SUPPORTING INFORMATIONS

Tristhienylphenylamine – extended dithiafulvene hybrids as bifunctionnal electroactive species

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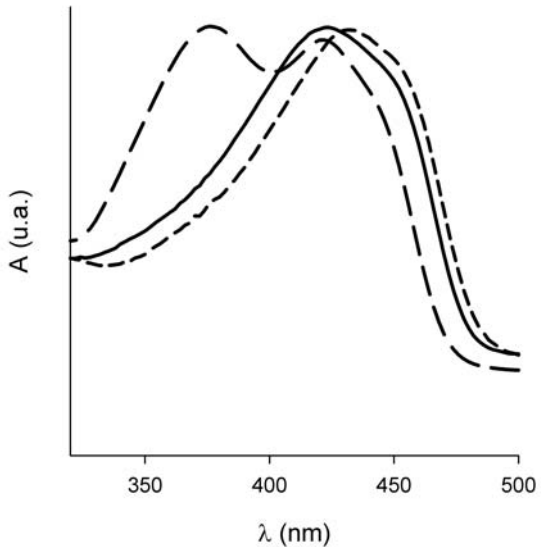


Figure S1. UV Vis. spectra of compounds **1** (dotted line), **2** (line) and **3** (short dashes), 10^{-5}M in CH_2Cl_2.

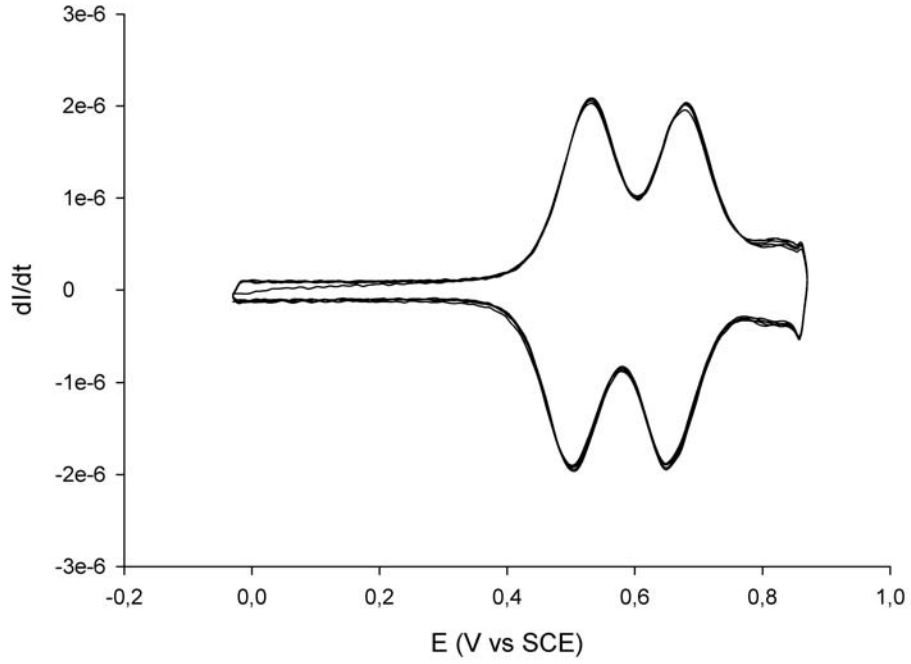


Figure S2. Deconvoluated CV of **1**, CH_2Cl_2 $TBAPF_6$ 0.1M 100mV/s

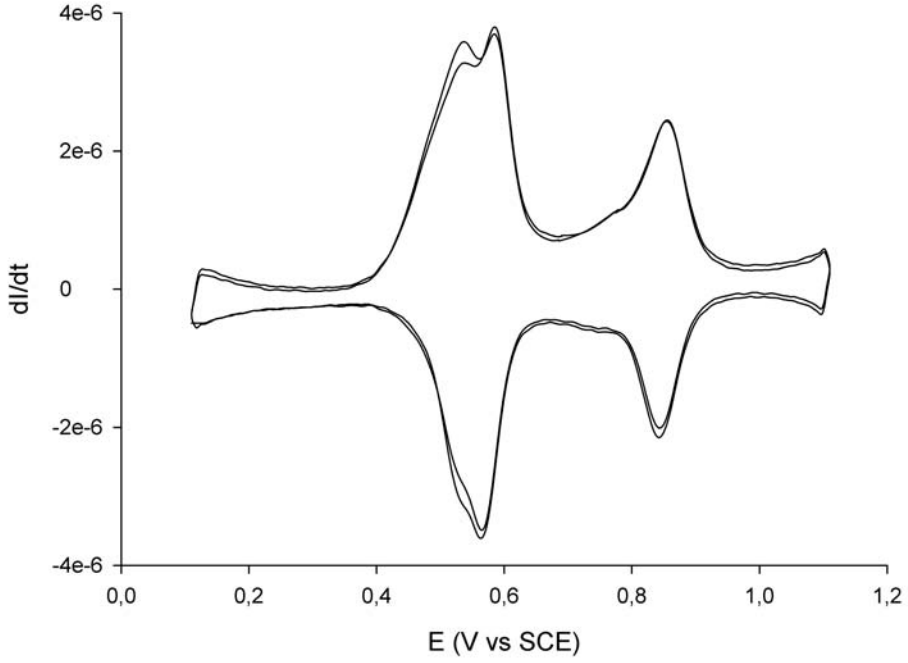


Figure S3. Deconvoluated CV of **2**, CH_2Cl_2 $TBAPF_6$ 0.1M 100mV/s

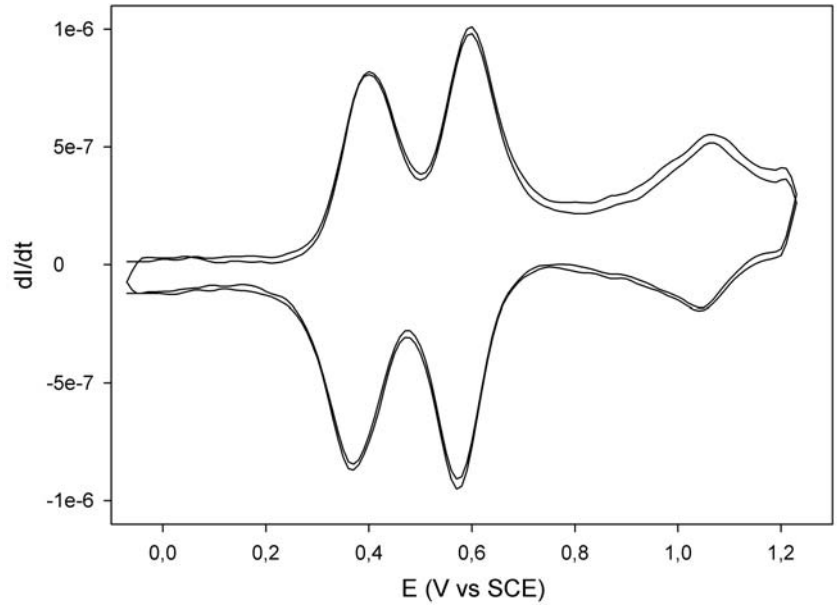


Figure S4. Deconvoluated CV of **8**, CH_2Cl_2 $TBAPF_6$ 0.1M 100mV/s

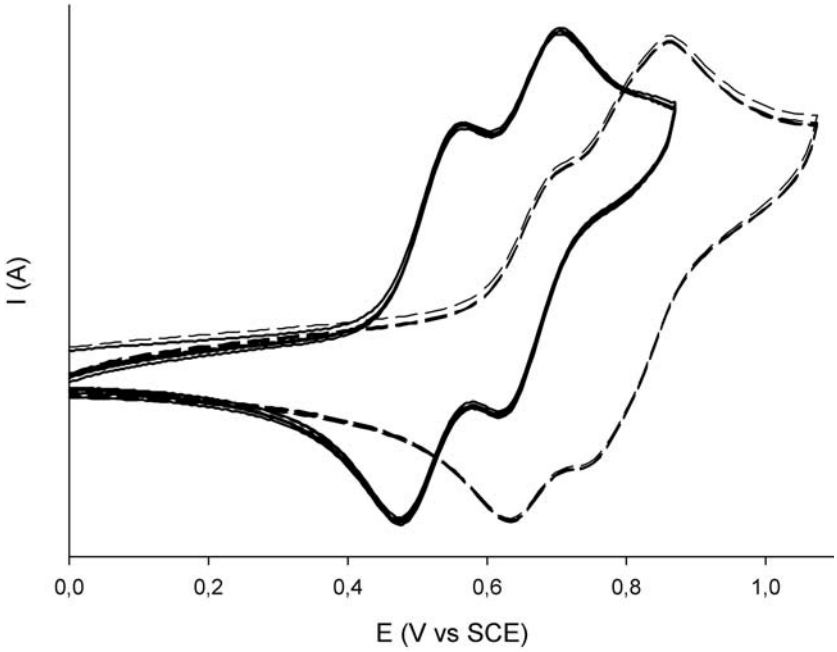


Figure S5 : normalized CV of compounds **1** (line) and **9** (dotted line)

