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SUPPLEMENTARY DATA

Anthraquinone-chalcone hybrids: Synthesis, preliminary antiproliferative evaluation and DNA-interaction studies

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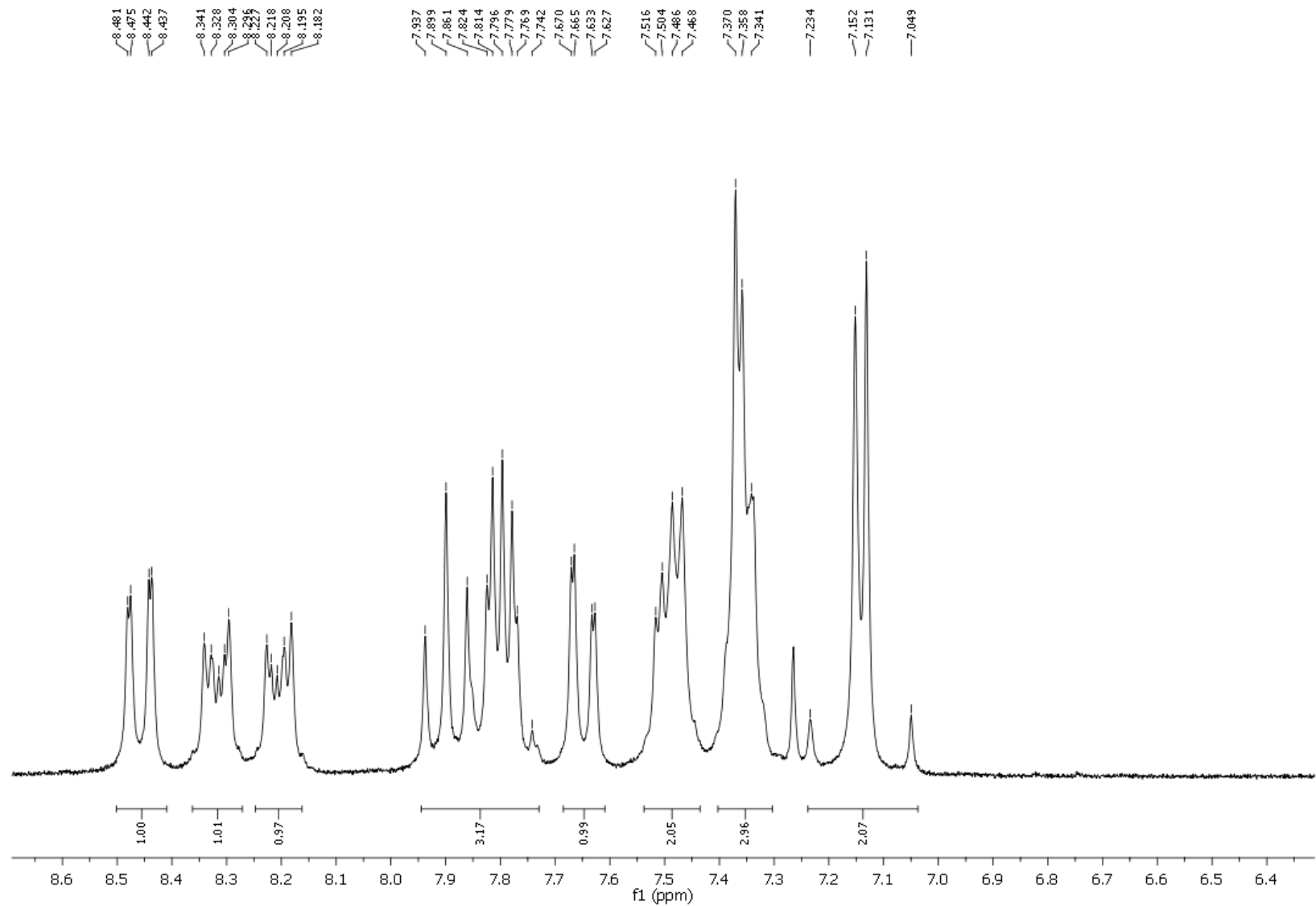


Fig. S1. ^1H NMR spectrum of **2a** in CDCl_3 (200 MHz).

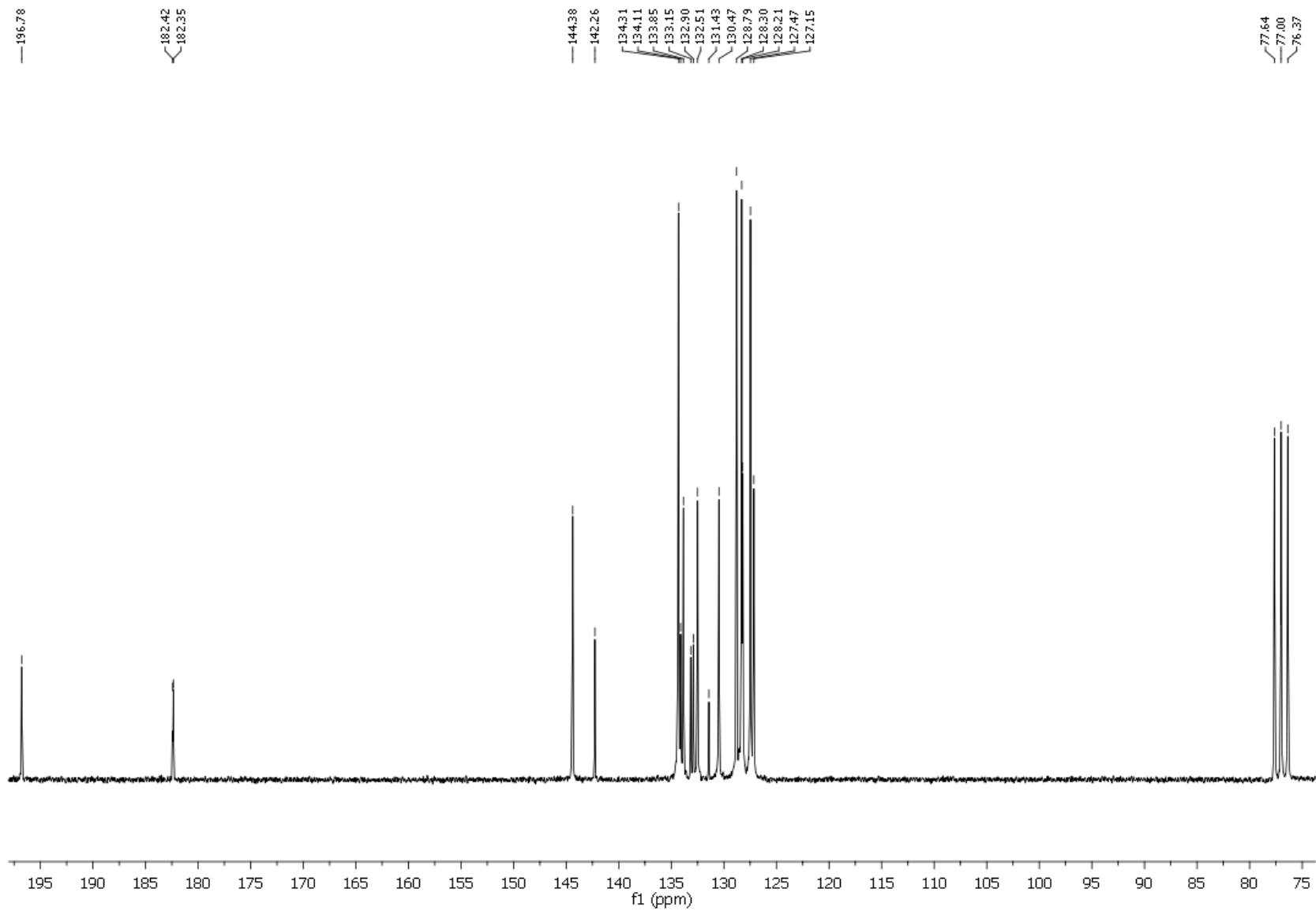


Fig. S2. ^{13}C NMR spectrum of **2a** in CDCl_3 (50 MHz).

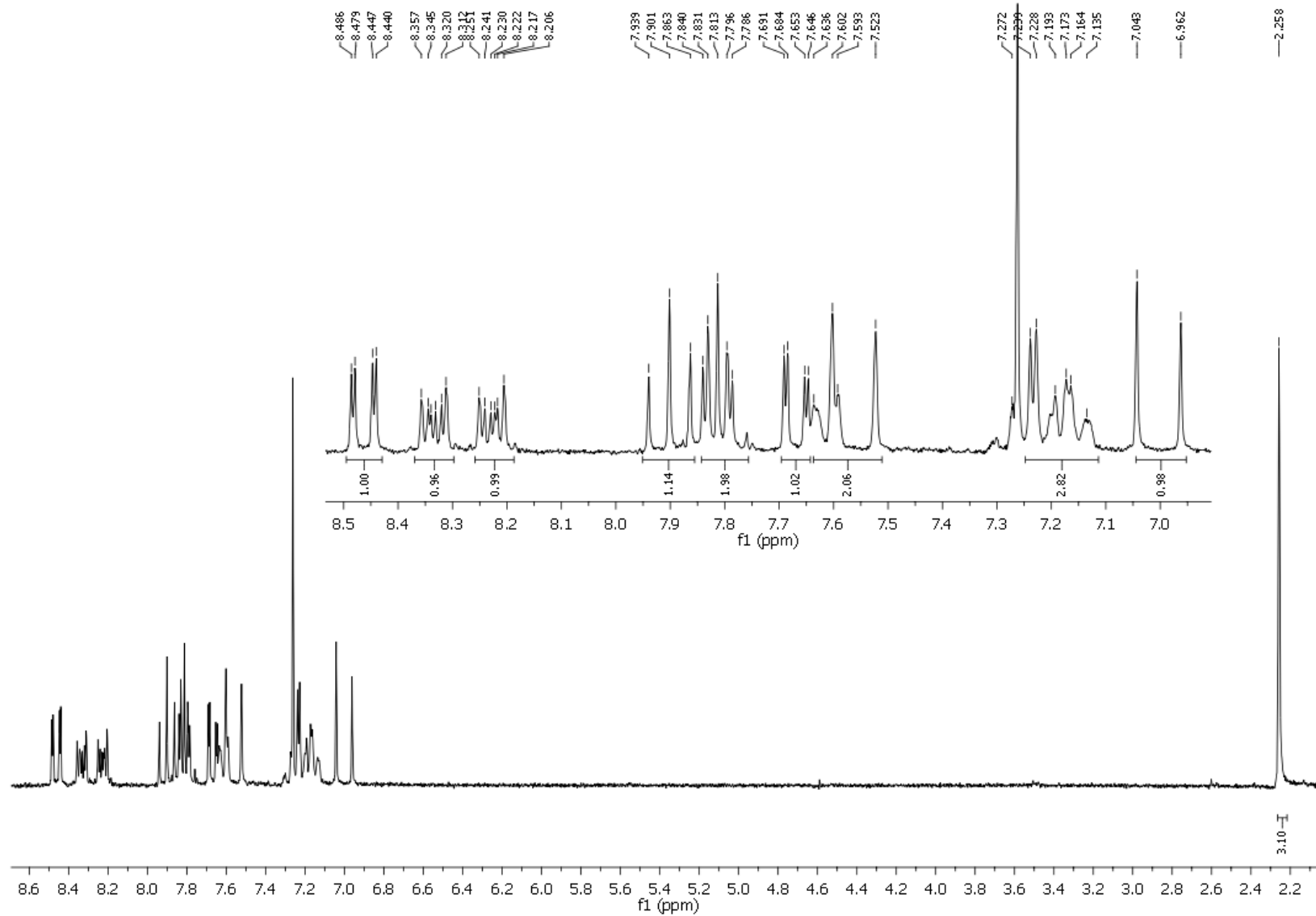


Fig. S3. ^1H NMR spectrum of **2b** in CDCl_3 (200 MHz).

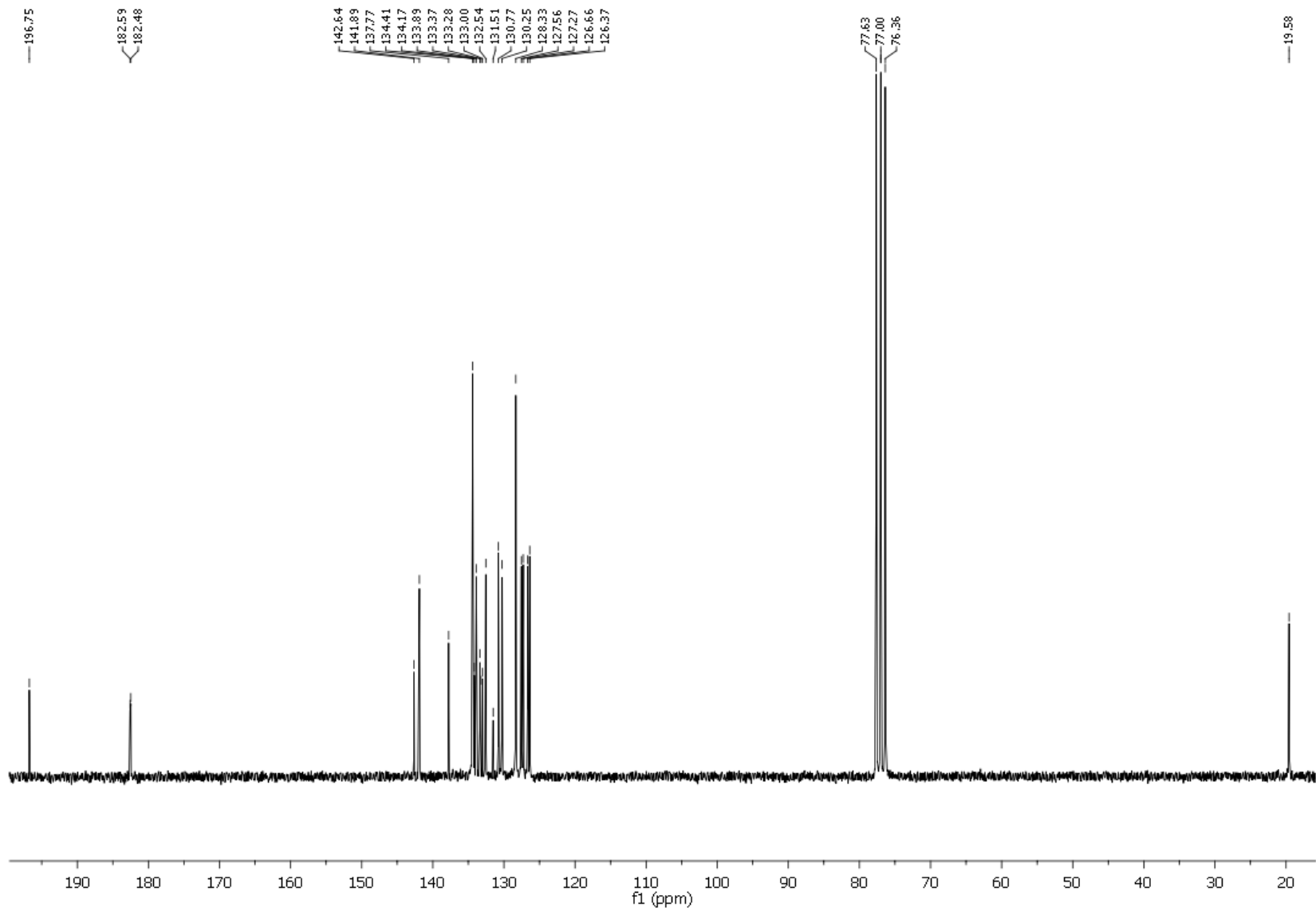


Fig. S4. ^{13}C NMR spectrum of **2b** in CDCl_3 (50 MHz).

