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Electronic Supplementary Information (ESI).

Experimental and theoretical insights on the formation of weak hydrogen bonds and dihydrogen interactions in the solid-state structure of two eucalyptol derivatives.

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Figure S1. Optimized molecular structures of compounds **4** (a) and **6** (b) at the B3LYP/6-311++G(d,p) level of theory.

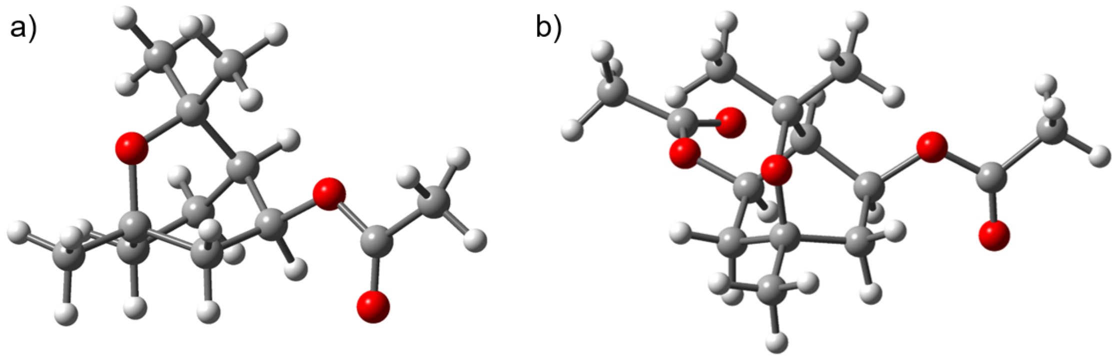

Figure S2. Full and decomposed two-dimensional fingerprint plots for **4**.

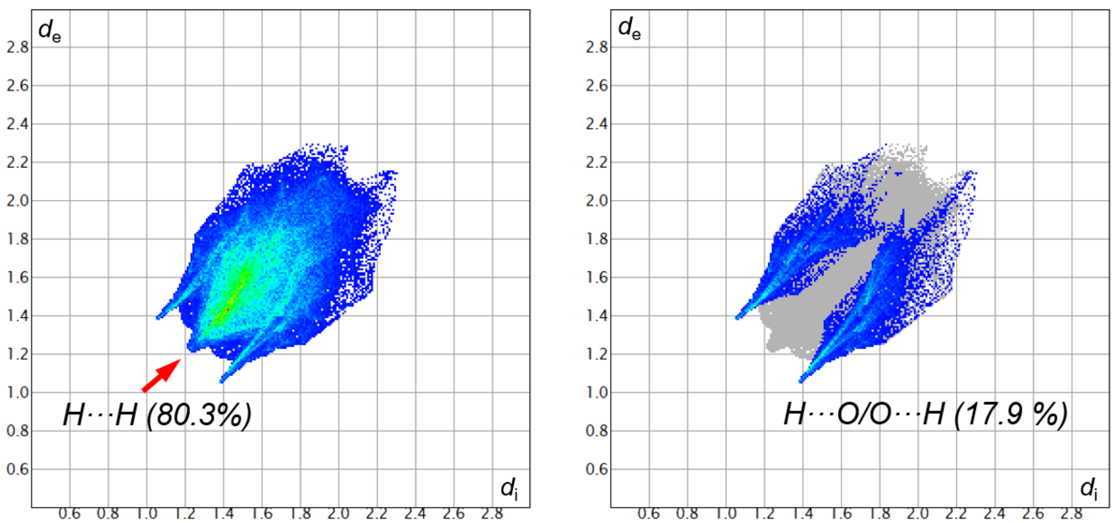

Figure S3. Full and decomposed two-dimensional fingerprint plots for **6**.

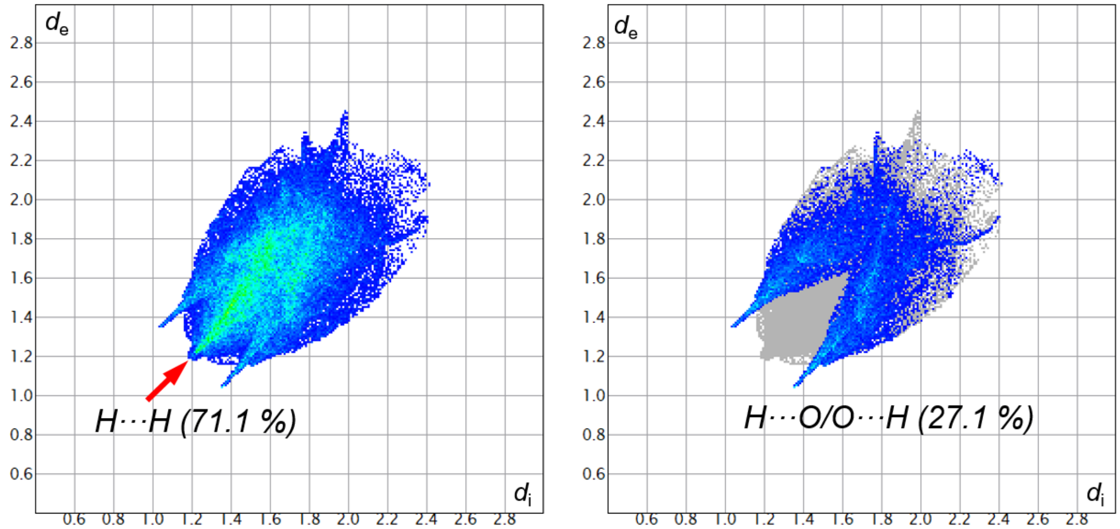

Figure S4. Combined QTAIM/NCI plot (0.5 a.u. isosurface) analysis for dimer D2 of compound **4**. The bond critical points are represented as red spheres.

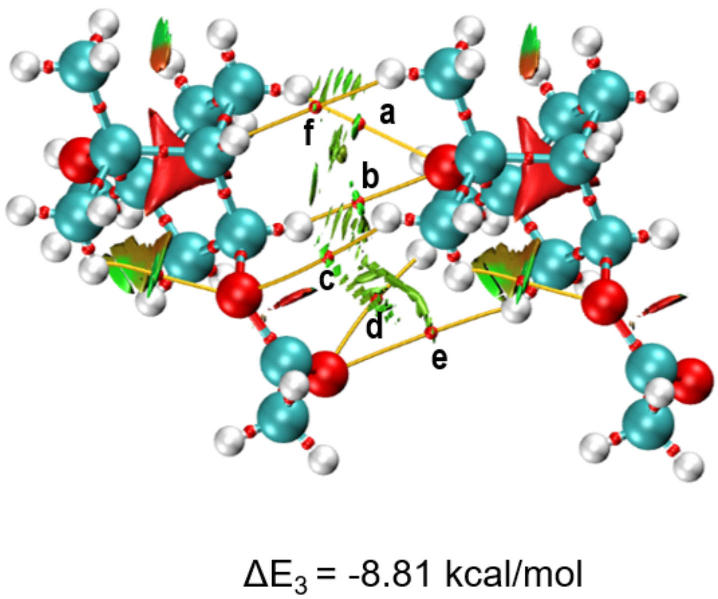

Figure S5. Experimental (black line) and calculated [B3LYP/6-311++G(d,p)] (red line) IR spectra of **4**.

