

## Supplementary Material

### Coumarin-carbazole based functionalized pyrazolines: Synthesis, characterization, anticancer investigation and molecular docking

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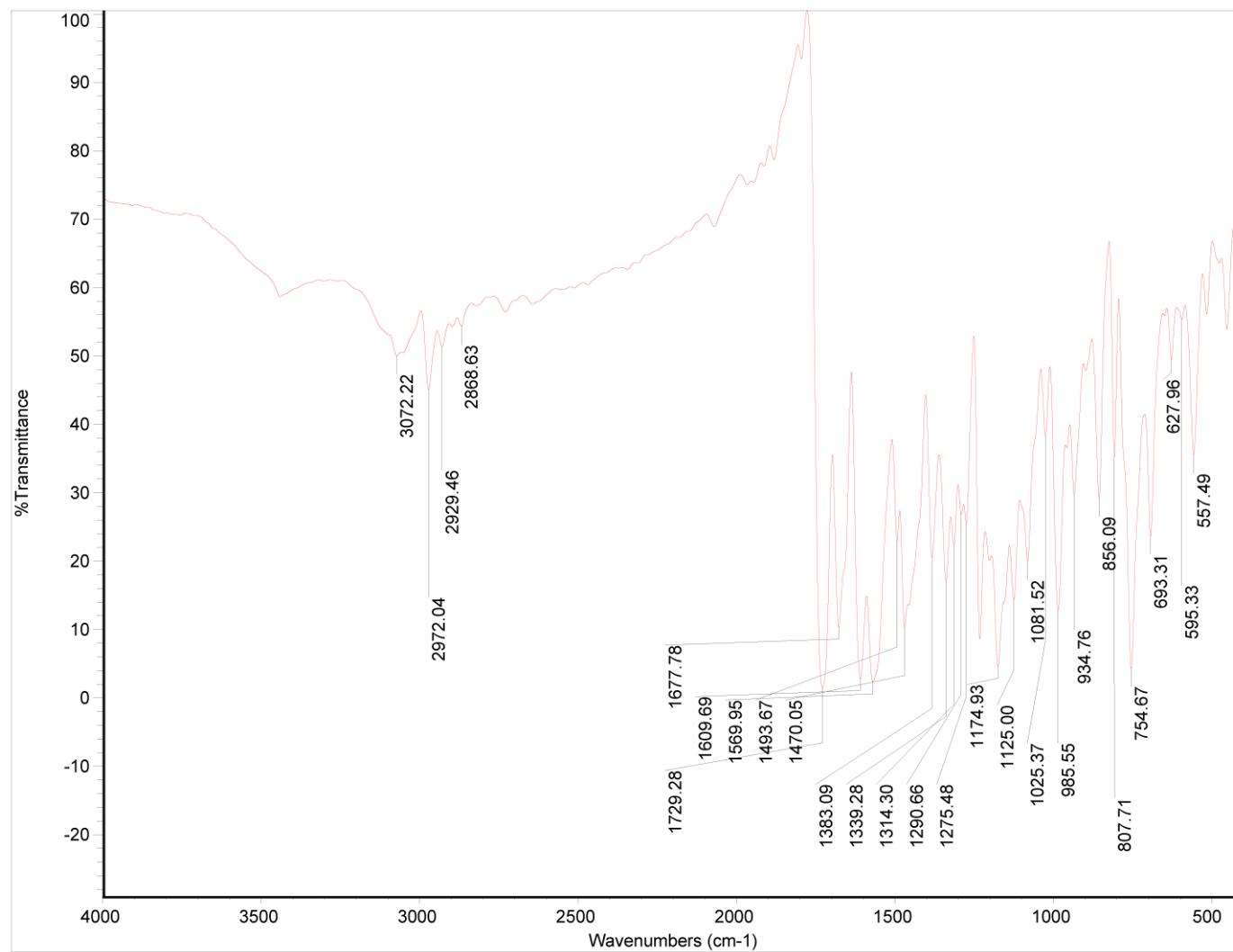
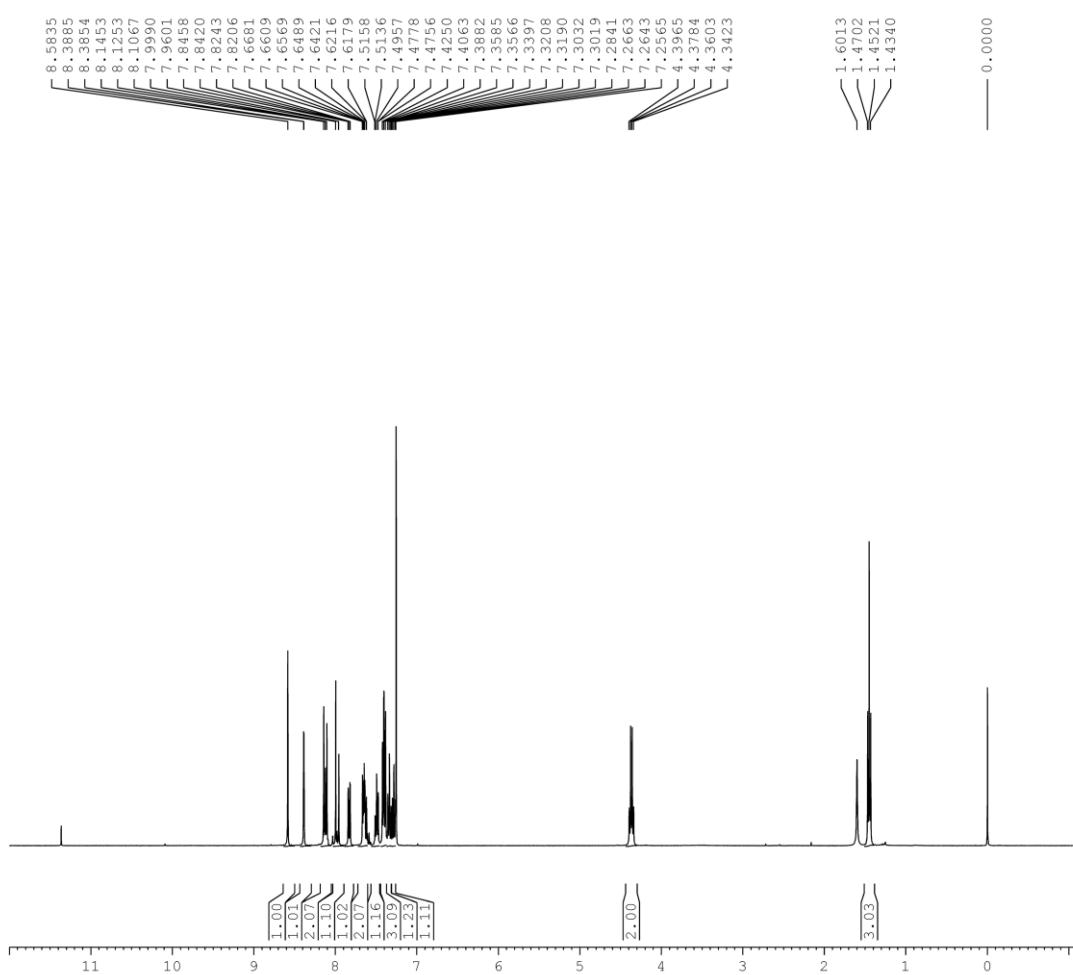