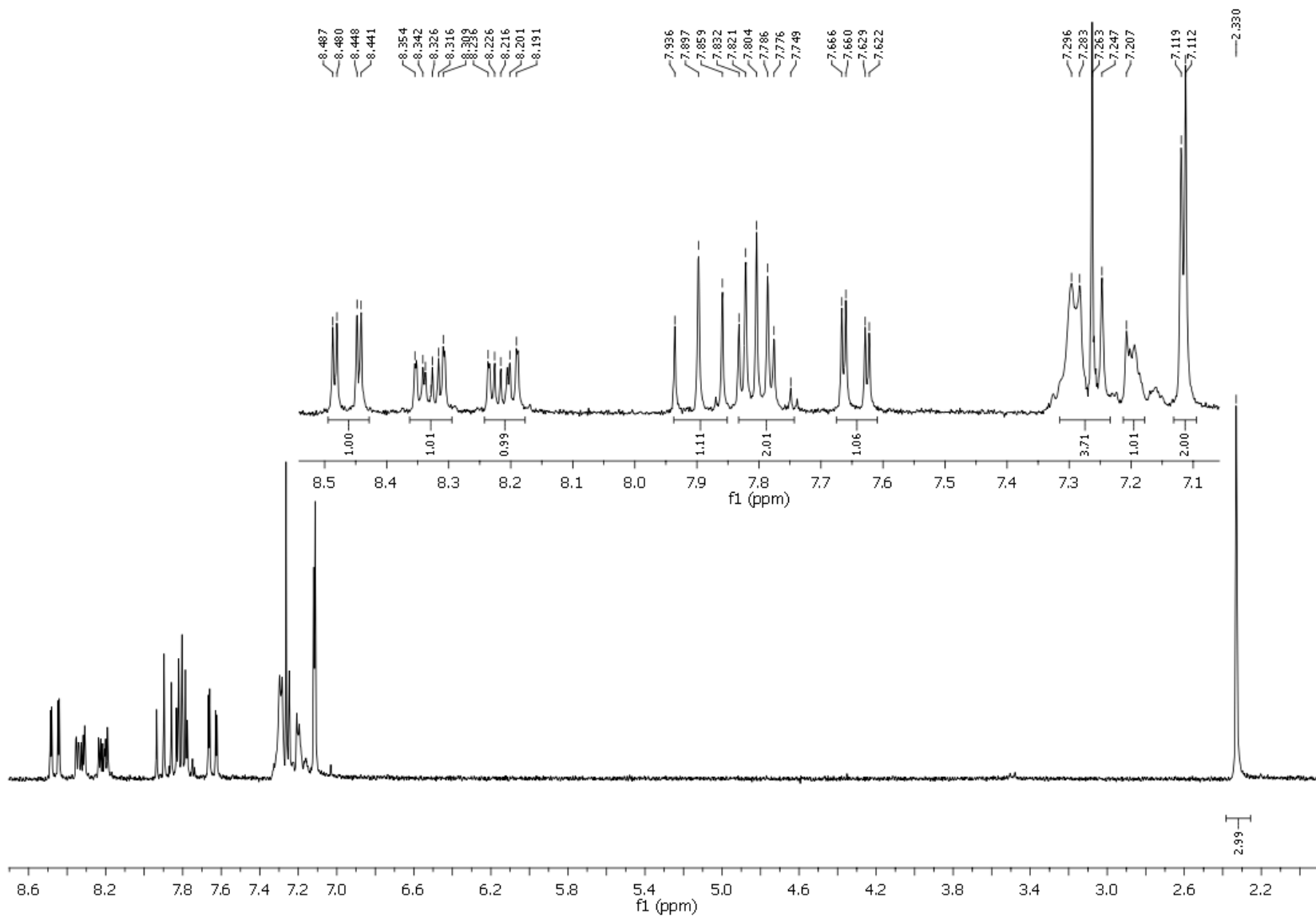


Fig. S5. ^1H NMR spectrum of **2c** in CDCl_3 (200 MHz).

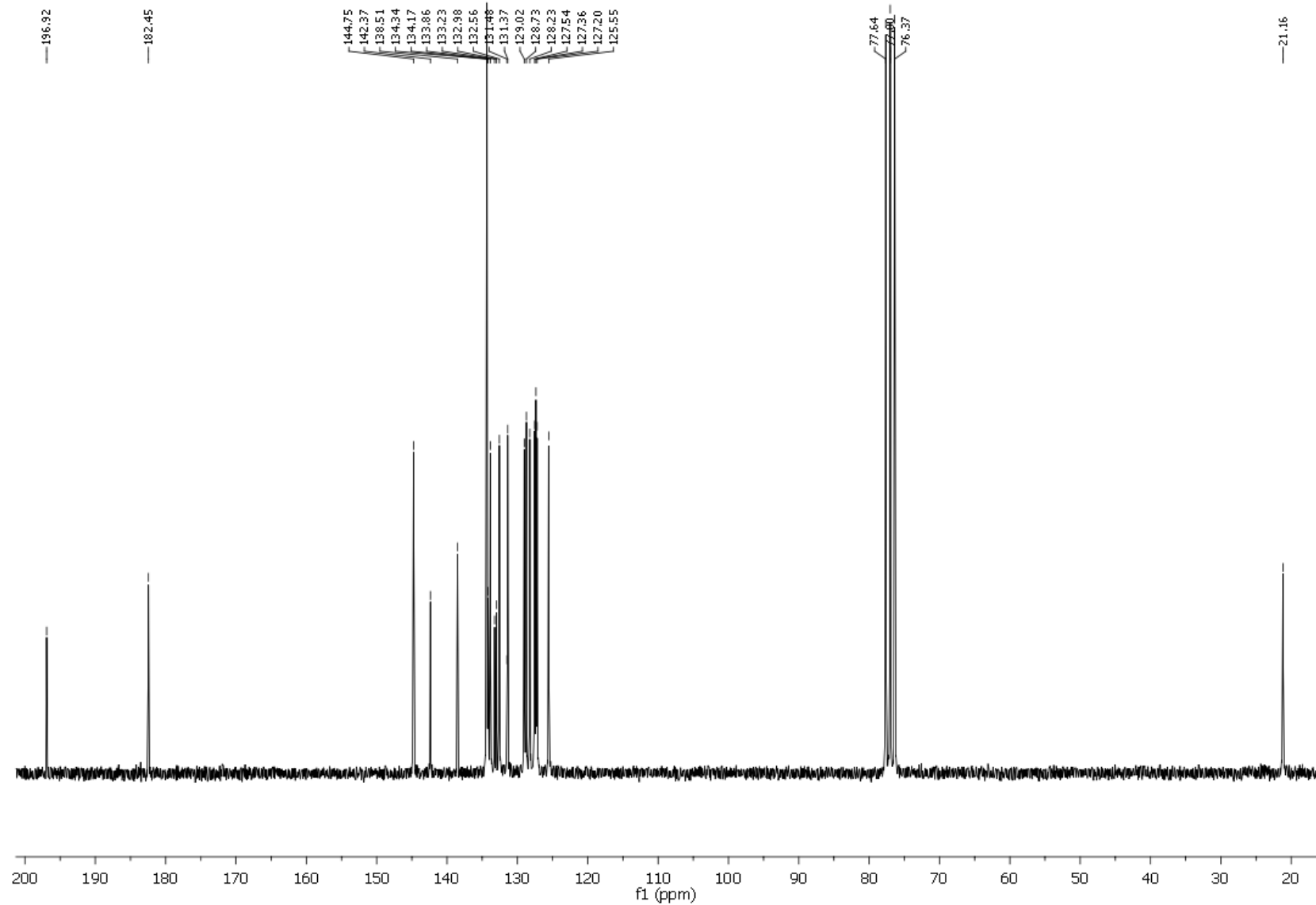


Fig. S6. ^{13}C NMR spectrum of **2c** in CDCl_3 (50 MHz).

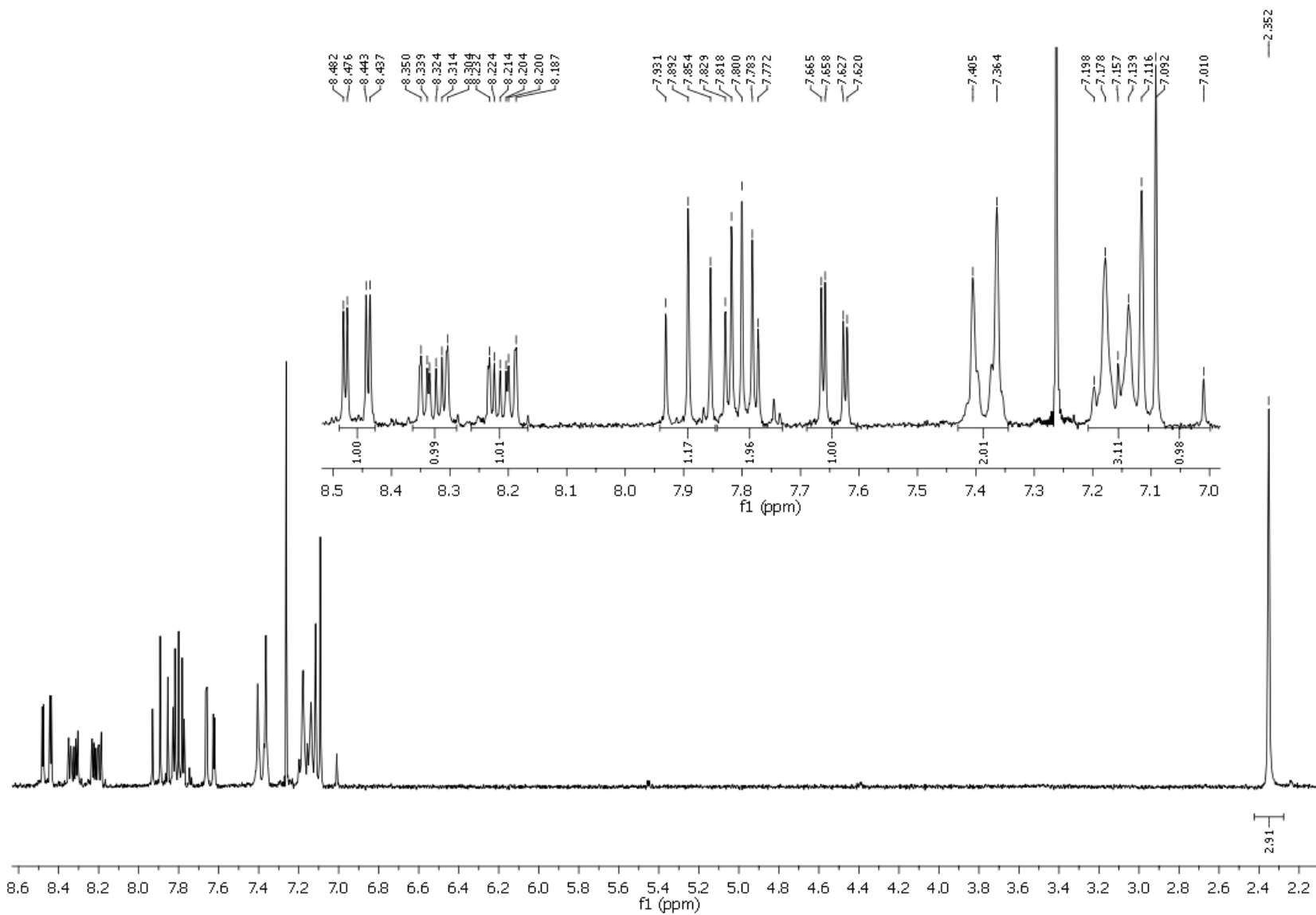


Fig. S7. ^1H NMR spectrum of **2d** in CDCl_3 (200 MHz).

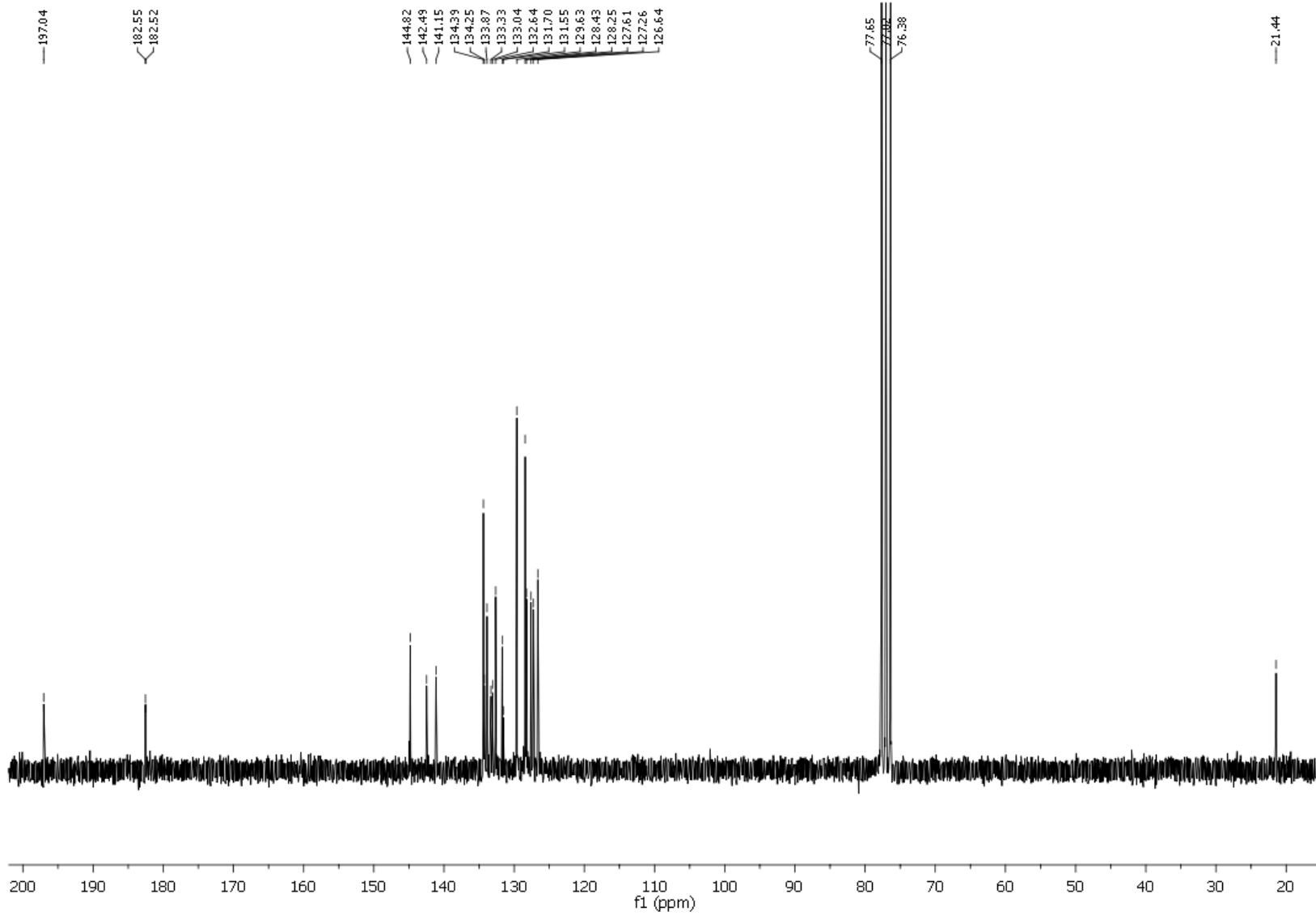


Fig. S8. ^{13}C NMR spectrum of **2d** in CDCl_3 (50 MHz).

