Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Structure of the Flavonoid Catechin in Solution: NMR and Quantum Chemical Investigation

Haroldo C. Da Silva[a] , Anna Nydia R. Da Silva[a], Theo L. S. Da Rocha[a], Isabel S. Hernandes[a], Hélio F. Dos Santos[b],Wagner B. De Almeida[a,*]

[a]Laboratório de Química Computacional e Modelagem Molecular (LQC-MM), Departamento de Química Inorgânica, Instituto de Química, Universidade Federal Fluminense (UFF), Outeiro de São João Batista s/n, Campus do Valonguinho, 24020-141, Centro, Niterói, RJ, Brazil.

[b] Núcleo de Estudos em Química Computacional (NEQC), Departamento de Química, ICE, Universidade Federal de Juiz de Fora (UFJF), Campus Universitário, Martelos, Juiz de Fora, MG, 36036-330, Brazil.

SUPPLEMENTARY MATERIAL

Methods: Molecular dynamics (MD) simulation was performed for catechin in aqueous solution. The solute plus 746 water molecules were placed inside a 30 Å cubic box. The simulation steps included minimizing the system, 100 ps of NVT heating up to 298.15 K, 1 ns of NPT density equilibration and 1 ns of NVT production. The GAFF2 force field with AM1 BCC charges was used for catechin and the TIP3P potential for water. For the MD simulation, we used the program AMBER-16 and the trajectory was analyzed with the CPPTRAJ module.

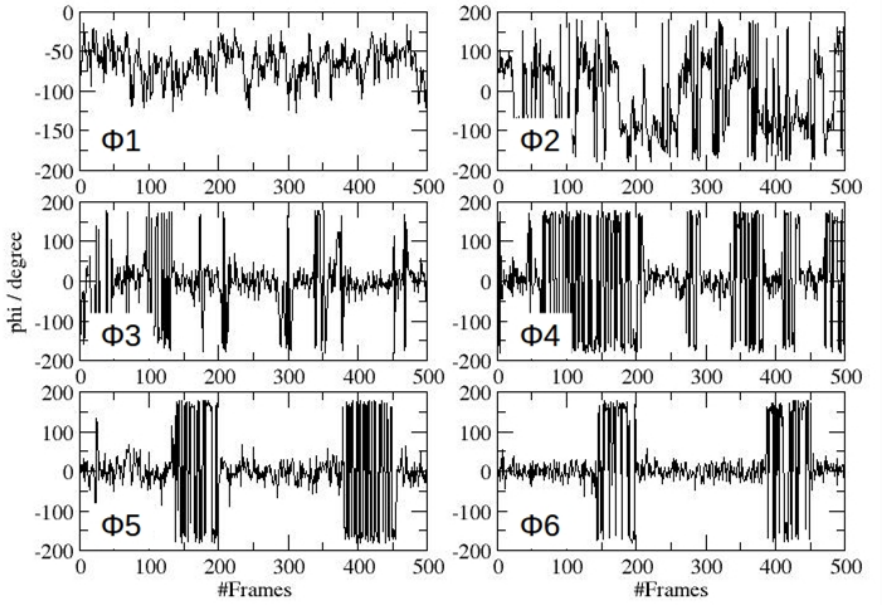


Figure S1. Variation of the dihedral angles that define the conformation of catechin in aqueous solution along the MD trajectory. ϕ_1:[C2', C1', C2, O], ϕ_2:[H, O, C3, C2], ϕ_3:[H, O, C5, C6], ϕ_4:[H, O, C7, C8], ϕ_5:[H, O, C3', C2'], ϕ_6:[H, O, C4', C3'].

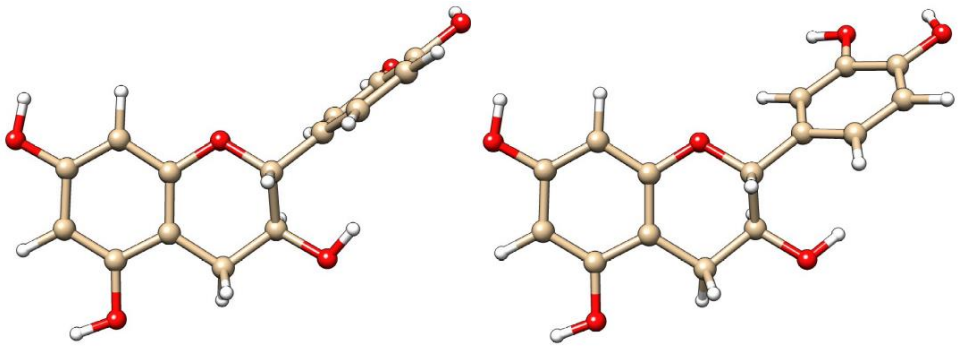


Figure S2. Catechin conformation obtained from the MD simulation (a) and optimized at wB97xD/6-31G(d,p)-PCM level (b). The MD geometry was used as starting point for the DFT geometry optimization (total energy: -1031.0827695 a.u.). The conformational difference is represented by the set of dihedrals ϕ_1:[C2', C1', C2, O], ϕ_2:[H, O, C3, C2], ϕ_3:[H, O, C5, C6], ϕ_4:[H, O, C7, C8], ϕ_5:[H, O, C3', C2'], ϕ_6:[H, O, C4', C3'] found equal to [-66, -23, -13, 6, 0.4, 13] (MD - a) and [-39, -62, 1, 0.9, 0.5, 0.1] (DFT - b).

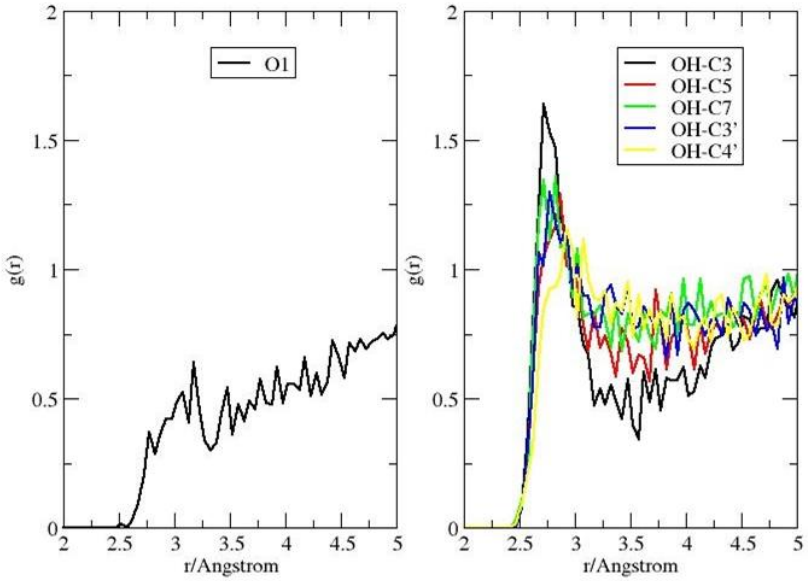


Figure S3. Radial distribution function (RDF) calculated for O-Ow pair of atoms in the catechin molecule.

