Supporting Information

Aggregation Induced Emission Based Fluorenes as Dual–Channel Fluorescent Probes for Rapid Detection of Cyanide: Applications of Smartphone and Logic Gate

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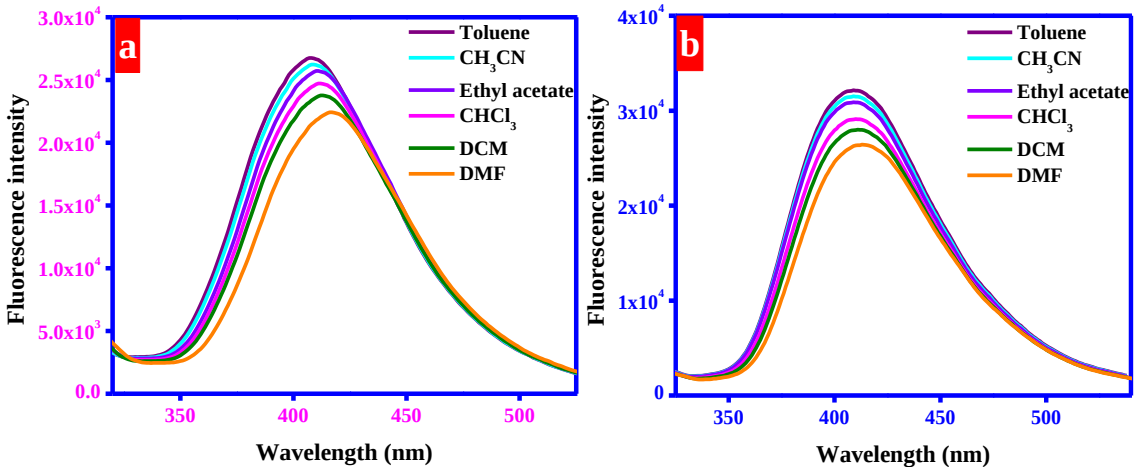
SI–1. Instruments and reagents

The NMR (^{1}H, ^{13}C, and DEPT–135) spectra of all newly synthesized compounds (**1a**, **1b**, **1c**, and **1d**) were recorded at Bruker Avance 400 MHz nuclear magnetic resonance (NMR) spectrometer using $CDCl_3$ as a solvent and tetramethylsilane (TMS) as a reference. Further, spectrofluorometer (model FluoroMax-Plus-P-C, Horiba Jobin Yvon Technology, USA) was used to record fluorescence emission spectra. The average particle size of compounds **1a** and **1b** was measured through Dynamic light scattering (DLS, model ZSP Malvern Analytical technology, UK). UV–visible studies were carried out at UV-Vis spectrophotometer (SPECORD 200 PLUS-223E2003C by Analytik Jena, Germany). All reagents and used chemicals were purchased from Alfa Aesar (UK), Daejung Chemicals & Metals (Korea), and Sigma Aldrich (USA) and were used without further purification. Solvents and chemicals utilized in this study include 9*H*–fluorene, ethanol, potassium tertiary butoxide, *N*,*N*–dimethylbenzaldehyde, 4–ethoxybenzaldehyde, 4–methoxybenzaldehyde, and 3–nitrobenzaldehyde, DCM, brine, distilled water, anhydrous $MgSO_4$, *n*-hexane, ethyl acetate, tetrahydrofuran (THF), ethanol, methanol, acetonitrile (CH_3CN), dichloromethane (DCM), chloroform ($CHCl_3$), toluene, CN^-, F^-, Cl^-, Br^-, I^-, ClO_4^-, N_3^-, NO_3^-, $H_2PO_4^-$, NO_2^-, and CH_3COO^-.



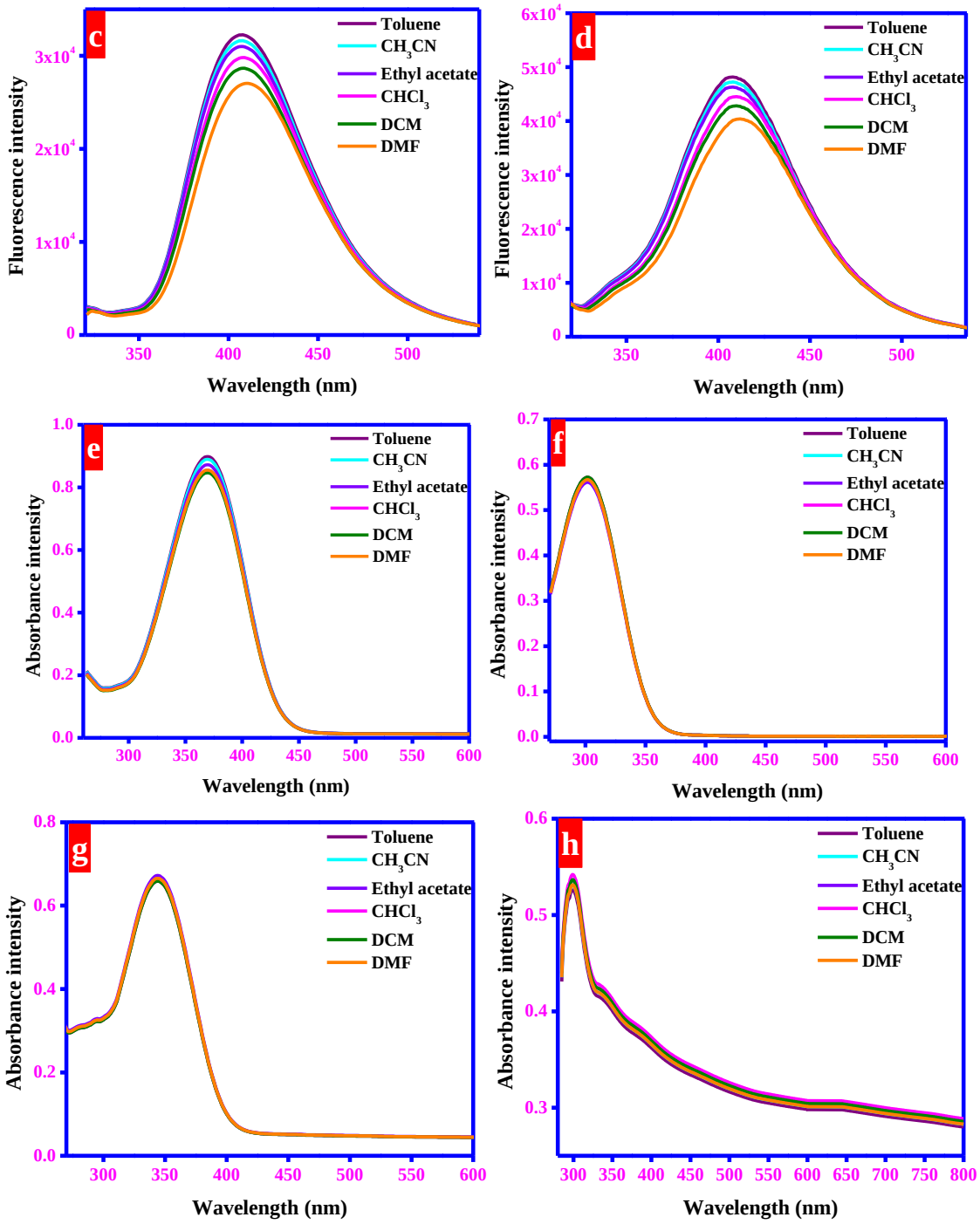


Fig. S1. Fluorescence and absorption spectra of probes **1a** (a and e), **1b** (b and f), **1c** (c and g), and **1d** (d and h) in different solvents (conc. = 20 μM (**1a**), 50 μM (**1b**), 10 μM (**1c**), and 20 μM (**1d**); for fluorescence, λ_{ex} = 390 nm; slit width 2/2).

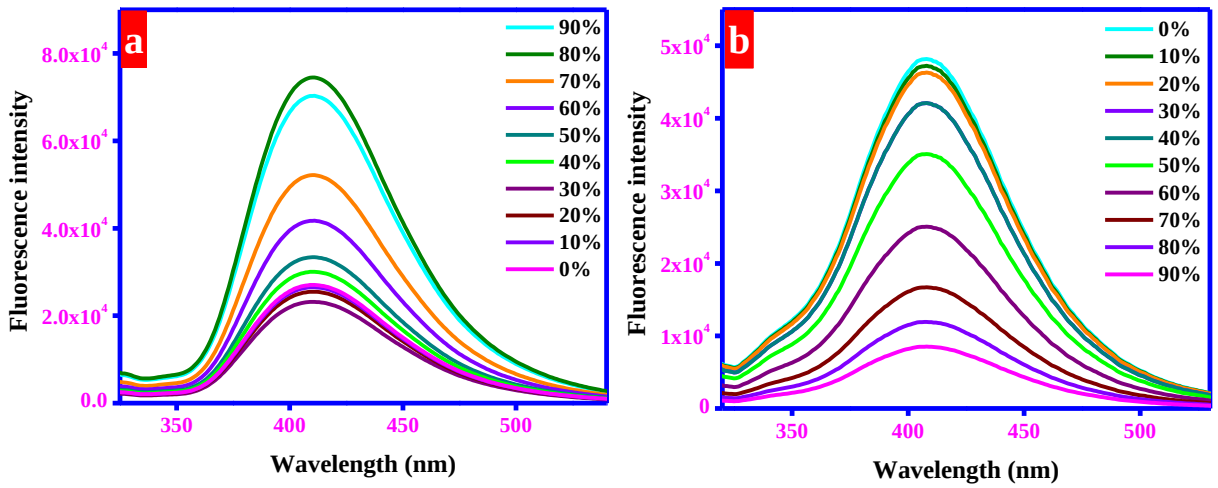
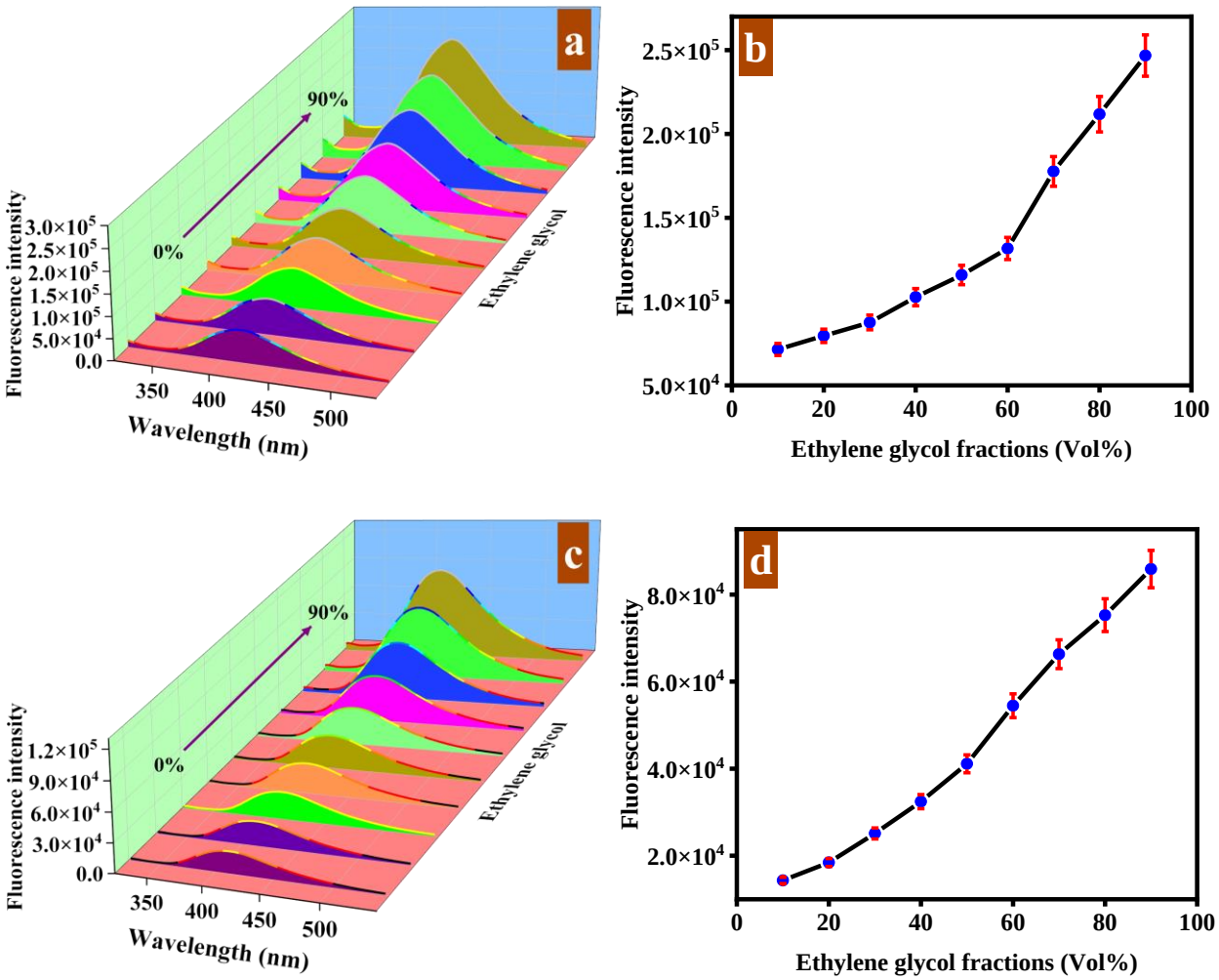


Fig. S2. Fluorescence spectra of probes **1c** (a) and **1d** (b) in DMF with increasing water contents from 0 to 90% (conc. = 10 μM (**1c**), and 20 μM (**1d**); λ_{ex}=390 nm; slit width 2/2).



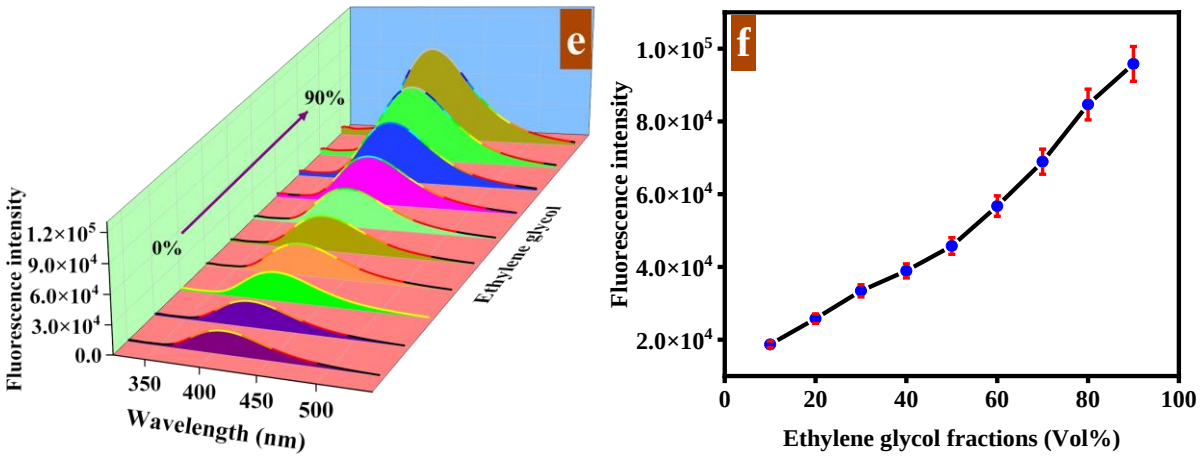


Fig. S3. Fluorescence spectra and linear fit plots of probes **1a** (a,b), **1b** (c,d), and **1c** (e,f) illustrating the constant increase in the fluorescence intensity upon regular increase of ethylene glycol contents from 0 to 90% (conc. = 20 μM (**1a**), 50 μM (**1b**), and 10 μM (**1c**); λ_{ex}=390 nm; slit width 2/2).

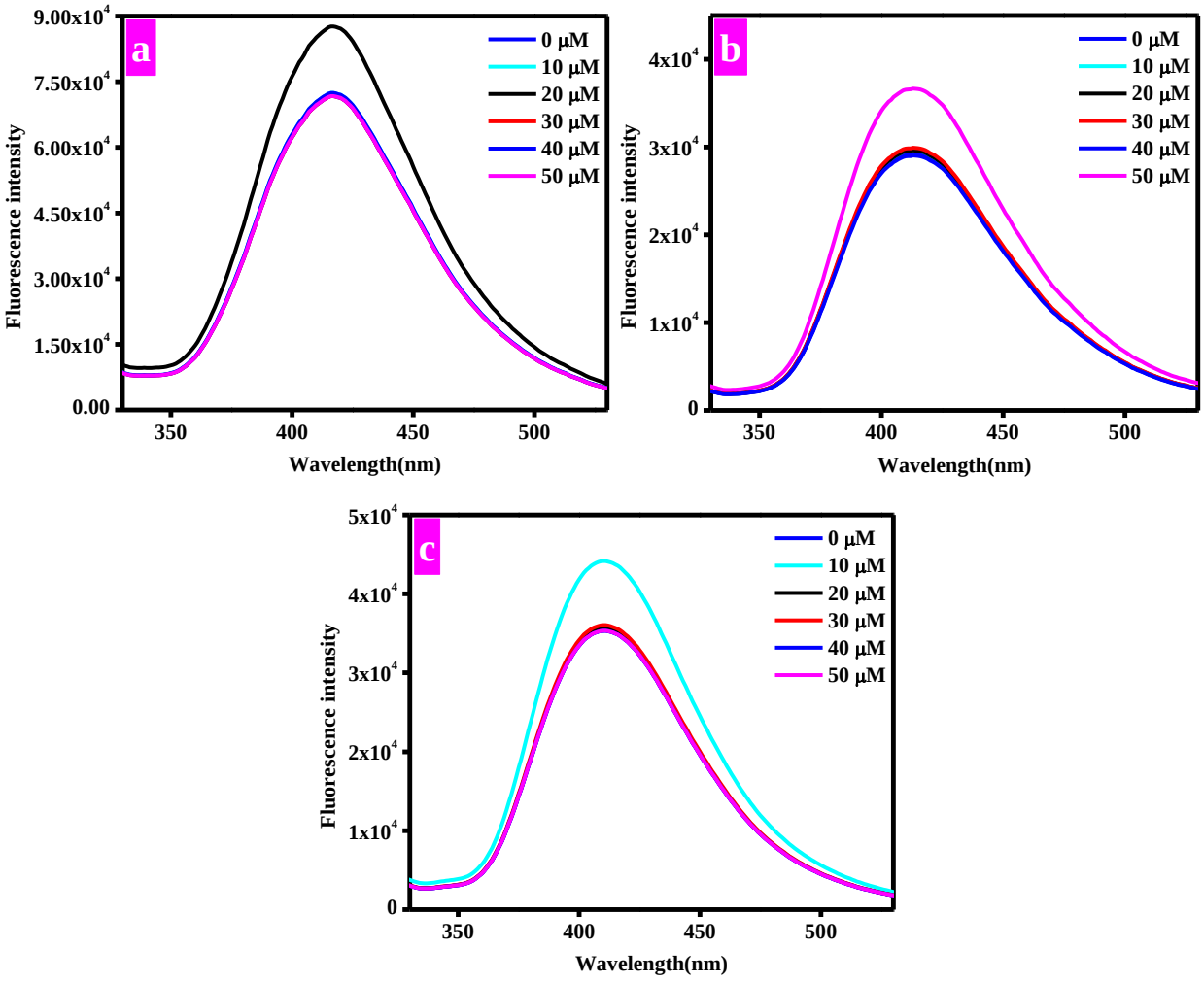


Fig. S4. Fluorescence spectra of probes **1a** (a), **1b** (b), and **1c** (c) in H_2O/DMF (4:1, v/v) with increasing concentrations from 0 to 50 μM (λ_{ex}=390 nm; slit width 2/2).

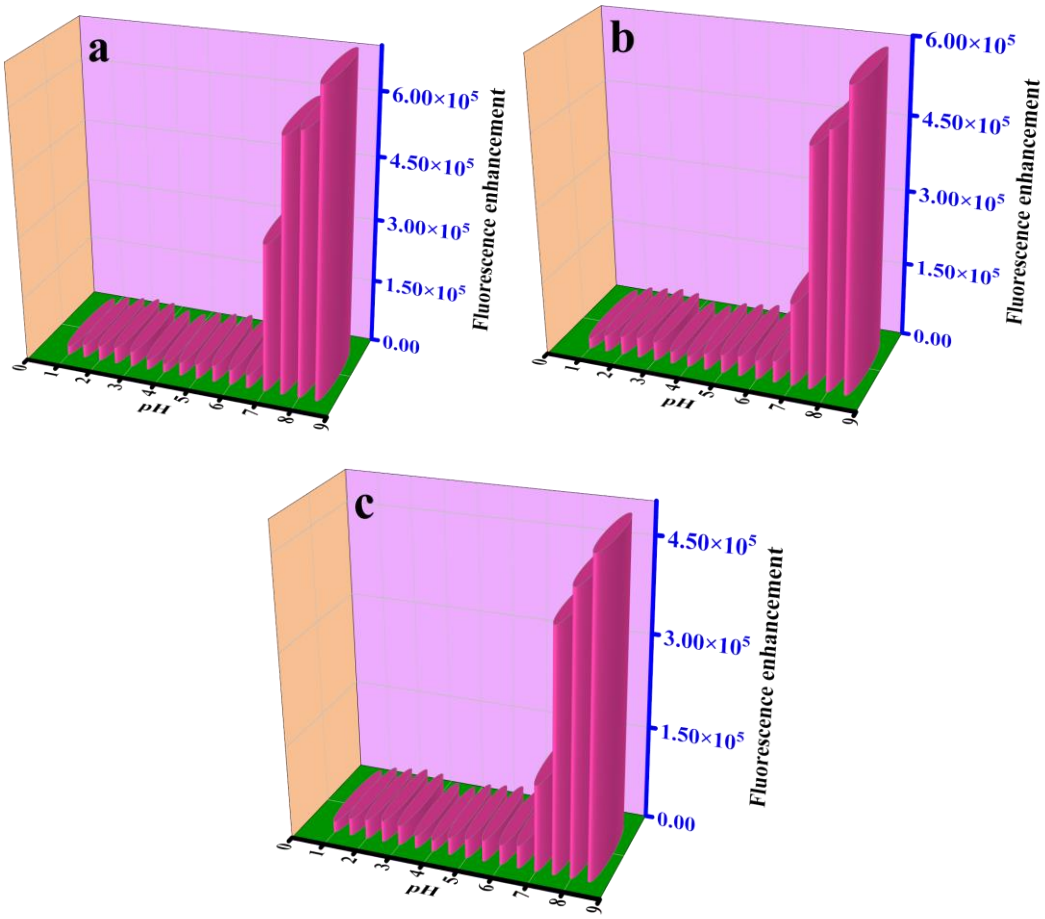


Fig. S5. Fluorescence spectra of probes **1a** (a), **1b** (b), and **1c** (c) before and after the addition of CN^- (500 nM) over a wide pH range (2.0–12.0) (conc. = 20 μM (**1a**), 50 μM (**1b**), and 10 μM (**1c**); λ_{ex} = 390 nm; slit width 2/2).

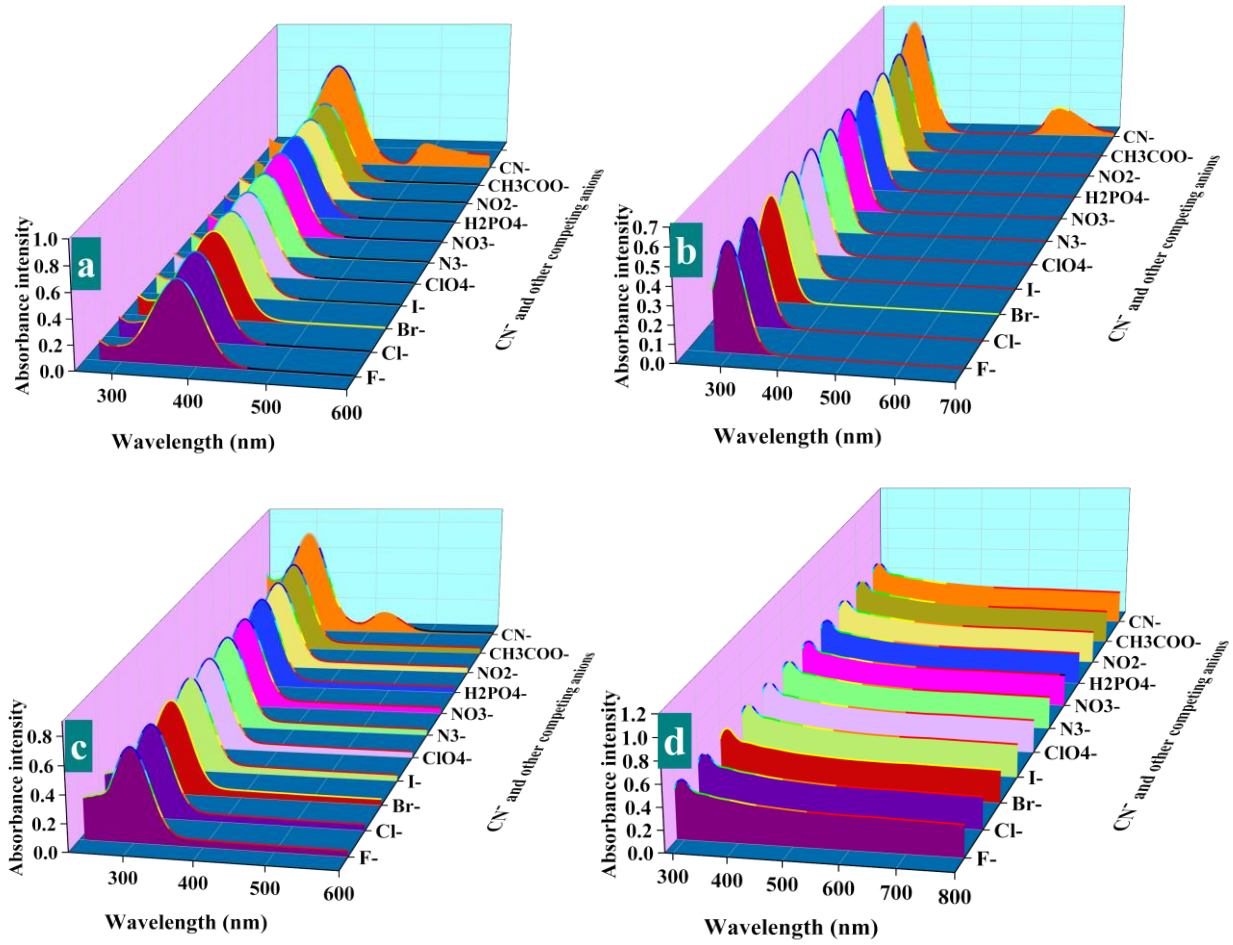
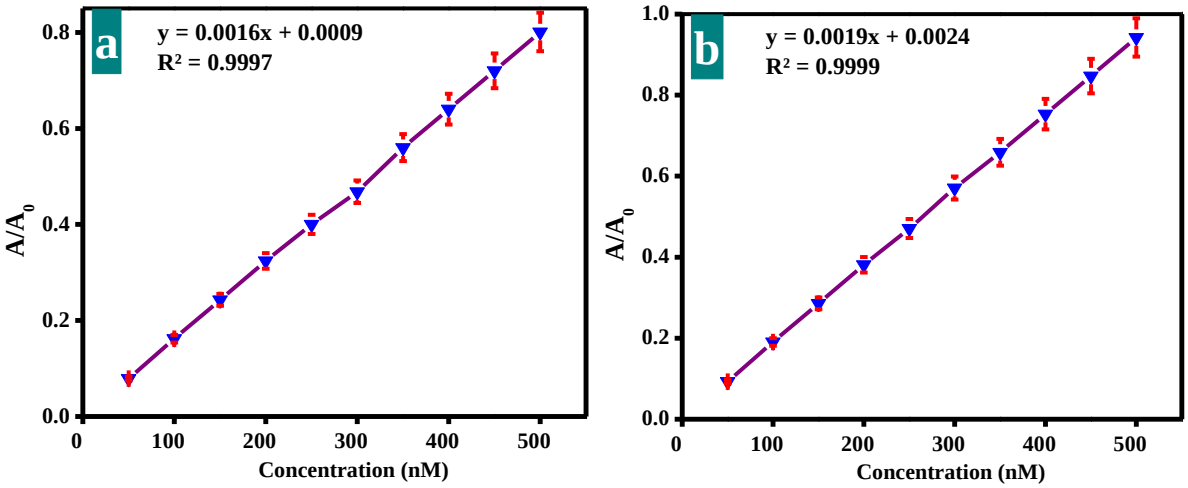


Fig. S6. Absorption spectra of probes **1a** (a), **1b** (b), **1c** (c), and **1d** (d) upon the addition of 500 nM of different anions (conc. = 20 μM (**1a**), 50 μM (**1b**), 10 μM (**1c**), and 20 μM (**1d**)).



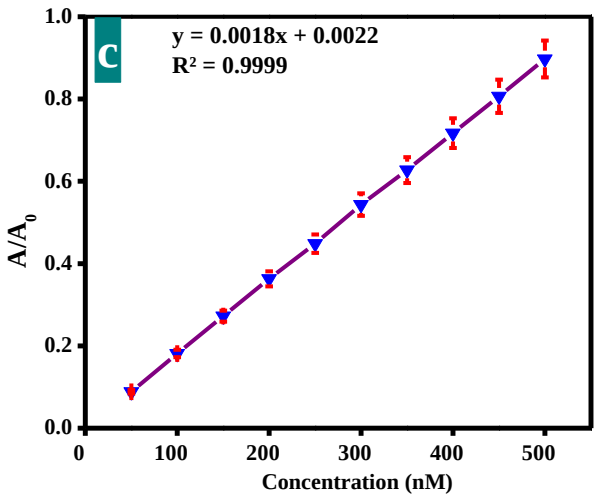


Fig. S7. Calibration curves demonstrating the steady elevation in the absorption intensity of probes **1a** (a), **1b** (b) and **1c** (c) upon constant addition (0–500 nM) of CN^-.

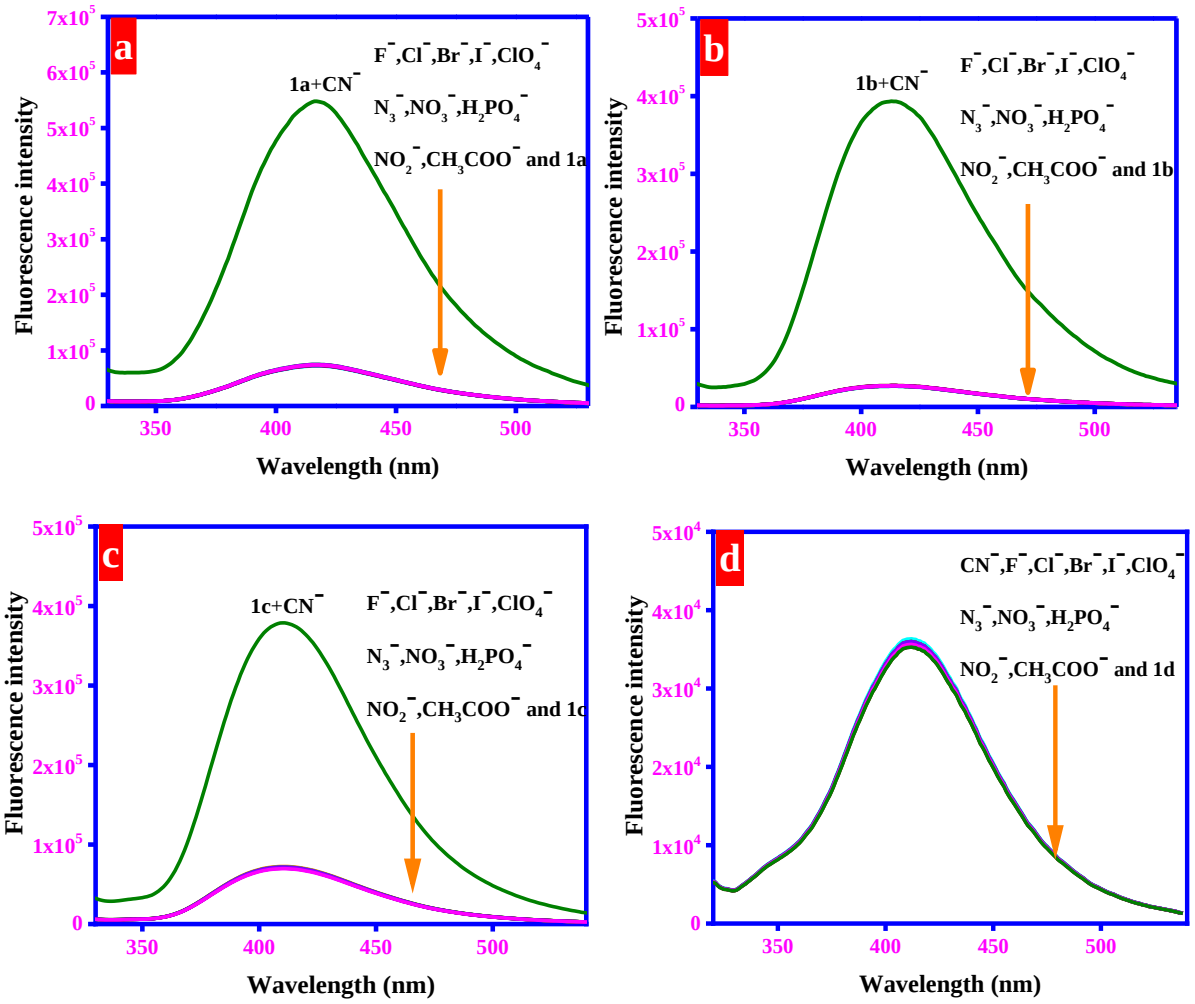


Fig. S8. Fluorescence spectra of probes **1a** (a), **1b** (b), **1c** (c), and **1d** (d) upon the addition of 500 nM of different anions (conc. = 20 μM (**1a**), 50 μM (**1b**), 10 μM (**1c**), and 20 μM (**1d**); λ_{ex} = 390 nm; slit width 2/2).

