

Electronic Supporting Information (ESI)

Synthesis and P-glycoprotein induction activity of colupulone analogs

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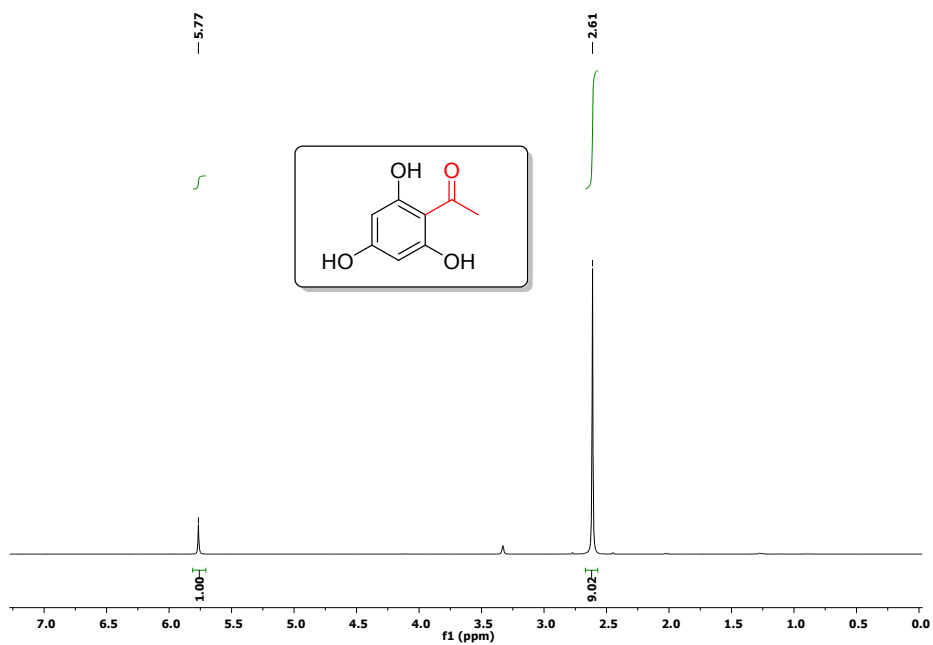
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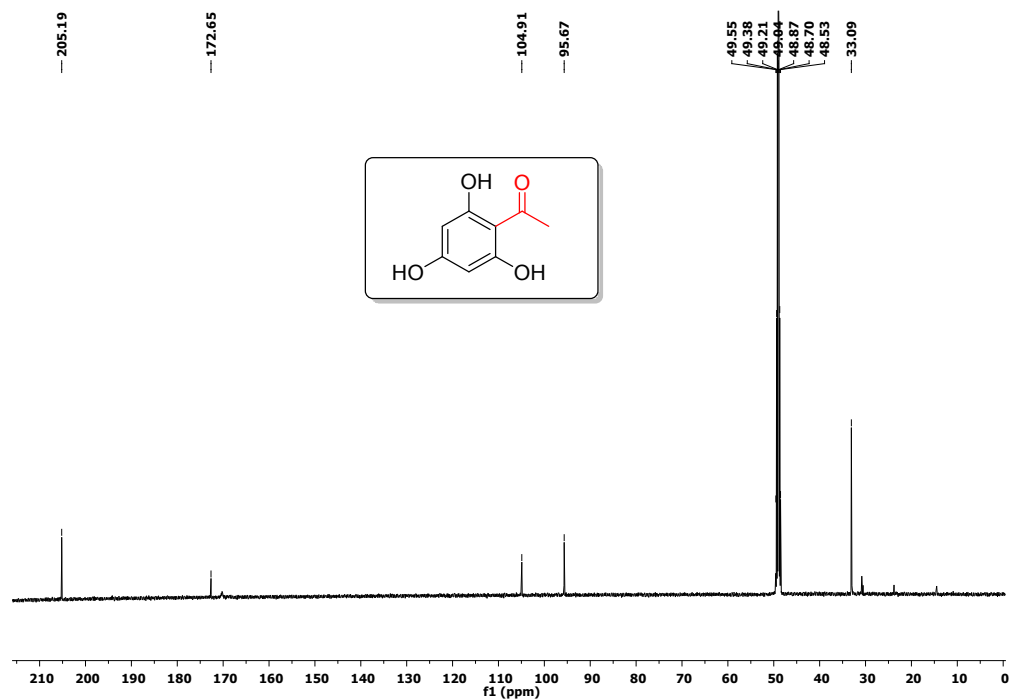
S.1. SPECTRAL DATA SCANS OF ALL COMPOUNDS

S1.a. ^1H , ^{13}C and DEPT-135 NMR spectrum of 1-acetyl-2,4,6-trihydroxy benzene (**2a**)

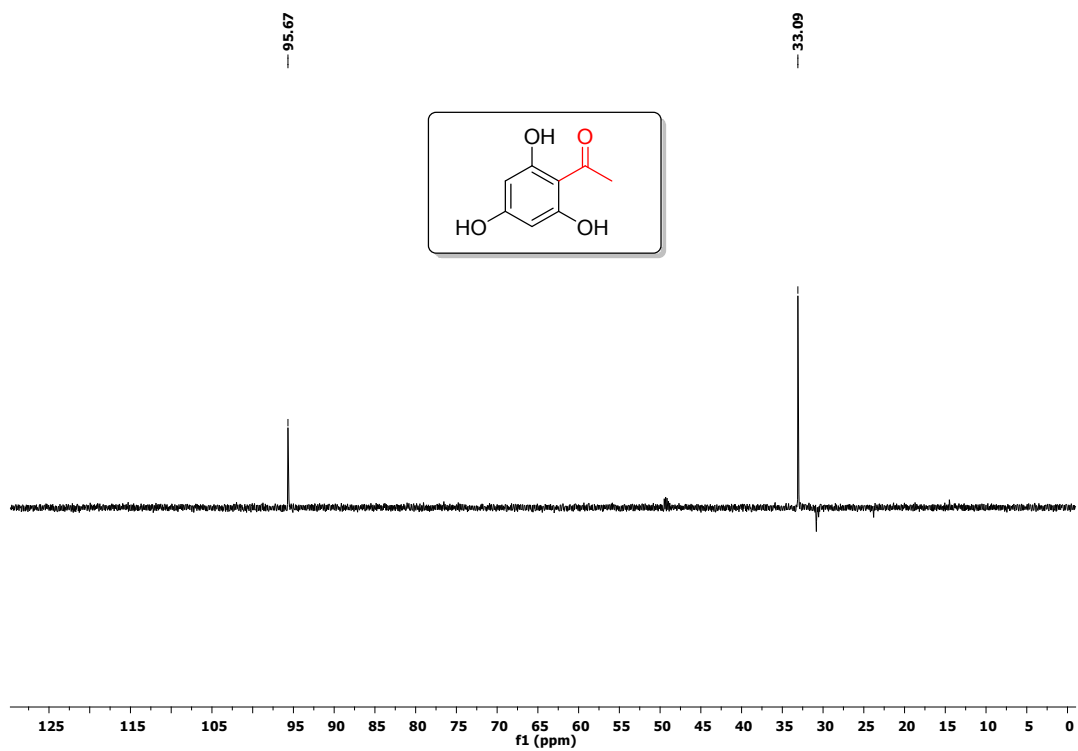
^1H NMR



^{13}C NMR

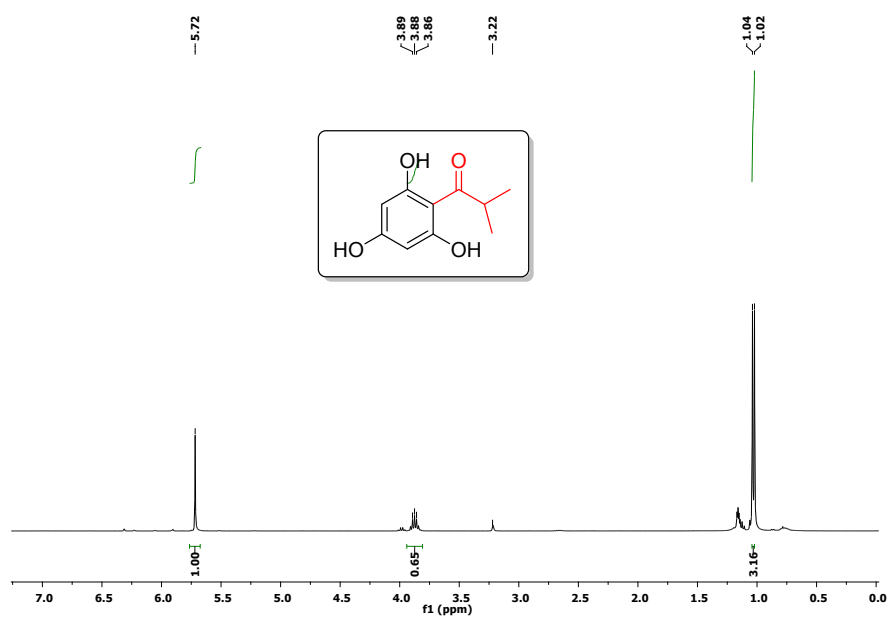


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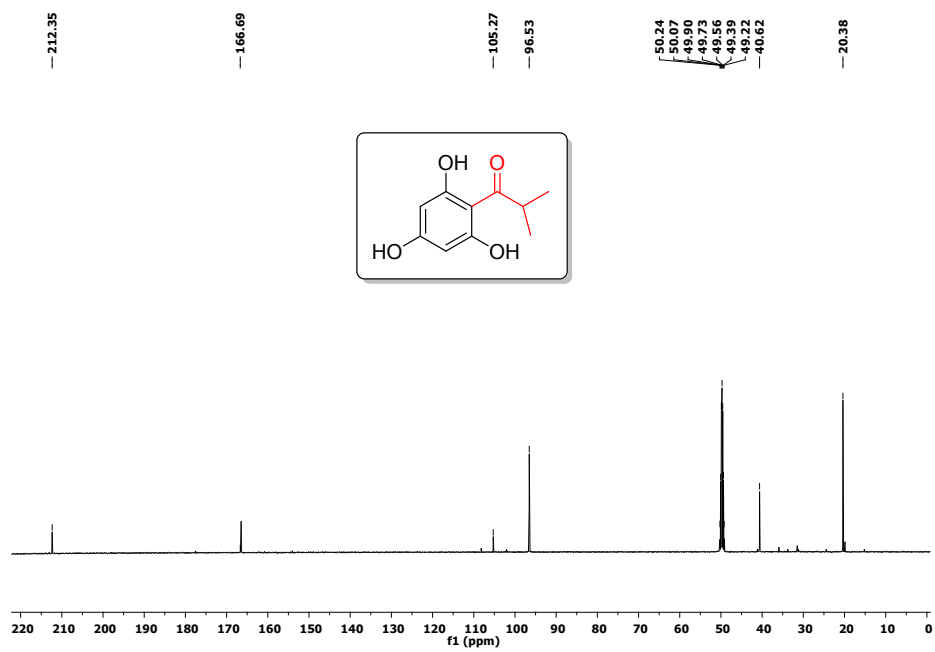


S1.b. ^1H , ^{13}C and DEPT-135 NMR spectrum of 1-isobutanoyl)-2,4,6-trihydroxy benzene (**2b**)

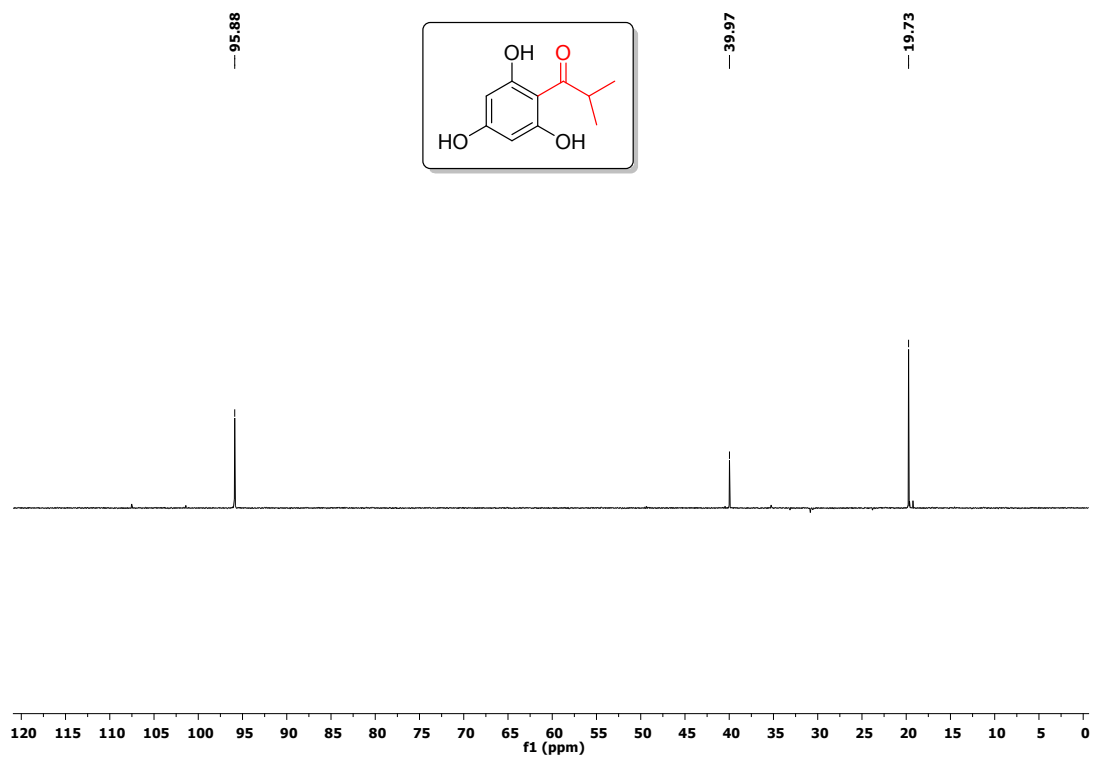
^1H NMR



^{13}C NMR

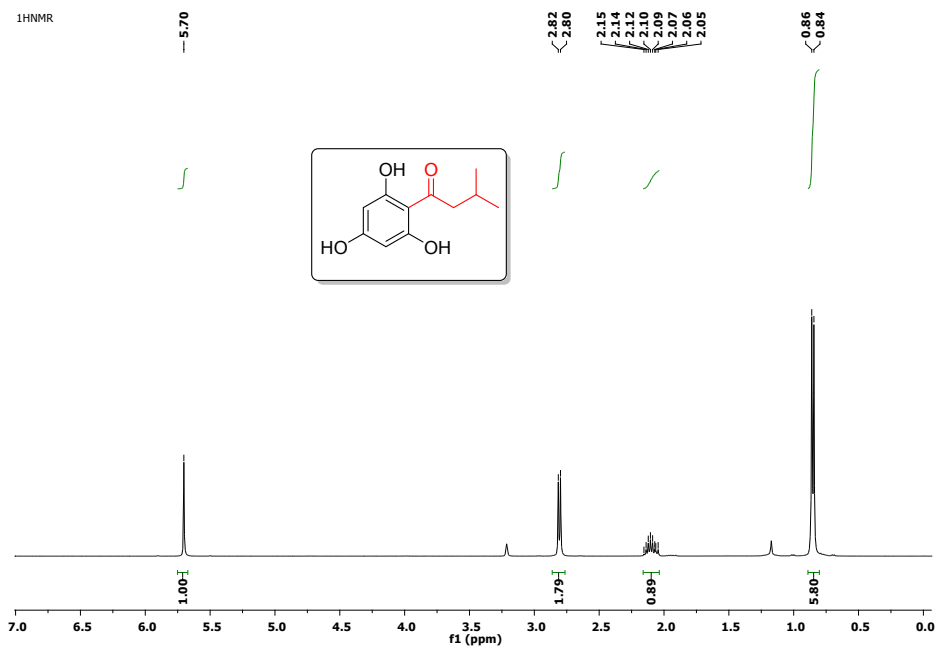


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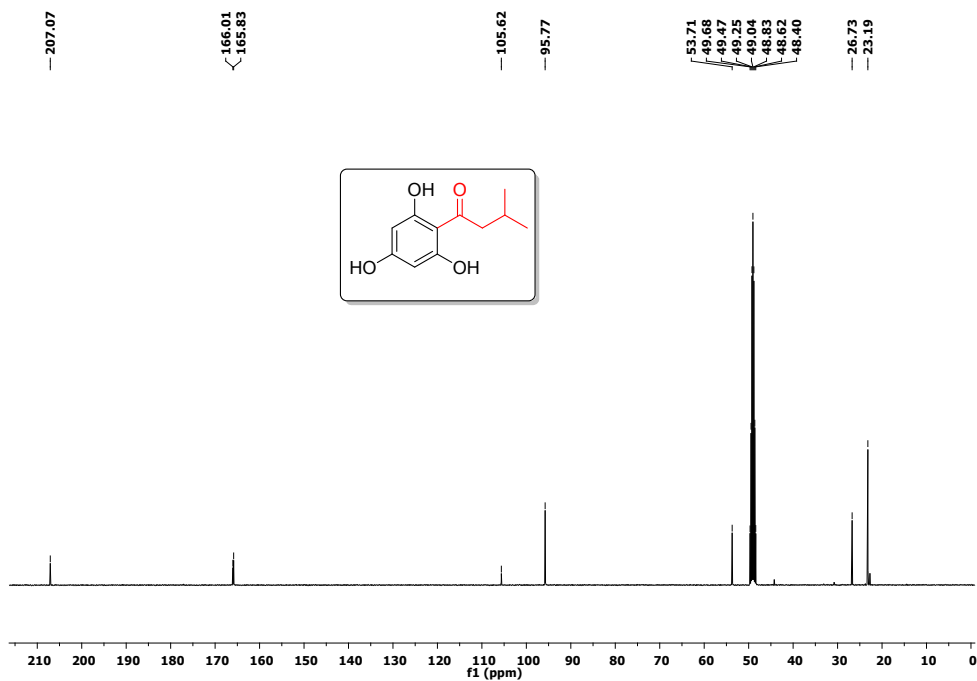


S1.c. ^1H , ^{13}C and DEPT-135 NMR spectrum of 1-(3-methyl-butanoyl)-2,4,6-trihydroxy benzene (2c)

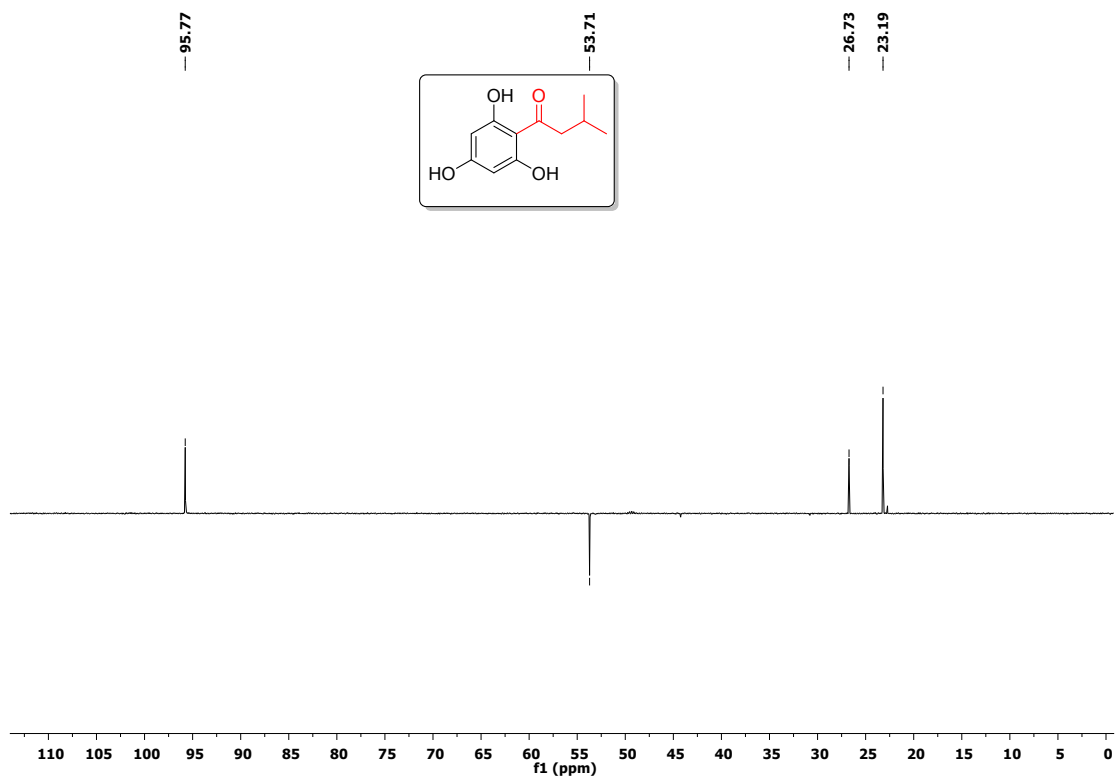
^1H NMR



^{13}C NMR

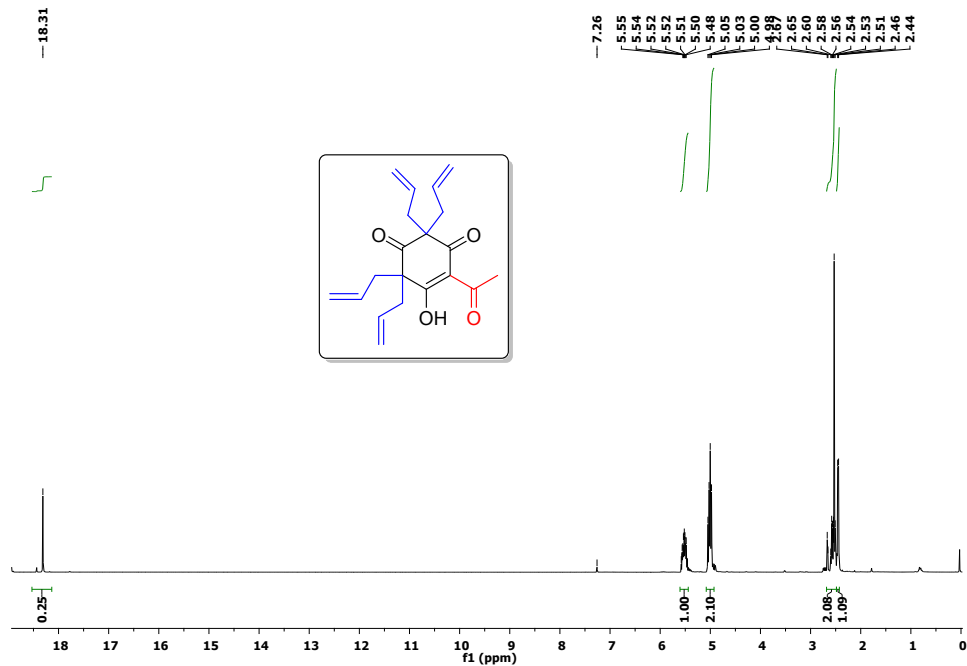


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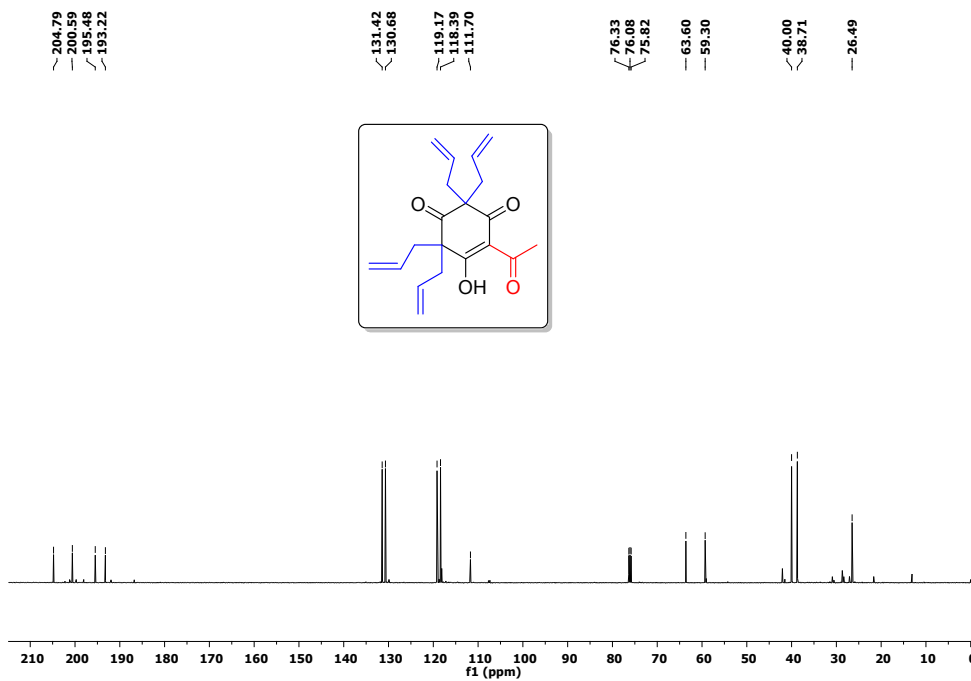