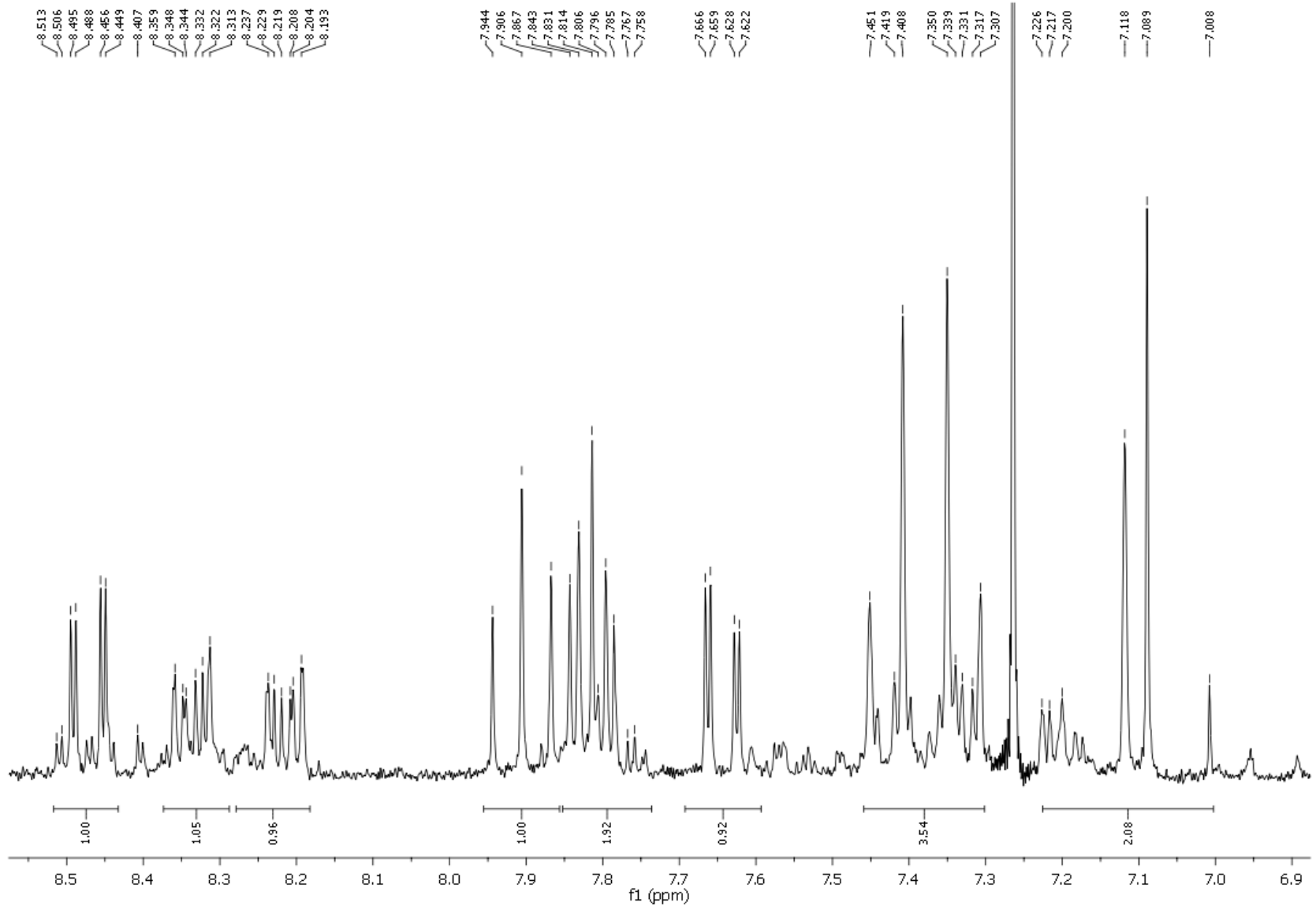


Fig. S9. ^1H NMR spectrum of **2e** in CDCl_3 (200 MHz).

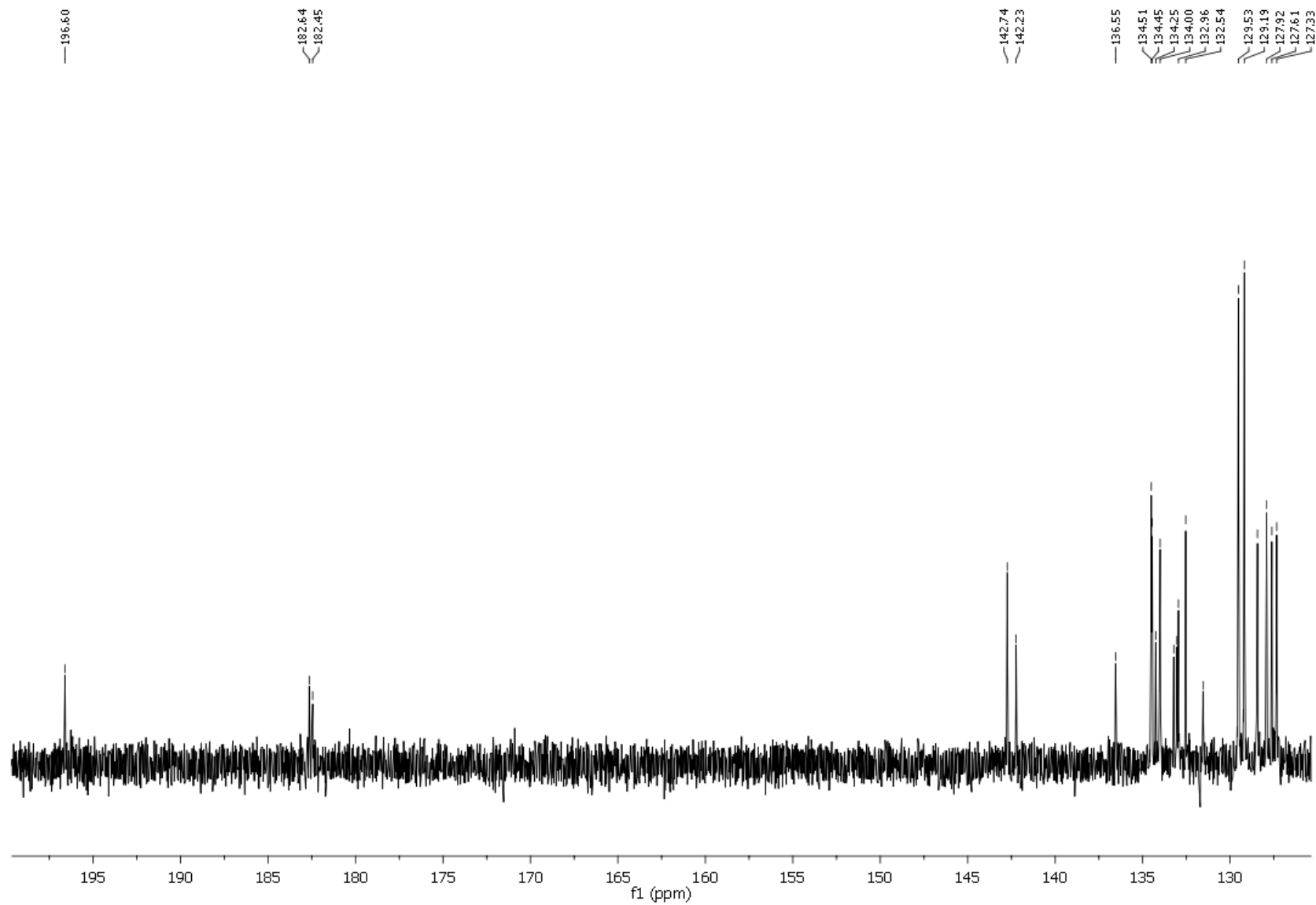


Fig. S10. ^{13}C NMR spectrum of **2e** in CDCl_3 (50 MHz).

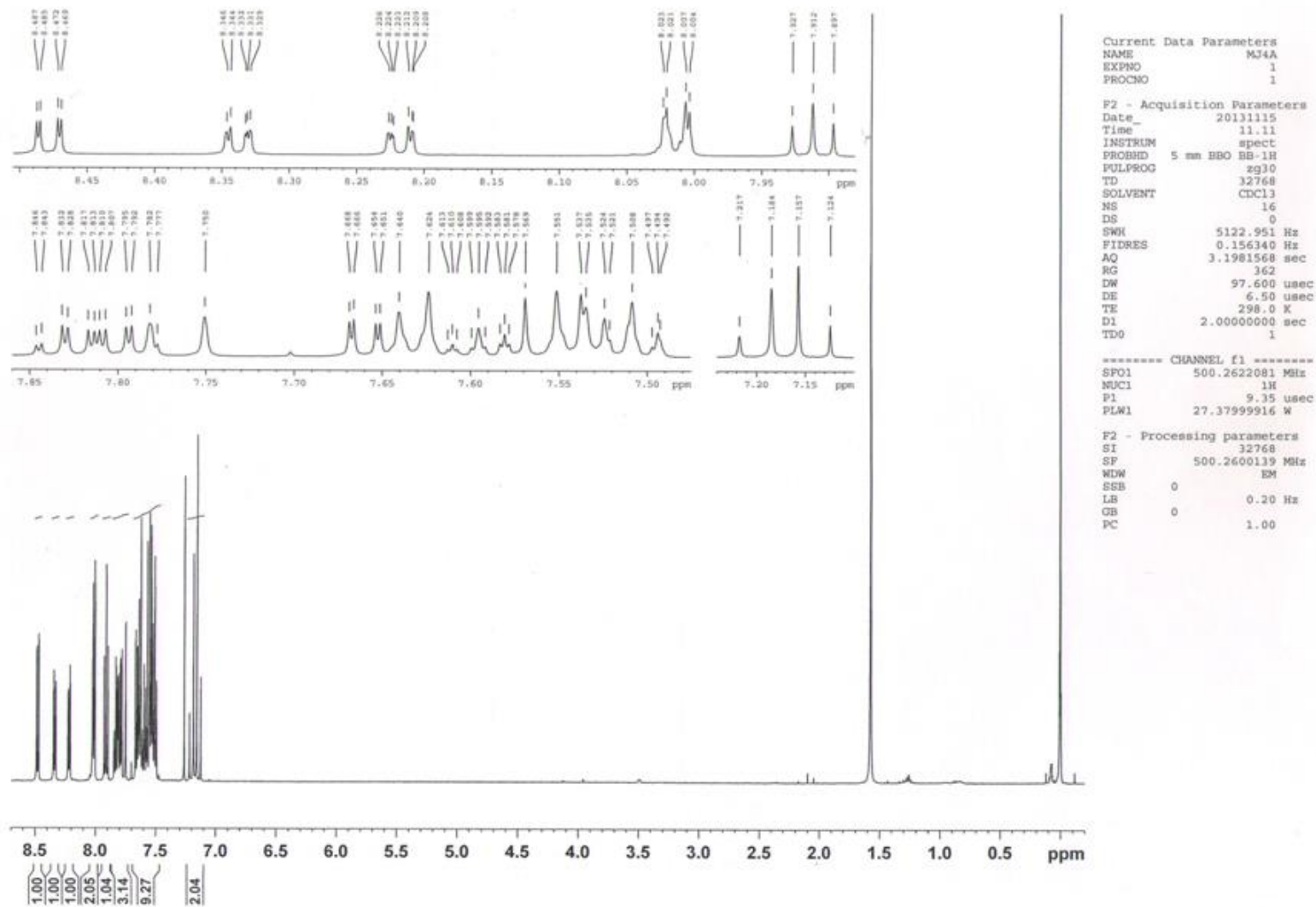
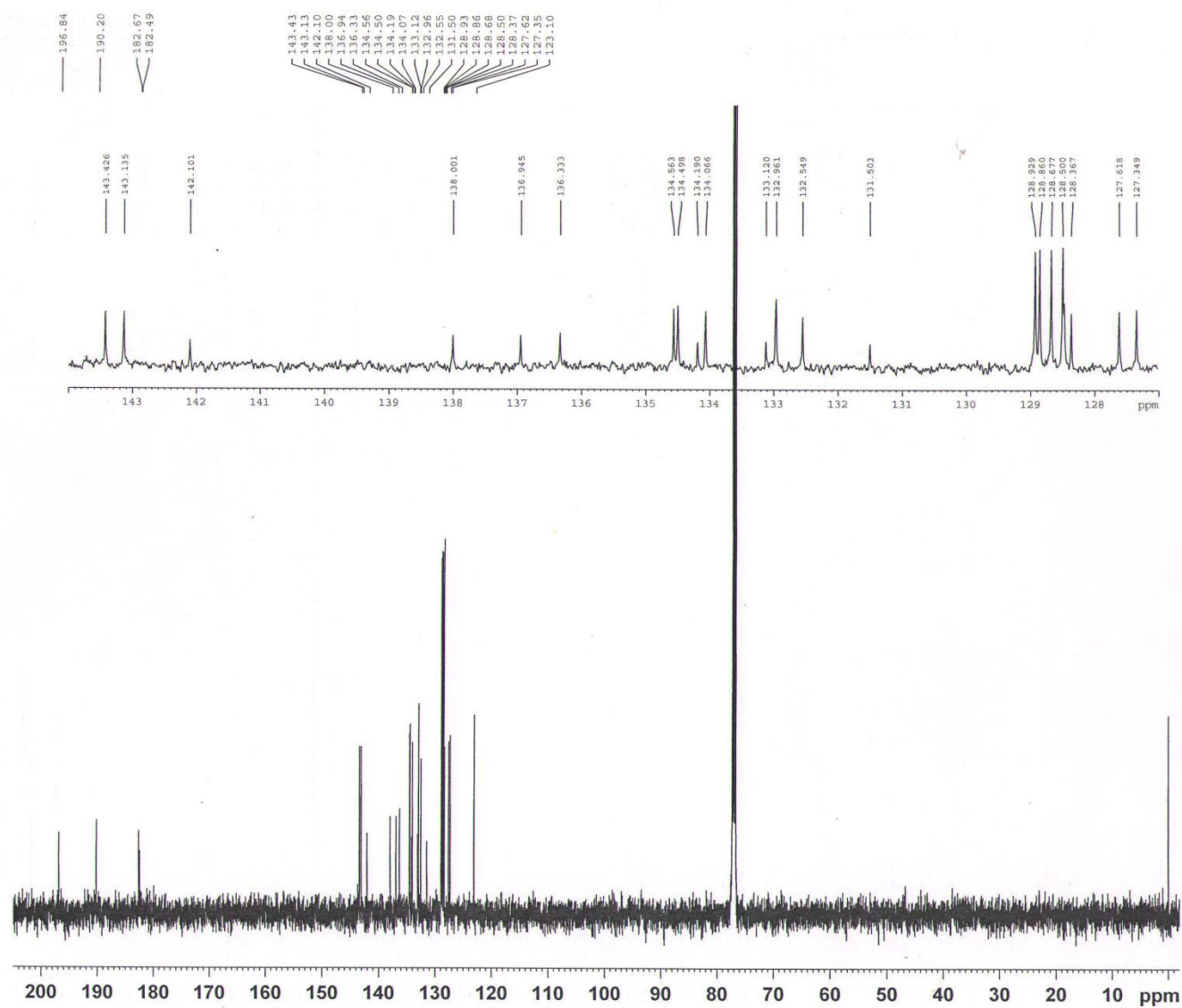


Fig. S11. ^1H NMR spectrum of **4a** in CDCl_3 (500 MHz).



