Supporting Information for:

Synthesis, Chiroptical and SHG Properties of Polarizable Push-Pull Dyes Built on π-Extended Binaphthyls

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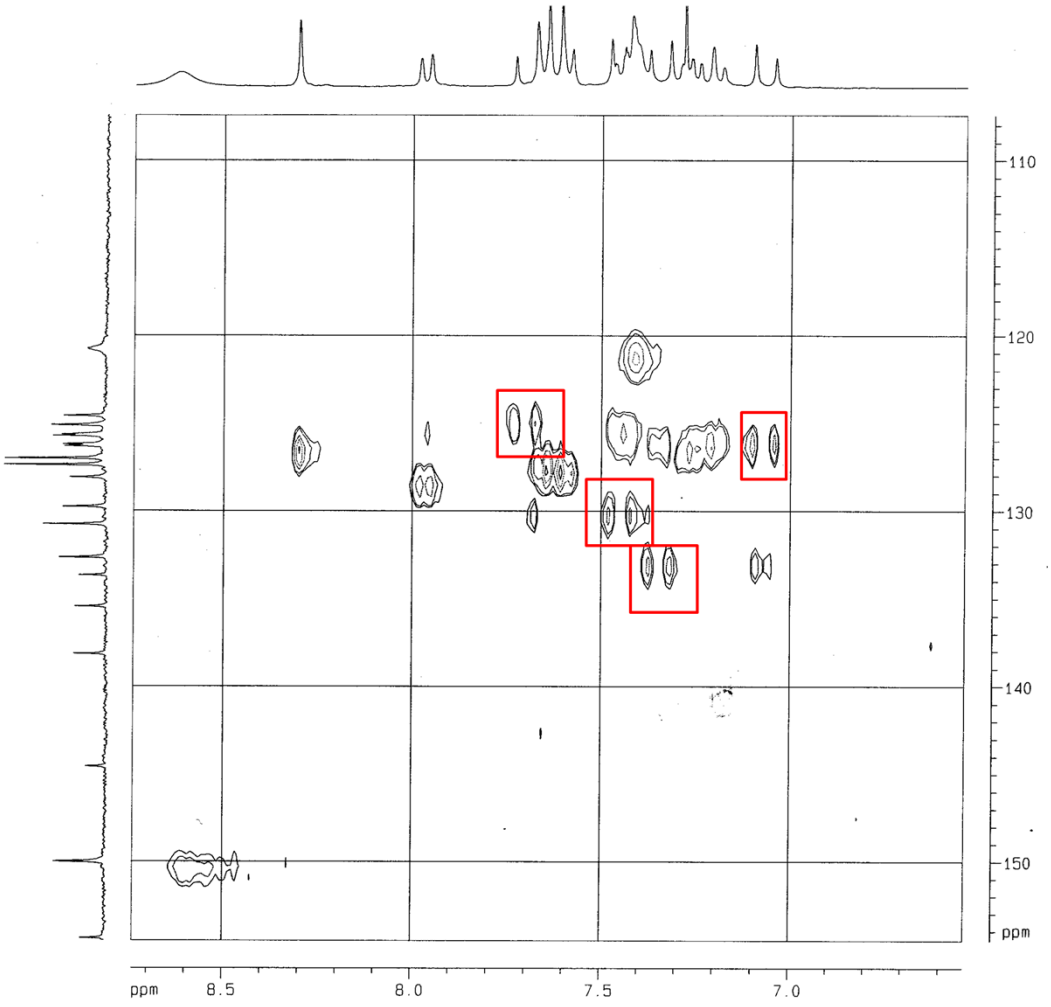


Figure S1. HETCOR 2D NMR experiment for compound (*R*)-**11** ($CDCl_3$, 300 MHz, 25 °C). Red boxes indicate the areas attributable to the four vinyl proton resonances.

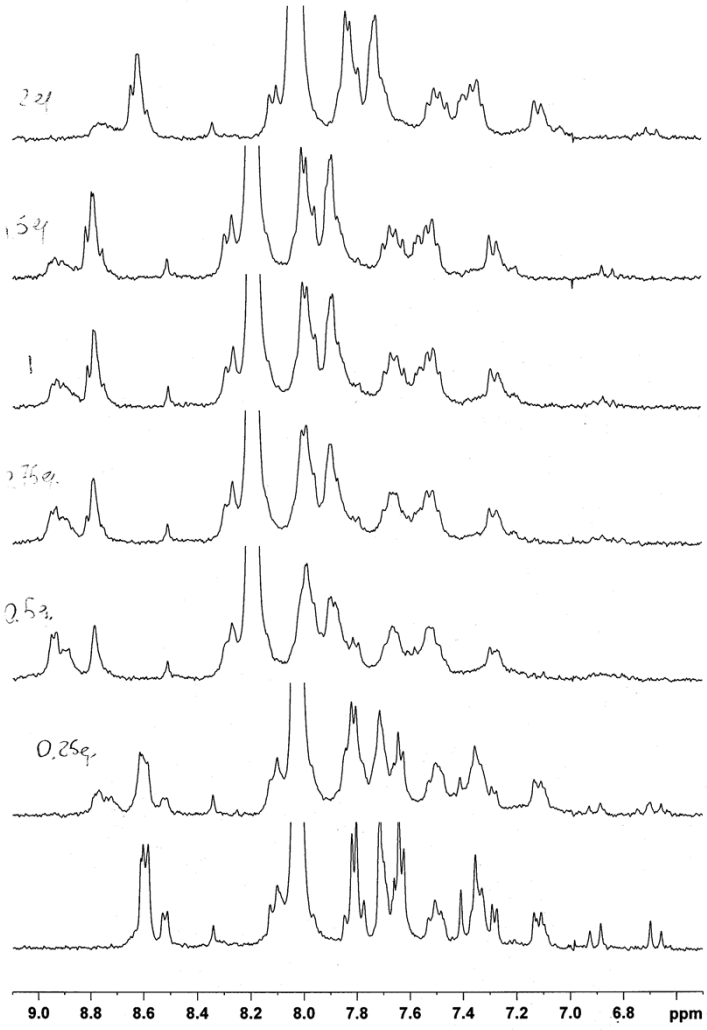


Figure S2. Titration of (*R*)-**11** with $Pd(MeCN)_2Cl_2$ (d_7-DMF, 300 MHz, 25 °C).