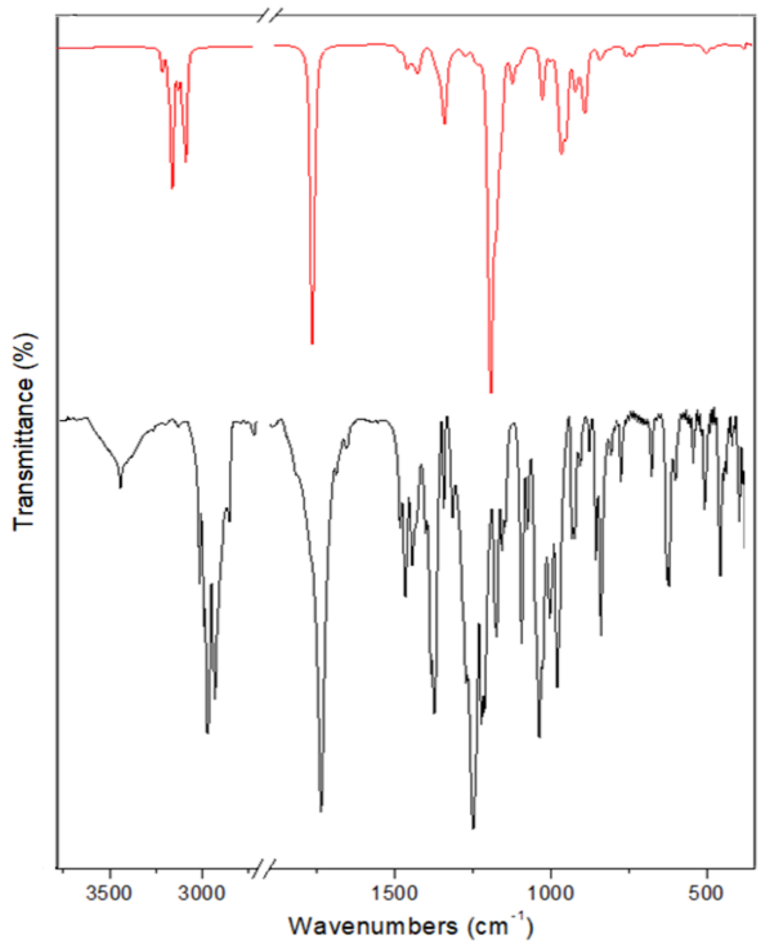

Figure S6. Experimental (black line) and calculated [B3LYP/6-311++G(d,p)] (red line) IR spectra of **6**.

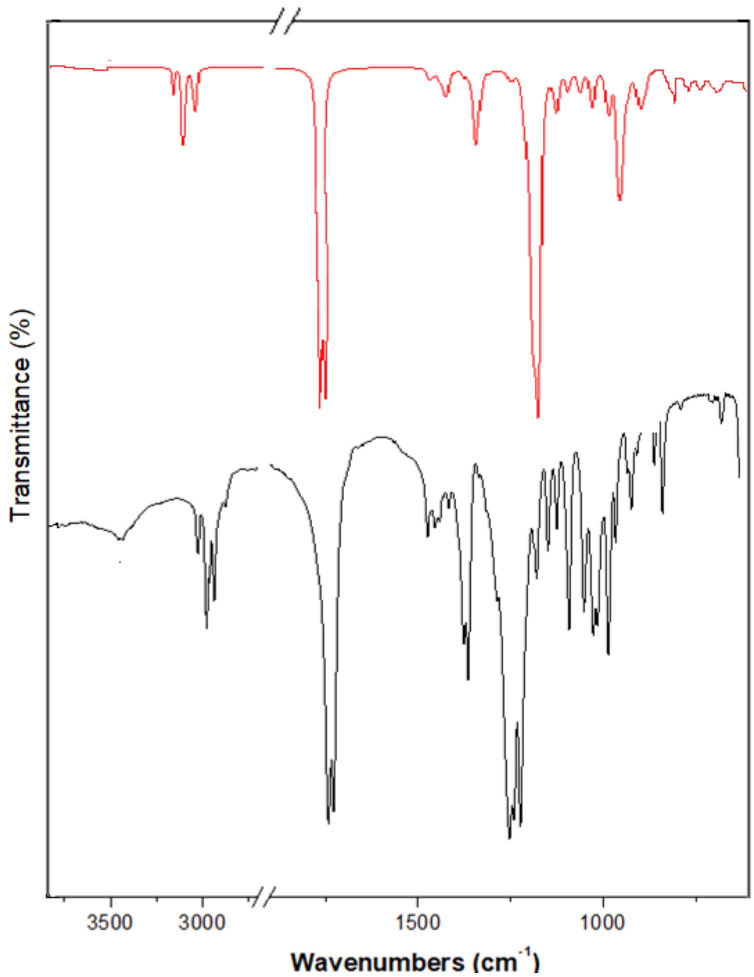

Figure S7. Experimental (black line) and calculated [B3LYP/6-311++G(d,p)] (red line) Raman spectra of **4**.

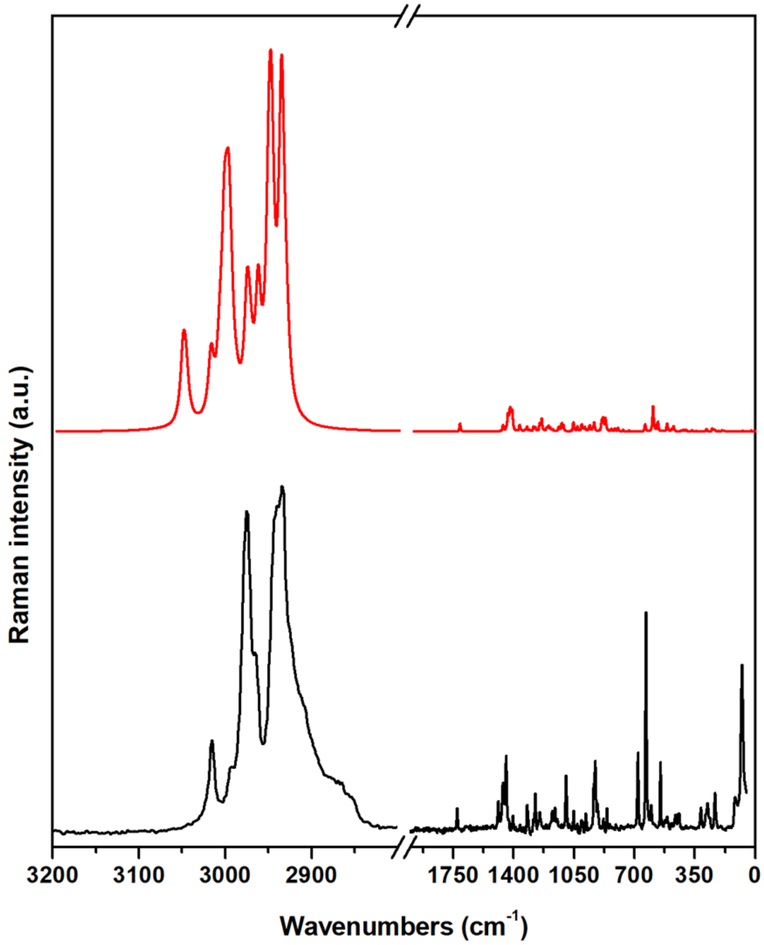

Figure S8. Experimental (black line) and calculated [B3LYP/6-311++G(d,p)] (red line) Raman spectra of **6**.