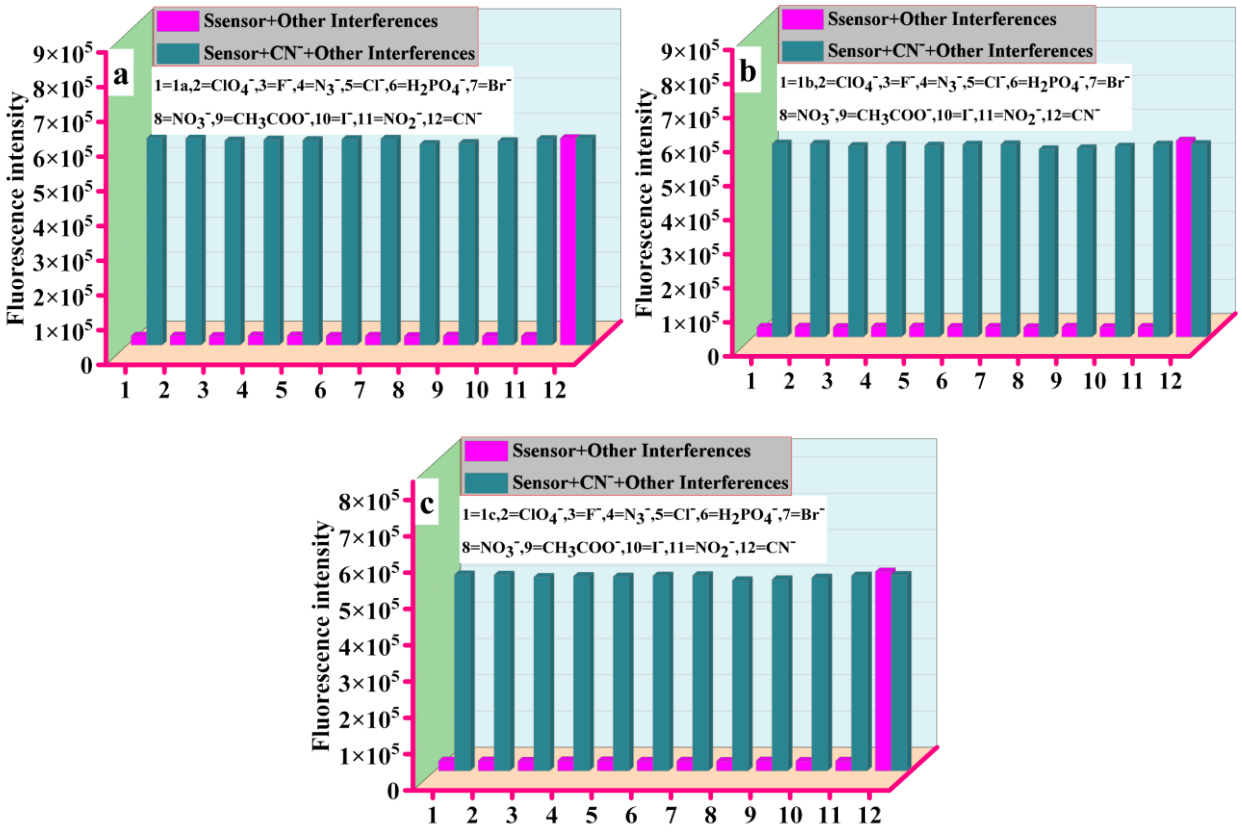


Fig. S9. Fluorescence spectra of probes **1a** (a), **1b** (b), and **1c** (c) upon the addition of CN^- (500 nM) in the presence of other interferences (20 equiv) (conc. = 20 μM (**1a**), 50 μM (**1b**), and 10 μM (**1c**); λ_{ex} = 390 nm; slit width 2/2).

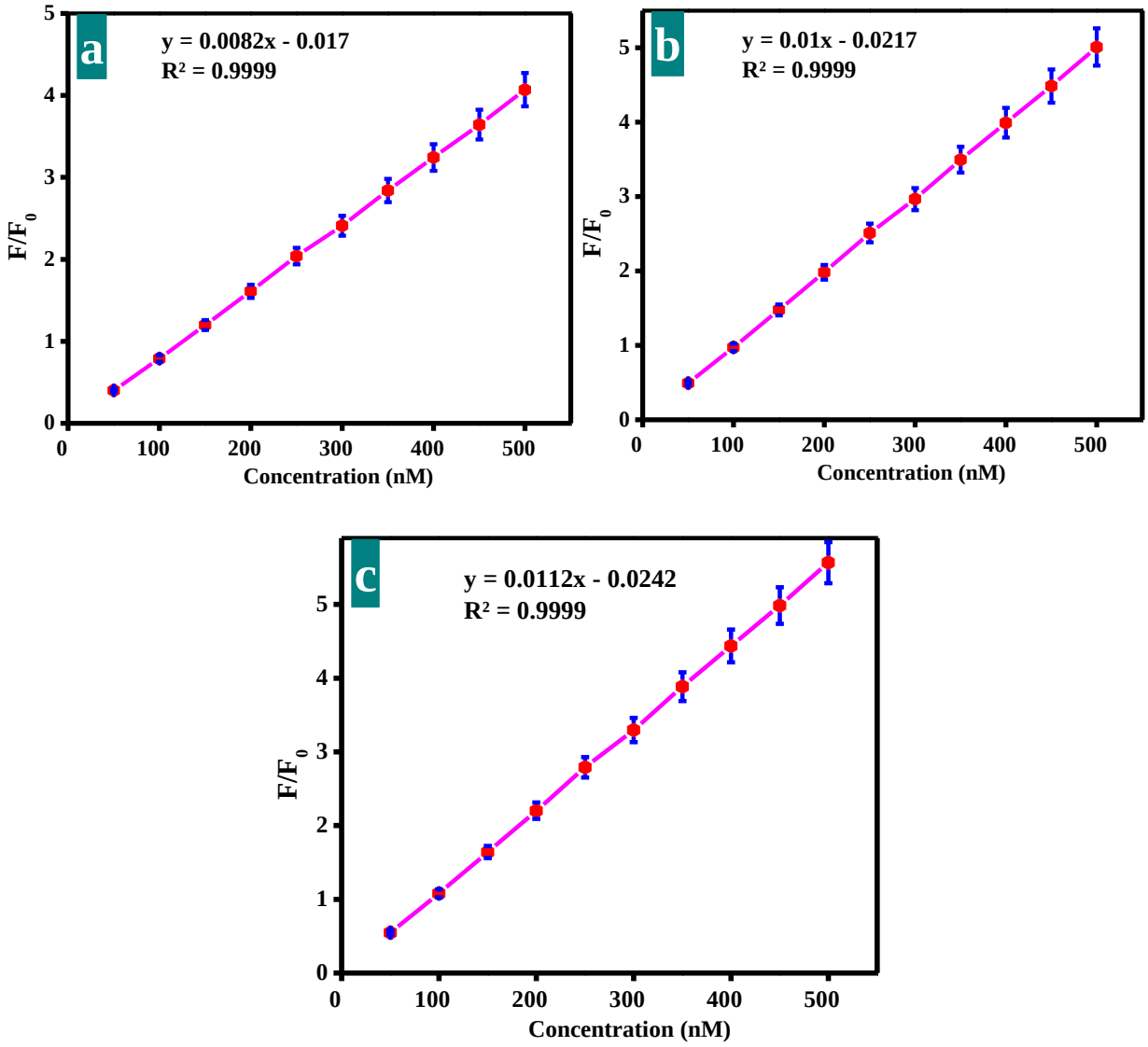


Fig. S10. Calibration curves demonstrating the linear fluorescence enhancement response probes **1a** (a), **1b** (b), and **1c** (c) towards CN^- ions in the range of 0–500 nM.

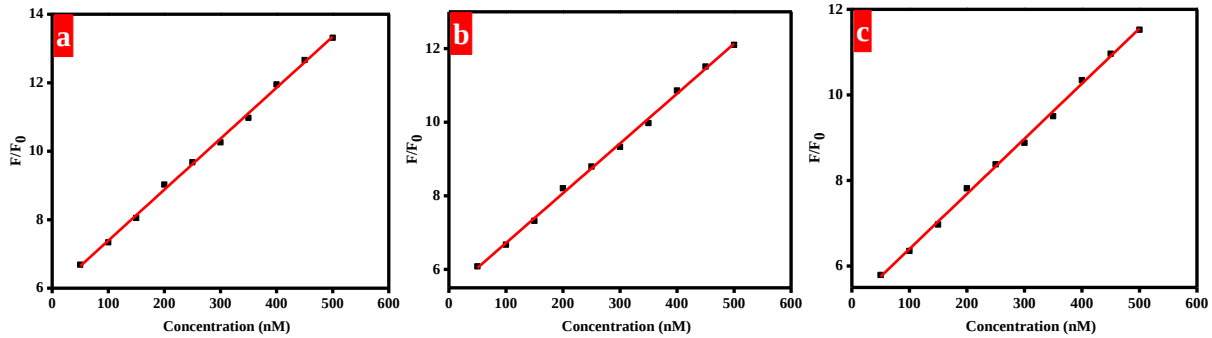


Fig. S11. Illustration of linear response of probes **1a** (a), **1b** (b), and **1c** (c) towards cyanide through the Benesi-Hildebrand plots.

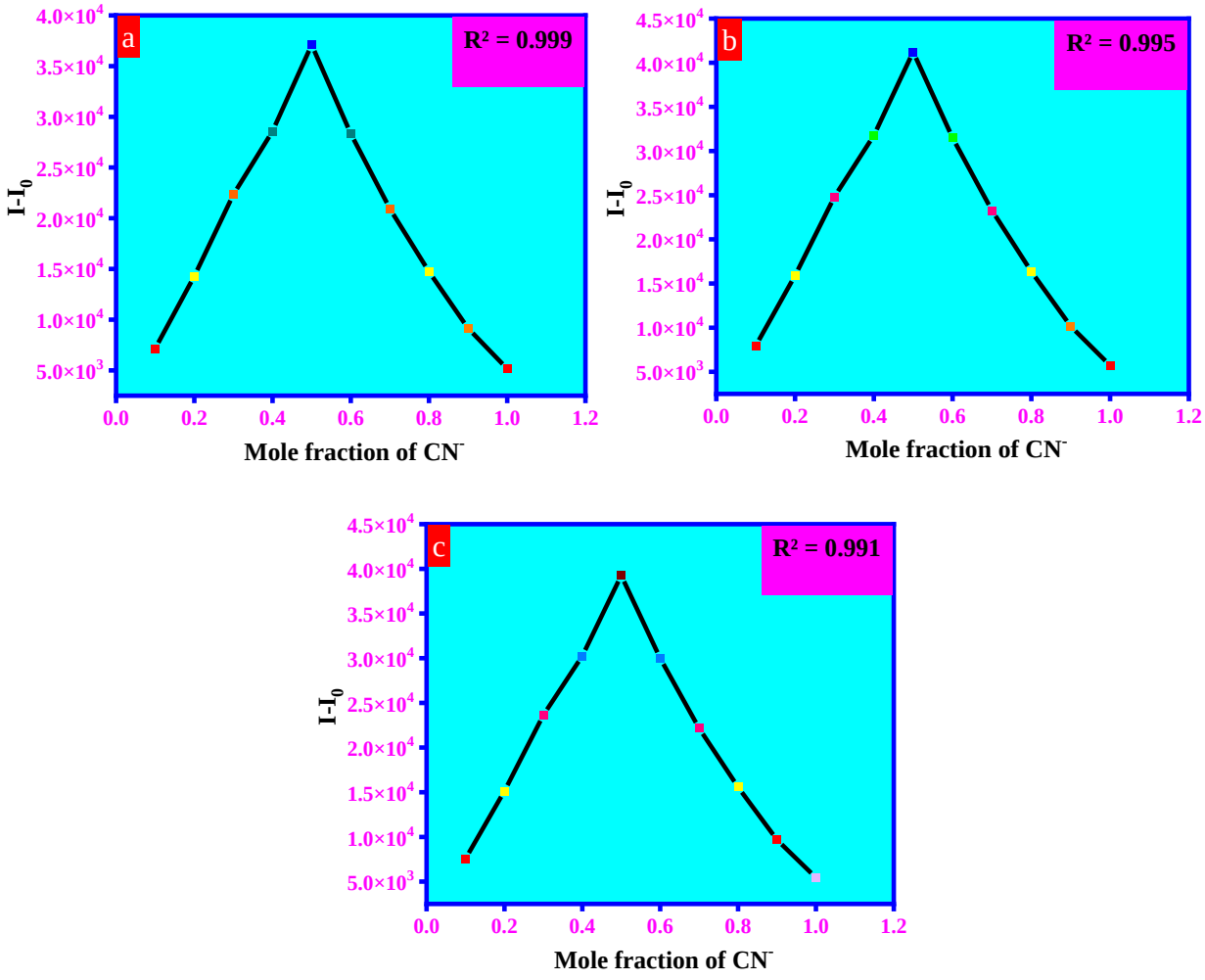


Fig. S12. Job's plots of probes **1a** (a), **1b** (b), and **1c** (c) upon the addition of 0–500 nM of CN^-.

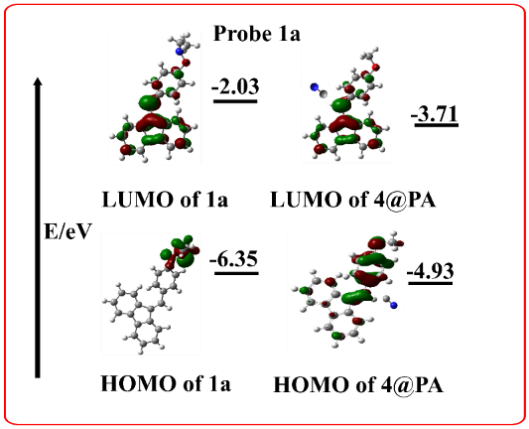


Fig. S13. The HOMO–LUMO energy level diagram for probe **1a** and their CN^- complexes.

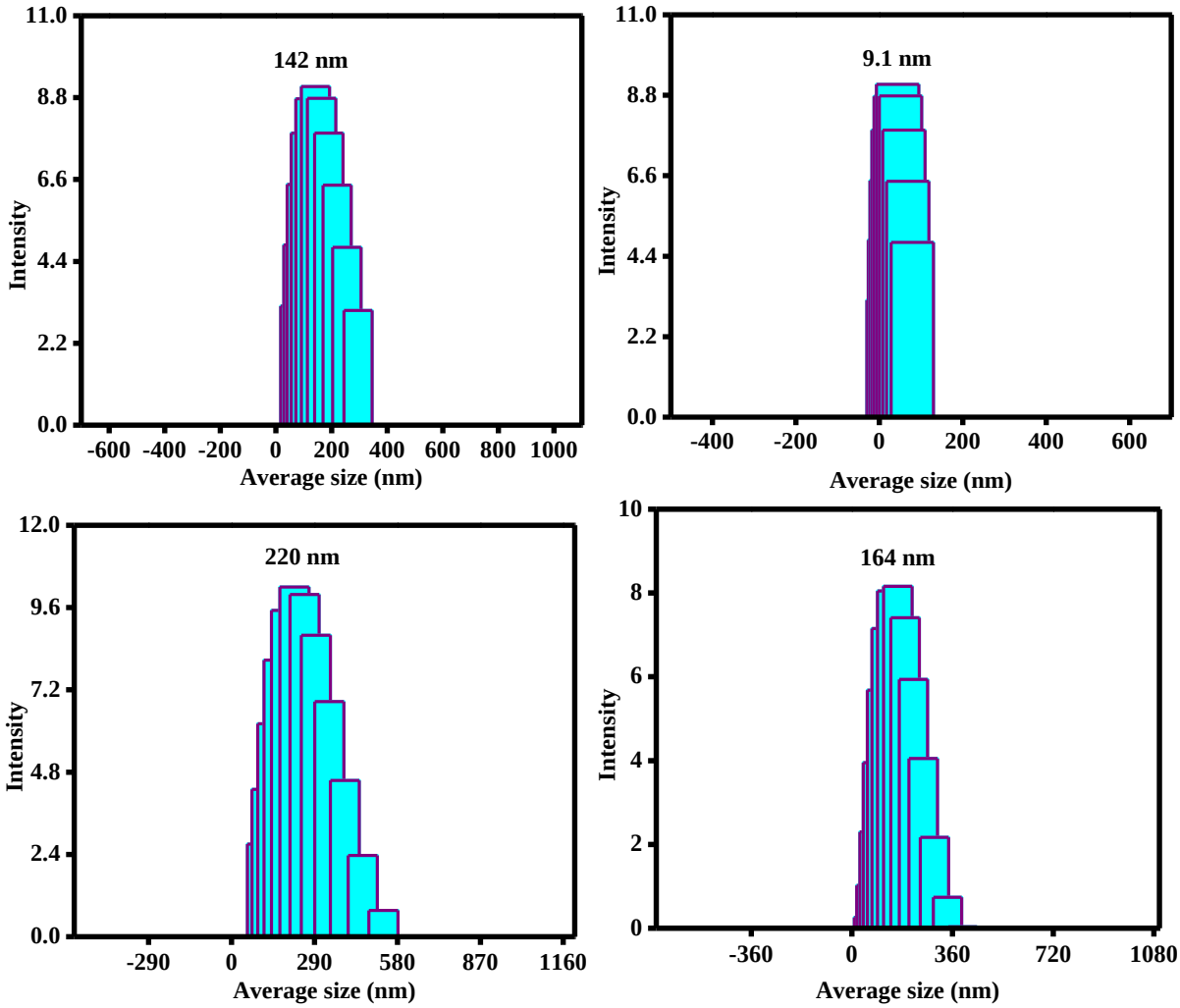


Fig. S14. Dynamic light scattering (DLS) measurements of probes **1a** and **1b** before and after the addition of 500 nM of CN^- (conc. = 20 μM (**1a**) and 50 μM (**1b**); solvent = H_2O/DMF (4:1, v/v).

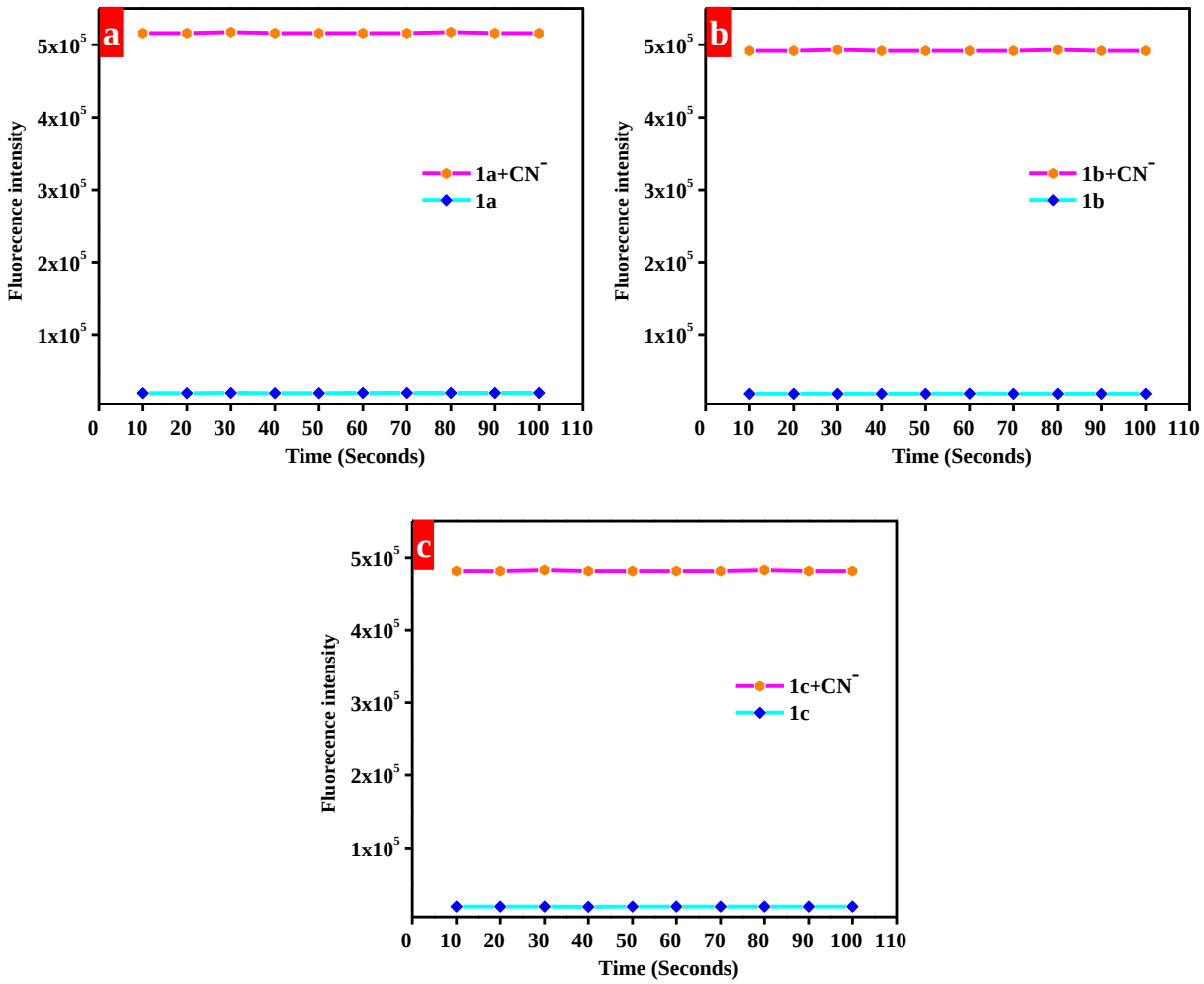
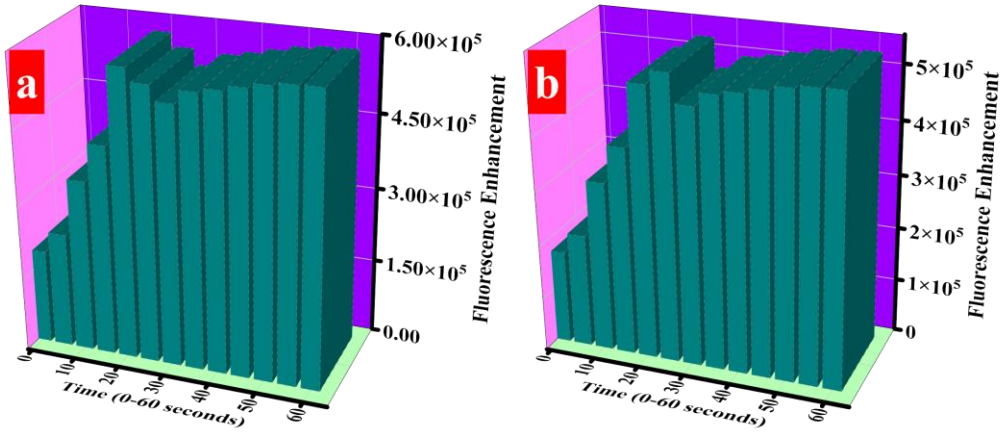


Fig. S15. Photostability test of probes **1a** (a), **1b** (b), and **1c** (c) and their probe–CN^- adducts.



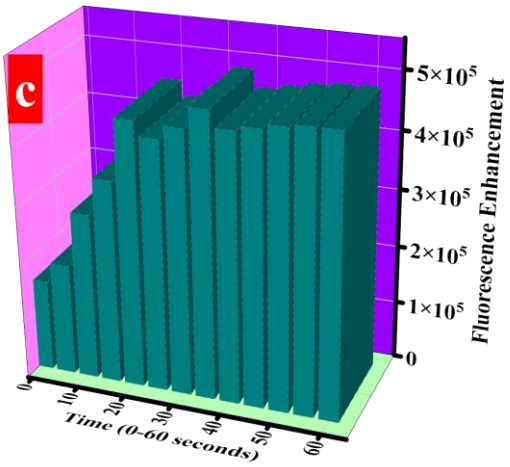


Fig. S16. Fluorescence spectra of probes **1a** (a), **1b** (b), and **1c** (c) as a function of time upon the addition of 500 nM of CN^- (conc. = 20 μM (**1a**), 50 μM (**1b**) and 10 μM (**1c**); λ_{ex} = 390 nm; slit width 2/2).

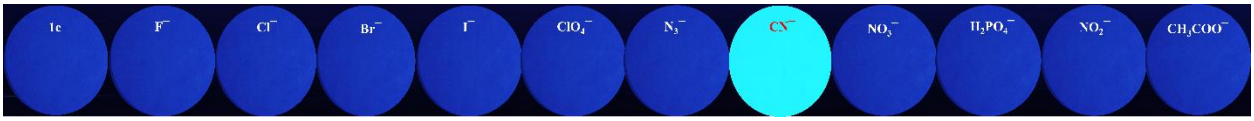


Fig. S17. Color change of probes' **1c** coated test strips upon dipping in THF solution of CN^- and other anions (500 nM).

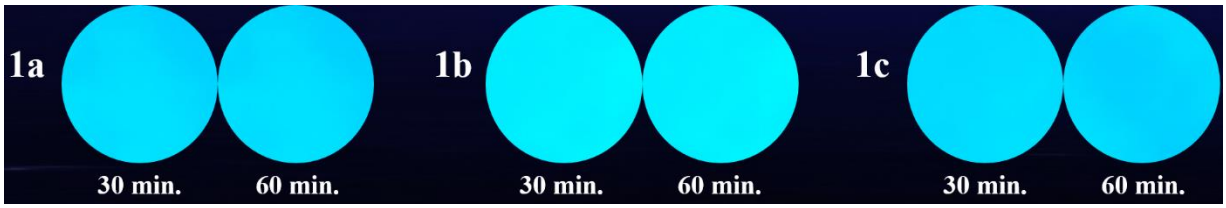


Fig. S18. Response of probes' coated tests strips when exposed to CN^- after regular interval of time.

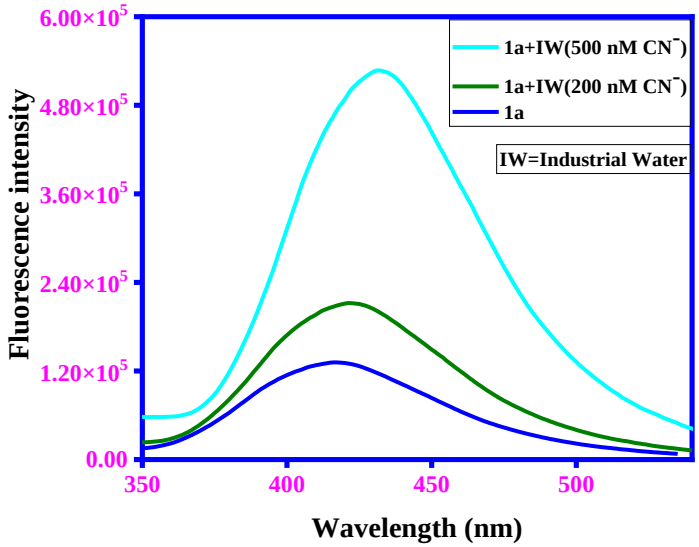


Fig. S19. Fluorescence spectra of probes **1a** upon the addition of industrial wastewater containing CN^- (200 and 500 nM) (conc. = 20 μM (**1a**); λ_{ex} = 390 nm; slit width 2/2).

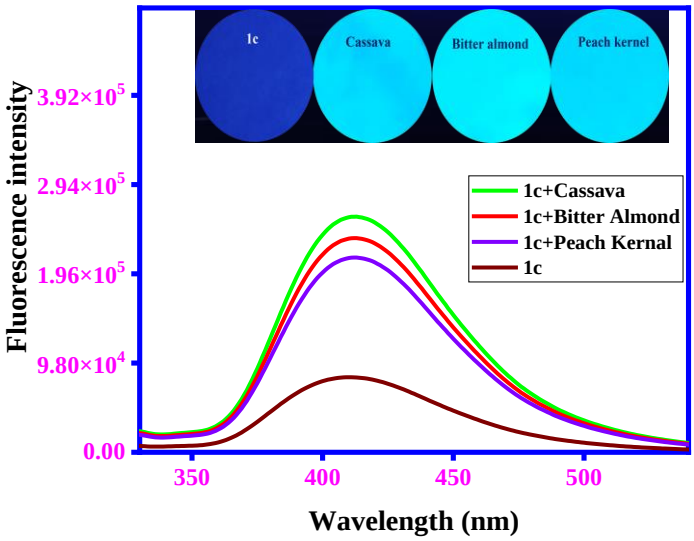


Fig. S20. Fluorescence spectra of probes **1c** upon the addition of H_2O/DMF (4:1, v/v) solution of peach kernel, bitter almond, and cassava powder (conc. = 20 μM (**1a**), 50 μM (**1b**) and 10 μM (**1c**); λ_{ex} = 390 nm; slit width 2/2).

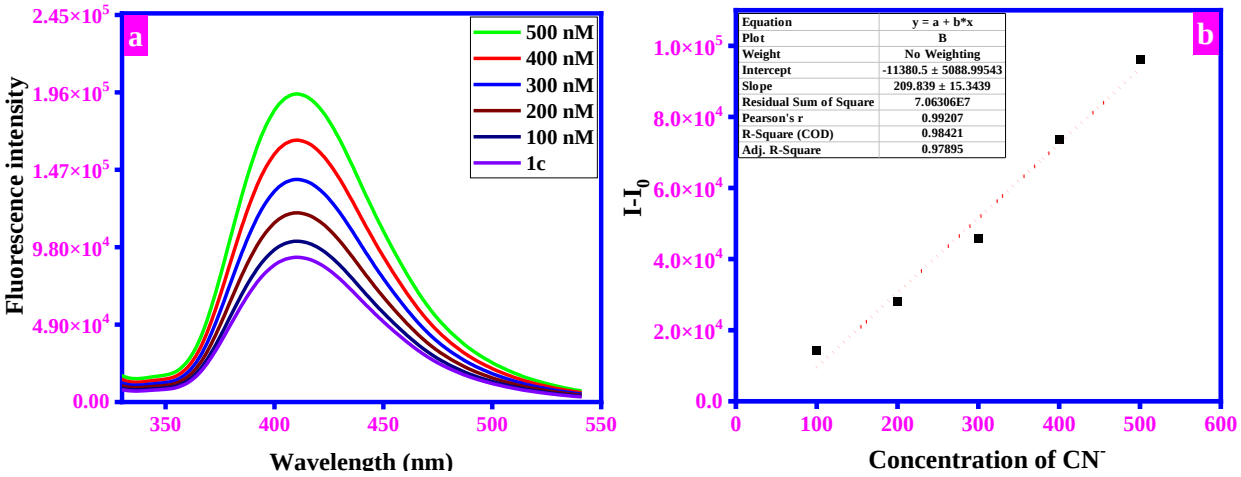


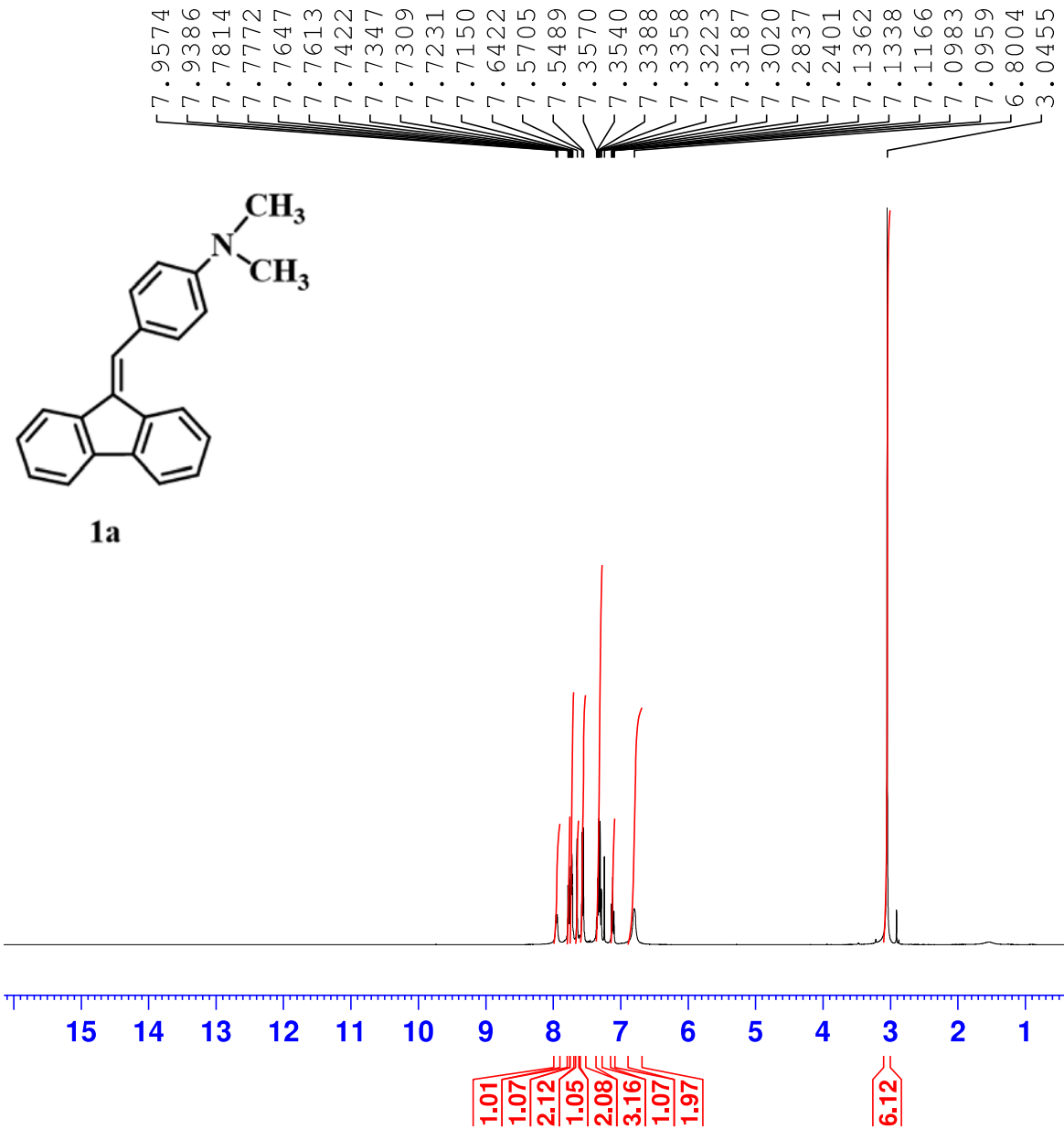
Fig. S21. Fluorescence spectra (a) and calibration curve (b) for the quantitation of CN^- ions in cassava food samples.

Table S1. Analysis of variance (ANOVA) for the linear fit model calculated for the method.