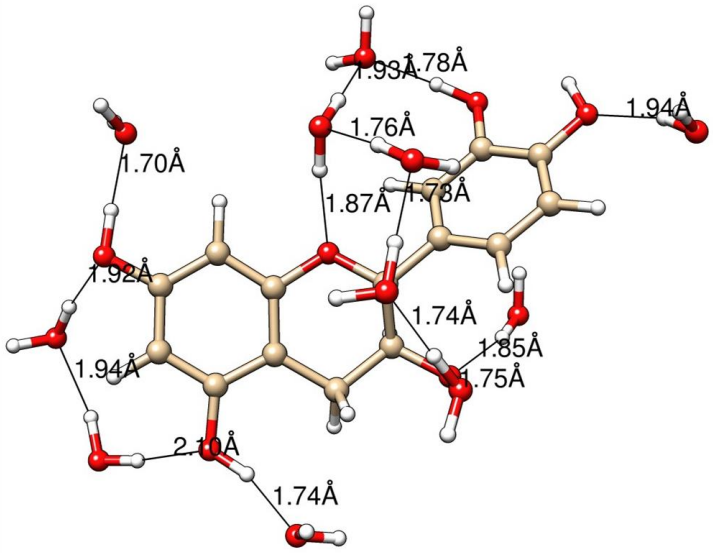


Figure S4. wB97xD/6-31G(d,p)-PCM optimized geometry for the cluster of catechin with 11 water molecules (total energy: -1871.7130978 a.u.). The catechin conformer is characterized by the dihedral angles [-22, 56, -161, 3, 39, 5] (values in degrees).

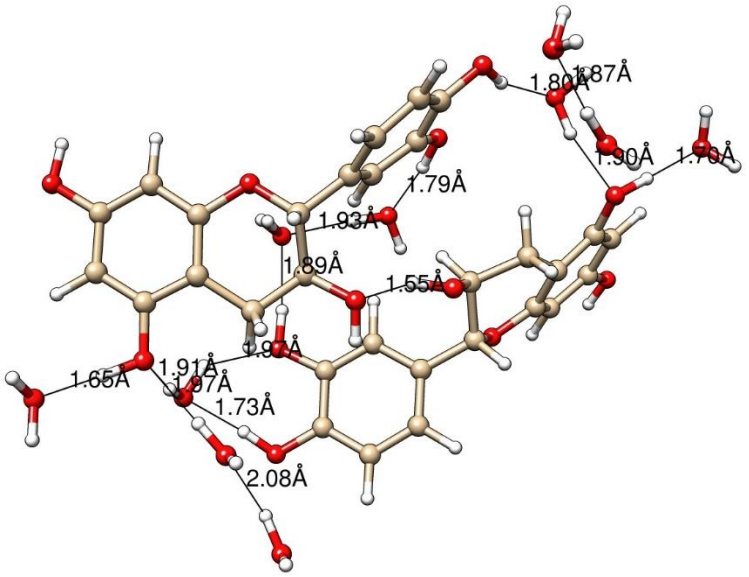
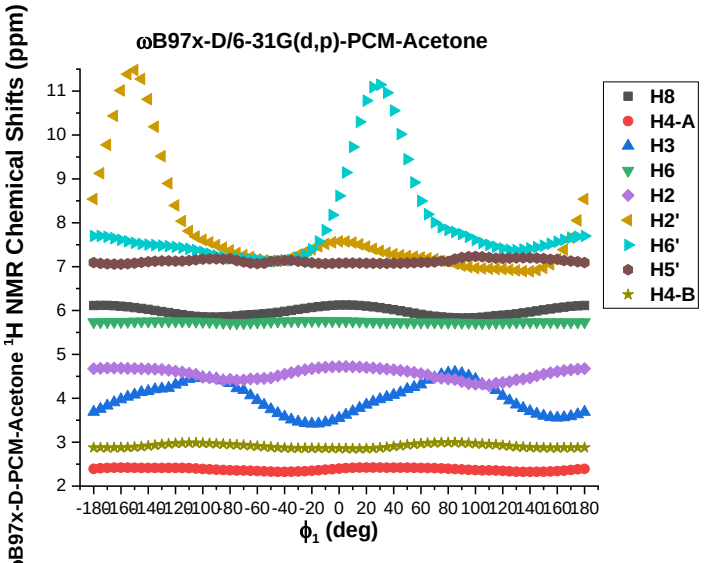
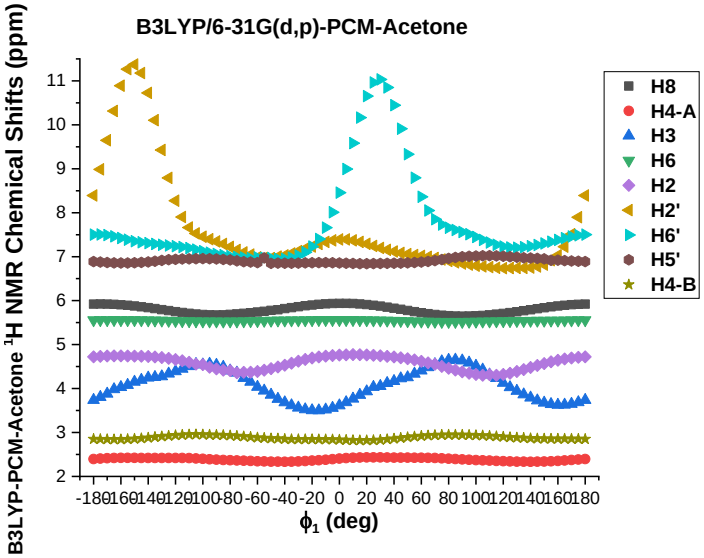


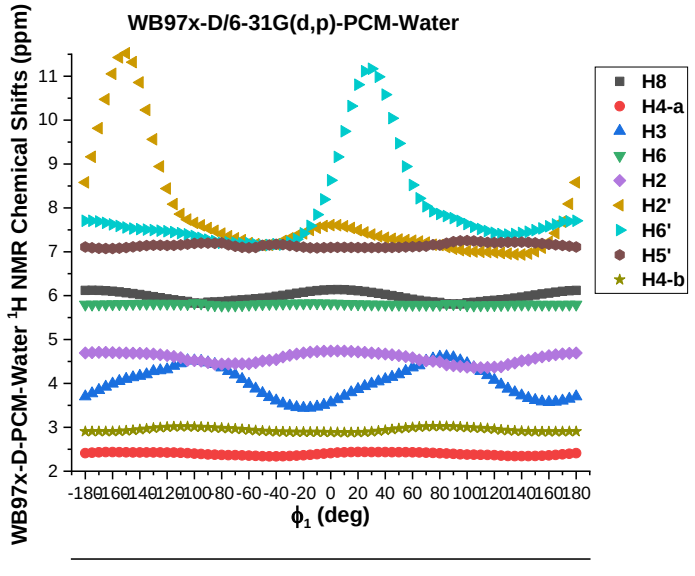
Figure S5. Catechin structures obtained from the solid-state experimental data. The dimer with 10 H_2O molecules with H-position and water arrangements optimized: [-79, 168, -21, 4, -13, -23]...[-79, -97, -12, 6, -9, -29]. The values inset are the O-H...O distances.