S1.d. ^1H , ^{13}C and DEPT-135 NMR spectrum of 4-acetyl-2,2,6,6-tetraallyl-5-hydroxycyclohex-4-ene-1,3-dione: (**3a**)

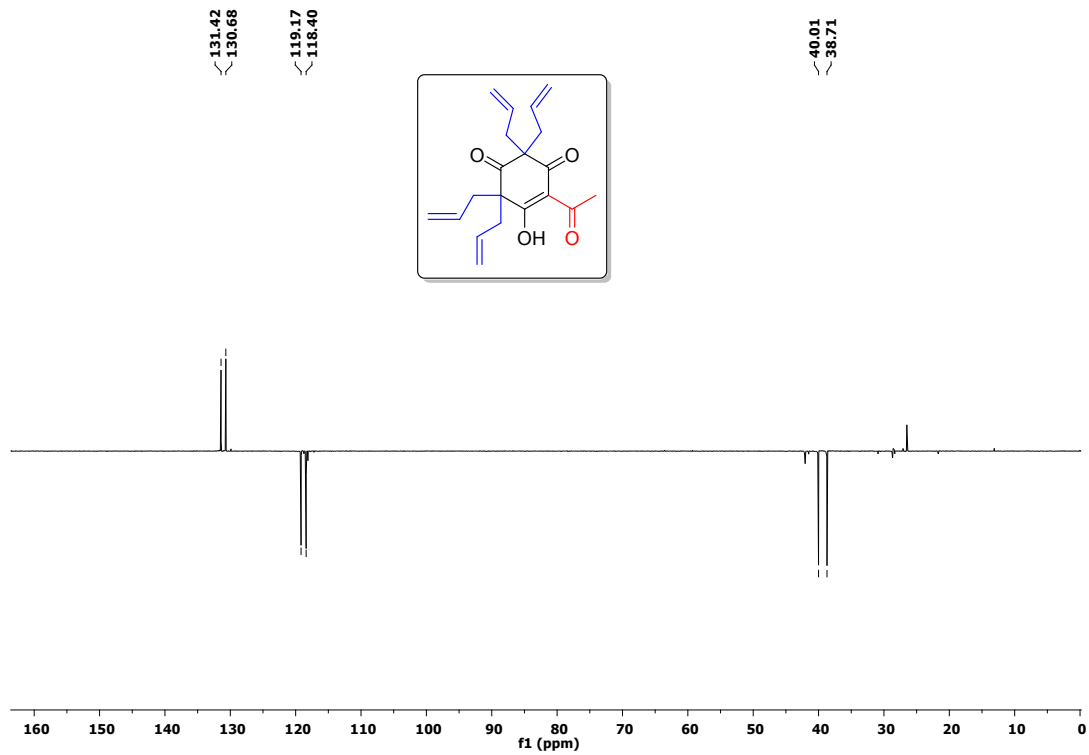
^1H NMR



^{13}C NMR

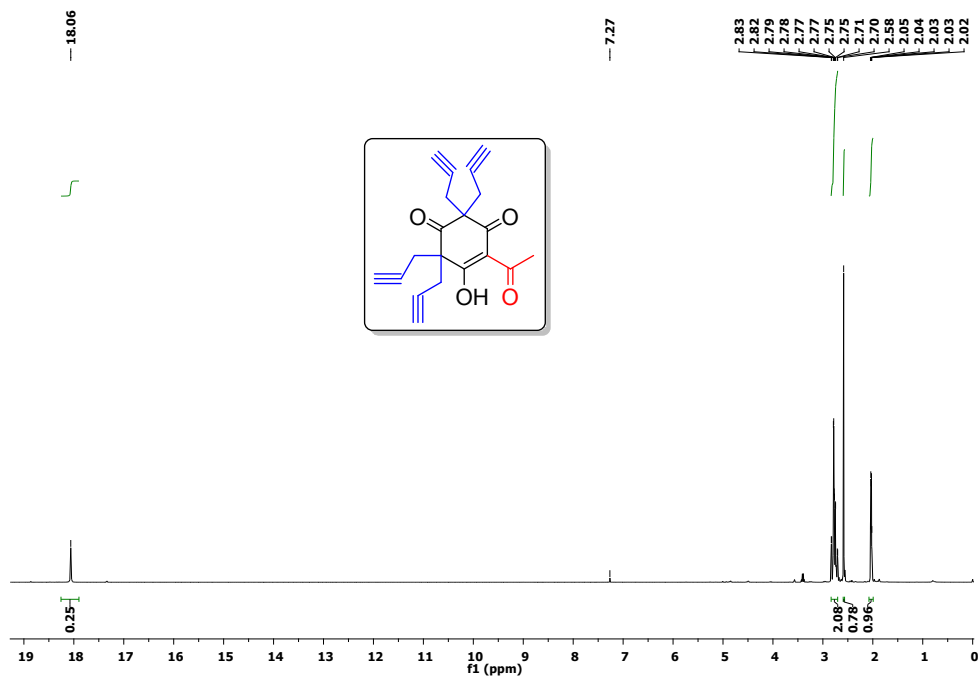


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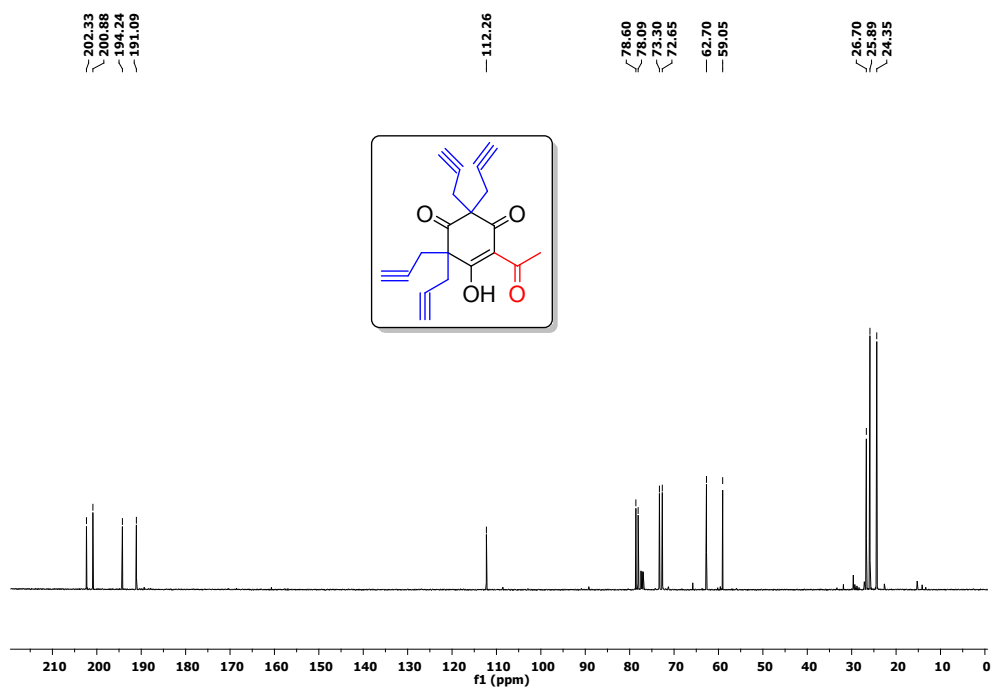


S1.e. ^1H , ^{13}C and DEPT-135 NMR spectrum of 4-acetyl-5-hydroxy-2,2,6,6-tetra(prop-2-ynyl)cyclohex-4-ene-1,3-dione (**3b**)

^1H NMR



^{13}C NMR

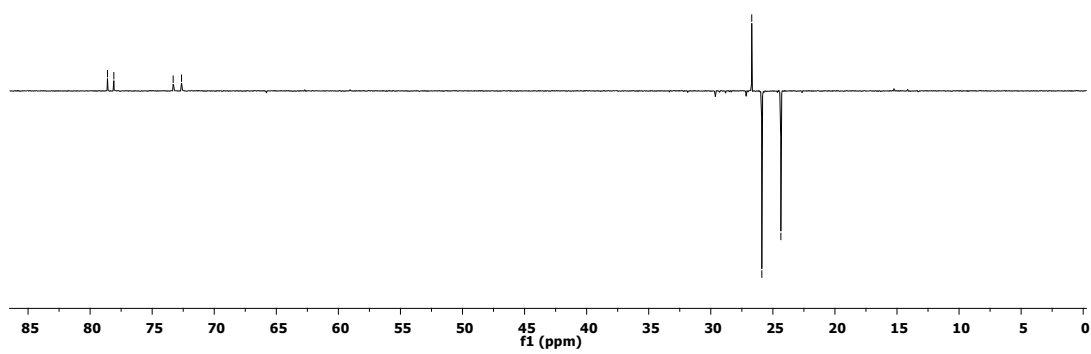
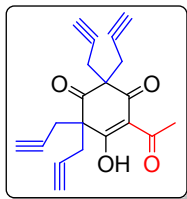


DEPT

78.60
78.09

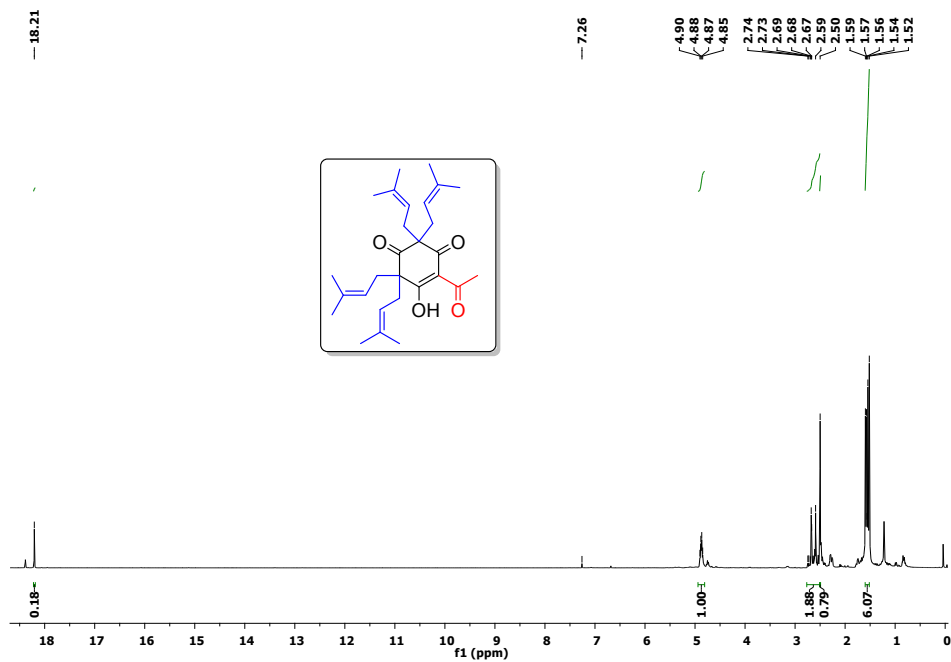
73.31
72.63

26.70
25.89
24.35

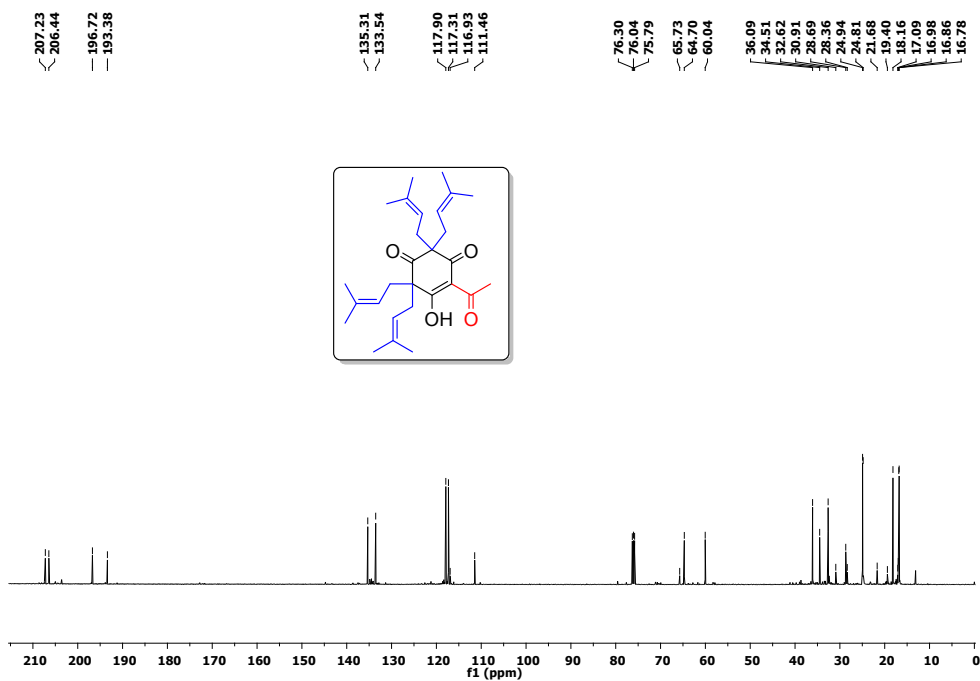


S1.f. ^1H , ^{13}C and DEPT-135 NMR spectrum of 4-acetyl-5-hydroxy-2,2,6,6-tetrakis(3-methylbut-2-enyl)cyclohex-4-ene-1,3-dione (**3c**)

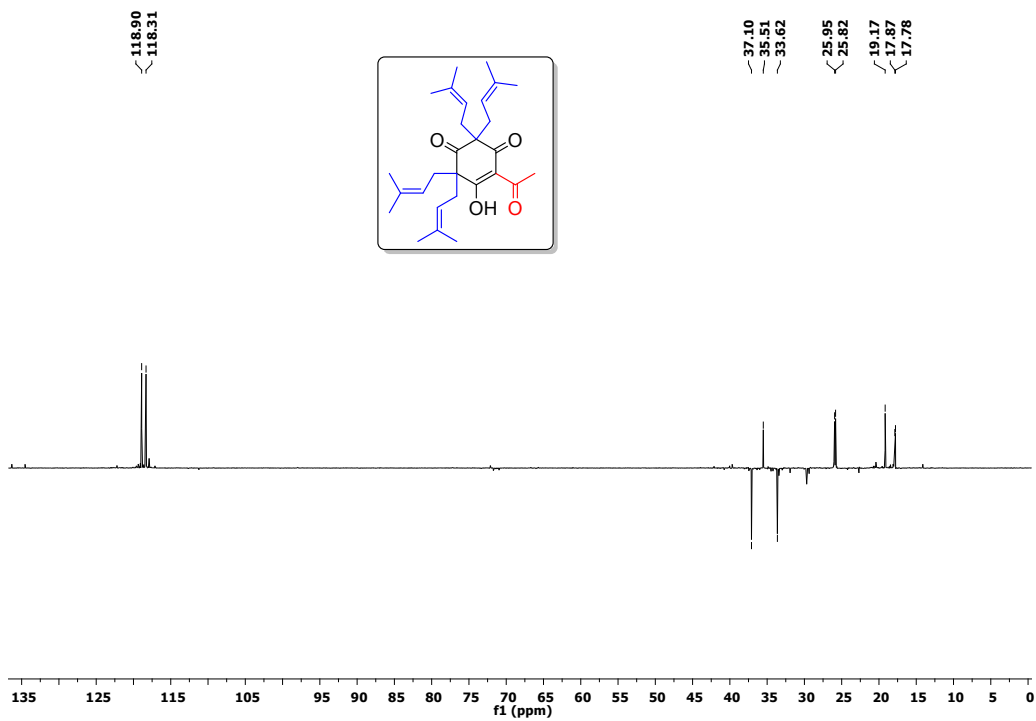
^1H NMR



^{13}C NMR

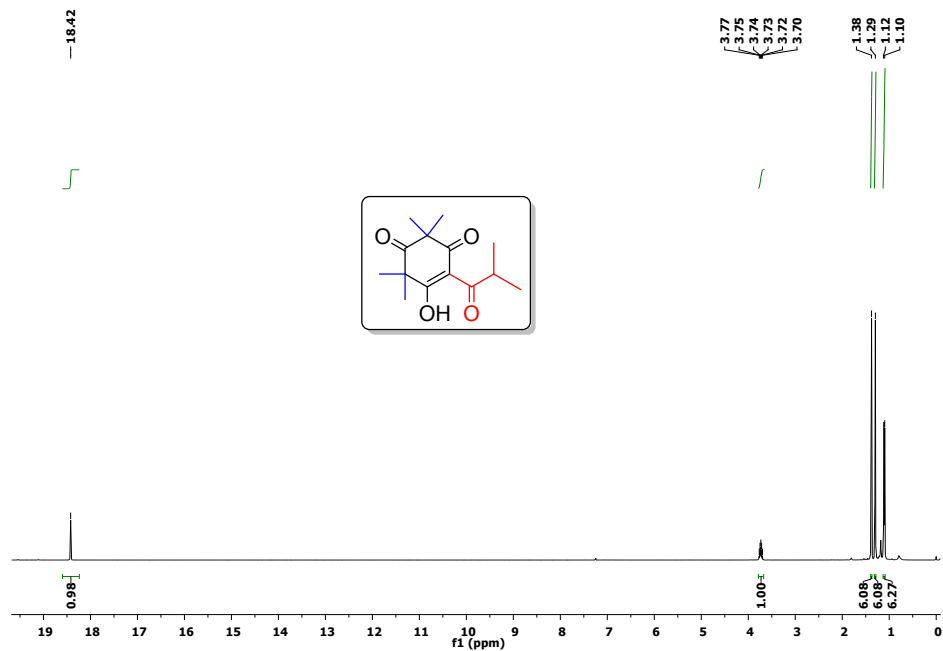


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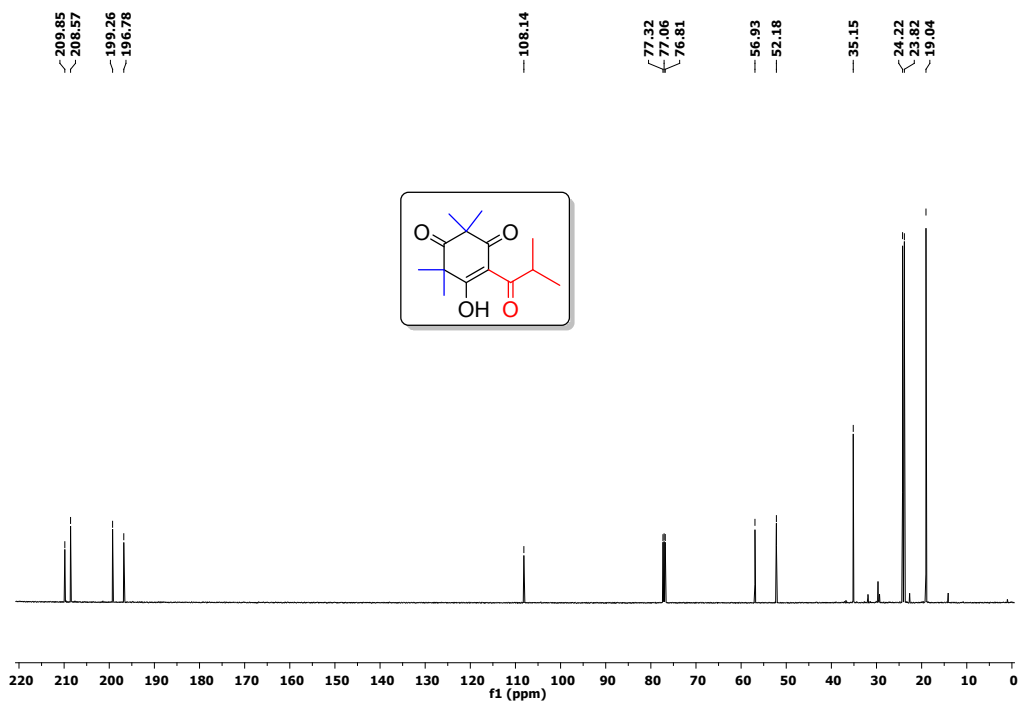


S1.g. ^1H , ^{13}C and DEPT-135 NMR spectrum of 5-hydroxy-4-(isobutyryl)-2,2,6,6-tetramethylcyclohex-4-ene-1,3-dione (**3d**)