Analyte	Parameter	[a]SS	[b]DF	[c]MS	[d]*F*
CN^-	Model	2340304.0	1	2452300.0	4860.9
	Residue	8244.35	12	8162.75	
	Lack of fit	2142.33	3	857.75	0.8955
	Pure error	6755.27	11	773.41	

[a]SS: sum of squares // [b]DF: Degrees of freedom // [c]MQ: mean of the squares // [d]F_{critic} = 3.631// [d]F_{critic} = 4.098

Compound 1a, 1H NMR (400 MHz, CDCl3)

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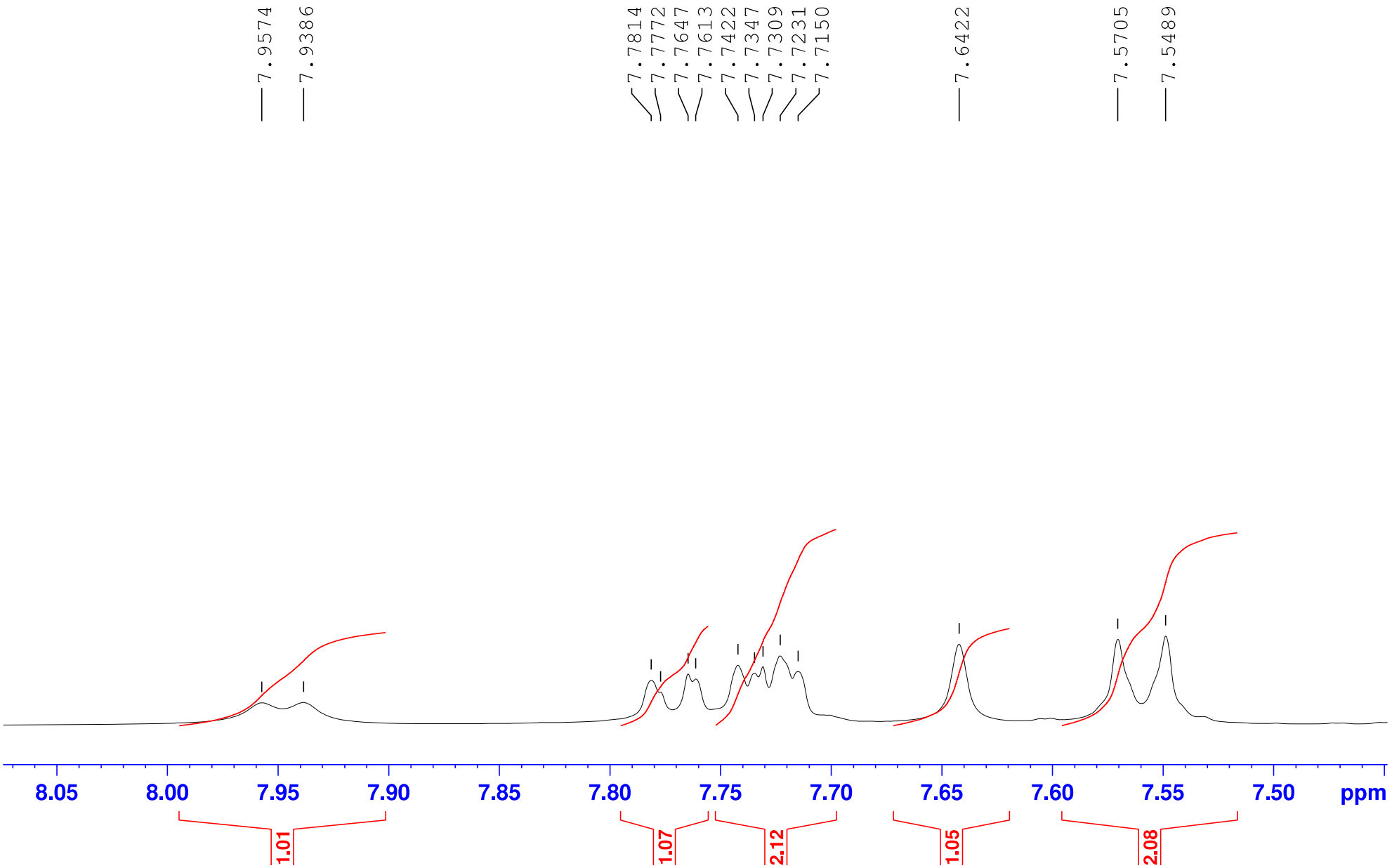

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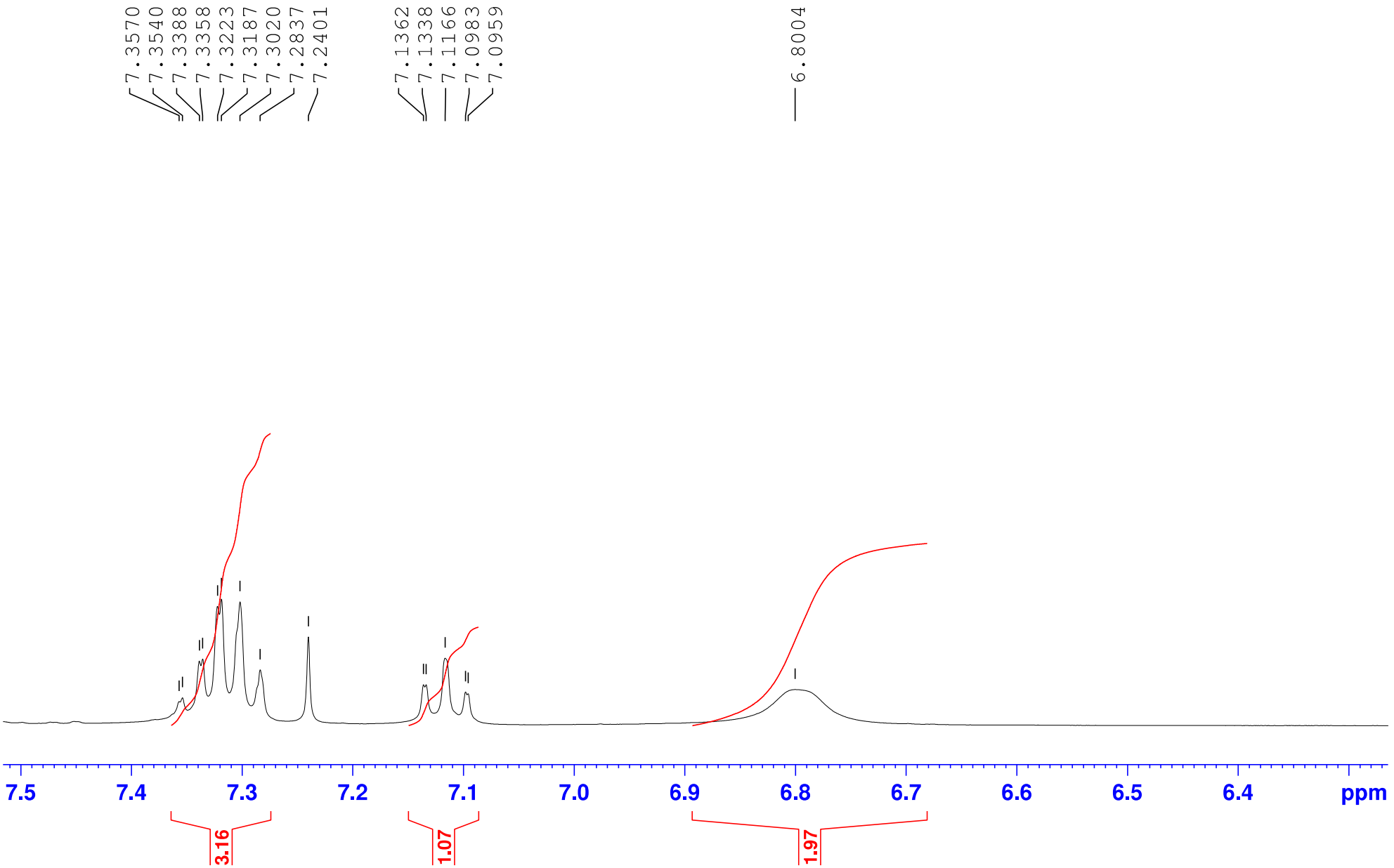

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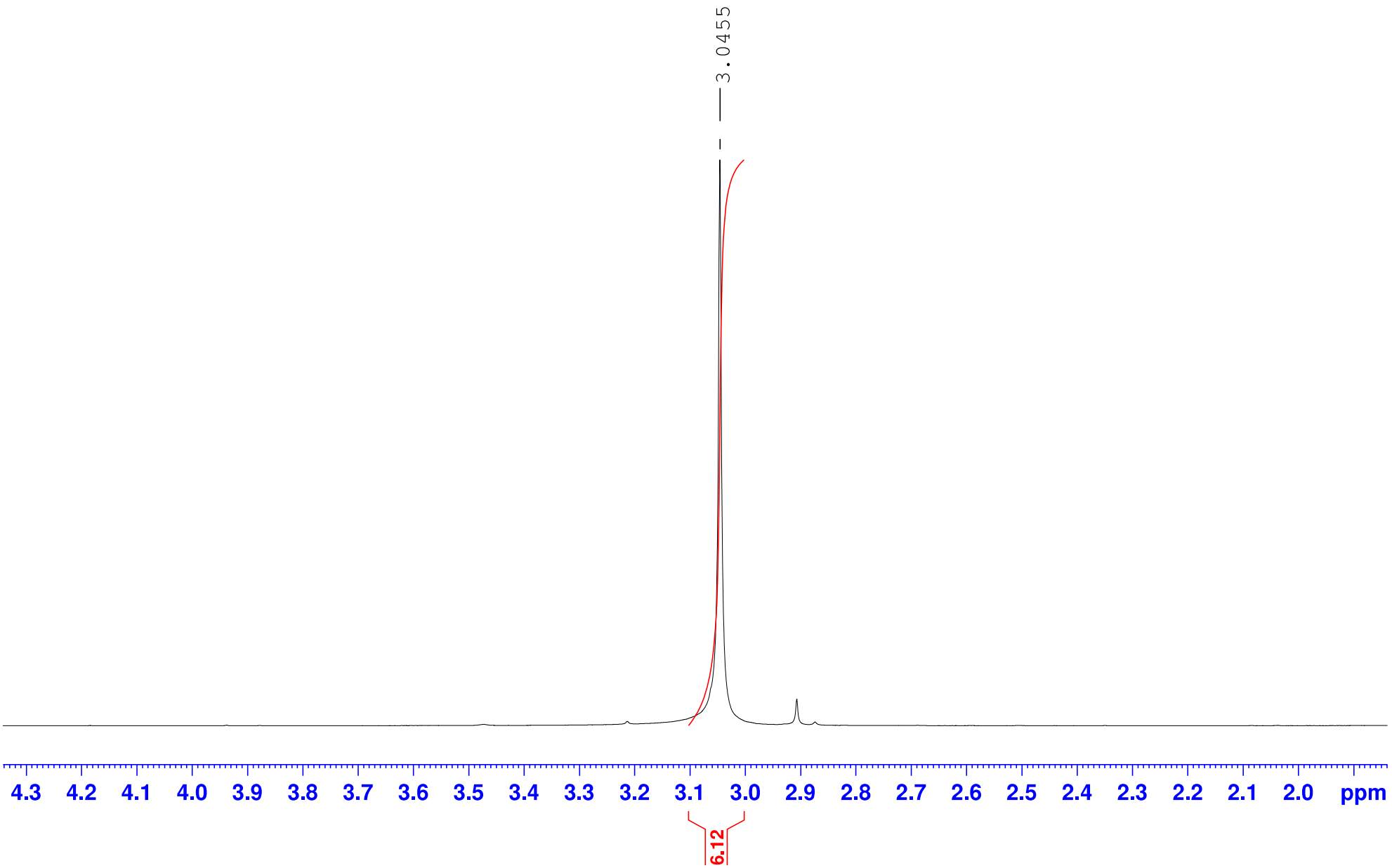

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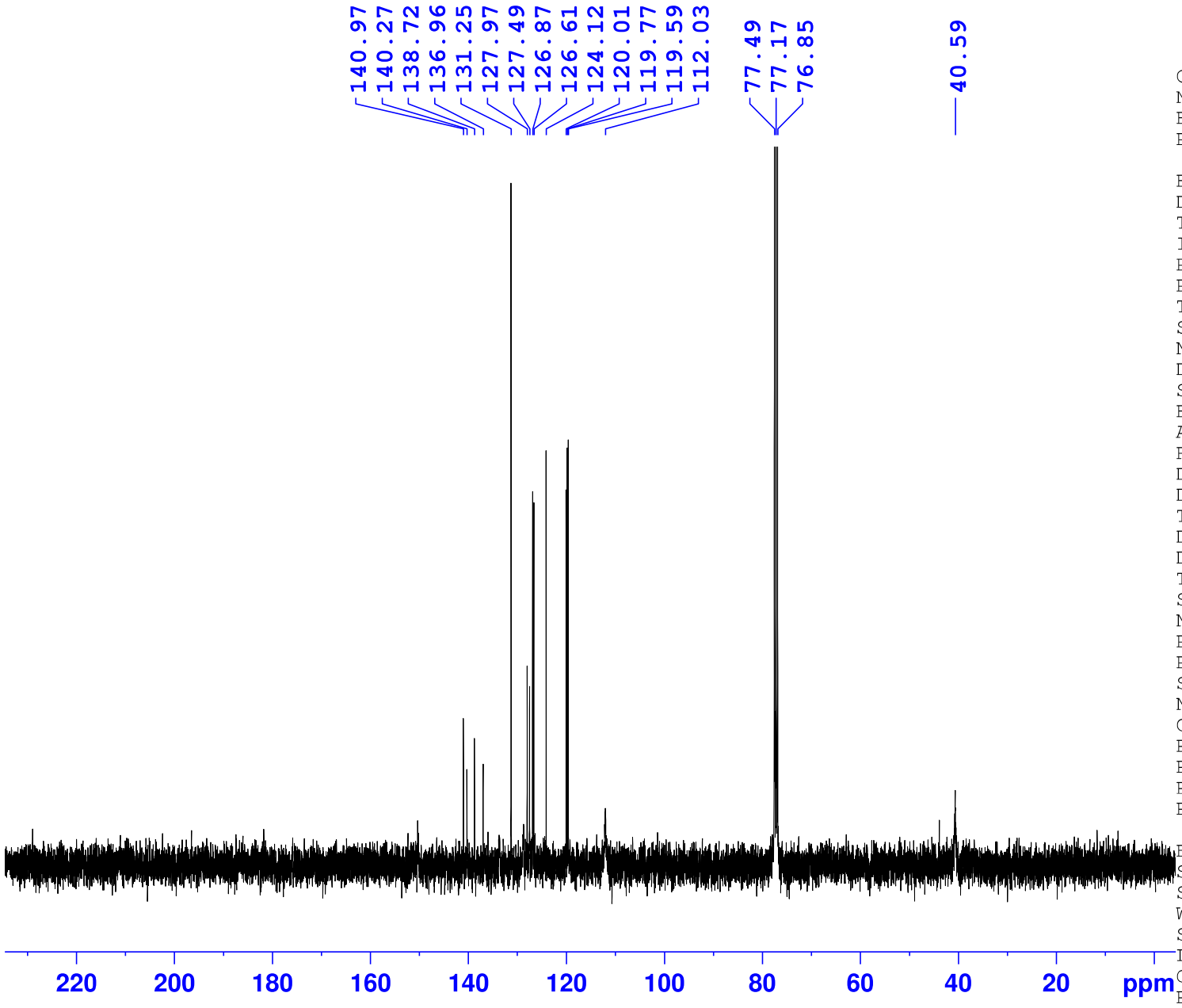


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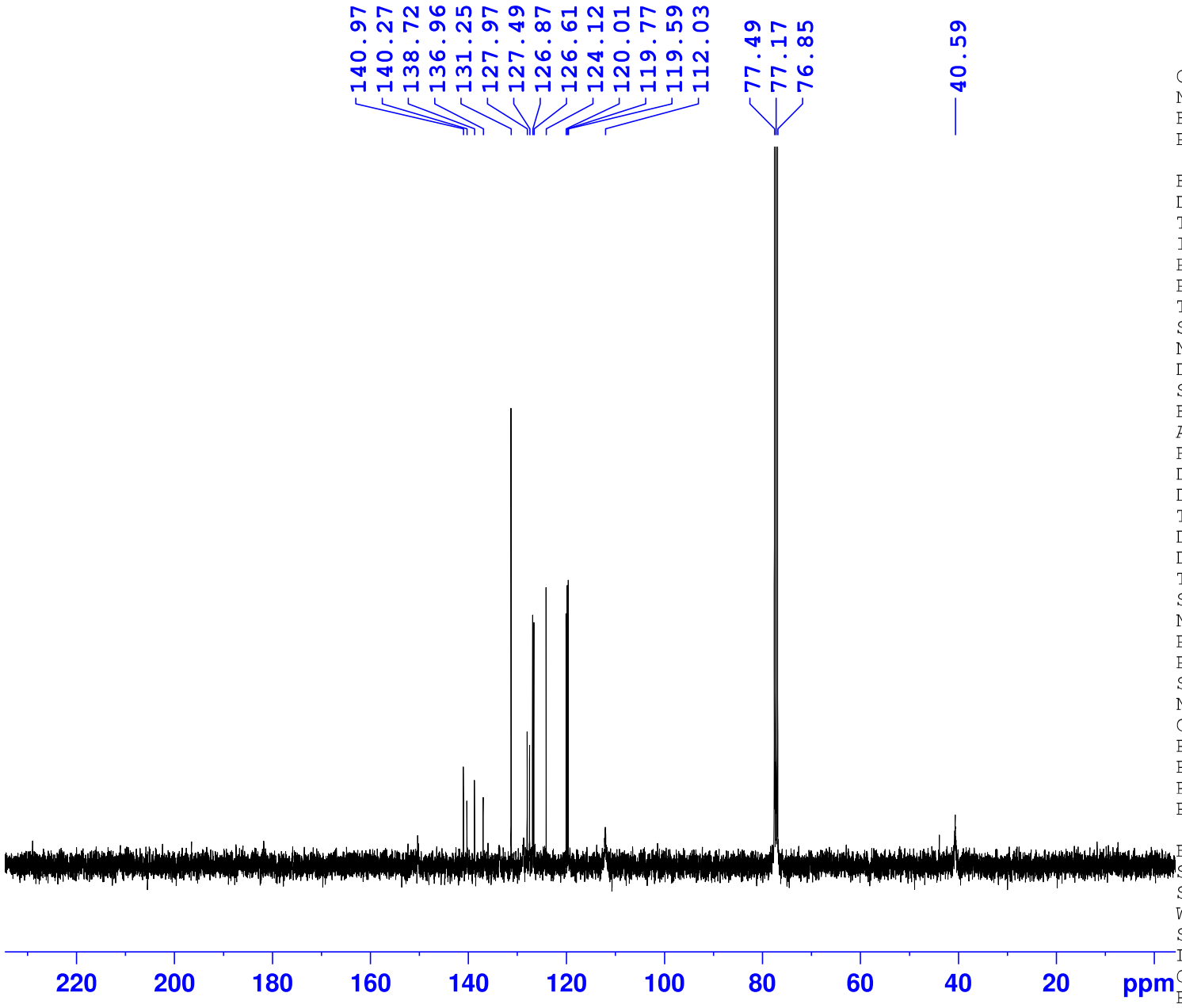


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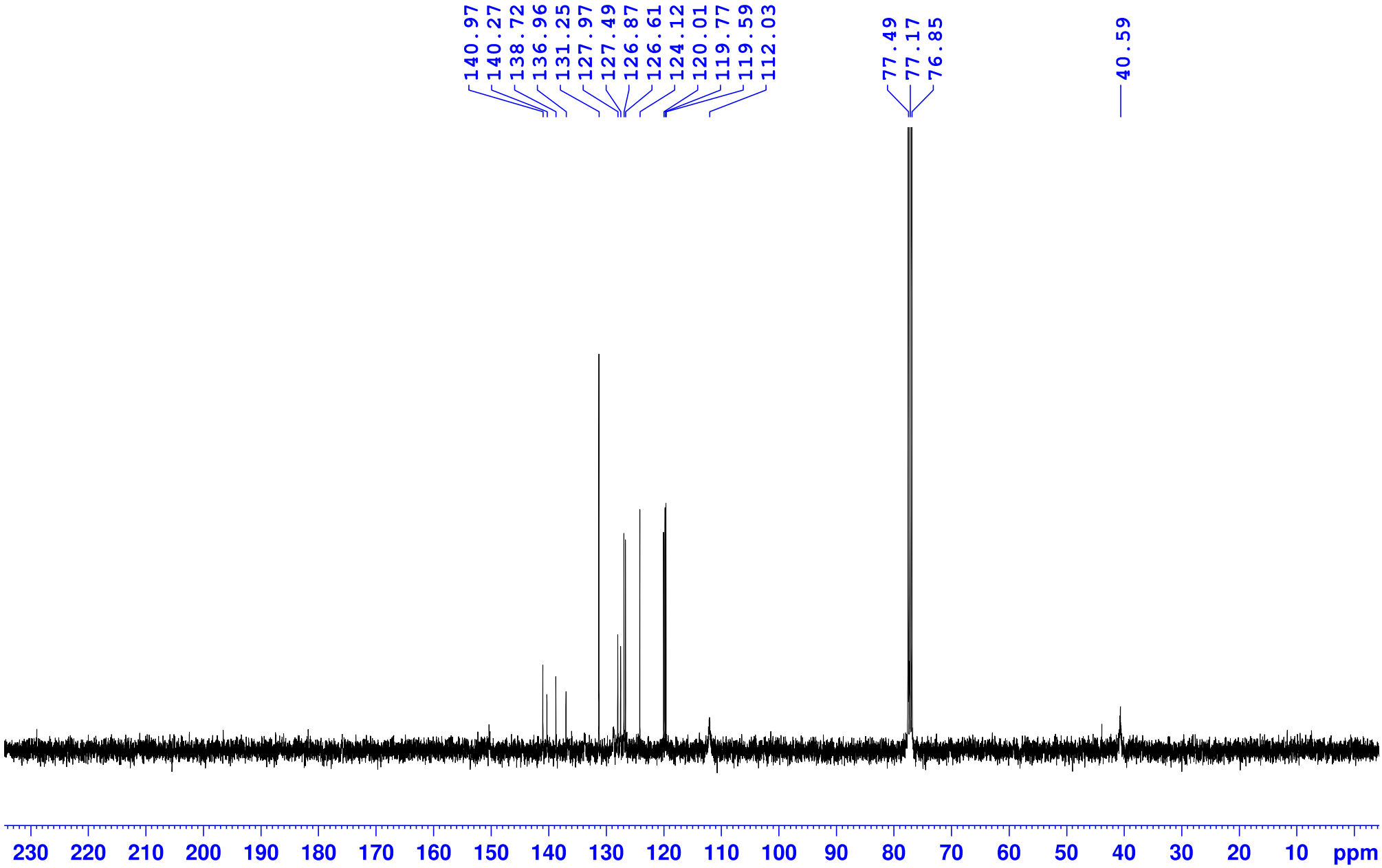

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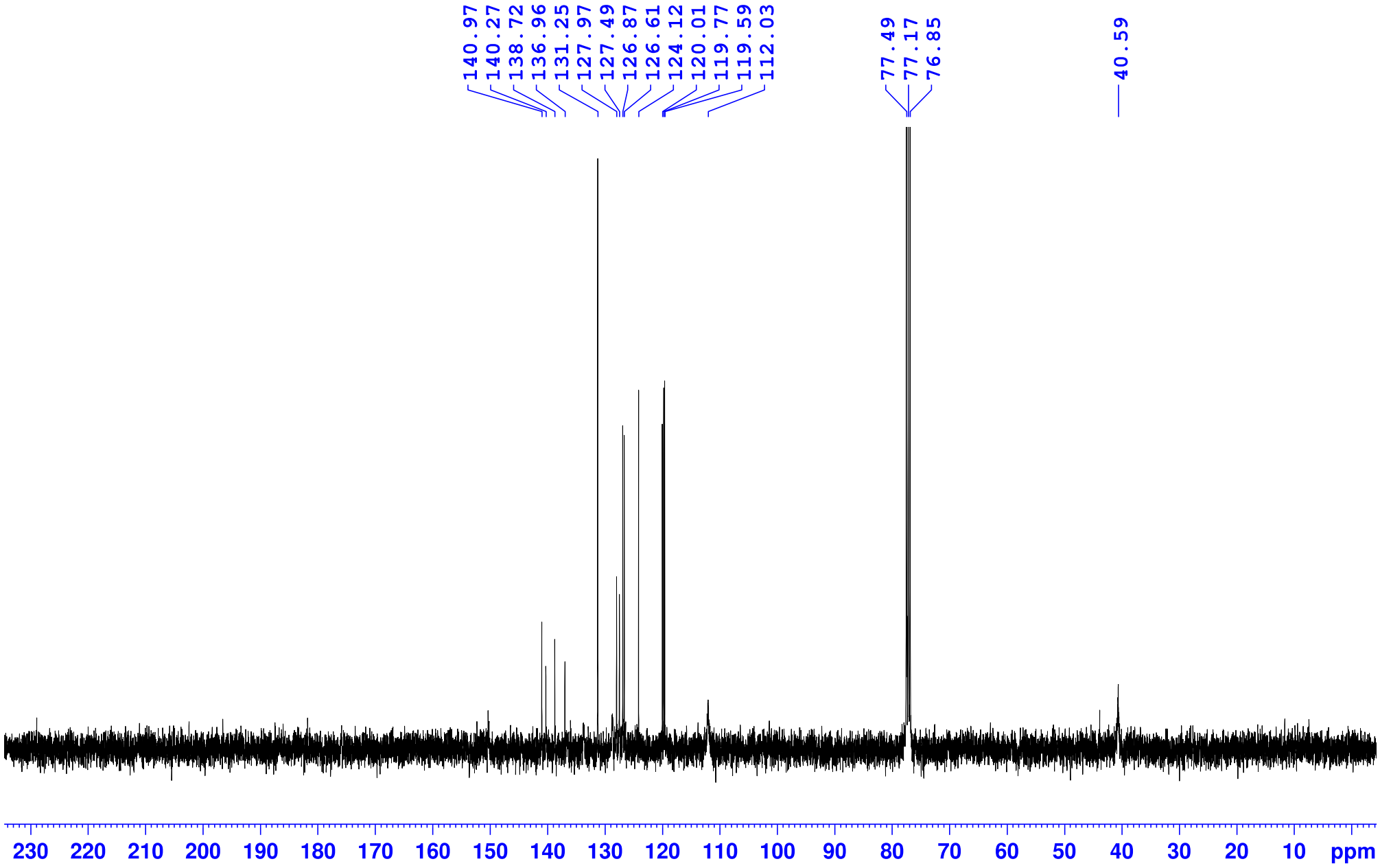

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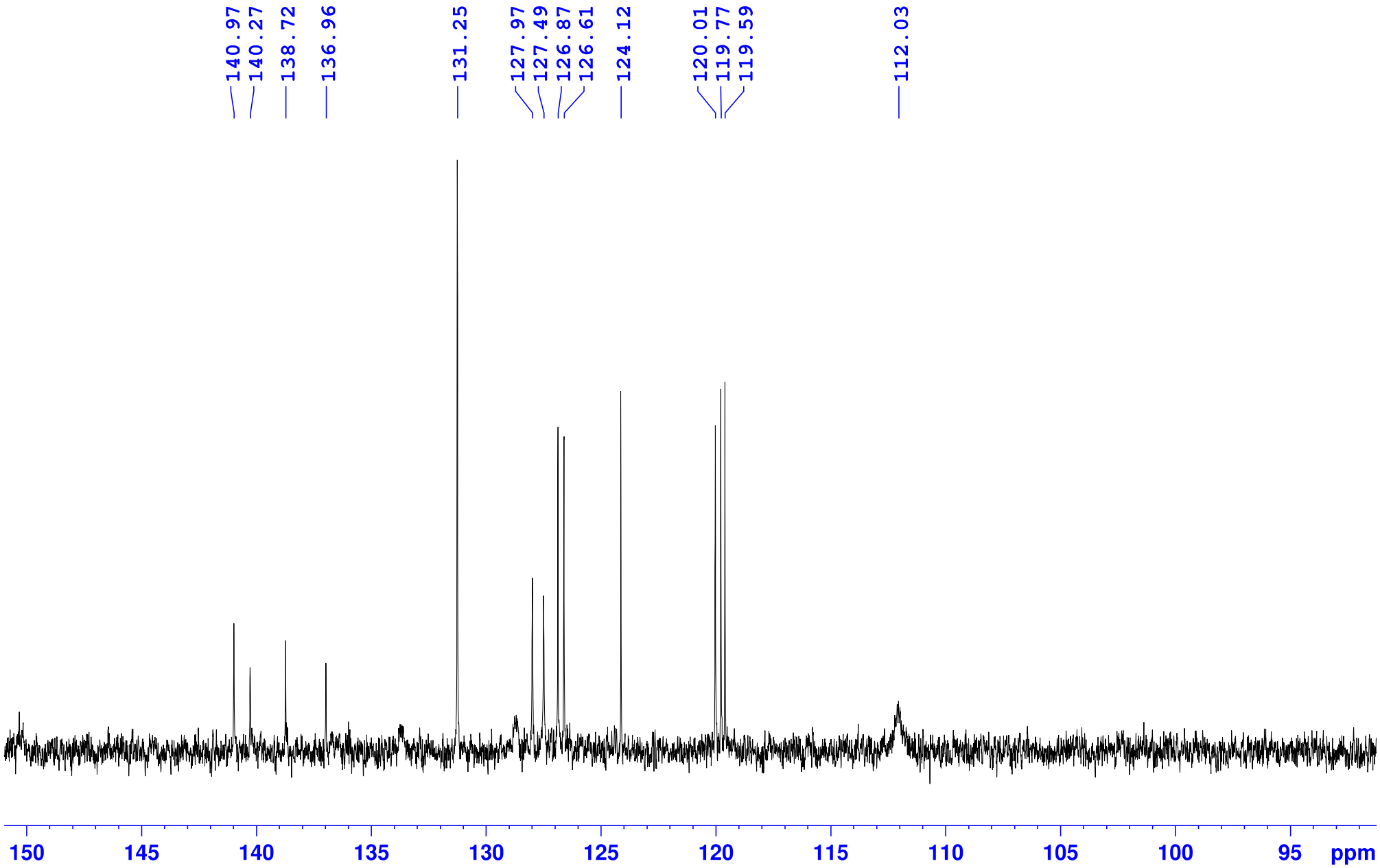

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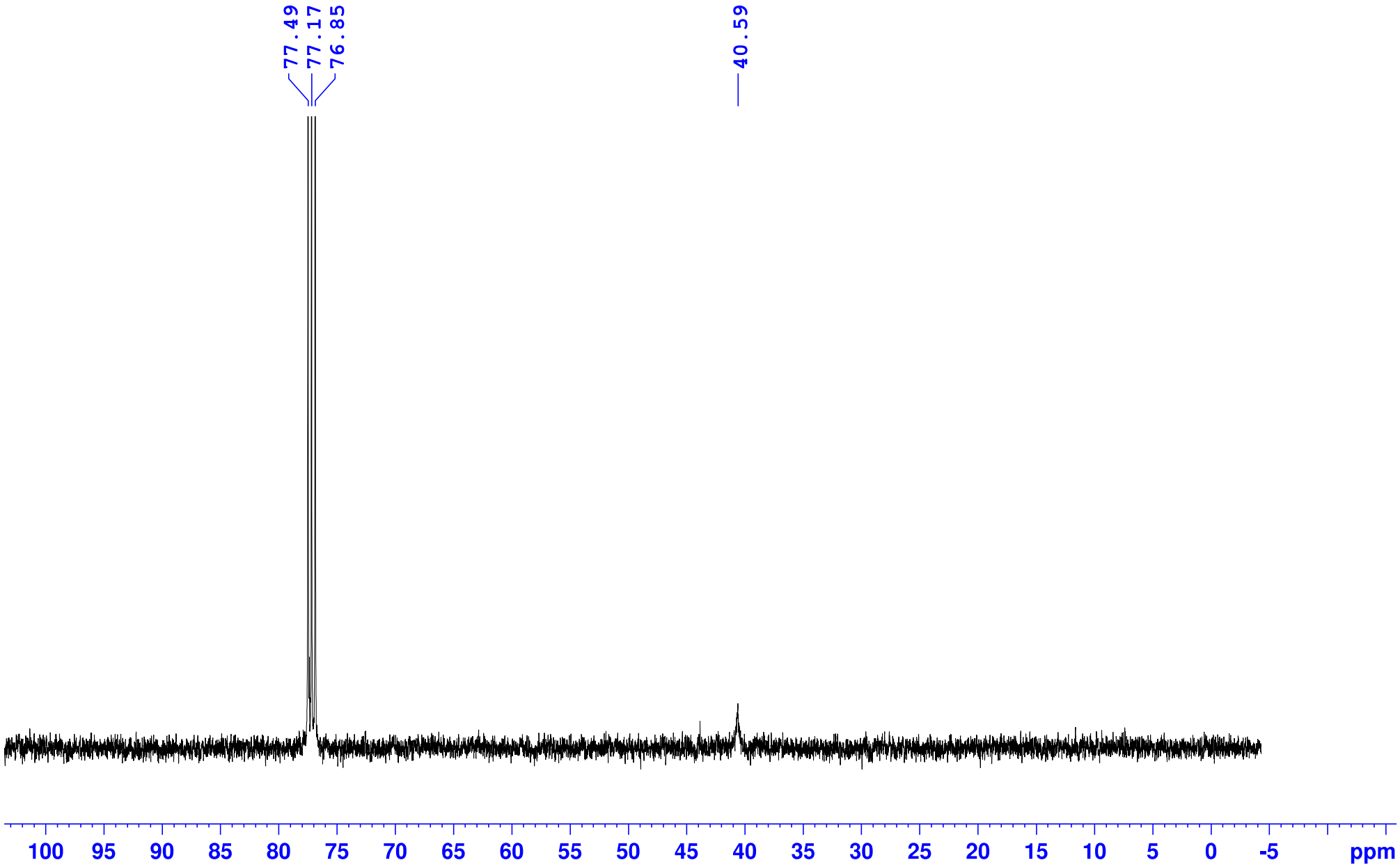

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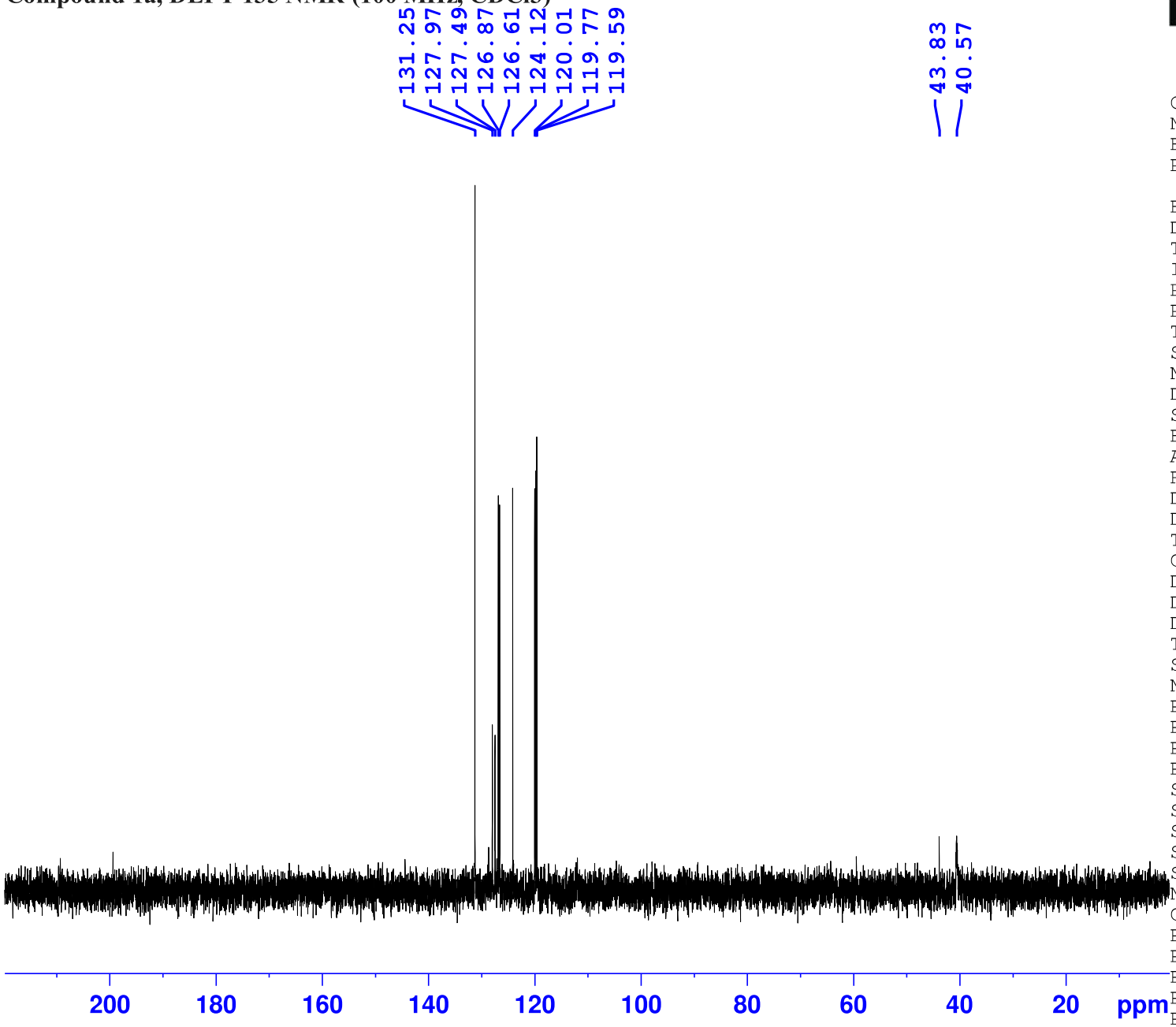