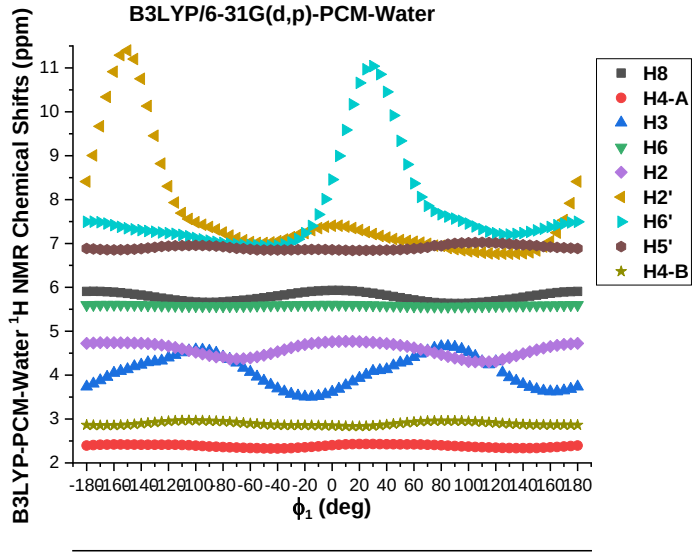
(a)



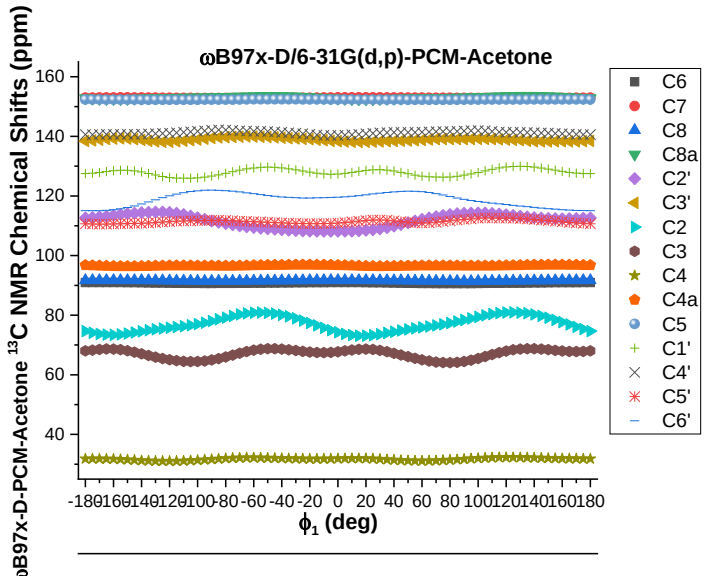
(b)


WB97x-D/6-31G(d,p)-PCM-Water
WB97x-D-PCM-Water ^{1}H NMR Chemical Shifts (ppm)
ϕ_1 (deg)
H8
H4-a
H3
H6
H2
H2'
H6'
H5'
H4-b

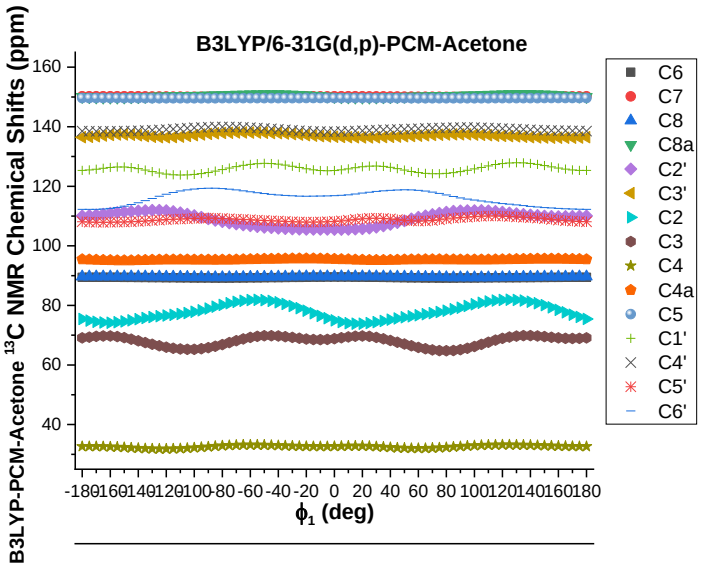
(c)


B3LYP/6-31G(d,p)-PCM-Water
B3LYP-PCM-Water ^{1}H NMR Chemical Shifts (ppm)
ϕ_1 (deg)
H8
H4-A
H3
H6
H2
H2'
H6'
H5'
H4-B

(d)

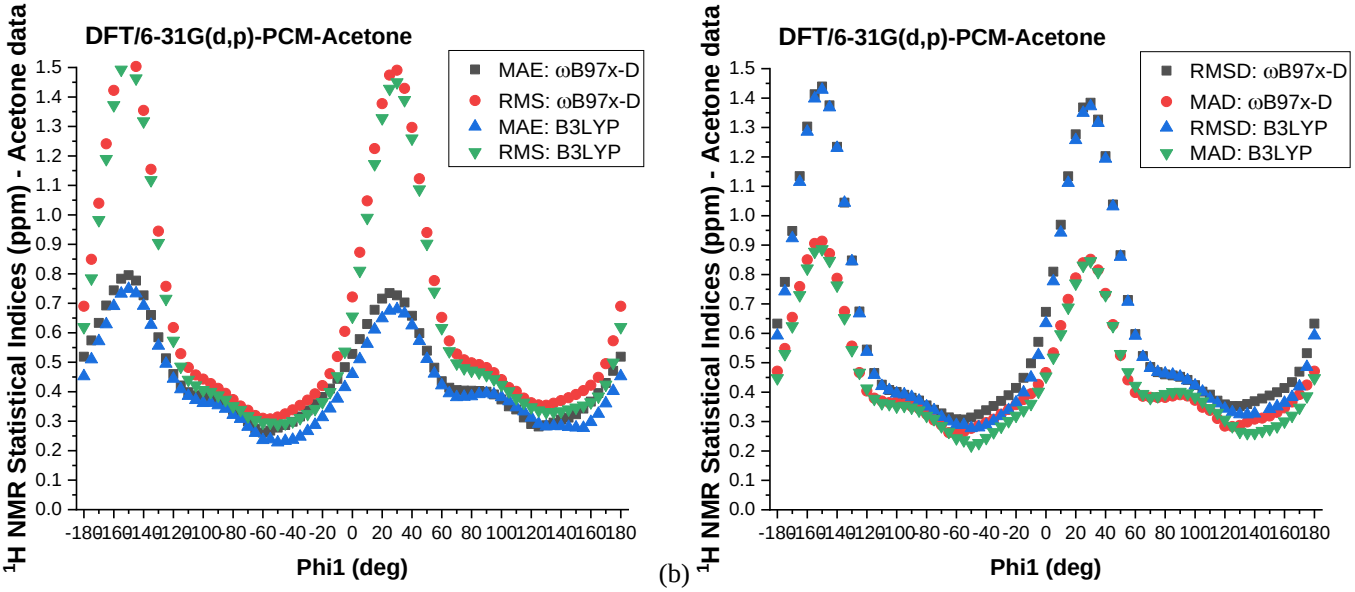

ωB97x-D/6-31G(d,p)-PCM-Acetone
ωB97x-D-PCM-Acetone ^{13}C NMR Chemical Shifts (ppm)
ϕ_1 (deg)
C6
C7
C8
C8a
C2'
C3'
C2
C3
C4
C4a
C5
C1'
C4'
C5'
C6'

(e)



(f)

Figure S6. DFT-PCM NMR chemical shifts scan varying the B-ring torsion angle from -180° do 180° in step size of 5º.
(a,c) ωB97x-d/6-31G(d,p)-PCM-Acetone and water ^{1}H NMR chemical shifts (b,d) B3LYP/6-31(d,p)-PCM-Acetone and water ^{1}H NMR chemical shifts (e) ωB97x-d/6-31G(d,p)-PCM-Acetone ^{13}C NMR chemical shifts.
(f) B3LYP6-31G(d,p)-PCM-Acetone ^{13}C NMR chemical shifts.