Current Data Parameters
 NAME MJ4A
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131115
 Time_ 11.19
 INSTRUM spect
 PROBD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 946
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505024 sec
 RG 1030
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8043140 MHz
 NUC1 13C
 P1 11.50 usec
 PLW1 32.22800064 W

===== CHANNEL f2 =====
 SFO2 500.2622081 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.77000046 W
 PLW12 0.39267001 W
 PLW13 0.25130999 W

F2 - Processing parameters
 SI 32768
 SF 125.7904802 MHz
 WDW EM
 SSB 0
 LB 1.50 Hz
 GB 0
 PC 1.40

Fig. S12. ^{13}C NMR spectrum of **4a** in CDCl_3 (125 MHz).

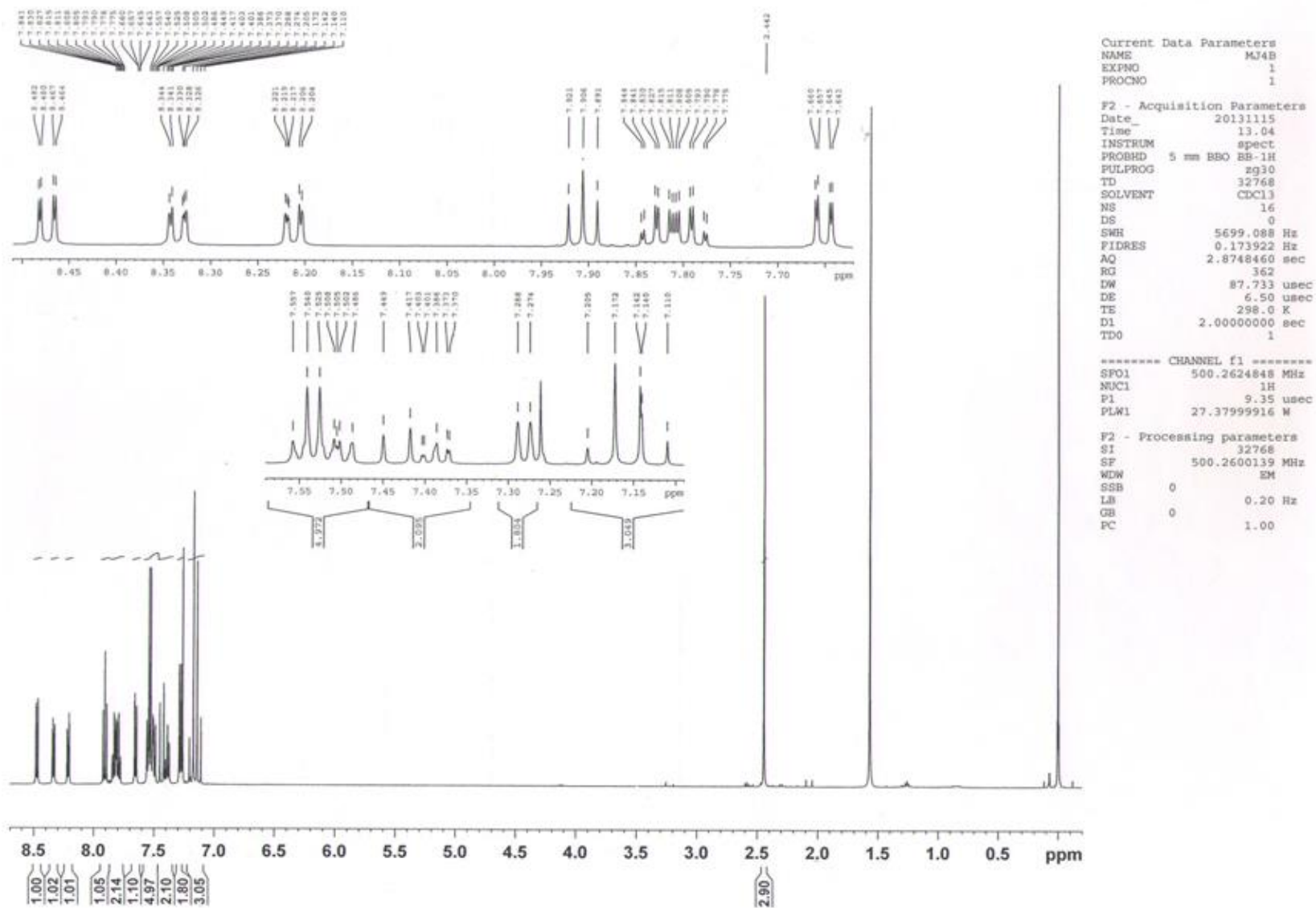
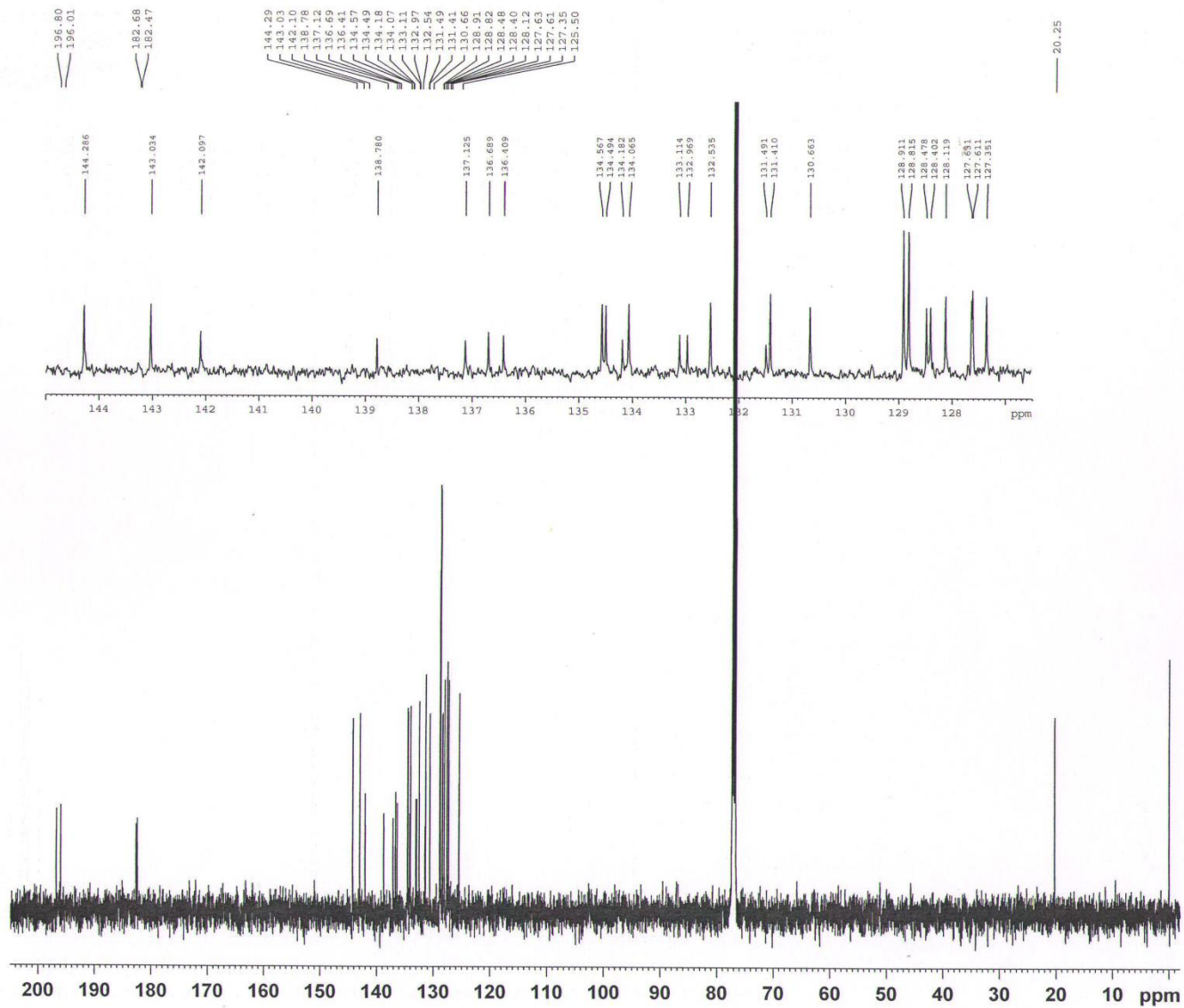


Fig. S13. ^1H NMR spectrum of **4b** in CDCl_3 (500 MHz).



Current Data Parameters
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 EXPNO 2
 PROCNO 1

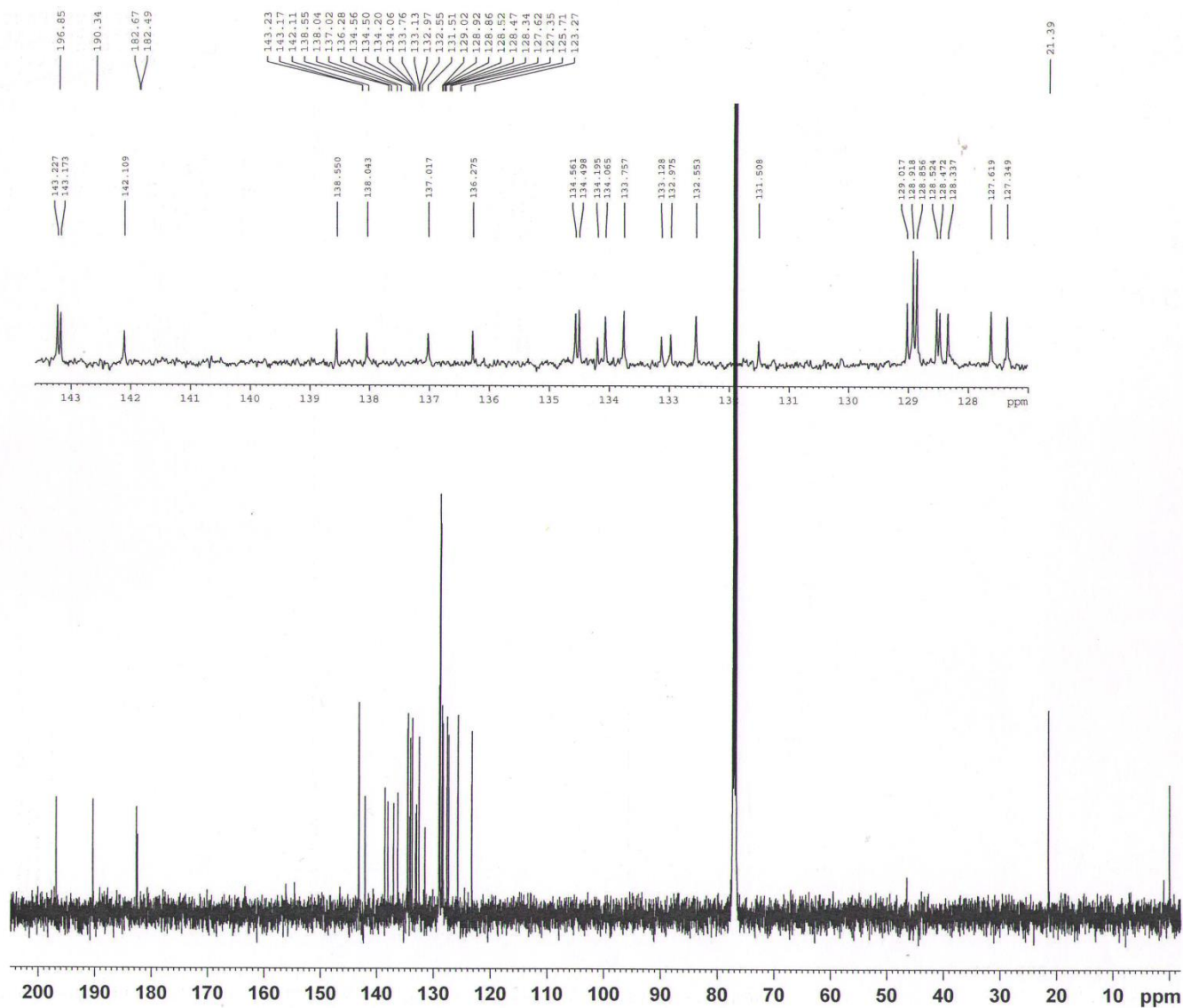
F2 - Acquisition Parameters
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 Time 13.13
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1214
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505024 sec
 RG 1030
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8043140 MHz
 NUC1 13C
 P1 11.50 usec
 PLW1 32.22800064 W

===== CHANNEL f2 =====
 SFO2 500.2624848 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.77000046 W
 PLW12 0.39267001 W
 PLW13 0.25130999 W

F2 - Processing parameters
 SI 32768
 SF 125.7904800 MHz
 WDW EM
 SSB 0
 LB 1.50 Hz
 GB 0
 PC 1.40

Fig. S14. ¹³C NMR spectrum of **4b** in CDCl₃ (125 MHz).



```

Current Data Parameters
NAME          MJ4C
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20131122
Time          14.15
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            1607
DS            4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            0.5505024 sec
RG            912
DW            16.800 usec
DE            6.50 usec
TE            298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          125.8043140 MHz
NUC1           13C
P1            11.50 usec
PLW1          32.22800064 W

===== CHANNEL f2 =====
SFO2          500.2623552 MHz
NUC2           1H
CPDPRG[2]     waltz16
PCPD2         80.00 usec
PLW2          20.77000046 W
PLW12         0.39267001 W
PLW13         0.25130999 W

F2 - Processing parameters
SI            32768
SF            125.7904801 MHz
WDW           EM
SSB           0
LB            1.50 Hz
GB            0
PC            1.40

```

Fig. S16. ^{13}C NMR spectrum of **4c** in CDCl_3 (125 MHz).