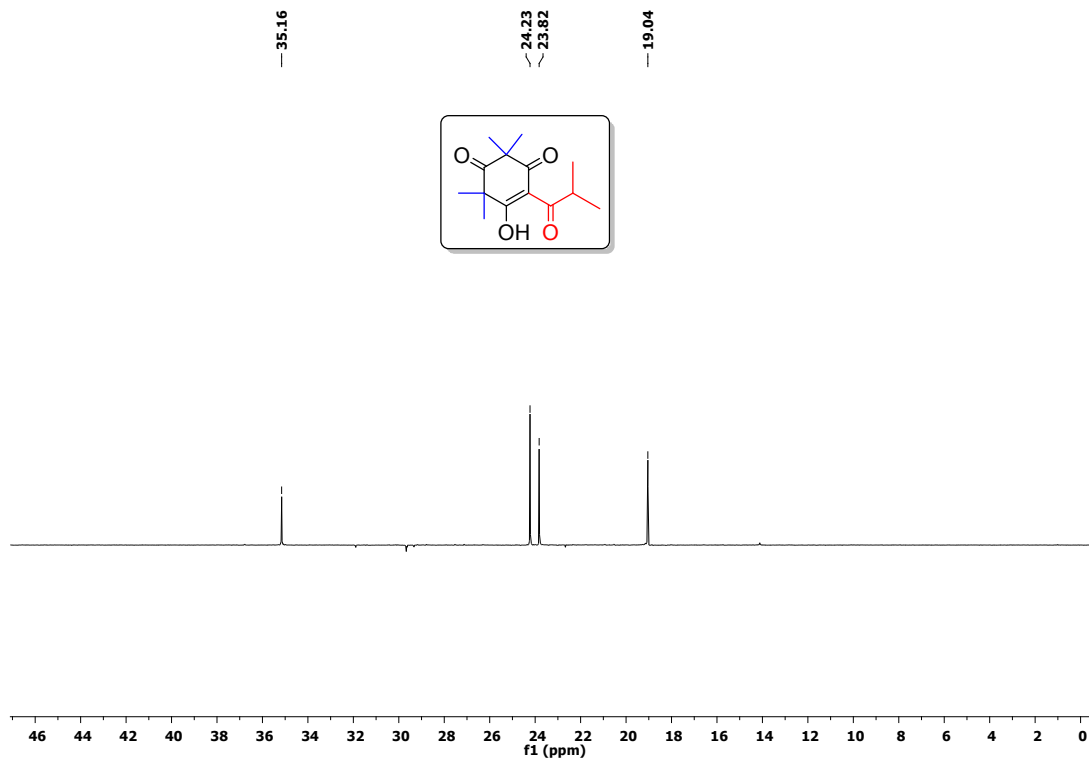
^1H NMR



^{13}C NMR

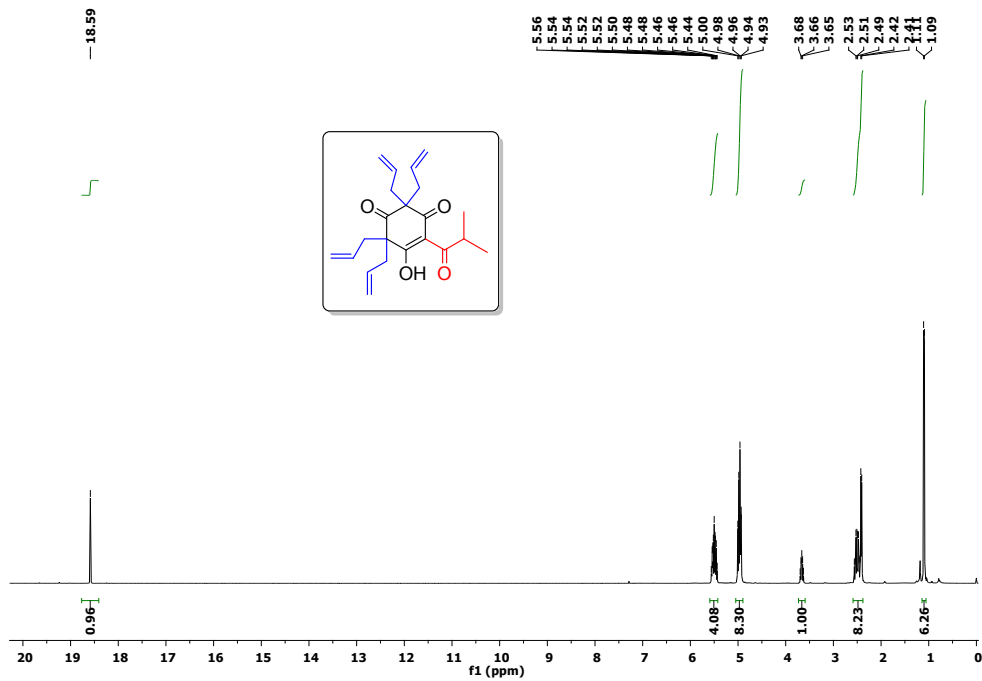


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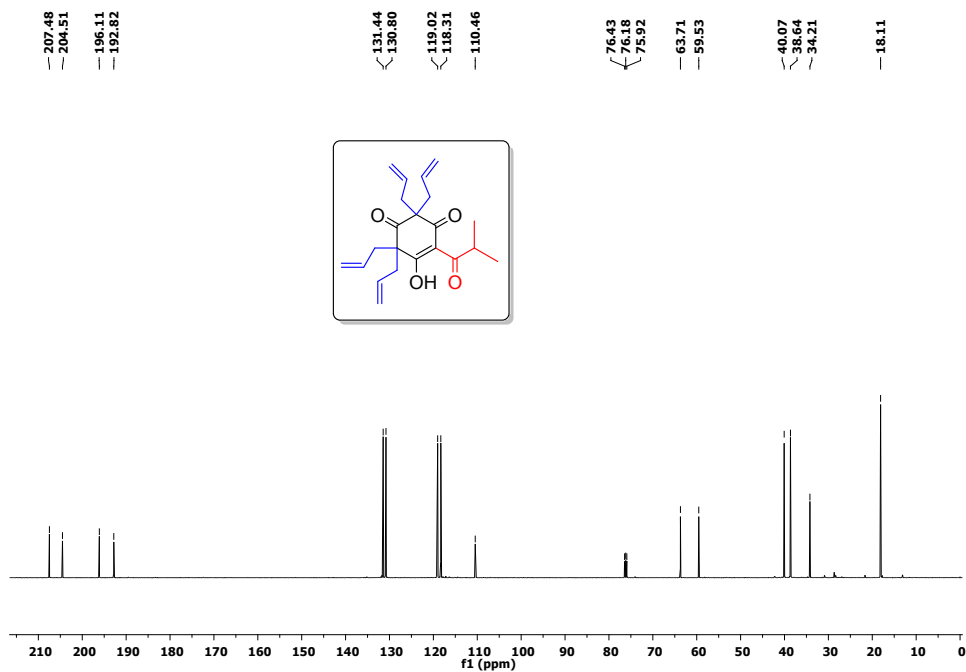


S1.h. ^1H , ^{13}C and DEPT-135 NMR spectrum of 2,2,6,6-tetraallyl-5-hydroxy-4-(isobutyryl)cyclohex-4-ene-1,3-dione (**3e**)

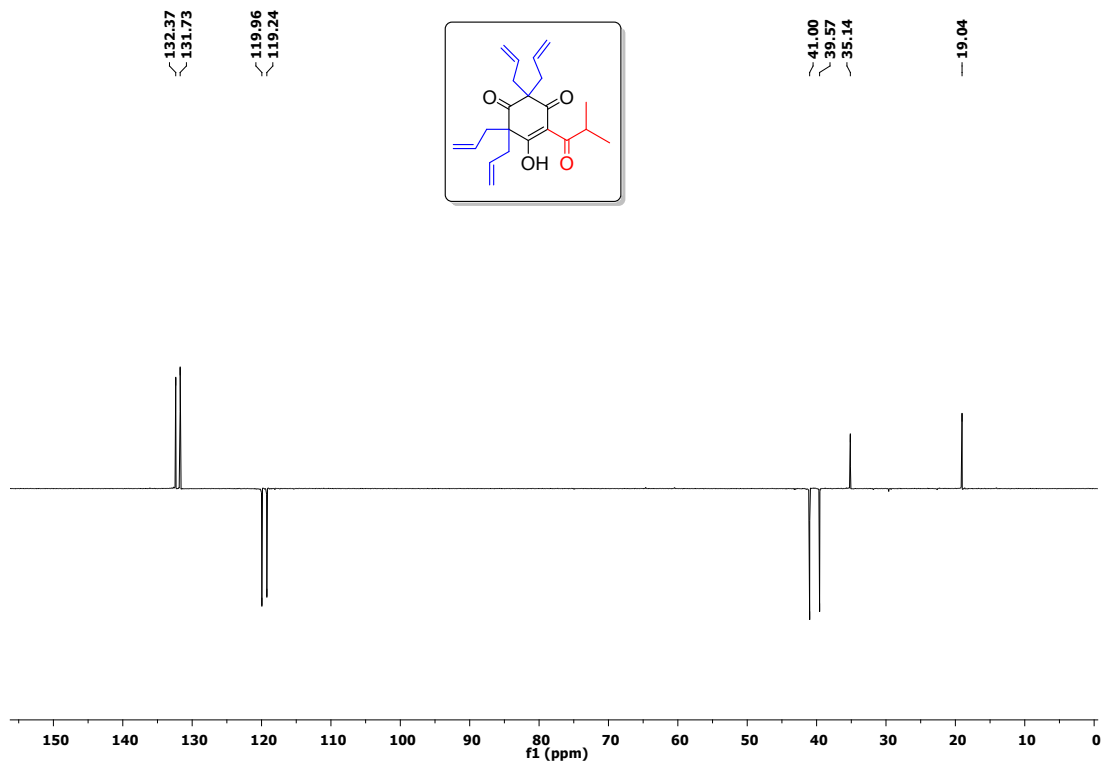
^1H NMR



^{13}C NMR

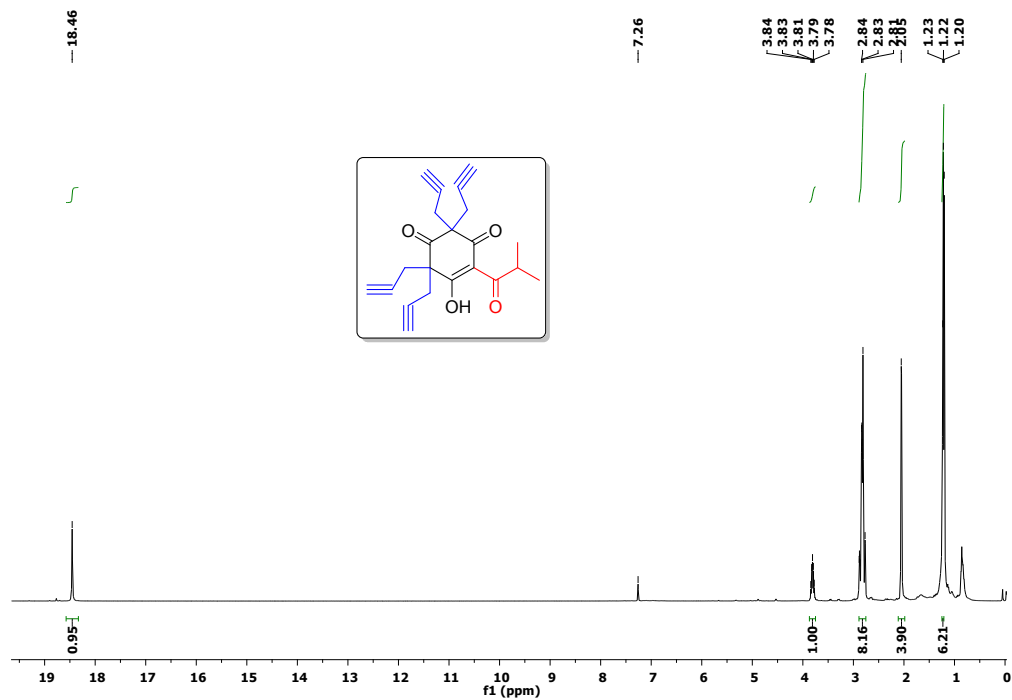


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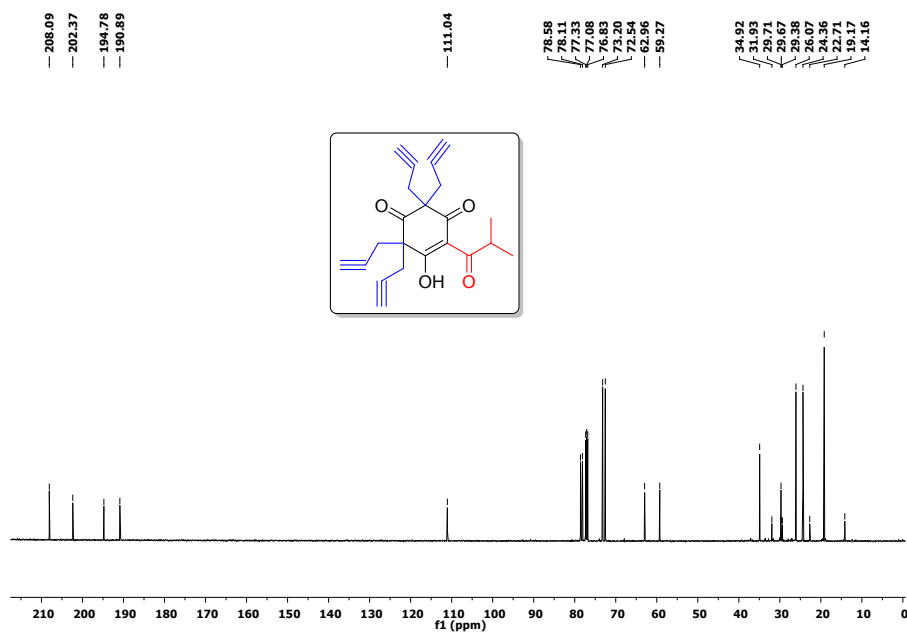


S1.i. ^1H , ^{13}C and DEPT-135 NMR spectrum of 5-hydroxy-4-(isobutyryl)-2,2,6,6-tetra(prop-2-ynyl)cyclohex-4-ene-1,3-dione (**3f**)

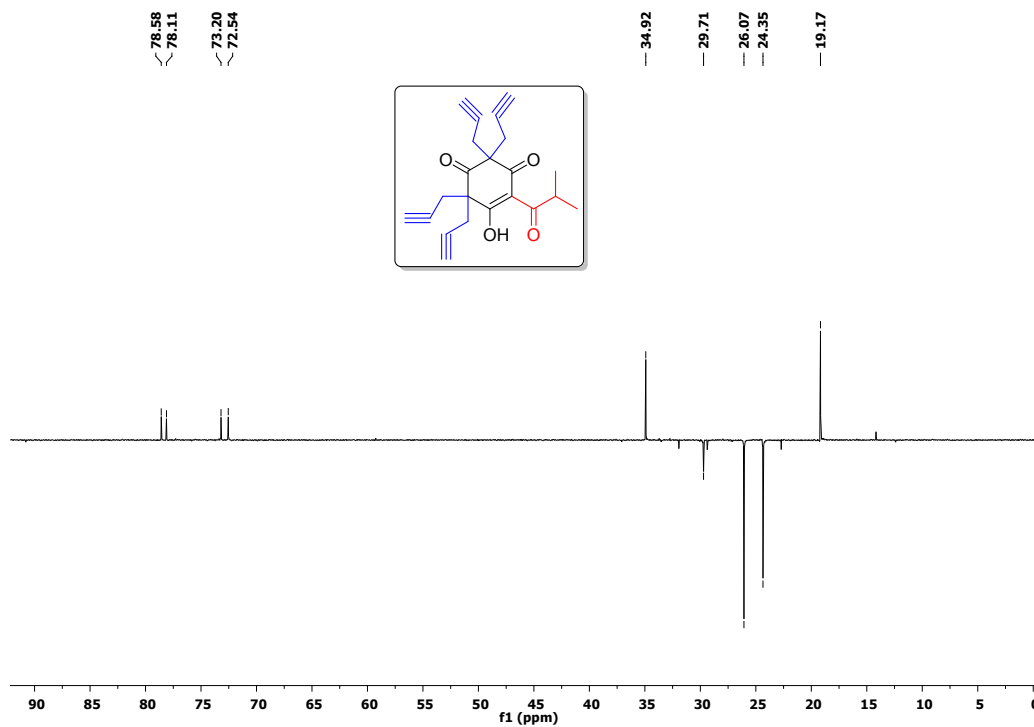
^1H NMR



^{13}C NMR

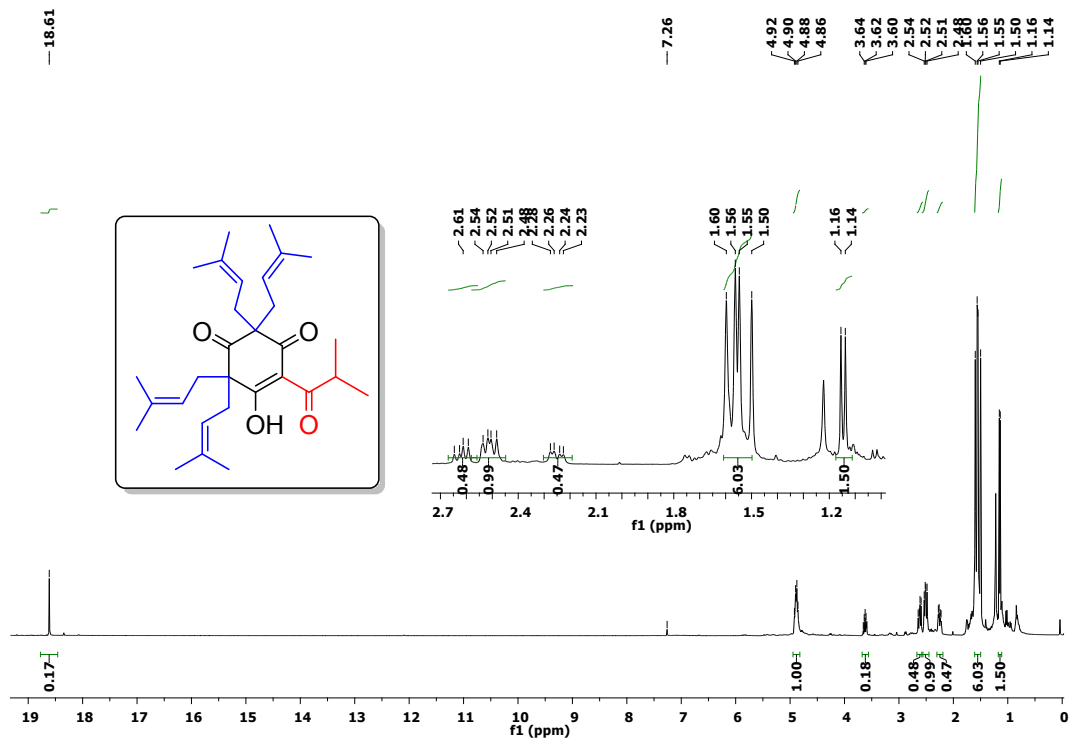


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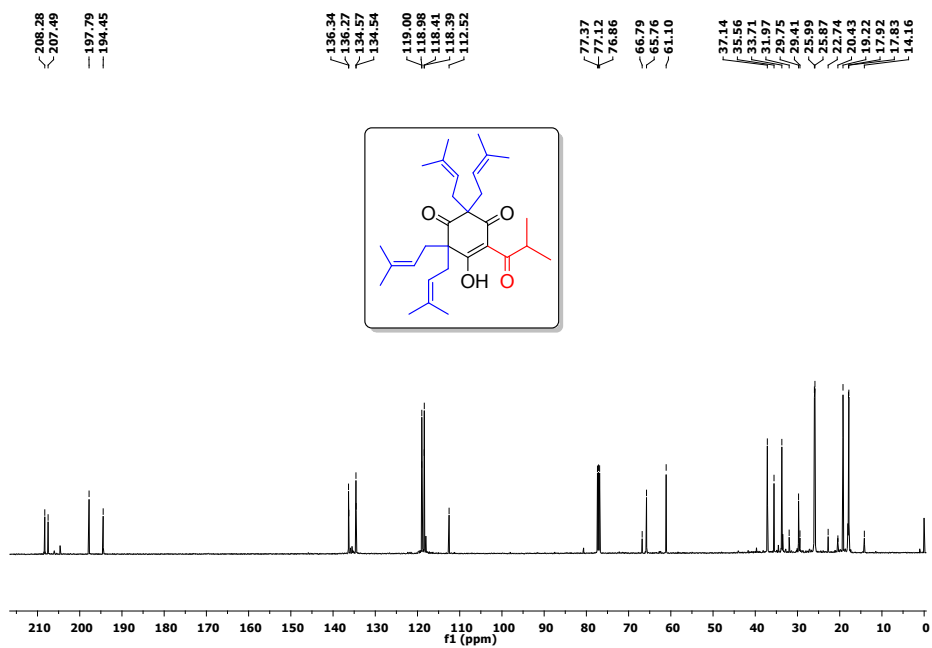


S1.j. ^1H , ^{13}C and DEPT-135 NMR spectrum of 5-hydroxy-4-isobutyryl-2,2,6,6-tetrakis(3-methylbut-2-en-1-yl)cyclohex-4-ene-1,3-dione (**3g**)

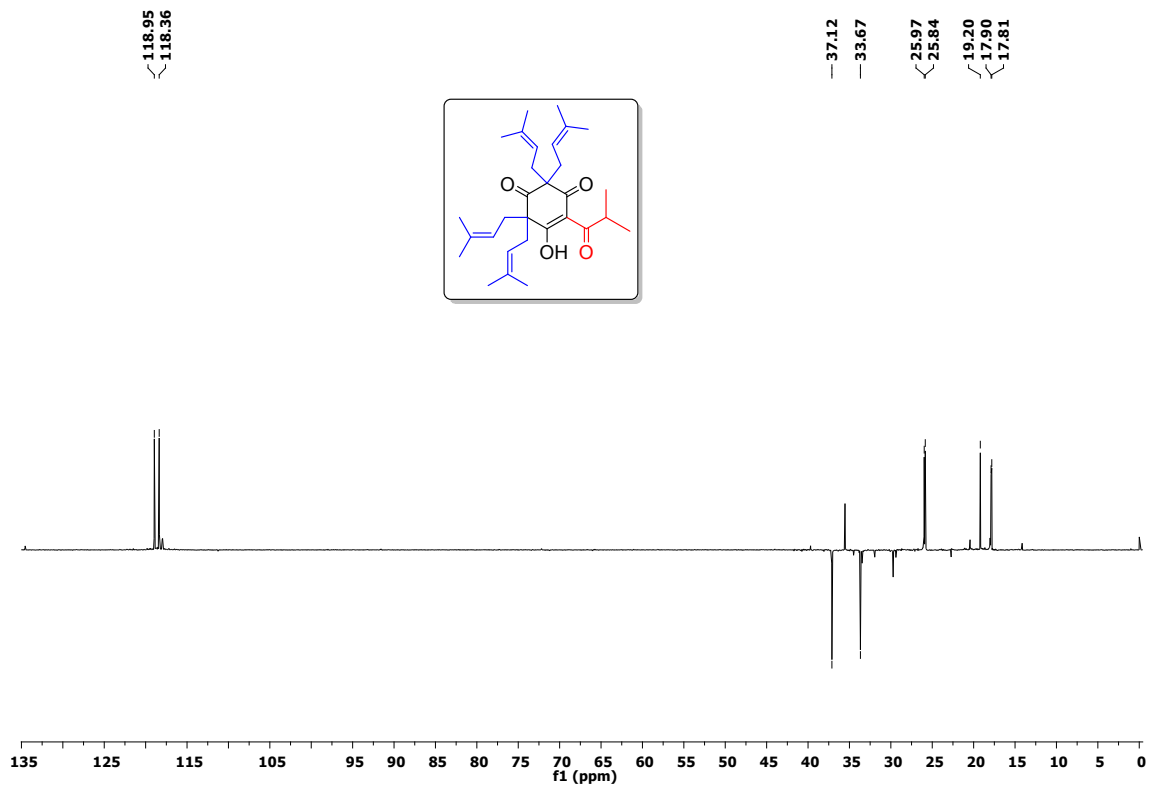
^1H NMR



^{13}C NMR

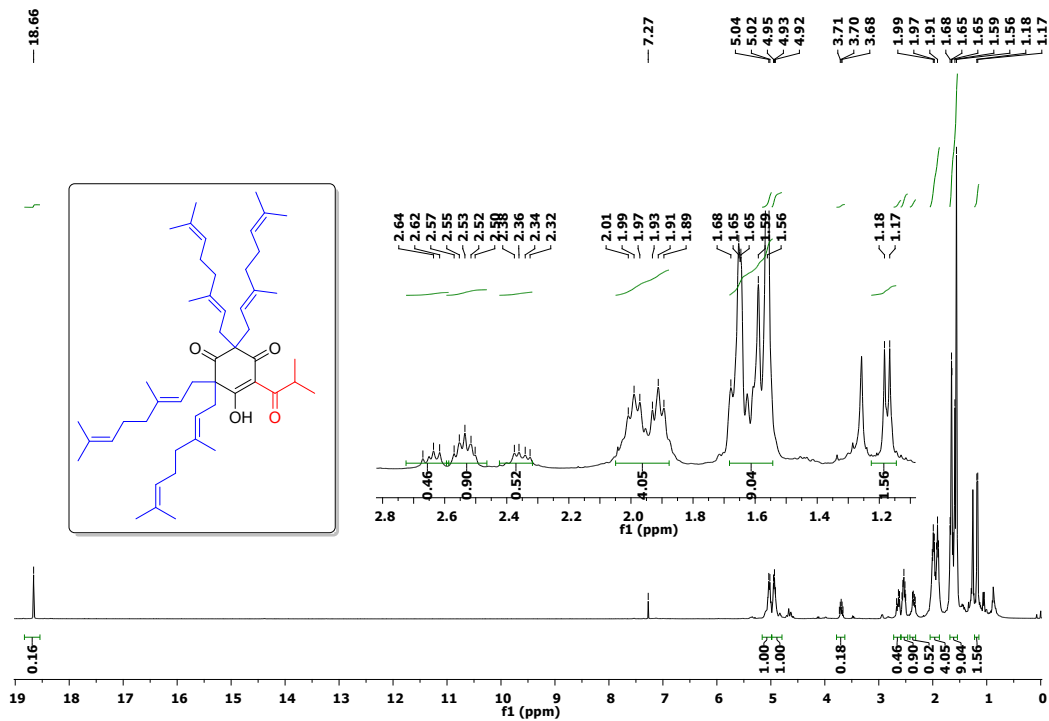


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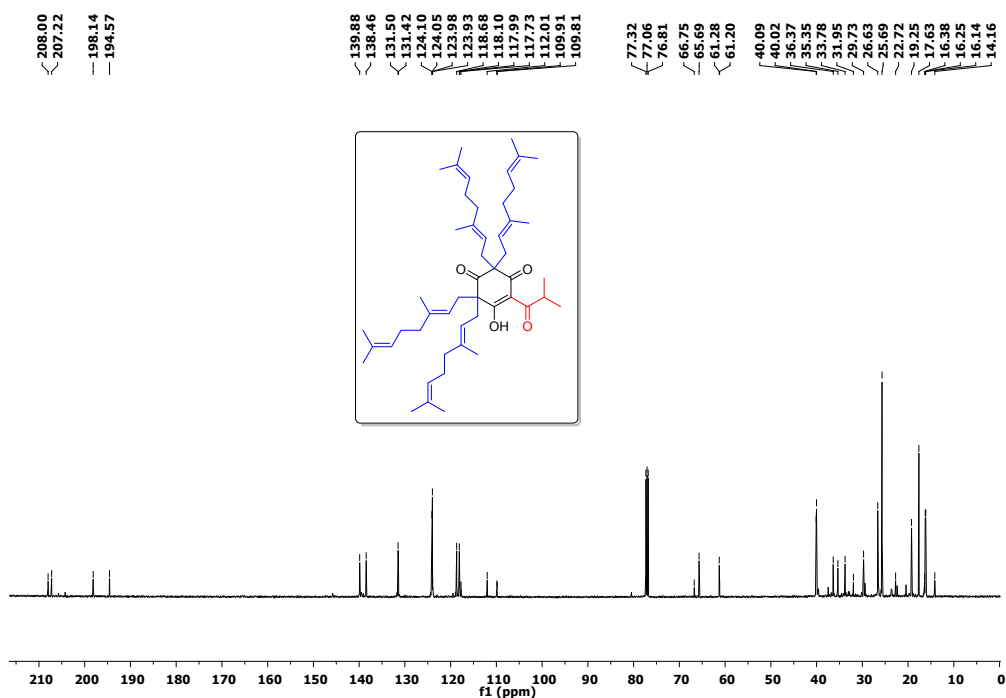