Fig. 1. IR spectrum of compound 3a



BRUKER  
AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

F2 - Acquisition Parameters  
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Time\_ 7.39  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.183399 Hz  
AQ 2.7263477 sec  
RG 724  
DW 41.600 usec  
DE 6.00 usec  
TE 299.9 K  
D1 1.0000000 sec  
TDO 1  
===== CHANNEL f1 ======  
NUC1 1H  
P1 10.90 usec  
PL1 -3.00 dB  
SF01 400.1324710 MHz  
F2 - Processing parameters  
SI 32768  
SF 400.1300108 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Fig. 2.  $^1\text{H}$  NMR spectrum of compound 3a

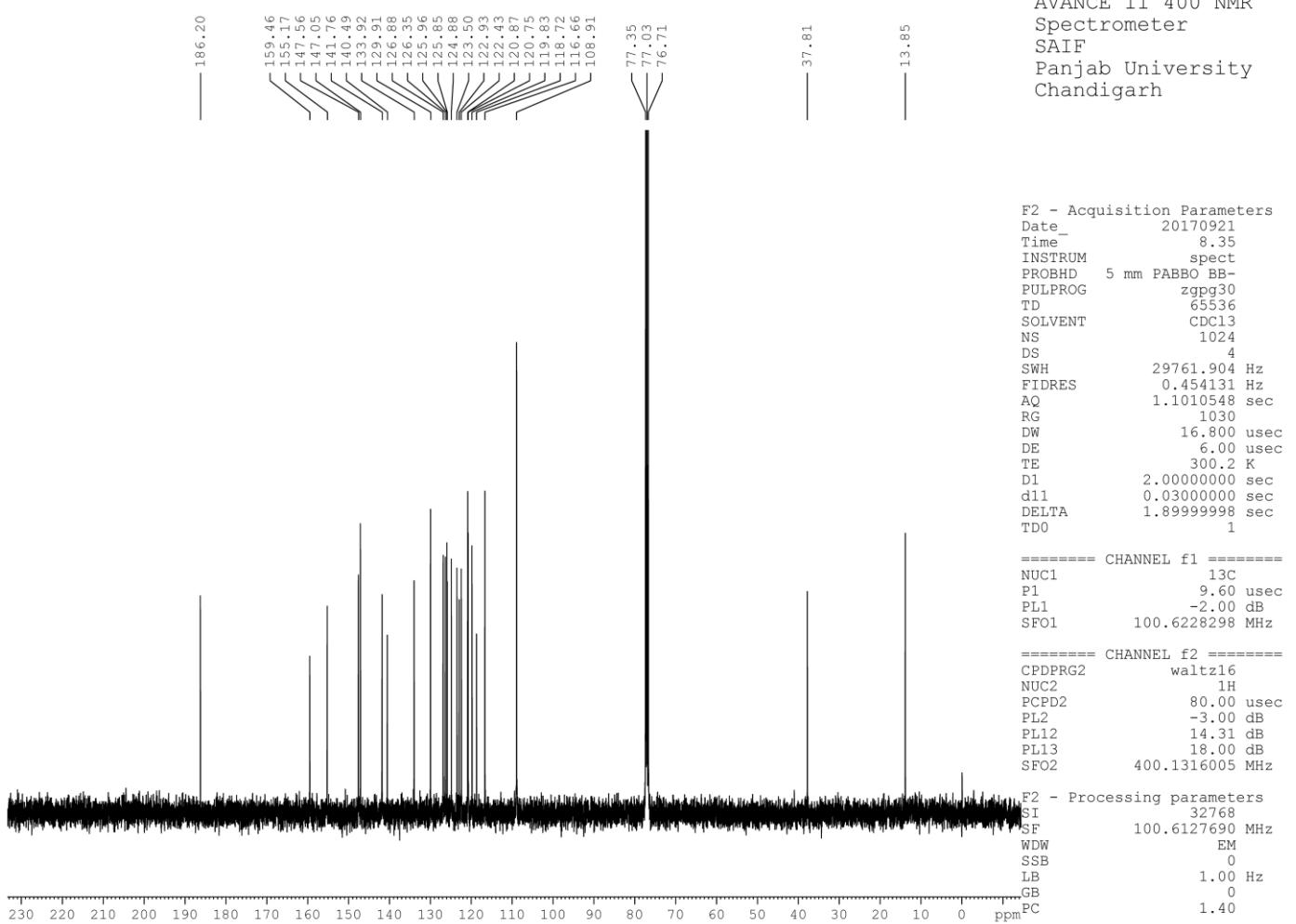


Fig. 3 <sup>13</sup>C NMR spectrum of compound 3a

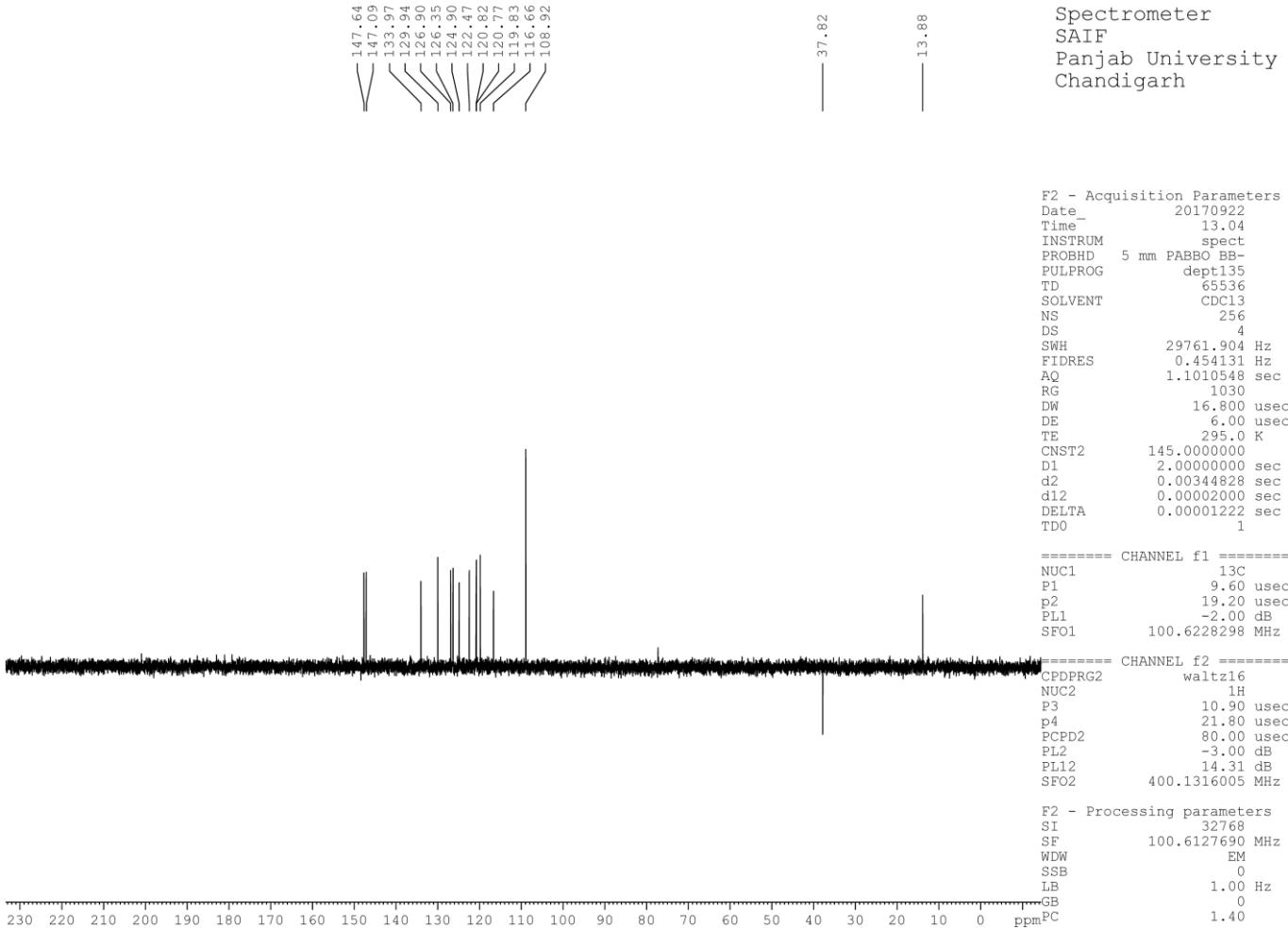


Fig. 4. DEPT-135 spectrum of compound 3a

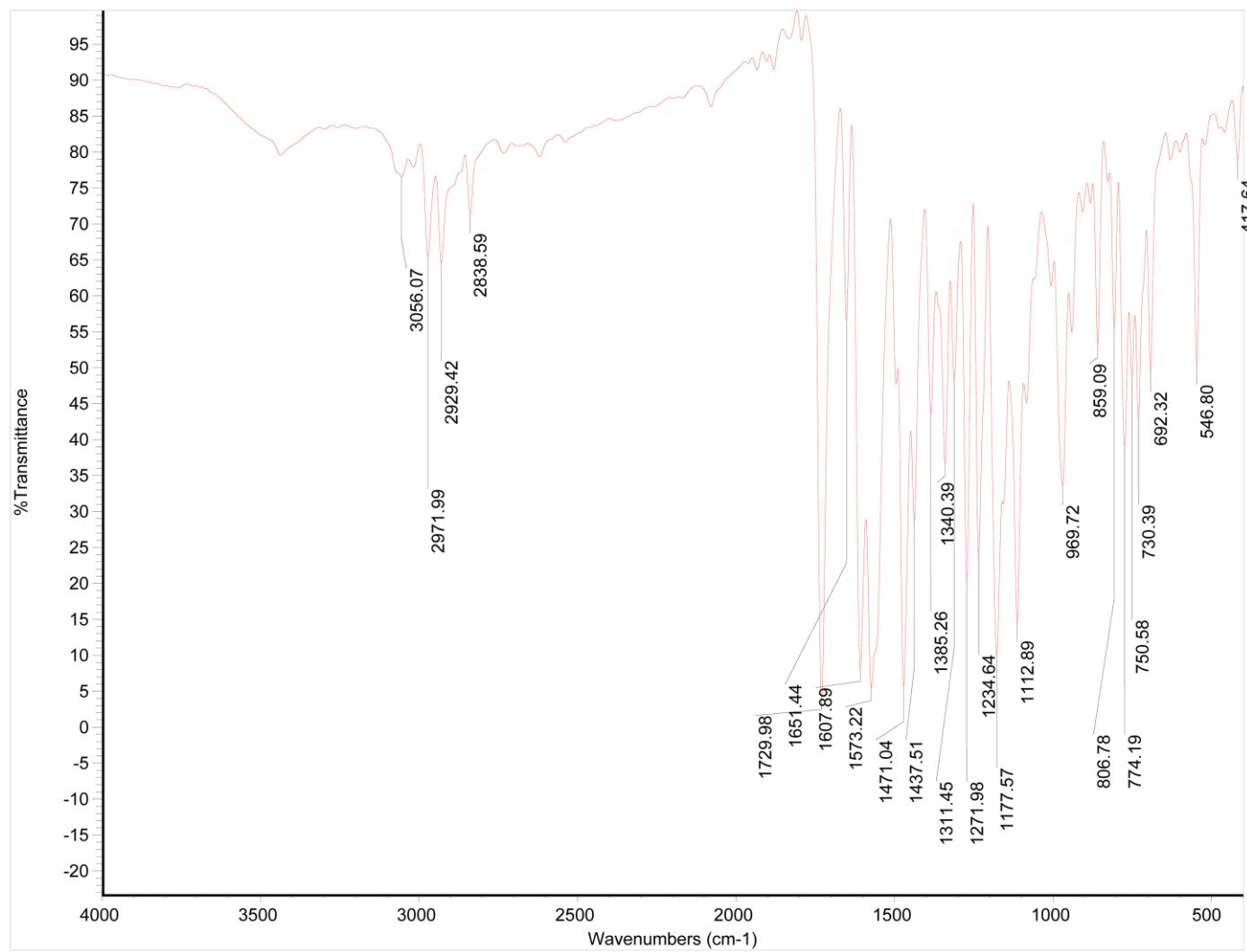


Fig. 5. IR spectrum of compound 3b

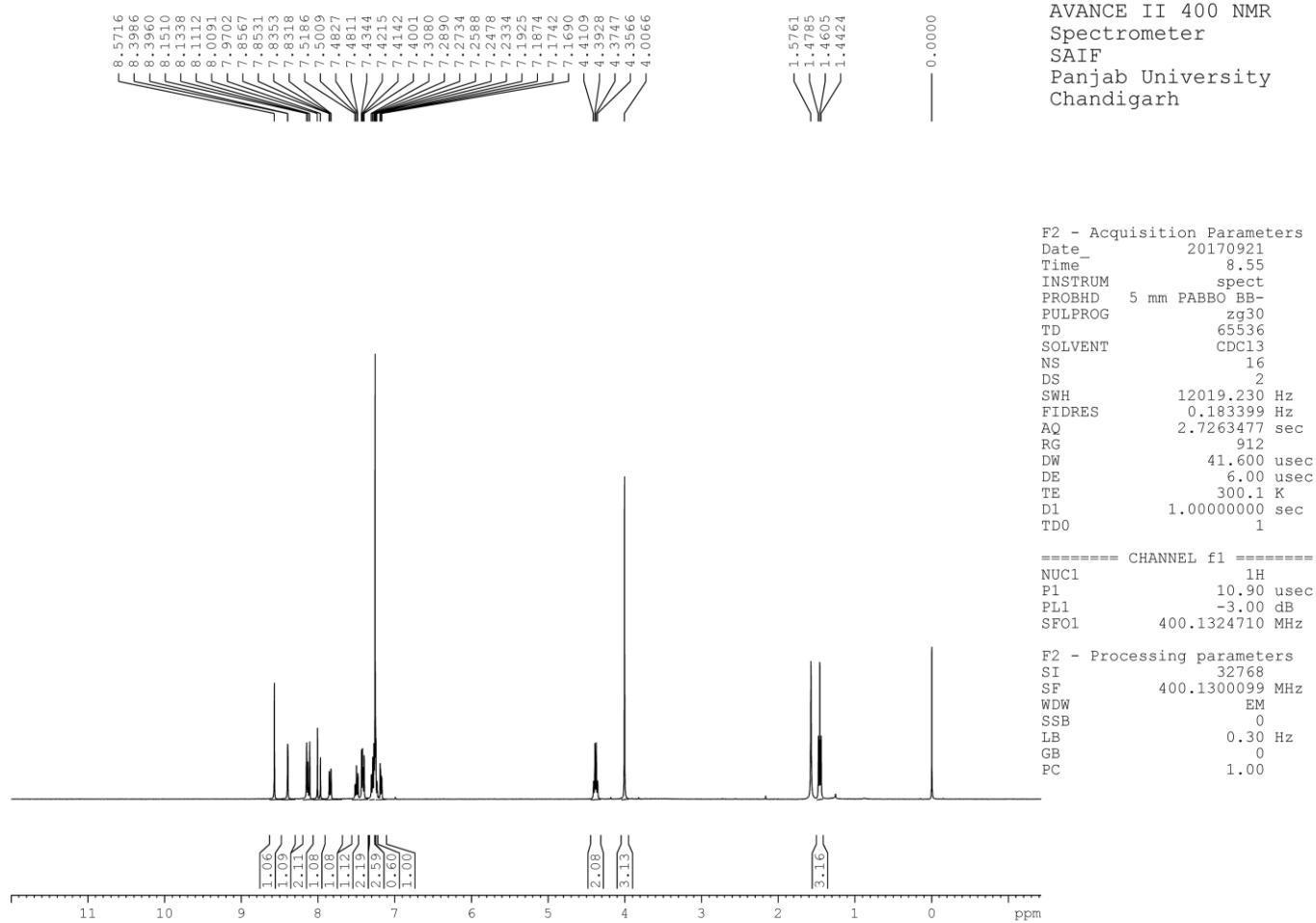