(a) (b)

Figure S7. DFT-PCM-Acetone ^{1}H NMR statistical indices (a) MAE, RMS (b) (RMSD, MAD)

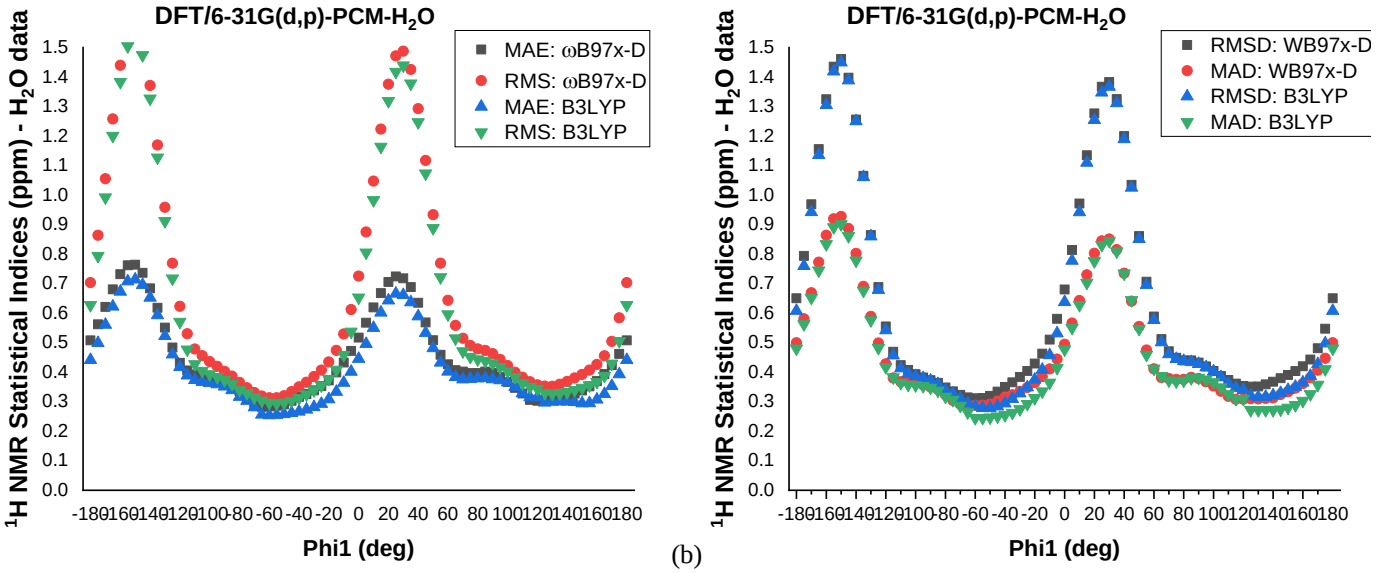


Figure S8. DFT-PCM-Water ^{1}H NMR statistical indices (a) MAE, RMS (b) (RMSD, MAD)

1. RMSD: *Root Mean Square Deviation*.

$$RMSD = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\Delta\delta_i - \overline{\Delta\delta}\right)^2}$$

2. MAD: *Root Mean Deviation*.

$$MAD = \frac{1}{N}\sum_{i=1}^{N}\left|\Delta\delta_i - \overline{\Delta\delta}\right|$$

3. MAE: *Mean Absolute Error*.

$$MAE = \frac{1}{N}\sum_{i=1}^{N}\left|\Delta\delta_i\right|$$

4. RMS: *Root Mean Square*.

$$RMS = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\Delta\delta_i)^2}$$

- Meaning of variables:
$\Delta\delta$: Difference between the calculated and experimental chemical shifts ($\delta_{Theoretical} - \delta_{Experimental}$).
$\overline{\Delta\delta}$: Average of $\Delta\delta$.
N: Total number of carbon or hydrogen atoms considered.
i: Index of the ith C or H atom in the sum.

Figure S9. Statistical Indices: RMSD, MAE, MAD and RMS

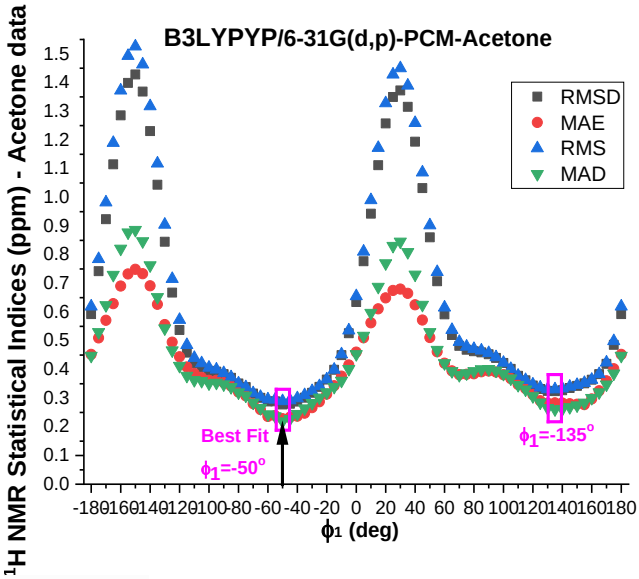


Figure S10. B3LYP/6-31(d,p)-PCM-Acetone statistical indices (RMSD, MAE, RMS and MAD) scan varying the B-ring torsion angle from -180° do 180° in step size of 5º.