S1.k. ^1H , ^{13}C and DEPT-135 NMR spectrum of 5-hydroxy-4-(isobutyryl)-2,2,6,6-tetrakis((E)-3,7-dimethylocta-2,6-dienyl)cyclohex-4-ene-1,3-dione (**3h**)

^1H NMR

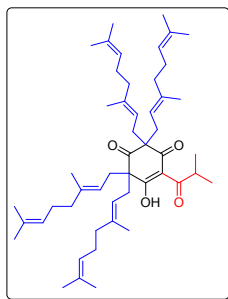


^{13}C NMR

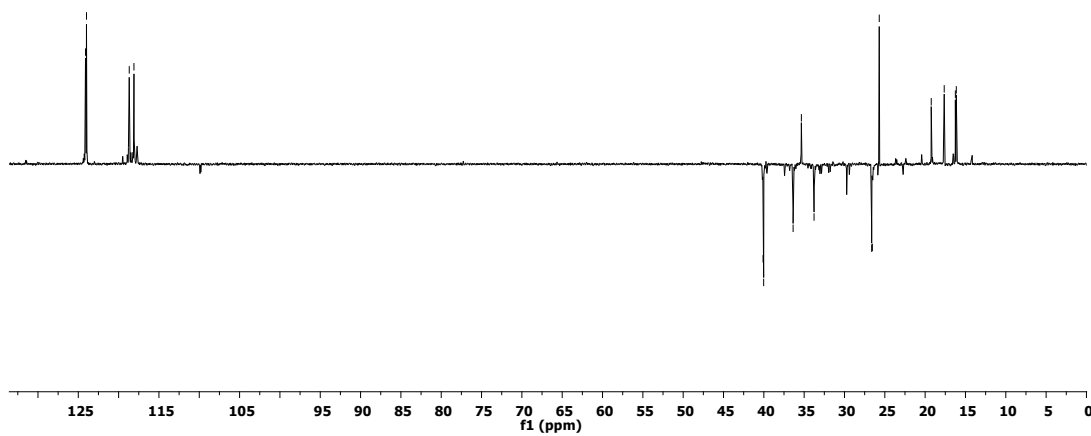


DEPT

124.10
123.98
118.68
118.10

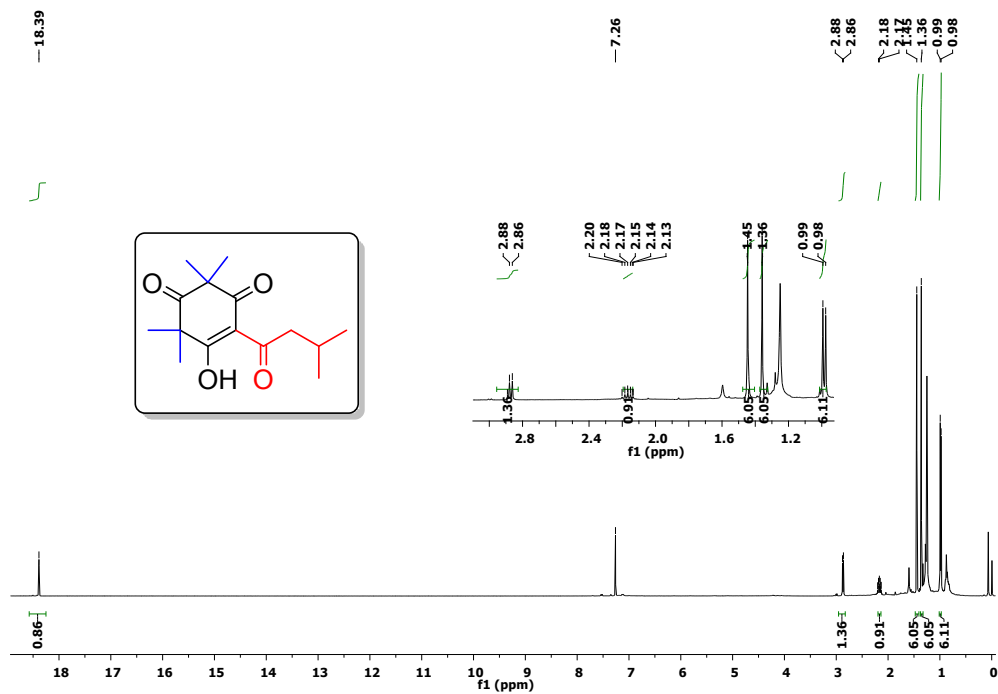


40.10
40.02
36.37
35.35
33.77
26.63
26.54
25.69
19.25
17.64
16.25
16.14

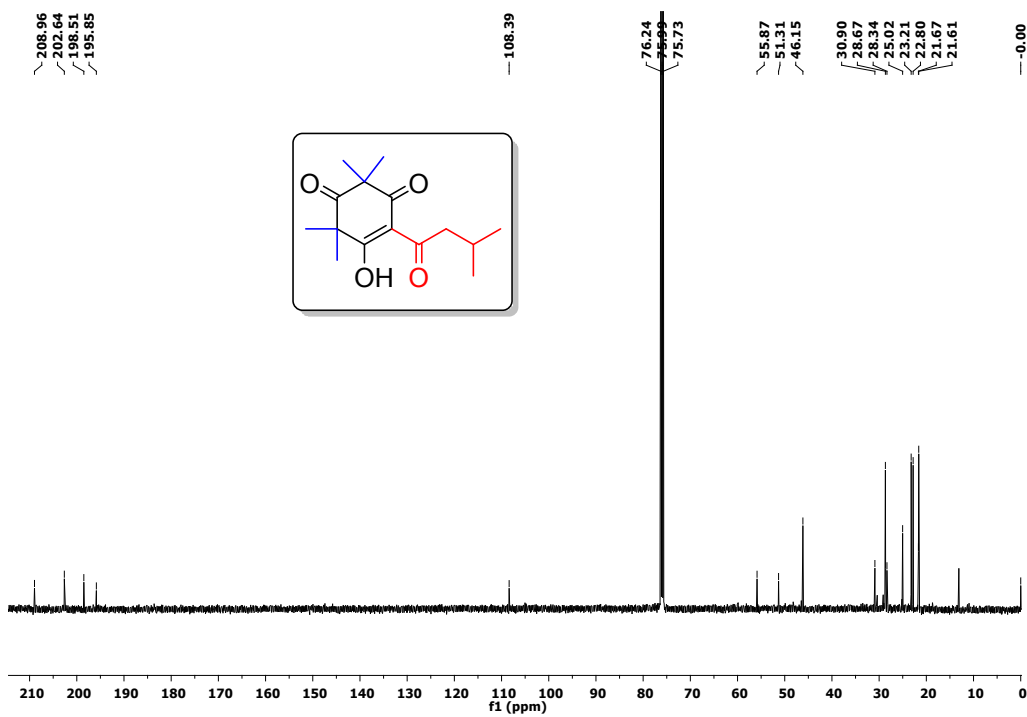


S1.1. ^1H , ^{13}C and DEPT-135 NMR spectrum of 4-(3-methylbutanoyl)-5-hydroxy-2,2,6,6-tetramethylcyclohex-4-ene-1,3-dione (**3i**)

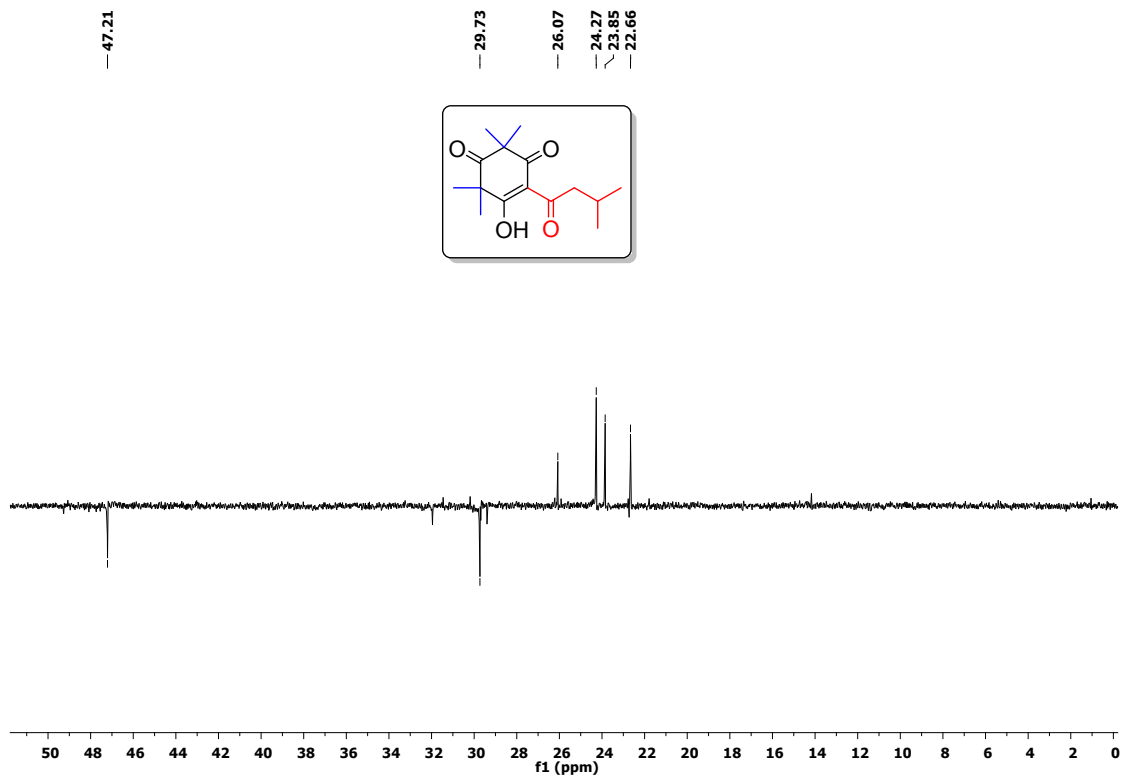
^1H NMR



^{13}C NMR

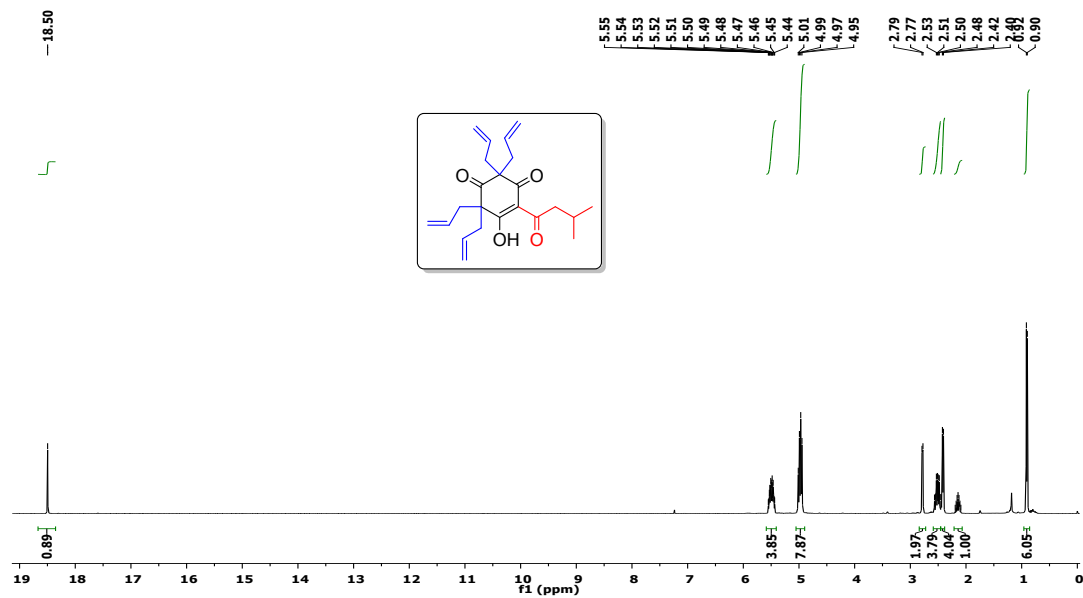


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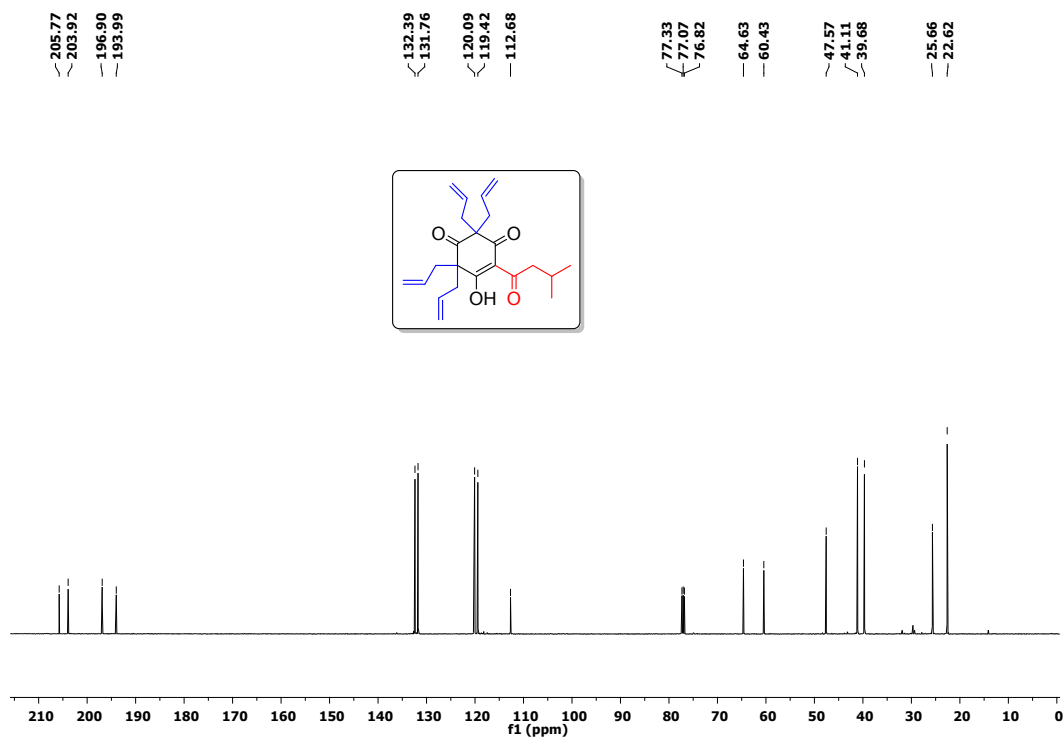


S1.m. ^1H , ^{13}C and DEPT-135 NMR spectrum of 4-(3-methylbutanoyl)-2,2,6,6-tetraallyl-5-hydroxycyclohex-4-ene-1,3-dione (**3j**)

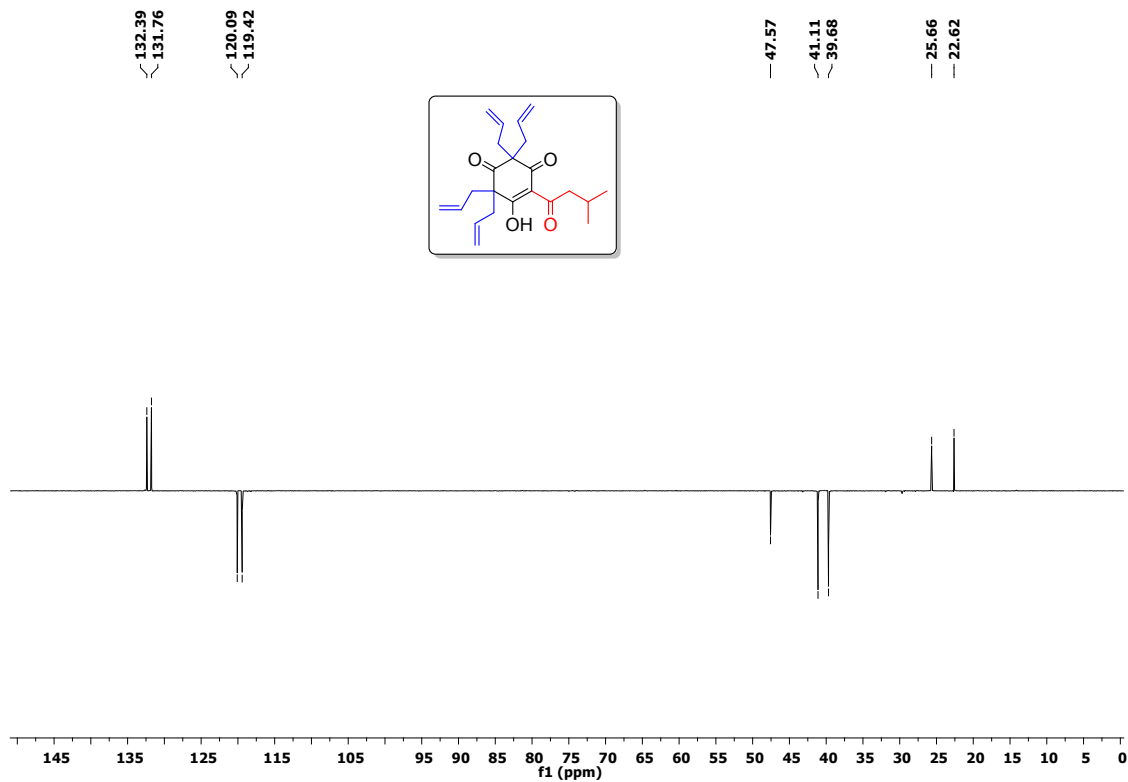
^1H NMR



^{13}C NMR

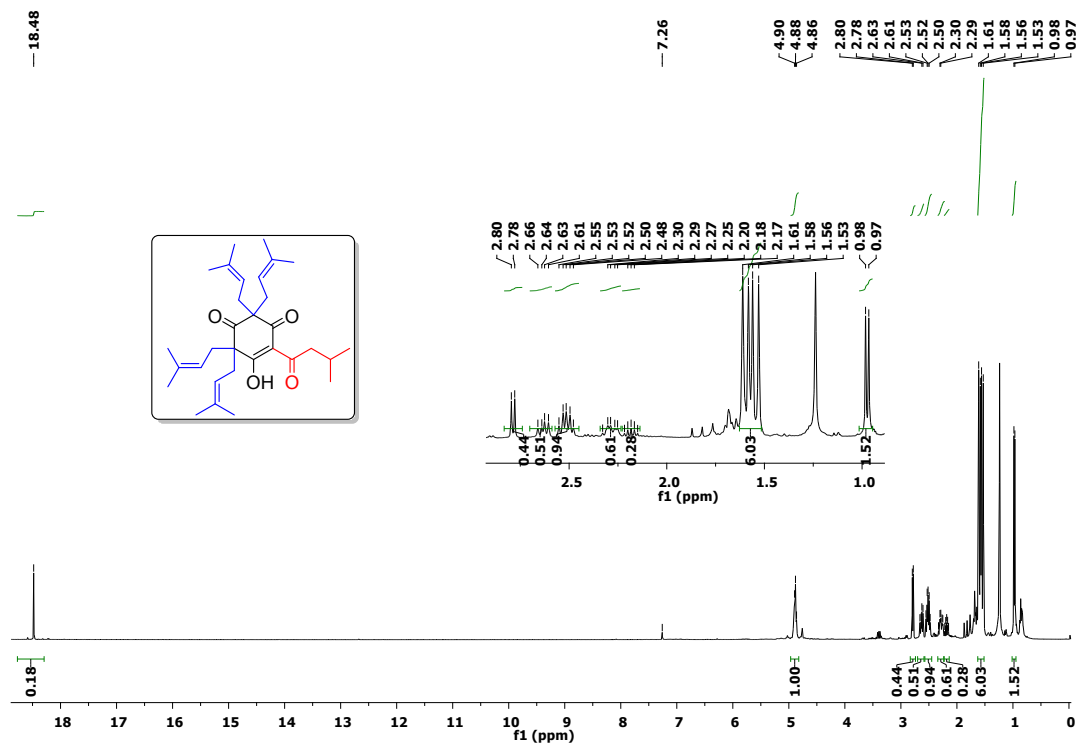


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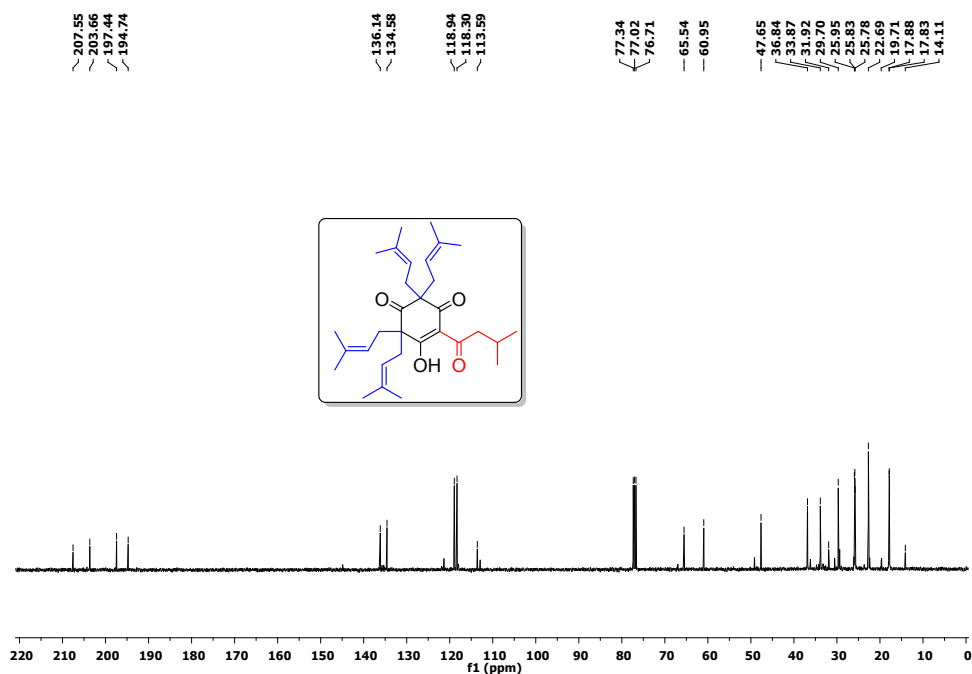


S1.n. ^1H , ^{13}C and DEPT-135 NMR spectrum of 4-(3-methylbutanoyl)-5-hydroxy-2,2,6,6-tetrakis(3-methylbut-2-enyl)cyclohex-4-ene-1,3-dione (**3k**)