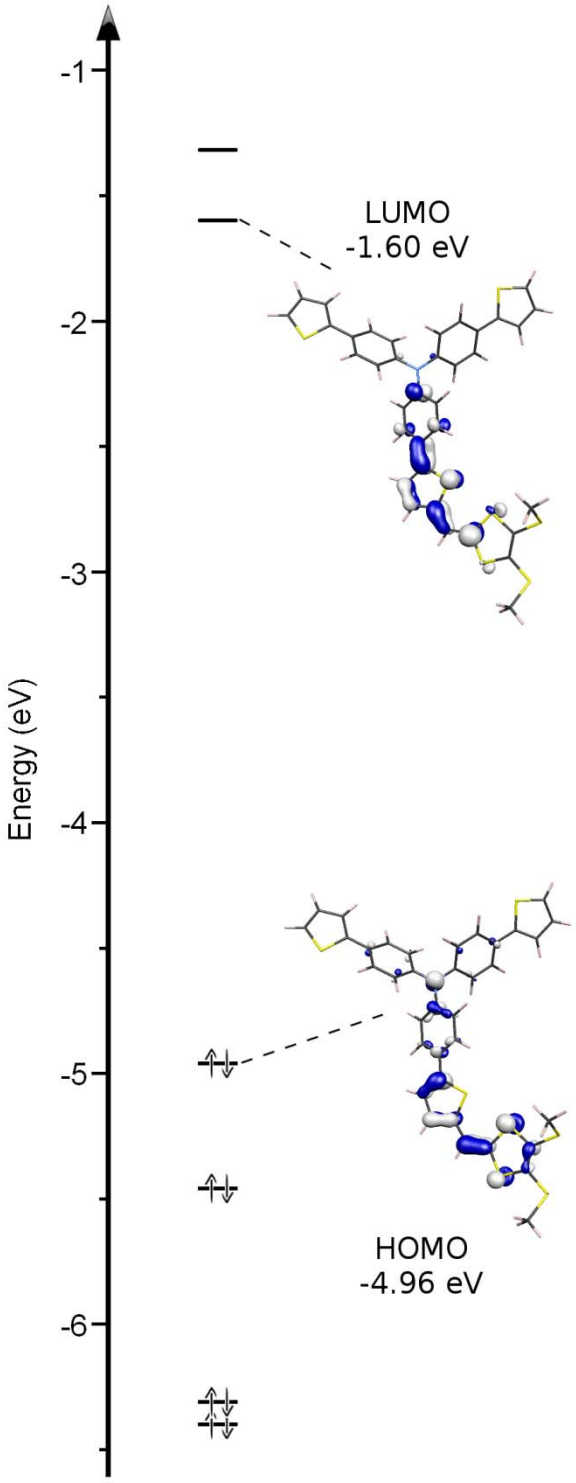


Fig S6. Molecular orbital diagram of **1**. Contour values are ±0.05 $[e/bohr^3]^{½}$

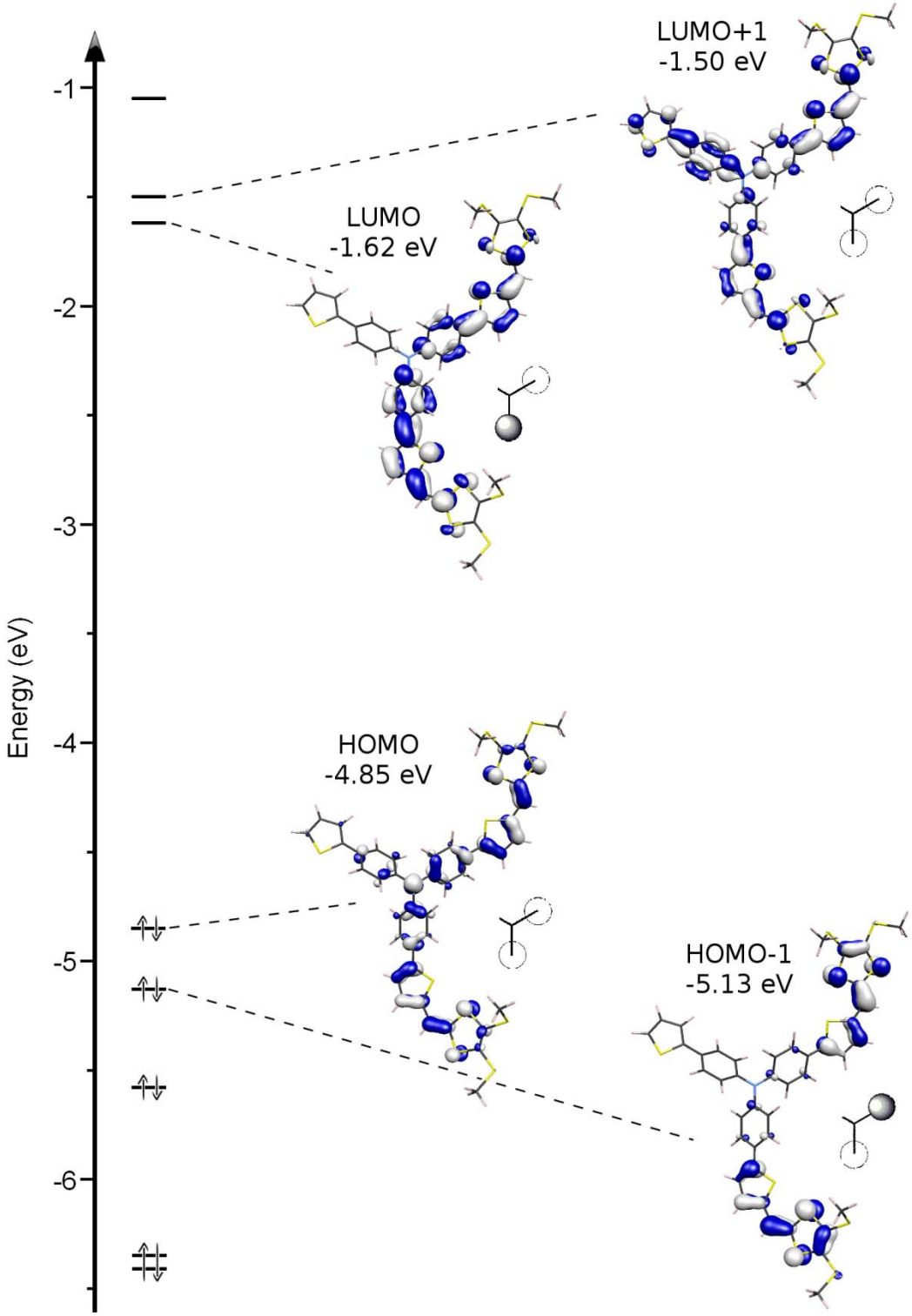


Fig S7. Molecular orbital diagram of **2**. Contour values of orbitals were chosen to match approximatively the volume of those in Fig SX. The cutoff values are ±0.035 $[e/bohr^3]^{½}$

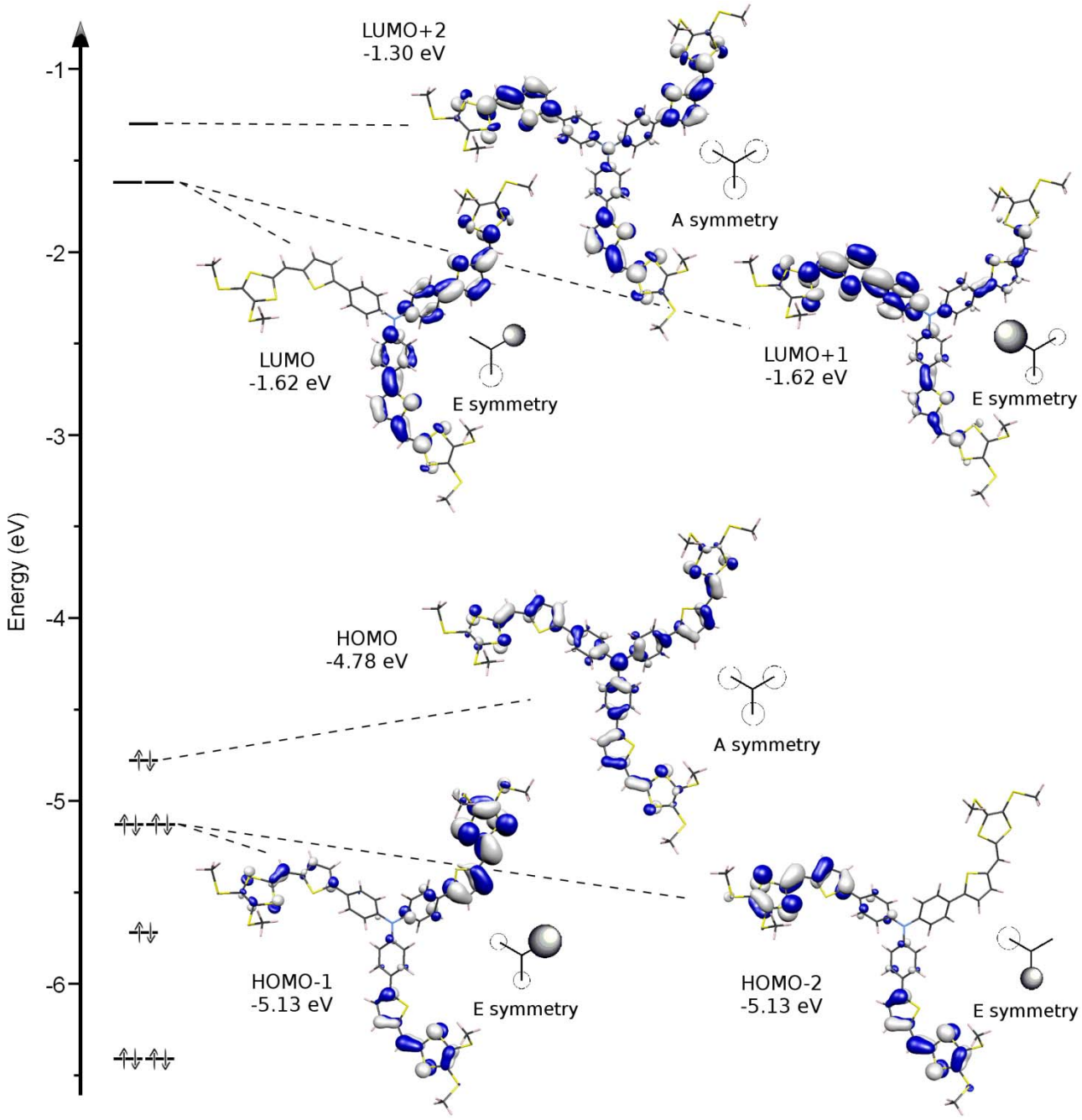


Fig S8. Molecular orbital diagram of **3**. Contour values of orbitals were chosen to match approximatively the volume of those in Fig SX and SX. The cutoff values are ±0.03 $[e/bohr^3]^{½}$