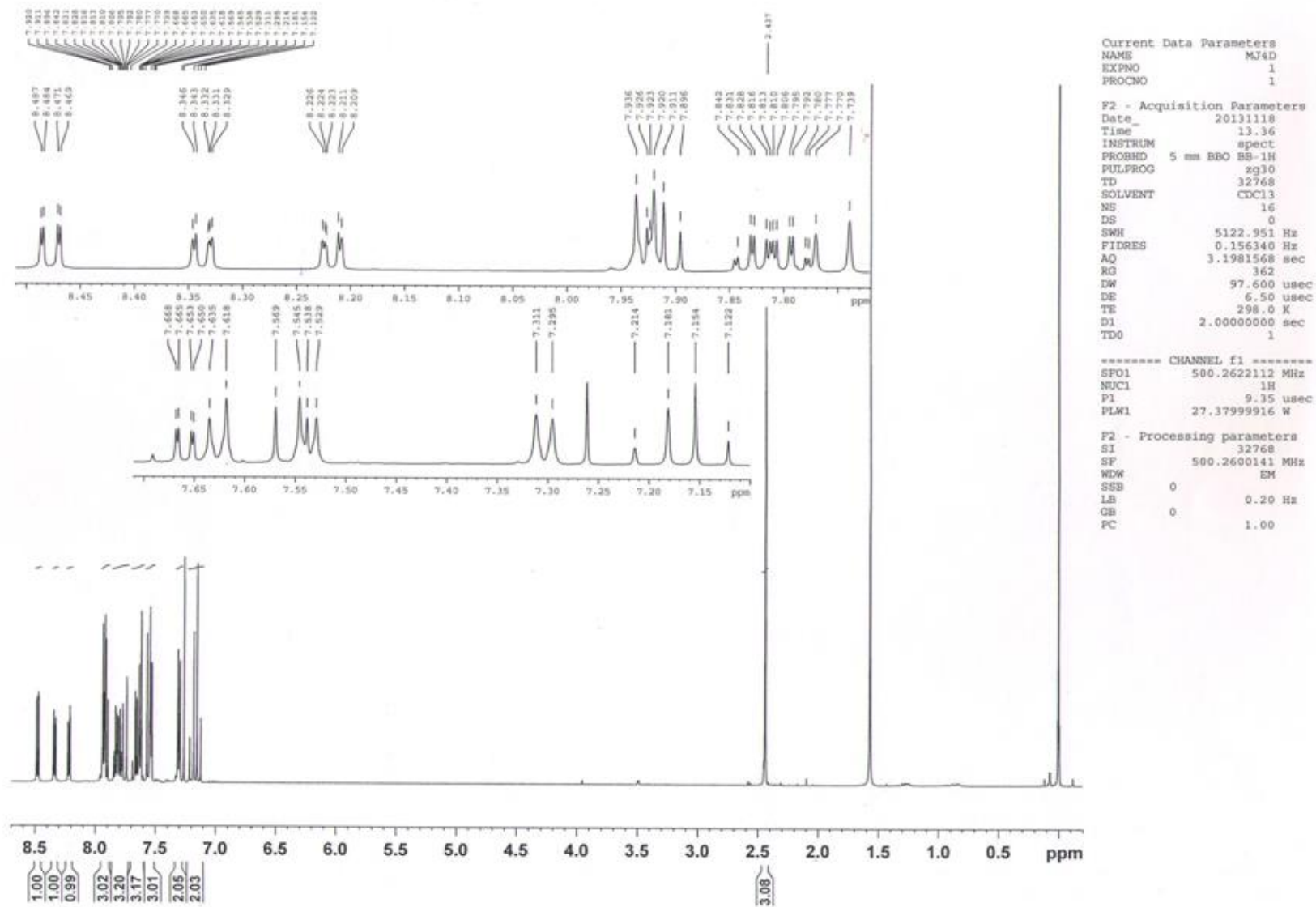
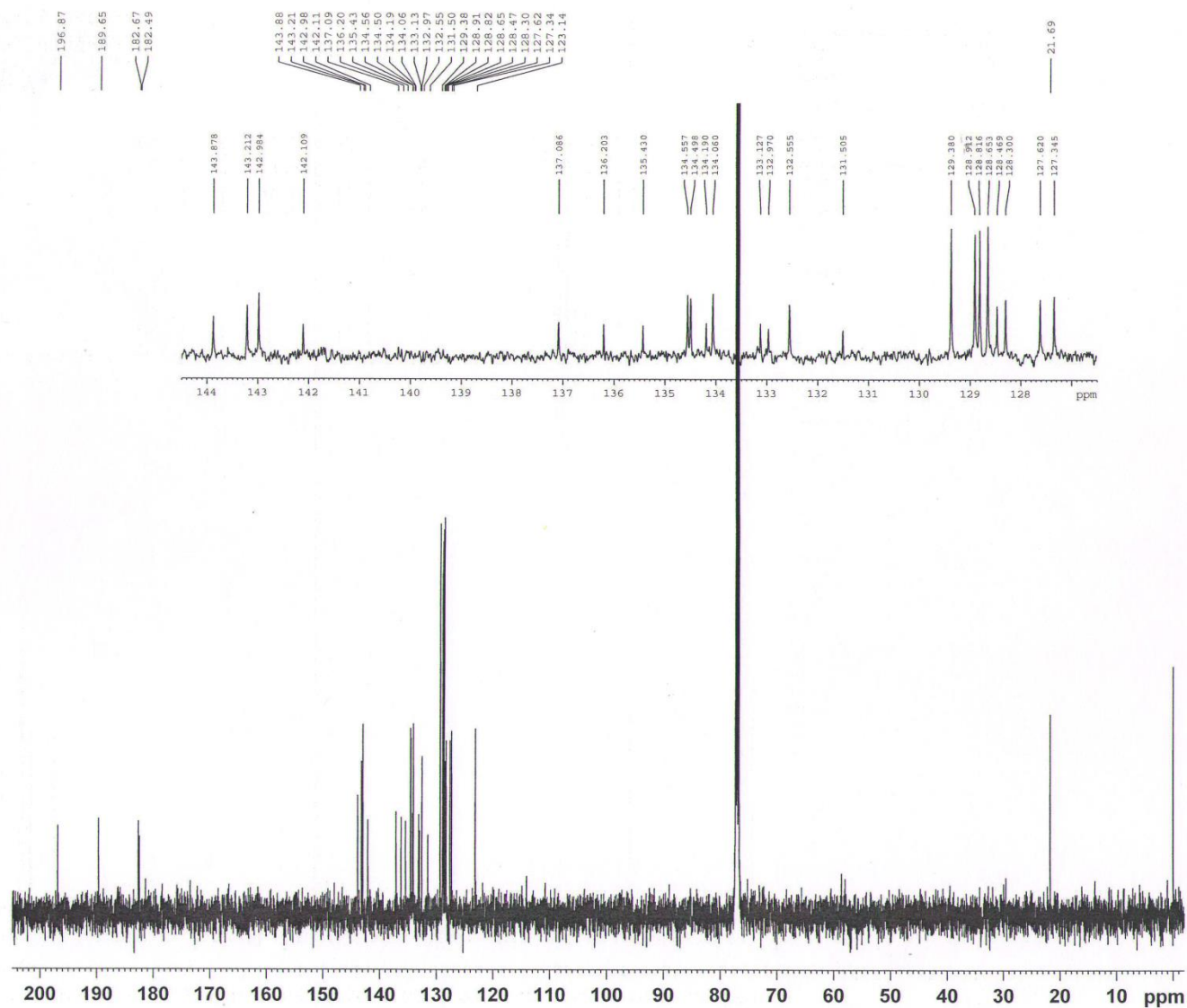


Fig. S17. ^1H NMR spectrum of **4d** in CDCl_3 (500 MHz).



Current Data Parameters
 NAME MJ4D
 EXPNO 2
 PROCNO 1

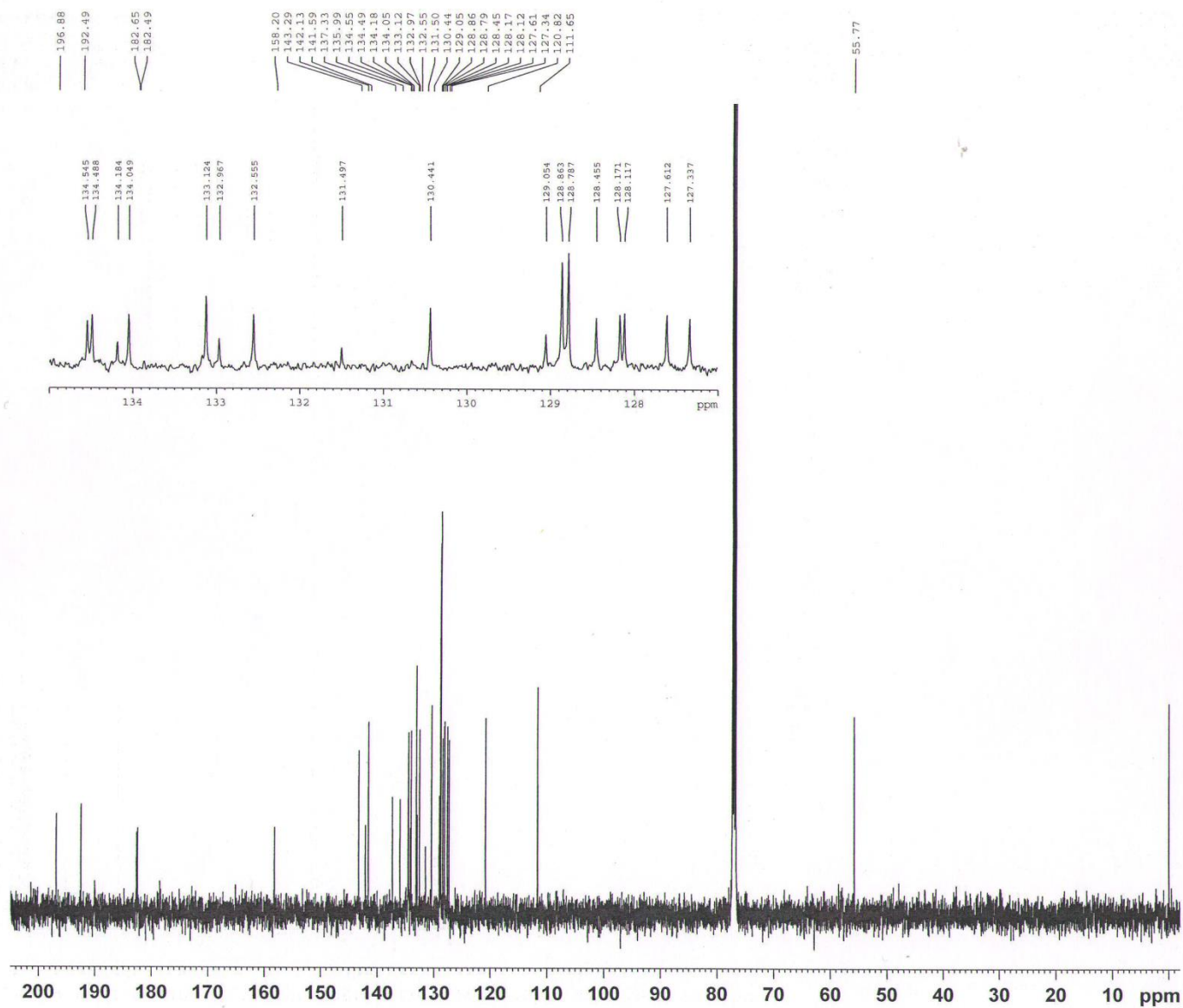
F2 - Acquisition Parameters
 Date 20131118
 Time 13.47
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 929
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505024 sec
 RG 1030
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 125.8043140 MHz
 NUC1 13C
 P1 11.50 usec
 PLW1 32.22800064 W

===== CHANNEL f2 =====
 SFO2 500.2622111 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.77000046 W
 PLW12 0.39267001 W
 PLW13 0.25130999 W

F2 - Processing parameters
 SI 32768
 SF 125.7904801 MHz
 WDW EM
 SSB 0
 LB 1.50 Hz
 GB 0
 PC 1.40

Fig. S18. ^{13}C NMR spectrum of **4d** in CDCl_3 (125 MHz).



Current Data Parameters
 NAME MJ4E
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131119
 Time 16.02
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505024 sec
 RG 1030
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8043140 MHz
 NUC1 13C
 P1 11.50 usec
 PLW1 32.22800064 W

===== CHANNEL f2 =====
 SFO2 500.2624568 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.77000046 W
 PLW12 0.39267001 W
 PLW13 0.25130999 W

F2 - Processing parameters
 SI 32768
 SF 125.7904802 MHz
 WDW EM
 SSB 0
 LB 1.50 Hz
 GB 0
 PC 1.40

Fig. S20. ^{13}C NMR spectrum of **4e** in CDCl_3 (125 MHz).

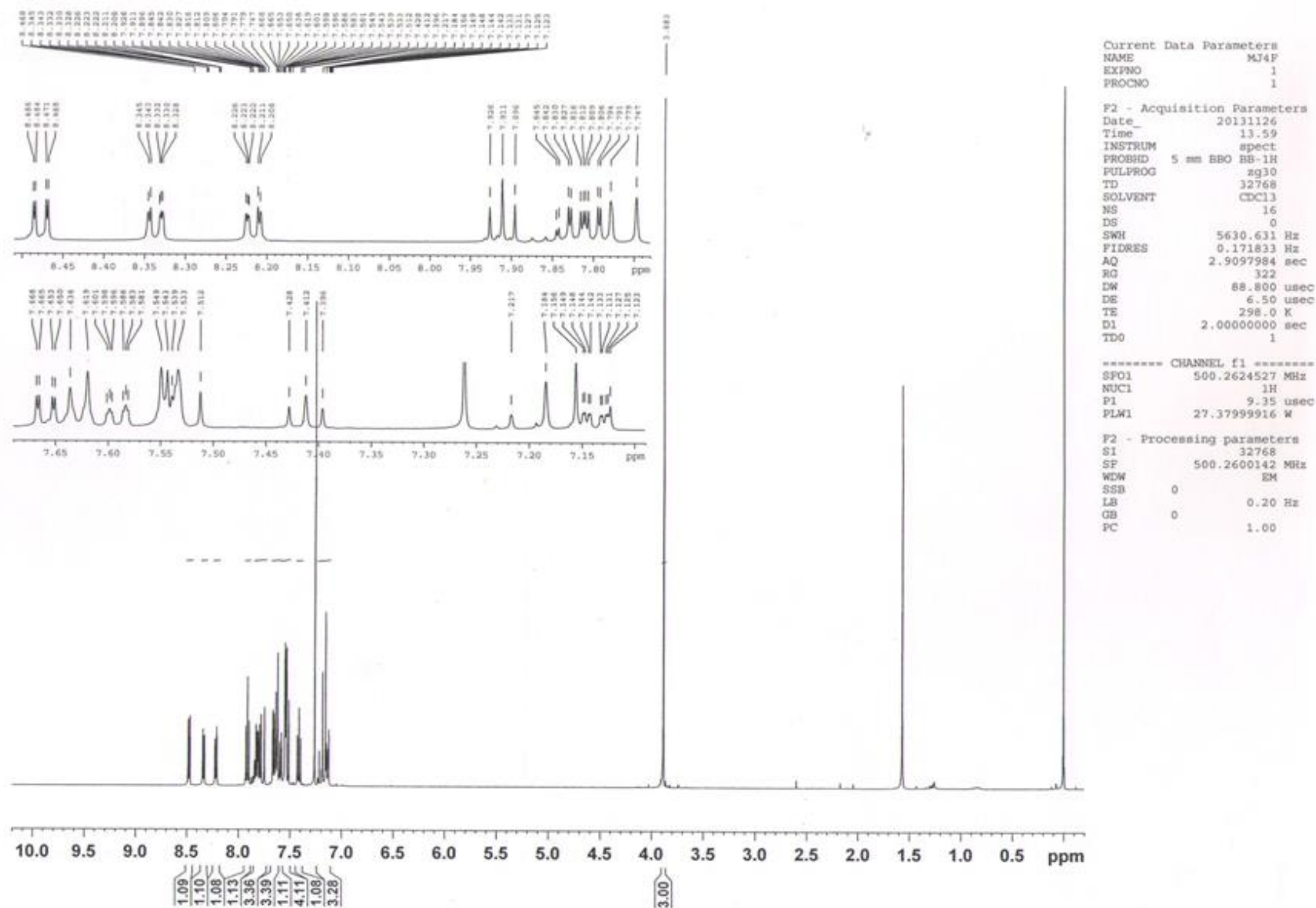
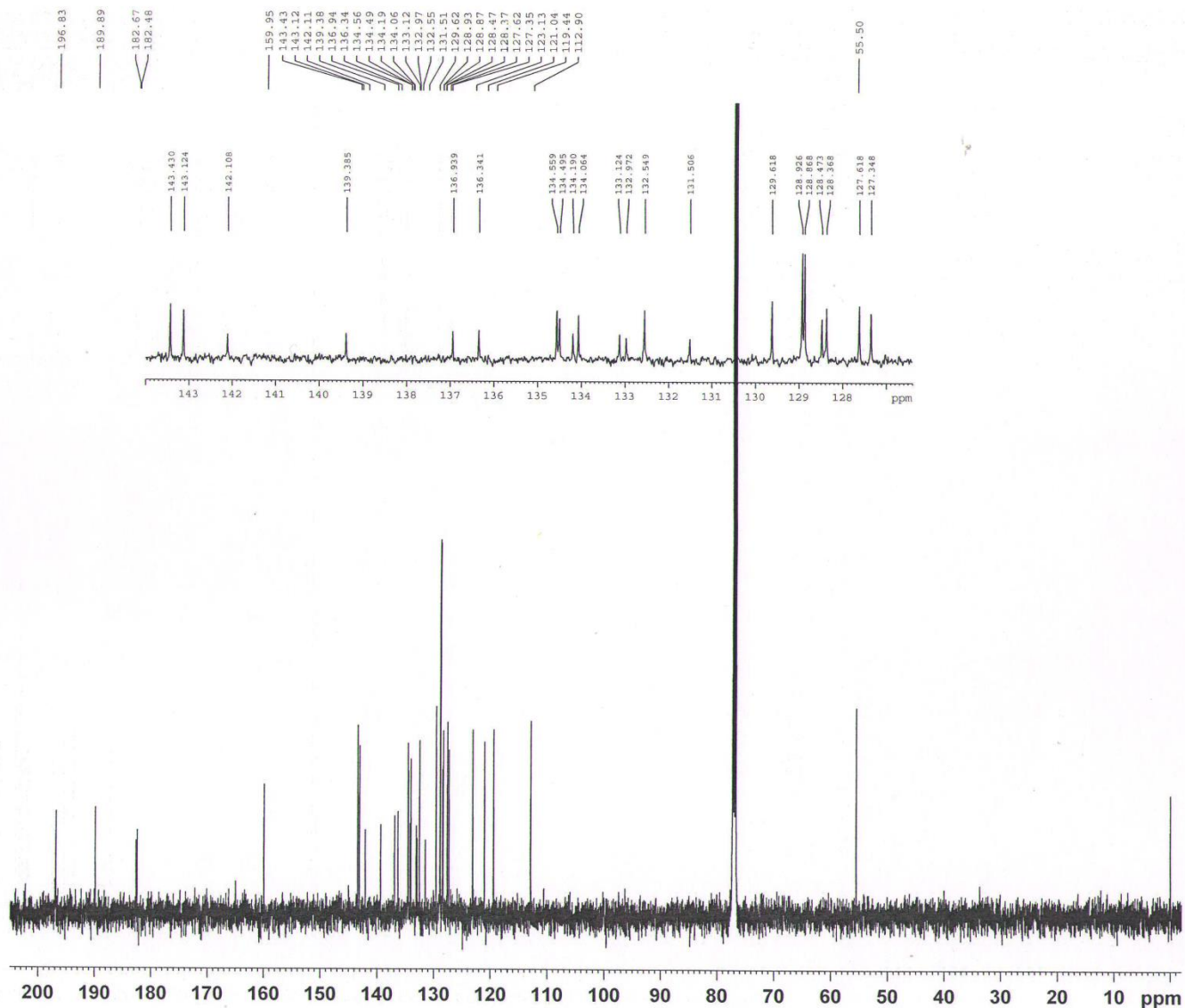