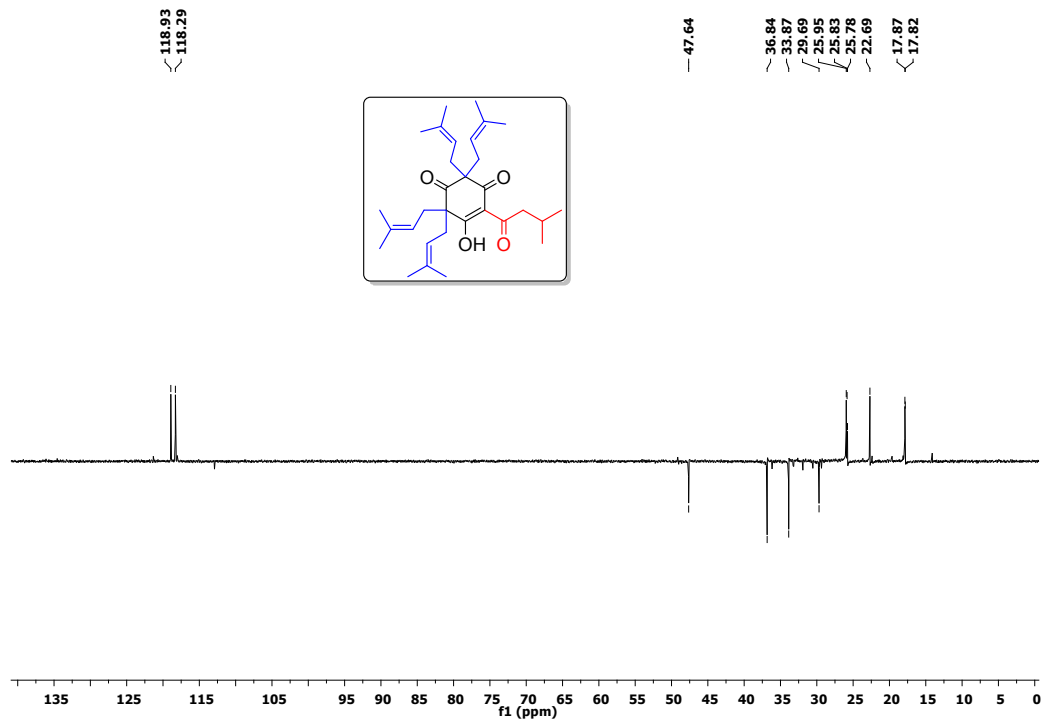
^1H NMR



^{13}C NMR

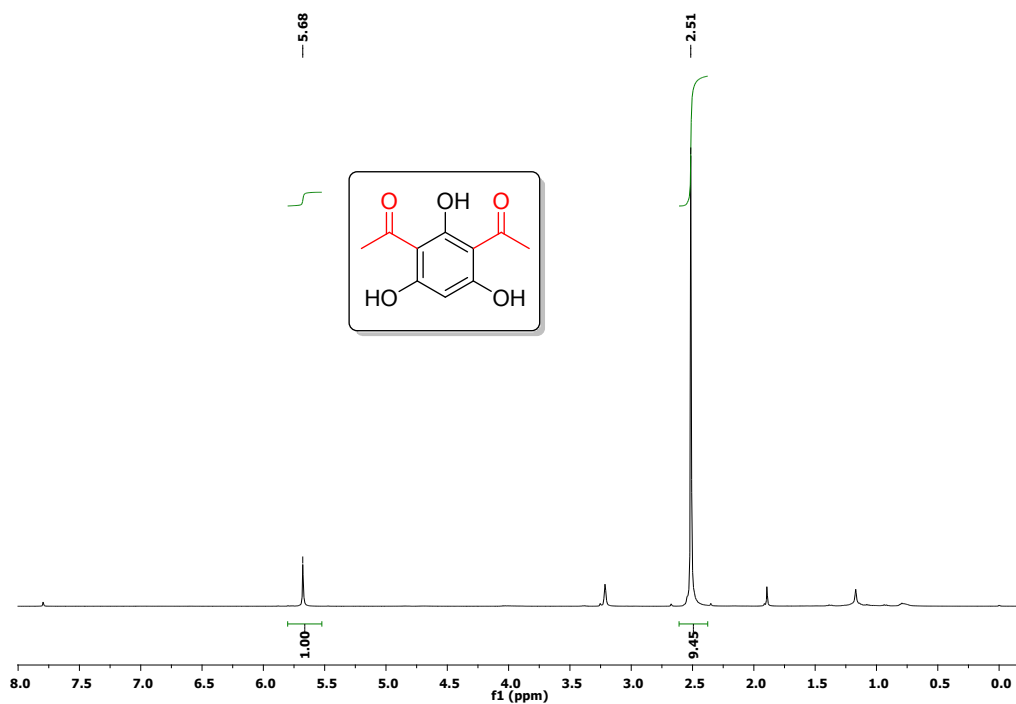


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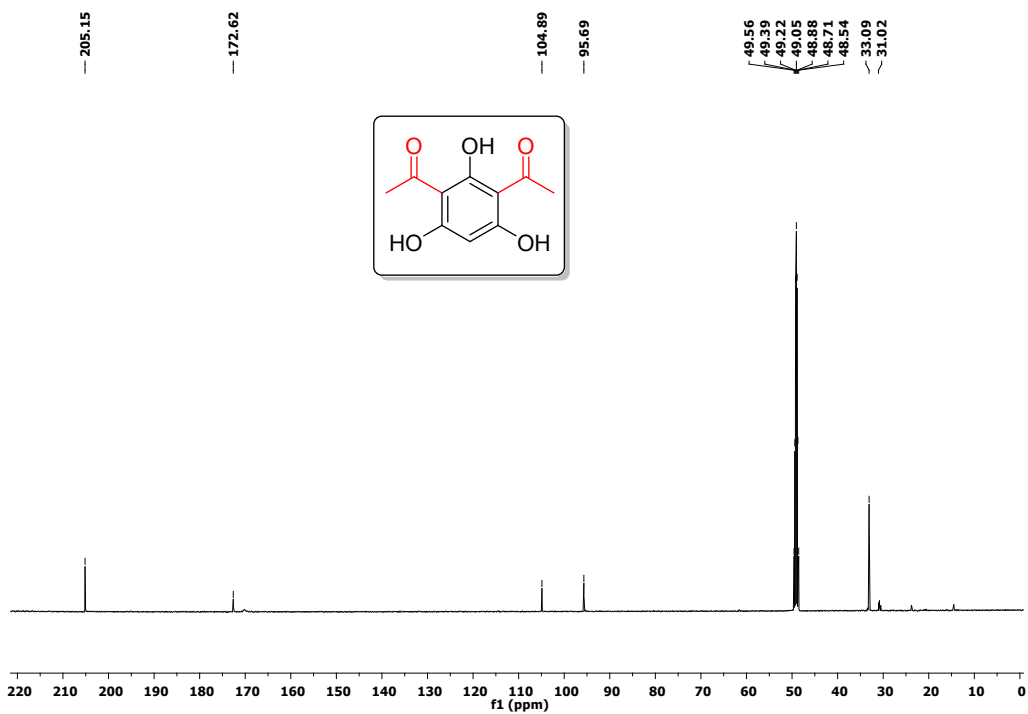


S1.0. ^1H , ^{13}C and DEPT-135 NMR spectrum of 1,3-diacetyl-2,4,6-trihydroxy benzene (**4a**)

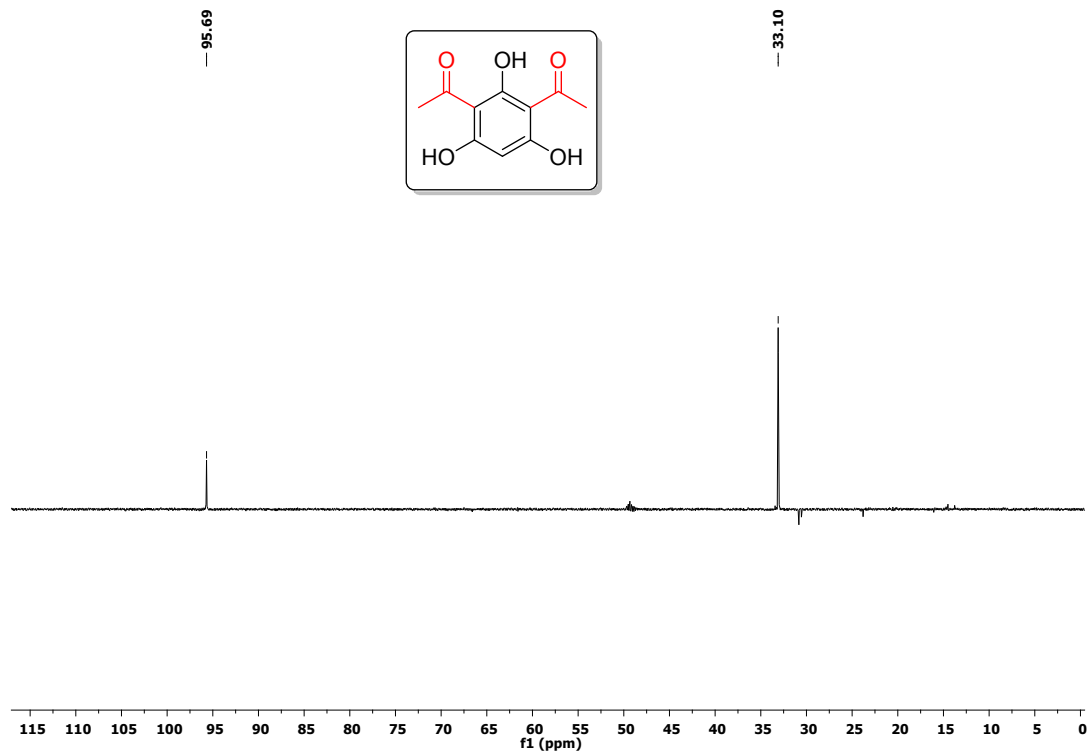
^1H NMR



^{13}C NMR

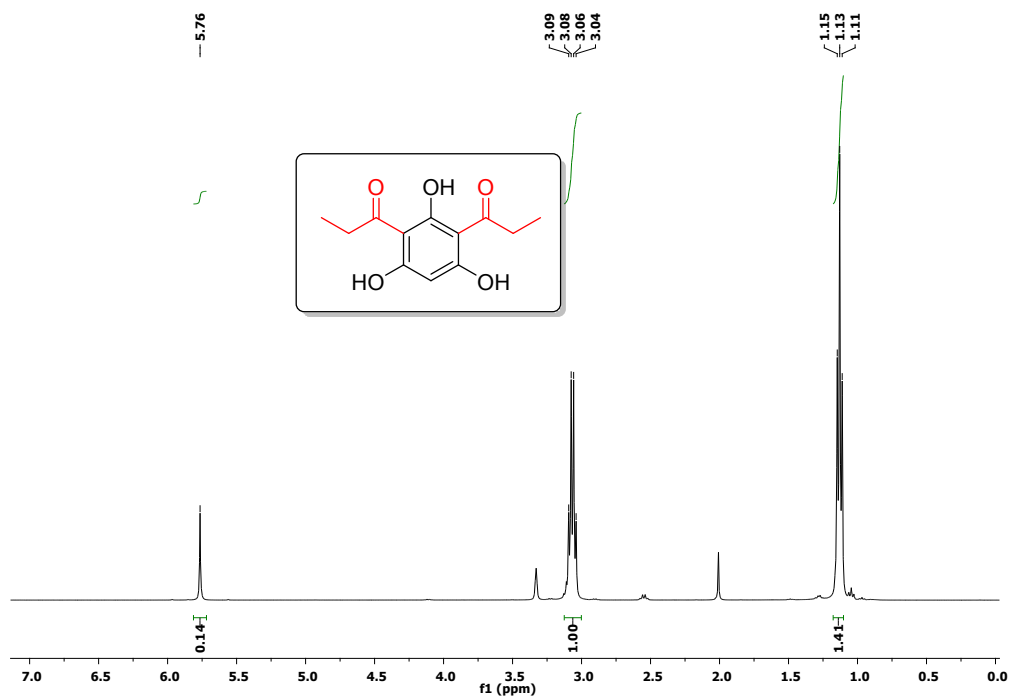


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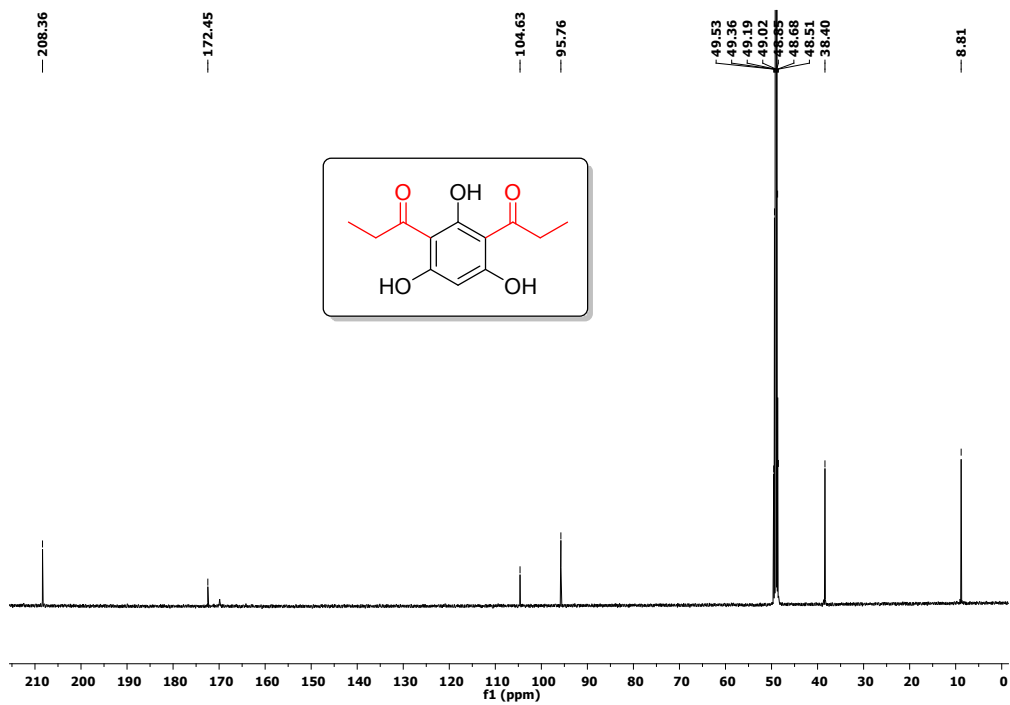


S1.p. ^1H , ^{13}C and DEPT-135 NMR spectrum of 1,3-dipropanoyl-2,4,6-trihydroxy benzene (**4b**)

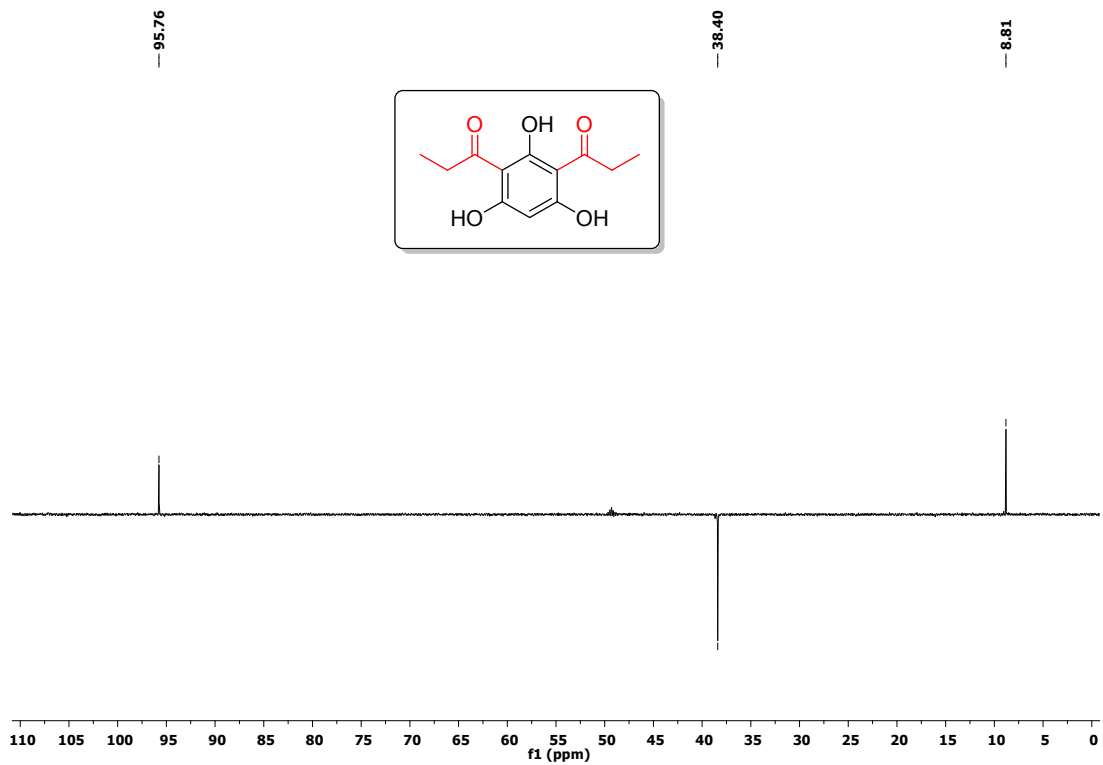
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^{13}C NMR

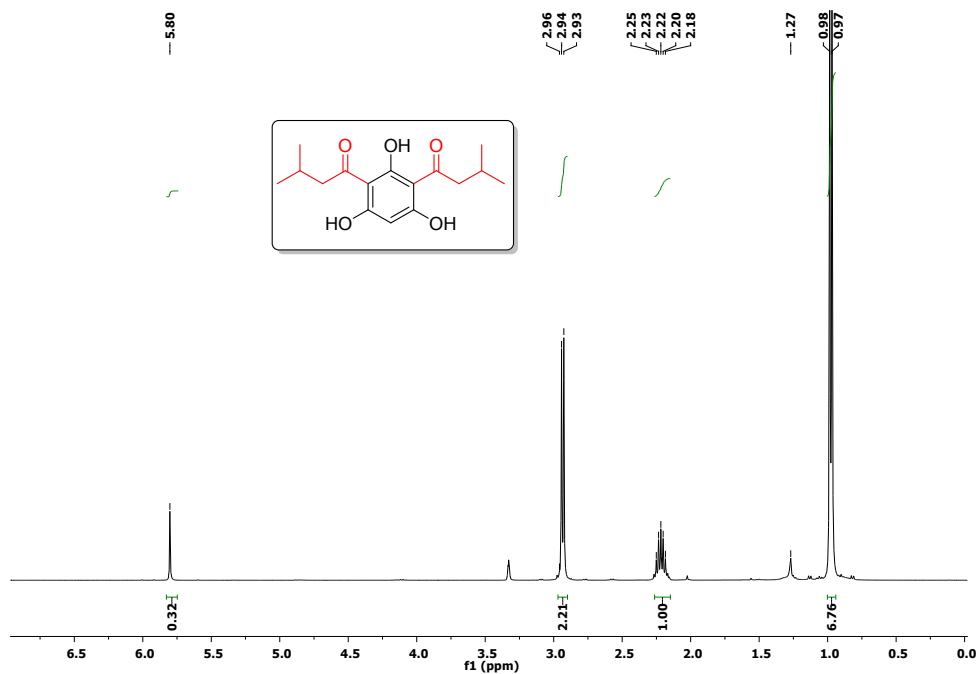


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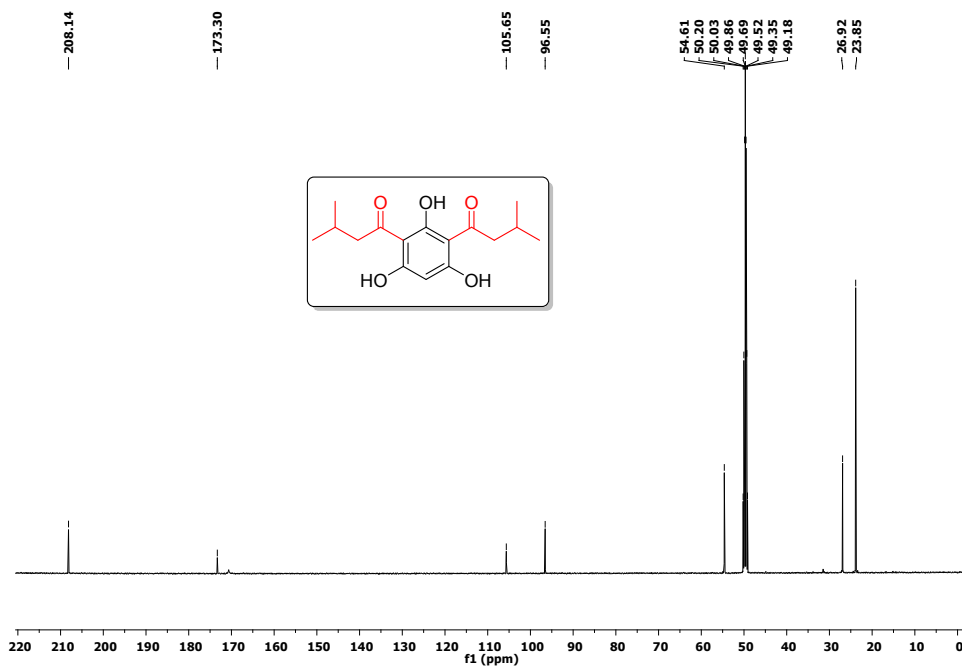


S1.q. ^1H , ^{13}C and DEPT-135 NMR spectrum of 1,3-di-(3-Methyl-butanoyl)-2,4,6-trihydroxy benzene (**4c**)