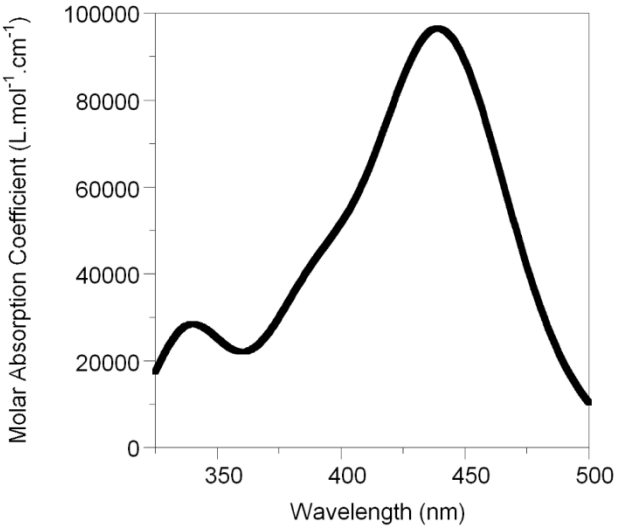


Fig S9. Theoretical absorption spectra of **1**.

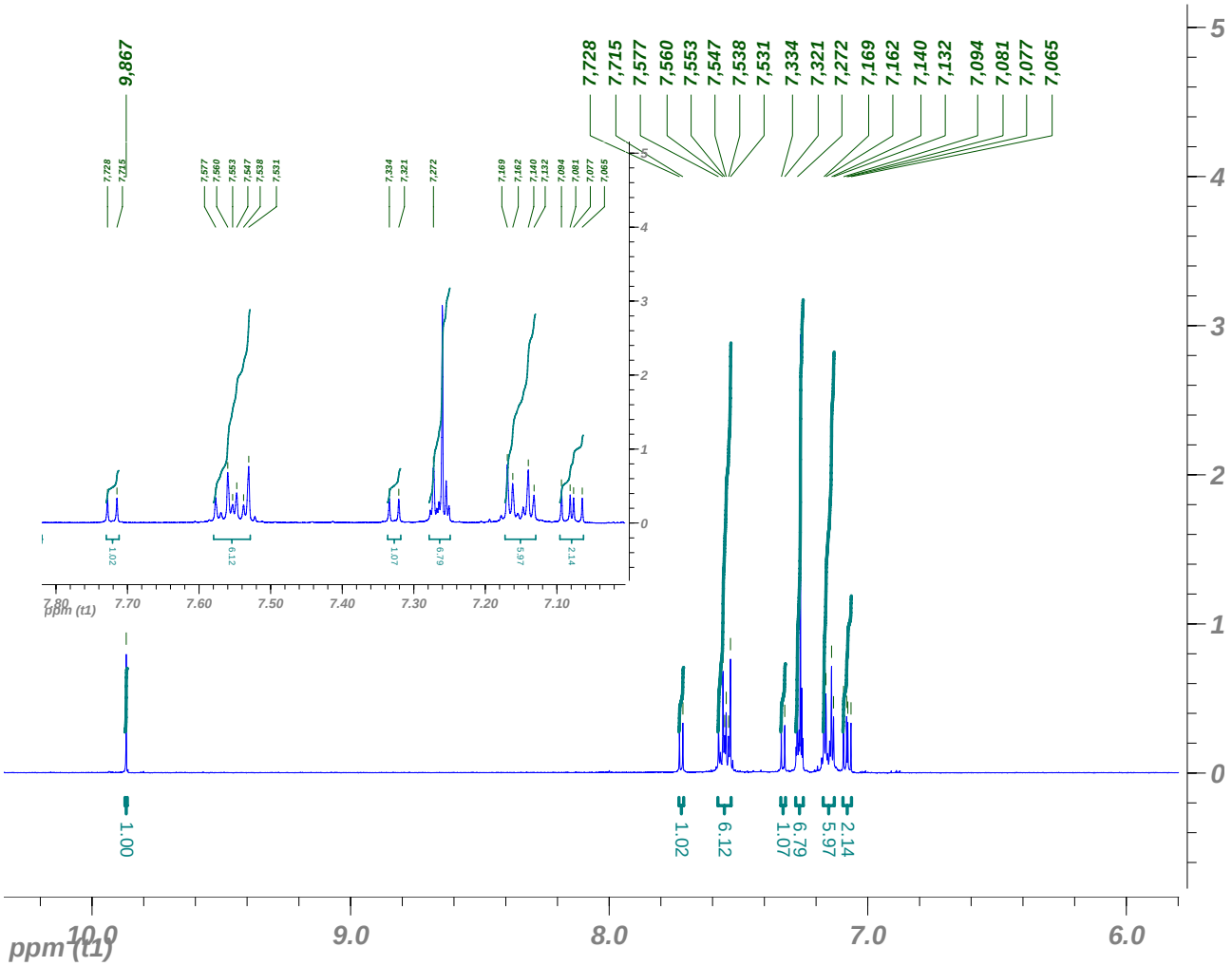
Table S1. TD-DFT calculated energies of the first low-lying electronic excitations associated with an oscillator factor *f*>0.05 of compound **1**.

Energy (cm-1)	λ (nm)	Osc.	Transitions
22682	441	1.28	HOMO→LUMO (96%)
25444	393	0.45	HOMO→LUMO+1 (91%)
29512	339	0.17	HOMO-1→LUMO+1 (71%), HOMO→LUMO+2 (14%)
29591	338	0.19	HOMO→LUMO+2 (51%), HOMO-1→LUMO+1 (19%), HOMO→LUMO+5 (13%),