Fig. S21. ¹H NMR spectrum of **4f** in CDCl₃ (500 MHz).



Current Data Parameters
 NAME MU4F
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131126
 Time_ 14.05
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 914
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505024 sec
 RG 912
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8043140 MHz
 NUC1 13C
 P1 11.50 usec
 PLW1 32.22800064 W

===== CHANNEL f2 =====
 SFO2 500.2624528 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.77000046 W
 PLW12 0.39267001 W
 PLW13 0.25130999 W

F2 - Processing parameters
 SI 32768
 SF 125.7904802 MHz
 WDW EM
 SSB 0
 LB 1.50 Hz
 GB 0
 PC 1.40

Fig. S22. ¹³C NMR spectrum of **4f** in CDCl₃ (125 MHz).

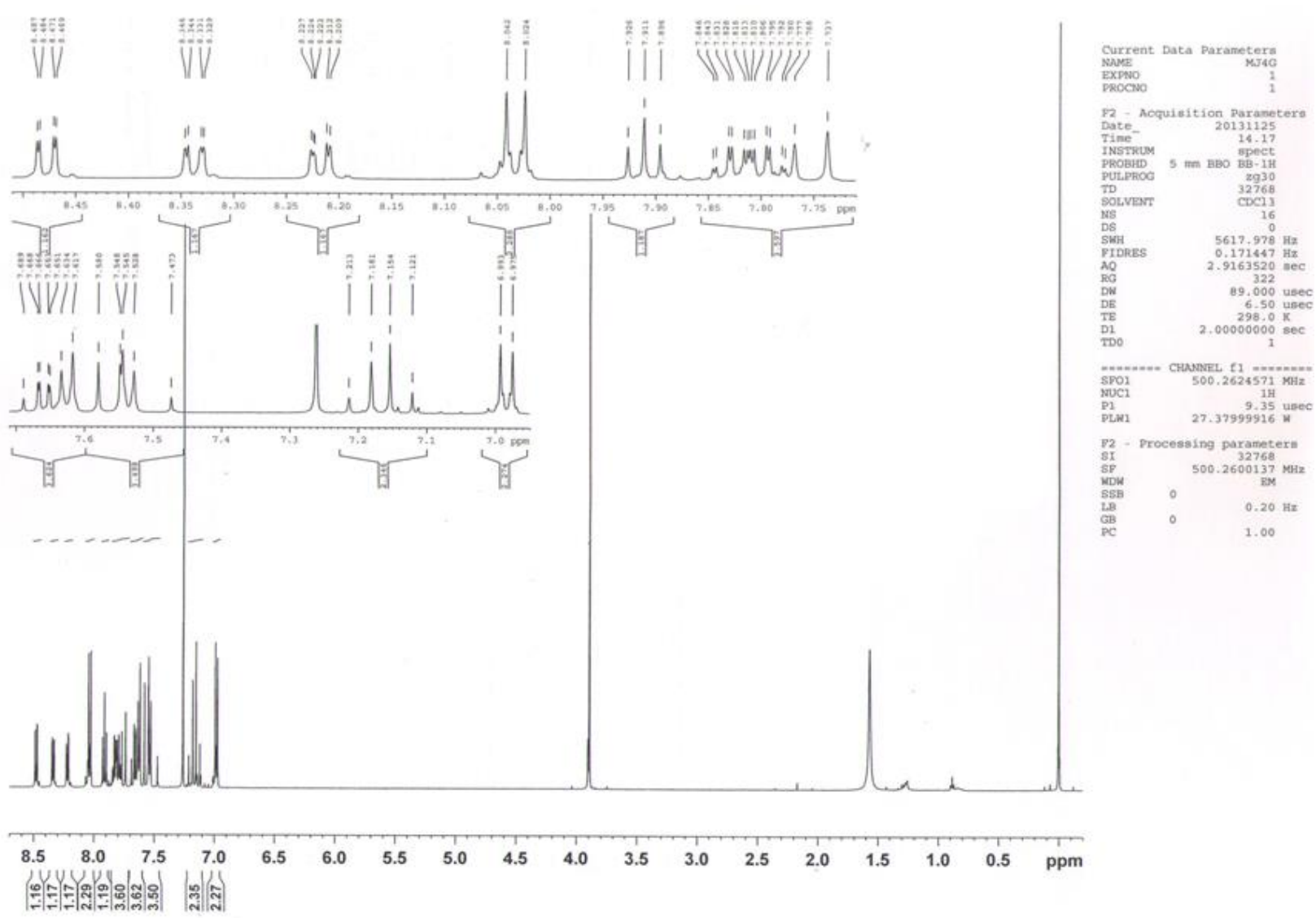
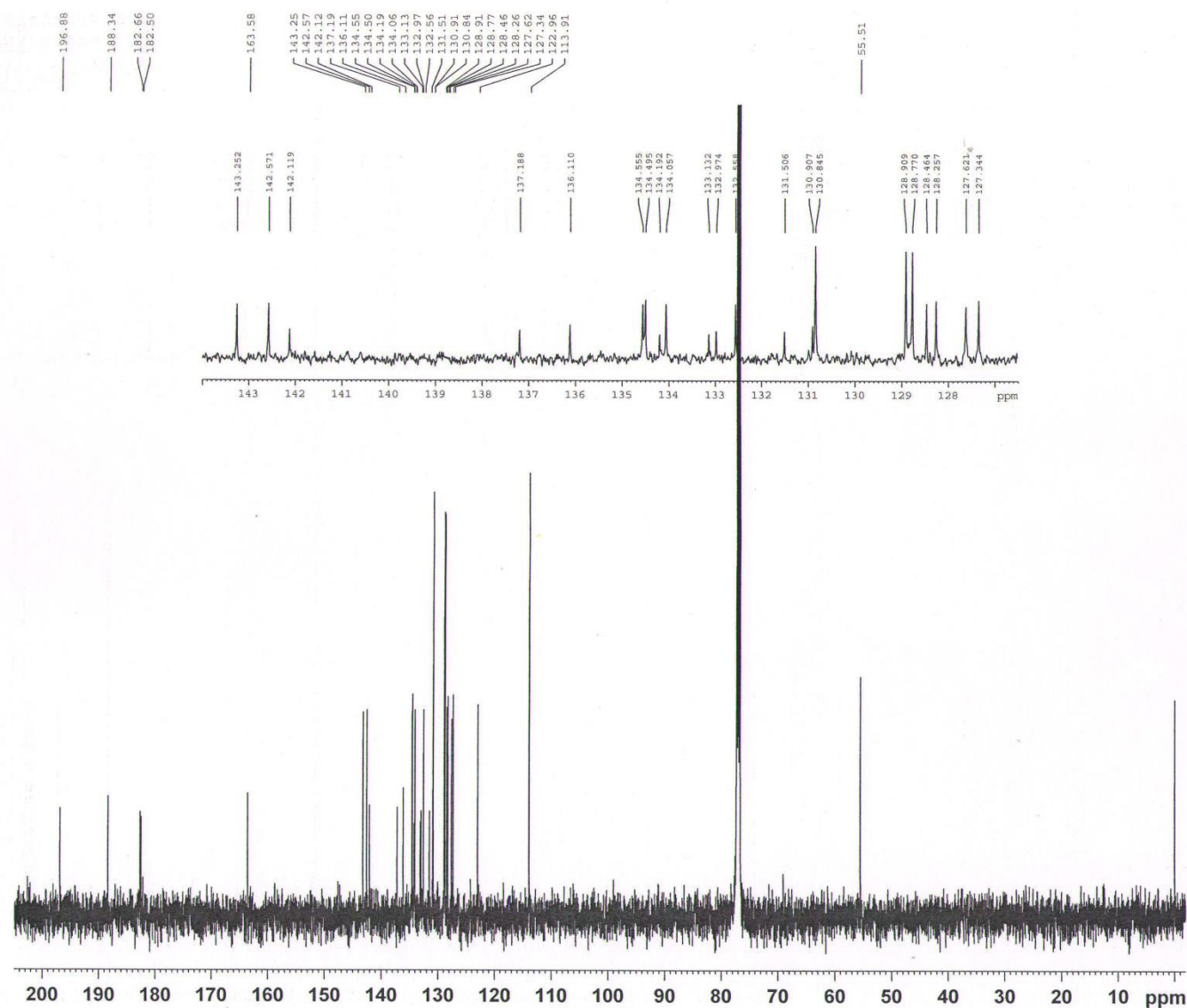


Fig. S23. ¹H NMR spectrum of **4g** in CDCl₃ (500 MHz).



Current Data Parameters
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 EXPNO 2
 PROCNO 1

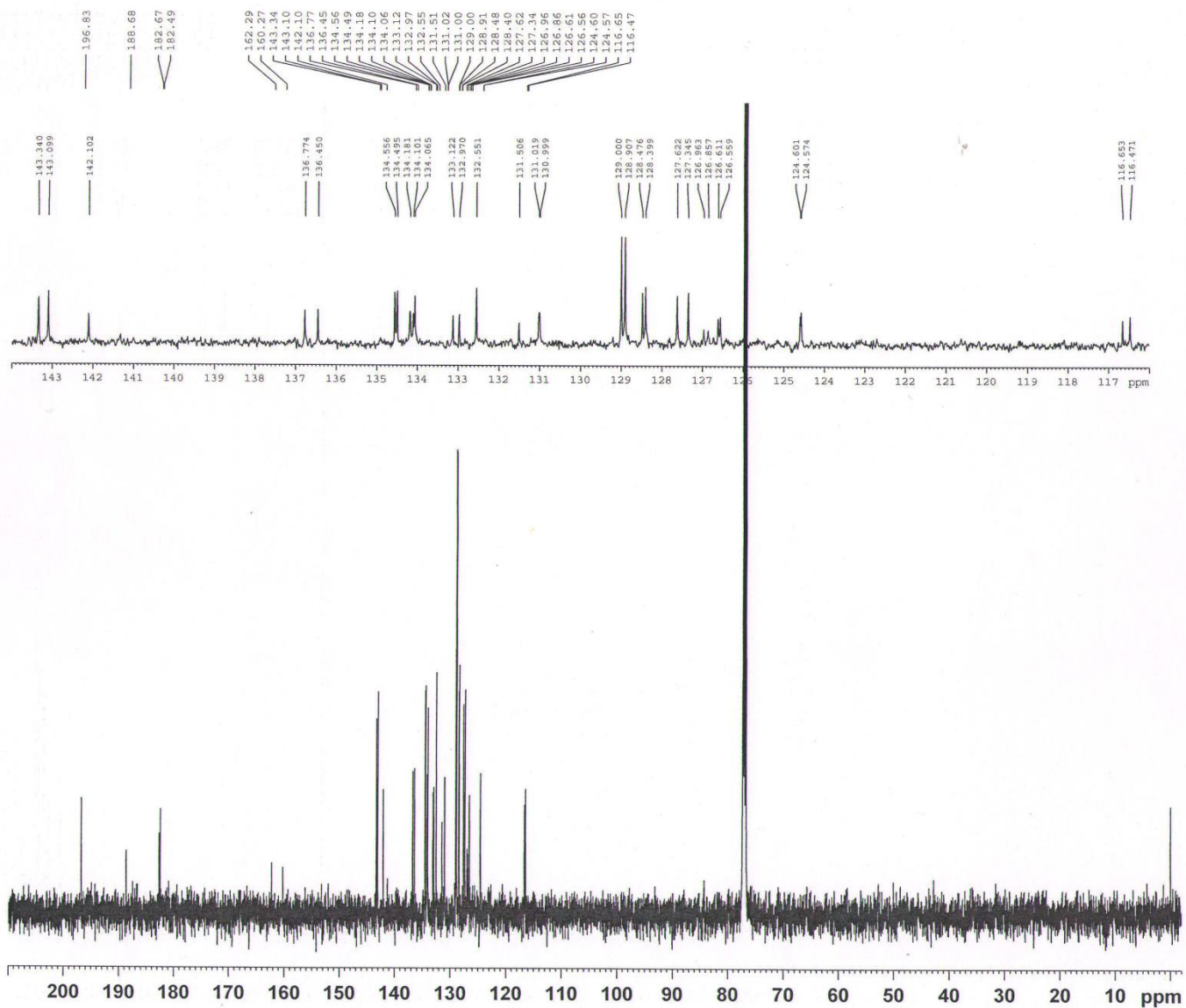
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 Time_ 14.26
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 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1611
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505024 sec
 RG 1030
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8043140 MHz
 NUC1 13C
 P1 11.50 usec
 PLW1 32.22800064 W

===== CHANNEL f2 =====
 SFO2 500.2624573 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.77000046 W
 PLW12 0.39267001 W
 PLW13 0.25130999 W

F2 - Processing parameters
 SI 32768
 SF 125.7904800 MHz
 WDW EM
 SSB 0
 LB 1.50 Hz
 GB 0
 PC 1.40

Fig. S24. ^{13}C NMR spectrum of **4g** in CDCl_3 (125 MHz).