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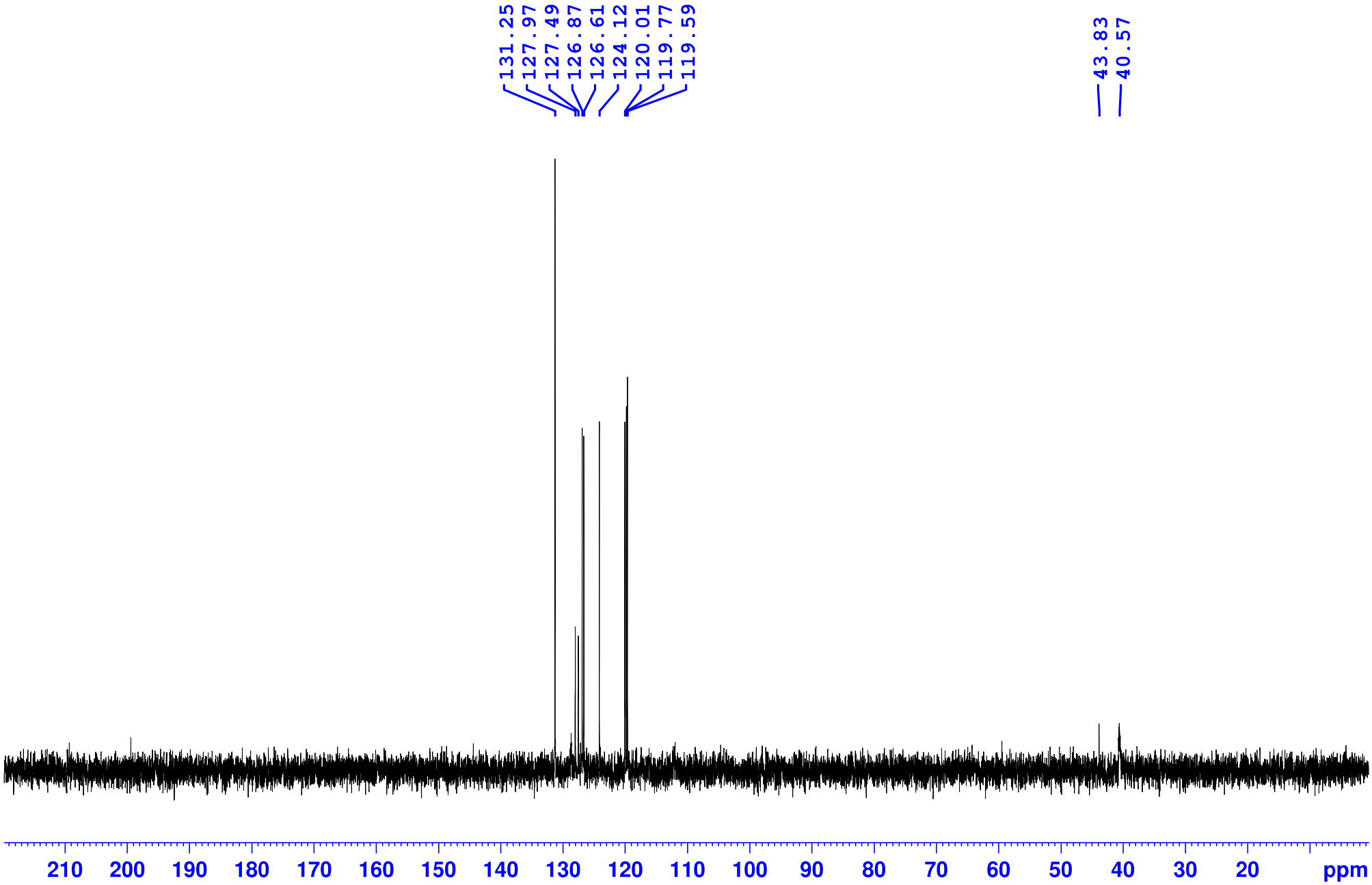
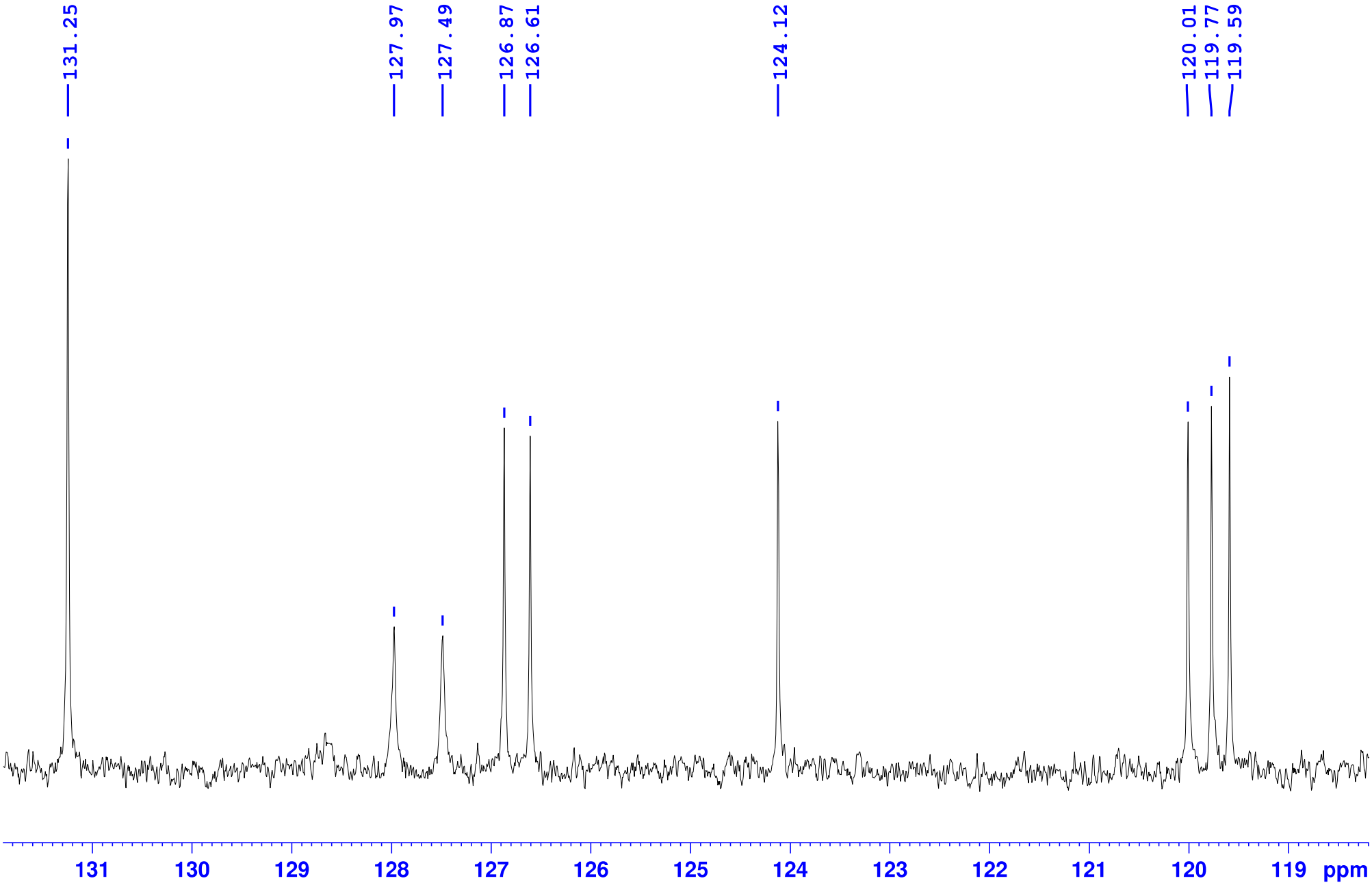
SFO1 100.6238359 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 72.56700134 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 11.08699989 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
P3 10.00 usec
P4 20.00 usec
PCPD2 90.00 usec
PLW2 16.68099976 W
PLW12 0.20593999 W

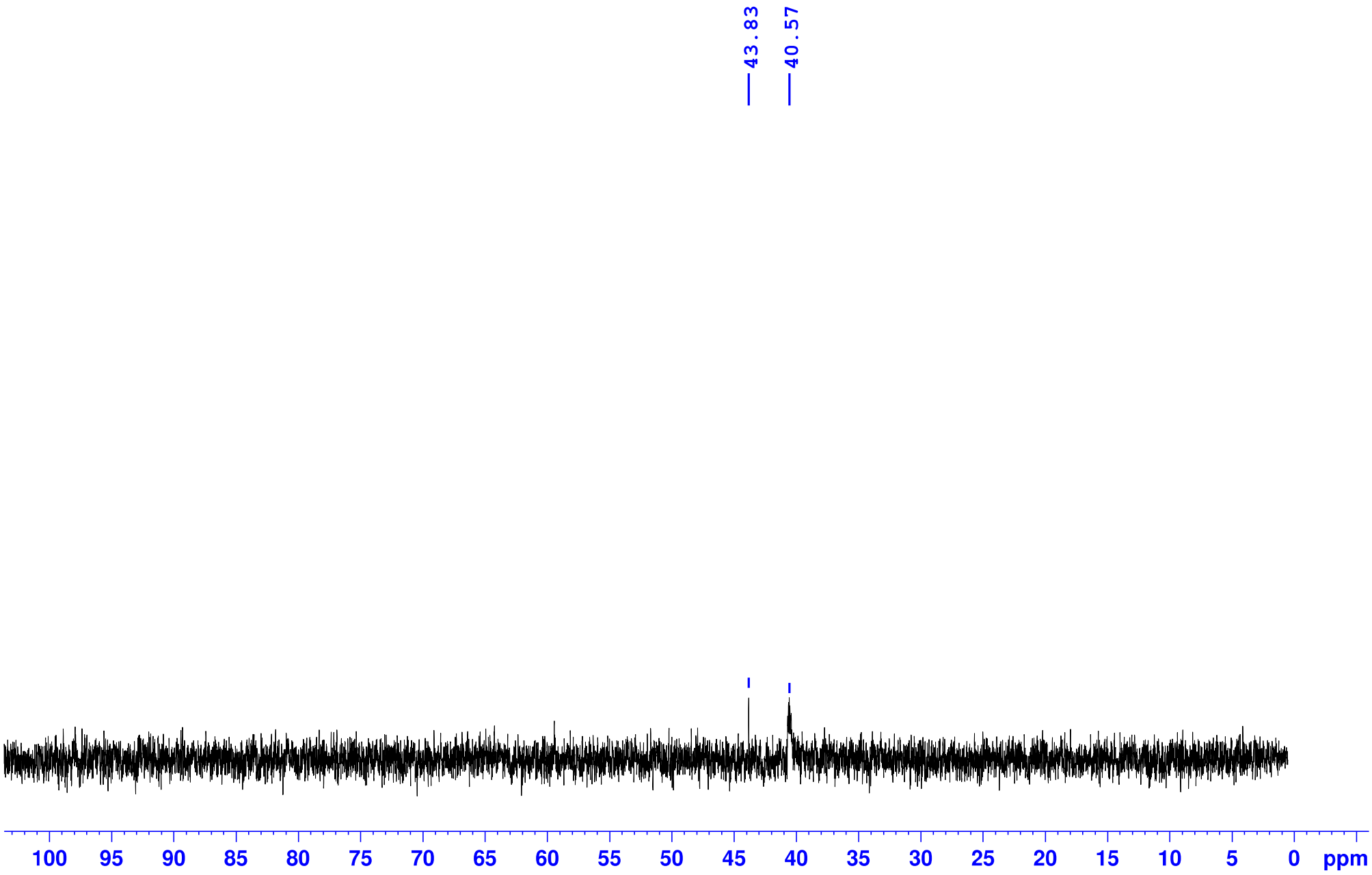
Compound 1a, DEPT 135 NMR (100 MHz, CDCl3)



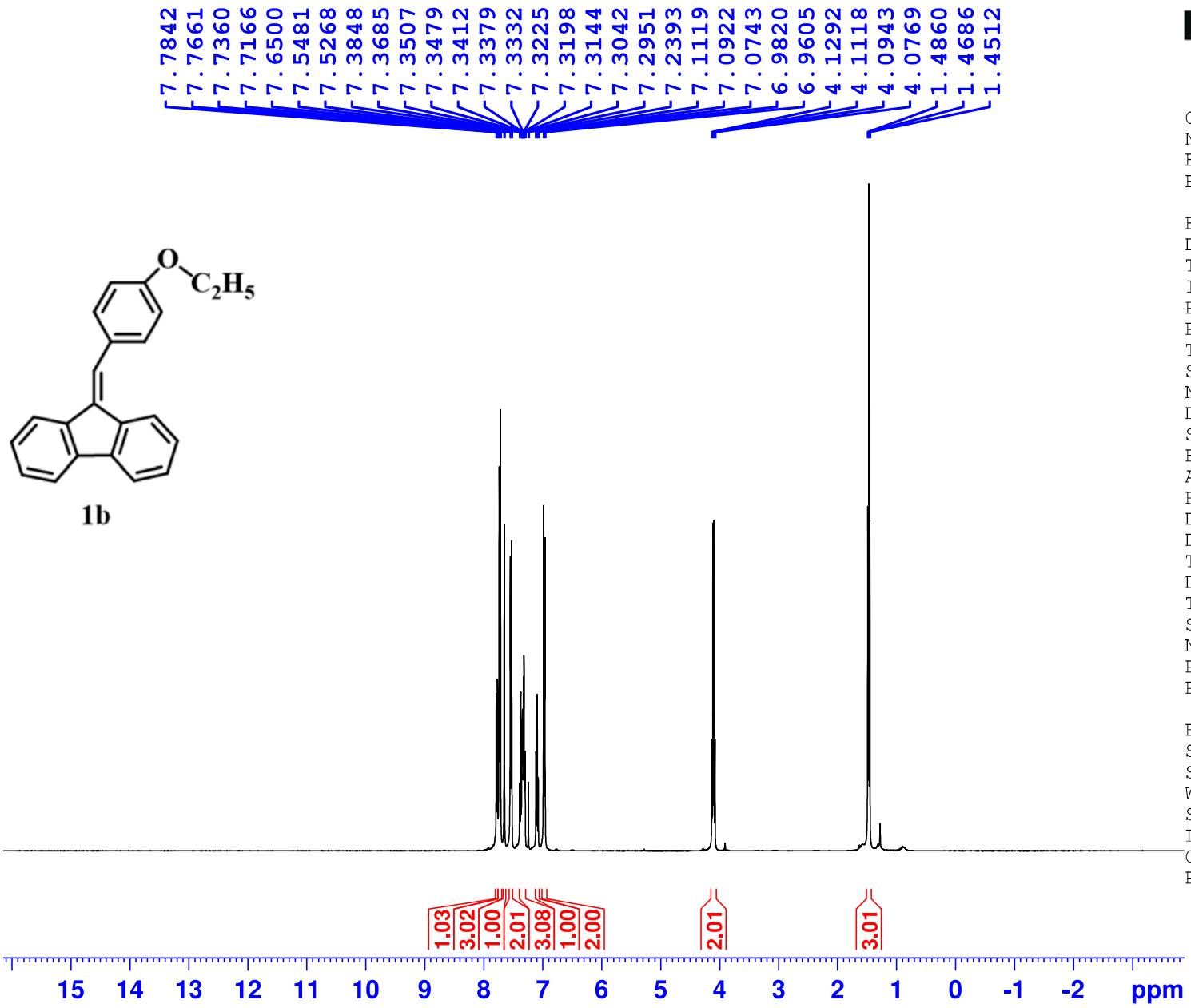
Compound 1a, DEPT 135 NMR (100 MHz, CDCl3)



Compound 1a, DEPT 135 NMR (100 MHz, CDCl3)



Compound 1b, 1H NMR (400 MHz, CDCl3)

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Current Data Parameters
NAME                  SMT-7
EXPNO                   156
PROCNO                    1

F2 - Acquisition Parameters
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Time                  15.45 h
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PROBHD    Z116098_0621 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES             0.244532 Hz
AQ                 4.0894465 sec
RG                     31.9
DW                    62.400 usec
DE                     6.50 usec
TE                    298.0 K
D1              1.00000000 sec
TD0                       1
SFO1           400.1324708 MHz
NUC1                    1H
P1                    10.00 usec
PLW1           16.68099976 W

F2 - Processing parameters
SI                    65536
SF             400.1300172 MHz
WDW                     EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
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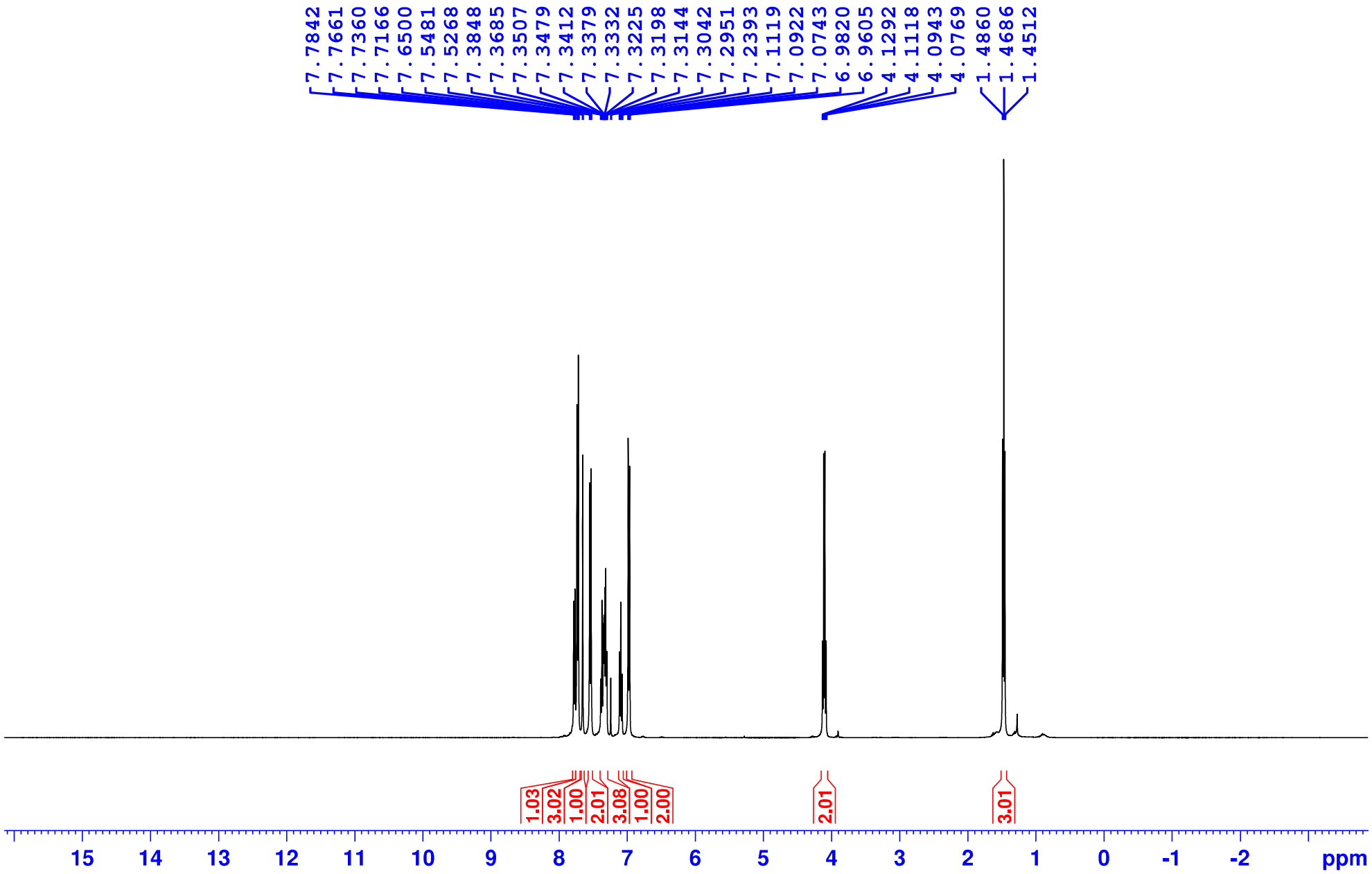
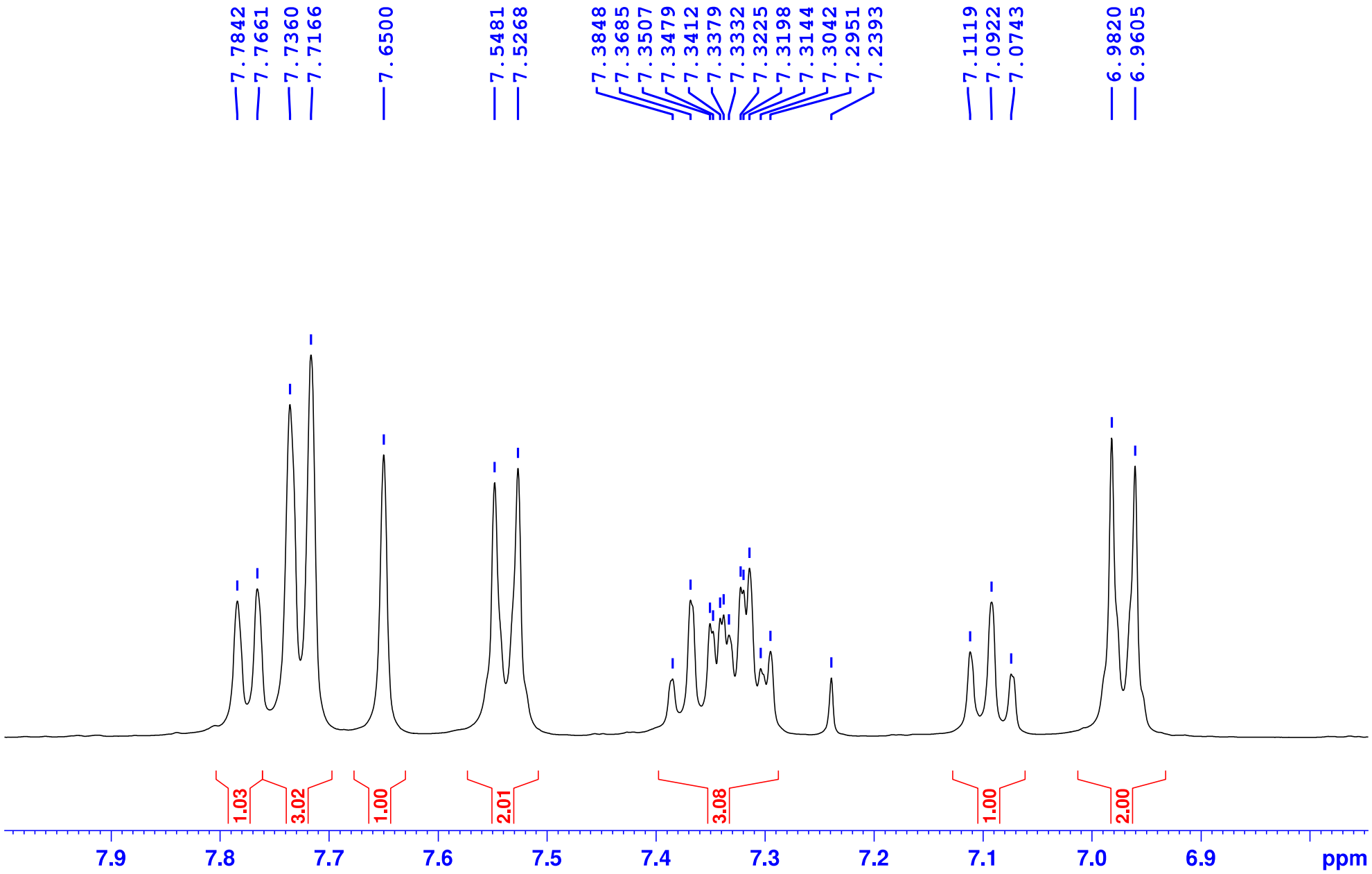
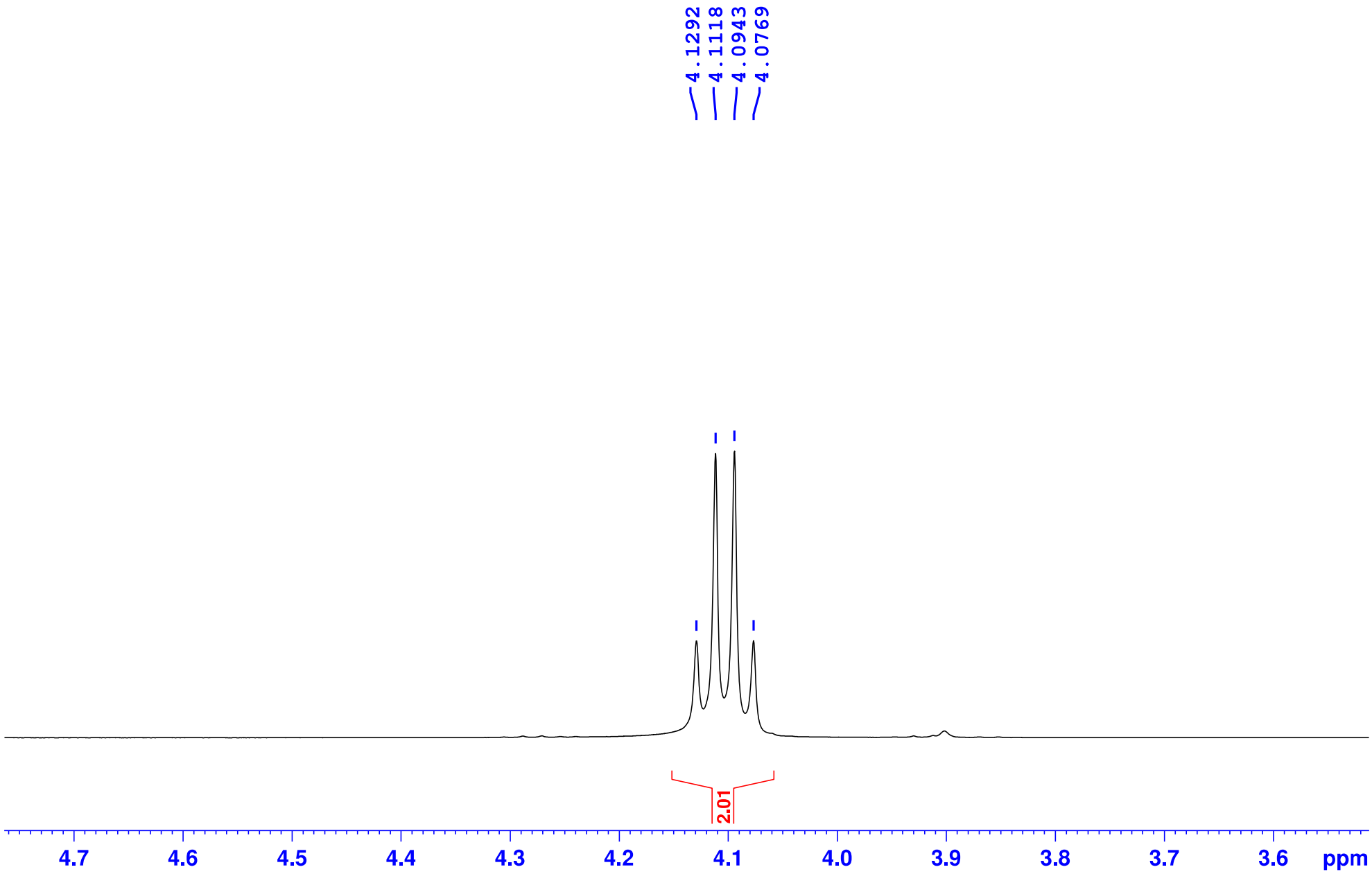
Compound 1b, 1H NMR (400 MHz, CDCl3)



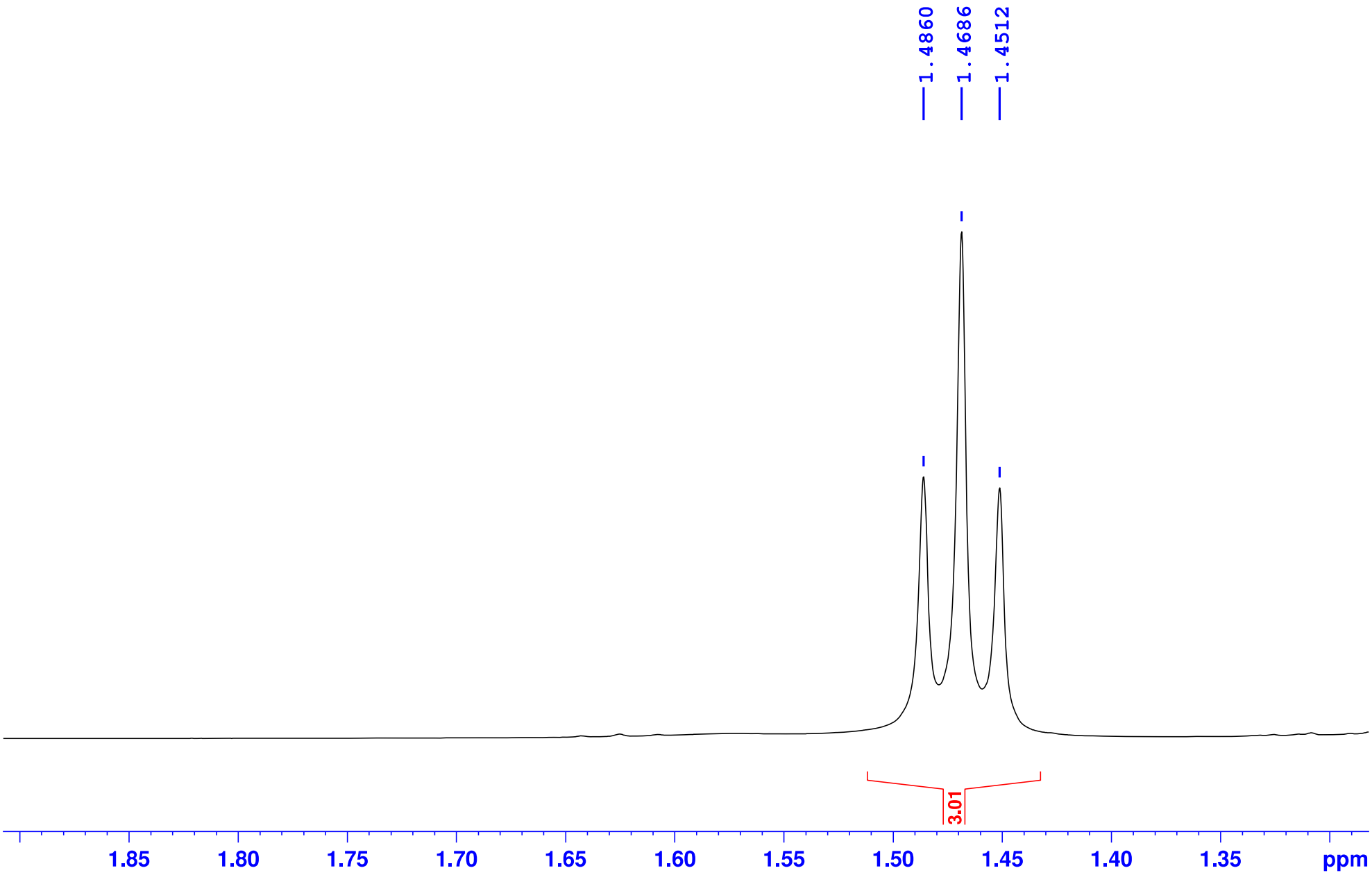
Compound 1b, 1H NMR (400 MHz, CDCl3)



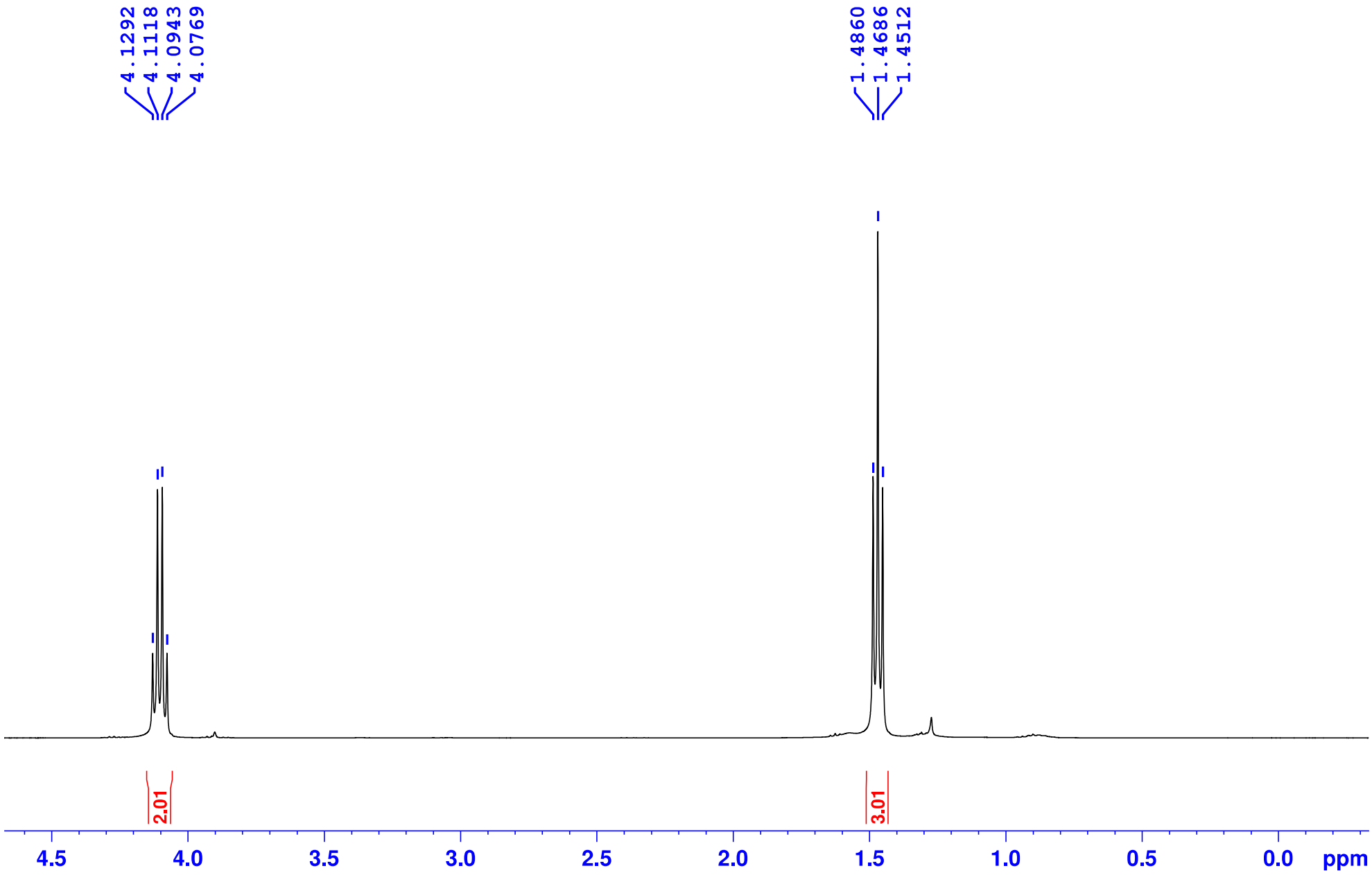
Compound 1b, 1H NMR (400 MHz, CDCl3)