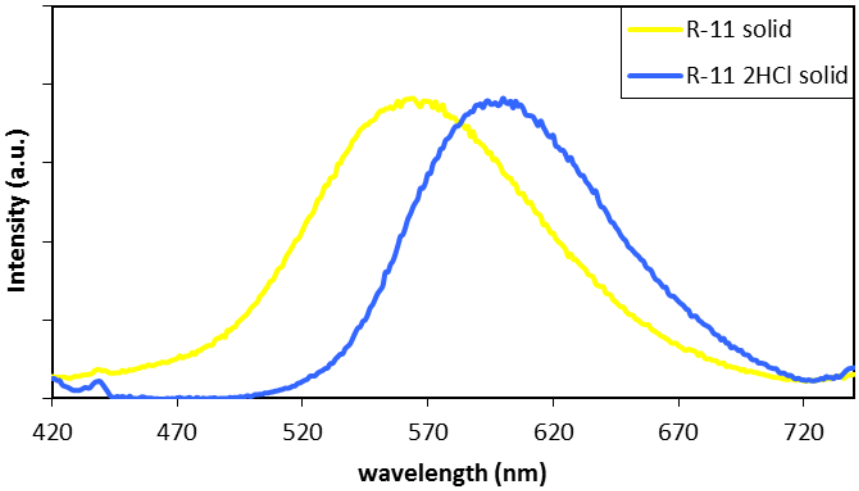


Figure S3. Normalized emission spectra of powders of **11** and **11.**2HCl.

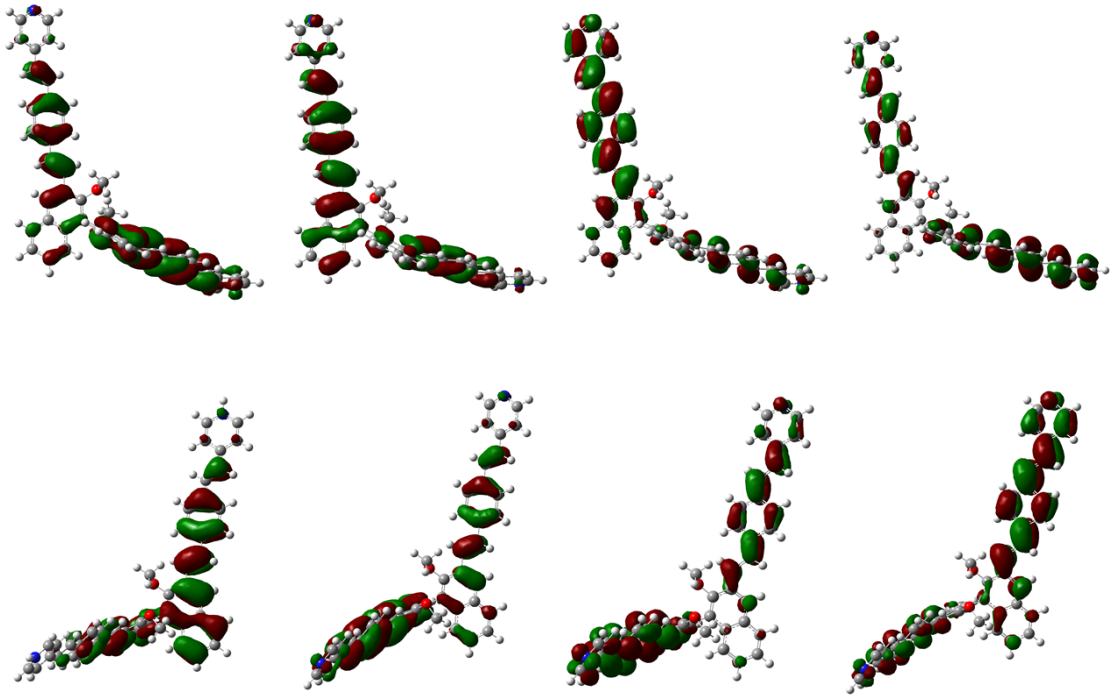


Fig. S4. Plots of the *ω*B97X/6-311++G** HOMO-1, HOMO, LUMO and LUMO+1 orbitals (from left to right) of compound **11** in $CHCl_3$, projected on the plane of one naphthalene arm (above) and on the plane of the other naphthalene arm (below). Isosurfaces value 0.02.