Current Data Parameters
 NAME MJ4H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131126
 Time_ 14.57
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1451
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505024 sec
 RG 724
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 125.8043140 MHz
 NUC1 13C
 P1 11.50 usec
 PLW1 32.22800064 W

===== CHANNEL f2 =====
 SFO2 500.2622016 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.77000046 W
 PLW12 0.39267001 W
 PLW13 0.25130999 W

F2 - Processing parameters
 SI 32768
 SF 125.7904800 MHz
 WDW EM
 SSB 0
 LB 1.50 Hz
 GB 0
 PC 1.40

Fig. S26. ^{13}C NMR spectrum of **4h** in CDCl_3 (125 MHz).

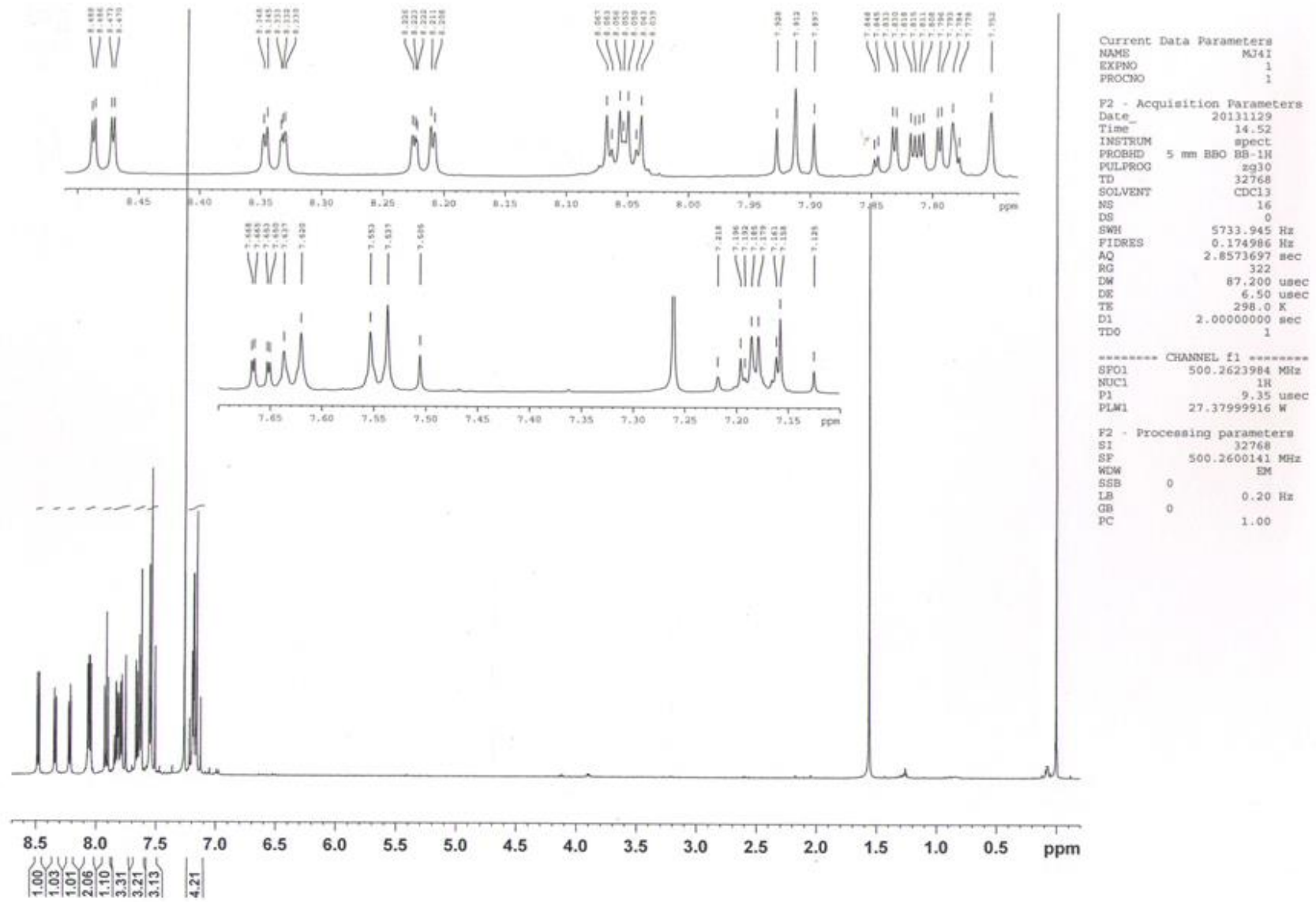
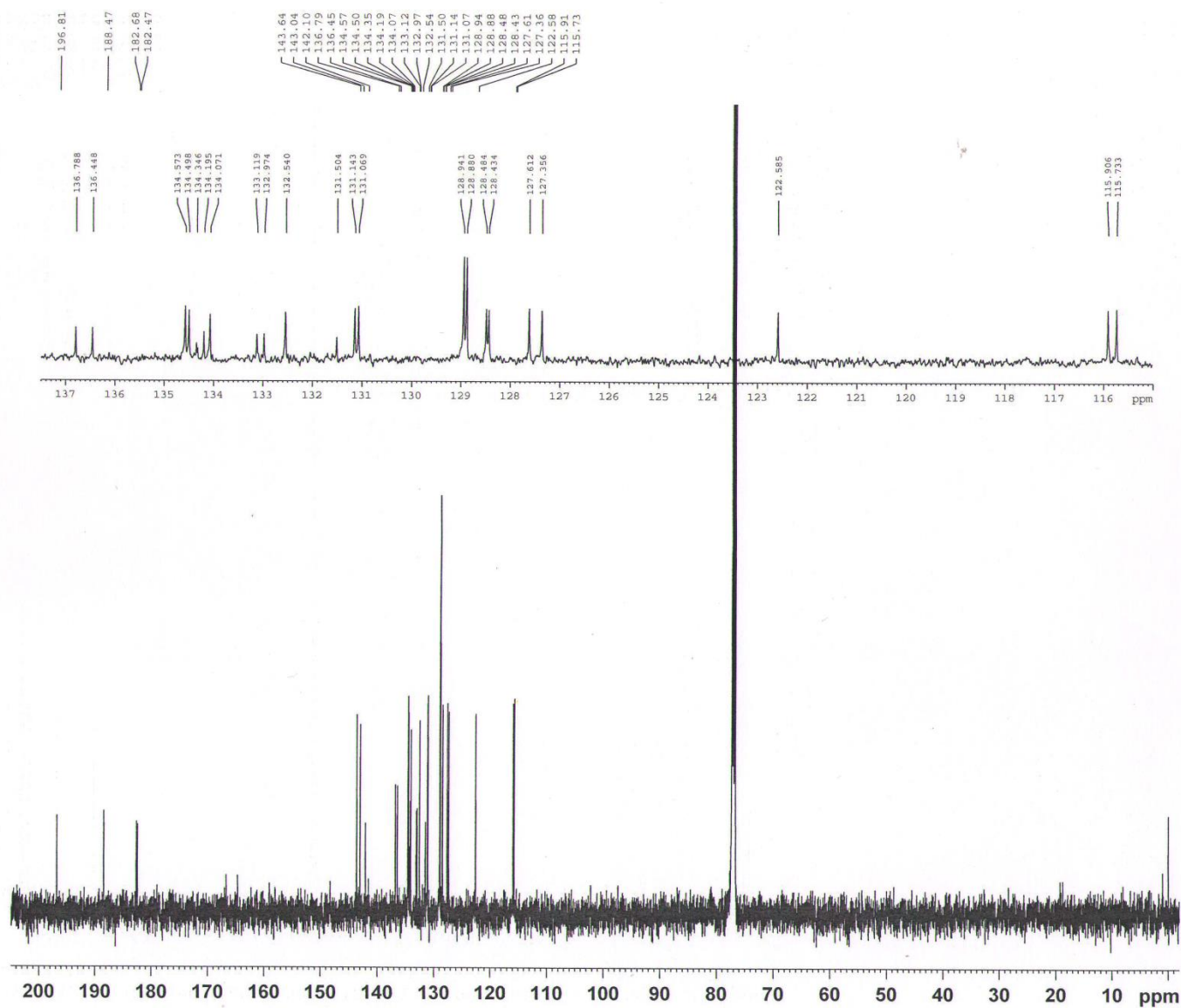


Fig. S27. ¹H NMR spectrum of **4i** in CDCl₃ (500 MHz).



Current Data Parameters
 NAME MJ4I
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131129
 Time 15.01
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1602
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505024 sec
 RG 812
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 125.8043140 MHz
 NUC1 13C
 P1 11.50 usec
 PLW1 32.22800064 W

===== CHANNEL f2 =====
 SFO2 500.2623982 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.77000046 W
 PLW12 0.39267001 W
 PLW13 0.25130999 W

F2 - Processing parameters
 SI 32768
 SF 125.7904802 MHz
 WDW EM
 SSB 0
 LB 1.50 Hz
 GB 0
 PC 1.40

Fig. S28. ^{13}C NMR spectrum of **4i** in CDCl_3 (125 MHz).

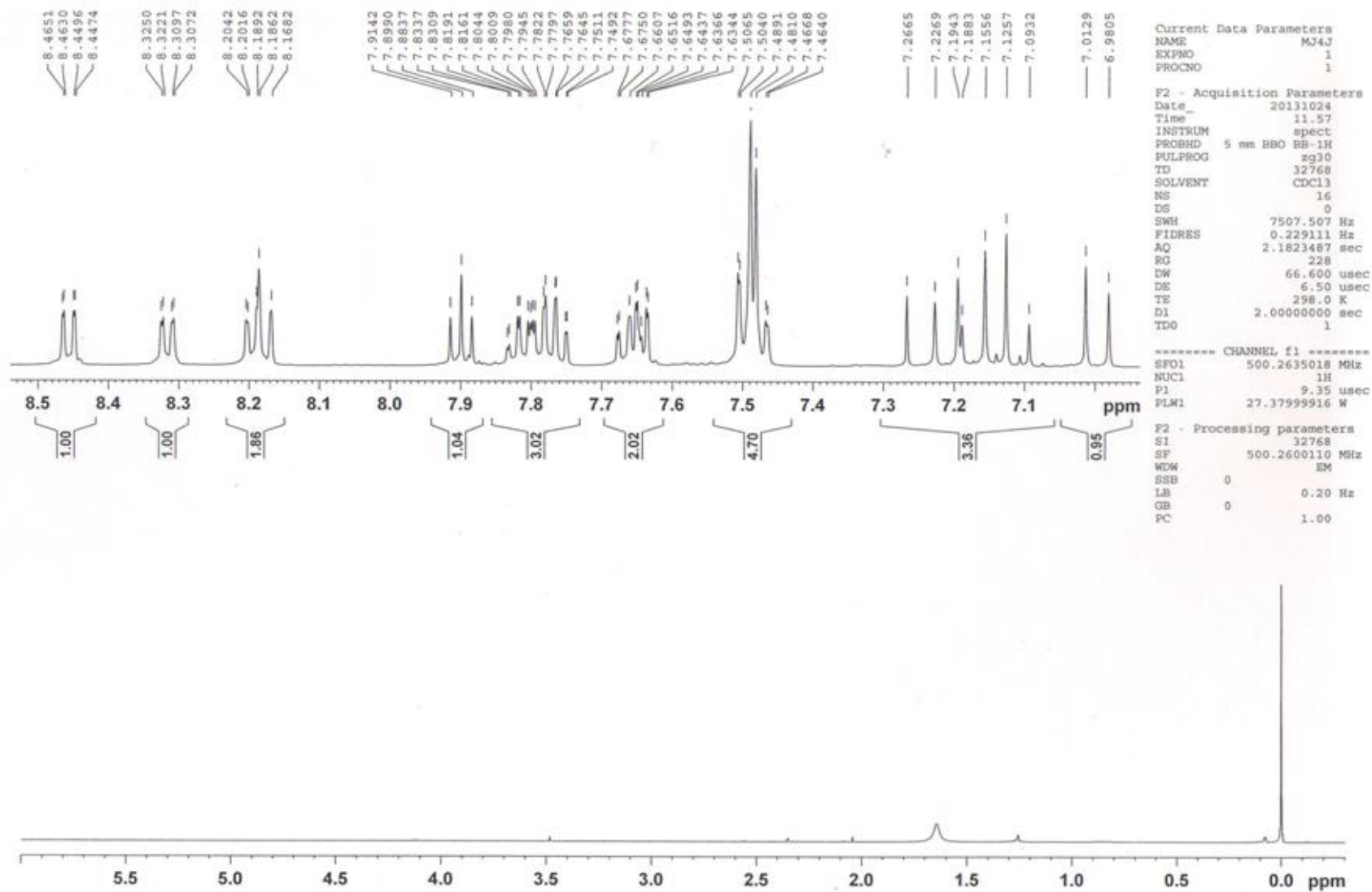
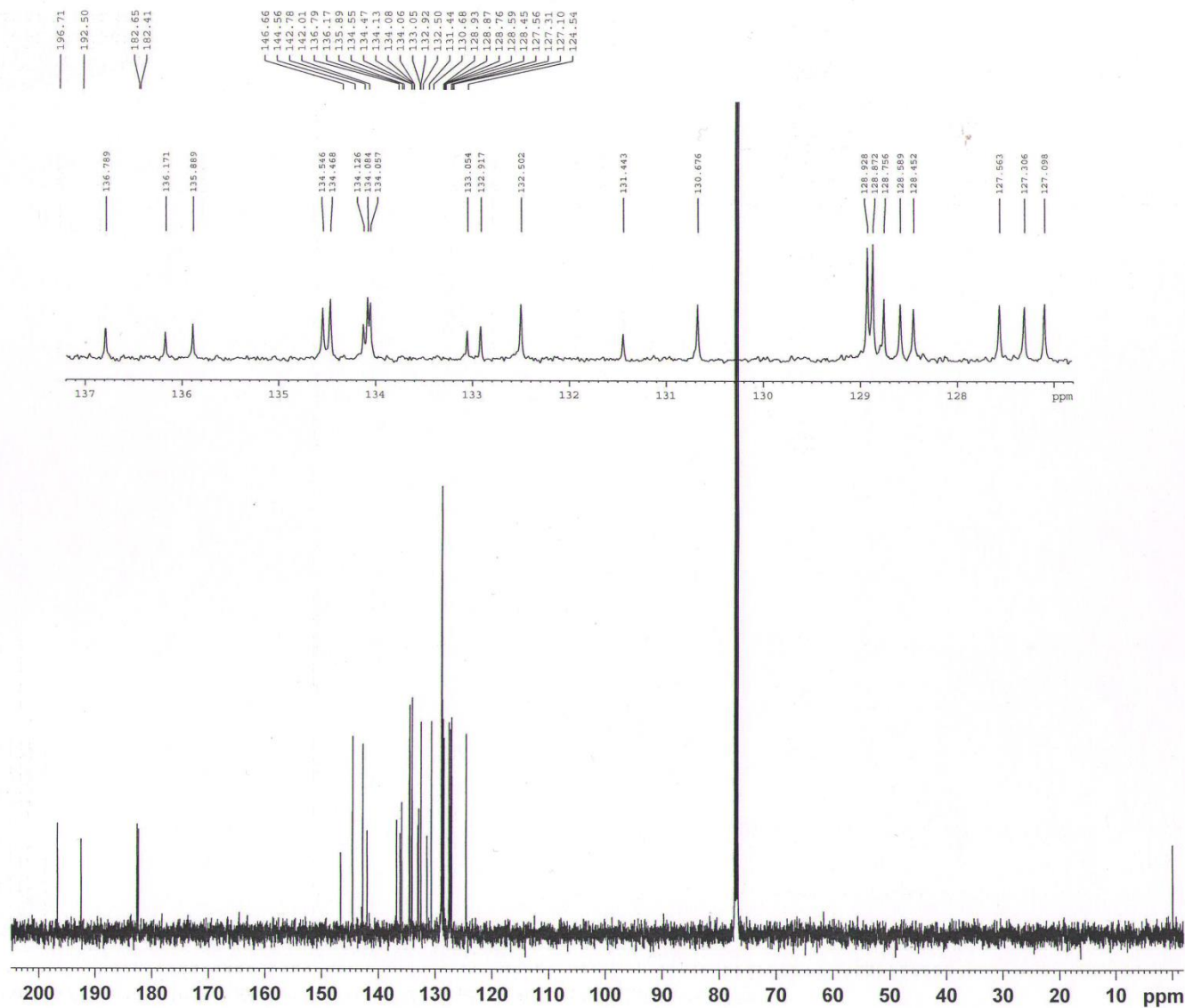


Fig. S29. ^1H NMR spectrum of **4j** in CDCl_3 (500 MHz).