Fig. 6.  $^1\text{H}$  NMR spectrum of compound 3b

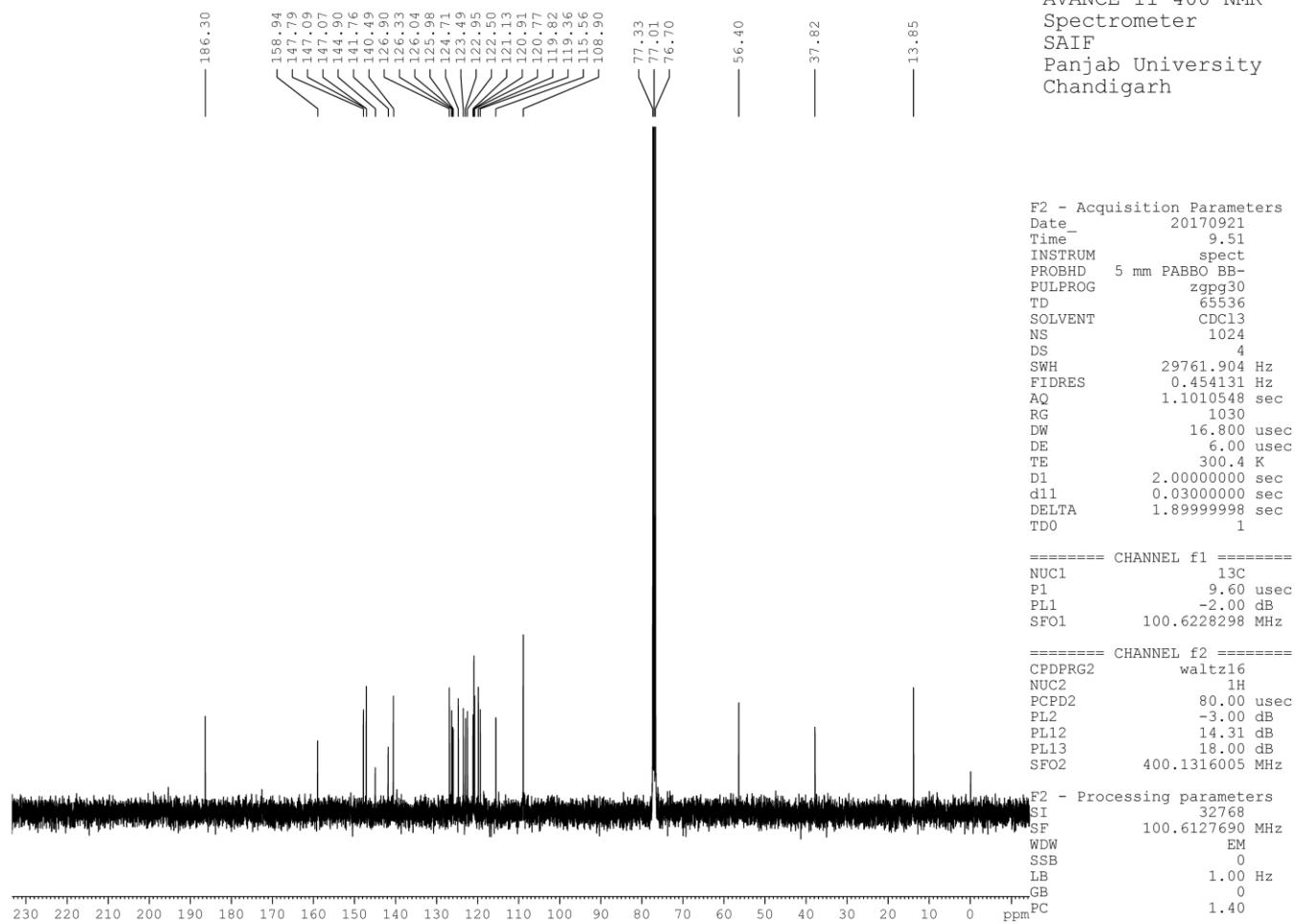


Fig. 7. <sup>13</sup>C NMR spectrum of compound 3b

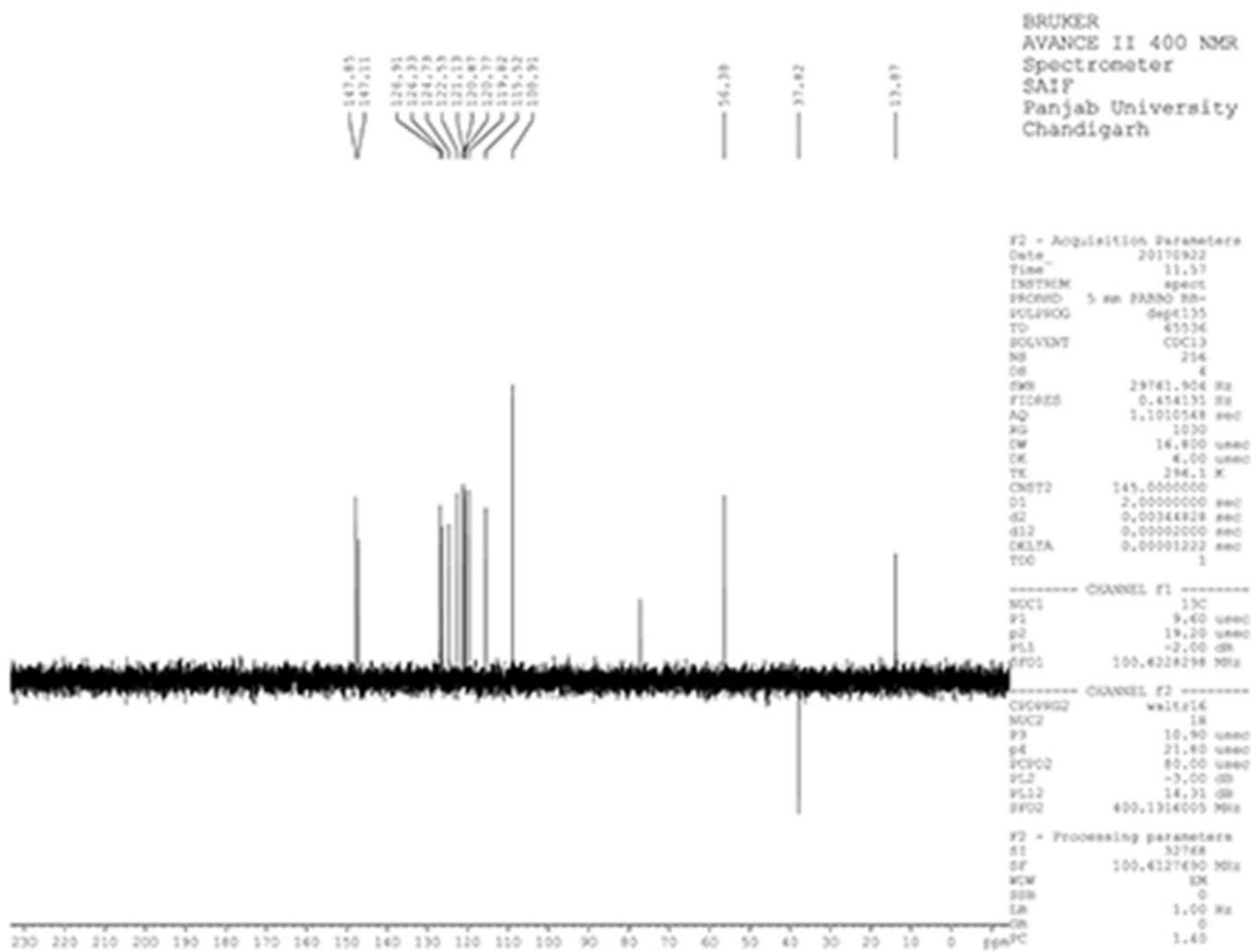


Fig. 8. DEPT-135 spectrum of compound 3b

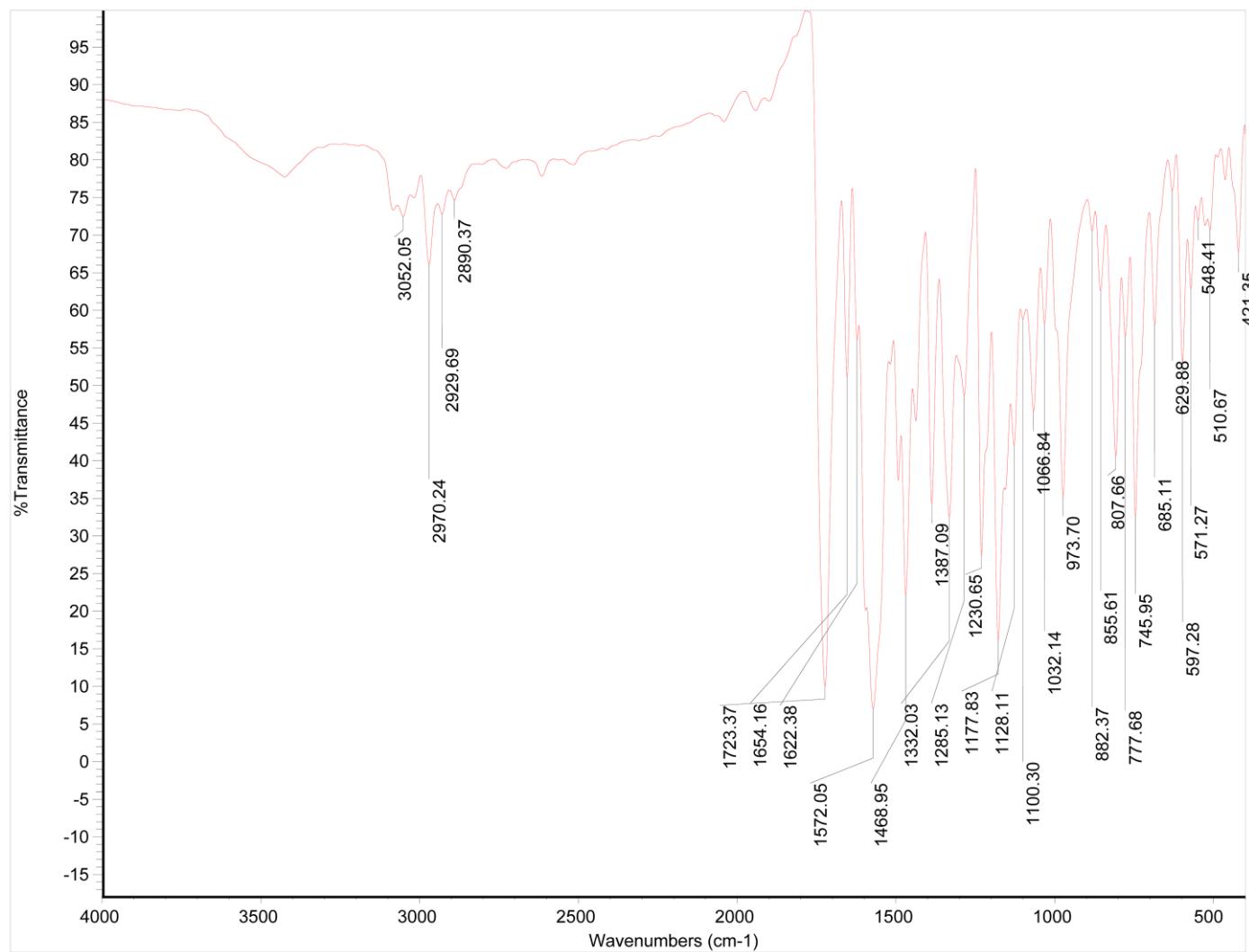
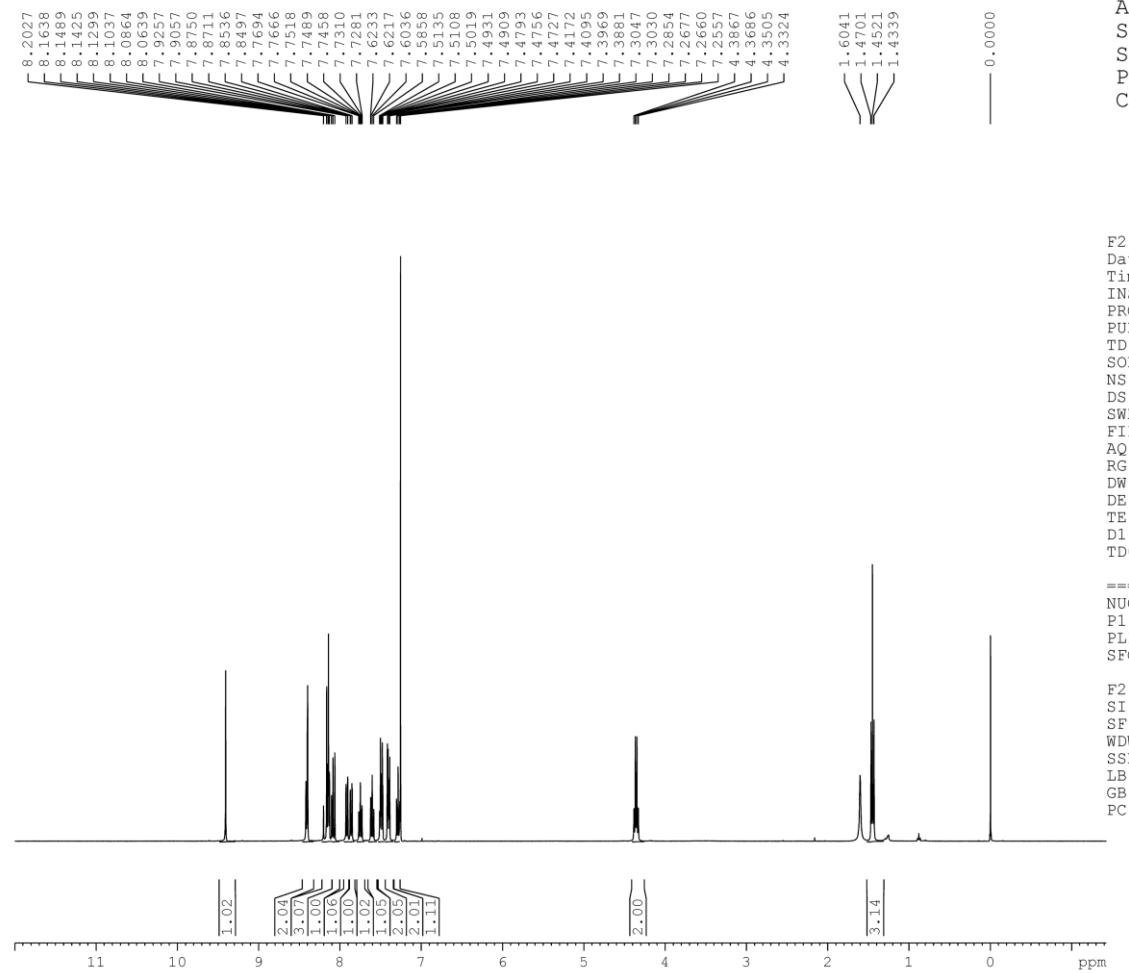