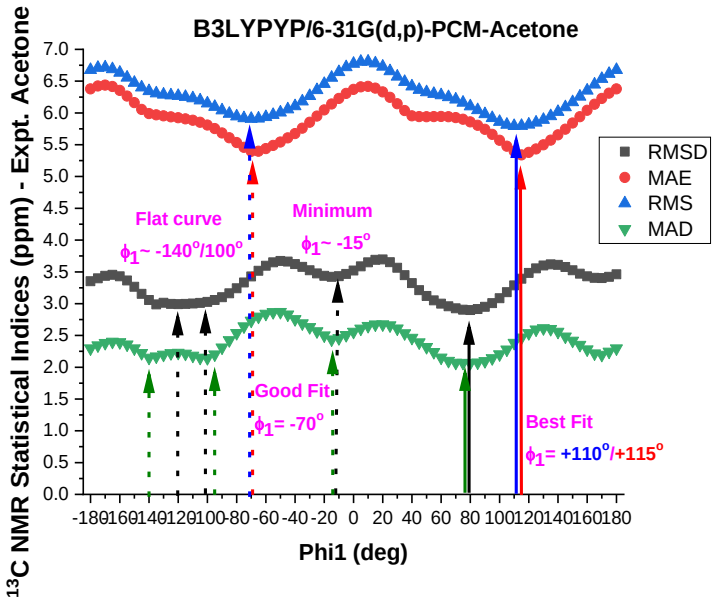


Figure S11. B3LYP/6-31G(d,p)-PCM-Acetone ^{13}C NMR statistical indices for various values of torsion angle ϕ_1 of flavonoid catechin (varying from -180° do 180° in step size of 5º), using as reference experimental Acetone-*d6* data

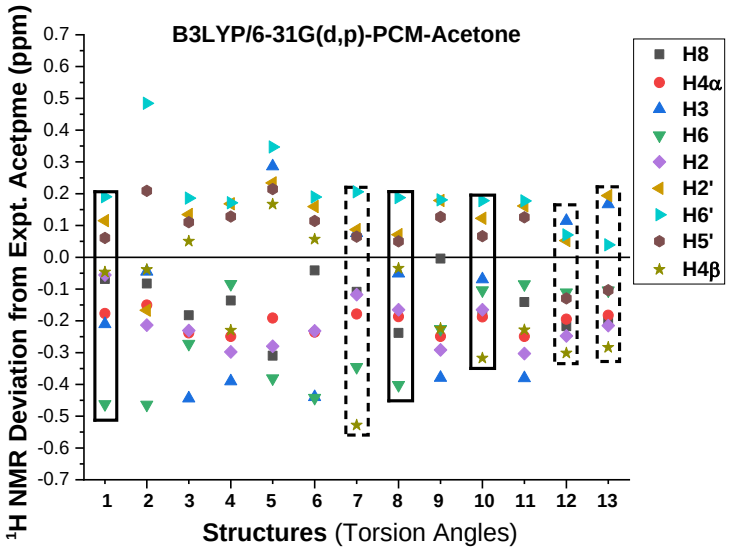


Figure S12. B3LYP/6-31(d,p)-PCM-Acetone deviation from experimental chemical shifts for all optimized catechin structures reported in Table 2.

Table S1. The RDF first peak position and coordination number (CN). The peak maximum (Max) and minimum (Min) are given.

	Max/Å	Min/Å	CN
O1	3.2	3.3	1
OH-C3	2.7	3.2	2
OH-C5	2.9	3.1	2
OH-C7	2.8	3.1	2
OH-C3’	2.8	3.2	2
OH-C4’	2.9	3.0	2

Table S2. ^{1}H and ^{13}C NMR shielding constant and chemical shift calculated for catechin in the solid state. The geometry was partially optimized at wB97xD/6-31G(d,p)-PCM (see Figures S5) and the NMR properties calculated at B3LYP/6-31G(d,p)-PCM.

	2Catechin.10H_2O – X-ray popt.			
	σ/ppm (A)	σ/ppm (B)	Average σ/ppm	Average δ/ppm
C2	111.1877	109.4412	110.3145	82.32
C3	126.4948	128.9930	127.7439	64.89
C4	157.4736	158.4182	157.9459	34.69
C4a	92.3285	92.1919	92.2602	100.37
C5	41.3582	38.9102	40.1342	152.50
C6	100.6408	100.7356	100.6882	91.95
C7	38.6359	38.5449	38.5904	154.04
C8	97.4361	99.6798	98.5579	94.08
C8a	35.3204	37.5891	36.45475	156.18
C1’	65.3122	63.5050	64.4086	128.23
C2’	83.0555	86.4159	84.7357	107.90
C3’	45.7114	52.0629	48.8872	143.75
C4’	45.7267	47.8162	46.7715	145.86
C5’	78.2350	76.7436	77.4893	115.14
C6’	72.0957	70.2621	71.1789	121.46
CH2	27.3751	27.6932	27.5342	4.24
OH3	31.6445	25.1028	28.3737	3.40
CH3	27.6235	27.4186	27.5211	4.26
CH4b	29.6167	29.8436	29.7302	2.05
CH4a	28.9126	29.0530	28.9828	2.79
OH5	20.7762	21.8079	21.2921	10.48
CH6	25.6085	25.5235	25.5660	6.21
OH7	27.5563	27.7301	27.6432	4.13
CH8	25.8639	26.0814	25.9727	5.80
CH2’	24.1277	24.5008	24.3143	7.46
OH3’	23.1035	24.5276	23.8156	7.96
OH4’	22.5570	22.4888	22.5229	9.25
CH5’	24.3776	24.3678	24.3727	7.40
CH6’	24.7574	24.7350	24.7462	7.03

Table S3. ^{1}H and ^{13}C NMR shielding constant and chemical shift calculated for catechin in aqueous solution. The geometry was optimized at wB97xD/6-31G(d,p)-PCM (see Figures S4) and the NMR properties calculated at B3LYP/6-31G(d,p)-PCM.

	Catechin.11H_2O (Fig. S4)	
	σ/ppm	δ/ppm
C2	114.3693	78.26
C3	125.2743	67.36
C4	158.5741	34.06
C4a	95.9273	96.71
C5	42.0515	150.58
C6	97.7084	94.93
C7	42.5860	150.05
C8	102.6768	89.96
C8a	43.7964	148.84
C1’	64.8903	127.74
C2’	81.2244	111.41
C3’	54.4771	138.16
C4’	52.7370	139.90
C5’	82.6528	109.98
C6’	75.5699	117.06
CH2	26.6083	5.17
OH3	25.2185	6.56
CH3	28.3035	3.47
CH4b	29.2939	2.48
CH4a	29.0719	2.70
OH5	22.5535	9.22
CH6	25.5513	6.23
OH7	21.9683	9.81
CH8	25.3200	6.46
CH2’	24.5285	7.25
OH3’	23.6736	8.10
OH4’	25.9091	5.87
CH5’	24.2365	7.54
CH6’	24.6075	7.17

OPTIMIZED CARTESIAN COORDINATES (Singlet State)

M1- Structure

ωB97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number	X	Y	Z
6	0.332208	0.608693	-0.598393
6	-1.762720	-0.507279	-0.280127
6	-2.380342	0.692045	0.077294
6	-1.579770	1.948172	0.278738
6	-0.108364	1.610646	0.473261
1	-1.972317	-2.604528	-0.719093
6	-2.480043	-1.691907	-0.438645
6	-3.765395	0.668141	0.269017
1	-1.660759	2.614666	-0.587647
1	0.040601	1.130019	1.451676
6	-4.511504	-0.497605	0.119185
6	-3.854144	-1.677583	-0.233692
1	-5.585853	-0.485854	0.277114
8	-0.418012	-0.601452	-0.472229
1	0.133080	1.056470	-1.580985
6	1.789737	0.250362	-0.489716
6	2.213736	-0.637261	0.504174
6	2.729414	0.836137	-1.328573
6	3.559630	-0.926229	0.646377
1	1.486156	-1.107010	1.158703
6	4.086522	0.550428	-1.184032
1	2.404576	1.526619	-2.098748
6	4.507756	-0.329862	-0.199423
1	4.826860	0.999594	-1.835336
8	0.712592	2.748702	0.334051
1	0.399926	3.408294	0.959945
8	-4.342430	1.846997	0.615189
1	-5.286191	1.716467	0.747382
8	-4.518528	-2.850051	-0.394894
1	-5.459371	-2.710079	-0.251758
8	5.825272	-0.618734	-0.051787
1	5.906468	-1.248200	0.675709
8	4.077569	-1.779977	1.575281
1	3.375462	-2.142818	2.122946
1	-1.960659	2.501085	1.142529