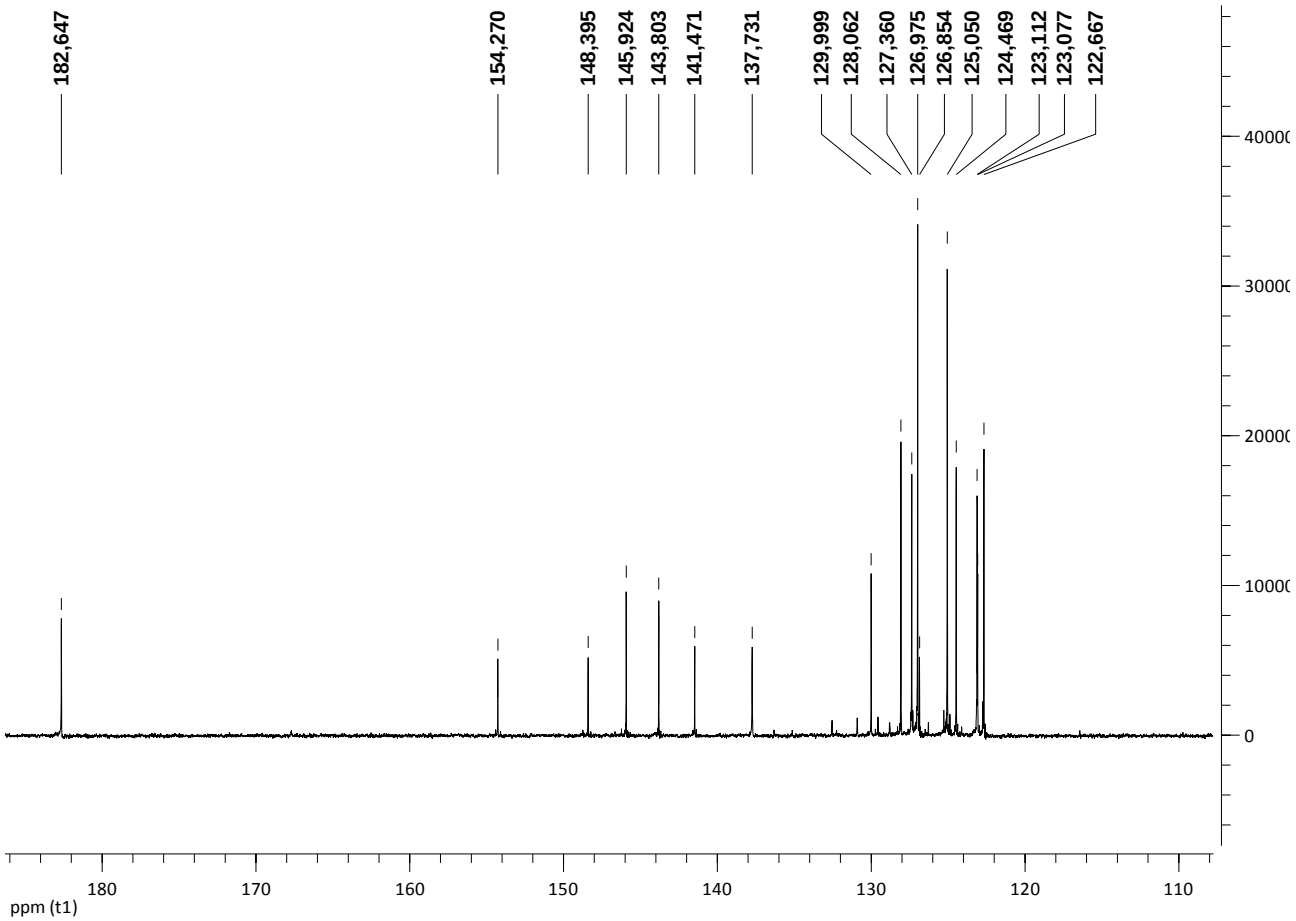
NMR data for compounds

Derivative 4

1H NMR

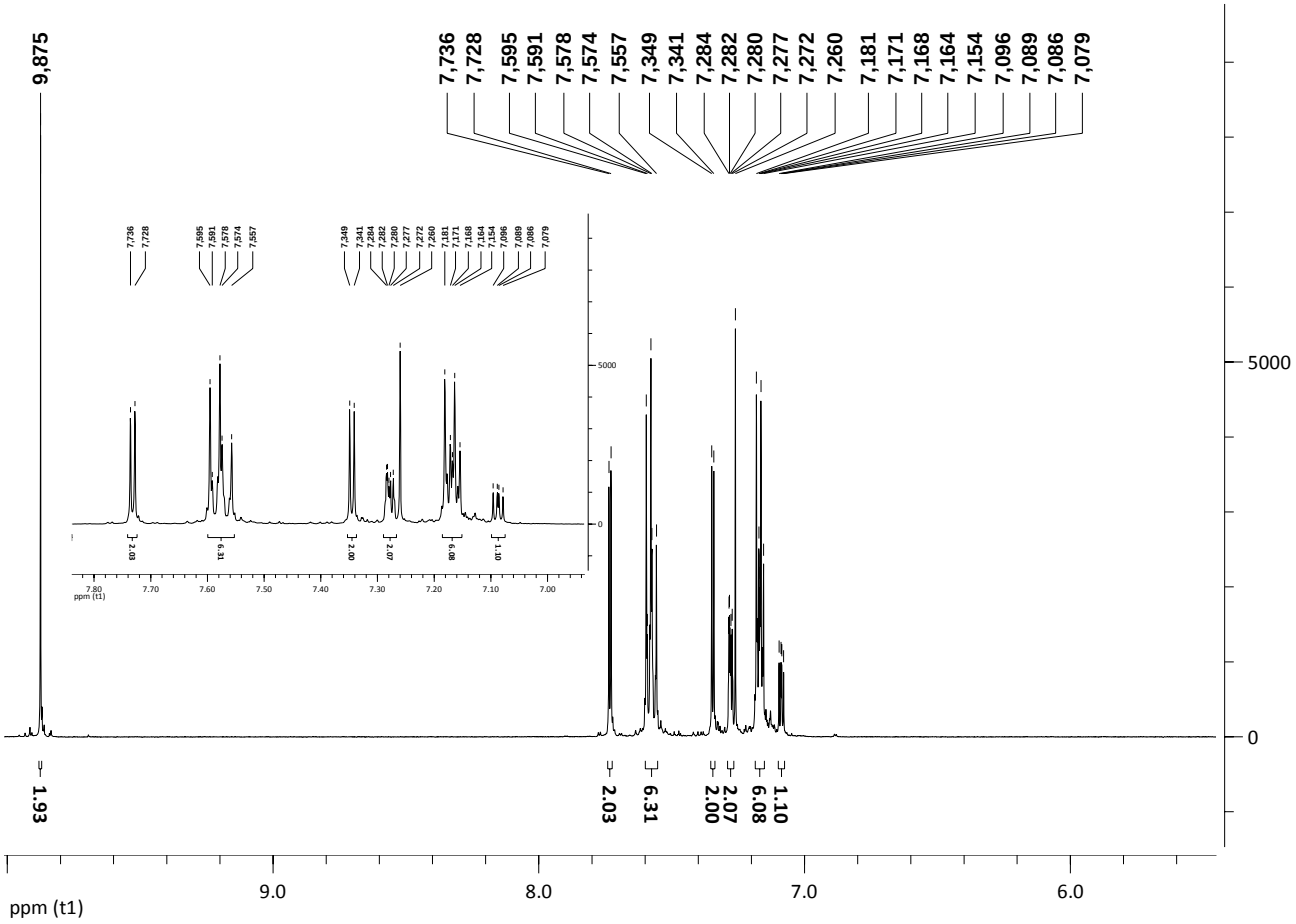


13C NMR

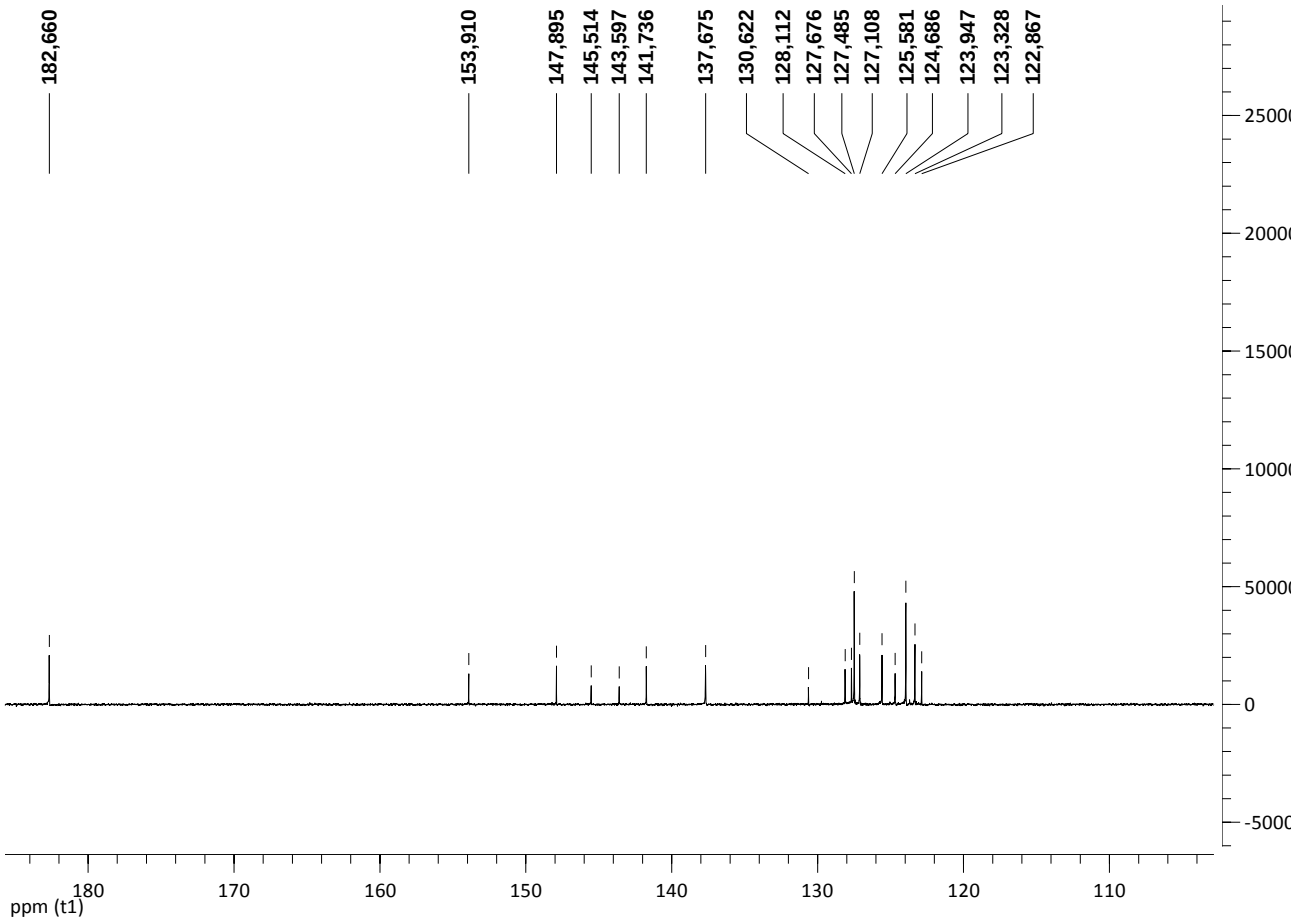


Derivative 5

1H NMR

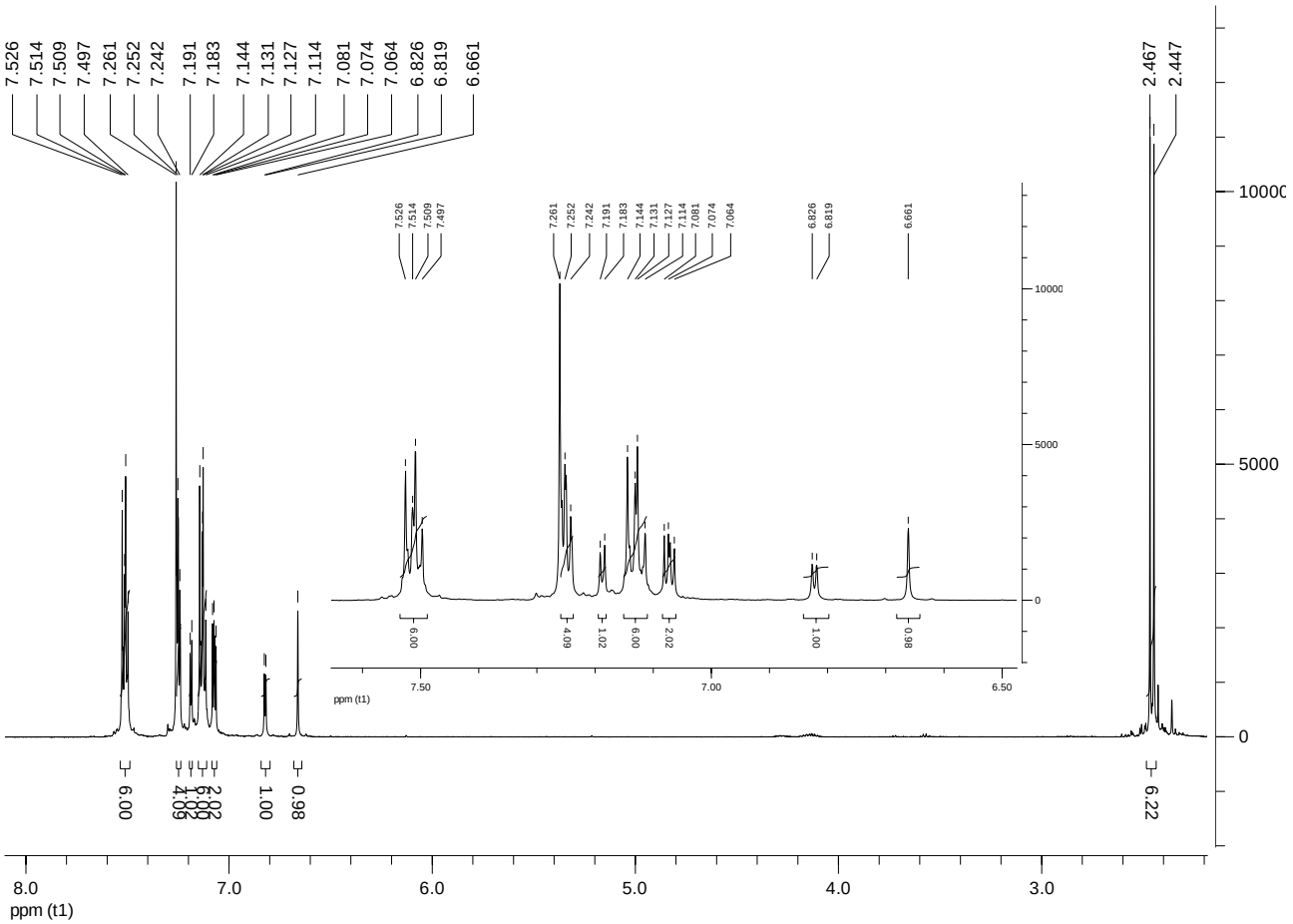