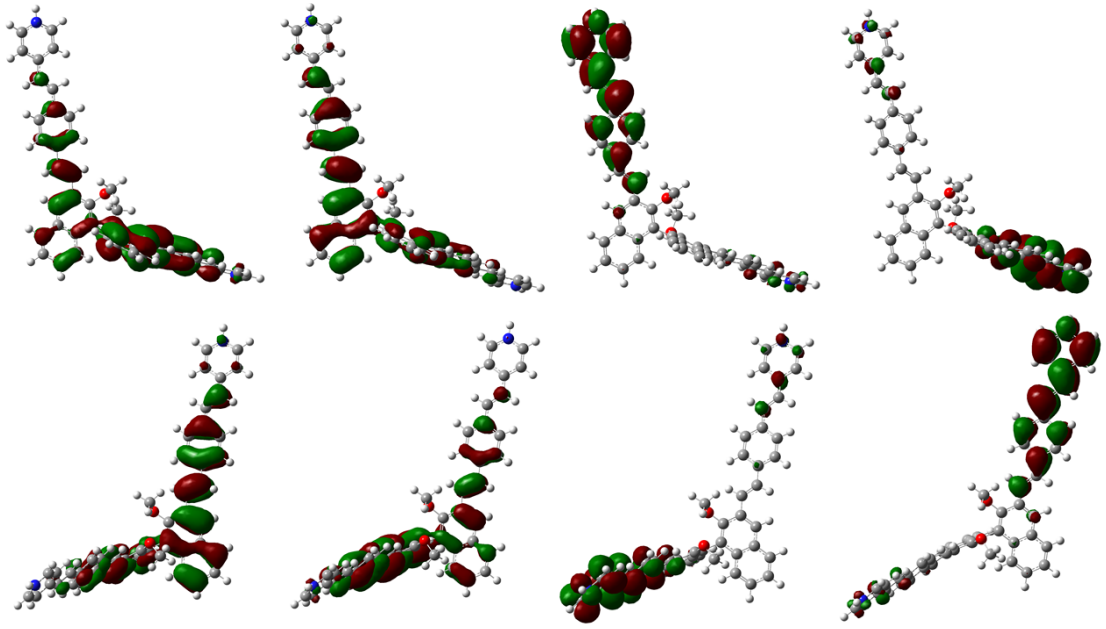
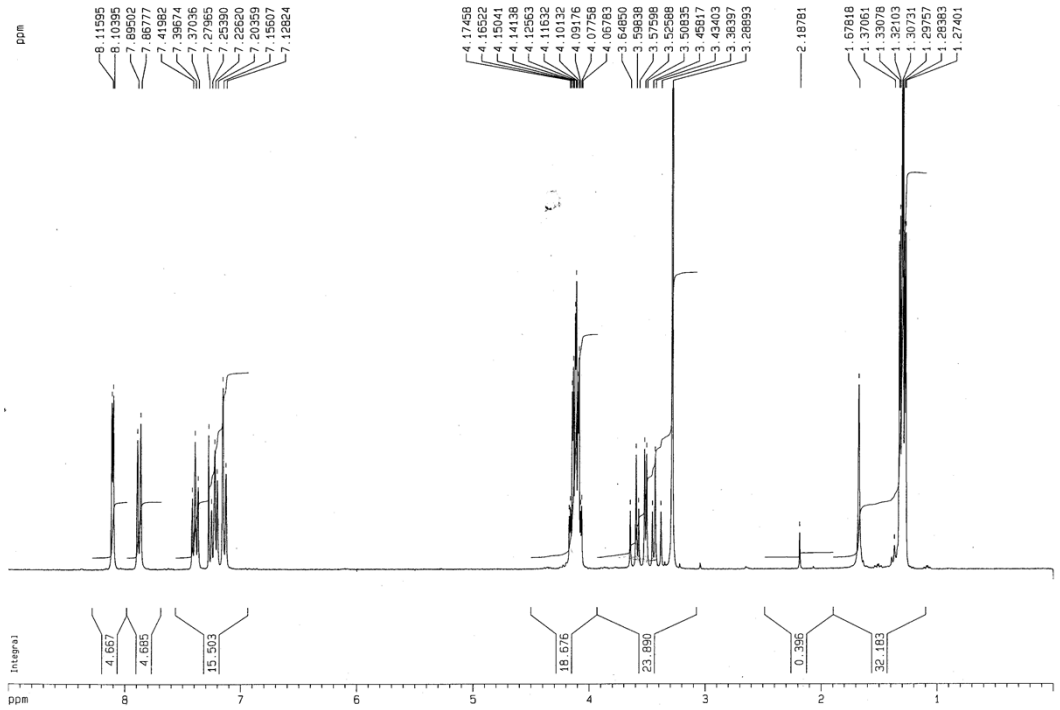
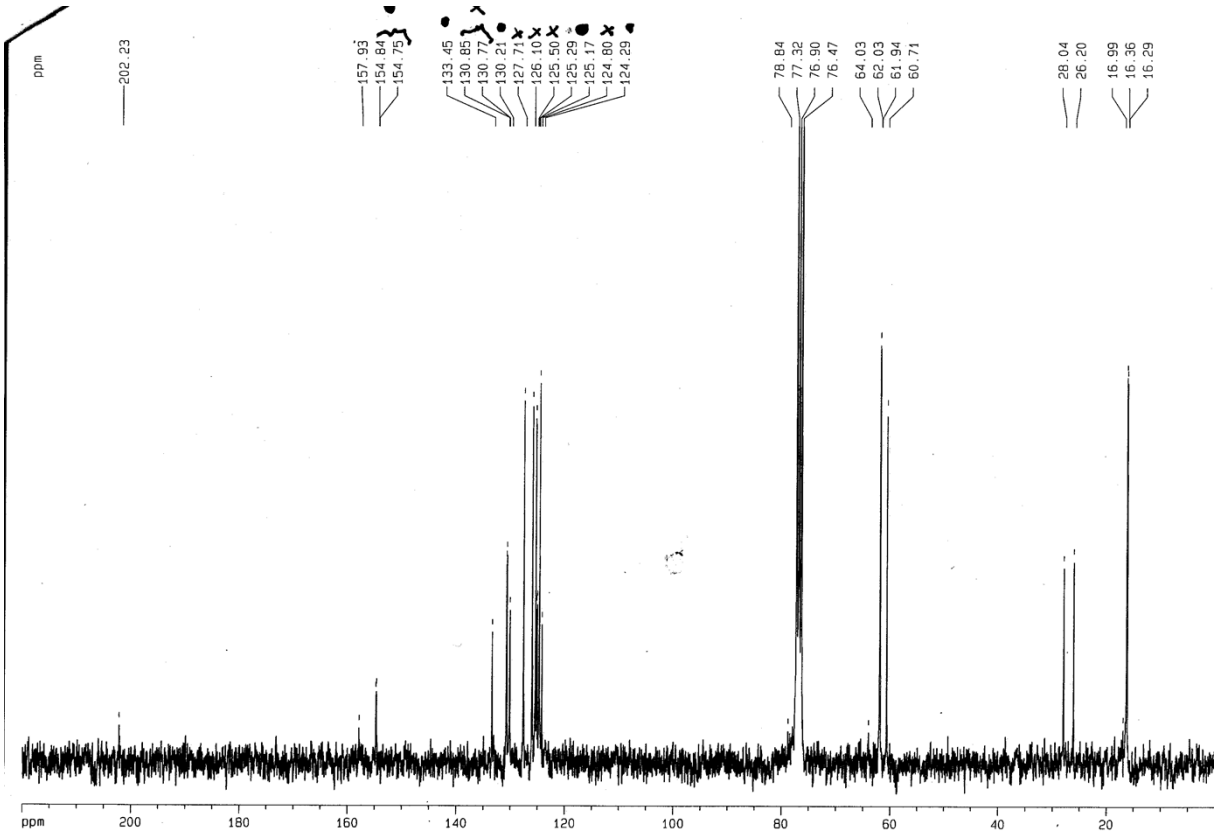