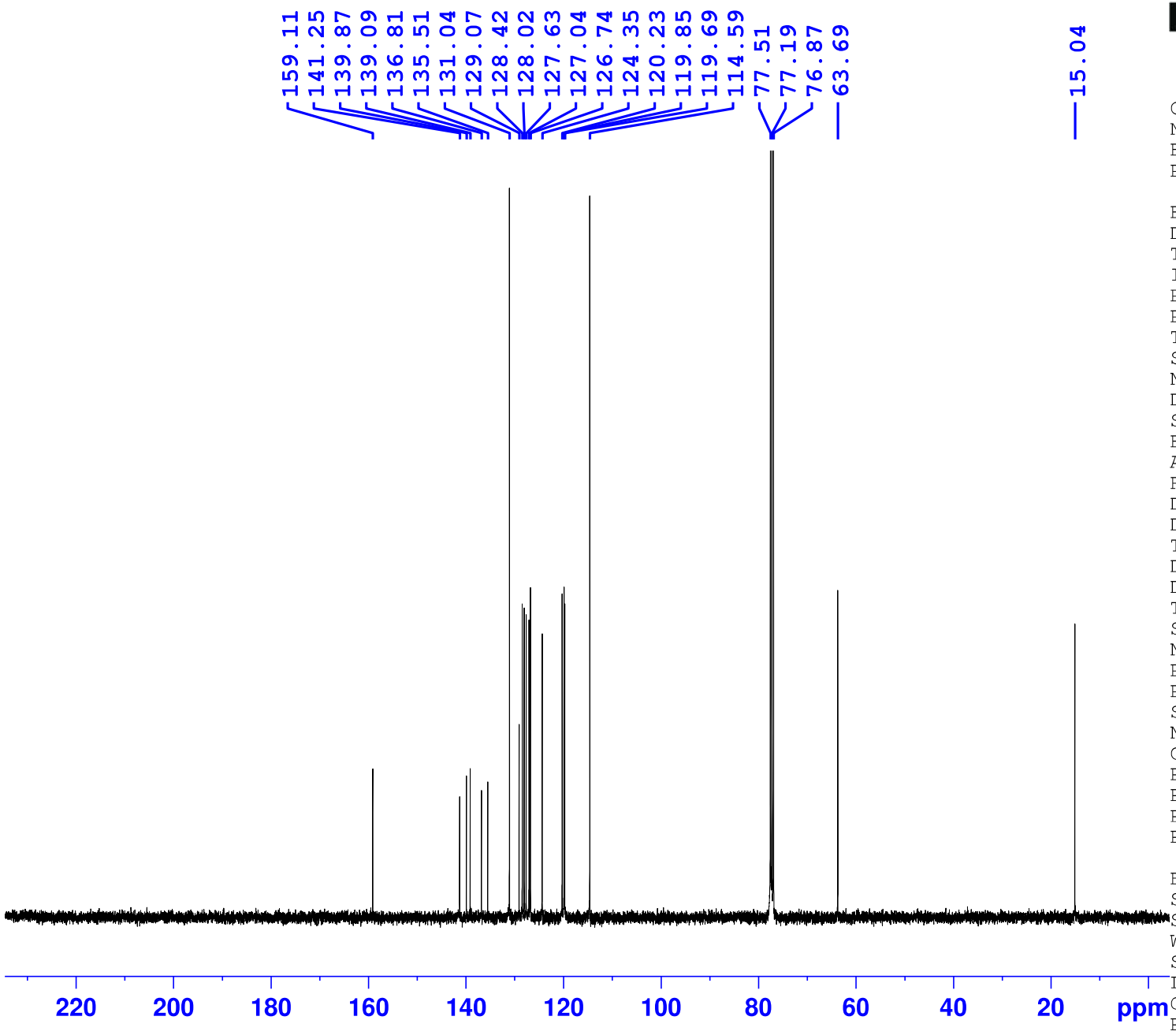
Compound 1b, 1H NMR (400 MHz, CDCl3)



Compound 1b, 1H NMR (400 MHz, CDCl3)



Compound 1b, 13C NMR (100 MHz, CDCl3)

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Current Data Parameters
NAME      Shumaila Majeed
EXPNO                 272
PROCNO                  1

F2 - Acquisition Parameters
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Time               14.39 h
INSTRUM             spect
PROBHD   Z116098_0621 (
PULPROG            zgpg30
TD                 65536
SOLVENT             CDCl3
NS                    400
DS                      2
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ             1.3631488 sec
RG                199.48
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1
SFO1         100.6243390 MHz
NUC1                 13C
P1                10.00 usec
PLW1         72.56700134 W
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         16.68099976 W
PLW12         0.20593999 W
PLW13         0.10342000 W

F2 - Processing parameters
SI                  32768
SF           100.6127547 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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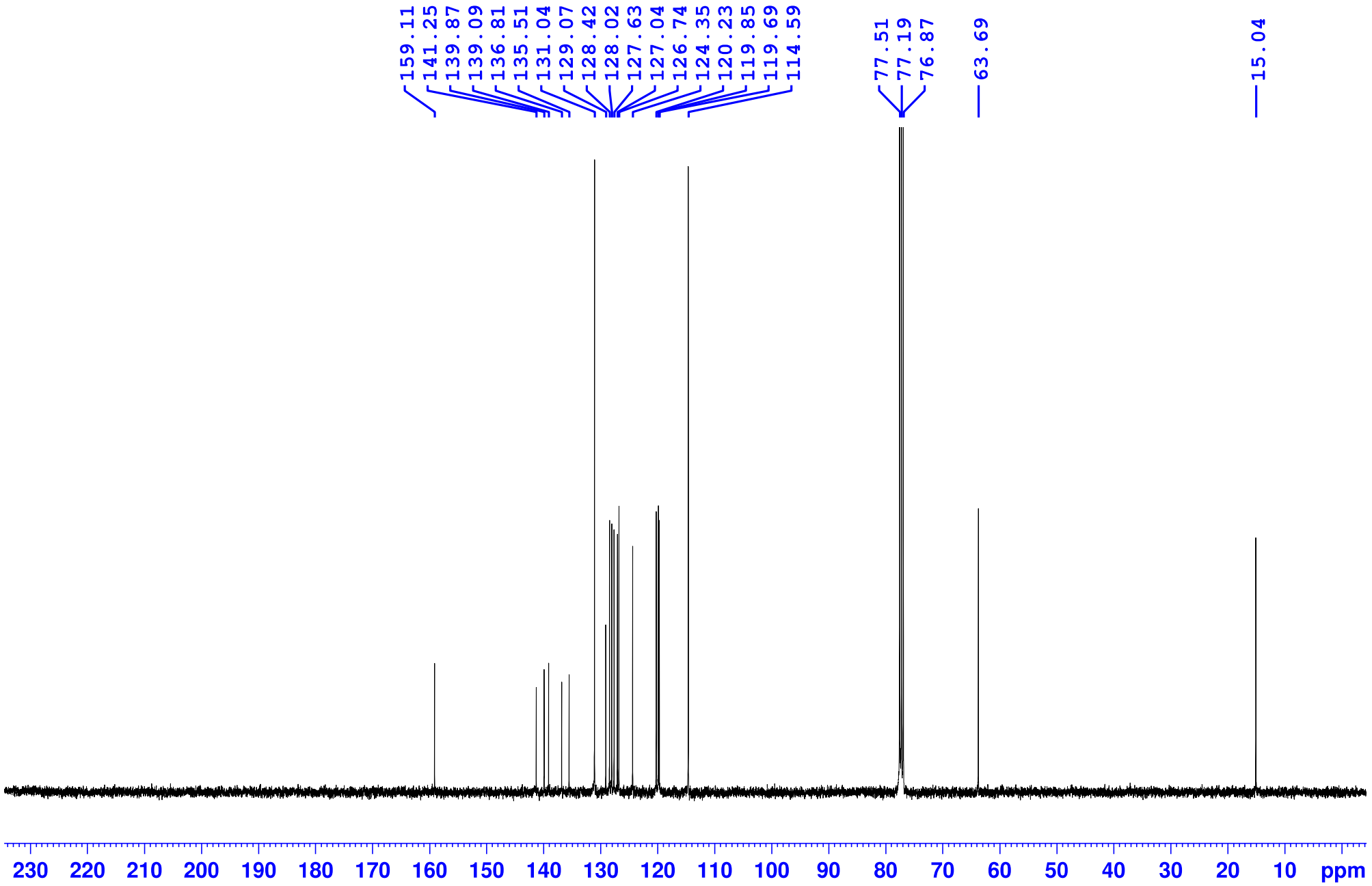
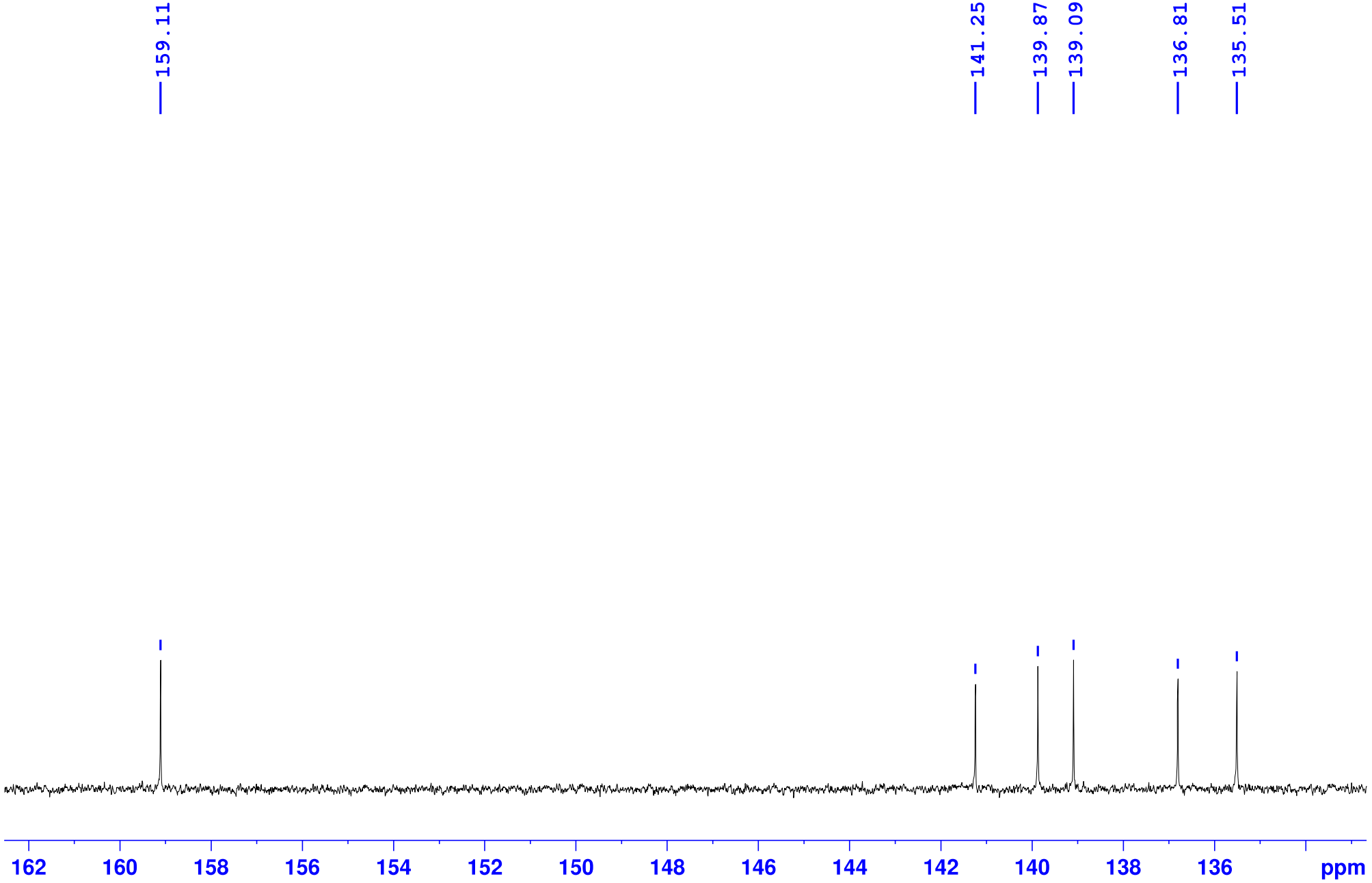
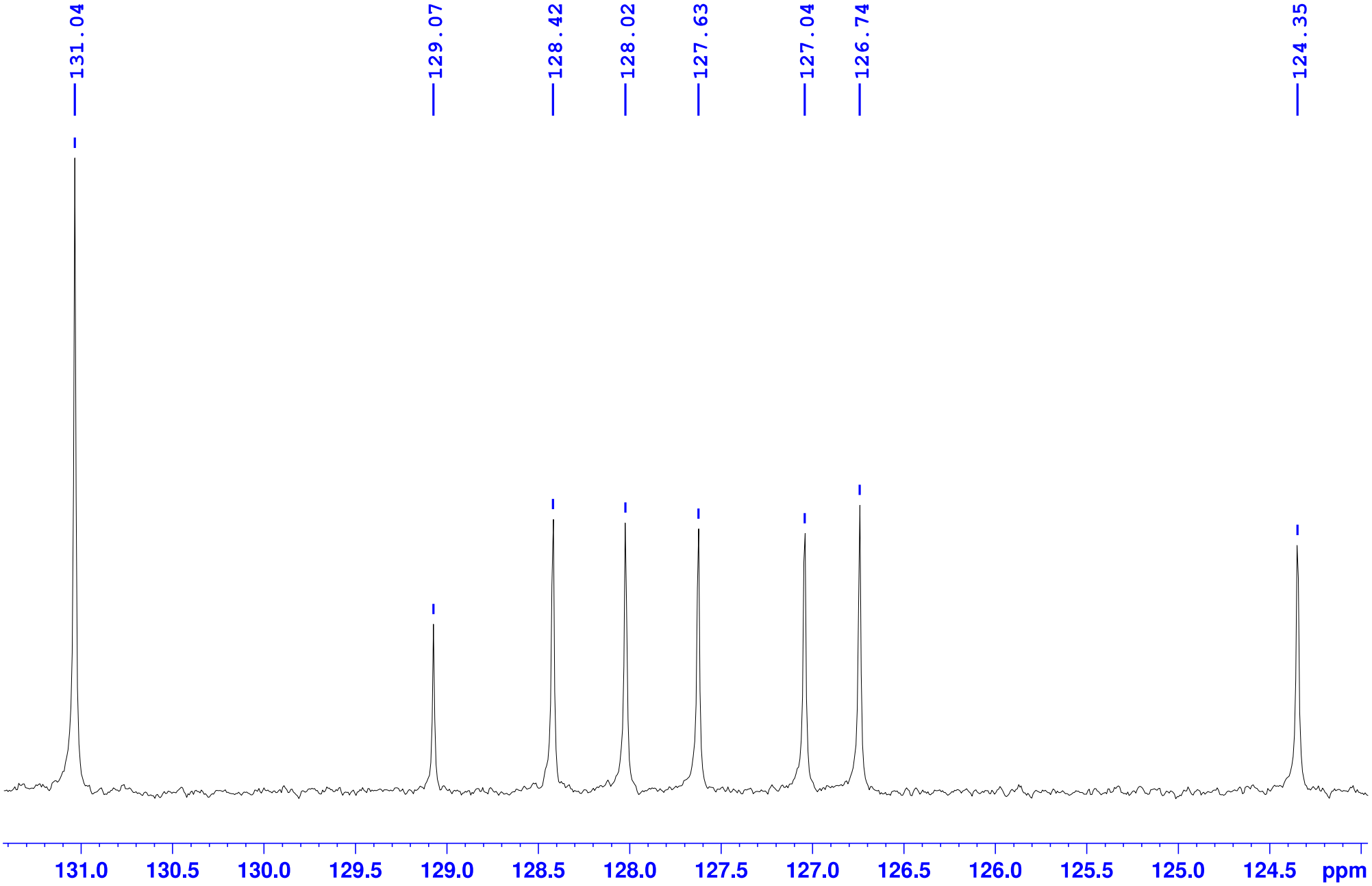
Compound 1b, 13C NMR (100 MHz, CDCl3)



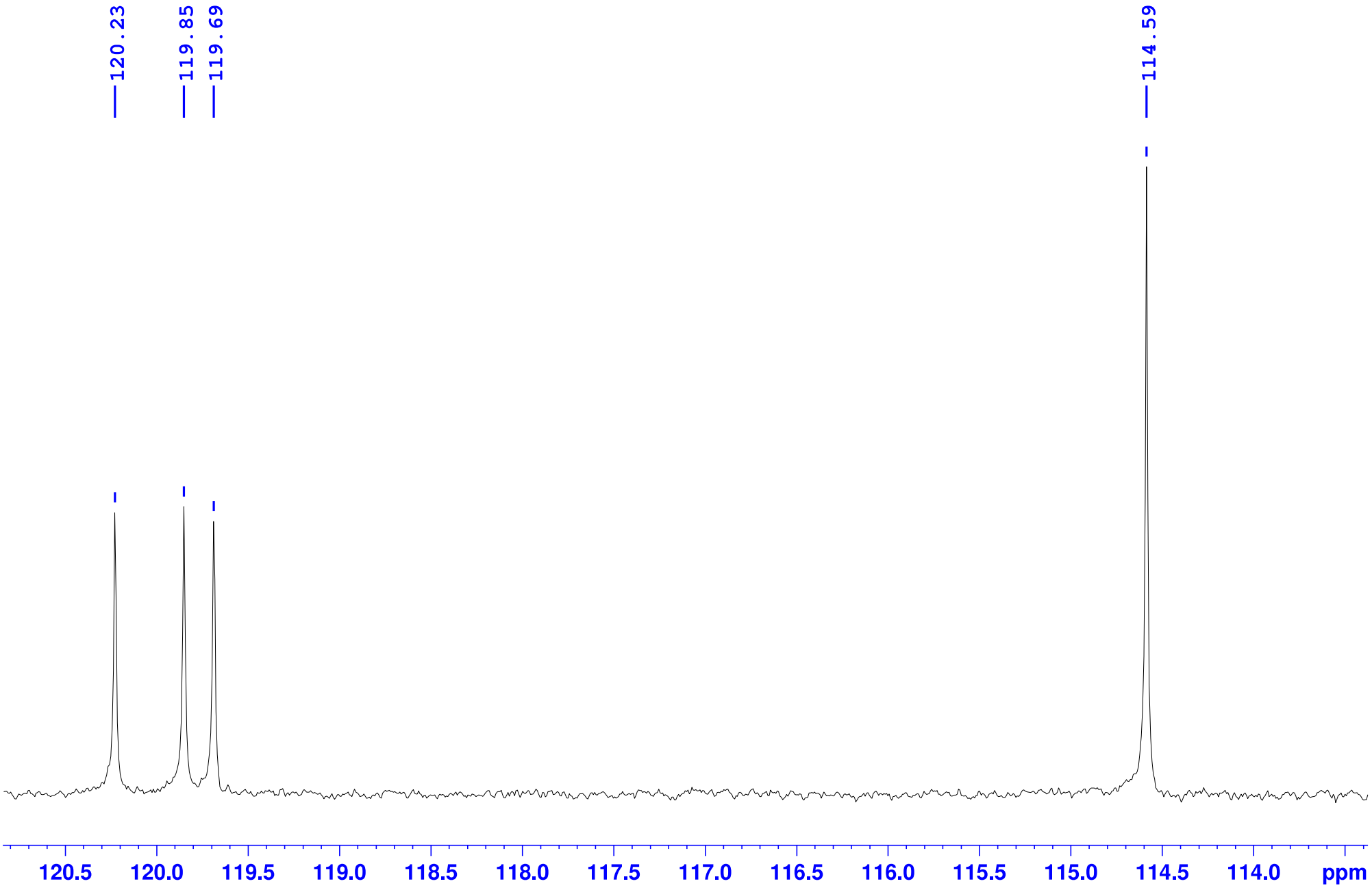
Compound 1b, 13C NMR (100 MHz, CDCl3)



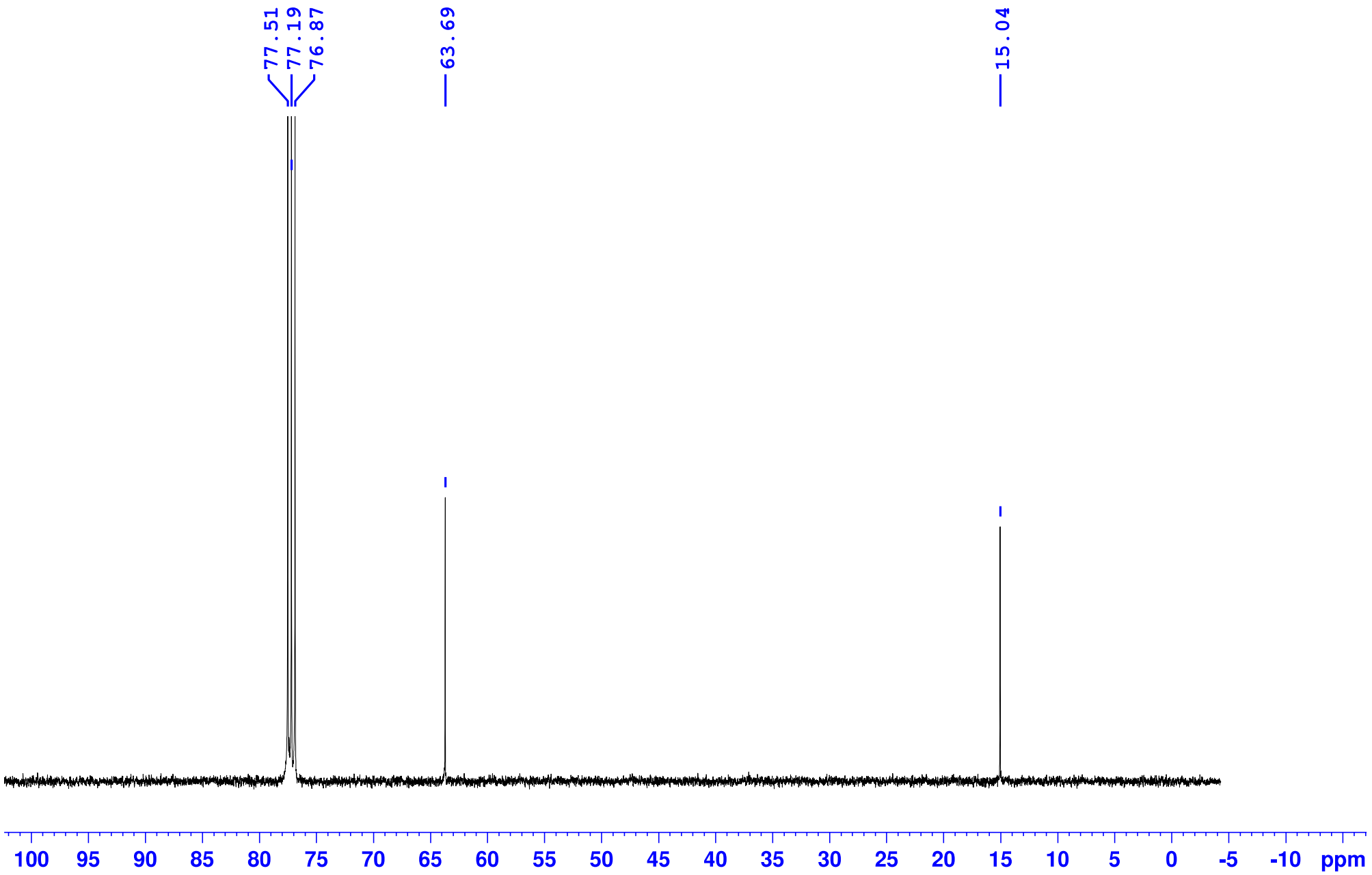
Compound 1b, 13C NMR (100 MHz, CDCl3)



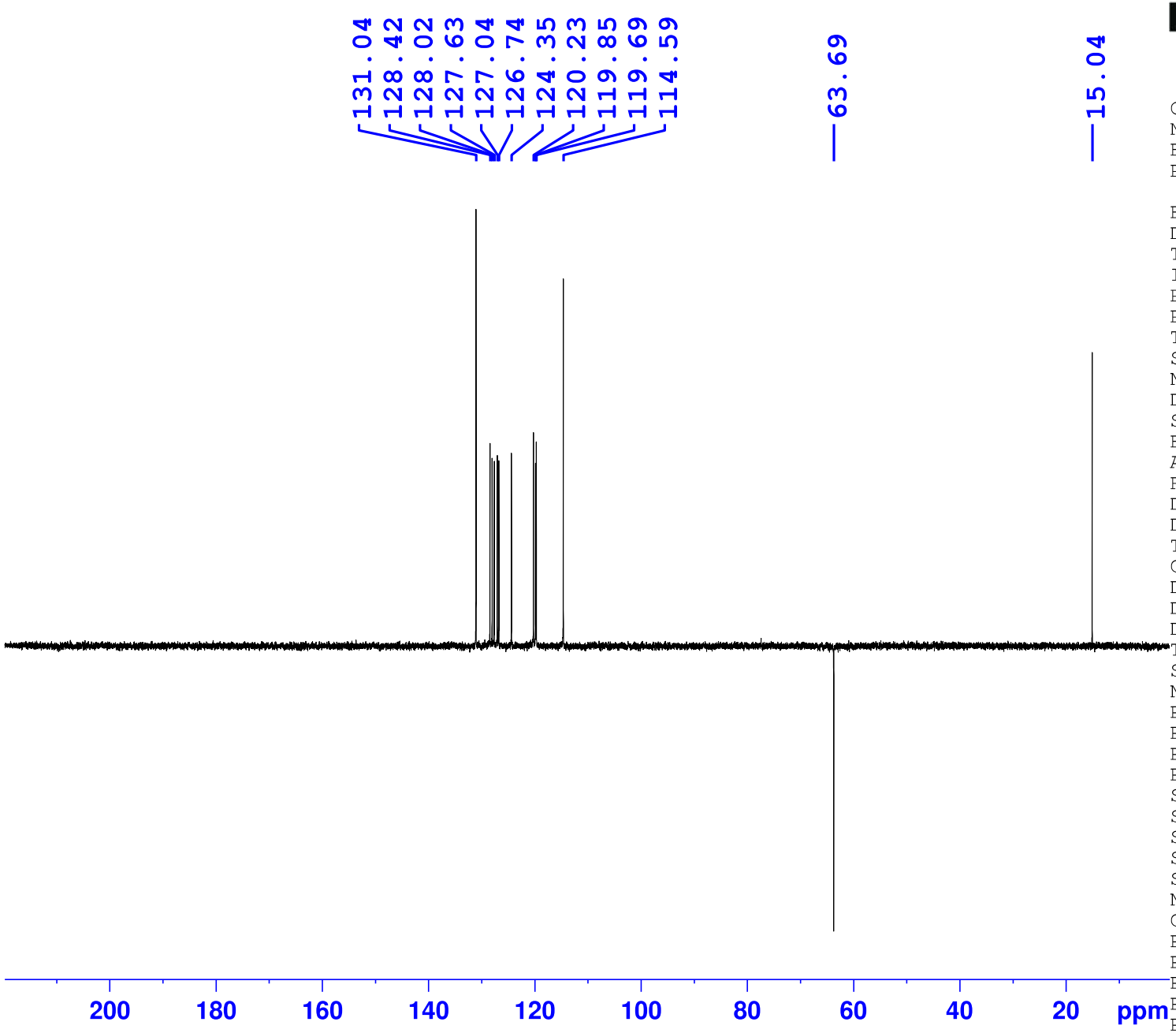
Compound 1b, 13C NMR (100 MHz, CDCl3)



Compound 1b, 13C NMR (100 MHz, CDCl3)



Compound 1b, DEPT 135 NMR (100 MHz, CDCl3)

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Current Data Parameters
NAME      Shumaila Majeed
EXPNO                 273
PROCNO                  1

F2 - Acquisition Parameters
Date_           20211013
Time               14.55 h
INSTRUM             spect
PROBHD   Z116098_0621 (
PULPROG        deptsp135
TD                 65536
SOLVENT             CDCl3
NS                    256
DS                      4
SWH            22058.824 Hz
FIDRES          0.673182 Hz
AQ             1.4854827 sec
RG                199.48
DW                22.667 usec
DE                 6.50 usec
TE                298.0 K
CNST2         145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                     1
SFO1          100.6238359 MHz
NUC1                  13C
P1                 10.00 usec
P13              2000.00 usec
PLW0      0 W
PLW1         72.56700134 W
SPNAM[5]     Crp60comp.4
SPOAL5             0.500
SPOFFS5   0 Hz
SPW5         11.08699989 W
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
P3                 10.00 usec
P4                 20.00 usec
PCPD2              90.00 usec
PLW2         16.68099976 W
PLW12         0.20593999 W
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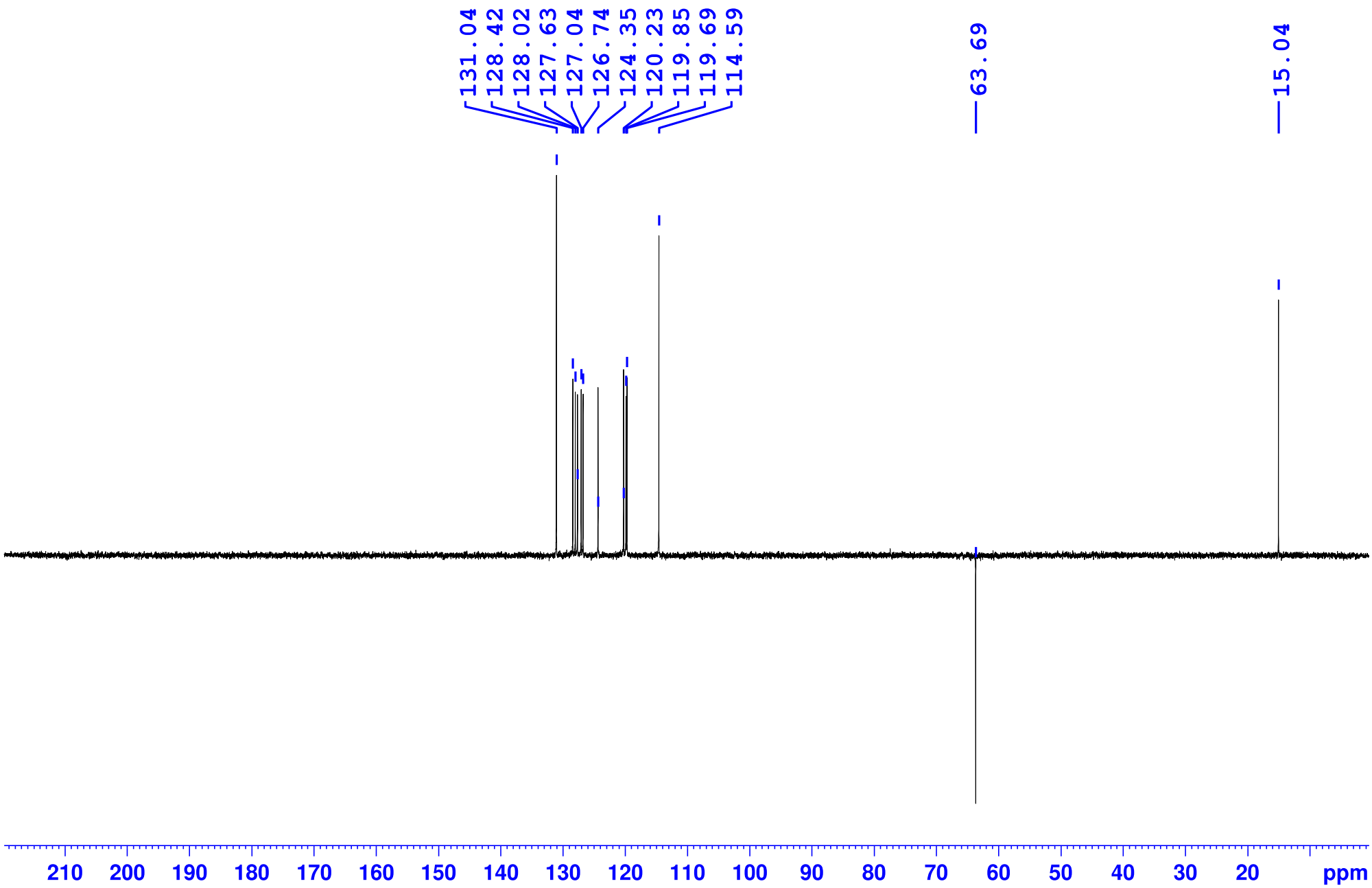
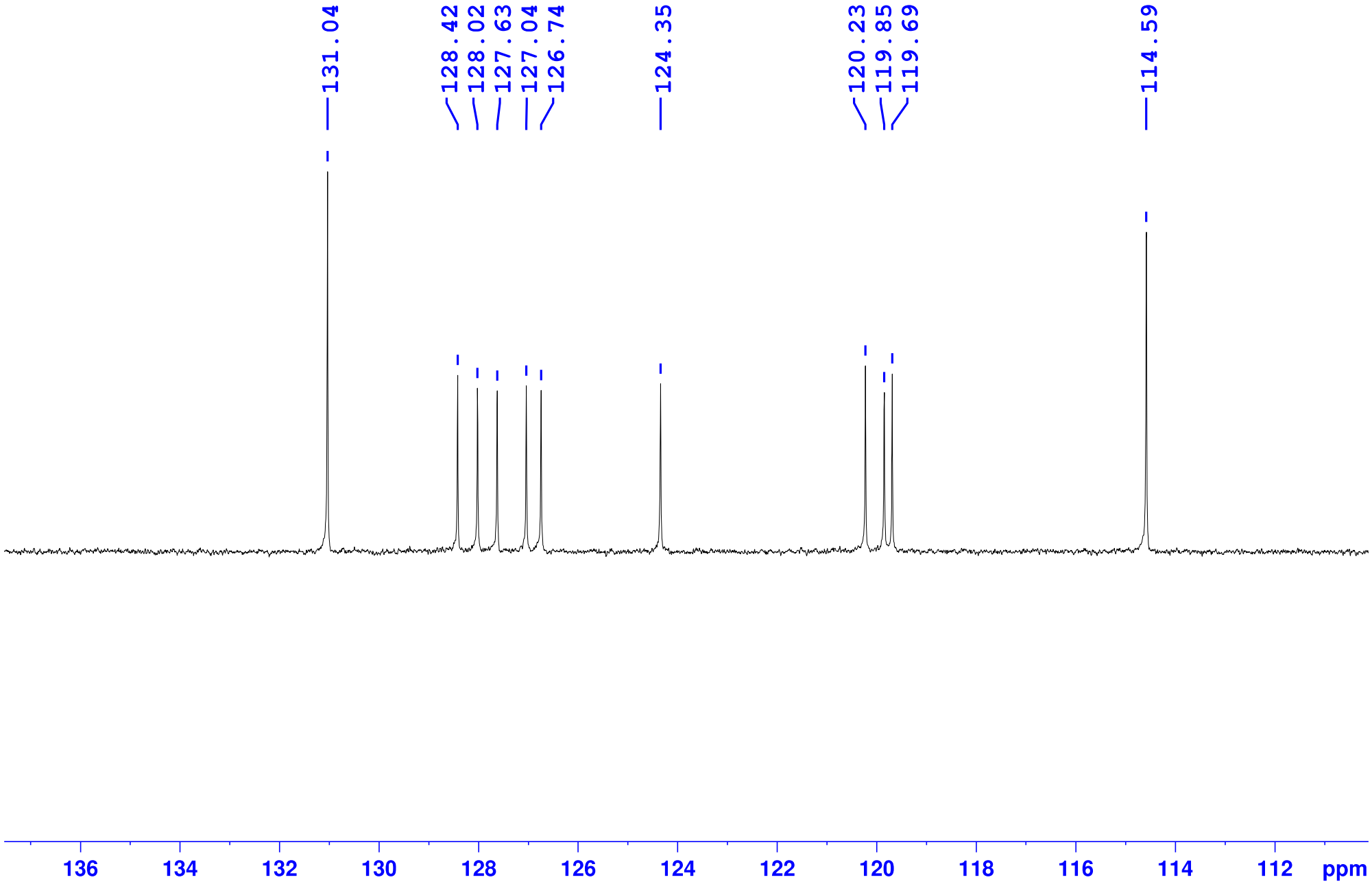
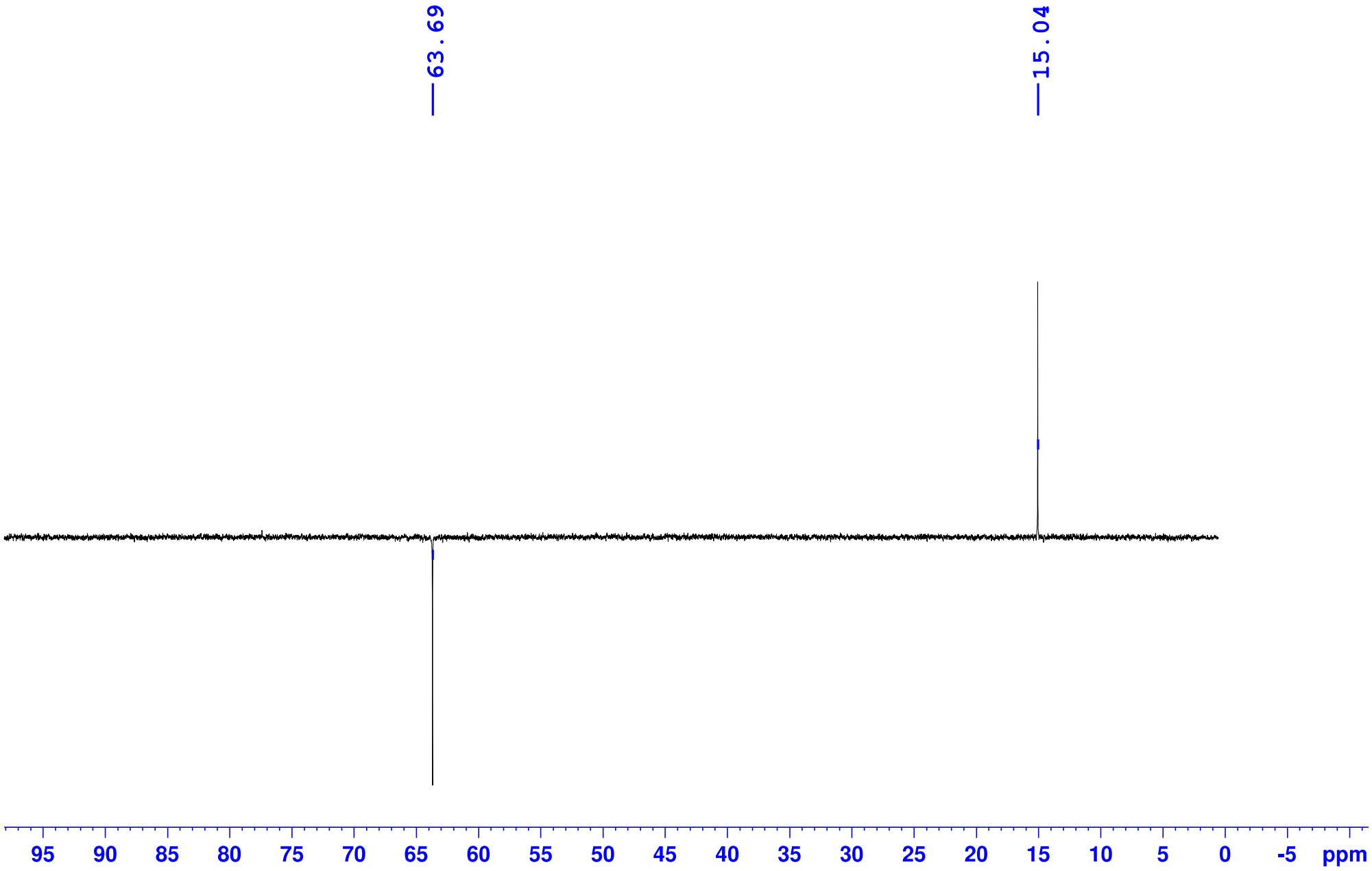
Compound 1b, DEPT 135 NMR (100 MHz, CDCl3)