13C NMR

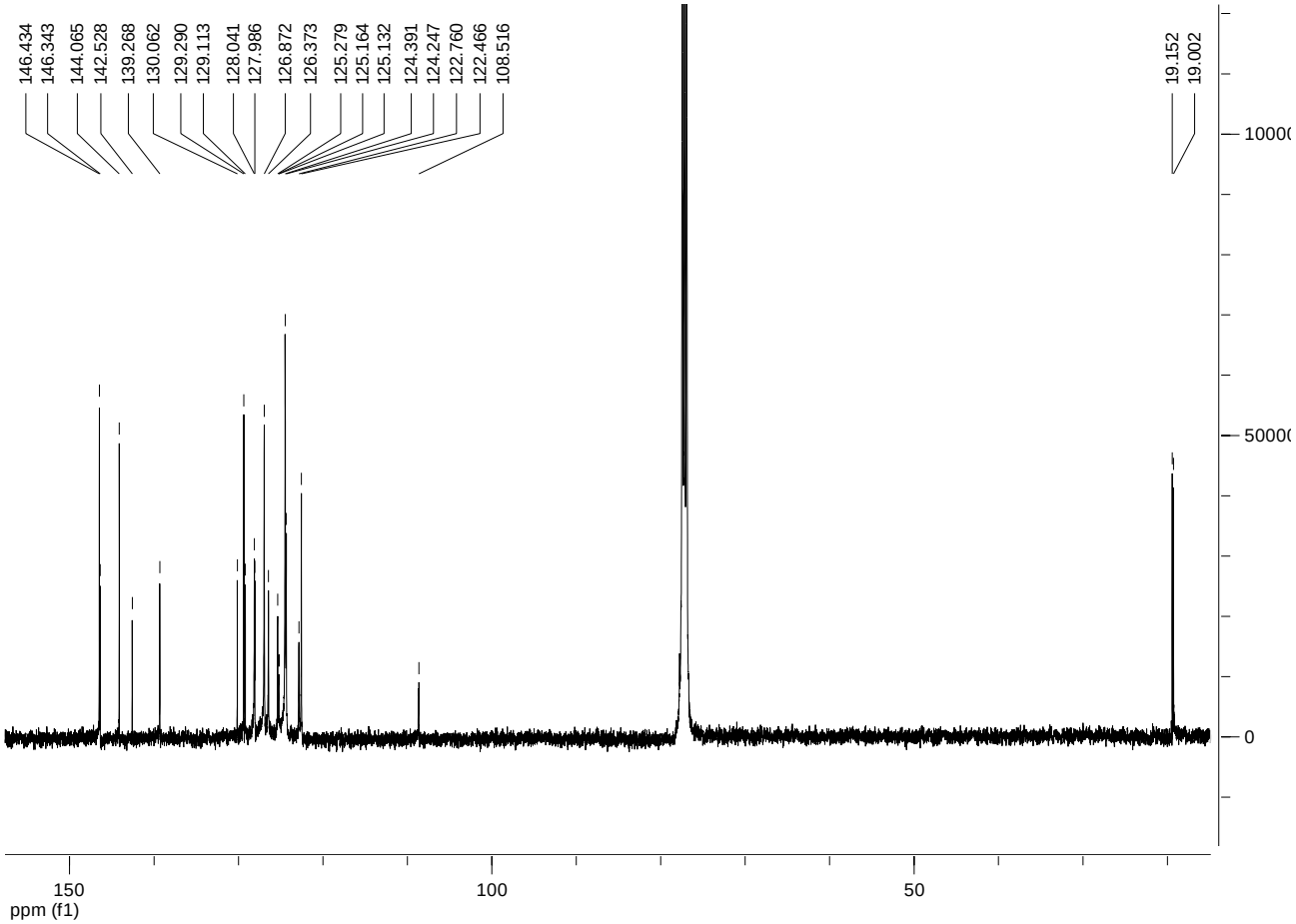


Derivative 1

1H NMR

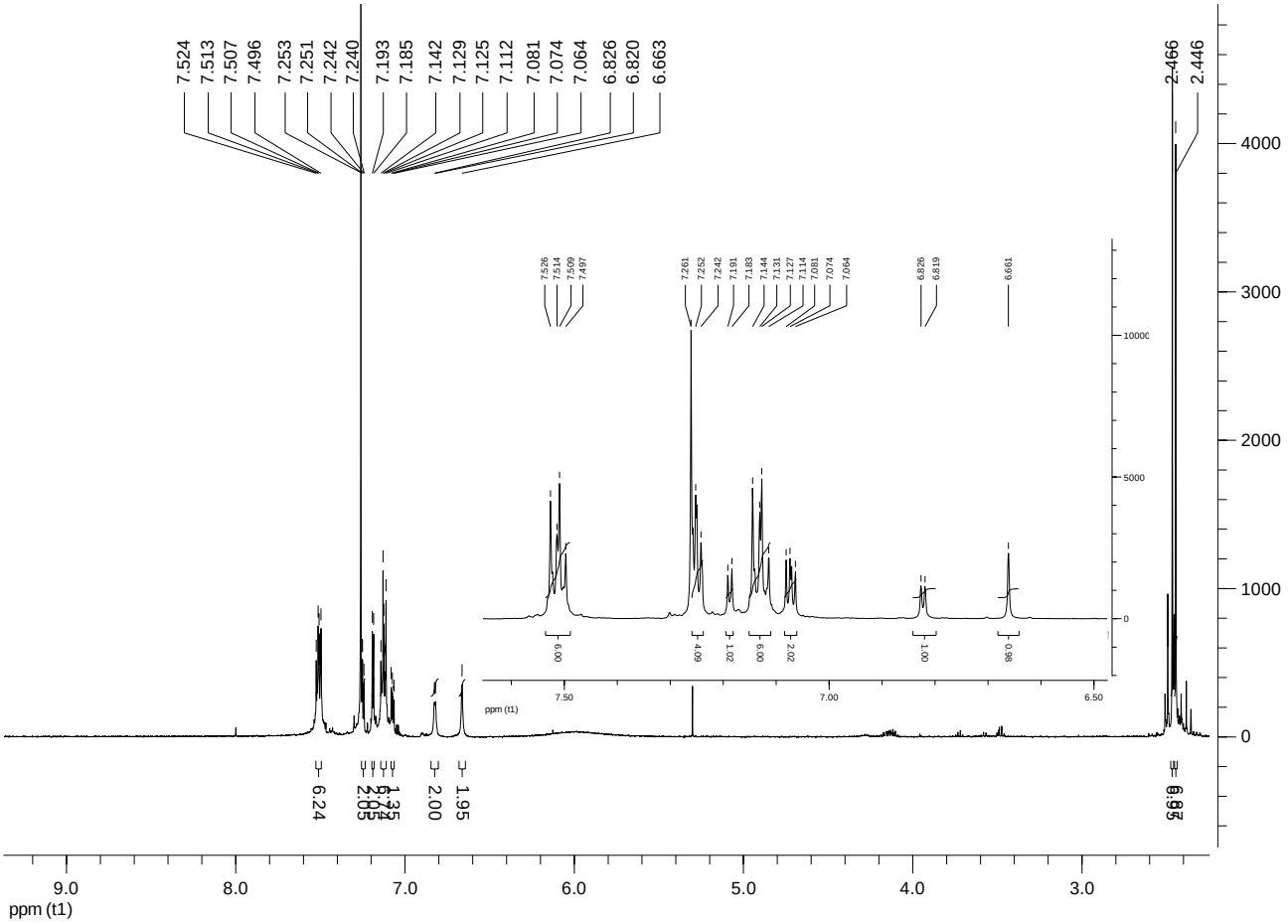


13c NMR

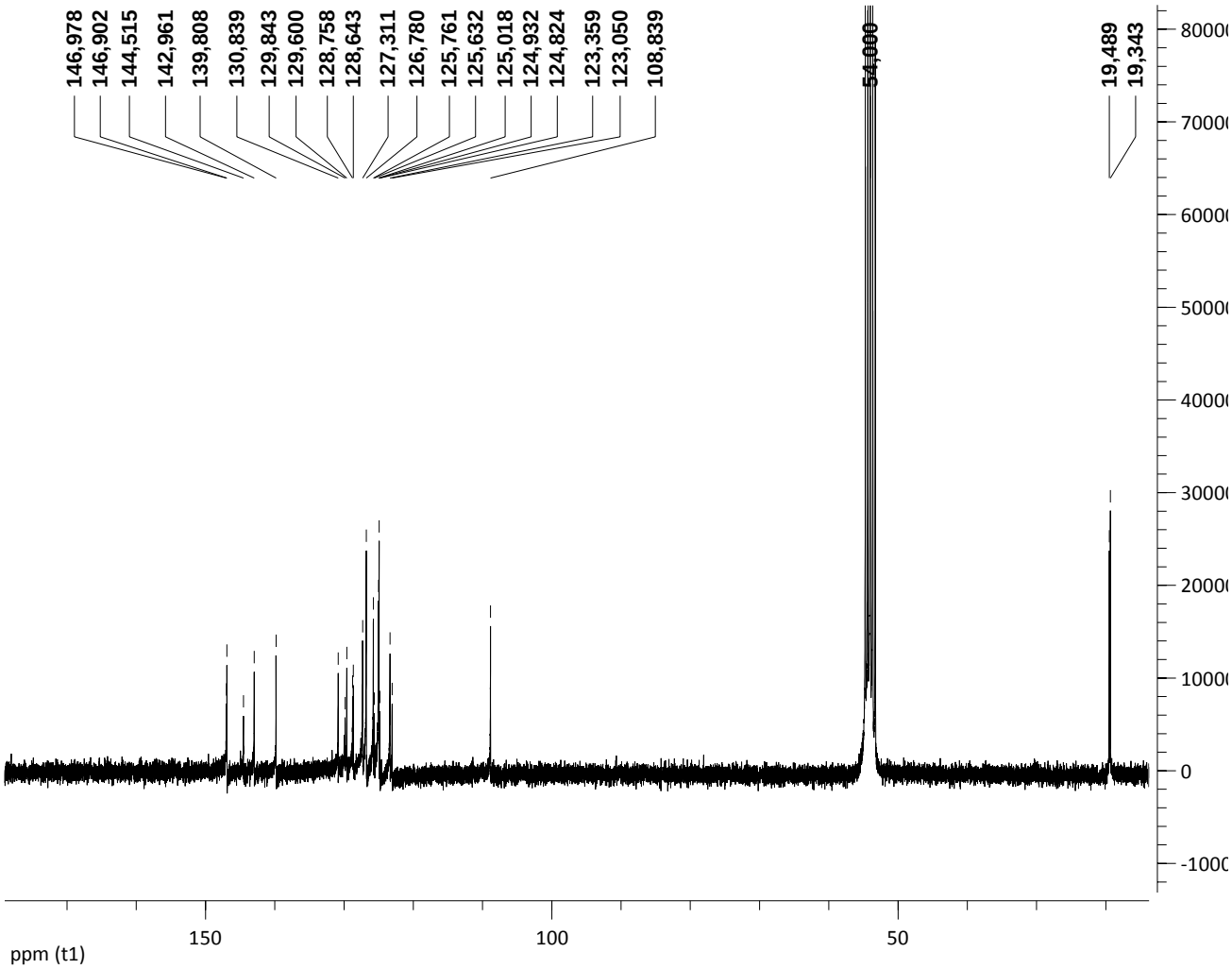

146.434
146.343
144.065
142.528
139.268
130.062
129.290