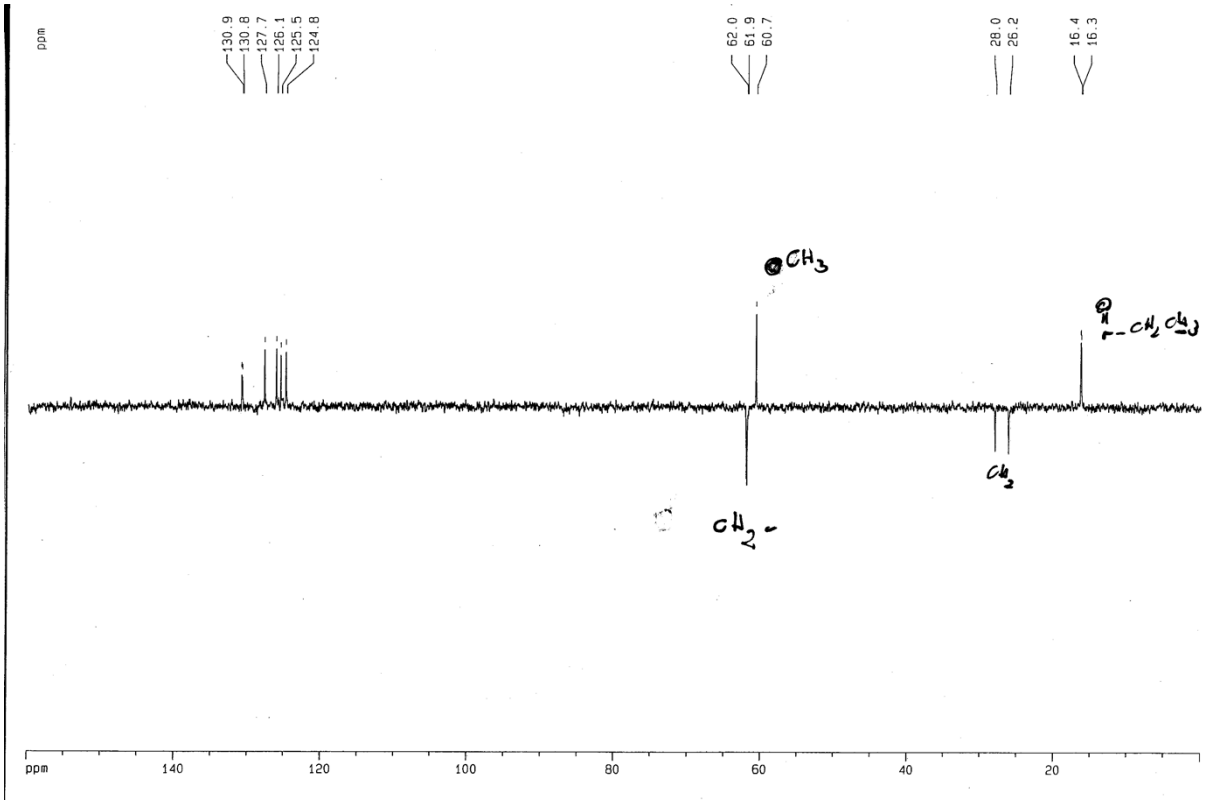
Fig. S5. Plots of the *ω*B97X/6-311++G** HOMO-1, HOMO, LUMO and LUMO+1 orbitals (from left to right) of compound **11** doubly protonated in $CHCl_3$, projected on the plane of one naphthalene arm (above) and on the plane of the other naphthalene arm (below). Isosurfaces value 0.02.

Copies of ^{1}H NMR, ^{13}C NMR and Mass Spectra for new compounds

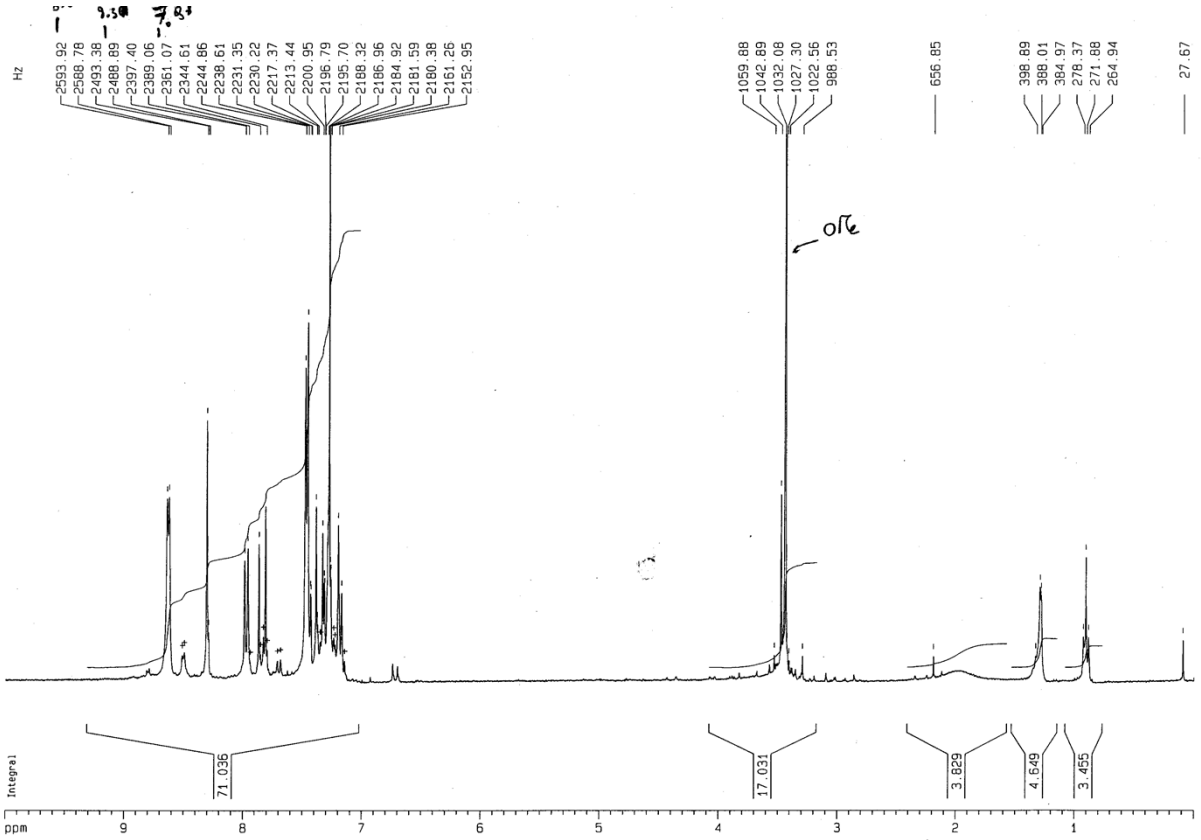
Compound **3**.