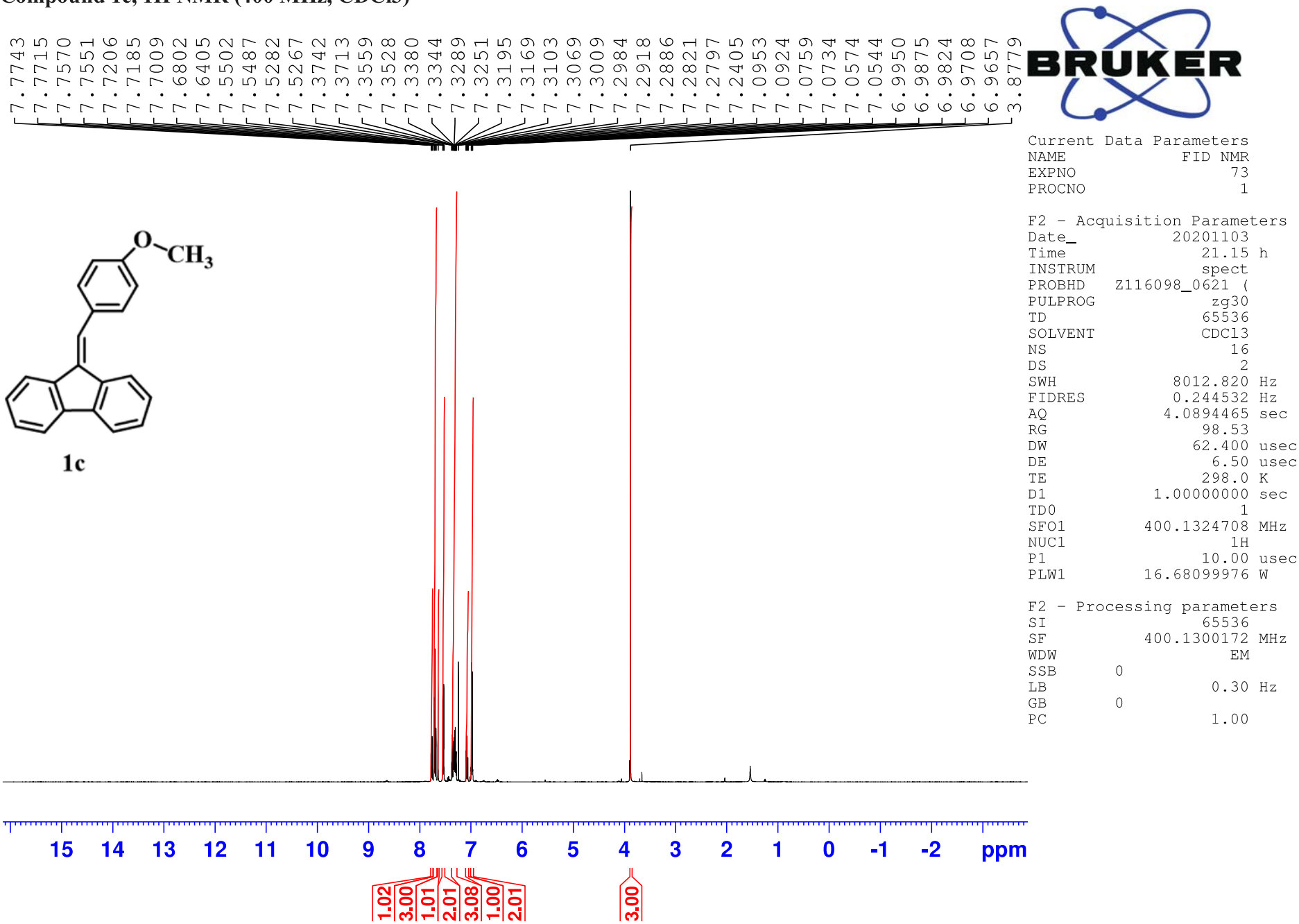
Compound 1b, DEPT 135 NMR (100 MHz, CDCl3)



Compound 1b, DEPT 135 NMR (100 MHz, CDCl3)



Compound 1c, 1H NMR (400 MHz, CDCl3)

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Current Data Parameters
NAME                  FID NMR
EXPNO                      73
PROCNO                      1

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Time                   21.15 h
INSTRUM                spect
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PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.244532 Hz
AQ                  4.0894465 sec
RG                     98.53
DW                    62.400 usec
DE                     6.50 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                        1
SFO1             400.1324708 MHz
NUC1                      1H
P1                    10.00 usec
PLW1             16.68099976 W

F2 - Processing parameters
SI                     65536
SF               400.1300172 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
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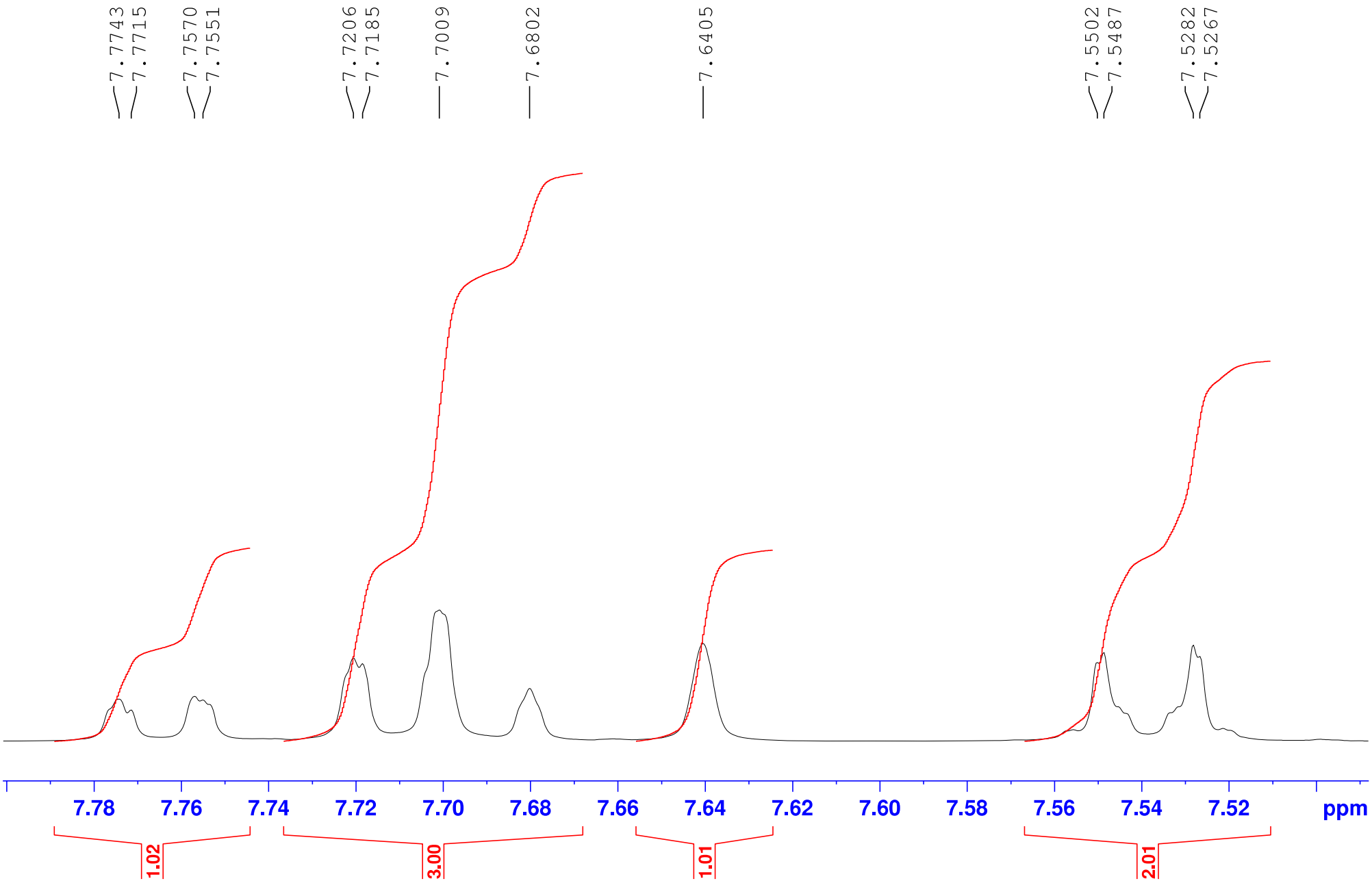
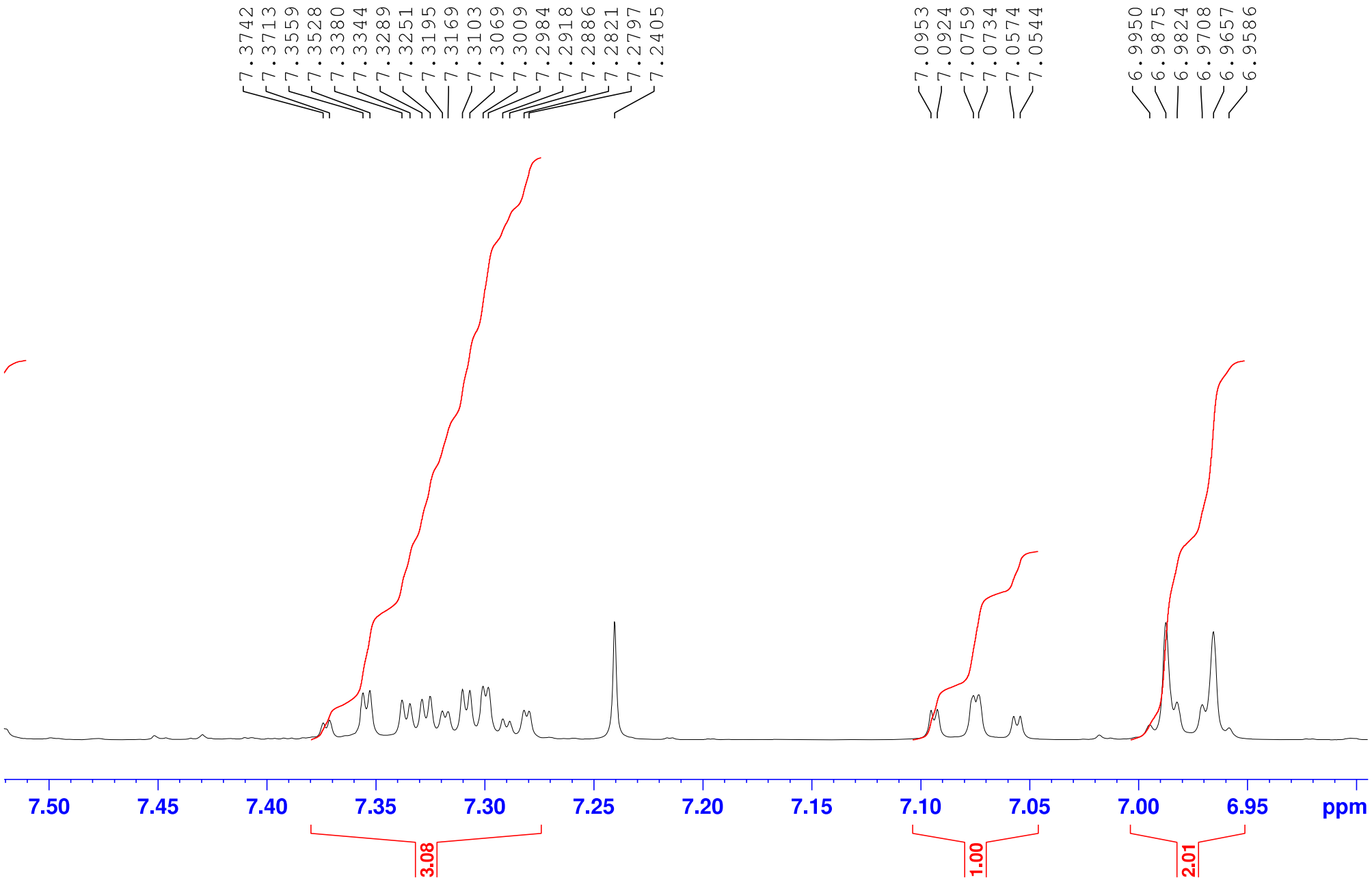
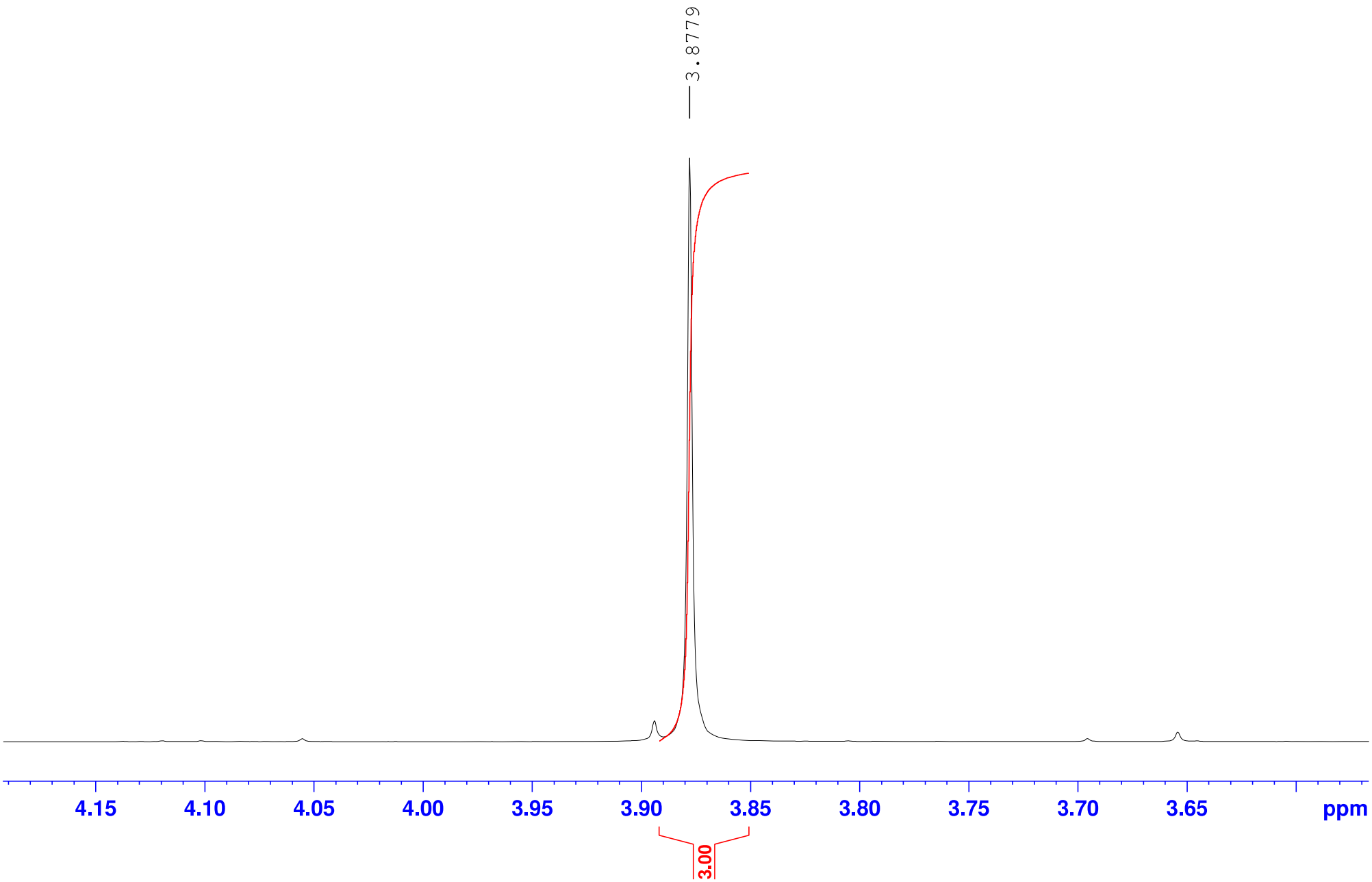
Compound 1c, 1H NMR (400 MHz, CDCl3)



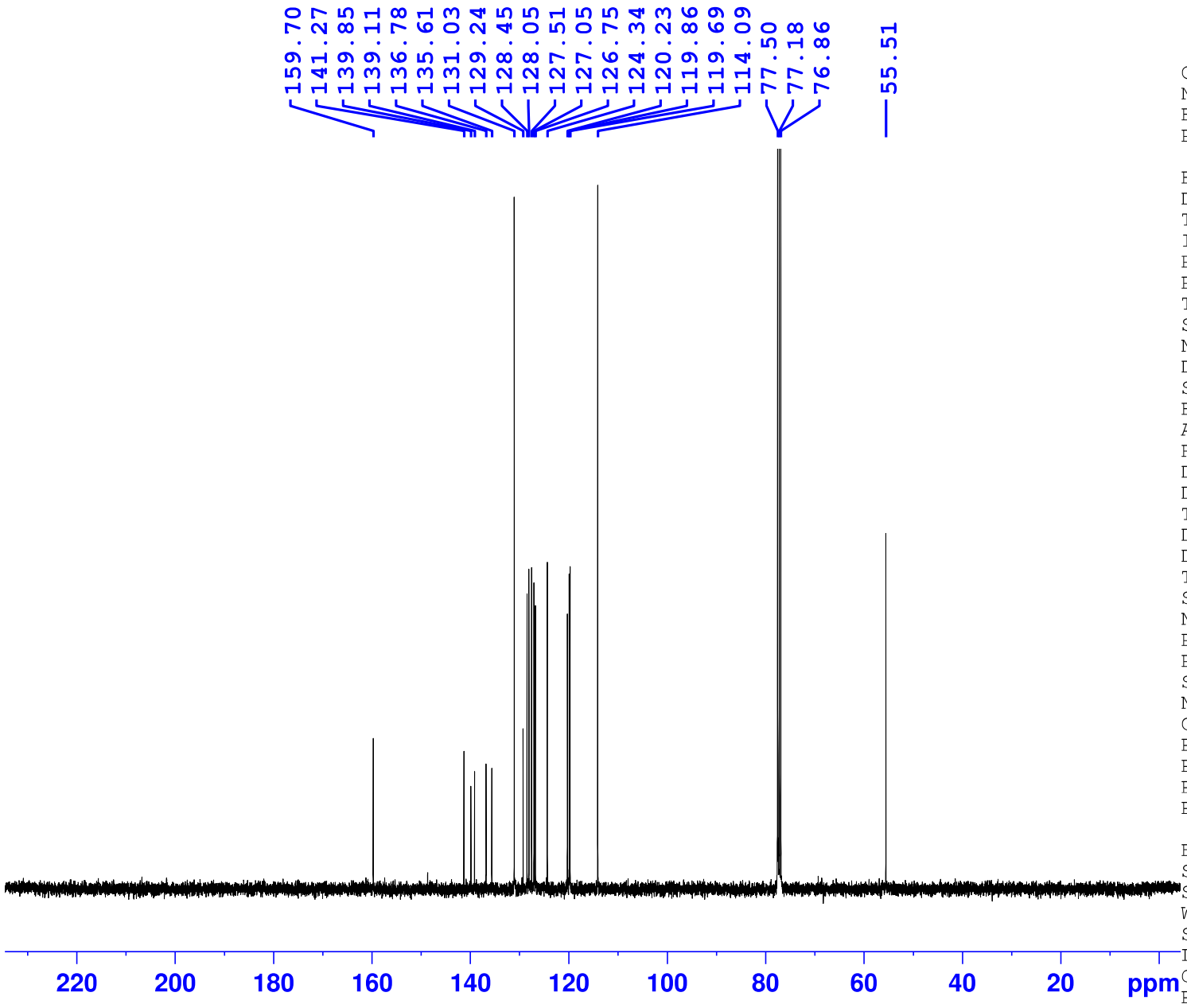
Compound 1c, 1H NMR (400 MHz, CDCl3)



Compound 1c, 1H NMR (400 MHz, CDCl3)



Compound 1c, 13C NMR (100 MHz, CDCl3)

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Current Data Parameters
NAME      Shumaila Majeed
EXPNO                 268
PROCNO                  1

F2 - Acquisition Parameters
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Time               13.13 h
INSTRUM             spect
PROBHD   Z116098_0621 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    400
DS                      2
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ             1.3631488 sec
RG                 199.48
DW                 20.800 usec
DE                  6.50 usec
TE                 298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         100.6243390 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         72.56700134 W
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         16.68099976 W
PLW12         0.20593999 W
PLW13         0.10342000 W

F2 - Processing parameters
SI                  32768
SF           100.6127547 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
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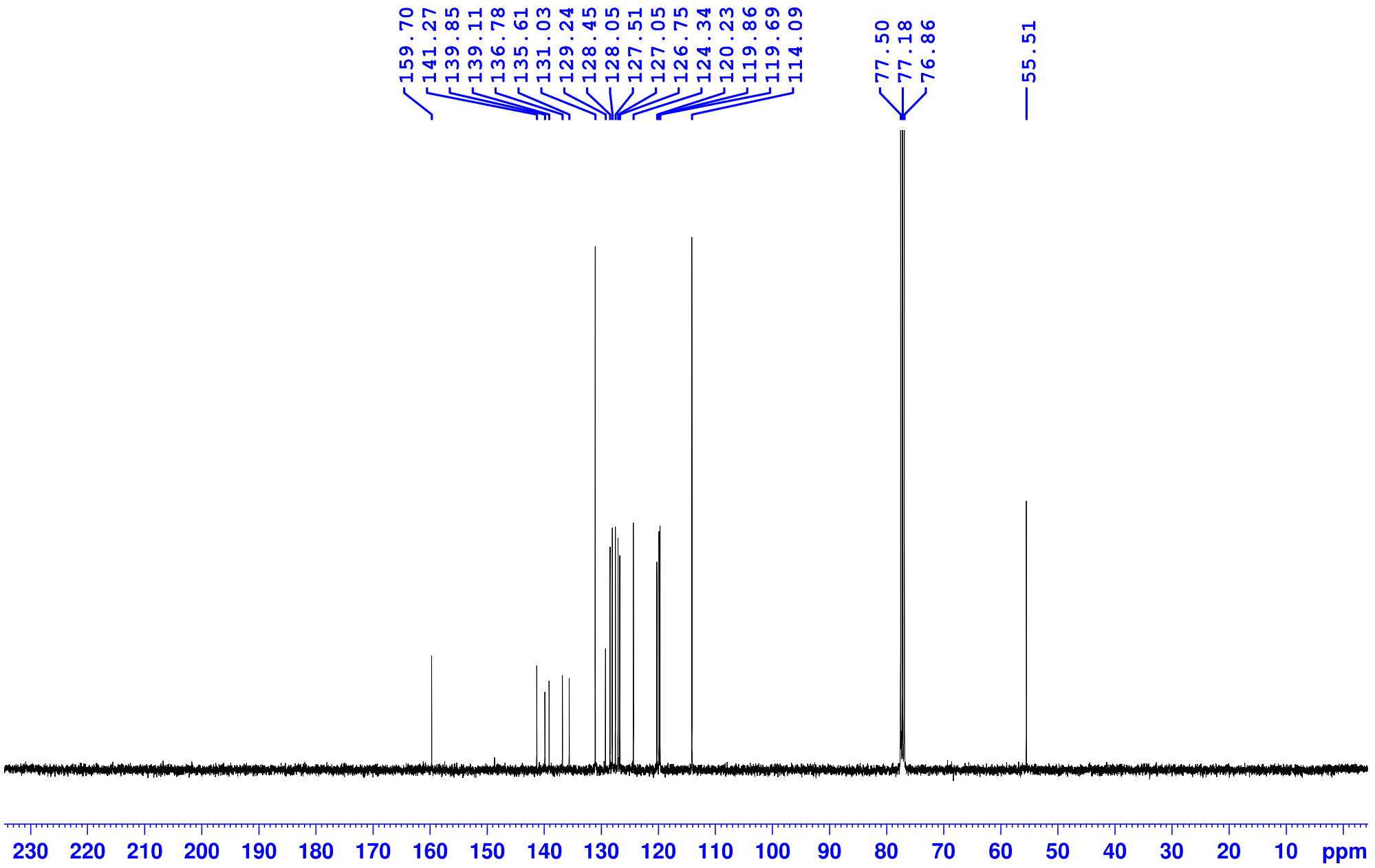
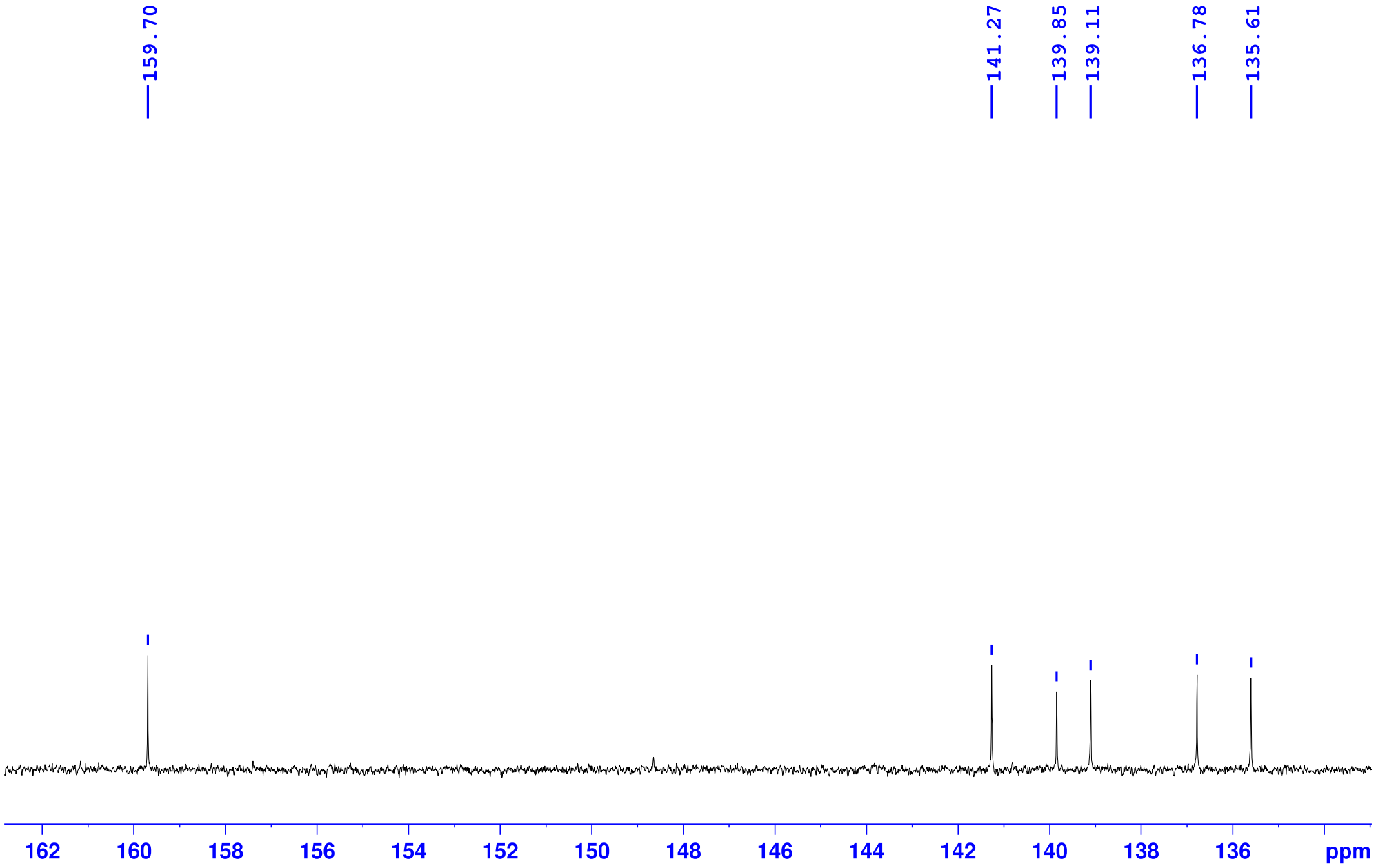
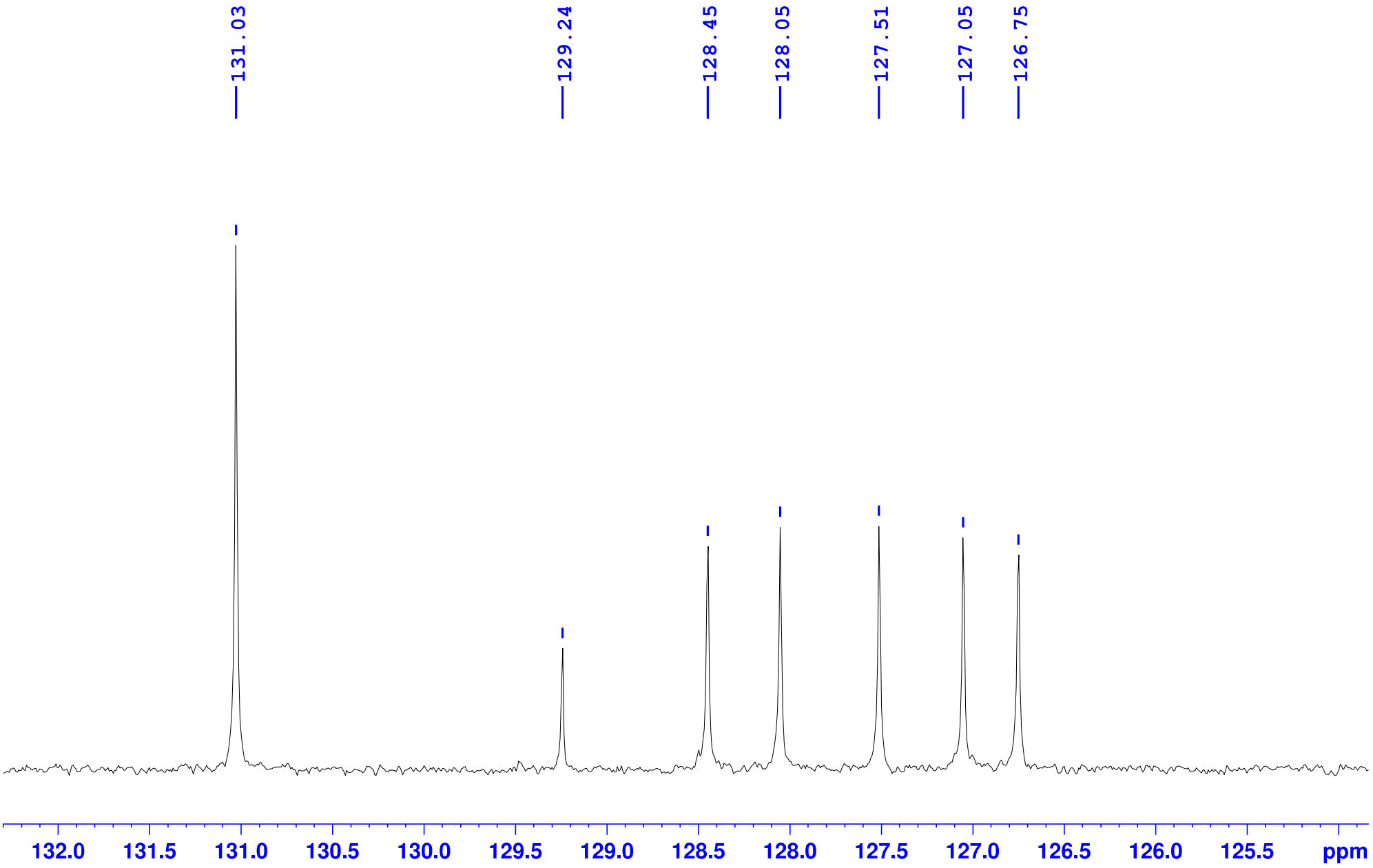
Compound 1c, 13C NMR (100 MHz, CDCl3)