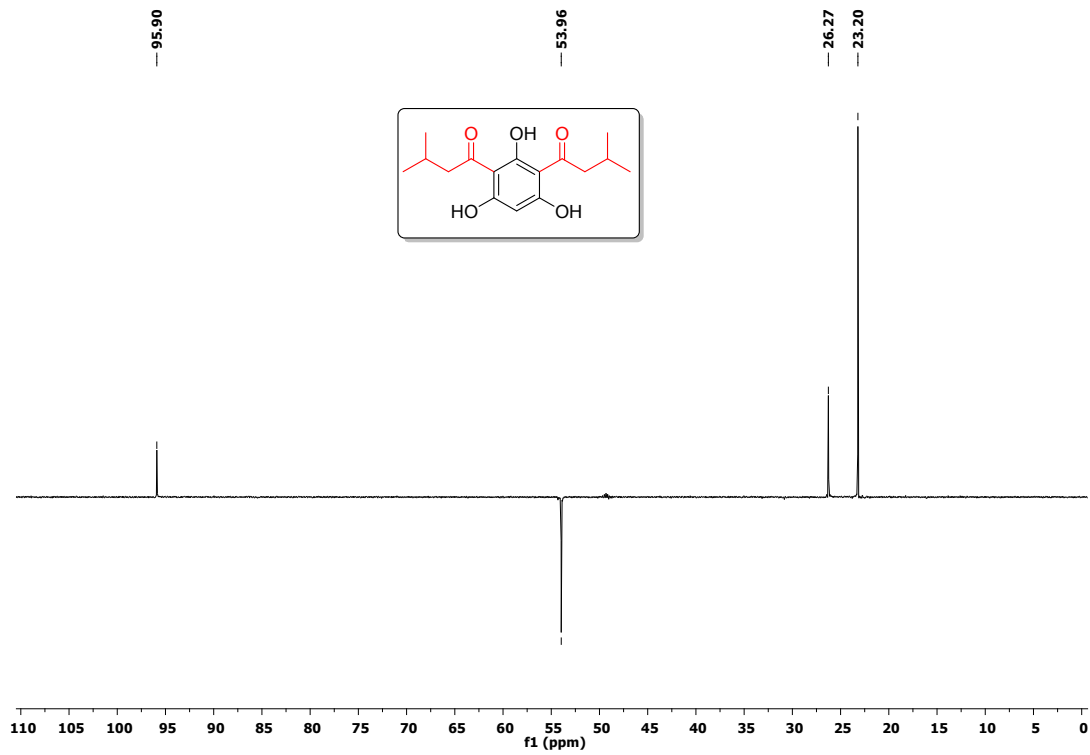
^1H NMR



^{13}C NMR

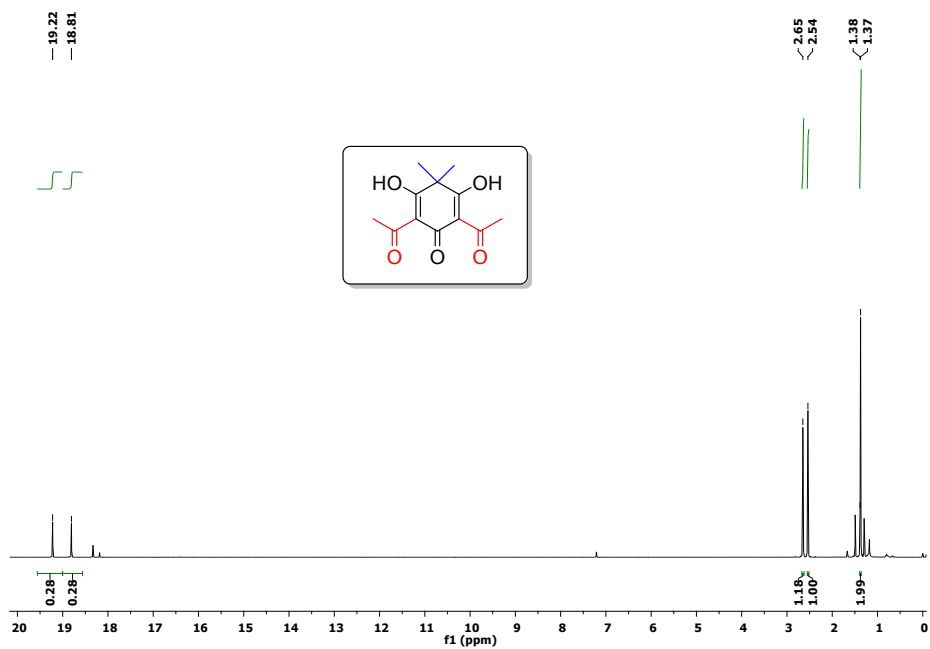


DEPT

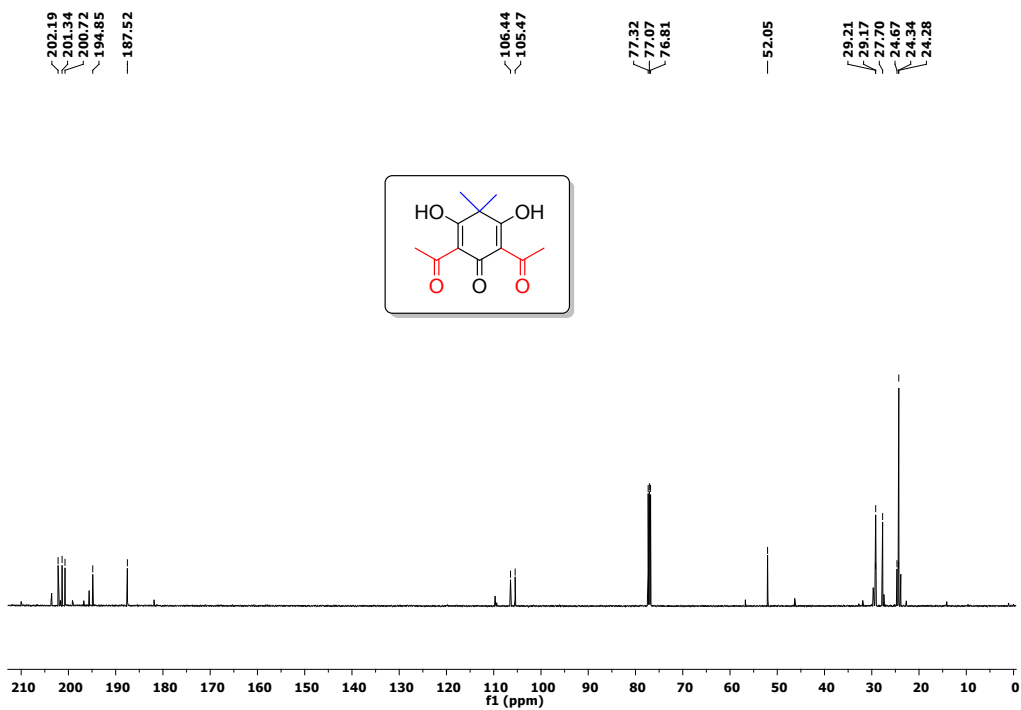


S1.r. ^1H , ^{13}C and DEPT-135 NMR spectrum of 2,6-diacetyl-3,5-dihydroxy-4,4-dimethylcyclohexa-2,5-dienone (**5a**)

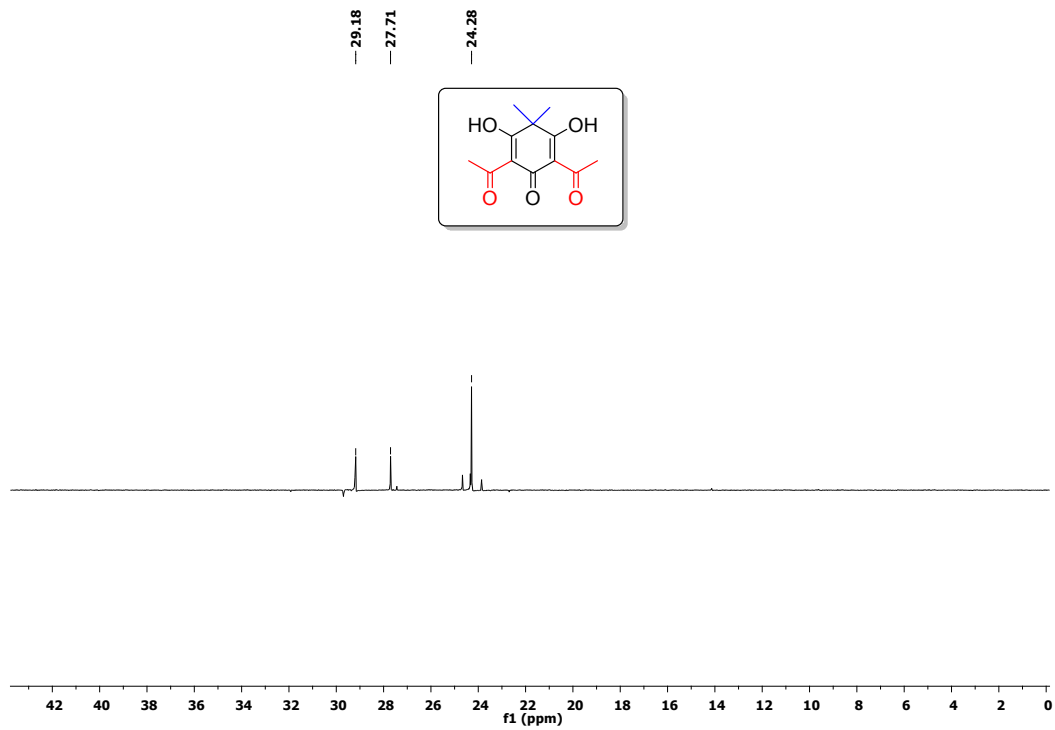
^1H NMR



^{13}C NMR

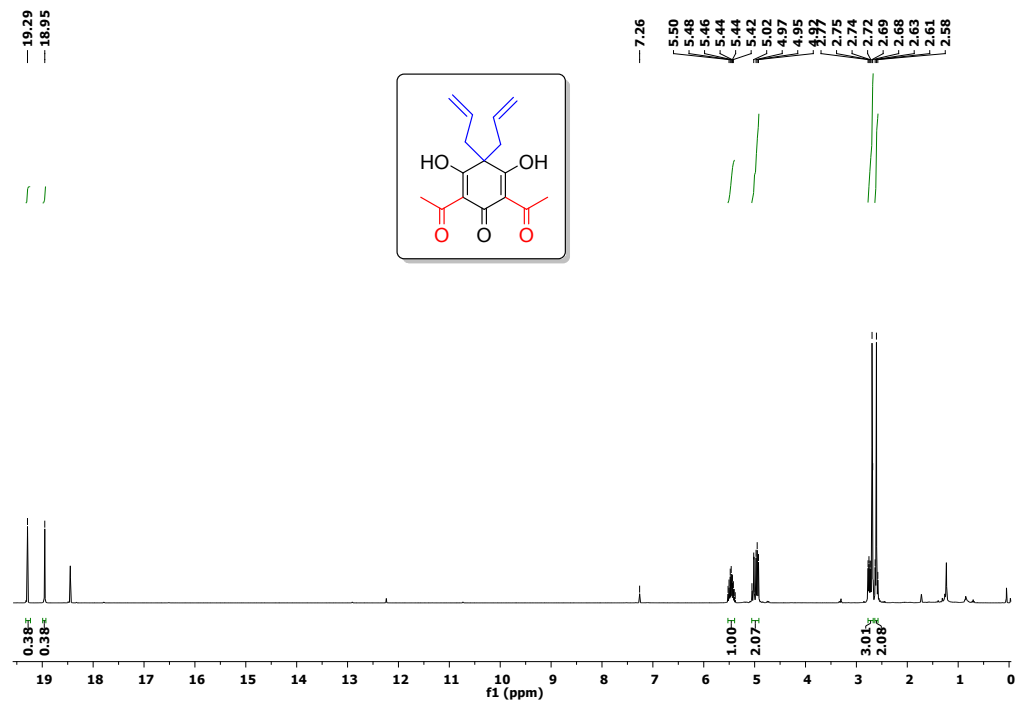


DEPT

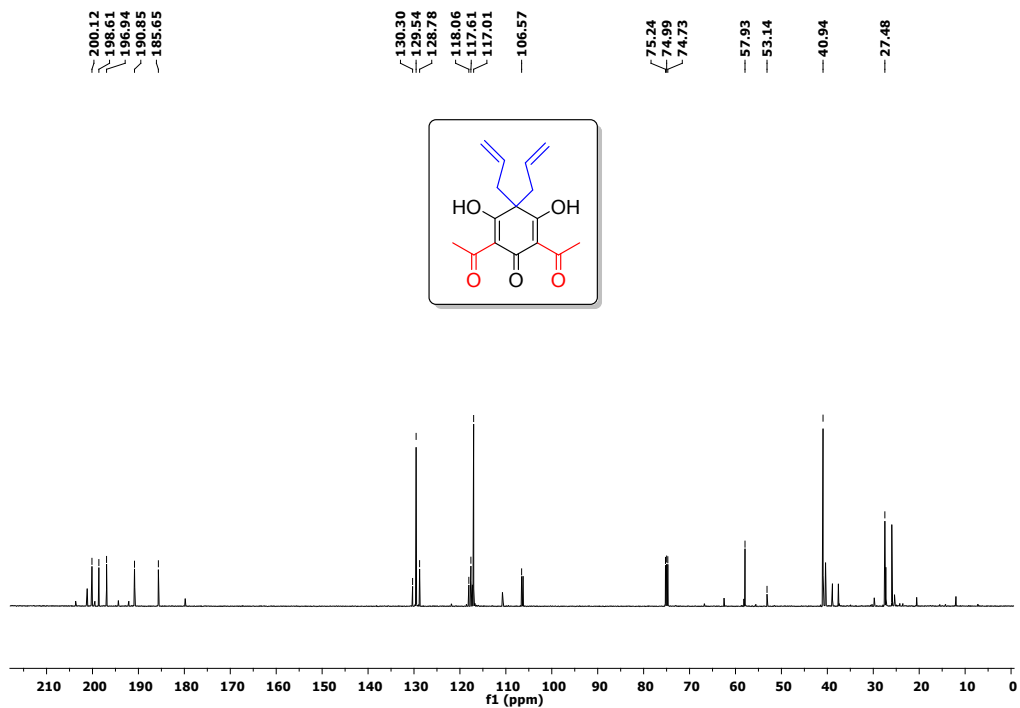


S1.s. ^1H , ^{13}C and DEPT-135 NMR spectrum of 2,6-diacetyl-4,4-diallyl-3,5-dihydroxycyclohexa-2,5-dienone (**5b**)

^1H NMR



^{13}C NMR



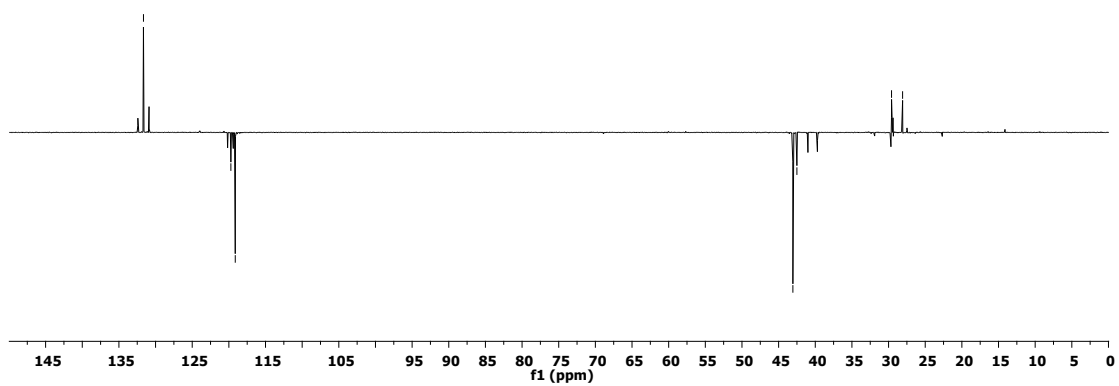
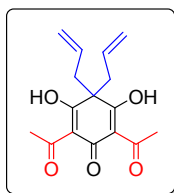
DEPT

131.65

119.73
119.13

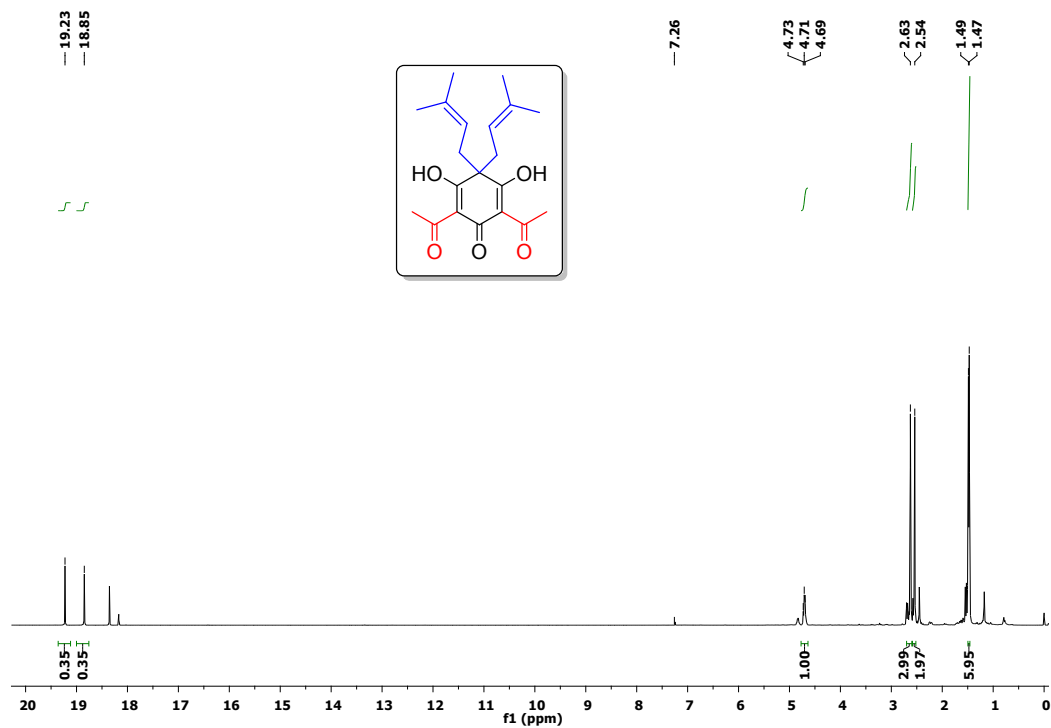
43.05
42.51

29.59
28.09

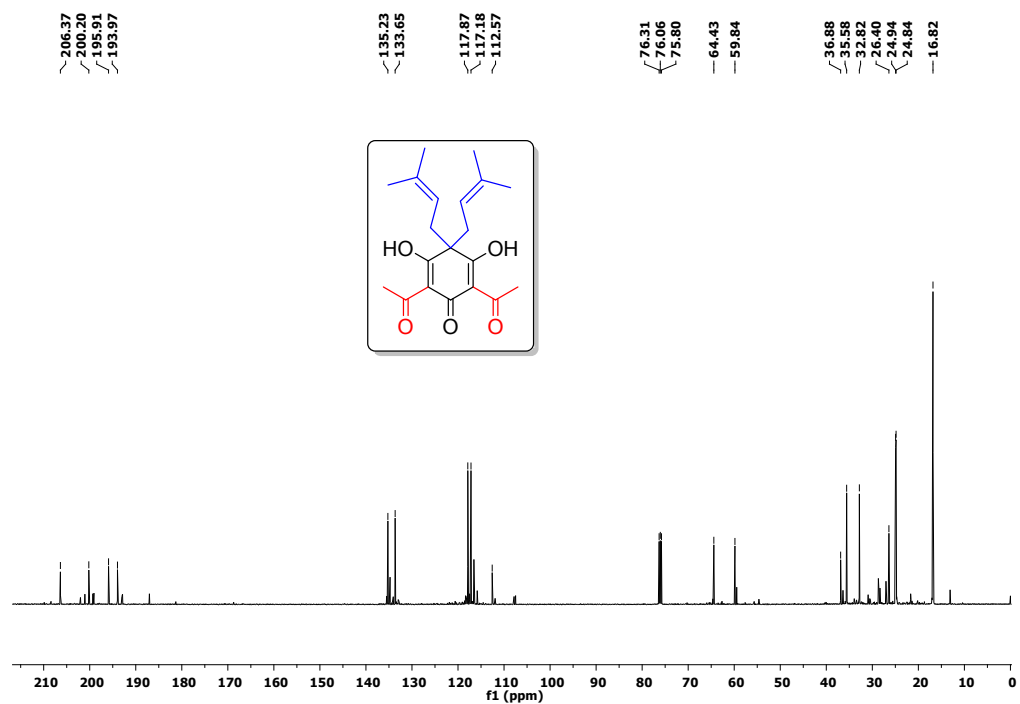


S1.t. ^1H , ^{13}C and DEPT-135 NMR spectrum of 2,6-diacetyl-3,5-dihydroxy-4,4-bis(3-methylbut-2-enyl)cyclohexa-2,5-dienone (**5c**)

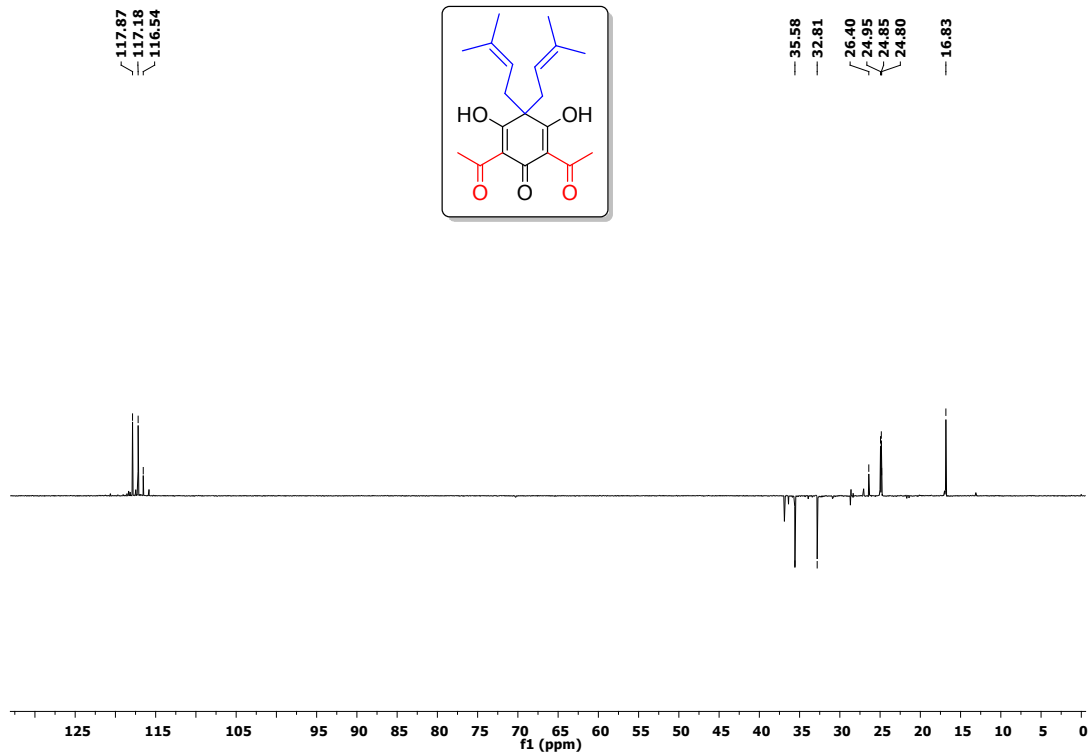
^1H NMR



^{13}C NMR

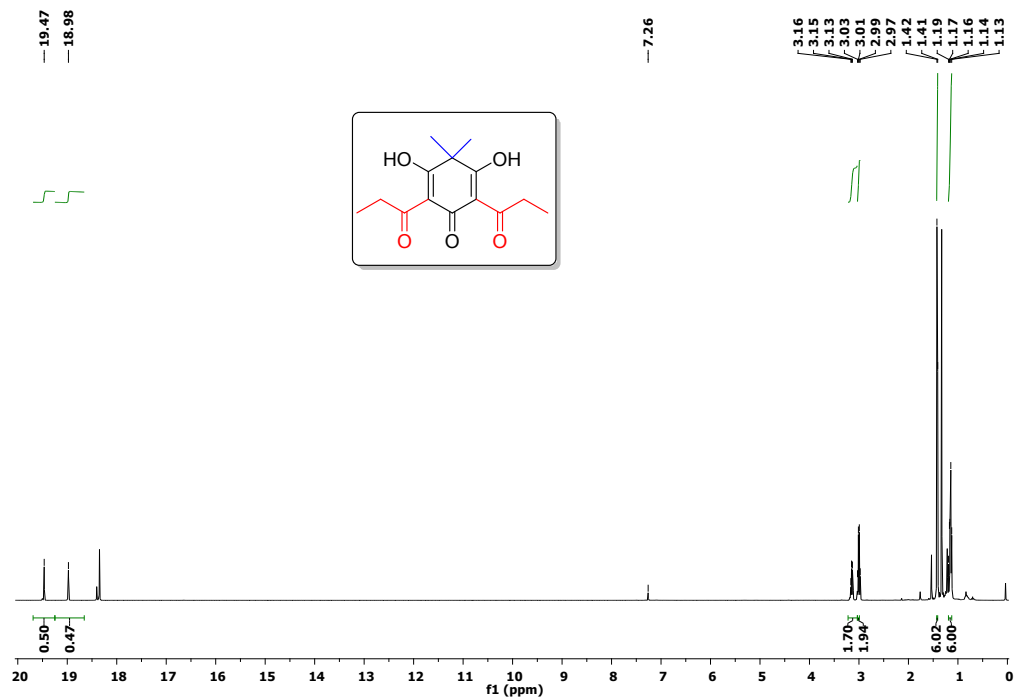


DEPT

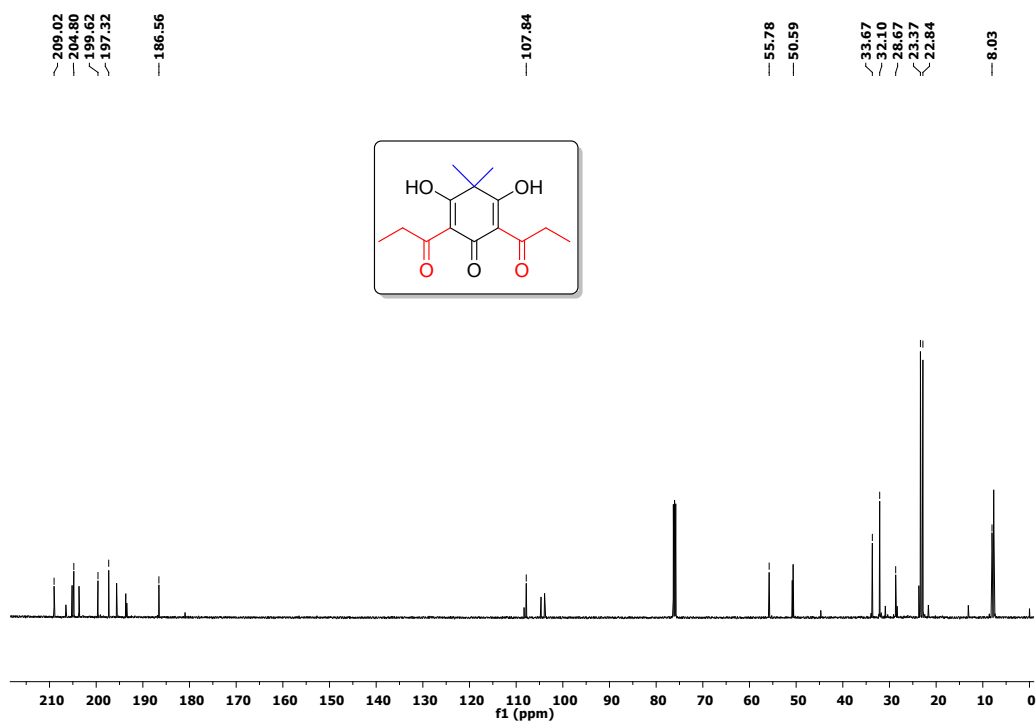


S1.u. ^1H , ^{13}C and DEPT-135 NMR spectrum of 3,5-dihydroxy-4,4-dimethyl-2,6-dipropionylcyclohexa-2,5-dienone (**5d**)

