo	1.615	2.475	145.51	0.411	176.830	3.444
in chloroform	1.619	2.478	145.51	0.698	175.477	4.711
in acetonitrile	1.622	2.480	145.47	0.847	174.703	5.432
in water	1.639	2.491	144.71	1.341	172.817	7.204
d-r						
in vacuo	1.616	2.476	145.31	0.227	177.641	2.716
in chloroform	1.619	2.478	145.49	0.438	176.620	3.687
in acetonitrile	1.620	2.479	145.48	0.507	176.213	4.120
in water	1.639	2.491	144.65	1.474	172.192	7.828
KT3#						
d-w						
in vacuo	1.638	2.489	144.38	0.336	179.570	1.799
in chloroform	1.643	2.494	144.46	0.274	179.933	1.567
in acetonitrile	1.643	2.494	144.50	0.340	179.495	1.978
in water	1.658	2.503	143.76	1.116	176.297	4.958
d-r						

in vacuo	1.644	2.493	144.17	0.164	–179.709	1.207
in chloroform	1.645	2.494	144.31	0.262	–179.990	1.534
in acetonitrile	1.646	2.495	144.34	0.337	179.430	2.091
in water	1.661	2.505	143.61	1.190	175.994	5.363
KT3[##]						
d-w						
in vacuo	1.637	2.493	143.80	0.182	178.153	2.369
in chloroform	1.652	2.498	143.91	0.226	177.887	2.659
in acetonitrile	1.652	2.499	143.97	0.278	177.621	2.919
in water	1.663	2.504	143.34	0.486	176.727	3.785
d-r						
in vacuo	1.654	2.498	143.55	0.066	178.651	1.915
in chloroform	1.651	2.497	143.87	0.118	178.399	2.215
in acetonitrile	1.651	2.498	143.94	0.105	178.439	2.173
in water	1.660	2.502	143.39	0.076	178.768	1.865
KT3*						
d-w						
in vacuo	1.616	2.477	145.65	0.007	178.632	1.916
in chloroform	1.617	2.478	145.73	–0.003	178.648	1.946
in acetonitrile	1.617	2.478	145.76	0.064	178.311	2.276
in water	1.625	2.482	145.18	0.148	178.128	2.470
KT3**						
d-w						
in vacuo	1.637	2.489	144.58	0.039	–178.577	0.376
in chloroform	1.637	2.491	144.77	–0.044	–178.488	0.301
in acetonitrile	1.638	2.491	144.83	–0.079	–178.464	0.271
in water	1.644	2.494	144.33	0.208	–179.683	1.396
KTT3						
d-w						
in vacuo						
in chloroform	1.649	2.496	143.92	–0.072	179.271	1.419
in acetonitrile	1.648	2.496	144.13	–0.094	179.362	1.342
in water	1.649	2.497	144.20	–0.082	179.335	1.376
in water	1.655	2.500	143.72	0.069	178.777	1.911
d-r						
in vacuo	1.651	2.497	143.74	–0.102	179.381	1.320
in chloroform	1.649	2.496	144.04	–0.084	179.306	1.418
in acetonitrile	1.648	2.496	144.14	–0.049	179.167	1.563
in water	1.657	2.501	143.62	–0.054	179.374	1.345
KT4						
d-w						
in vacuo	1.613	2.484	146.88	0.267	–178.431	4.304
in chloroform	1.612	2.485	147.17	0.343	–178.498	4.077
in acetonitrile	1.611	2.484	147.36	0.384	–178.341	3.588

in water	1.611	2.483	147.19	0.387	−178.224	2.432
d-r						
in vacuo	1.591	2.470	147.69	–0.008	−177.748	3.319
in chloroform	1.605	2.479	147.34	0.107	−177.768	3.095
in acetonitrile	1.593	2.472	148.07	0.151	−177.743	2.734
in water	1.611	2.483	147.19	0.219	−177.652	1.975