129.113
128.041
127.986
126.872
126.373
125.279
125.164
125.132
124.391
124.247
122.760
122.466
108.516
19.152
19.002
10000
50000
0
150
100
50
ppm (f1)

Derivative 2

1H NMR

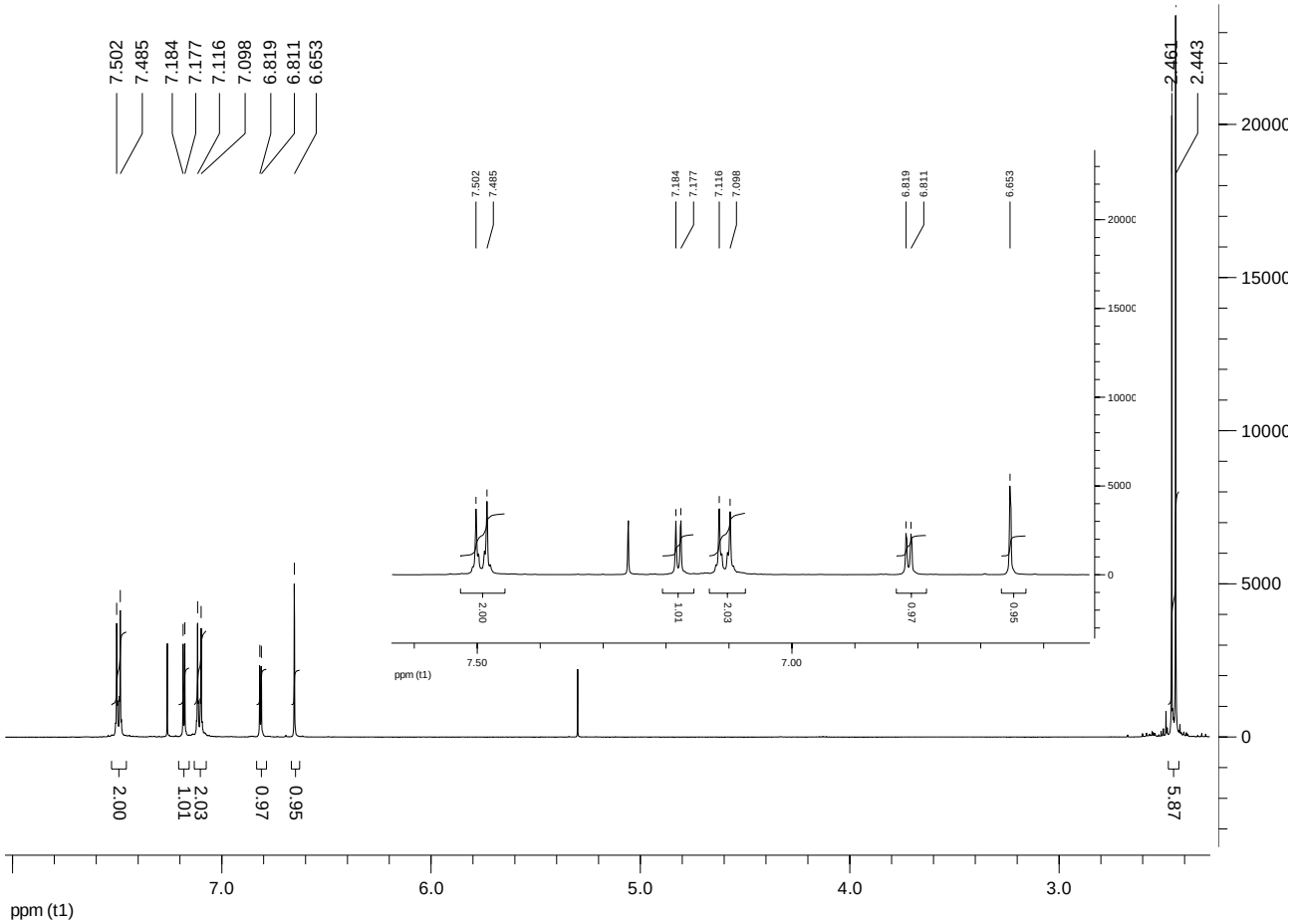


13C NMR (CD_2Cl_2)