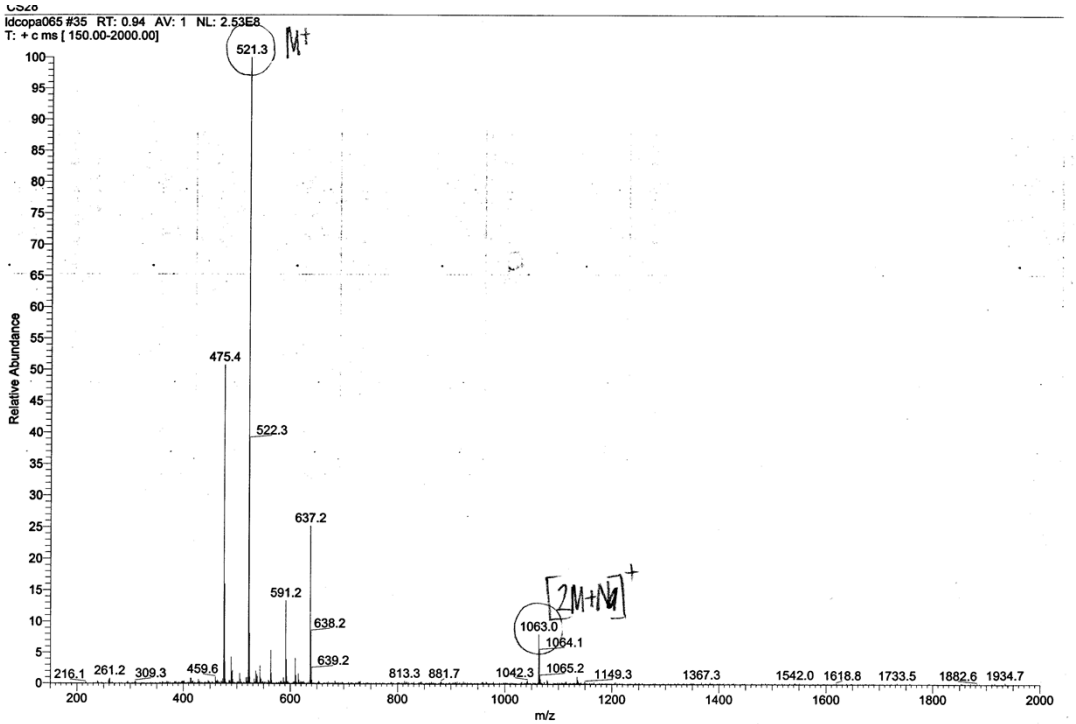




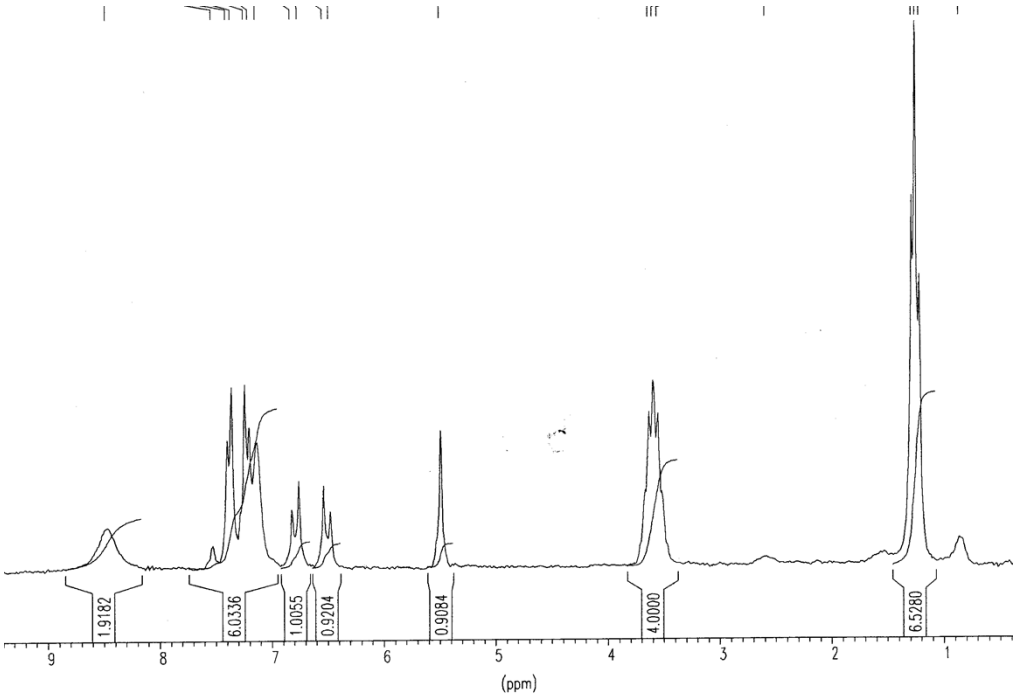

ppm
130.9
130.8
127.7
126.1
125.5
124.8
62.0
61.9
60.7
28.0
26.2
16.4
16.3
CH3
CH2
CH2
CH3
ppm
140
120
100
80
60
40
20

Compound **7**.

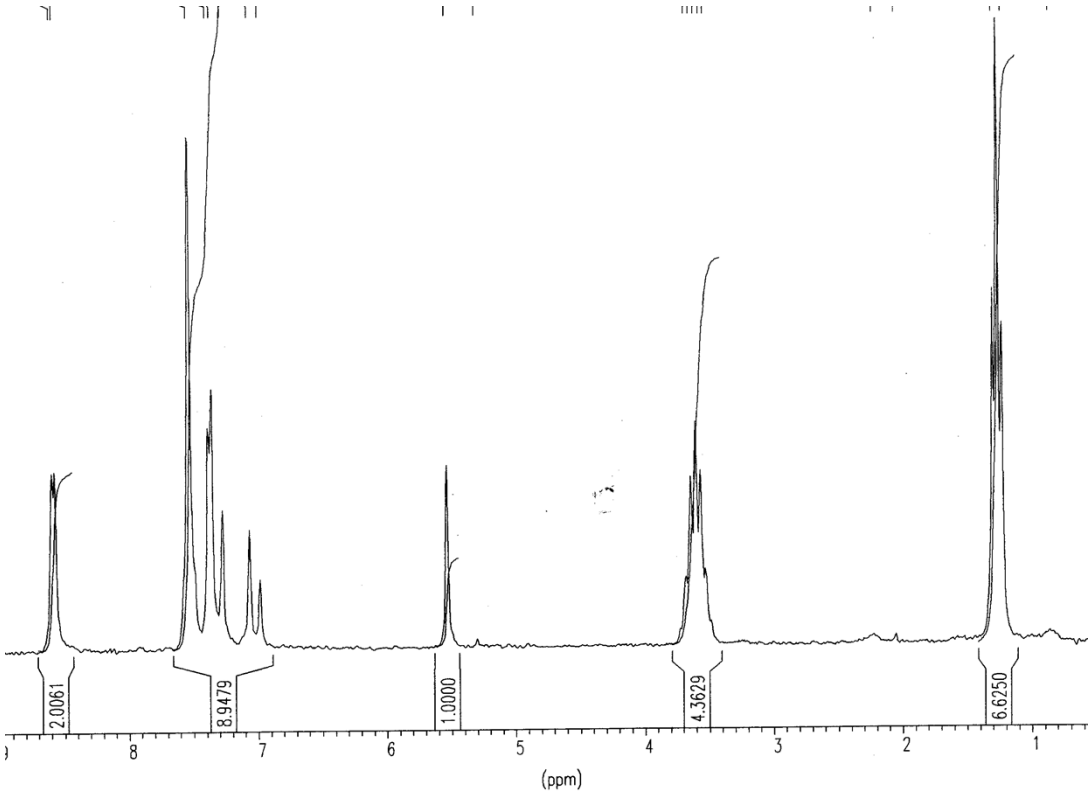

Hz
2593.92
2568.78
2493.38
2488.69
2397.40
2389.06
2361.07
2344.61
2244.86
2238.61
2231.35
2230.22
2217.37
2213.44
2200.95
2196.79
2195.70
2188.32
2186.96
2184.92
2181.59
2180.38
2161.26
2152.95
1059.88
1042.89
1032.08
1027.30
1022.56
988.53
656.85
398.89
388.01
384.97
278.37
271.88
264.94
27.67
Integral
71.036
17.031
3.829
4.649
3.455
ppm
9
8
7
6
5
4
3
2
1