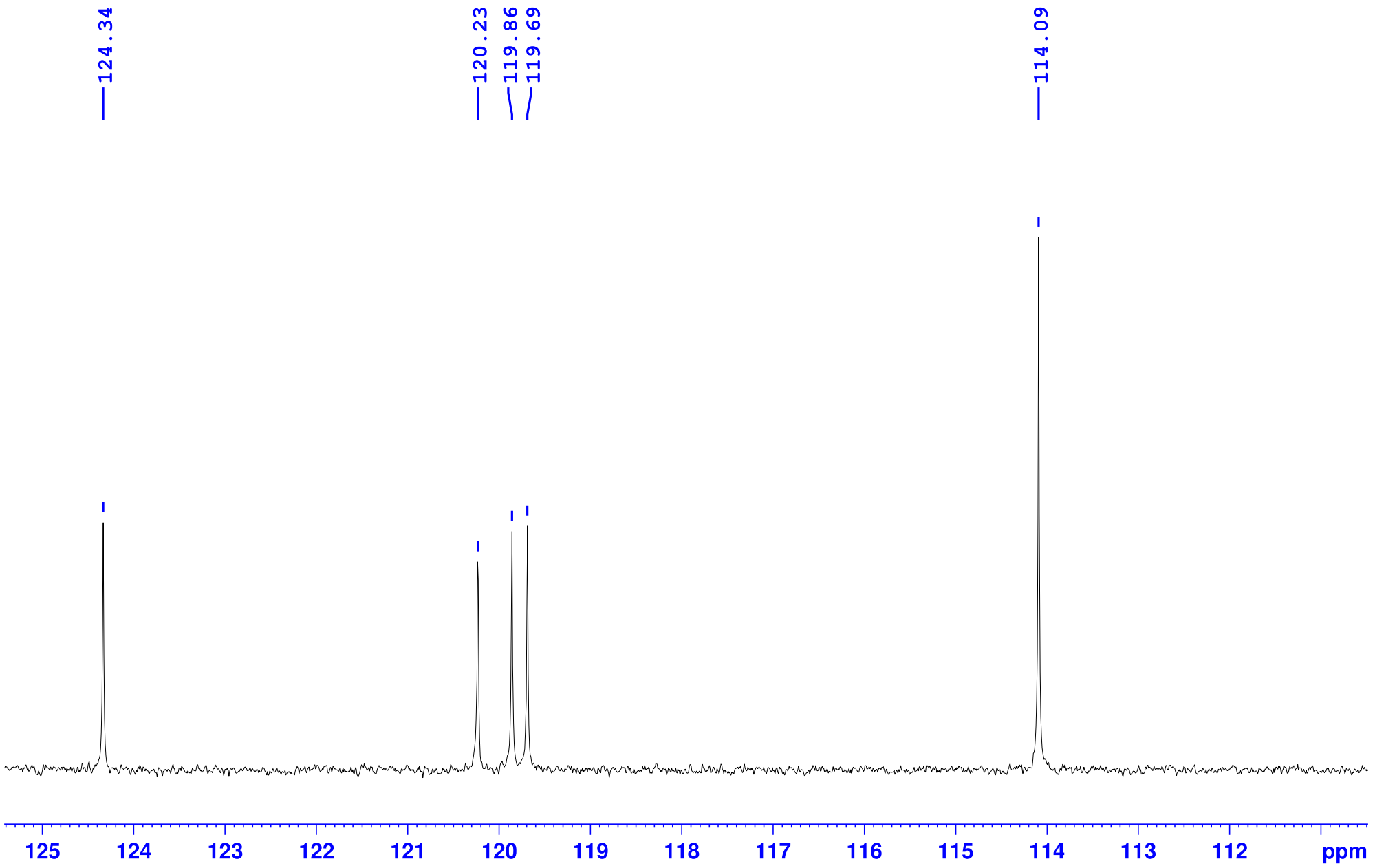
Compound 1c, 13C NMR (100 MHz, CDCl3)



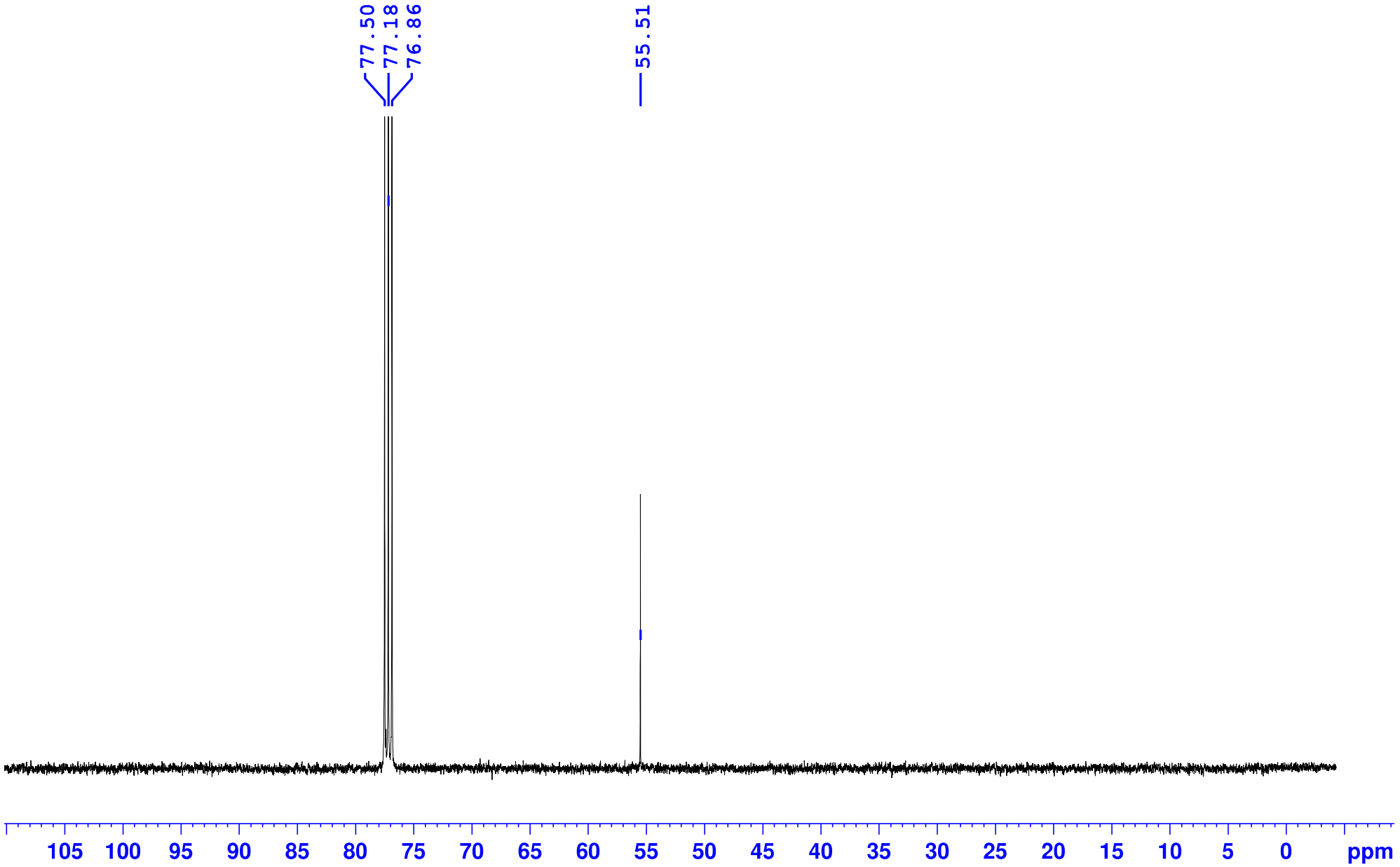
Compound 1c, 13C NMR (100 MHz, CDCl3)



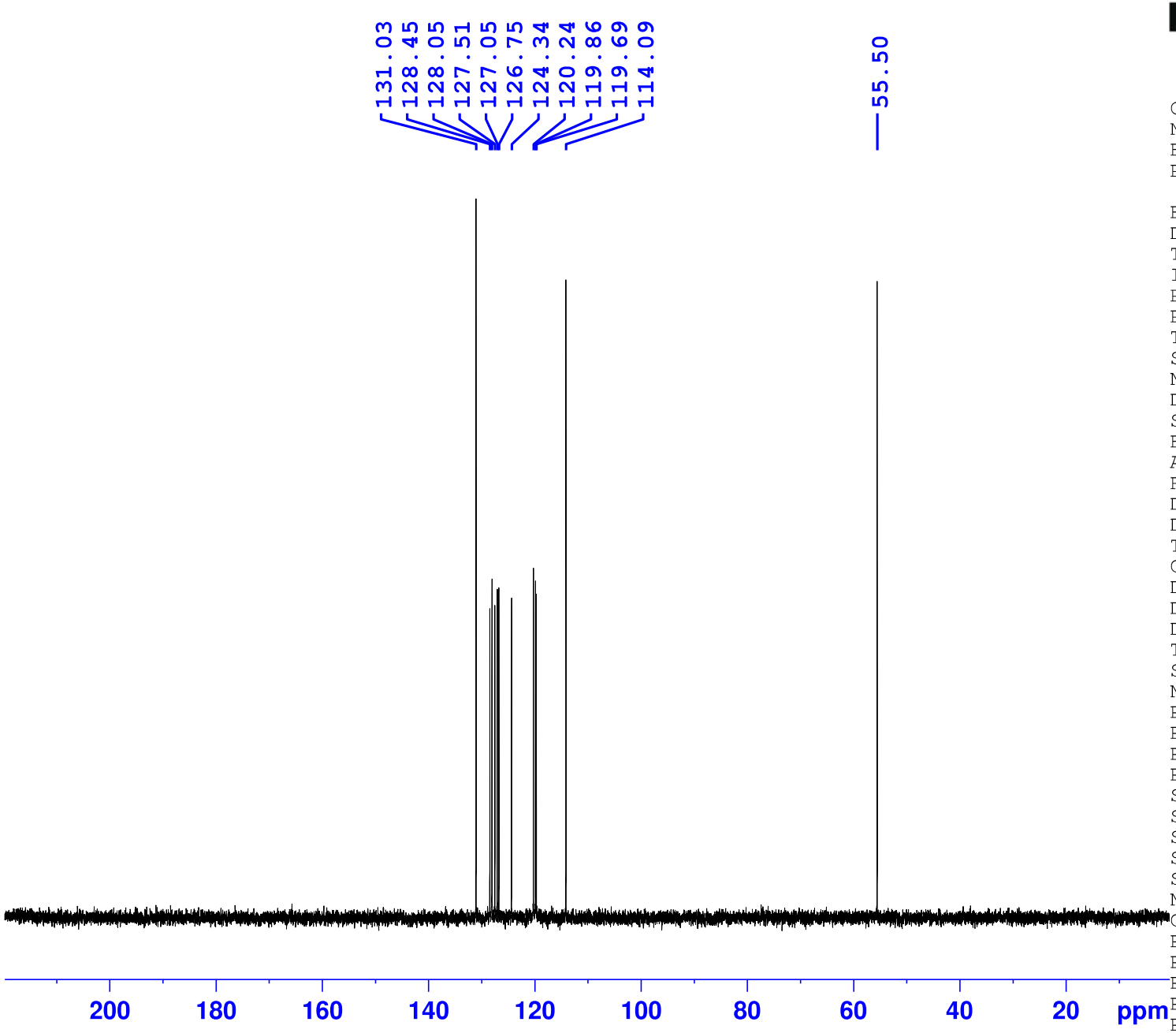
Compound 1c, 13C NMR (100 MHz, CDCl3)



Compound 1c, 13C NMR (100 MHz, CDCl3)



Compound 1c, DEPT 135 NMR (100 MHz, CDCl3)

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Current Data Parameters
NAME      Shumaila Majeed
EXPNO                 269
PROCNO                  1

F2 - Acquisition Parameters
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Time               13.29 h
INSTRUM             spect
PROBHD   Z116098_0621 (
PULPROG        deptsp135
TD                 65536
SOLVENT             CDCl3
NS                    256
DS                      4
SWH            22058.824 Hz
FIDRES          0.673182 Hz
AQ             1.4854827 sec
RG                199.48
DW                22.667 usec
DE                 6.50 usec
TE                298.0 K
CNST2         145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                     1
SFO1          100.6238359 MHz
NUC1                  13C
P1                 10.00 usec
P13              2000.00 usec
PLW0      0 W
PLW1         72.56700134 W
SPNAM[5]     Crp60comp.4
SPOAL5             0.500
SPOFFS5   0 Hz
SPW5         11.08699989 W
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
P3                 10.00 usec
P4                 20.00 usec
PCPD2              90.00 usec
PLW2         16.68099976 W
PLW12         0.20593999 W
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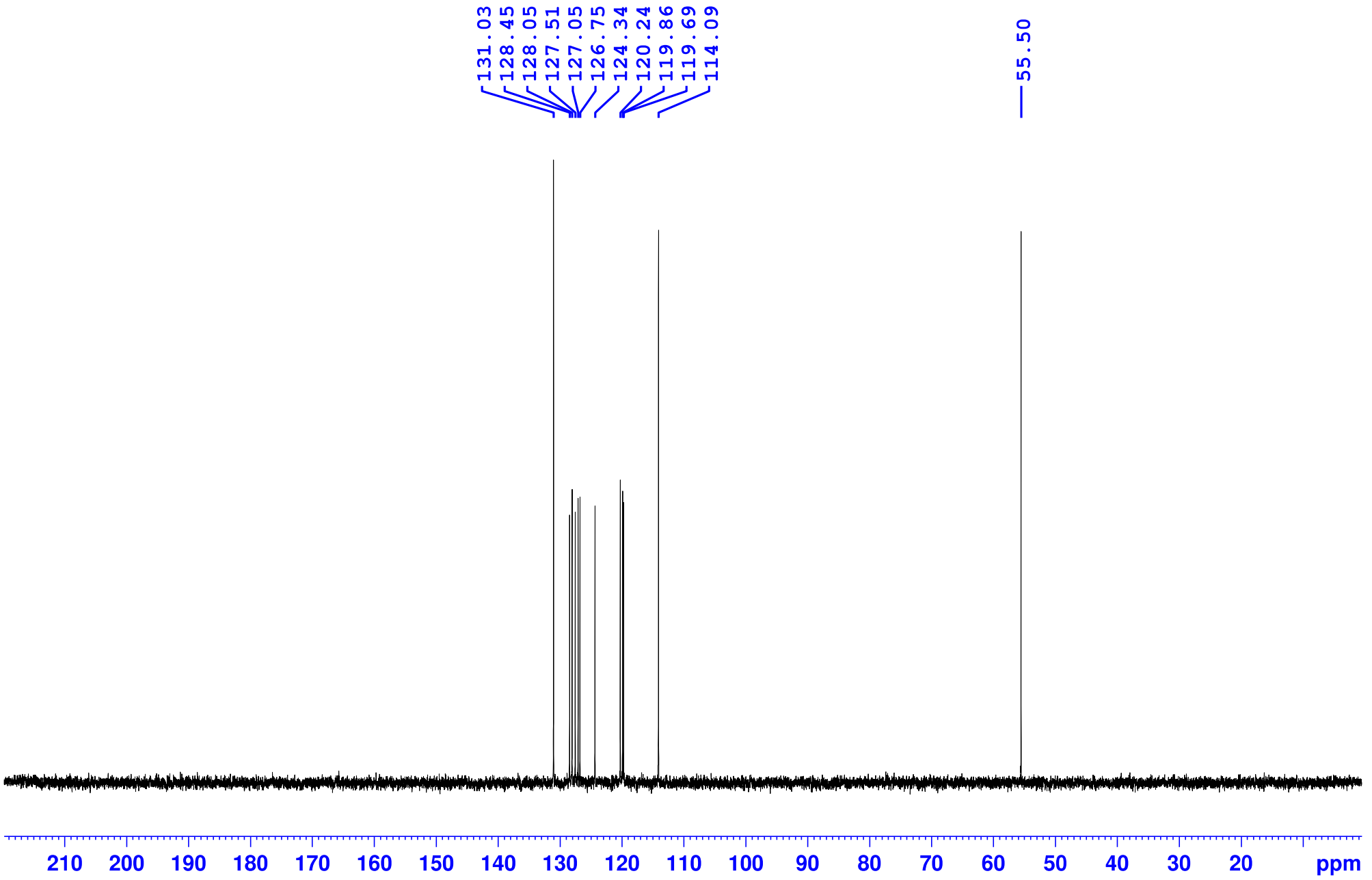
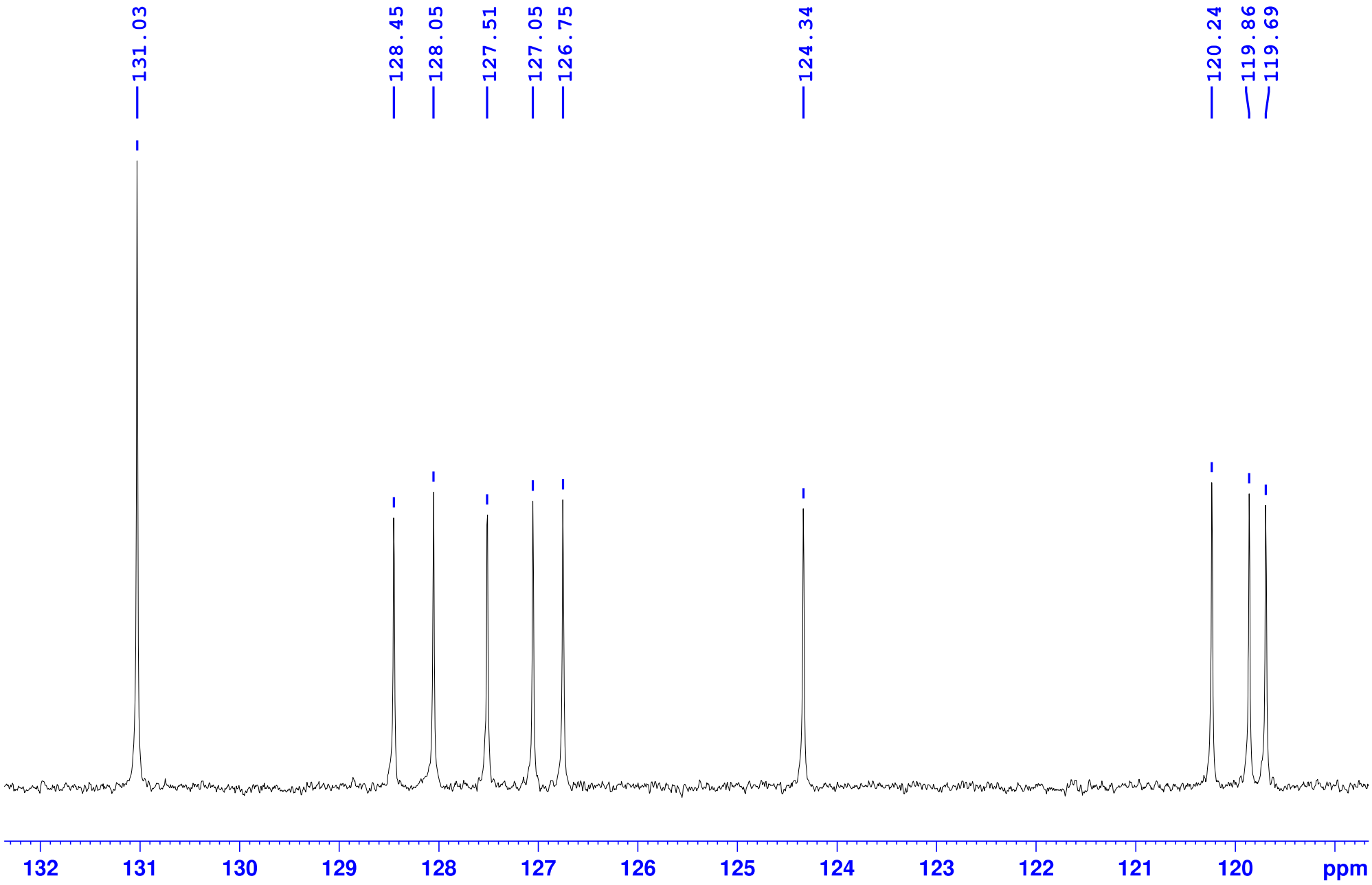
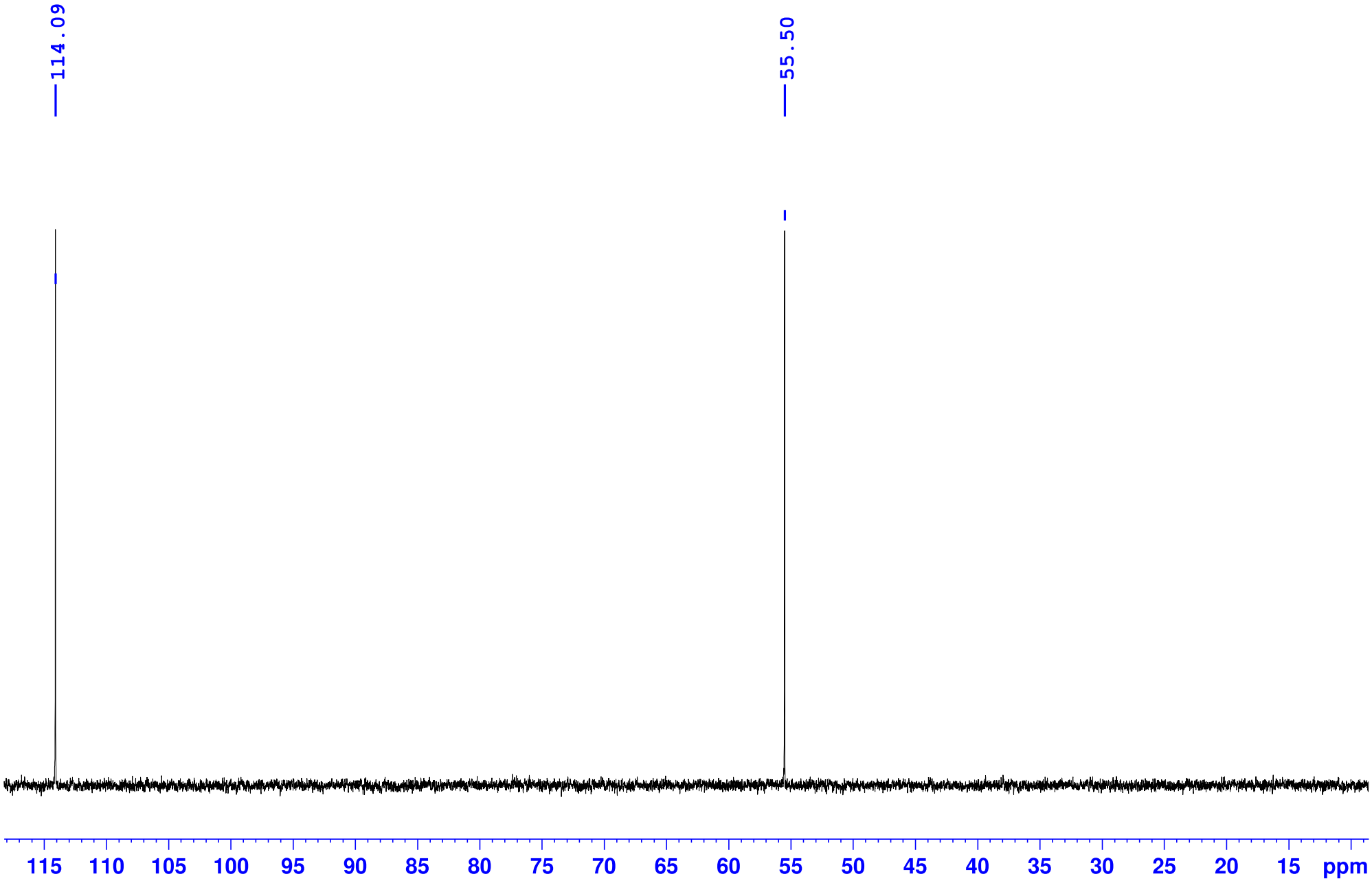
Compound 1c, DEPT 135 NMR (100 MHz, CDCl3)



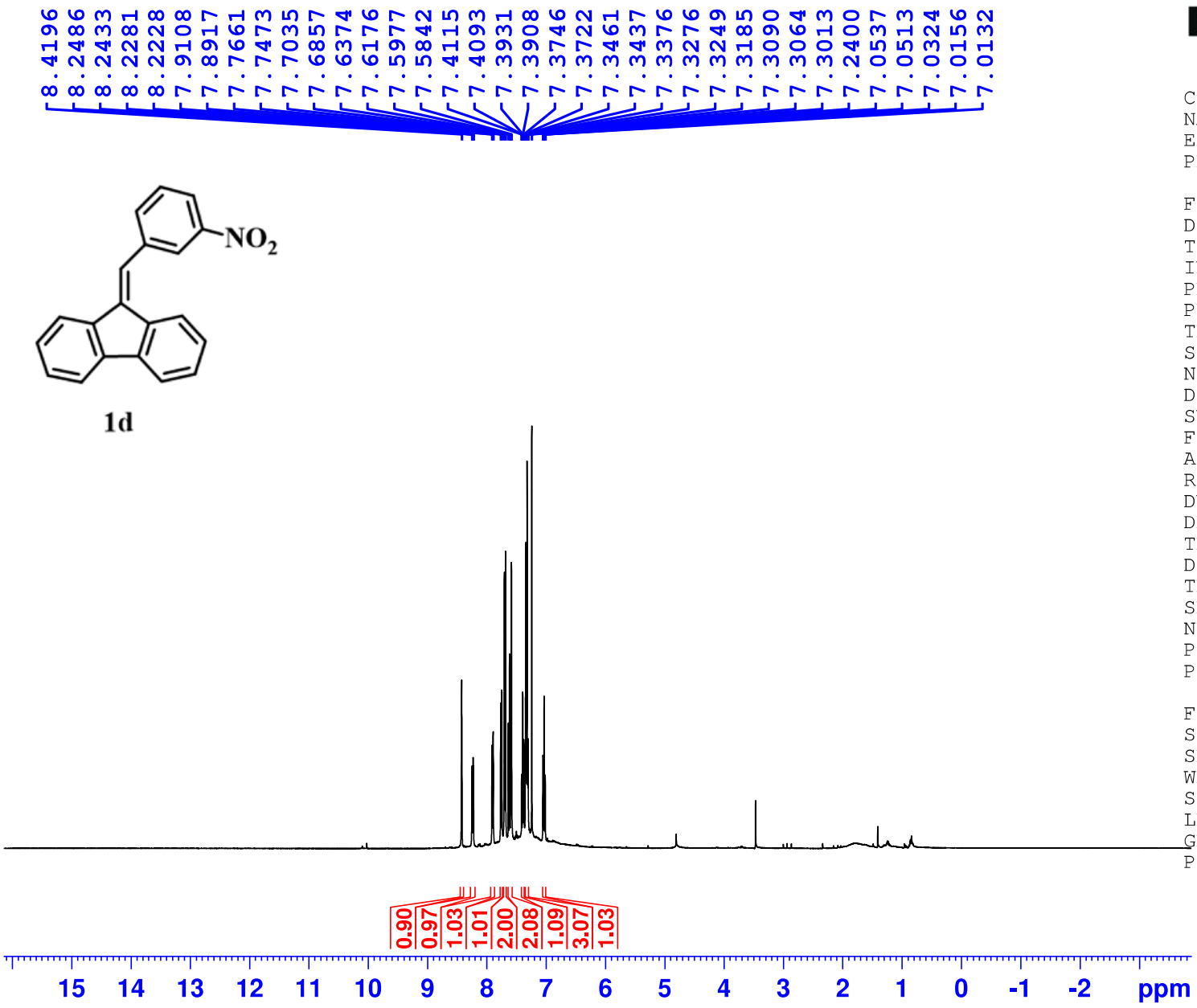
Compound 1c, DEPT 135 NMR (100 MHz, CDCl3)



Compound 1c, DEPT 135 NMR (100 MHz, CDCl3)



Compound 1d, 1H NMR (400 MHz, CDCl3)

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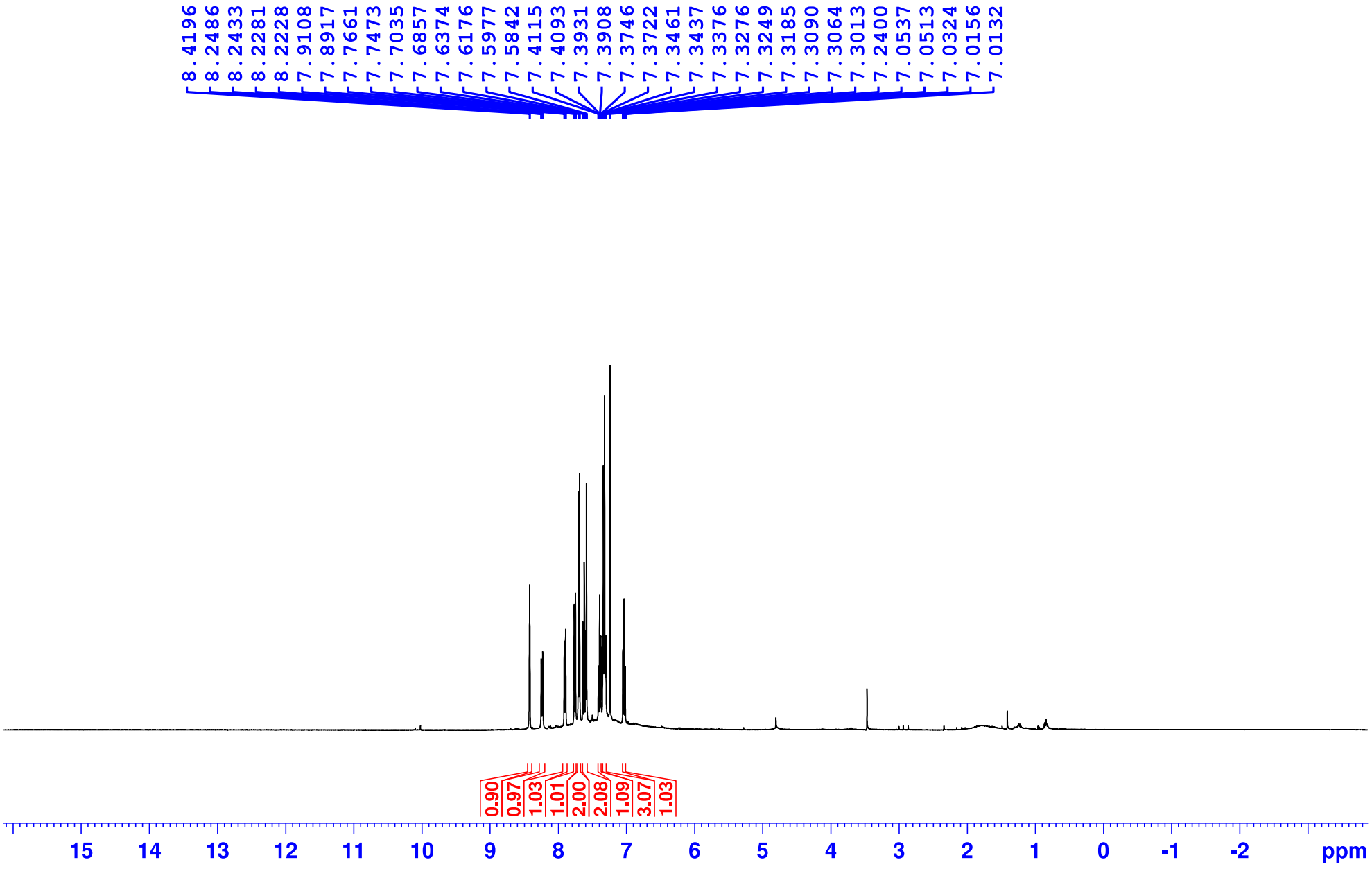
Current Data Parameters
NAME                  SMT-8
EXPNO                   157
PROCNO                    1