Current Data Parameters
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 EXPNO 2
 PROCNO 1

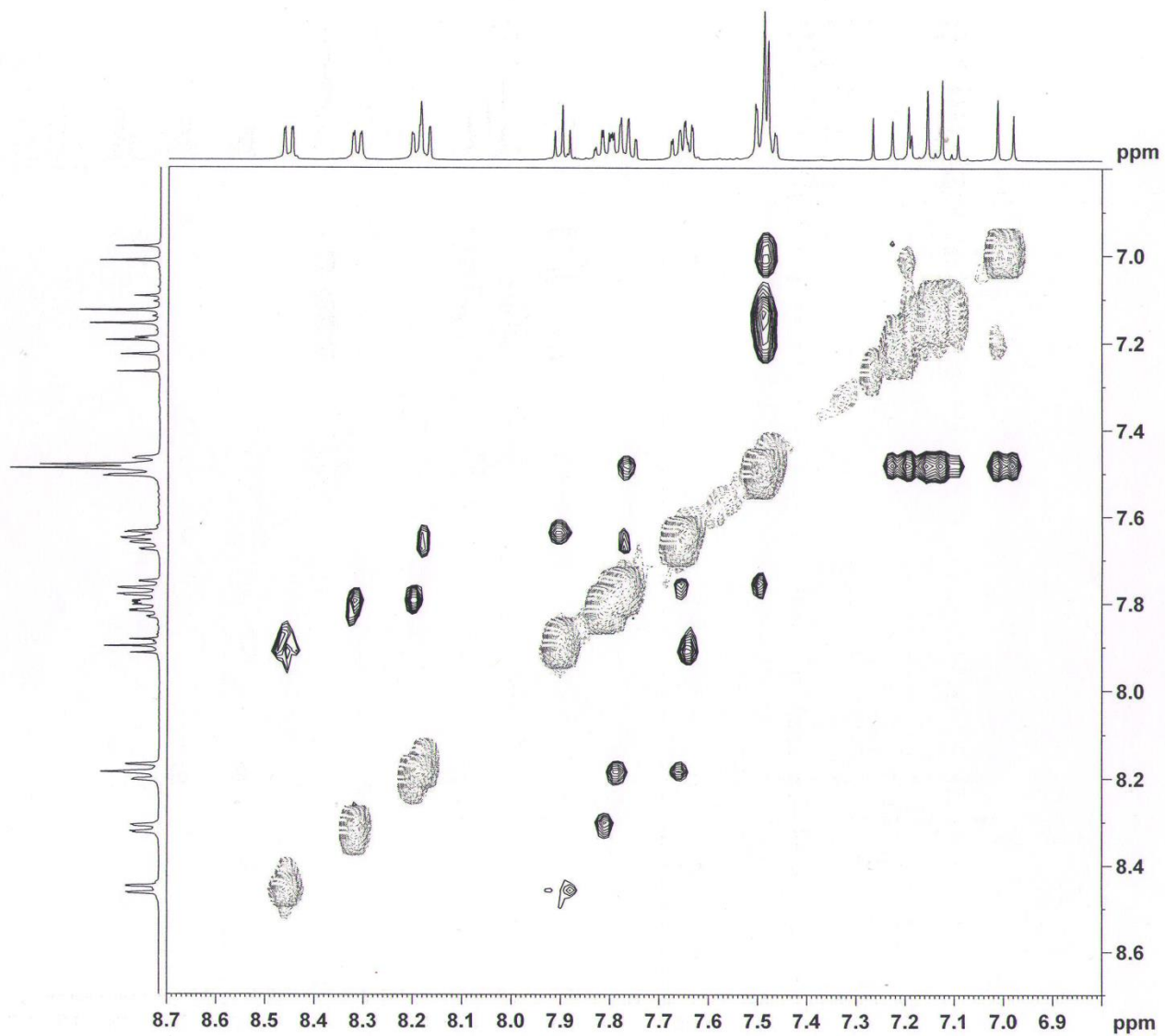
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 Time 12.02
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 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 220
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.5505024 sec
 RG 2050
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8043140 MHz
 NUC1 13C
 P1 11.50 usec
 PLW1 32.22800064 W

===== CHANNEL f2 =====
 SFO2 500.2619835 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.77000046 W
 PLW12 0.39267001 W
 PLW13 0.25130999 W

F2 - Processing parameters
 SI 32768
 SF 125.7904832 MHz
 WDW EM
 SSB 0
 LB 1.50 Hz
 GB 0
 PC 1.40

Fig. S30. ^{13}C NMR spectrum of **4j** in CDCl_3 (125 MHz).



```

Current Data Parameters
NAME          MJ4J
EXPNO         5
PROCNO        1

F2 - Acquisition Parameters
Date_         20131024
Time          12.14
INSTRUM       5 mm BBO BB-1H
PROBHD        spect
PULPROG       noesygpph
TD            1024
SOLVENT       CDCl3
NS            2
DS            16
SWH           5000.000 Hz
FIDRES        4.882813 Hz
AQ            0.1024000 sec
RG            144
DW            100.000 usec
DE            6.50 usec
TE            298.0 K
D0            0.0000800 sec
D1            2.0000000 sec
D8            1.0000000 sec
D16           0.0002000 sec
INO           0.00019980 sec

===== CHANNEL f1 =====
SF01          500.2621511 MHz
NUC1           1H
P1             9.35 usec
P2            18.70 usec
PLW1           27.37999916 W

===== GRADIENT CHANNEL =====
GPNAM[1]      SINE.100
GPZ1           40.00 %
P16            1000.00 usec

F1 - Acquisition parameters
TD            256
SF01          500.2622 MHz
FIDRES        19.550800 Hz
SW            10.005 ppm
FnMODE        States-TPPI

F2 - Processing parameters
SI            1024
SF            500.260083 MHz
WDW           QSINE
SSB           2
LB            0 Hz
GB            0
PC            1.00

F1 - Processing parameters
SI            256
MC2           States-TPPI
SF            500.260018 MHz
WDW           QSINE
SSB           2
LB            0 Hz
GB            0

```

Fig. S31. NOESY spectrum of **4j** in CDCl₃ (500 MHz).

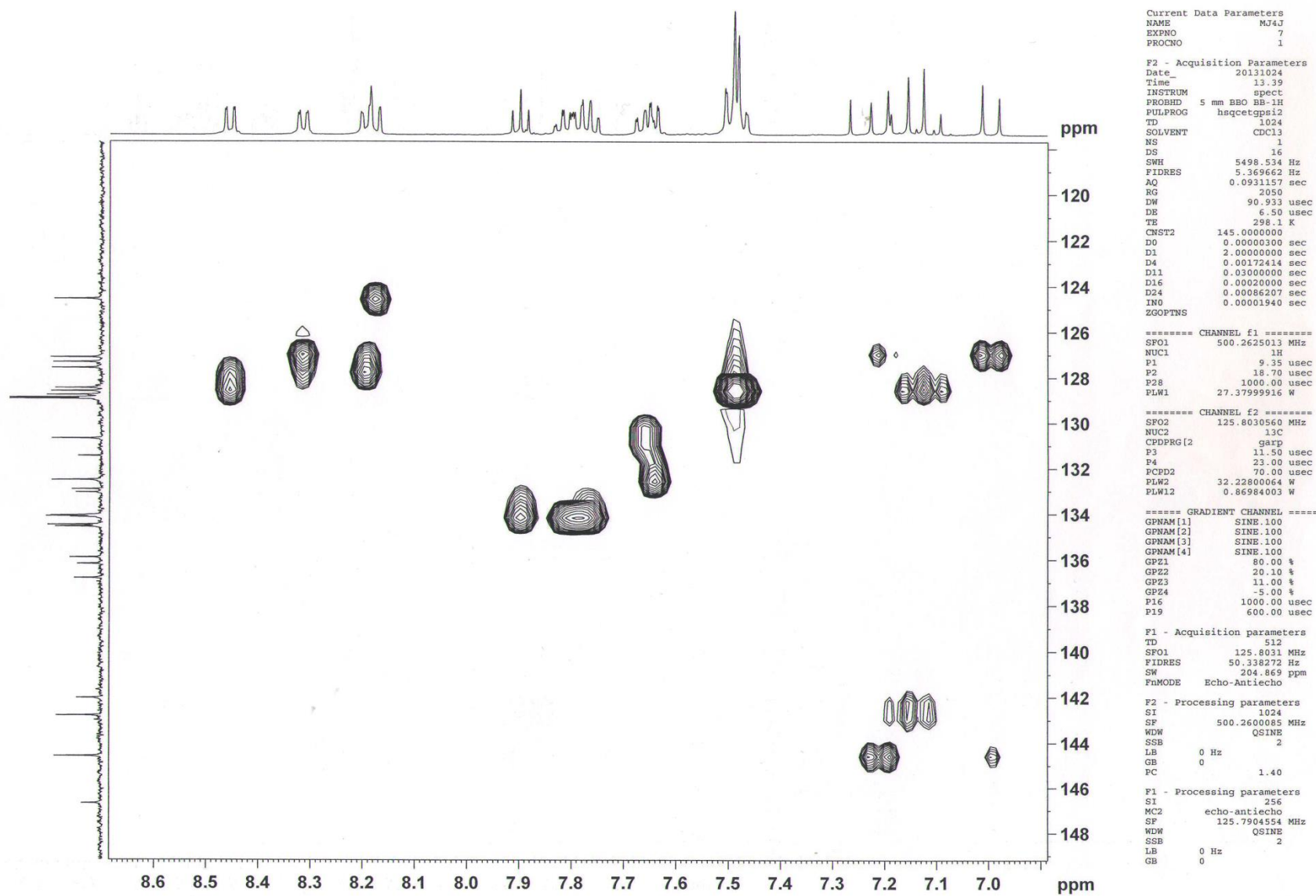


Fig. S32. HSQC spectrum of **4j** in CDCl₃ (500 MHz).

MJ4J 6 1 C:\Bruker\TopSpin3.1\BBO\Guest

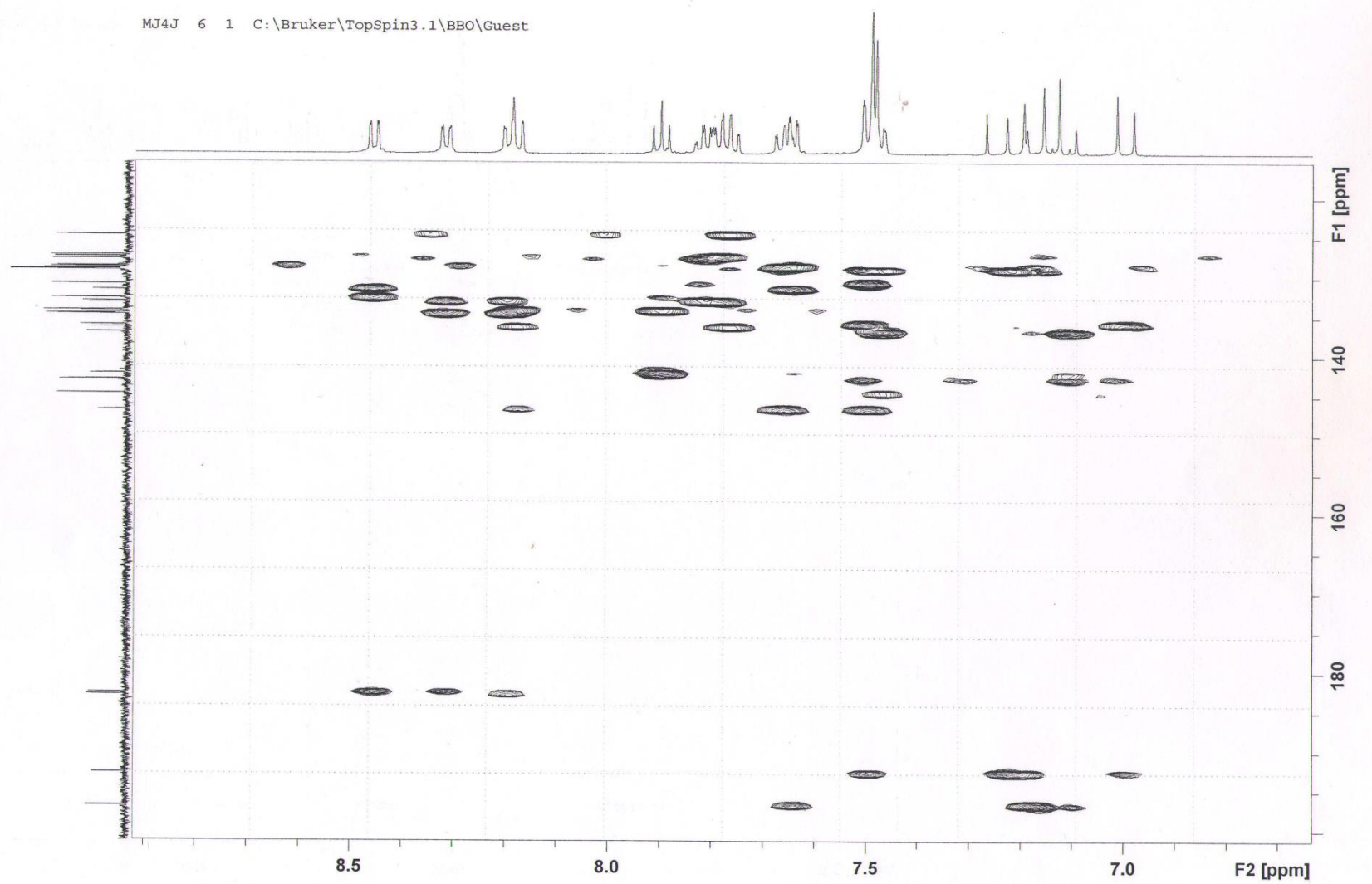


Fig. S33. HMBC spectrum of **4j** in CDCl₃ (500 MHz).