Idcopa065 #35 RT: 0.94 AV: 1 NL: 2.53E8
T: + c ms [150.00-2000.00]
Relative Abundance
m/z
521.3
475.4
522.3
637.2
591.2
638.2
639.2
1063.0
1064.1
1065.2
216.1
261.2
309.3
459.6
813.3
881.7
1042.3
1149.3
1367.3
1542.0
1618.8
1733.5
1882.6
1934.7

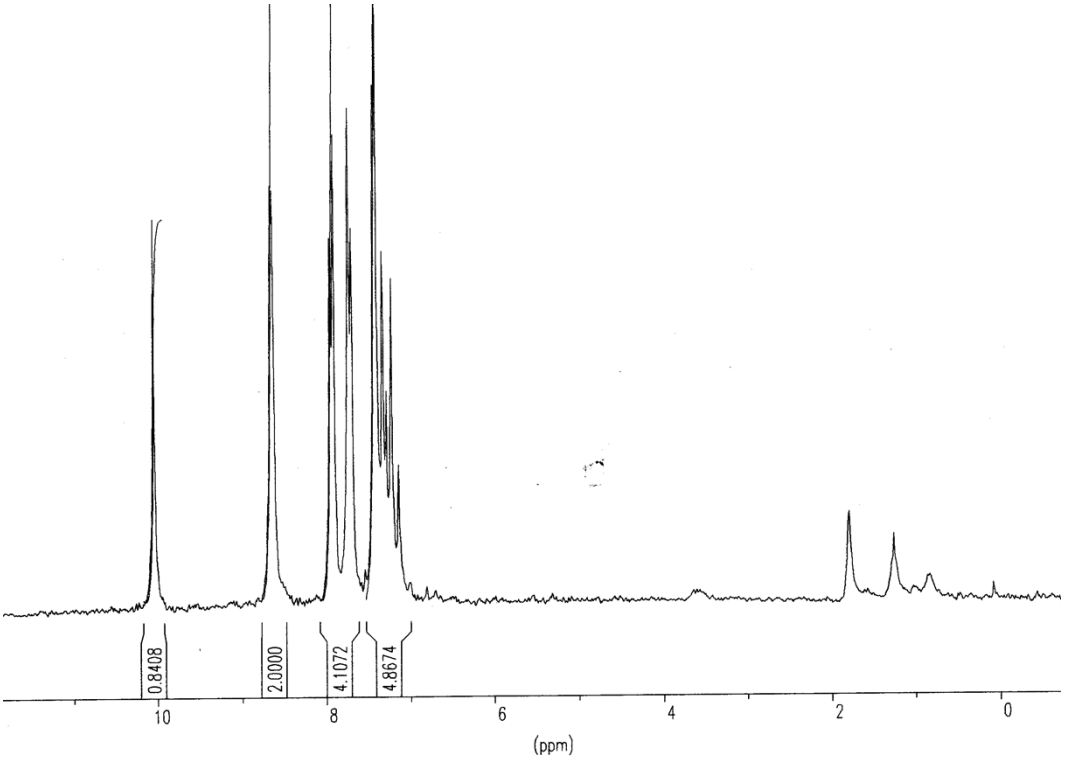
Compound *cis* **9**.



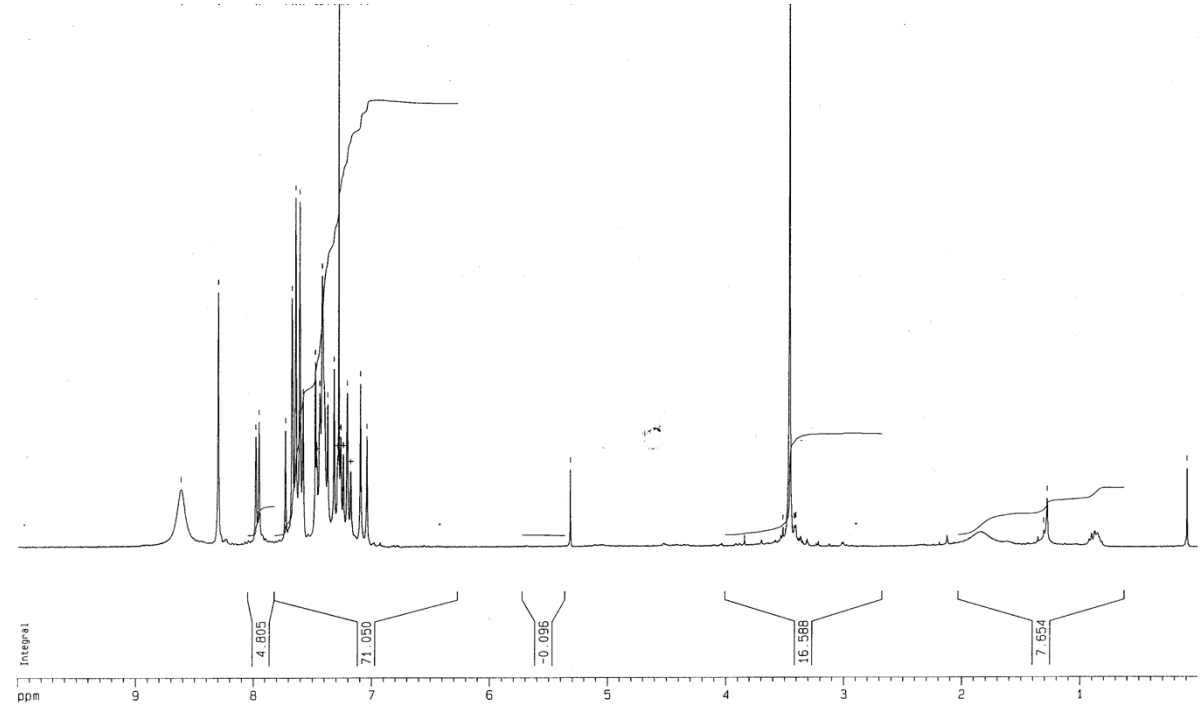
Compound *trans* **9**.