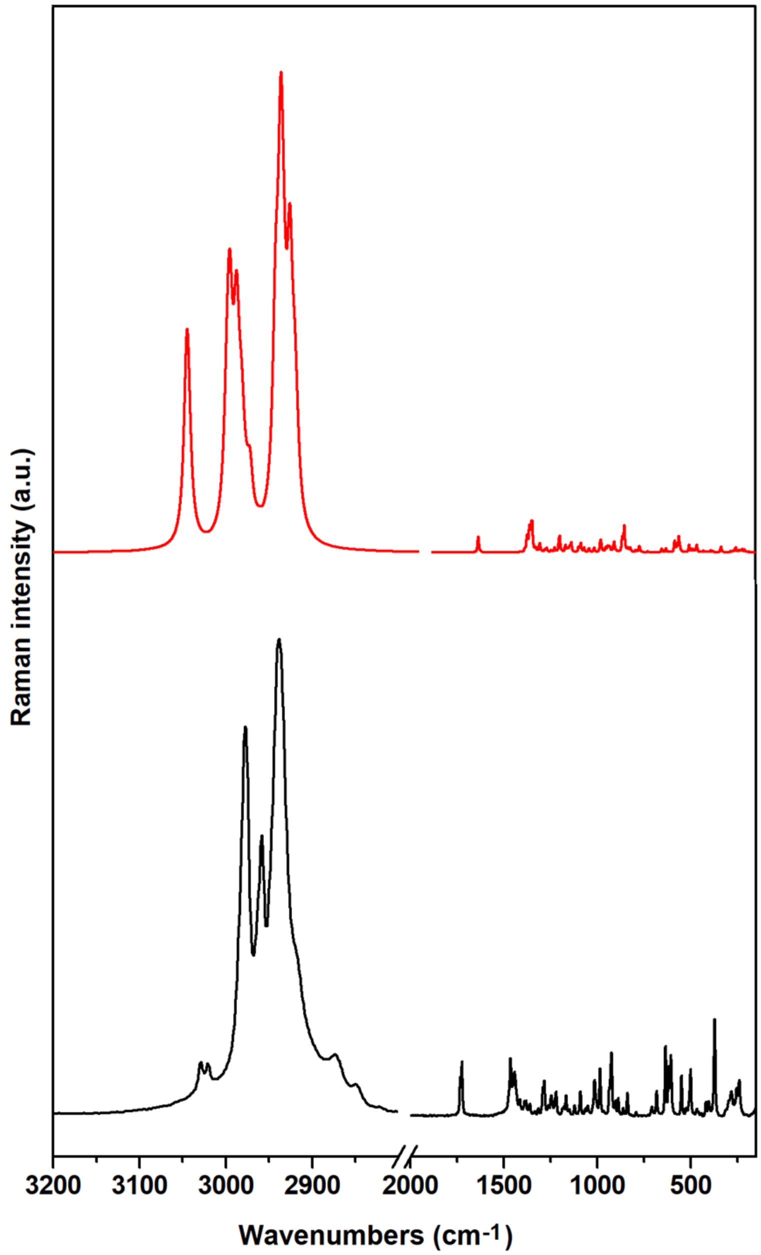

Figure S9. Experimental ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

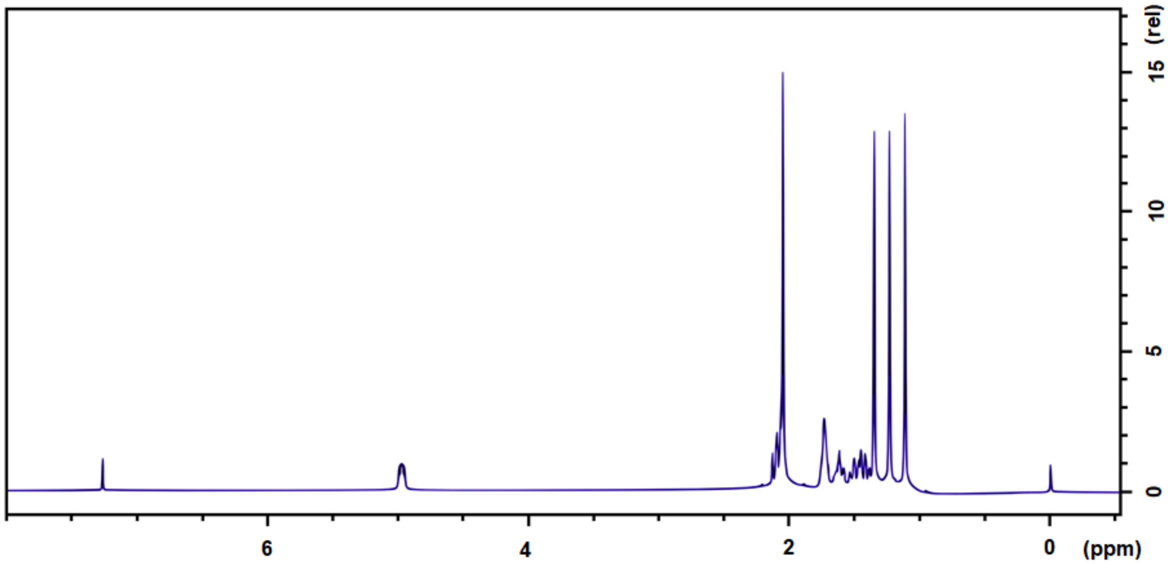

Figure S10. Experimental ^{1}H NMR spectrum of compound **6** in $CDCl_3$.

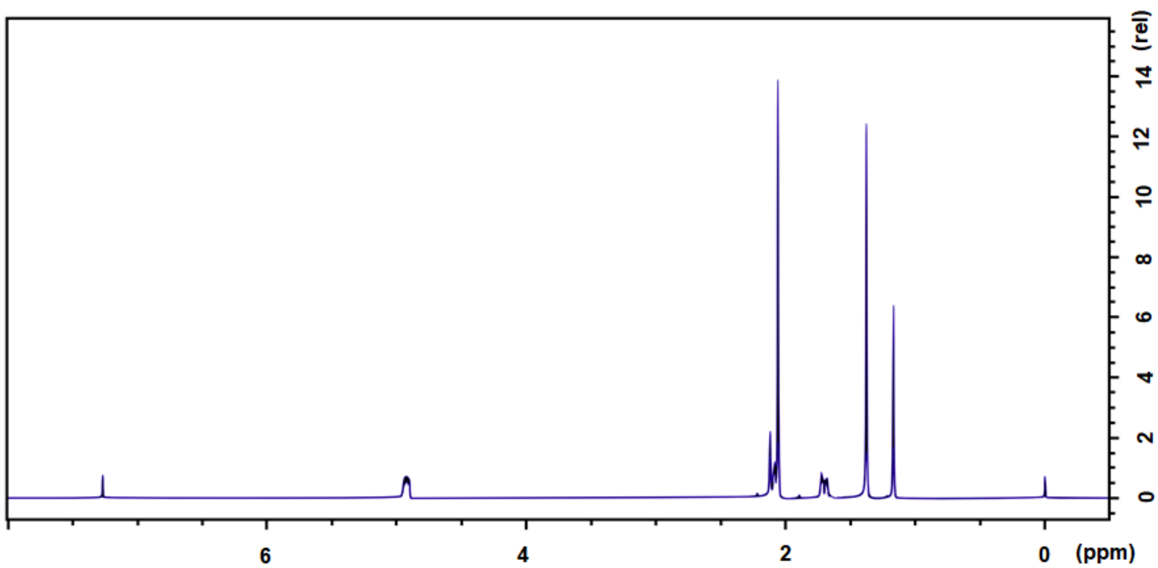

Figure S11. Experimental ^{13}C NMR spectrum of compound **4** in $CDCl_3$.