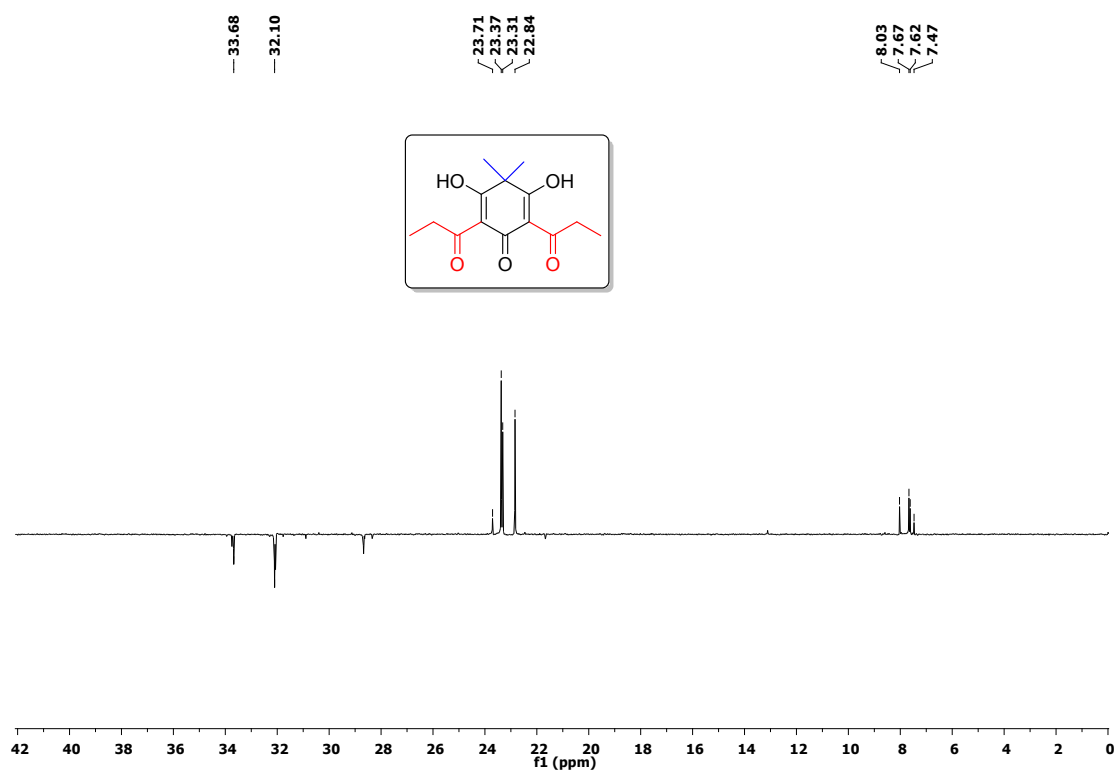
^1H NMR



^{13}C NMR

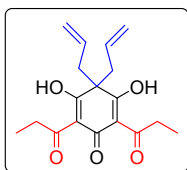
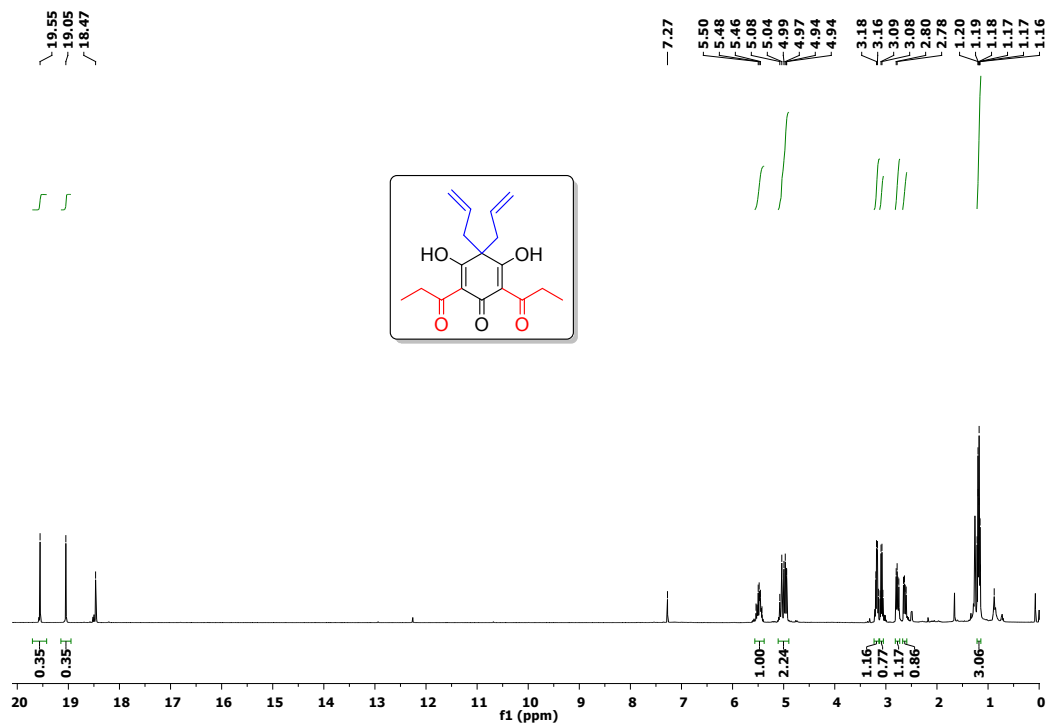


DEPT

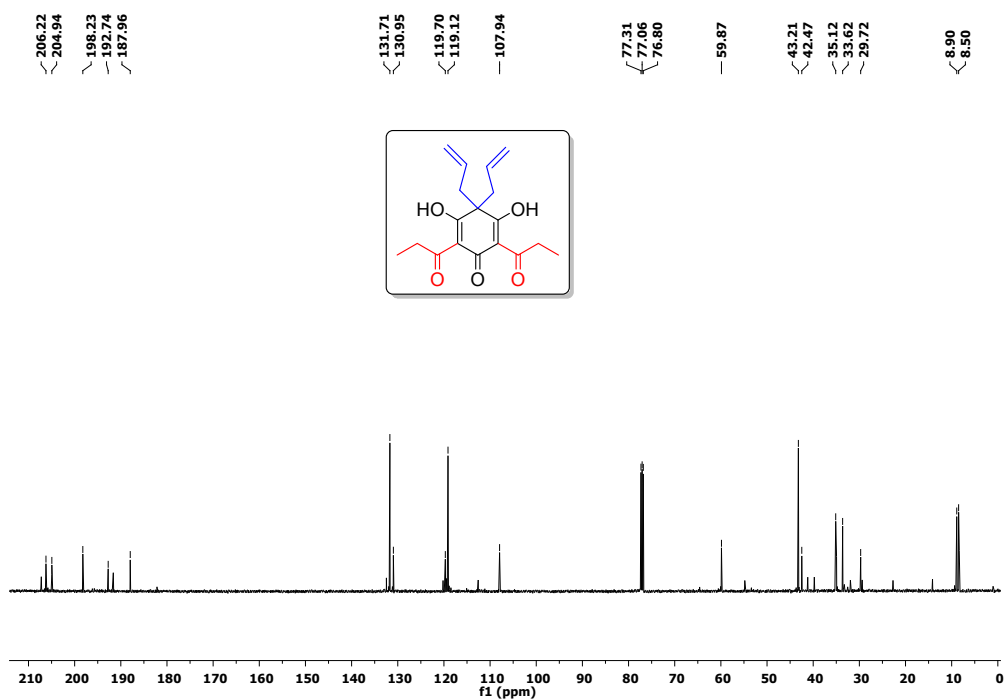


S1.v. ^1H , ^{13}C and DEPT-135 NMR spectrum of 4,4-diallyl-3,5-dihydroxy-2,6-dipropionylcyclohexa-2,5-dienone (**5e**)

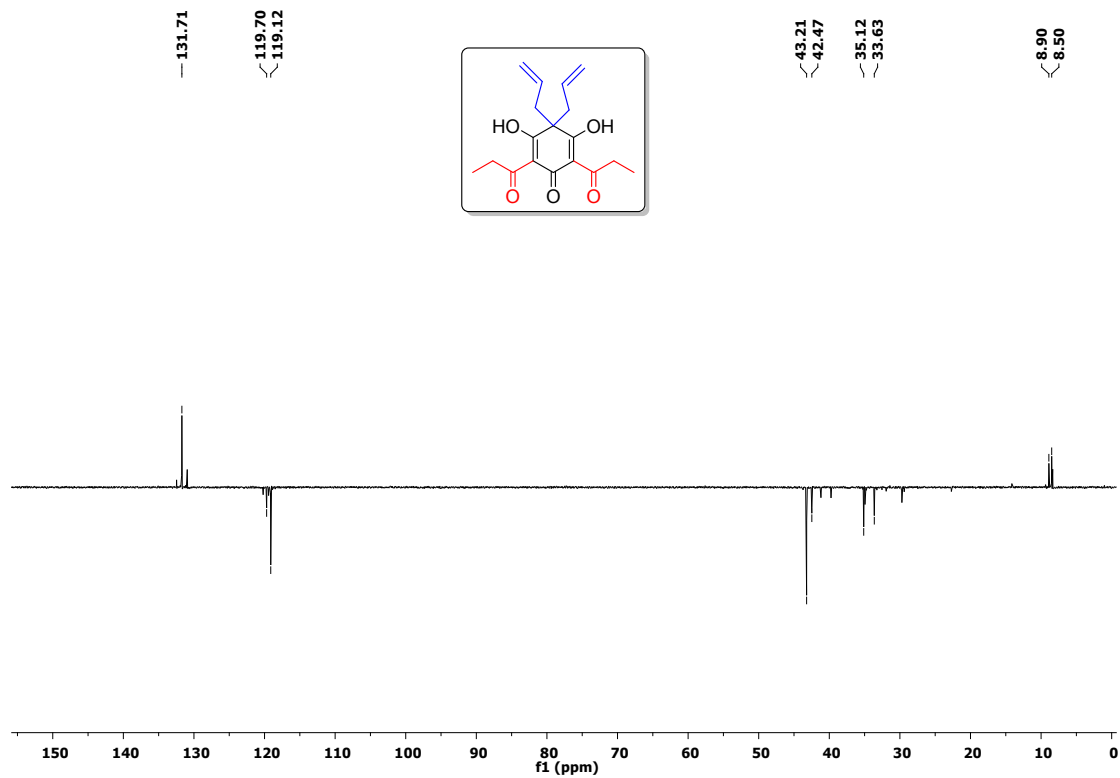
^1H NMR



^{13}C NMR

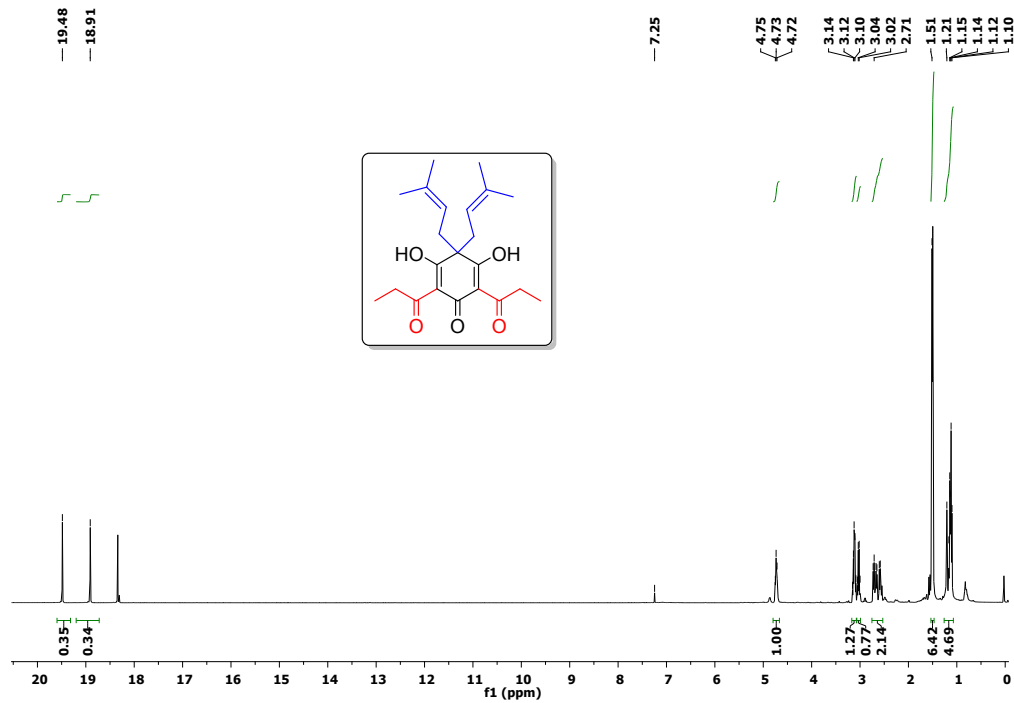


DEPT

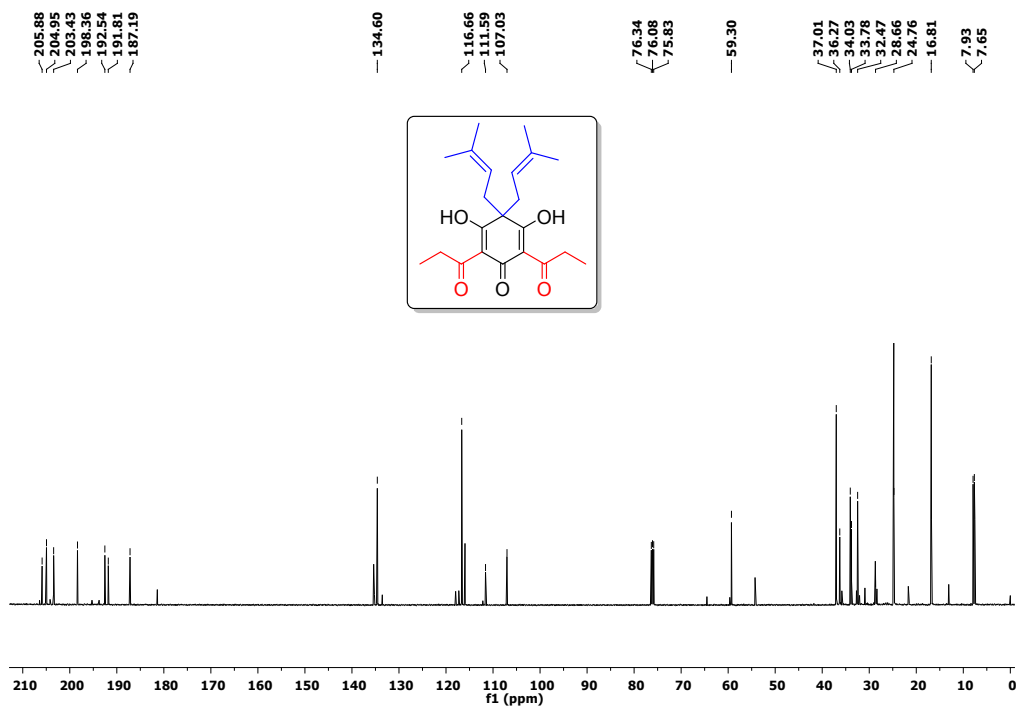


S1.w. ^1H , ^{13}C and DEPT-135 NMR spectrum of 3,5-dihydroxy-4,4-bis(3-methylbut-2-enyl)-2,6-dipropionylcyclohexa-2,5-dienone (**5f**)

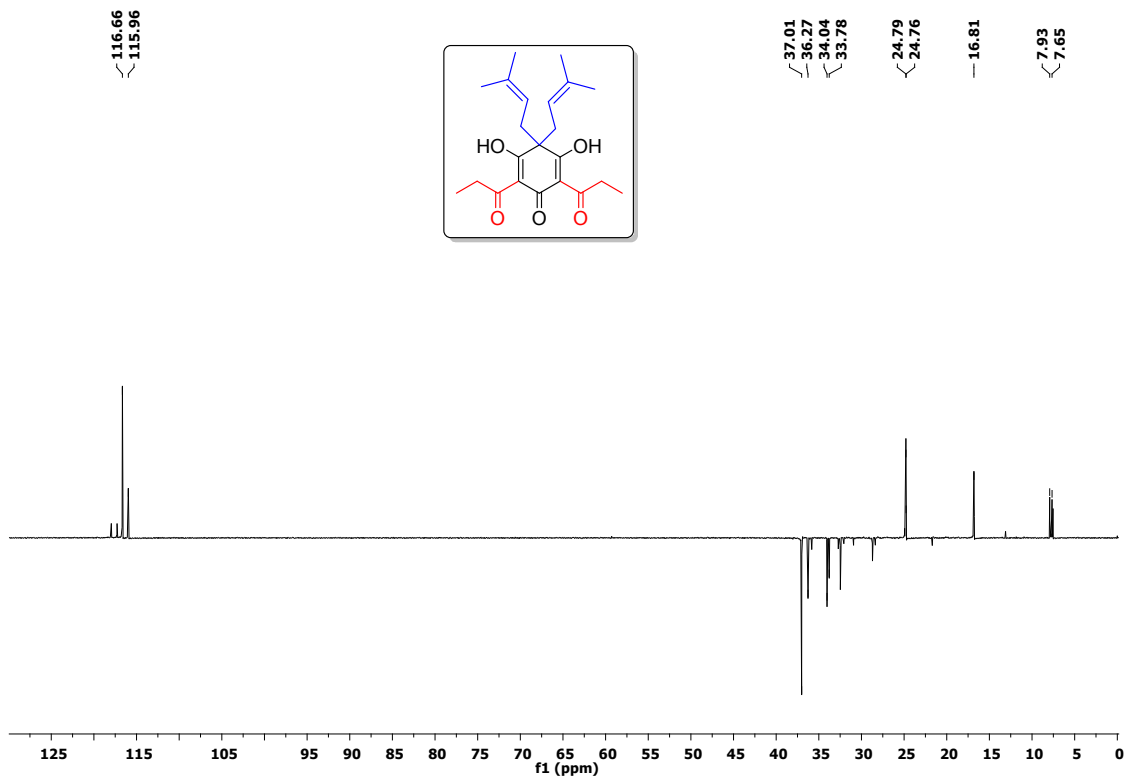
^1H NMR



^{13}C NMR

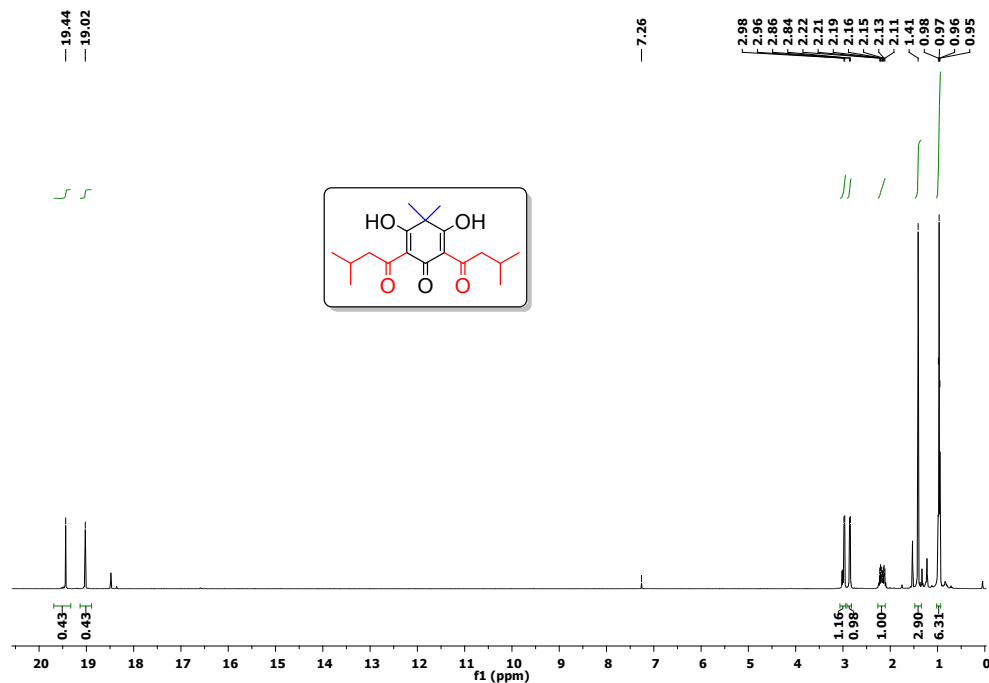


DEPT

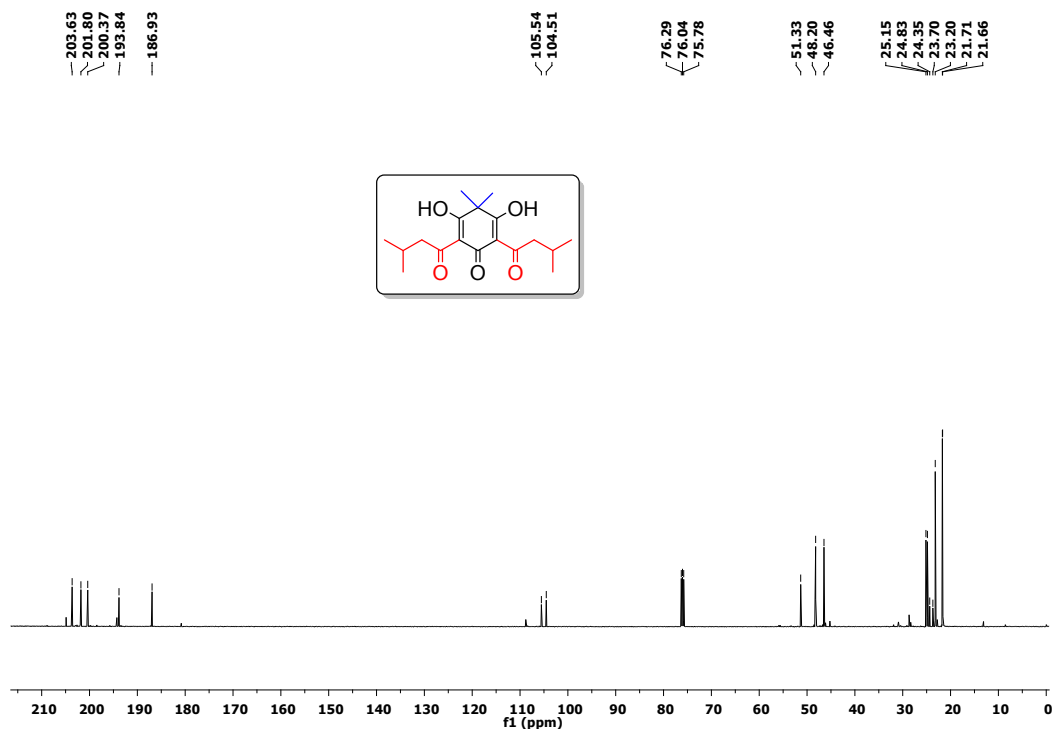


S1.x. ^1H , ^{13}C and DEPT-135 NMR spectrum of 1,1'-(4,6-dihydroxy-5,5-dimethyl-2-oxocyclohexa-3,6-diene-1,3-diyl) bis (3-methylbutan-1-one) (**5g**)