Compound **10**.



Compound **11**.


Integral
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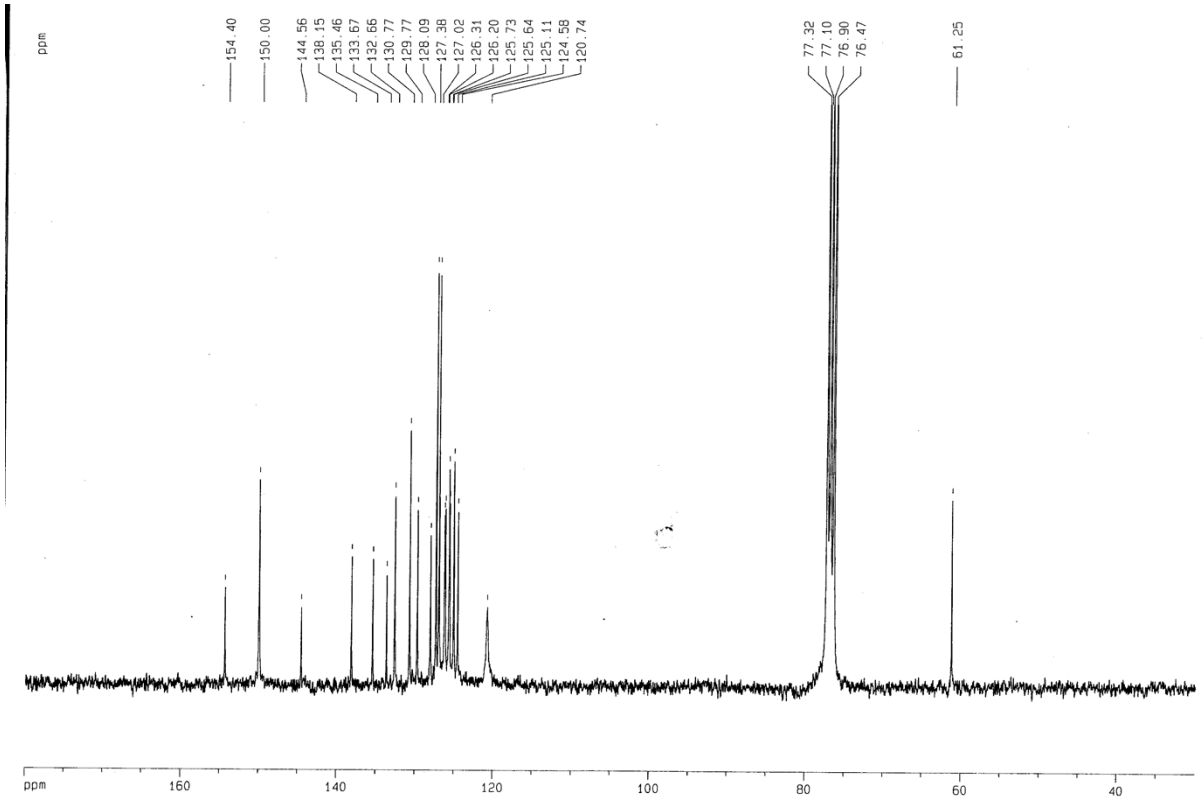
-0.096
16.588
7.654
ppm
9
8
7
6
5
4
3
2
1