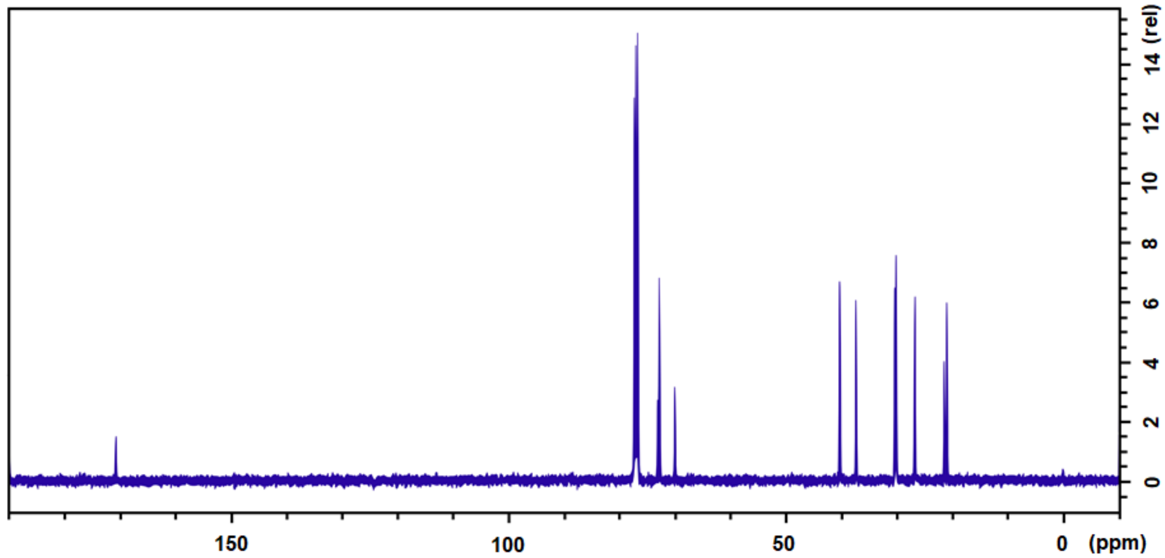

Figure S12. Experimental ^{13}C NMR spectrum of compound **6** in $CDCl_3$.

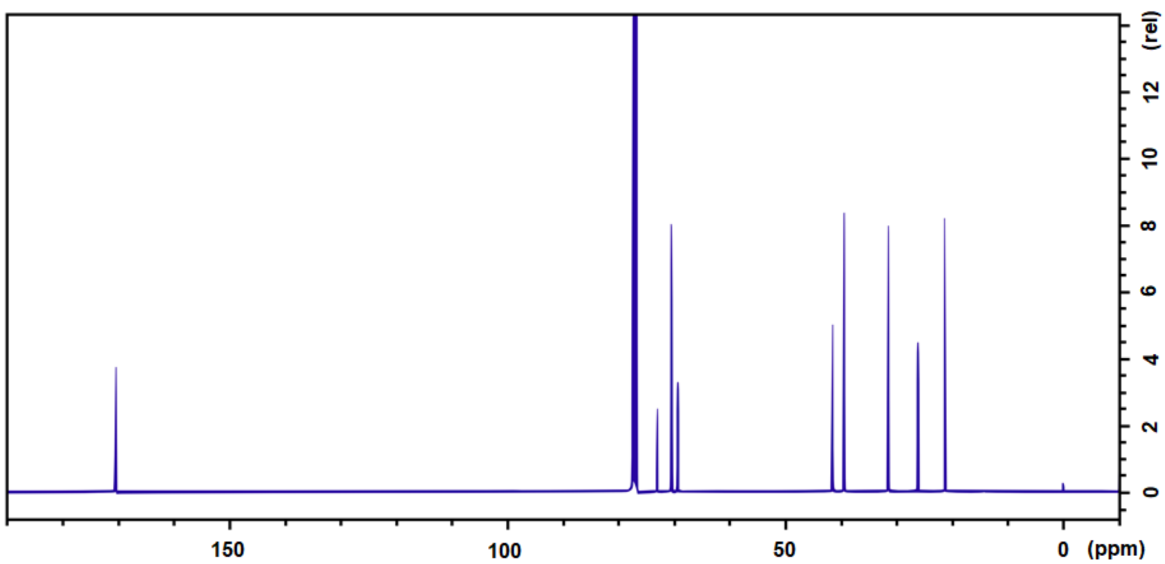

Figure S13. Experimental 2D (^1H-^1H) COSY NMR spectrum of compound **4** in $CDCl_3$

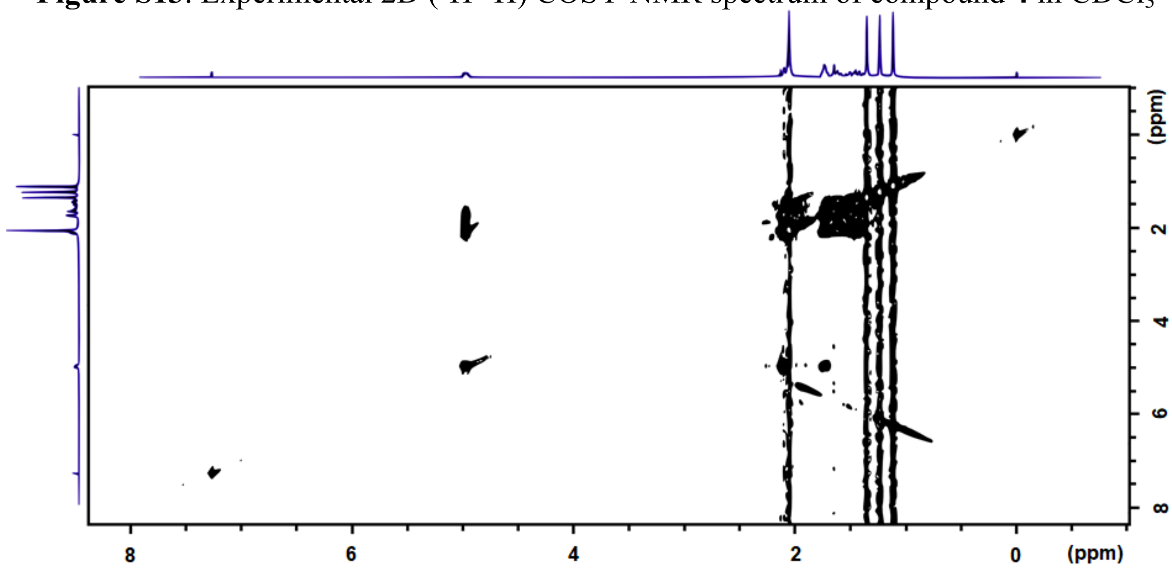

Figure S14. Experimental 2D (^1H-^1H) COSY NMR spectrum of compound **6** in $CDCl_3$.

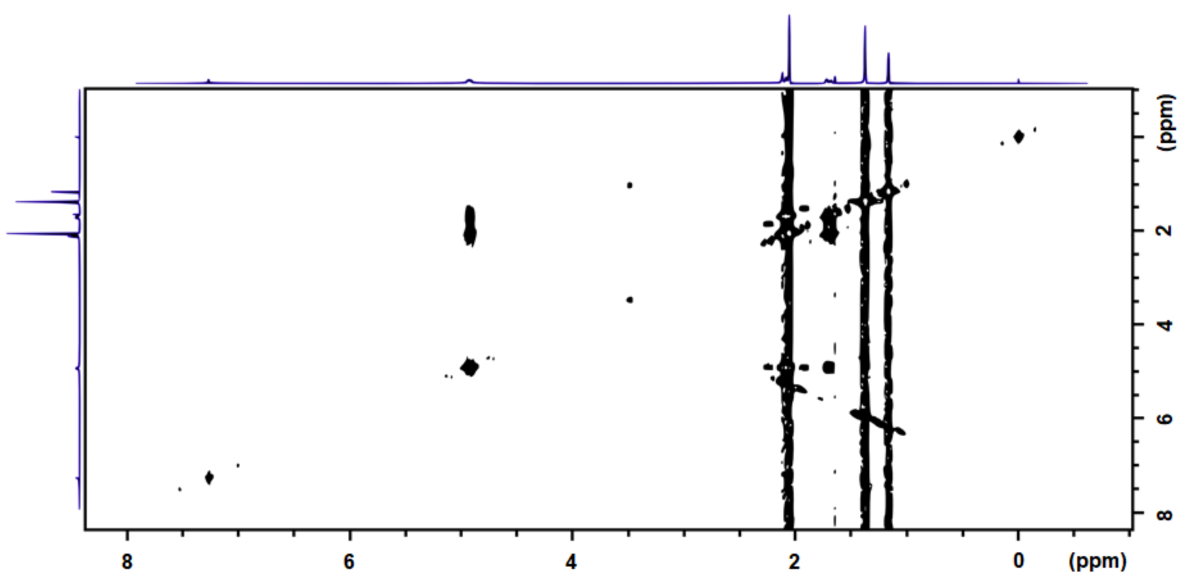

Figure S15. Experimental 2D (^1H-^{13}C) HSQC NMR spectrum of compound **4** in $CDCl_3$.