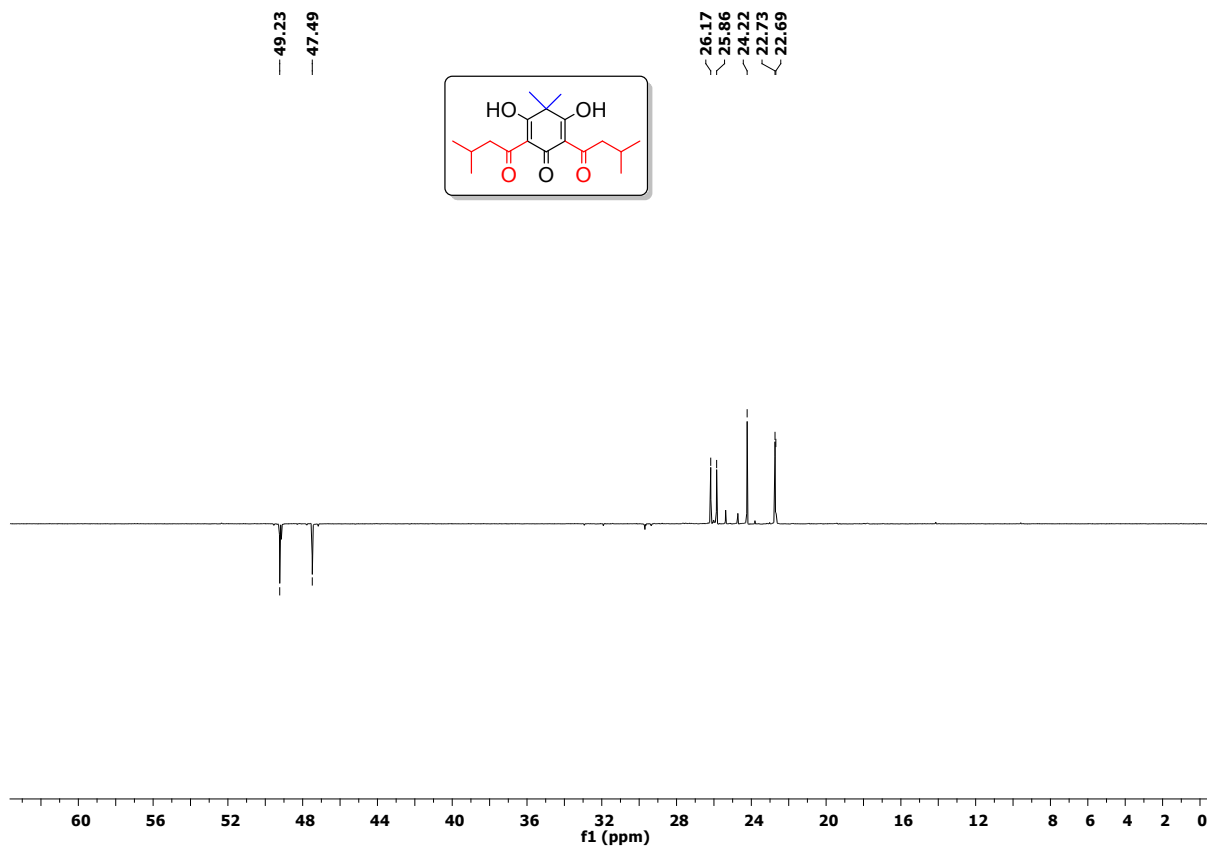
^1H NMR



^{13}C NMR

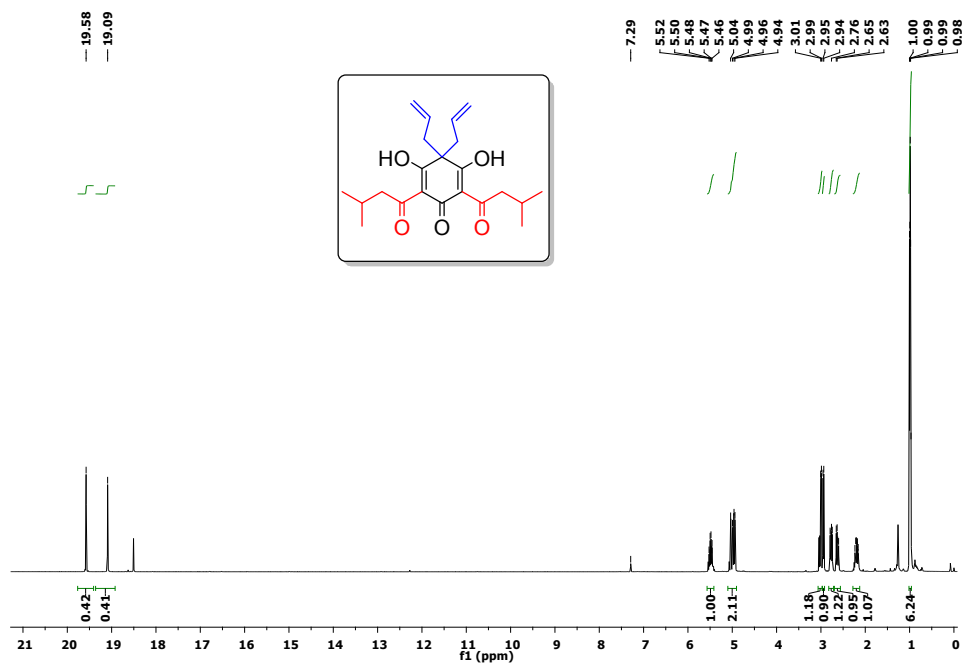


DEPT

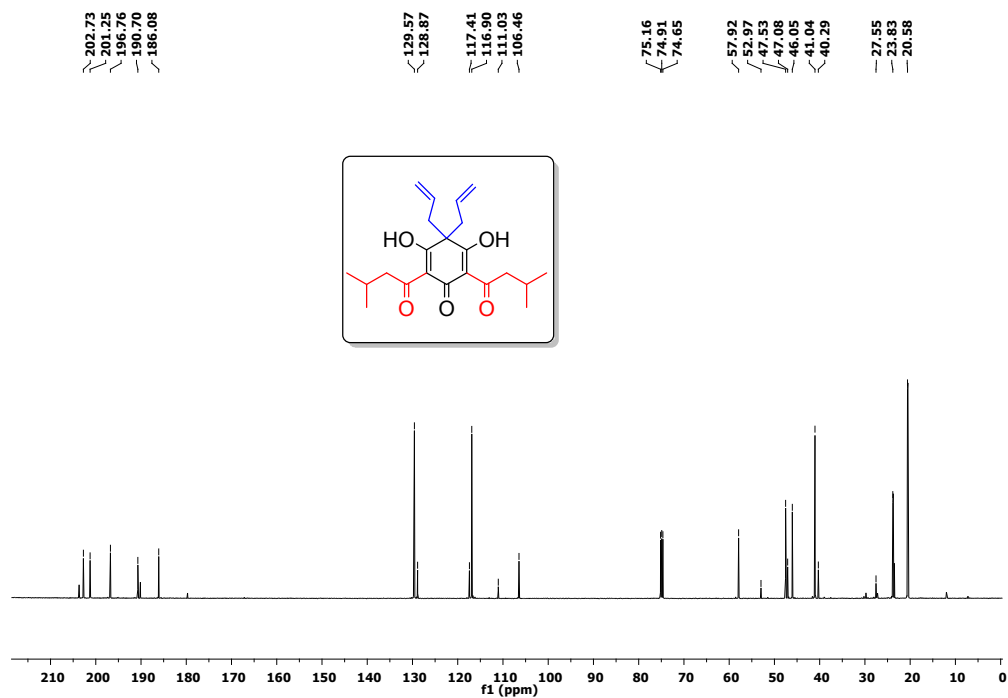


S1.y. ^1H , ^{13}C and DEPT-135 NMR spectrum of 2,6-bis(3-methylbutanoyl)-4,4-diallyl-3,5-dihydroxycyclohexa-2,5-dienone (**5h**)

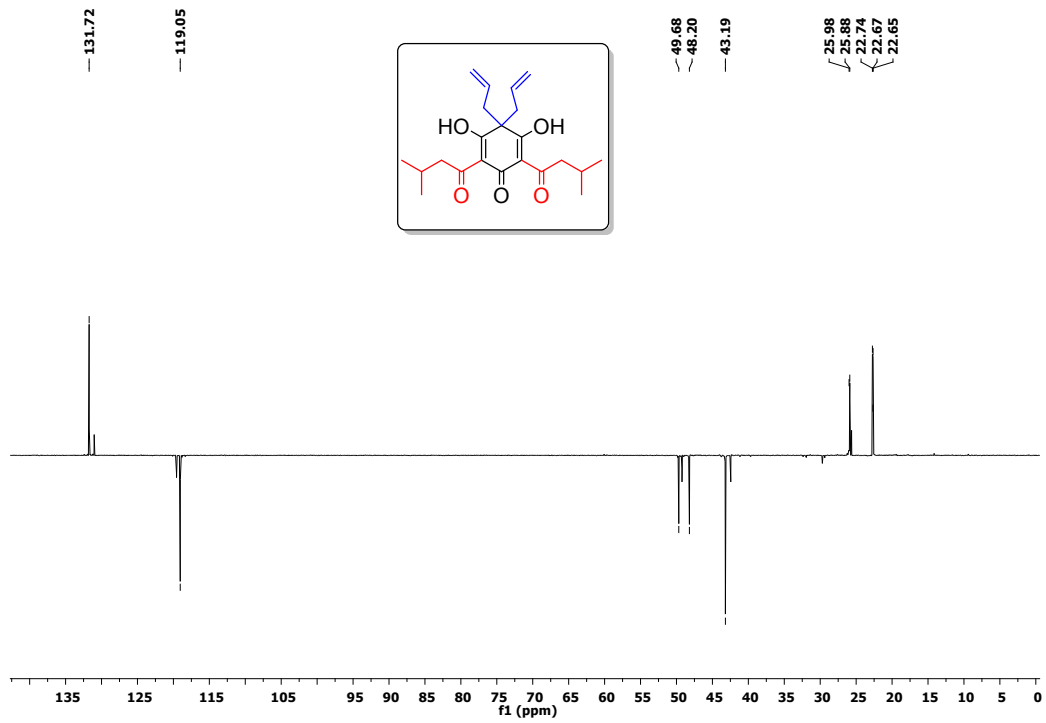
^1H NMR



^{13}C NMR

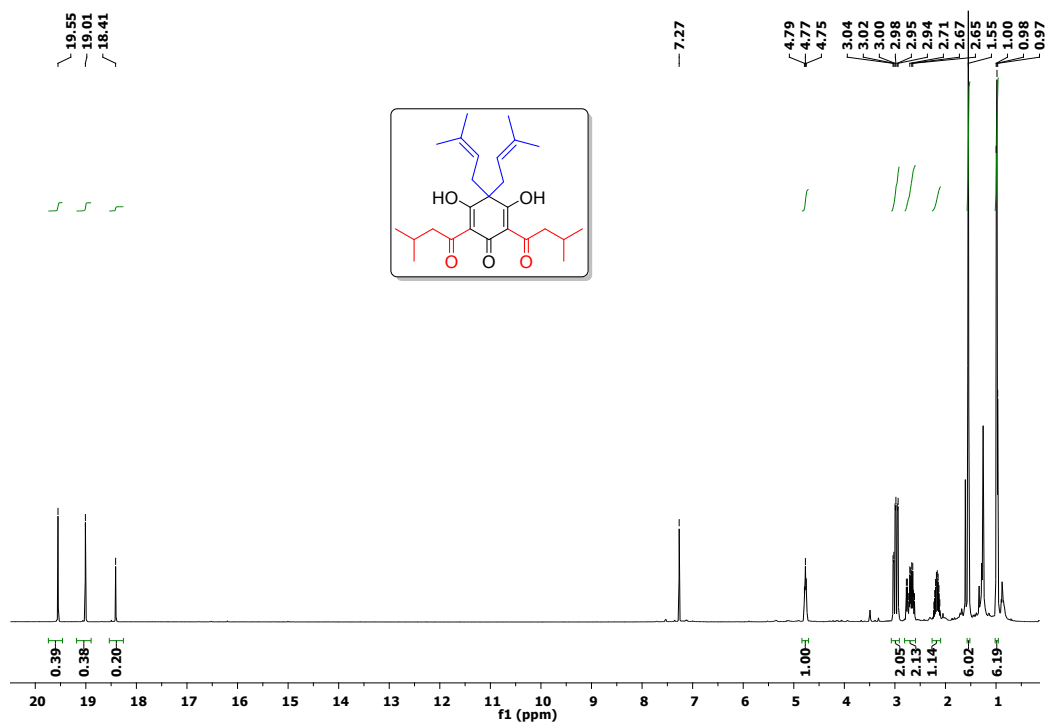


DEPT

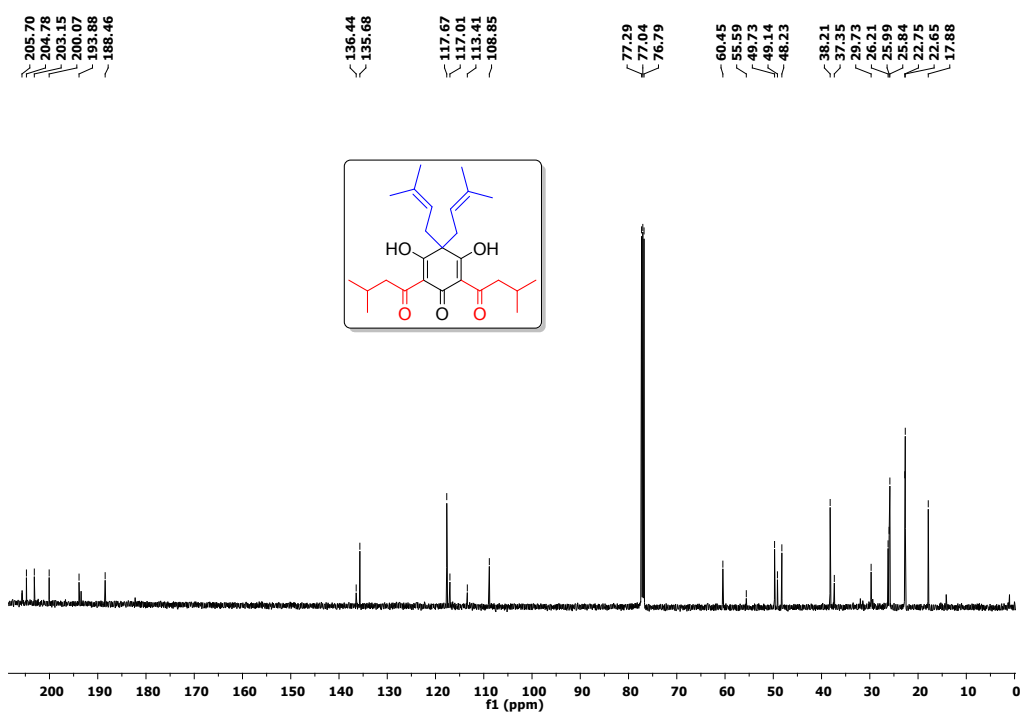


S1.z. ^1H , ^{13}C and DEPT-135 NMR spectrum of 2,6-bis(3-methylbutanoyl)-3,5-dihydroxy-4,4-bis(3-methylbut-2-enyl)cyclohexa-2,5-dienone (**5i**)

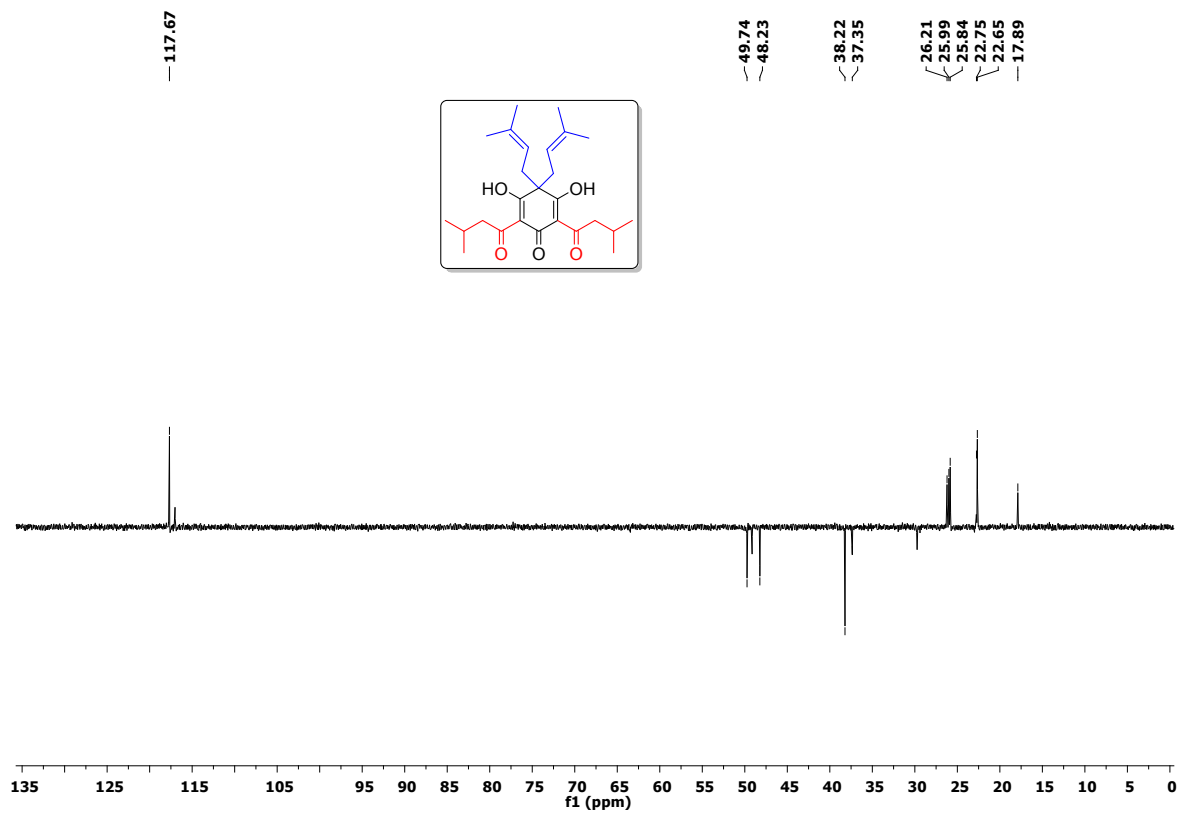
^1H NMR



^{13}C NMR

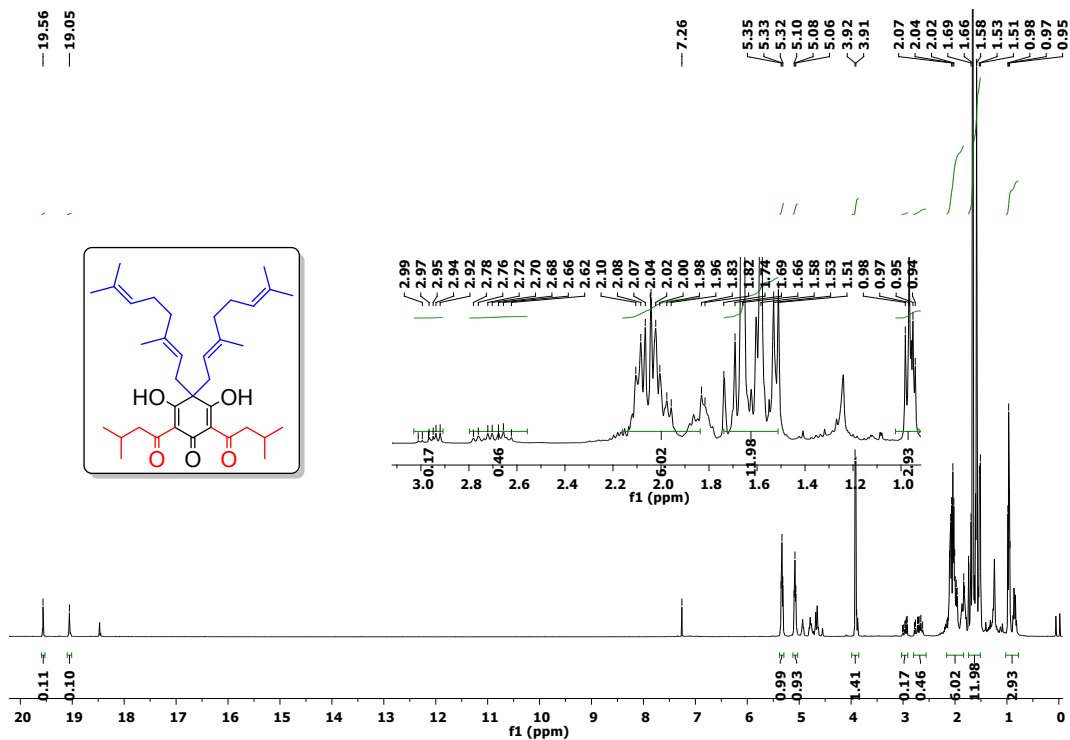


DEPT

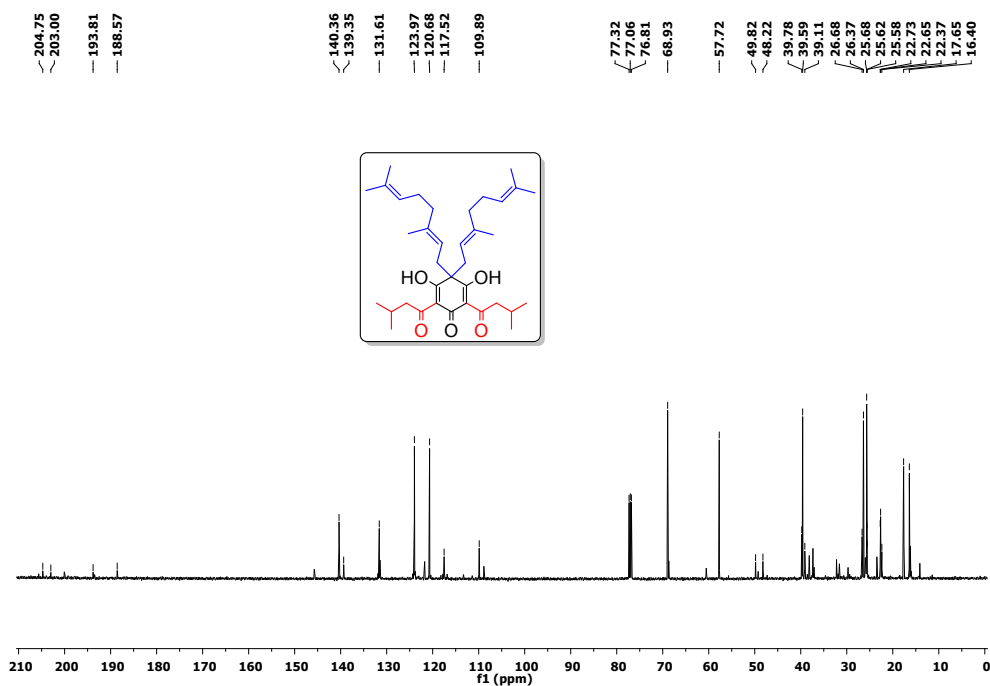


S2.a. ^1H , ^{13}C and DEPT-135 NMR spectrum of 2,6-bis(3-methylbutanoyl)-3,5-dihydroxy-4,4-bis((E)-3,7-dimethylocta-2,6-dienyl)cyclohexa-2,5-dienone (**5j**)

^1H NMR



^{13}C NMR



DEPT

123.97
123.83
120.67
117.52

57.72
49.82
48.22
39.78
39.59
38.15
37.35
26.67
26.37
25.68
22.72
22.64
17.65
16.40