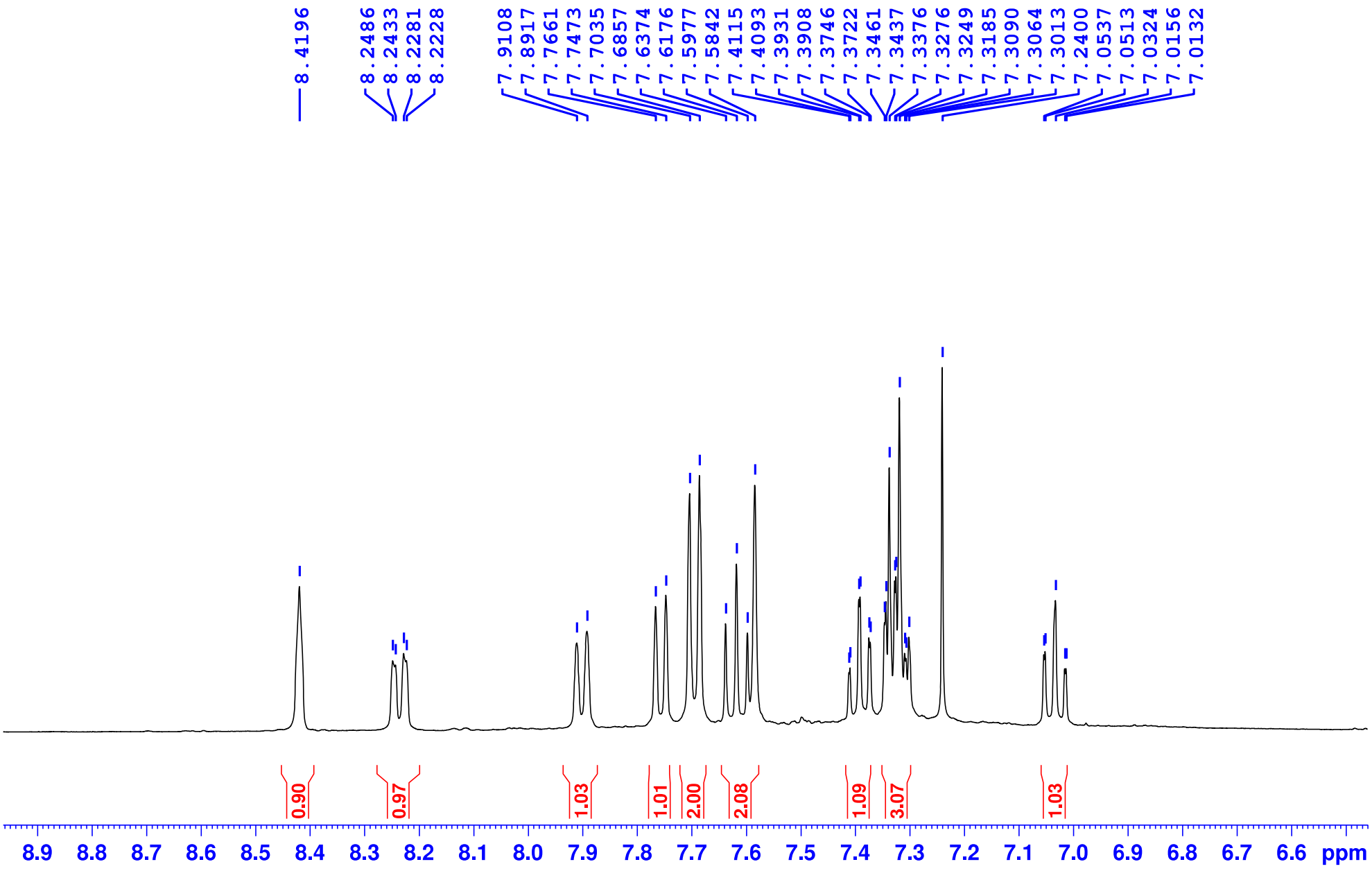
F2 - Acquisition Parameters
Date_              20210305
Time                  15.50 h
INSTRUM               spect
PROBHD    Z116098_0621 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES            0.244532 Hz
AQ                4.0894465 sec
RG                    98.53
DW                   62.400 usec
DE                    6.50 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                       1
SFO1           400.1324708 MHz
NUC1                    1H
P1                   10.00 usec
PLW1           16.68099976 W

F2 - Processing parameters
SI                    65536
SF             400.1300172 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

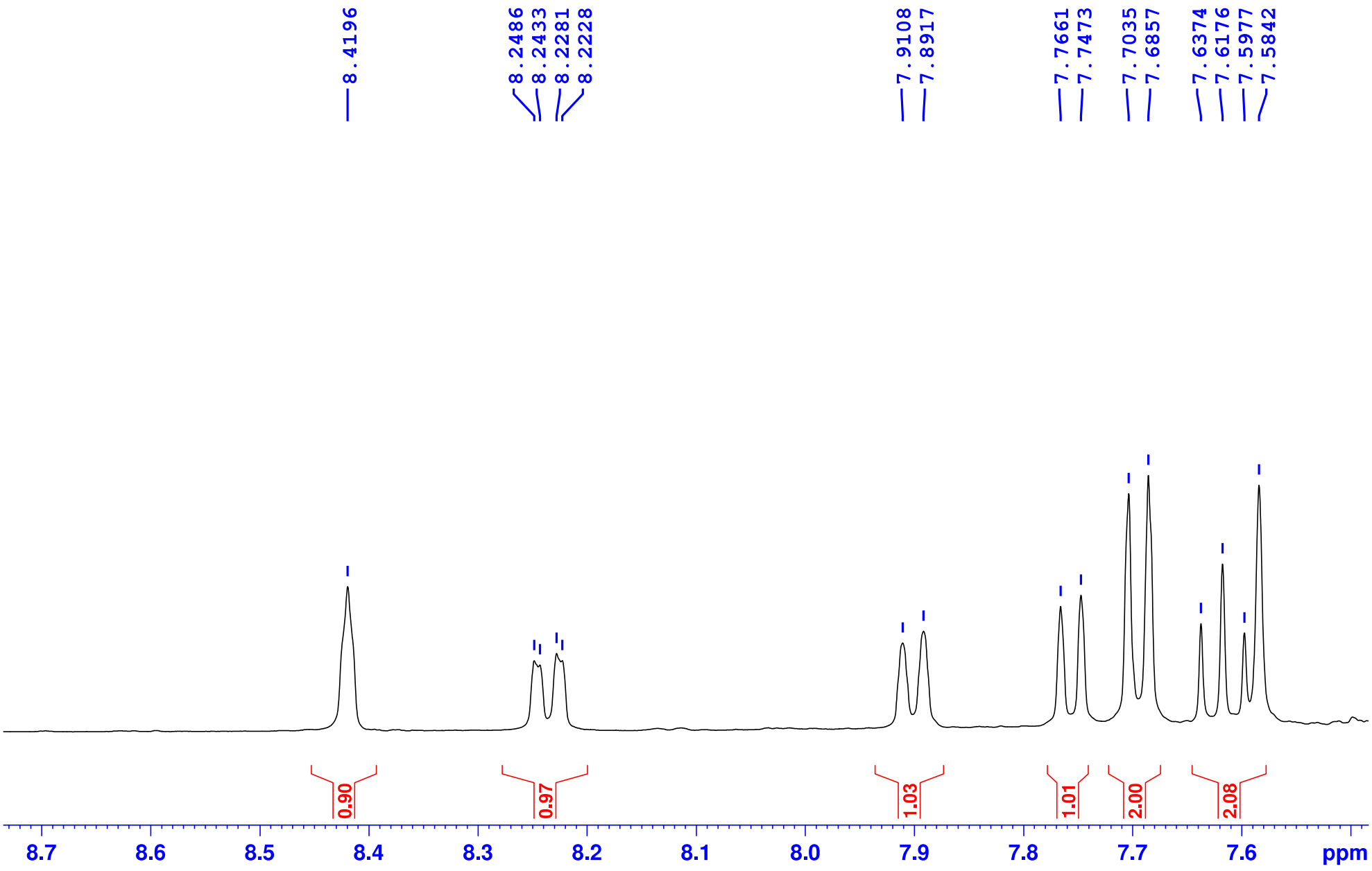
Compound 1d, 1H NMR (400 MHz, CDCl3)



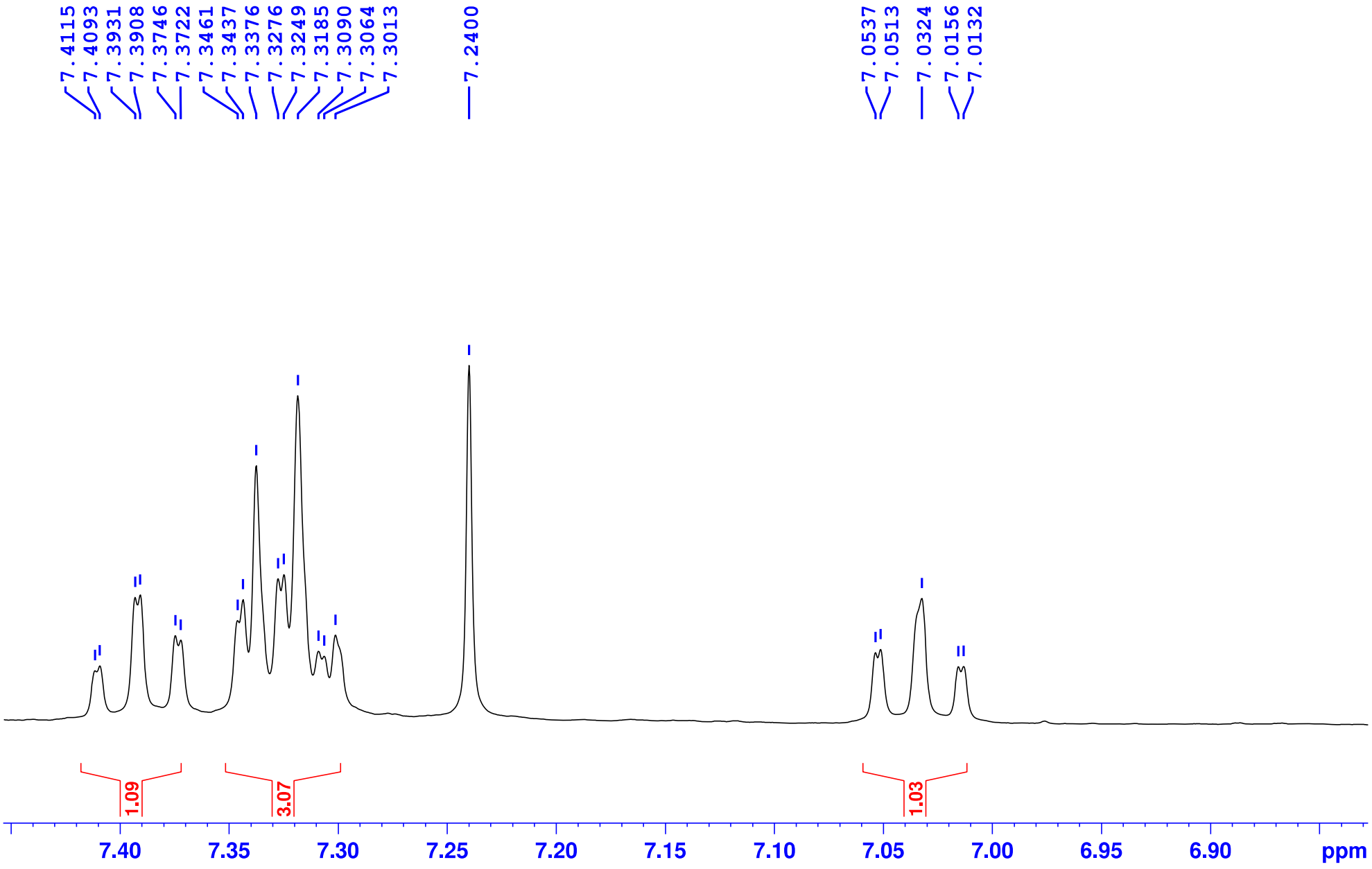
Compound 1d, 1H NMR (400 MHz, CDCl3)



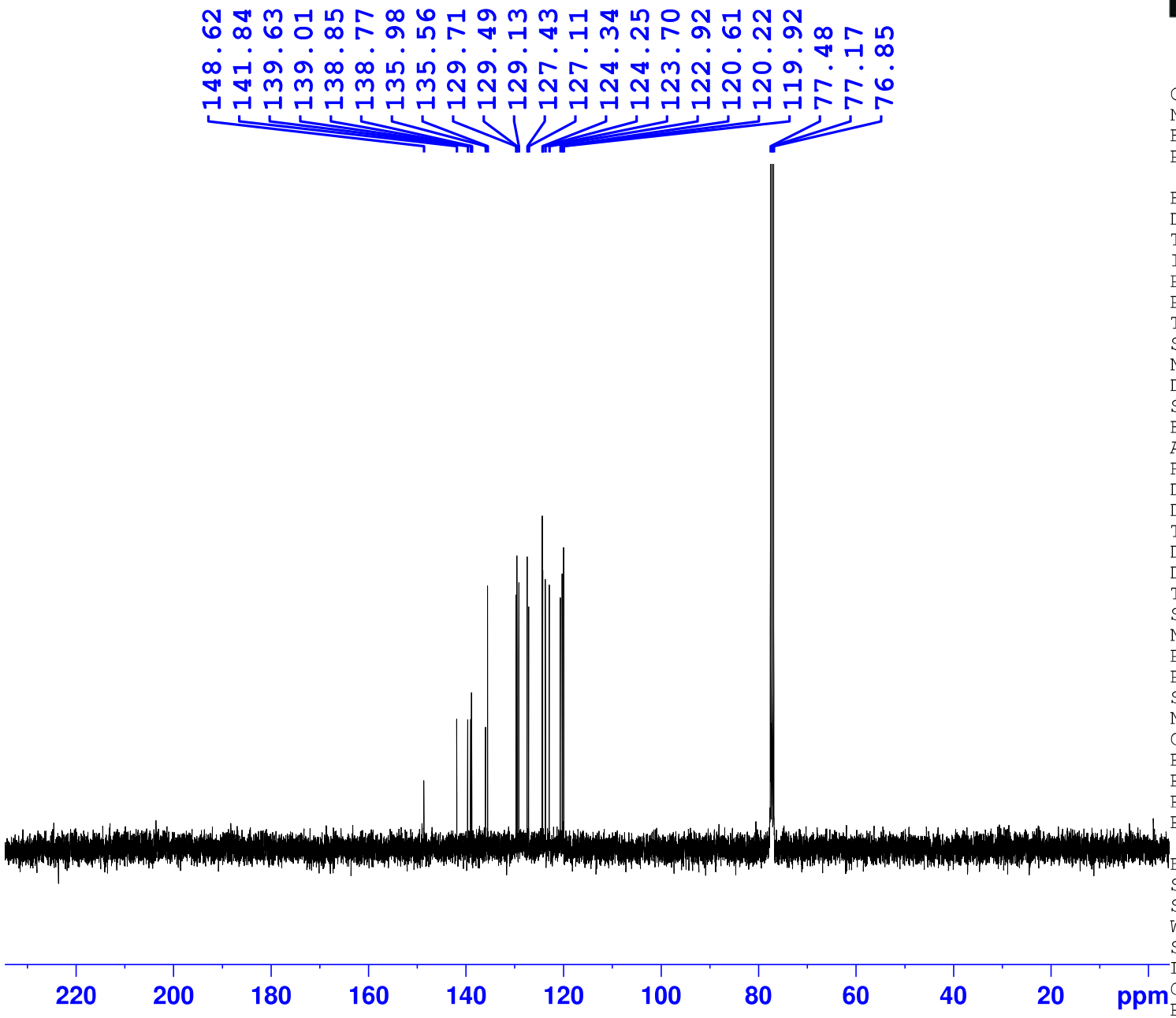
Compound 1d, 1H NMR (400 MHz, CDCl3)



Compound 1d, 1H NMR (400 MHz, CDCl3)



Compound 1d, 13C NMR (100 MHz, CDCl3)

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Current Data Parameters
NAME      Shumaila Majeed
EXPNO                 274
PROCNO                  1

F2 - Acquisition Parameters
Date_           20211013
Time               15.22 h
INSTRUM             spect
PROBHD   Z116098_0621 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    400
DS                      2
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ             1.3631488 sec
RG                 199.48
DW                 20.800 usec
DE                  6.50 usec
TE                 298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         100.6243390 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         72.56700134 W
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         16.68099976 W
PLW12         0.20593999 W
PLW13         0.10342000 W

F2 - Processing parameters
SI                  32768
SF           100.6127547 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
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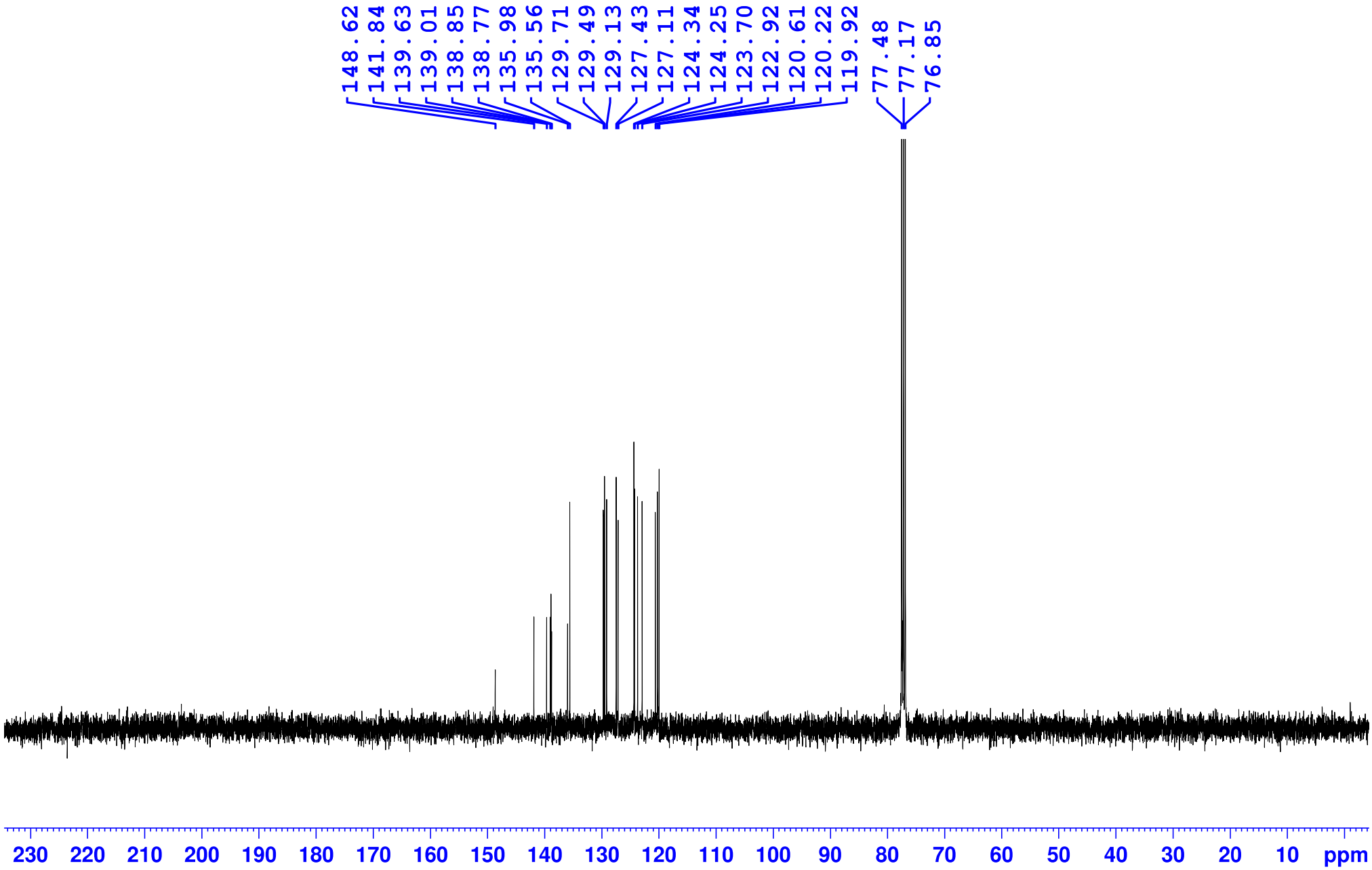
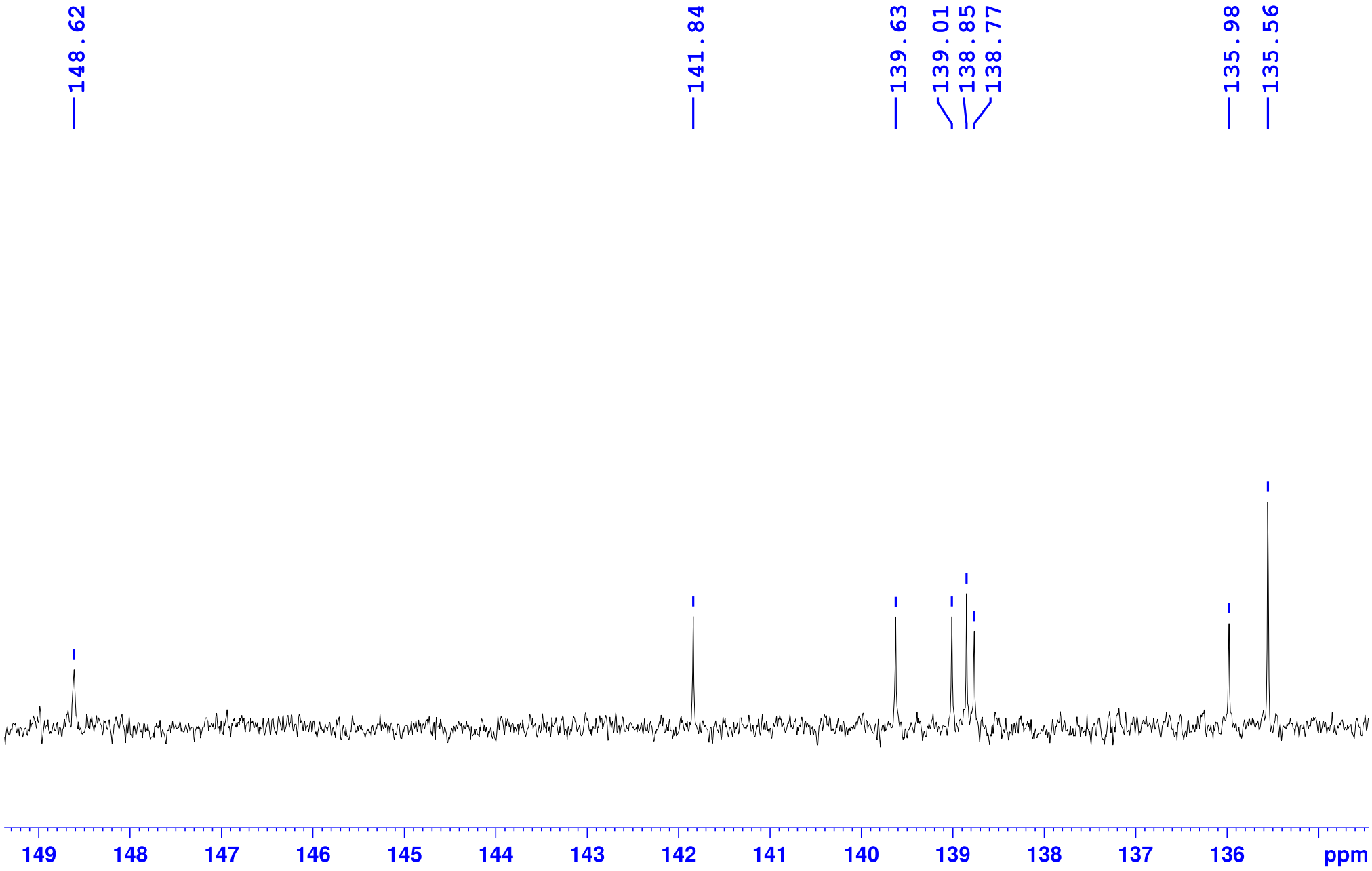
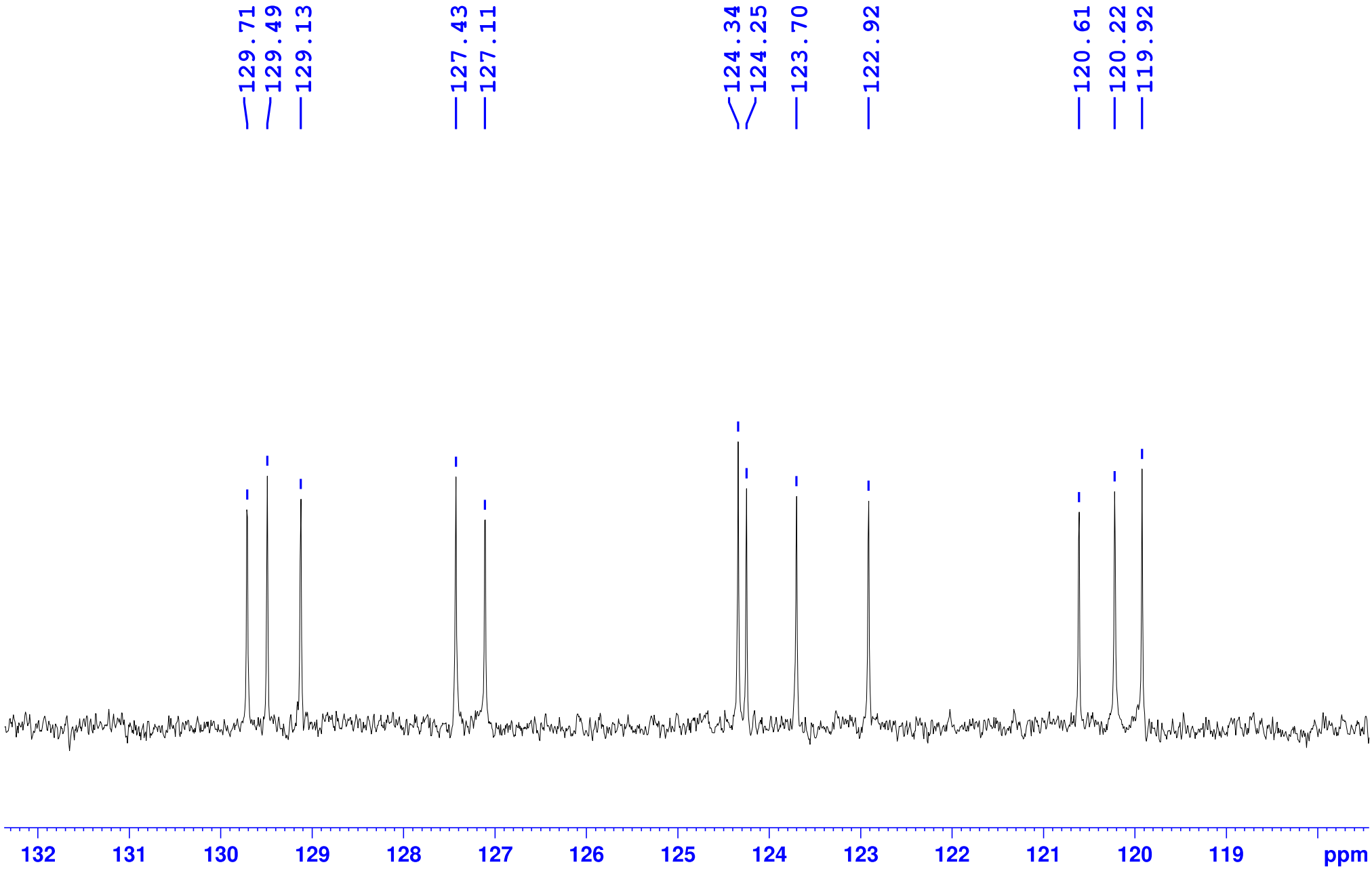
Compound 1d, 13C NMR (100 MHz, CDCl3)



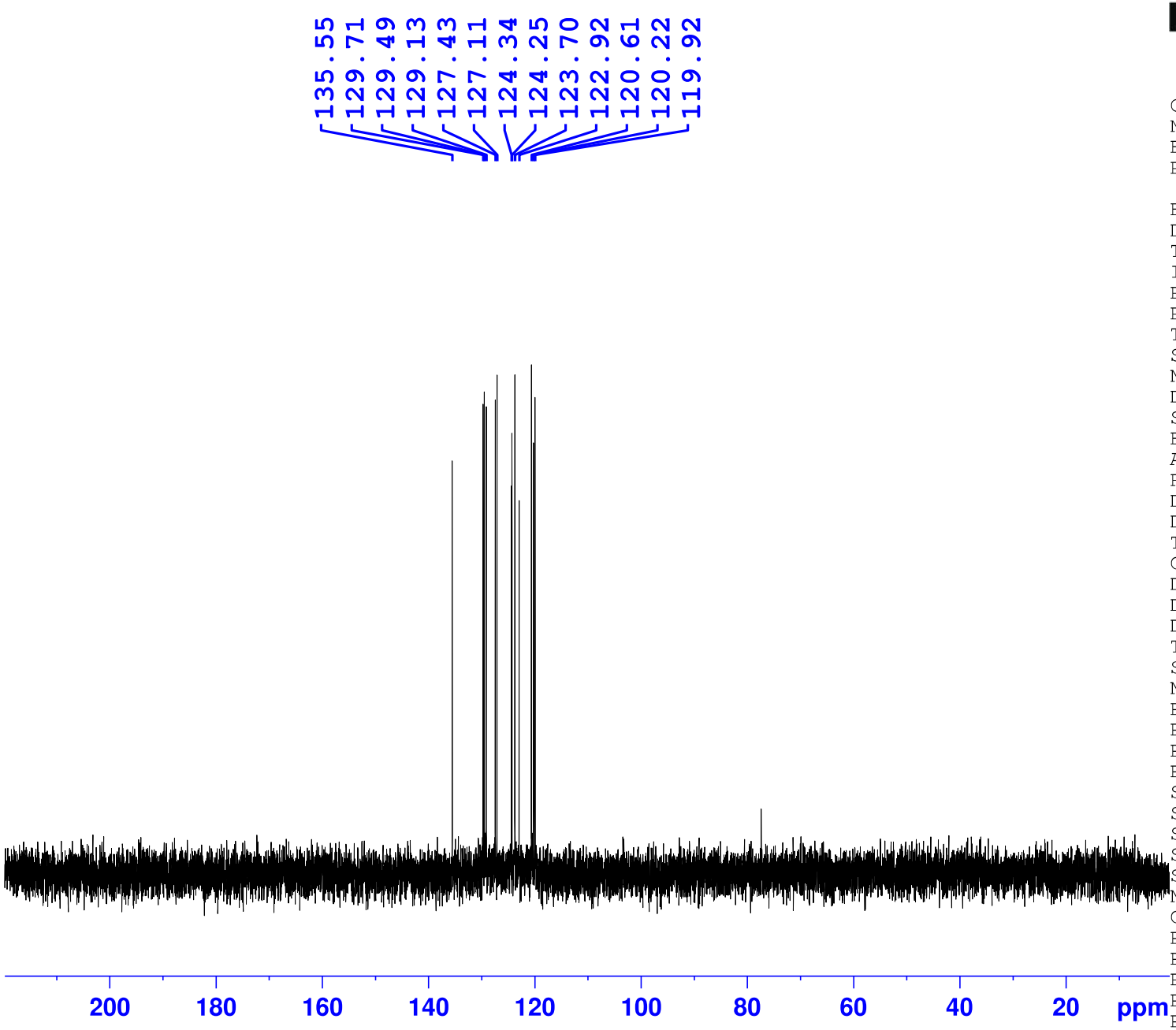
Compound 1d, 13C NMR (100 MHz, CDCl3)



Compound 1d, 13C NMR (100 MHz, CDCl3)



Compound 1d, DEPT 135 NMR (100 MHz, CDCl3)

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Current Data Parameters
NAME      Shumaila Majeed
EXPNO                 275
PROCNO                  1

F2 - Acquisition Parameters
Date_           20211013
Time              15.38 h
INSTRUM             spect
PROBHD   Z116098_0621 (
PULPROG        deptsp135
TD                 65536
SOLVENT             CDCl3
NS                    256
DS                      4
SWH           22058.824 Hz
FIDRES         0.673182 Hz
AQ             1.4854827 sec
RG                199.48
DW                22.667 usec
DE                 6.50 usec
TE                298.0 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                    1
SFO1         100.6238359 MHz
NUC1                13C
P1                10.00 usec
P13             2000.00 usec
PLW0      0 W
PLW1         72.56700134 W
SPNAM[5]    Crp60comp.4
SPOAL5             0.500
SPOFFS5   0 Hz
SPW5         11.08699989 W
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
P3                10.00 usec
P4                20.00 usec
PCPD2             90.00 usec
PLW2         16.68099976 W
PLW12         0.20593999 W
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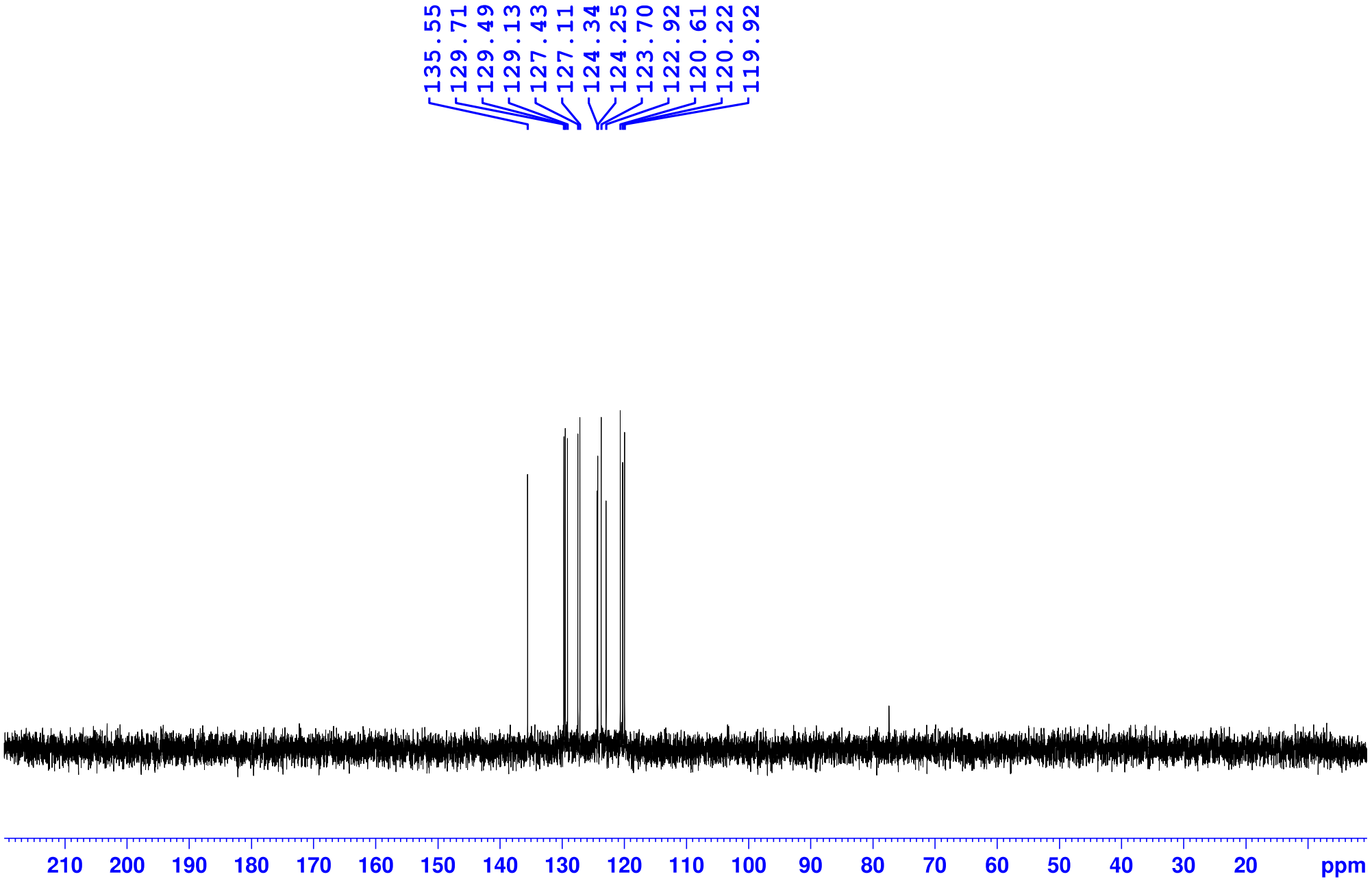
Compound 1d, DEPT 135 NMR (100 MHz, CDCl3)



Compound 1d, DEPT 135 NMR (100 MHz, CDCl3)