ppm
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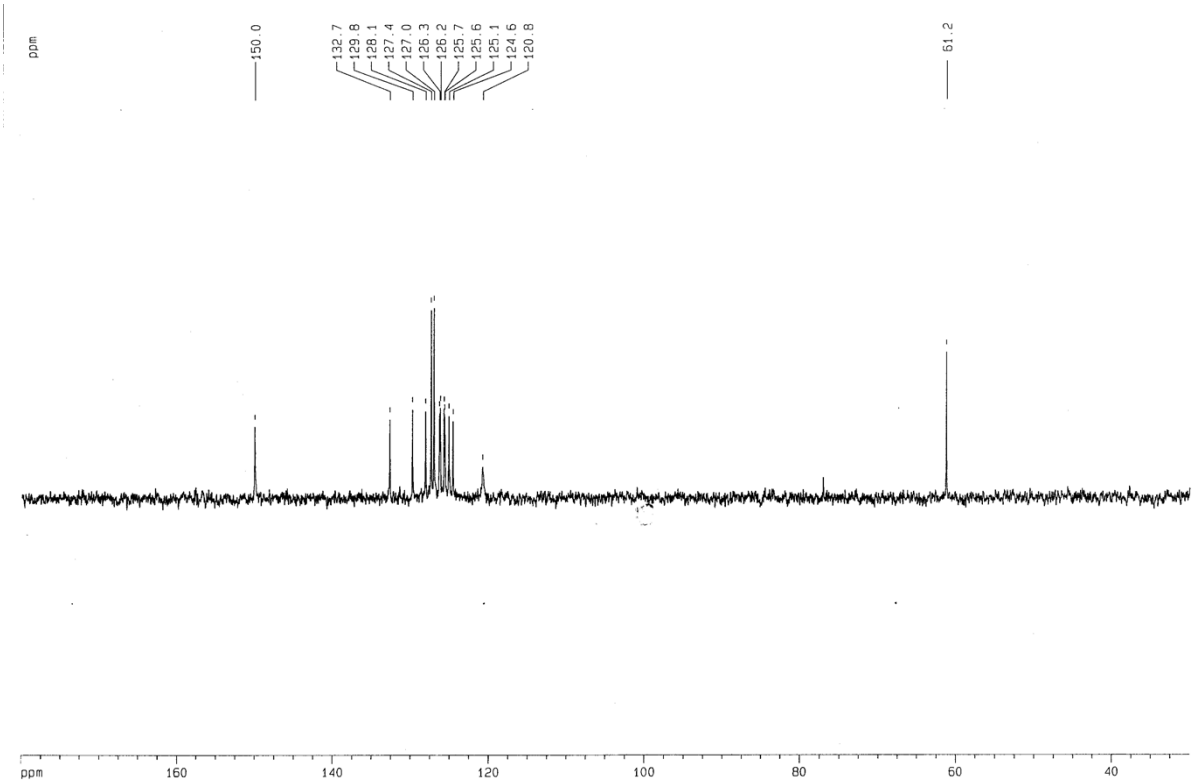
150.00
144.56
138.15
135.46
133.67
132.66
130.77
129.77
128.09
127.38
127.02
126.31
126.20
125.73
125.64
125.11
124.58
120.74
77.32
77.10
76.90
76.47
61.25
ppm
160
140
120
100
80
60
40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132.7
129.8
128.1
127.4
127.0
126.3
126.2
125.7
125.6
125.1
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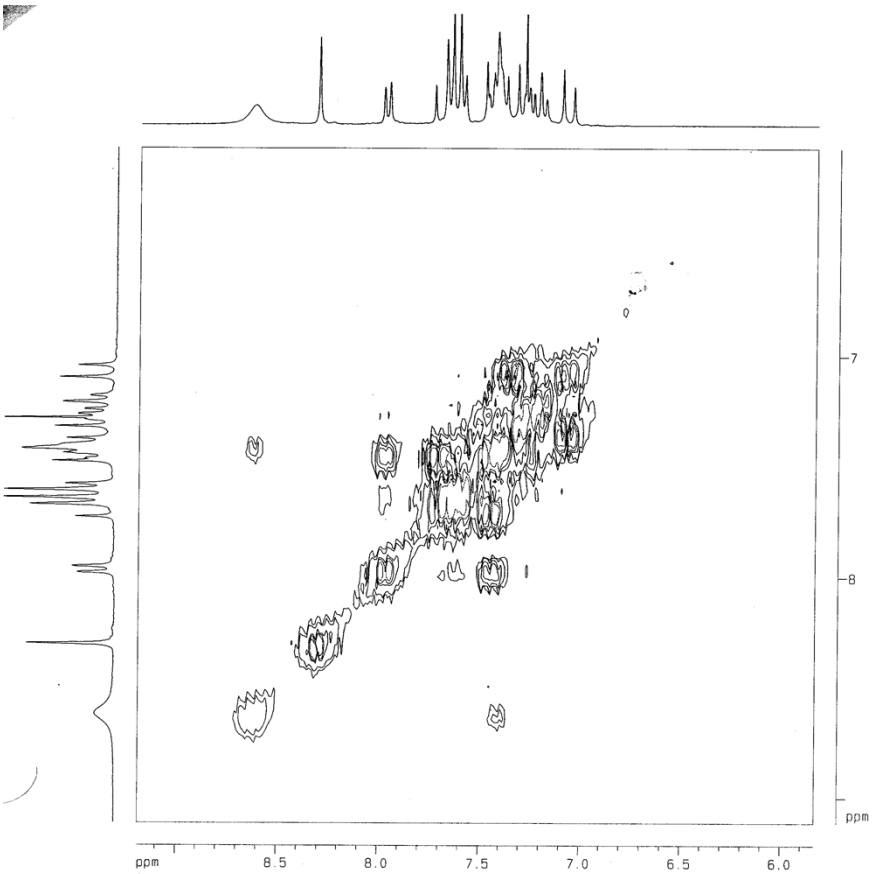
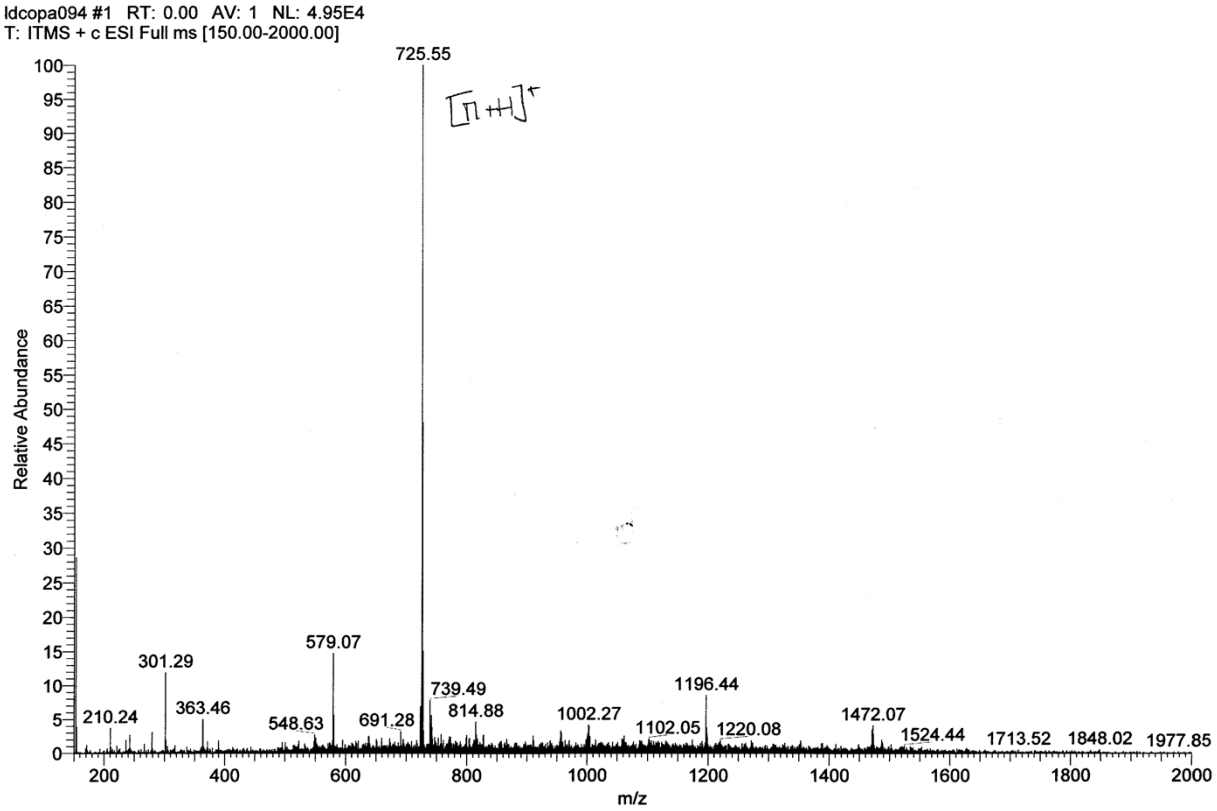
61.2
ppm
160
140
120
100
80
60
40


7
8
ppm
ppm
8.5
8.0
7.5
7.0
6.5
6.0


ldcopa094 #1 RT: 0.00 AV: 1 NL: 4.95E4
T: ITMS + c ESI Full ms [150.00-2000.00]
725.55
[M+H]+
Relative Abundance
m/z
579.07
301.29
739.49
1196.44
363.46
814.88
210.24
548.63
691.28
1002.27
1102.05
1220.08
1472.07
1524.44
1713.52
1848.02
1977.85