M2- Structure

ωB97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number	X	Y	Z
6	-0.328975	0.372241	0.332910
6	1.847348	-0.572786	0.088972
6	2.414057	0.697846	-0.025818
6	1.553192	1.924272	-0.160773
6	0.128991	1.541557	-0.542947
1	2.152136	-2.694098	0.290384
6	2.623777	-1.724875	0.199040
6	3.810092	0.779973	-0.018829
1	1.507794	2.473060	0.787710
1	0.096215	1.196475	-1.587373
6	4.615087	-0.350901	0.092249
6	4.007801	-1.603607	0.194561
1	5.696401	-0.255478	0.093334

8	0.498722	-0.765147	0.079535
1	-0.216282	0.671674	1.383564
6	-1.752970	-0.035661	0.068922
6	-2.750054	0.272492	0.995152
6	-2.094836	-0.685632	-1.113541
6	-4.069368	-0.063326	0.735963
1	-2.496644	0.775329	1.923711
6	-3.419831	-1.023492	-1.376920
1	-1.320089	-0.937085	-1.828816
6	-4.412476	-0.712344	-0.458019
1	-3.698838	-1.529762	-2.293540
8	-0.774977	2.602353	-0.327355
1	-0.451728	3.362401	-0.819288
8	4.339022	2.025065	-0.129269
1	5.299131	1.965818	-0.144605
8	4.732361	-2.746205	0.300902
1	5.670723	-2.535897	0.277524
8	-5.706292	-1.036157	-0.708057
1	-6.231988	-0.738933	0.045407
8	-5.114605	0.184594	1.576319
1	-4.808094	0.628171	2.372521
1	1.976417	2.607756	-0.902672

M3- Structure

*ω*B97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number	**X**	**Y**	**Z**
6	-0.312656	-0.557403	-0.595534
6	1.783679	0.516615	-0.255882
6	2.373277	-0.695540	0.099640
6	1.554491	-1.939536	0.315345
6	0.090061	-1.581997	0.479025
1	2.028155	2.601421	-0.708350
6	2.530396	1.683958	-0.426035
6	3.762923	-0.703283	0.279160
1	1.642053	-2.622187	-0.537636
1	-0.075375	-1.108612	1.458187
6	4.535817	0.440607	0.118338
6	3.905763	1.634864	-0.233102
1	5.610347	0.417688	0.262193
8	0.439871	0.645003	-0.442845
1	-0.097947	-0.998535	-1.577884
6	-1.774151	-0.211884	-0.498970
6	-2.214256	0.696374	0.471076
6	-2.707685	-0.862480	-1.299046
6	-3.565941	0.951293	0.617701
1	-1.493206	1.208566	1.099979
6	-4.071869	-0.611209	-1.146957
1	-2.372369	-1.569560	-2.049783
6	-4.506644	0.296969	-0.195481
1	-4.805368	-1.109221	-1.769230
8	-0.663365	-2.764659	0.346073
1	-1.593537	-2.527790	0.430847
8	4.312787	-1.895008	0.625854
1	5.261295	-1.786383	0.745423
8	4.696440	2.727391	-0.381522
1	4.149030	3.483754	-0.609014
8	-5.828371	0.556070	-0.045409
1	-5.920966	1.216097	0.652955
8	-4.100030	1.819667	1.520853
1	-3.405996	2.223775	2.049840
1	1.915986	-2.480818	1.192773

M4- Structure

*ω*B97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number	X	Y	Z
6	0.293494	0.519948	-0.490815
6	-1.789603	-0.546130	-0.143098
6	-2.390471	0.682702	0.137955
6	-1.568856	1.921812	0.392377
6	-0.097245	1.578459	0.553649
1	-2.015758	-2.641019	-0.539196
6	-2.530303	-1.712570	-0.322718
6	-3.792185	0.709324	0.192616
1	-1.648203	2.630583	-0.441278
1	0.081005	1.135278	1.543729
6	-4.559057	-0.435618	0.013138
6	-3.917548	-1.646776	-0.235406
1	-5.638305	-0.381047	0.066647
8	-0.436348	-0.679101	-0.246410
1	0.031819	0.911805	-1.482792
6	1.762997	0.203408	-0.441249
6	2.255717	-0.729577	0.477760
6	2.653527	0.903273	-1.250015
6	3.617145	-0.964020	0.561314
1	1.569440	-1.282955	1.110267
6	4.026394	0.674289	-1.158814
1	2.276957	1.627841	-1.963786
6	4.513632	-0.260353	-0.259632
1	4.725598	1.210732	-1.788404
8	0.637019	2.766506	0.379816
1	1.571521	2.548779	0.471368
8	-4.469230	1.860690	0.433162
1	-3.857375	2.600435	0.495805
8	-4.703266	-2.740222	-0.402136
1	-4.149218	-3.508683	-0.568812
8	5.844398	-0.500894	-0.172146
1	5.975789	-1.186159	0.495176
8	4.201043	-1.856266	1.408149
1	3.534155	-2.300039	1.940112
1	-1.912179	2.439739	1.295300

M5- Structure

*ω*B97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number	X	Y	Z
6	0.305713	0.398644	-0.711477
6	-1.819894	-0.562165	-0.168700
6	-2.392728	0.703761	-0.042306
6	-1.550430	1.946526	-0.100409
6	-0.089068	1.603927	0.146568
1	-2.104737	-2.695219	-0.197472
6	-2.577840	-1.729160	-0.091134
6	-3.773613	0.764794	0.168313
1	-1.620362	2.428299	-1.081980
1	0.059096	1.320479	1.198966
6	-4.559420	-0.380991	0.252465
6	-3.947115	-1.628415	0.121917
1	-5.629507	-0.300980	0.417720
8	-0.482238	-0.738311	-0.352193
1	0.112512	0.655208	-1.761068

6	1.751094	0.019779	-0.537901
6	2.314688	0.007082	0.741693
6	2.549625	-0.257477	-1.639987
6	3.658248	-0.281147	0.902931
1	1.697518	0.217029	1.609362
6	3.904881	-0.544020	-1.480273
1	2.115068	-0.244591	-2.632858
6	4.463990	-0.559153	-0.212088
1	4.535891	-0.765501	-2.332395
8	0.765139	2.664032	-0.220864
1	1.664475	2.391870	-0.017109
8	-4.306684	2.006690	0.290471
1	-5.251047	1.934460	0.457745
8	-4.651188	-2.786109	0.193491
1	-4.050453	-3.533752	0.121141
8	5.779707	-0.842874	-0.042362
1	5.965935	-0.806332	0.904223
8	4.305415	-0.324802	2.101741
1	3.697262	-0.115039	2.816302
1	-1.901638	2.673152	0.637473