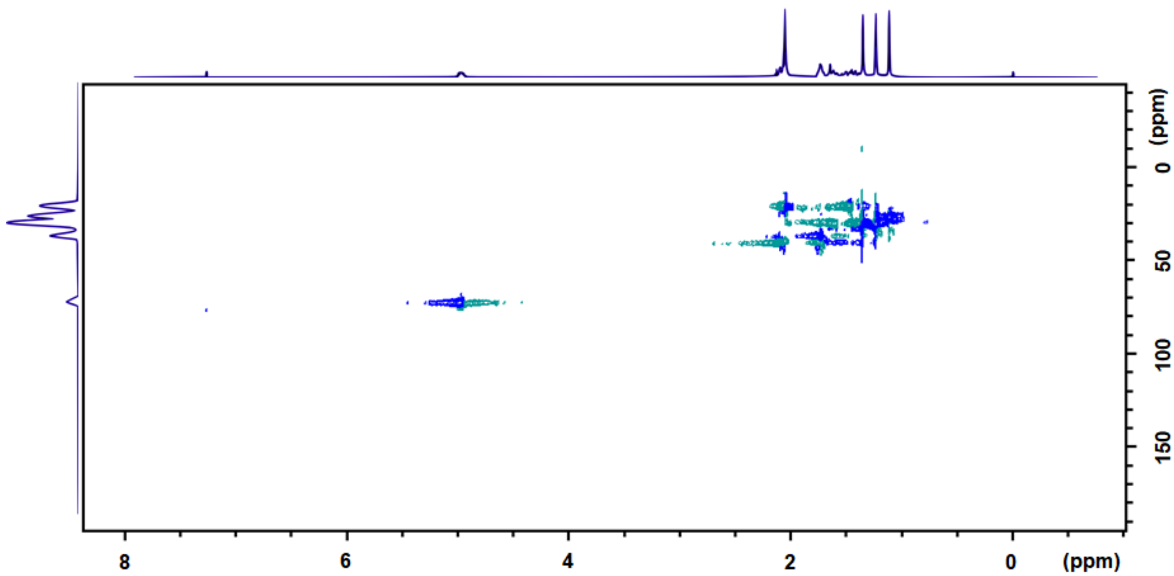

Fig. S16. Experimental 2D (^1H-^{13}C) HSQC NMR spectrum of compound **6** in $CDCl_3$.

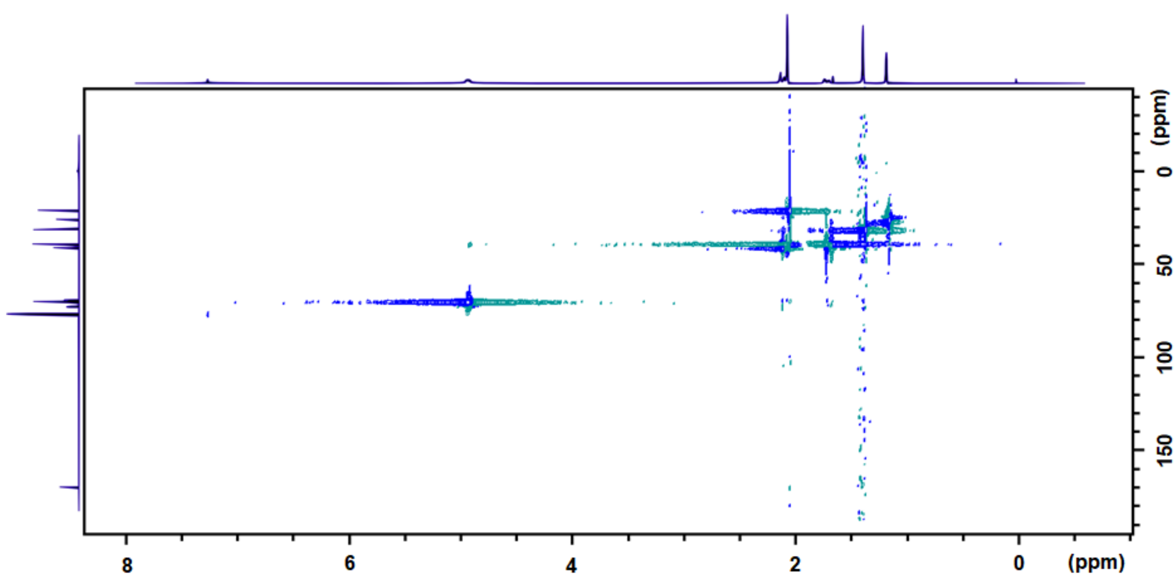

Figure S17. Experimental 2D (^1H-^{13}C) HMBC NMR spectrum of compound **4** in $CDCl_3$.

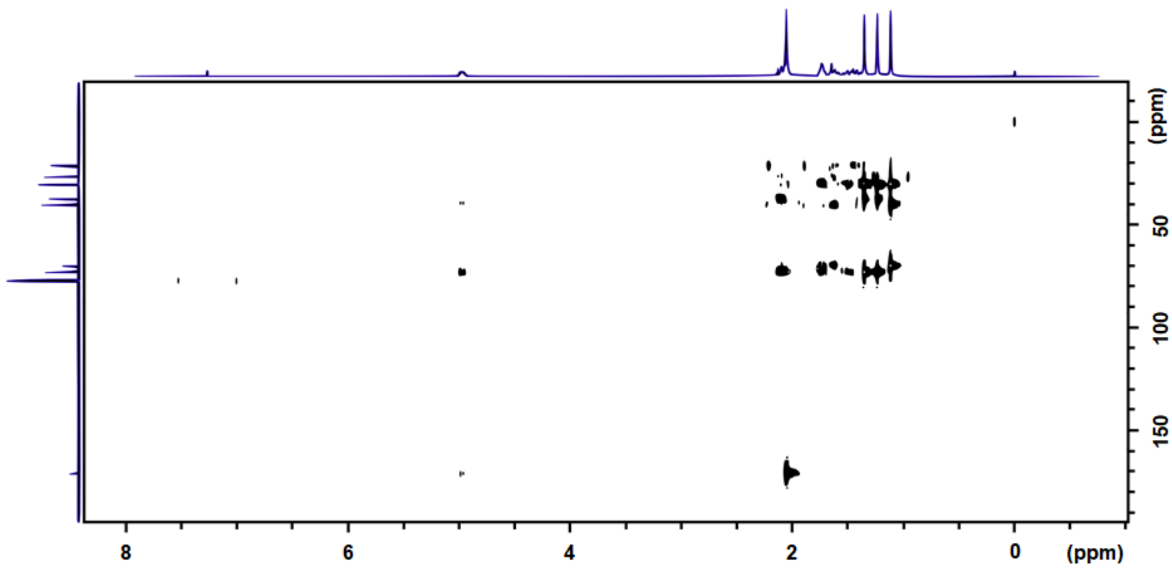

Figure S18. Experimental 2D (^1H-^{13}C) HMBC NMR spectrum of compound **6** in $CDCl_3$.