Fig. 9. IR spectrum of compound 3c



BRUKER  
AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

F2 - Acquisition Parameters  
 Date\_ 20170921  
 Time\_ 10.11  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 12019.230 Hz  
 FIDRES 0.183399 Hz  
 AQ 2.7263477 sec  
 RG 724  
 DW 41.600 usec  
 DE 6.00 usec  
 TE 300.2 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 ======

NUC1 1H  
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 PL1 -3.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
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Fig. 10.  $^1\text{H}$  NMR spectrum of compound 3c

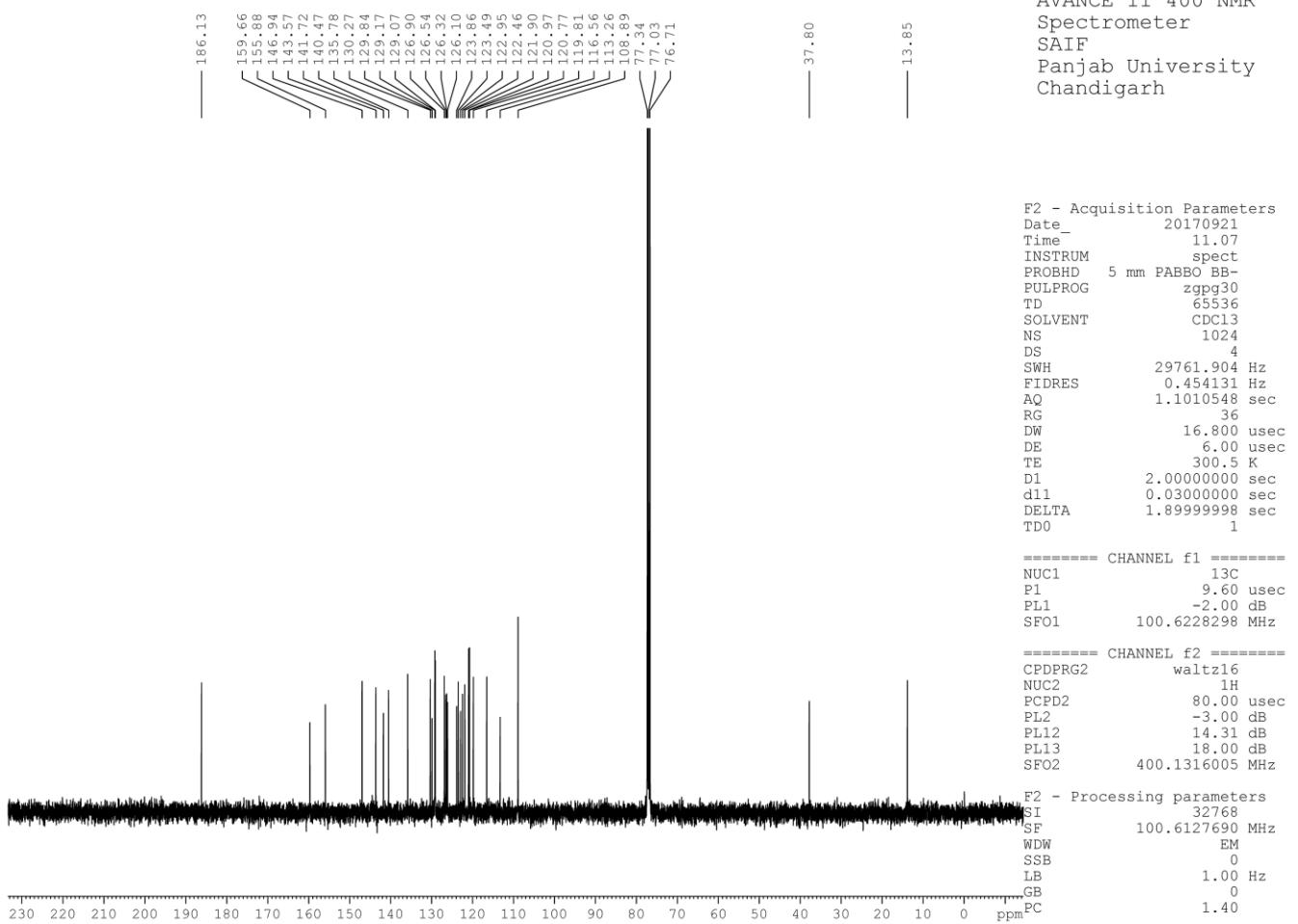


Fig. 11. <sup>13</sup>C NMR spectrum of compound 3c

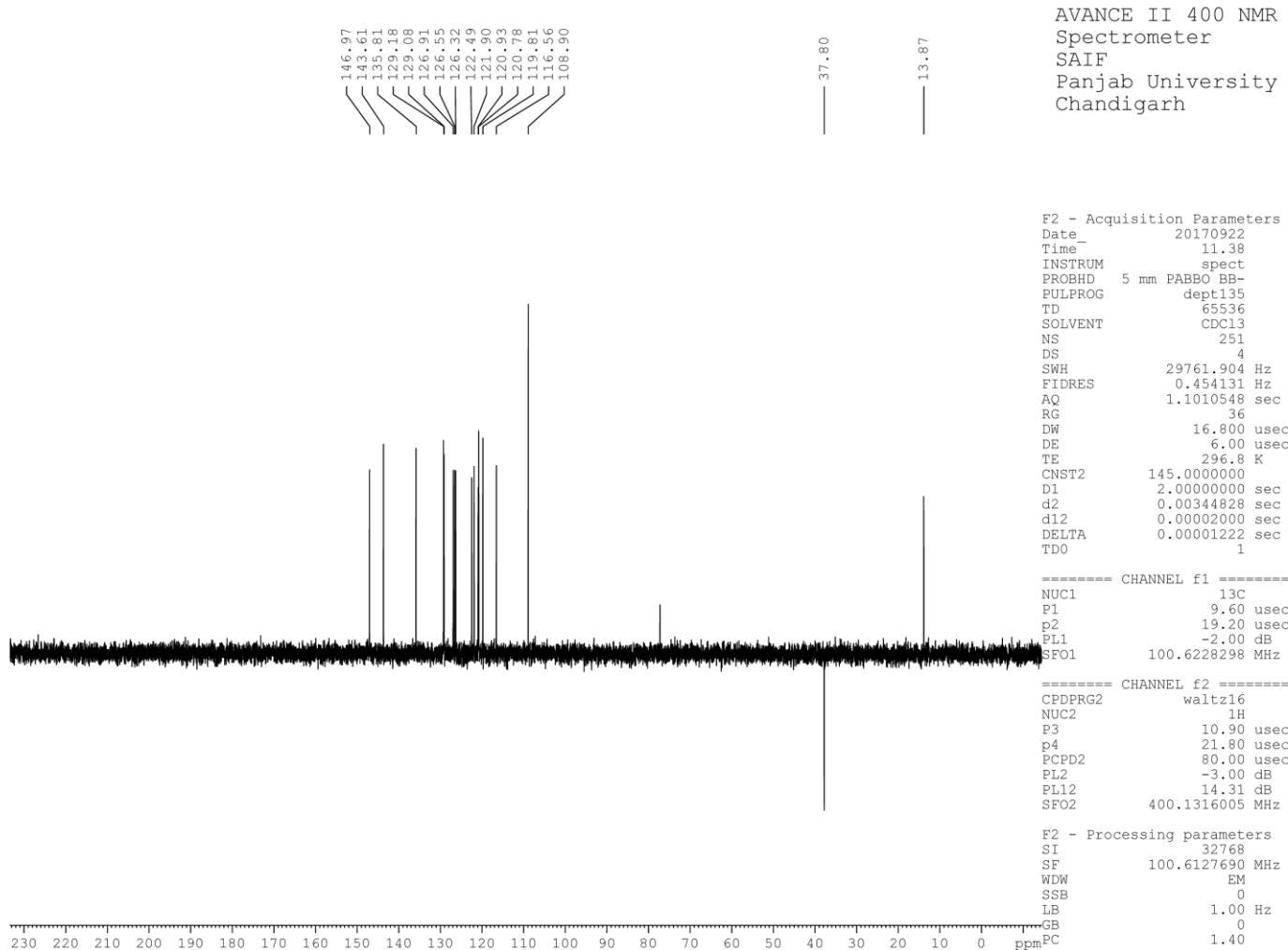


Fig. 12. DEPT-135 spectrum of compound 3c

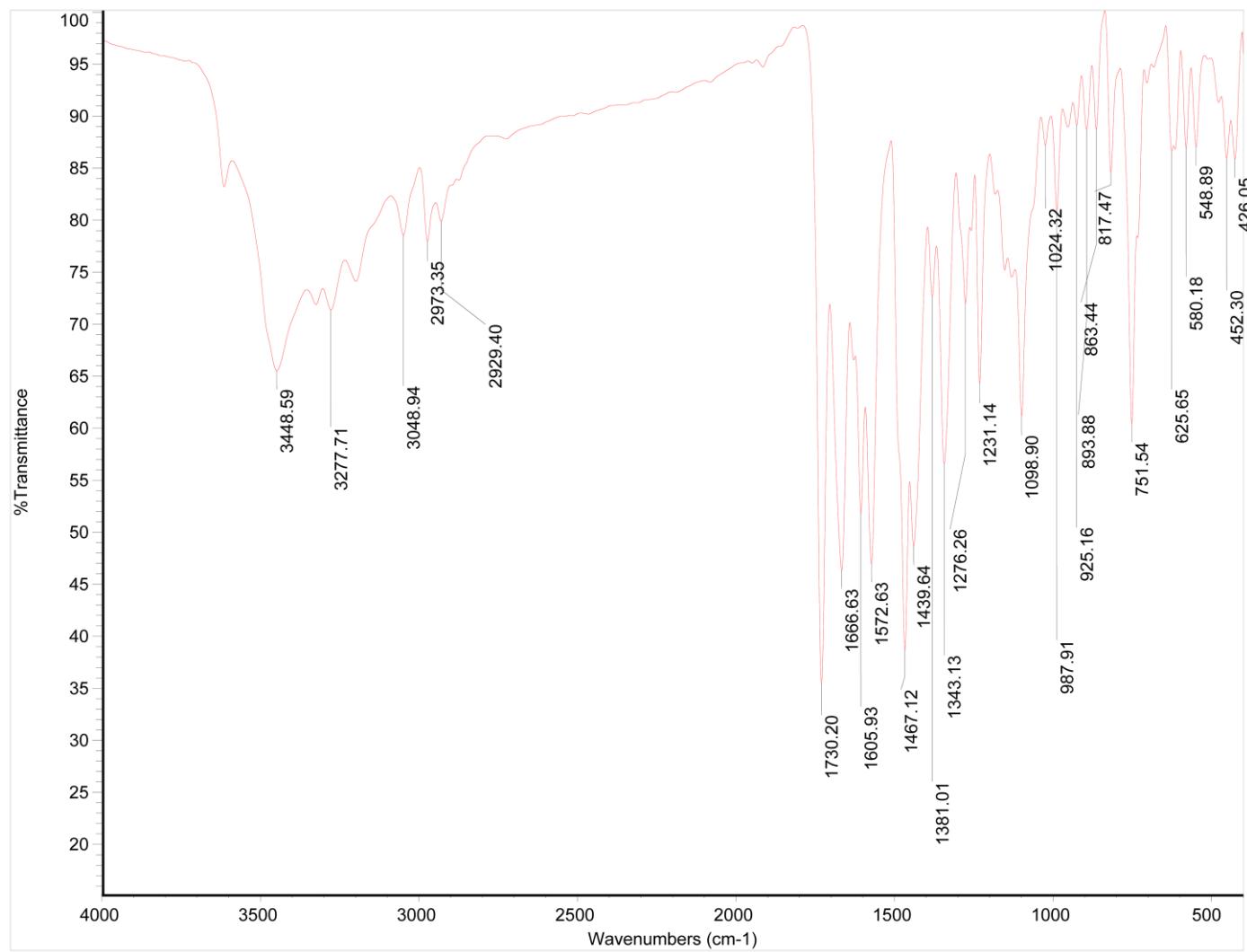


Fig. 13. IR spectrum of compound 4a

Line#:1 R.Time:----(Scan#-----)  
MassPeaks:7

MS Spectrum

Spectrum Mode:Averaged 0.415-0.747(61-109) Base Peak:473.2(18452366)  
BG Mode:Averaged 0.000-0.415(1-61) Segment 1 - Event 1