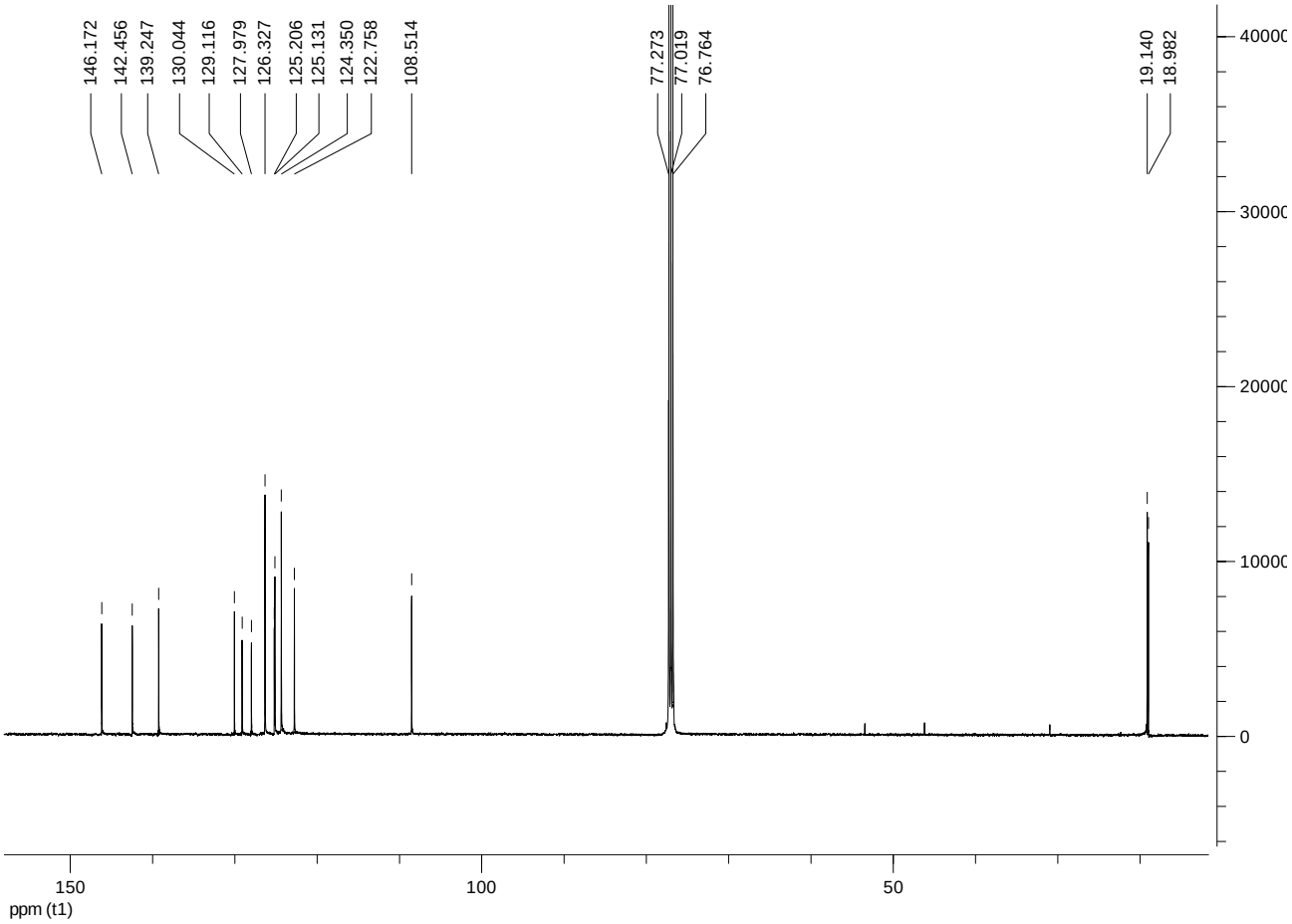


Derivative 3

1H NMR

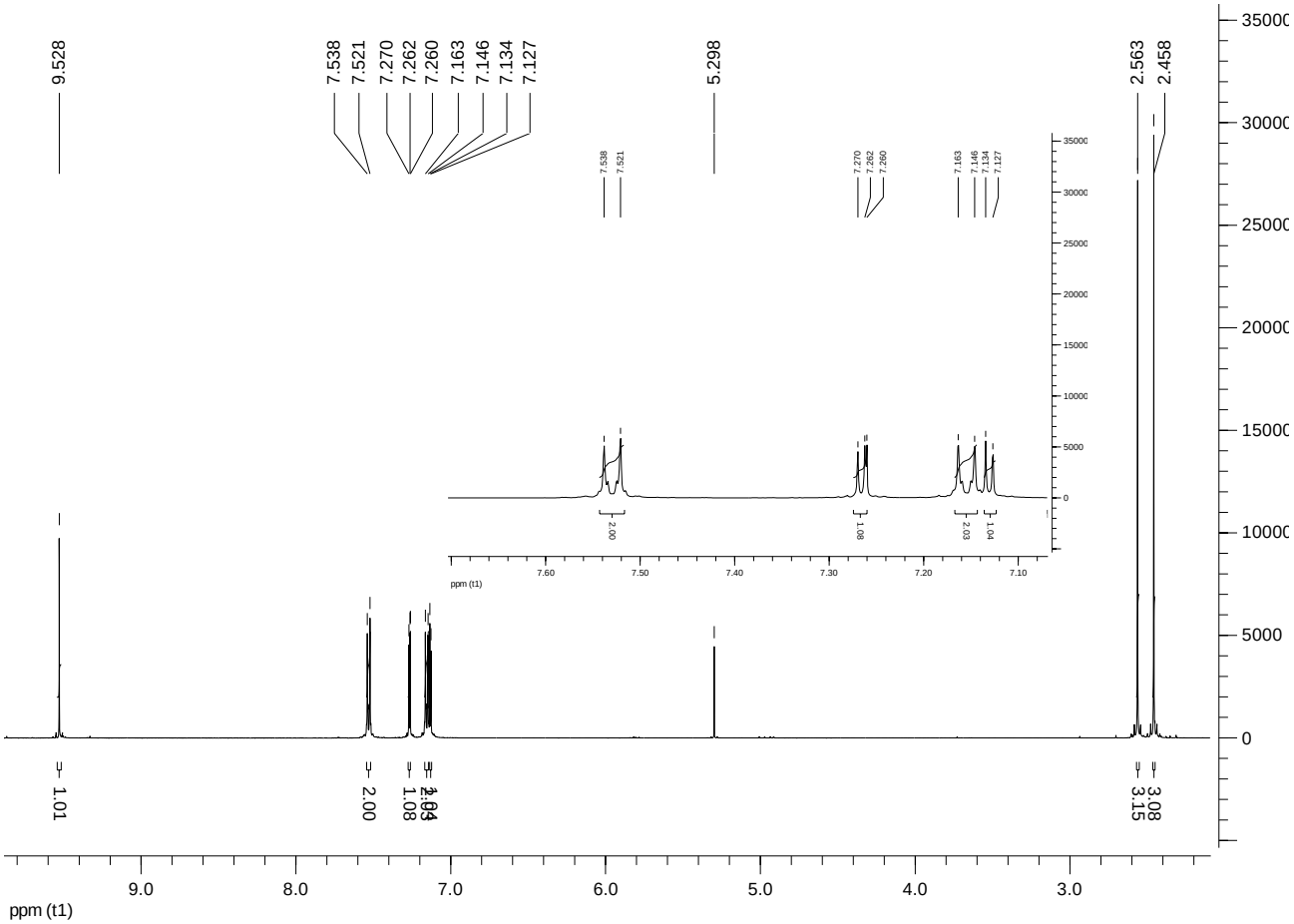


13C NMR

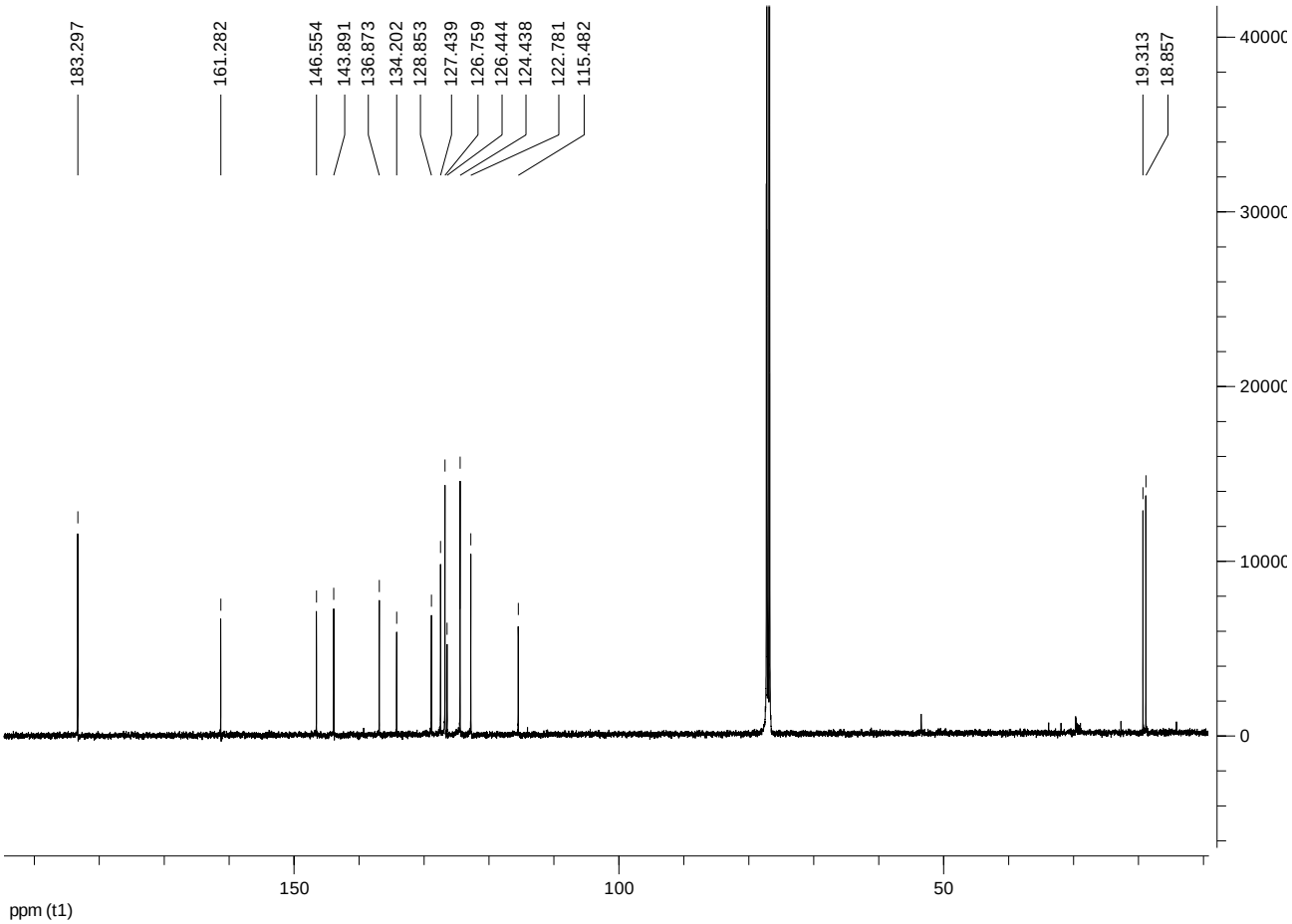

146.172
142.456
139.247
130.044
129.116
127.979
126.327
125.206
125.131
124.350
122.758
108.514
77.273
77.019
76.764
19.140
18.982
40000
30000
20000
10000
0
150
100
50
ppm (t1)