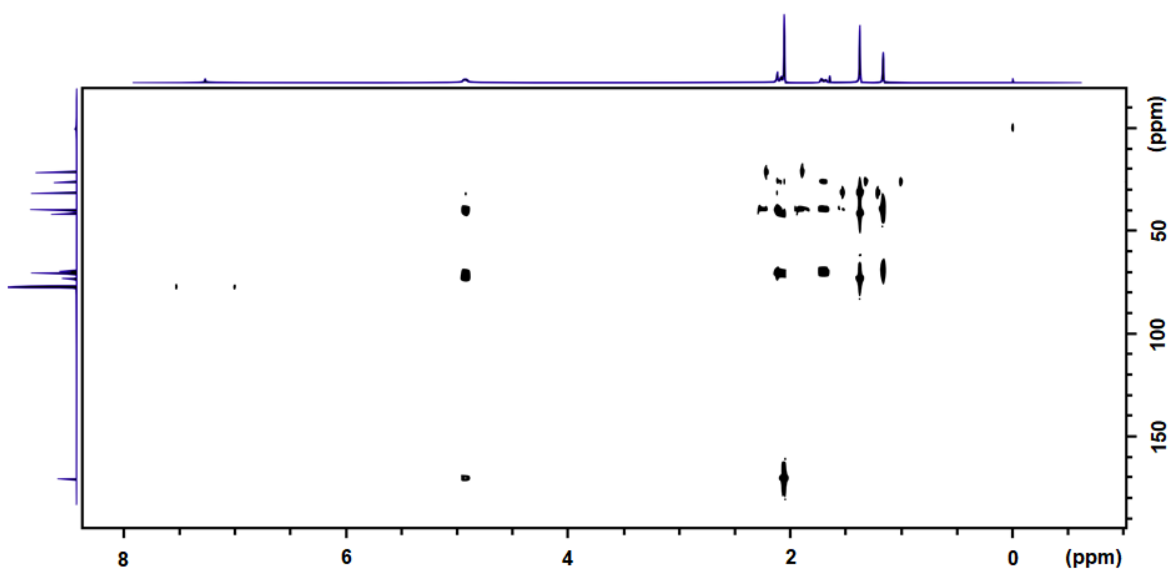

Table S1: Topological parameters[a] for intramolecular interactions observed in the structures of compounds **4** and **6**.

CP[b]	Interaction	d(H···O)[b]	ρ(r)	$\nabla^2(\rho)$	G(r)	H(r)	V(r)	|V/G|	DE[c]
Compound 4									
1	C9-H9C···O2	2.405	0.0121	0.0545	0.0108	-0.0023	-0.0085	0.79	2.91
Compound 6									
1	C9-H9C···O2	2.295	0.0144	0.0622	0.0129	-0.0026	-0.0104	0.81	3.47
2	C9-H8A···O4	2.339	0.0136	0.0572	0.0119	-0.0024	-0.0095	0.80	3.20

[a] ρ: electron density(a.u.), $\nabla^2(\rho)$: Laplacian of electron density (a.u.), G: Kinetic energy density (a.u.), H: Total electronic density (a.u.), V: potential energy density (a.u.).
[b] See Fig. 5 for labels of CPs.
[c] DE: dissociation energy (kcal/mol) computed with the formula [DE = 0.429 x G(r)].

Table S2. Experimental and calculated wavenumbers of compound **4** monomer and tentative assignment of fundamental vibrational modes.

Mode N°	Approximate description [a]	Experimental [b]		B3LYP/6-311++G(d,p) [c]			
		IR (solid)	Raman (solid)	Unscaled	Scaled	Int. IR	Act. Raman
	ν O···H dimer	3442 m	-				
1	ν_{as} C(12)H_3	-	-	3154	3028	3	30
2	ν_{as} C(9)H_3	3014 m	3016 m	3151	3025	6	18
3	ν_{as} C(8)H_3 + ν_{as} C(5)H_2	2991 m	2993 sh	3121	2996	11	26
4	ν_{as} C(12)H_3	-	-	3111	2986	2	20
5	ν_{as} C(10)H_3	-	-	3106	2982	17	35
6	ν_{as} C(10)H_3 + ν_{as} C(2)H_2	2973 s	2975 s	3105	2981	18	31
7	ν_{as} C(8)H_3 + ν_{as} C(5)H_2	-	-	3102	2978	3	24
8	ν_{as} C(8)H_3 + ν_{as} C(9)H_3	2964 sh	2965 sh	3100	2976	14	56
9	ν C(3)H + ν_{as} C(2)H_2	-	-	3096	2972	1	16
10	ν_s C(2)H_2	-	-	3090	2966	1	4
11	ν C(4)H + ν C(3)H	-	-	3078	2955	6	46
12	ν_{as} C(6)H_2 + ν_{as} C(5)H_2	-	-	3074	2951	3	18
13	ν C(3)H + ν C(4)H	2941 m	2941 sh	3065	2942	5	48
14	ν_s C(2)H_2 + ν_s C(6)H_2	2931 m	2934 m	3052	2930	8	67
15	ν_s C(12)H_3	-	-	3049	2927	1	64
16	ν_s C(5)H_2 + ν_s C(6)H_2	-	-	3048	2926	13	32
17	ν_s C(9)H_3 + ν_s C(8)H_3	2912 sh	2912 sh	3037	2916	11	100
18	ν_s C(10)H_3 + ν_s C(6)H_2	2896 sh	2896 sh	3036	2914	16	37
19	ν_s C(6)H_3 + ν_s C(10)H_2	-	-	3031	2910	1	21
20	ν_s C(8)H_3 + ν_s C(9)H_3	2854 m	2854 sh	3030	2909	4	5
	Fermi resonance	2720 w	2722 w				
21	ν C(11)O(3)	1737 vs	1726 w	1786	1714	100	3
22	δ C(5)H_2 + δ_{as} C(8)H_3	1483 m	1488 w	1529	1468	2	2

23	δ_{as} C(9)H_3 + δ_{as} C(8)H_3	1466 m	1460 m	1509	1449	6	1
24	δ_{as} C(10)H_3	1444 m	1443 m	1500	1440	1	2
25	δ_{as} C(8)H_3 + δ_{as} C(9)H_3	-	-	1498	1438	<1	2
26	δ C(6)H_2 + δ_{as} C(9)H_3	-	-	1492	1432	1	1
27	δ C(2)H_2 + δ_{as} C(10)H_3	1432 sh	1427 sh	1488	1428	4	3
28	δ C(5)H_2 + δ_{as} C(8)H_3	-	-	1485	1426	<1	4
29	ω C(10)H_3 + δ C(2)H_2	-	-	1478	1419	<1	<1
30	δ_{as} C(12)H_3	1402 m	1404 w	1478	1418	4	3
31	ω C(8)H_3 + ω C(9)H_3	-	-	1474	1415	1	2
32	ω C(12)H_3	-	-	1471	1412	5	2
33	δ C(3)H	-	-	1429	1372	2	2
34	δ_s C(8)H_3 + δ_s C(9)H_3	-	-	1421	1364	4	<1
35	δ_s C(10)H_3	-	-	1410	1354	5	<1
36	δ C(4)H + δ C(5)H_2	-	-	1400	1344	7	<1
37	δ_s C(8)H_3 + δ_s C(9)H_3	1385 s	1387 vw	1397	1341	18	<1
38	δ_s C(12)H_3	1374 vs	-	1385	1330	3	2
39	δ C(3)H + ω C(2)H_2	1360 sh	1361 w	1369	1314	1	<1
40	ω C(5)H_2 + δ C(4)H	1344 m	1343 vw	1346	1292	<1	1
41	ω C(2)H_2 + δ C(3)H	-	-	1335	1282	3	1
42	δ C(6)H_2 + δ C(4)H	1315 m	1320 m	1309	1257	2	2
43	$\tau\omega$ C(6)H_2 + $\tau\omega$ C(5)H_2	-	-	1297	1245	4	3
44	$\tau\omega$ C(2)H_2	1284 sh	1284 w	1268	1217	11	1
45	ω C(12)H_3 + ν C(11)O(2)	1272 m	1273 m	1262	1212	87	<1
46	ν C(11)O(2) + ν CC ring	1249 vs	1248 w	1256	1206	24	1
47	ν C(3)O(2) + ν CC ring	1223 s	-	1246	1196	42	1
48	ν CC ring	1214 s	1212 vw	1232	1183	34	1
49	ν C-CH_3	-	-	1198	1150	5	<1
50	ν C-CH_3	-	-	1194	1146	6	1
51	ν C-CH_3	1174 m	1175 w	1176	1129	6	2
52	ν CC ring	1157 m	1160 w	1167	1120	1	2
53	ν CCC	1147 m	1145 w	1107	1063	16	2
54	ν_{as} C(1)O(1)C(7)	1095 m	1095 m	1084	1041	3	1
55	δ C(12)C(11)O3	1075 m	1076 vw	1065	1022	2	<1
56	ν CC ring	-	-	1057	1015	12	2
57	ν C(3)O(2)	1049 sh	1052 w	1050	1008	23	<1
58	ν CC ring + ν C(11)O(2)	1038 s	1040 vw	1038	996	28	1
59	$\tau\omega$ C(8)H_3 + $\tau\omega$ C(9)H_3	1027 m	1028 w	1014	973	1	1
60	ν CC ring + ω C(10)H_3	1005 m	1005 w	1009	969	14	1
61	ρ C(10)H_3 + ρ C(2)H_2	980 s	980 w	992	952	5	1
62	ν CC ring + ν_{as} C(1)O(1)C(7)	974 sh	975 sh	982	943	23	2
63	ρ C(8)H_3 + ρ C(9)H_3	933 m	935 m	938	900	4	2
64	ρ C(9)H_3 + ρ C(8)H_3	-	-	932	895	<1	1