M6- Structure

ωB97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number	X	Y	Z
6	0.315039	0.554225	-0.587180
6	-1.779323	-0.522474	-0.248384
6	-2.370014	0.692230	0.104293
6	-1.552347	1.936570	0.322781
6	-0.086624	1.582171	0.484641
1	-2.034344	-2.610367	-0.703060
6	-2.523819	-1.687552	-0.423824
6	-3.758290	0.701223	0.274622
1	-1.641793	2.620430	-0.529109
1	0.082395	1.111334	1.464472
6	-4.531727	-0.444239	0.106888
6	-3.900429	-1.639158	-0.241938
1	-5.607581	-0.404001	0.247654
8	-0.433374	-0.648589	-0.423078
1	0.095020	0.989969	-1.570725
6	1.777394	0.211626	-0.494425
6	2.220436	-0.697830	0.473065
6	2.708569	0.863789	-1.296347
6	3.572371	-0.953934	0.614298
1	1.501215	-1.211145	1.103271
6	4.073140	0.611224	-1.149684
1	2.371290	1.571471	-2.045702
6	4.510617	-0.298906	-0.201179
1	4.804625	1.109626	-1.774117
8	0.663719	2.766108	0.346595
1	1.594830	2.530915	0.427303
8	-4.310748	1.891840	0.619960
1	-5.259406	1.784079	0.737148
8	-4.592422	-2.792543	-0.422940
1	-5.531136	-2.629797	-0.290025
8	5.832551	-0.559647	-0.056494
1	5.926978	-1.222667	0.638921
8	4.108644	-1.824409	1.514109
1	3.415618	-2.231853	2.041993
1	-1.914633	2.476156	1.200997

M7- Structure

*ω*B97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number	X	Y	Z
6	0.319162	0.561200	-0.632663
6	-1.783822	-0.527108	-0.273483
6	-2.386859	0.685127	0.063441
6	-1.574318	1.938820	0.222617
6	-0.105609	1.593147	0.415886
1	-2.017714	-2.630087	-0.666749
6	-2.513872	-1.707520	-0.400098
6	-3.769144	0.677318	0.273572
1	-1.654126	2.579059	-0.662935
1	0.047568	1.138023	1.405449
6	-4.527564	-0.483969	0.156902
6	-3.885500	-1.676353	-0.180741
1	-5.599518	-0.458140	0.327321
8	-0.442054	-0.638322	-0.476735
1	0.121597	0.988317	-1.624295
6	1.772878	0.191938	-0.517989
6	2.226158	-0.492654	0.613837
6	2.682439	0.577459	-1.494303
6	3.571783	-0.782047	0.754441
1	1.522229	-0.802841	1.379405
6	4.039651	0.290655	-1.352690
1	2.333187	1.111286	-2.370573
6	4.489653	-0.389961	-0.232250
1	4.757040	0.583161	-2.109745
8	0.723688	2.719891	0.239213
1	0.414470	3.401414	0.842791
8	-4.331851	1.867524	0.602454
1	-3.650224	2.545214	0.636236
8	-4.561904	-2.845331	-0.311372
1	-5.500537	-2.692458	-0.167555
8	5.806532	-0.680976	-0.085433
1	5.908797	-1.155651	0.748992
8	4.117533	-1.446579	1.812000
1	3.435400	-1.674003	2.450295
1	-1.943930	2.520730	1.071481

M8- Structure

*ω*B97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number	X	Y	Z
6	0.319492	0.568950	-0.633808
6	-1.783004	-0.518582	-0.269456
6	-2.386765	0.695077	0.060983
6	-1.574926	1.950015	0.213803
6	-0.106082	1.606137	0.409231
1	-2.015686	-2.623710	-0.651785
6	-2.512398	-1.700026	-0.390079
6	-3.769097	0.687633	0.270817
1	-1.654856	2.585577	-0.675101
1	0.047093	1.156270	1.401196
6	-4.526873	-0.474649	0.160031
6	-3.884096	-1.668441	-0.171221
1	-5.598883	-0.448499	0.330053
8	-0.441127	-0.630145	-0.471799
1	0.121944	0.990775	-1.627706
6	1.773375	0.201064	-0.516854

6	2.226740	-0.477365	0.618644
6	2.682972	0.581960	-1.494948
6	3.572483	-0.765306	0.761085
1	1.522787	-0.783921	1.385652
6	4.040301	0.296621	-1.351508
1	2.333653	1.111016	-2.374080
6	4.490387	-0.377894	-0.227419
1	4.757721	0.585547	-2.109908
8	0.722662	2.732381	0.226875
1	0.412936	3.416885	0.826809
8	-4.332514	1.879243	0.593338
1	-5.275128	1.757943	0.740932
8	-4.559849	-2.838444	-0.295906
1	-3.946493	-3.541712	-0.528918
8	5.807384	-0.667439	-0.078763
1	5.909695	-1.137694	0.758154
8	4.118326	-1.424013	1.822234
1	3.436156	-1.648461	2.461543
1	-1.945054	2.536157	1.059525

M9- Structure

*ω*B97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number	X	Y	Z
6	0.299243	0.520850	-0.509154
6	-1.786621	-0.546423	-0.164070
6	-2.384332	0.682759	0.133556
6	-1.559376	1.919352	0.389365
6	-0.088703	1.570804	0.544348
1	-2.032349	-2.642187	-0.574577
6	-2.528561	-1.709356	-0.344870
6	-3.782884	0.708938	0.206059
1	-1.639205	2.631175	-0.441839
1	0.090040	1.118407	1.530265
6	-4.552654	-0.436910	0.028683
6	-3.914223	-1.645990	-0.238217
1	-5.631496	-0.366637	0.100854
8	-0.434059	-0.678558	-0.278259
1	0.042804	0.922998	-1.498244
6	1.767662	0.199625	-0.454789
6	2.253510	-0.718434	0.482888
6	2.663705	0.881232	-1.272703
6	3.613411	-0.956699	0.576336
1	1.562148	-1.255939	1.123598
6	4.035396	0.647771	-1.172569
1	2.292876	1.595226	-2.000007
6	4.515623	-0.272399	-0.254852
1	4.739250	1.169252	-1.809506
8	0.649506	2.757712	0.379242
1	1.583366	2.534572	0.464069
8	-4.460677	1.855565	0.466976
1	-3.856849	2.604057	0.485525
8	-4.603538	-2.800249	-0.421115
1	-5.545730	-2.628611	-0.329347
8	5.845028	-0.516469	-0.157965
1	5.971337	-1.190160	0.522014
8	4.190683	-1.834443	1.442629
1	3.520139	-2.265937	1.980028
1	-1.899049	2.434592	1.295026