Derivative 7

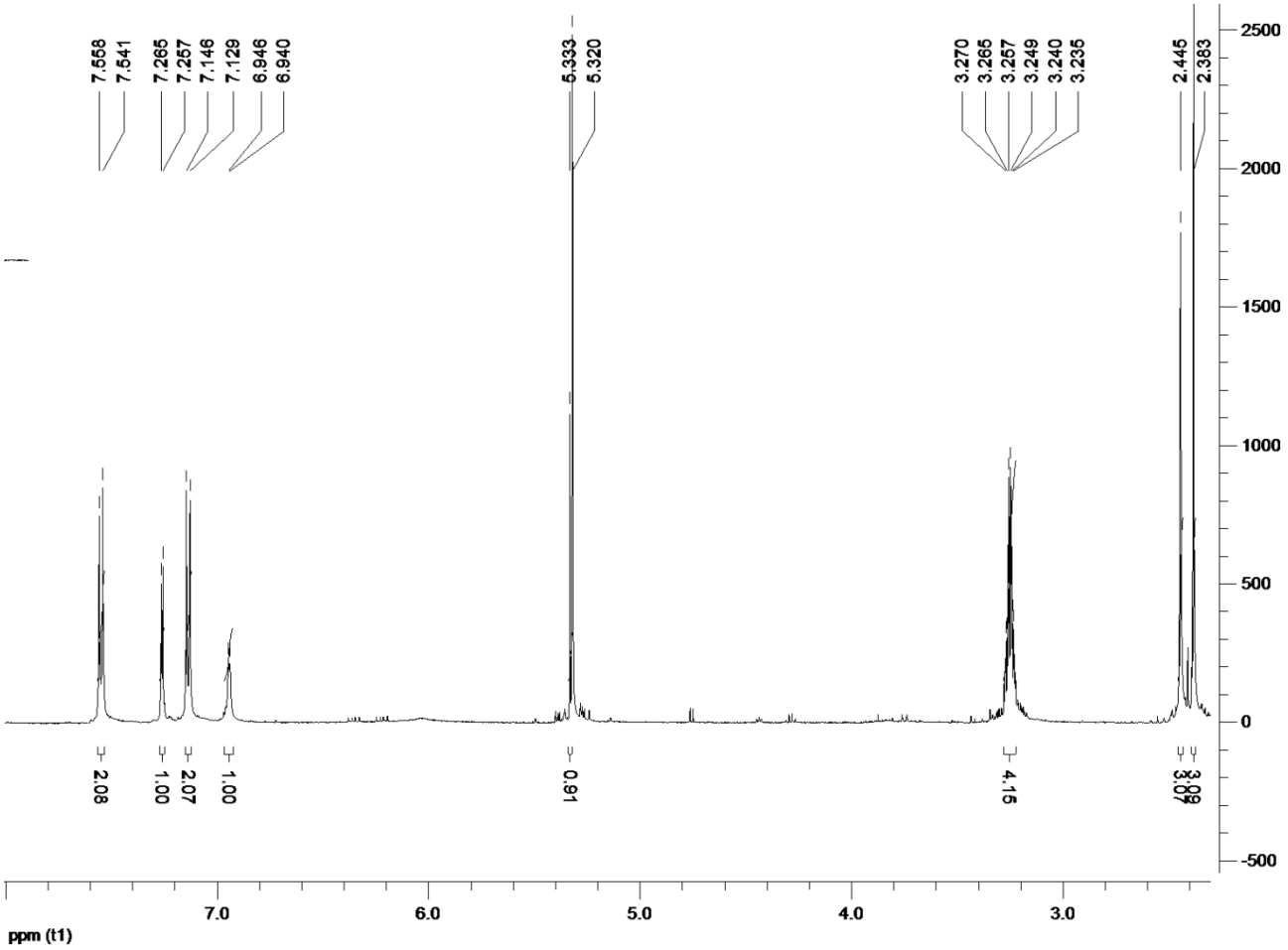
1H NMR



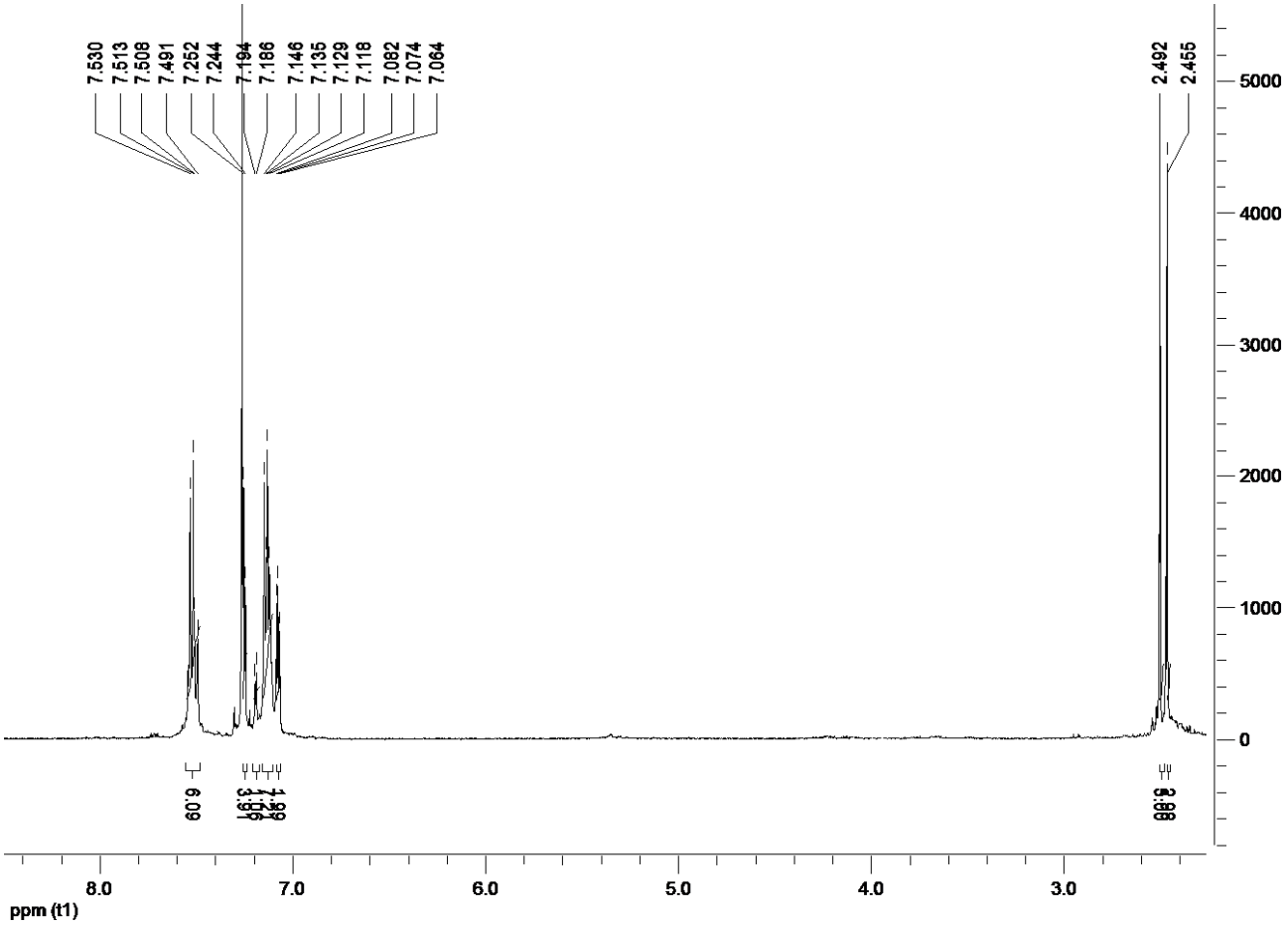
13C NMR



Derivative 8
1H NMR



Derivative 9
1H NMR


7.530
7.513
7.508
7.491
7.252
7.244
7.194
7.186
7.146
7.135
7.129
7.118
7.082
7.074
7.064
2.492
2.455
5000
4000
3000
2000
1000
0
6.09
3.91
1.98
1.98
8.0
7.0
6.0
5.0
4.0
3.0
ppm (t1)