65	δ CCH ring	923 m	925 m	928	891	2	2
66	δ CCH ring	-	915 w	915	878	<1	3
67	ρ $C(10)H_3$ + ν CC ring	907 w	909 sh	910	874	1	1
68	ν CCC	878 w	879 w	880	845	1	1
69	ρ $C(2)H_2$ + ρ $C(6)H_2$	857 m	860 w	859	825	3	1
70	ρ $C(6)H_2$ + ρ $C(2)H_2$	840 m	843 vw	840	806	5	1
71	ν_s C(1)O(1)C(7)	808 w	809 vw	811	779	<1	<1
72	ν CCC ring	777 w	-	776	745	<1	<1
73	δ CCH ring +ν_s C(1)O(1)C(7)	679 w	680 m	678	651	<1	2
74	δ O(2)C(11)O(3)	632 m	630 s	630	605	1	6
75	ω C(11)O(3)	622 m	-	622	597	2	<1
76	ρ $C(12)H_3$	601 w	603 w	601	577	1	2
77	δ C(10)C(1)O(1)	545 w	548 m	546	524	<1	2
78	δ O(2)C(11)O(3)	518 w	522 vw	522	501	<1	<1
79	δ C(8)C(7)C(9) ring + δ CCO ring	508 m	511 w	508	488	1	1
80	δ CCO ring	459 m	463 w	462	444	4	<1
81	δ CCC ring	448 w	447 w	448	430	<1	<1
82	δ $CCCH_2$	440 w	440 w	433	416	<1	<1
83	δ C(2)C(1)C(6)	421 w	-	401	385	<1	<1
84	δ CCC ring	397 m	-	396	380	1	<1
85	δ C(5)C(4)C(7)	375 m	-	372	357	<1	<1
86	τ CC ring	-	316 w	310	298	<1	1
87	τ $C(9)H_3$	-	275 w	276	265	<1	1
88	τ CH_3	-	261 w	268	257	<1	<1
89	τ CC ring	-	-	258	248	<1	<1
90	τ CH_3	-	232 w	238	228	<1	<1
91	τ $C(8)H_3$	-	-	219	210	1	<1
92	τ $C(10)H_3$	-	-	209	201	<1	<1
93	τ CC ring	-	-	201	193	<1	<1
94	τ CH_3	-	116	181	174	<1	<1
95	τ $C(12)H_3$	-	-	96	92	1	<1
96	τ skeletal	-	76	89	85	<1	<1
97	τ skeletal	-	-	56	54	<1	<1
98	τ C(3)O(2)	-	-	43	41	<1	<1
99	τ skeletal	-	-	11	11	1	<1

[a] Main contributors to fundamental vibrational modes. ν: stretching; δ: bending; ρ: rocking; ω: wagging; τω: twisting; τ: torsional modes; s: symmetric; as: asymmetric.
[b] s: strong; vs: very strong; m: medium; w: weak; vw: very weak; sh: shoulder.
[c] Shaded columns show the best correlation with experimental frequencies observed. Higher frequency values were scaled with 0.9676 factor [Ref. 55]. Relative infrared intensities and Raman activities were normalized to 100%.

Table S3. Experimental and calculated wavenumbers of **6** monomer and tentative assignment of fundamental vibrational modes.

Mode N°	Approximate description [a]	Experimental [b]		B3LYP/6-311++G(d,p) [c]			
		IR (solid)	Raman (solid)	unscaled	scaled	Int. IR	Act. Raman
	ν O···H dimer	3455 w	-				
	ν O···H dimer	3433 w	-				
1	ν_{as} C(9)H_3	-	-	3156	3030	3	21
2	ν_{as} C(14)H_3	3029 m	3029 w	3156	3030	1	30
3	ν_{as} C(12)H_3	3021 m	3021 w	3156	3030	1	33
4	ν_{as} C(8)H_3	-	-	3153	3027	2	16
5	ν_{as} C(12)H	-	-	3111	2987	1	20
6	ν_{as} C(14)H_3	-	-	3110	2986	1	20
7	ν_{as} C(10)H_3	-	-	3108	2984	6	35
8	ν_{as} C(10)H_3 + ν_{as} C(6)H_2 + ν_{as} C(2)H_2	2977 s	2977 s	3107	2983	9	47
9	ν_{as} C(10)H_3	-	-	3101	2977	1	15
10	ν_{as} C(8)H_3 + ν_{as} C(9)H_3	2965 s	2958 s	3100	2976	9	62
11	ν_{as} C(6)H_2 + ν_{as} C(2)H_2	-	-	3098	2974	1	7
12	ν C(4)H	-	-	3094	2970	1	36
13	ν_{as} C(8)H_3 + ν_{as} C(9)H_3	-	-	3090	2966	<1	5
14	ν C(3)H + ν C(4)H + ν C(5)H	-	-	3085	2962	1	23
15	ν C(3)H + ν C(5)H	-	-	3074	2951	1	2
16	ν_s C(2)H_2 + ν_s C(6)H_2	-	-	3056	2934	4	75
17	ν_s C(12)H_3	-	-	3050	2928	<1	71
18	ν_s C(14)H_3	-	-	3050	2928	<1	72
19	ν_s C(6)H_2 + ν_s C(2)H_2	-	-	3047	2925	4	34
20	ν_s C(8)H_3 + ν_s C(9)H_3	2918 sh	2919 sh	3040	2918	8	100
21	ν_s C(10)H_3	2876 m	2874 w	3034	2913	3	42
22	ν_s C(9)H_3 + ν_s C(8)H_3	-	2850 vw	3031	2910	2	9
	Fermi resonance	2710 vw	2710 vw				
23	ν C(11)O(3)	1741 vs	1734 s	1791	1719	74	4
24	ν C(13)O(5)	1728 vs	1725 vs	1788	1716	32	1
25	δ_{as} C(9)H_3 + δ_{as} C(8)H_3	1474 w	-	1516	1455	4	1
26	δ_{as} C(8)H_3 + δ_{as} C(9)H_3	1455 w	1451 sh	1504	1444	1	3
27	δ_{as} C(10)H_3	1440 w	1443 s	1500	1440	<1	3
28	δ_{as} C(8)H_3 + δ_{as} C(9)H_3	-	-	1489	1429	<1	2
29	δ_s C(2)H_2 + δ_{as} C(10)H_3	-	-	1488	1429	2	3
30	δ_s C(6)H_2 + δ_{as} C(10)H_3	-	-	1488	1429	1	1
31	δ_{as} C(8)H_3 + δ_{as} C(9)H_3 + δ_{as} C(10)H_3	-	-	1481	1422	<1	2