M10- Structure

*ω*B97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number	X	Y	Z
6	0.306903	0.554857	-0.509561
6	-1.777256	-0.538922	-0.162321
6	-2.398877	0.680698	0.111339
6	-1.588617	1.930165	0.344128
6	-0.109003	1.602271	0.527032
1	-1.970068	-2.643733	-0.527417
6	-2.498486	-1.721223	-0.318678
6	-3.800008	0.682844	0.182441
1	-1.664449	2.622083	-0.503908
1	0.058972	1.159774	1.519150
6	-4.547318	-0.478244	0.027031
6	-3.885083	-1.680575	-0.211536
1	-5.626835	-0.444020	0.092290
8	-0.424099	-0.649583	-0.274144
1	0.055029	0.941997	-1.505894
6	1.771638	0.219824	-0.453117
6	2.264373	-0.588134	0.576317
6	2.651986	0.743388	-1.391981
6	3.619426	-0.859787	0.653803
1	1.583708	-1.012435	1.308062
6	4.018109	0.477499	-1.310990
1	2.273098	1.368221	-2.192894
6	4.508330	-0.321196	-0.289351
1	4.713077	0.881455	-2.037337
8	0.699770	2.738395	0.329624
1	0.463239	3.386494	0.999312
8	-4.494964	1.824369	0.421172
1	-3.904665	2.583723	0.410938
8	-4.651246	-2.791683	-0.349982
1	-4.084069	-3.551751	-0.511677
8	5.835399	-0.588639	-0.201357
1	5.970705	-1.142698	0.577665
8	4.200216	-1.644723	1.605756
1	3.541980	-1.937976	2.241806
1	-1.947020	2.462967	1.234024

M11- Structure

*ω*B97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number	X	Y	Z
6	0.294574	0.519910	-0.504124
6	-1.790759	-0.544144	-0.155821
6	-2.388602	0.684164	0.134206
6	-1.563935	1.921197	0.388837
6	-0.093504	1.572684	0.546544
1	-2.021931	-2.637257	-0.558490
6	-2.534017	-1.709370	-0.333881
6	-3.789873	0.711387	0.200837
1	-1.642726	2.631770	-0.443502
1	0.083951	1.122424	1.533653
6	-4.558791	-0.432716	0.025645
6	-3.920237	-1.643434	-0.232779
1	-5.637456	-0.377578	0.088600
8	-0.438444	-0.679070	-0.268121
1	0.035873	0.918391	-1.494084
6	1.763261	0.200185	-0.451893
6	2.252602	-0.715855	0.485892

6	2.656364	0.881776	-1.273166
6	3.613121	-0.952253	0.576133
1	1.563631	-1.253142	1.129358
6	4.028541	0.650242	-1.176256
1	2.282784	1.594421	-2.000397
6	4.512287	-0.267987	-0.258380
1	4.730139	1.171698	-1.815707
8	0.645436	2.758699	0.379268
1	1.578907	2.535823	0.468073
8	-4.464724	1.861883	0.452194
1	-3.857154	2.606850	0.479231
8	-4.708092	-2.735941	-0.395642
1	-4.156080	-3.503993	-0.571075
8	5.842255	-0.510091	-0.164616
1	5.971335	-1.182254	0.516334
8	4.193781	-1.828253	1.441915
1	3.525590	-2.257567	1.983988
1	-1.904758	2.437878	1.293259

M12- Structure

ωB97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number			X	Y	Z
1	6	0	0.307152	0.508728	-0.531004
2	6	0	-1.786299	-0.551667	-0.141481
3	6	0	-2.395581	0.683616	0.086604
4	6	0	-1.572772	1.932642	0.274300
5	6	0	-0.096118	1.597191	0.467240
6	1	0	-2.001330	-2.666283	-0.431145
7	6	0	-2.519933	-1.731100	-0.257084
8	6	0	-3.796635	0.702942	0.155996
9	1	0	-1.643067	2.594766	-0.597524
10	1	0	0.068346	1.189963	1.474944
11	6	0	-4.556011	-0.454994	0.040428
12	6	0	-3.906203	-1.671888	-0.153960
13	1	0	-5.635103	-0.406863	0.103449
14	8	0	-0.434179	-0.679967	-0.247472
15	1	0	0.055160	0.858698	-1.541071
16	6	0	1.768546	0.162496	-0.467724
17	6	0	2.296538	-0.432383	0.681998
18	6	0	2.614984	0.466505	-1.523750
19	6	0	3.649994	-0.716222	0.779059
20	1	0	1.638231	-0.684949	1.508370
21	6	0	3.978440	0.188512	-1.433531
22	1	0	2.217381	0.925330	-2.421940
23	6	0	4.505543	-0.399723	-0.292036
24	1	0	4.641030	0.427652	-2.259457
25	8	0	0.724027	2.717315	0.228695
26	1	0	0.496063	3.390334	0.876356
27	8	0	-4.479837	1.859448	0.352927
28	1	0	-3.880756	2.611189	0.319261
29	8	0	-4.684273	-2.778898	-0.253819
30	1	0	-4.125351	-3.551078	-0.383455
31	8	0	5.820886	-0.699674	-0.137928
32	1	0	6.298246	-0.436323	-0.930691
33	8	0	4.217153	-1.295143	1.869514
34	1	0	3.535746	-1.445379	2.532222
35	1	0	-1.924677	2.500357	1.145018

M13- Structure

*ω*B97x-D/6-31G(d,p)-PCM-Acetone fully optimized XYZ coordinates

Atomic Number			X	Y	Z
1	6	0	0.296258	0.502248	-0.521117
2	6	0	-1.798284	-0.555898	-0.129595
3	6	0	-2.409135	0.680979	0.085016
4	6	0	-1.587777	1.932133	0.264558
5	6	0	-0.111504	1.599437	0.465905
6	1	0	-2.010550	-2.673396	-0.399862
7	6	0	-2.530449	-1.737012	-0.236321
8	6	0	-3.810502	0.699930	0.148770
9	1	0	-1.655052	2.586443	-0.613441
10	1	0	0.049392	1.201420	1.477882
11	6	0	-4.568541	-0.459731	0.041626
12	6	0	-3.917144	-1.677986	-0.138422
13	1	0	-5.647947	-0.411825	0.099698
14	8	0	-0.445655	-0.684118	-0.229675
15	1	0	0.048121	0.843284	-1.535124
16	6	0	1.757369	0.156139	-0.449015
17	6	0	2.277902	-0.428696	0.709982
18	6	0	2.608083	0.449788	-1.506992
19	6	0	3.630639	-0.705833	0.797944
20	1	0	1.620191	-0.675367	1.538005
21	6	0	3.972775	0.176711	-1.418915
22	1	0	2.207654	0.899602	-2.408630
23	6	0	4.490359	-0.398932	-0.269206
24	1	0	4.645698	0.404247	-2.236938
25	8	0	0.708610	2.717917	0.220258
26	1	0	0.477203	3.397062	0.860308
27	8	0	-4.495365	1.857695	0.331777
28	1	0	-3.897225	2.609874	0.290340
29	8	0	-4.693809	-2.786719	-0.229686
30	1	0	-4.133618	-3.559216	-0.352316
31	8	0	5.815908	-0.670439	-0.171817
32	1	0	6.232893	-0.394077	-0.997549
33	8	0	4.238442	-1.279217	1.875361
34	1	0	5.181353	-1.375958	1.713693
35	1	0	-1.943447	2.507269	1.128870