32	δ_{as} C(12)H_3	-	-	1478	1419	2	3
33	δ_{as} C(14)H_3	-	-	1476	1417	1	2
34	δ_s C(2)H_2 +δ_s C(6)H_2	-	-	1474	1415	<1	1
35	ω C(14)H_3	-	-	1471	1412	3	3
36	ω C(12)H_3	-	-	1471	1412	3	3
37	δ C(3)H + δ C(5)H	-	-	1451	1393	1	1
38	δ C(5)H + δ C(3)H	-	-	1428	1371	<1	3
39	δ_s C(8)H_3 + δ_s C(9)H_3	-	-	1424	1367	2	<1
40	δ_s C(10)H_3	1416 w	1414 m	1411	1354	2	<1
41	δ_s C(8)H_3 + δ_s C(9)H_3	-	-	1404	1348	3	<1
42	δ_s C(12)H_3 + δ_s C(14)H_3	-	-	1400	1344	5	<1
43	δ_s C(14)H_3 + δ_s C(12)H_3	1390 sh	1389 m	1398	1342	16	<1
44	δ C(3)H + δ C(4)H+ δ C(5)H	1376 m	1380 m	1387	1332	4	1
45	δ CH_2 + δ CH	1364 s	1361 m	1363	1308	1	<1
46	δ CH_2 + δ CH	1336 vw	1335 vw	1340	1286	<1	1
47	δ CH_2 + δ CH	1316 s	1315 m	1314	1261	2	2
48	δ CH_2 + δ CH	-	-	1309	1257	1	4
49	ω C(10)H_3	1286 sh	1283 m	1277	1226	13	2
50	τω C(2)H_2 + τω C(6)H_2	-	-	1266	1215	5	<1
51	ν C(11)O(3) + ν CC ring	1253 vs	1261 w	1260	1210	42	1
52	ν C(13)O(4) + ν CC ring	1241 vs	1246 m	1252	1202	44	1
53	ν CC ring	-	-	1246	1196	5	1
54	δ CH_3 + ν CC ring	1223 vs	1220 m	1241	1191	100	2
55	ν C-CH_3	-	-	1199	1151	2	<1
56	δ CH_3 + δ CH_2	1187 sh	1186 w	1198	1150	9	1
57	δ CH_3 + δ CH_2	1179 m	1179 w	1186	1139	<1	3
58	τω C(6)H_2 + τω C(2)H_2	-	1167 m	1167	1120	6	1
59	ν CC ring	1149 m	1149 w	1137	1092	8	1
60	ν CCC	1125 m	1121 m	1107	1063	11	1
61	ν_{as} C(1)O(1)C(7)	1092 m	1090 s	1070	1027	2	2
62	δ CCO	-	1064 w	1067	1024	11	1
63	τω C(14)H_3	-	-	1065	1022	1	<1
64	τω C(12)H_3	1052 m	1051 w	1065	1022	1	1
65	ν C(11)O(2) + ν C(13)O(4)	-	1034 vw	1039	997	45	1
66	ν CC ring + ν_{as} C(1)O(1)C(7)	1027 m	1026 sh	1028	987	8	1
67	τω C(8)H_3 + τω C(9)H_3	1015 m	1015 s	1020	979	1	1
68	ν CC ring	-	-	1014	973	4	1
69	ν CC ring + ω C(10)H_3	-	1002 sh	995	955	2	1
70	ν CC ring + ν_{as} C(1)O(1)C(7)	986 m	985 s	988	948	9	3
71	ρ C(10)H_3 + ρ C(2)H_2	967 m	967 w	976	937	9	<1

72	ρ $C(8)H_3$ + ρ $C(9)H_3$	-	-	942	904	2	3
73	ρ $C(9)H_3$ + ρ $C(8)H_3$	934 w	934 m	937	900	1	2
74	δ CCH ring	924 m	924 s	929	892	3	6
75	δ CCH ring	909 vw	-	914	877	1	<1
76	ν CC ring	902 sh	902 m	906	870	<1	1
77	ν CCC	888 w	888 m	893	857	<1	1
78	ρ $C(2)H_2$ + ρ $C(6)H_2$	862 m	861 w	863	828	1	<1
79	ρ $C(6)H_2$ + ρ $C(2)H_2$	-	-	842	808	1	1
80	ν_s C(1)O(1)C(7)	840 m	838 m	837	804	3	1
81	ν CCC ring	791 vw	791 vw	791	759	<1	<1
82	δ CCH ring	-	708 w	709	681	<1	1
83	δ CCH ring + δ C(3)O(2)C(11)	680 w	681 m	684	657	1	1
84	δ O(2)C(11)O(3)	632 m	633 s	632	607	3	3
85	ω C(13)O(5)	617 m	617 s	619	594	2	1
86	ρ $C(14)H_3$	-	-	608	584	1	3
87	ω C(11)O(3)	604 m	605 ws	602	578	1	1
88	δ C(10)C(1)O(1)	548 w	548 m	546	524	<1	2
89	δ O(5)C(13)C(14) + δ CCC ring	525 m	525 w	528	507	1	1
90	δ CCO ring	509 m	-	515	494	1	<1
91	δ CCC ring	500 m	500 m	502	482	1	2
92	δ CCC ring	464 sh	466 w	465	446	1	<1
93	δ CCO ring	456 m	458 vw	453	435	2	<1
94	δ CCC ring	442 w	442 w	439	421	<1	<1
95	δ C(4)C(7)C(9)	418 w	418 m	420	403	<1	<1
96	δ CCC ring	-	402 m	404	388	<1	<1
97	δ CCC ring	-	371 m	359	345	<1	1
98	τ CC ring	-	-	304	292	1	<1
99	τ CC ring + τ CH_3	-	296 sh	290	278	<1	<1
100	δ CCC ring	-	281 w	275	264	<1	<1
101	τ CC ring + τ CH_3	-	-	272	261	<1	1
102	τ CC ring	-	252 w	251	241	<1	<1
103	τ $C(9)H_3$ + τ $C(8)H_3$	-	239 w	241	231	<1	<1
104	τ $C(8)H_3$ + τ $C(9)H_3$	-	-	236	227	1	<1
105	τ CH_3	-	-	222	213	1	<1
106	τ $C(10)H_3$	-	-	219	210	<1	<1
107	τ CC ring + τ CH_3	-	-	207	199	<1	<1
108	τ CH_3	-	-	191	183	<1	<1
109	τ skeletal	-	140 vw	121	116	<1	<1
110	τ skeletal	-	103 sh	94	90	<1	<1
111	τ CC ring	-	71 m	78	75	<1	<1
112	τ CC ring	-	-	75	72	1	<1

113	τ skeletal	-	-	55	53	1	<1
114	τ $C(14)H_3$	-	-	48	46	<1	<1
115	τ C(5)O(4)	-	-	42	40	<1	<1
116	τ $C(12)H_3$	-	-	39	37	<1	<1
117	τ skeletal +	-	-	34	33	<1	<1

[a] Main contributors to fundamental vibrational modes. ν: stretching; δ: bending; ρ: rocking; ω: wagging; τω: twisting; τ: torsional modes; s: symmetric; as: asymmetric.

[b] s: strong; vs: very strong; m: medium; w: weak; vw: very weak; sh: shoulder.

[c] Shaded columns show the best correlation with experimental frequencies observed. Higher frequency values were scaled with 0.9676 factor [Ref. 55]. Relative infrared intensities and Raman activities were normalized to 100%.