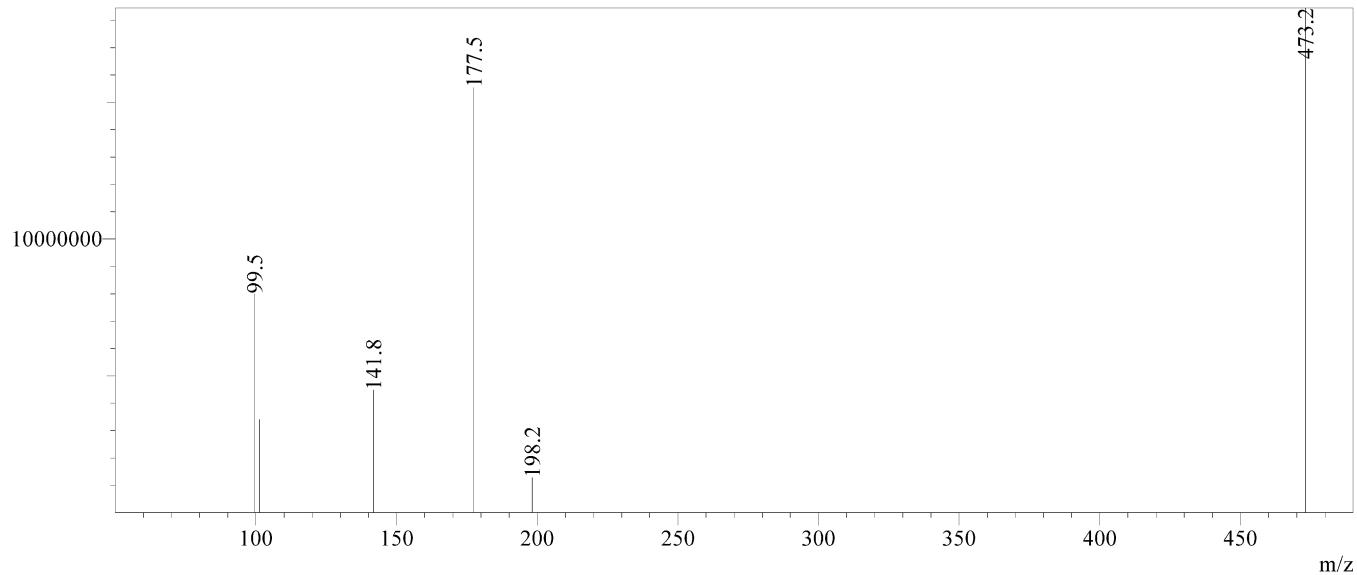


Fig. 14. Mass spectrum of compound 4a

## LCMS Analysis Report

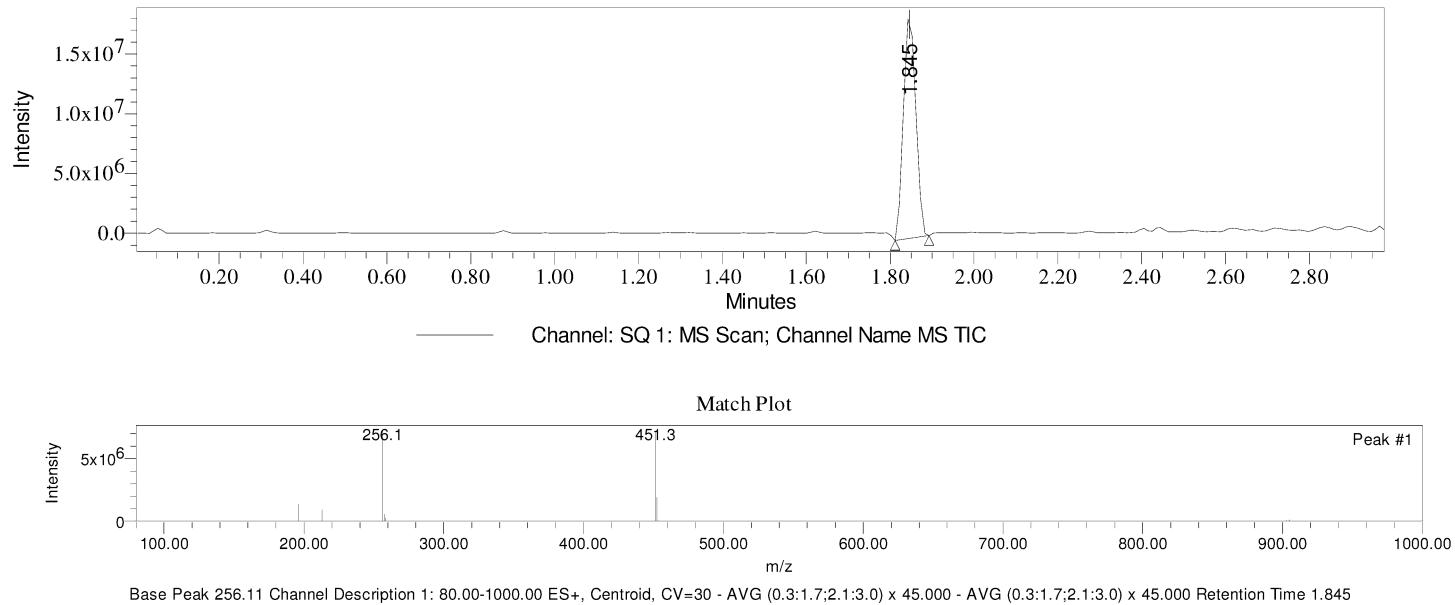


Fig. 4.15 LCMS spectrum of compound 4a

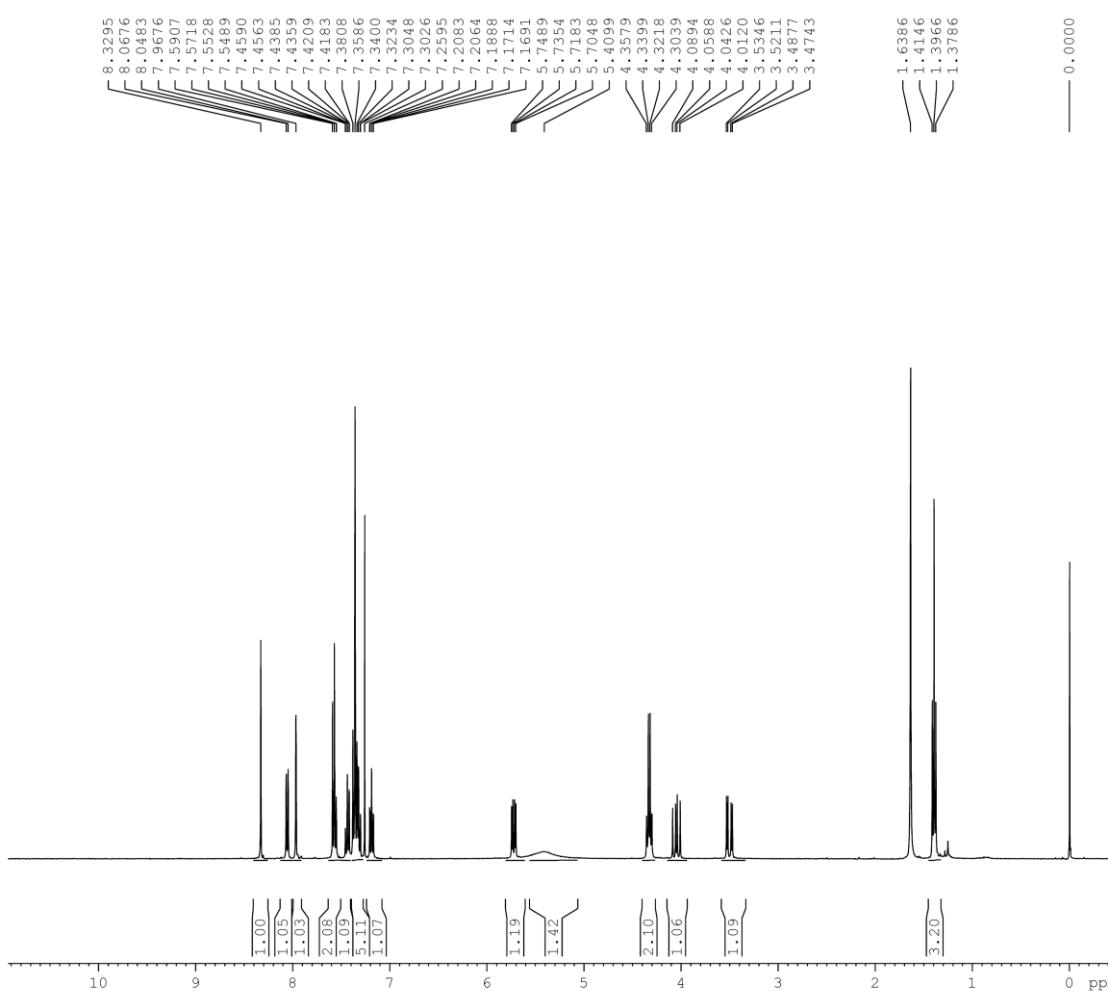


Fig. 16.  $^1\text{H}$  NMR spectrum of compound 4a

BRUKER  
AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

F2 - Acquisition Parameters  
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 Time\_ 20.00  
 INSTRUM spect  
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 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 8  
 DS 2  
 SWH 12019.230 Hz  
 FIDRES 0.183399 Hz  
 AQ 2.7263477 sec  
 RG 406  
 DW 41.600 usec  
 DE 6.00 usec  
 TE 295.7 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.90 usec  
 PL1 -3.00 dB  
 SFO1 400.1324710 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 400.1300096 MHz  
 WDW EM  
 SSB 0  
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 GB 0  
 PC 1.00

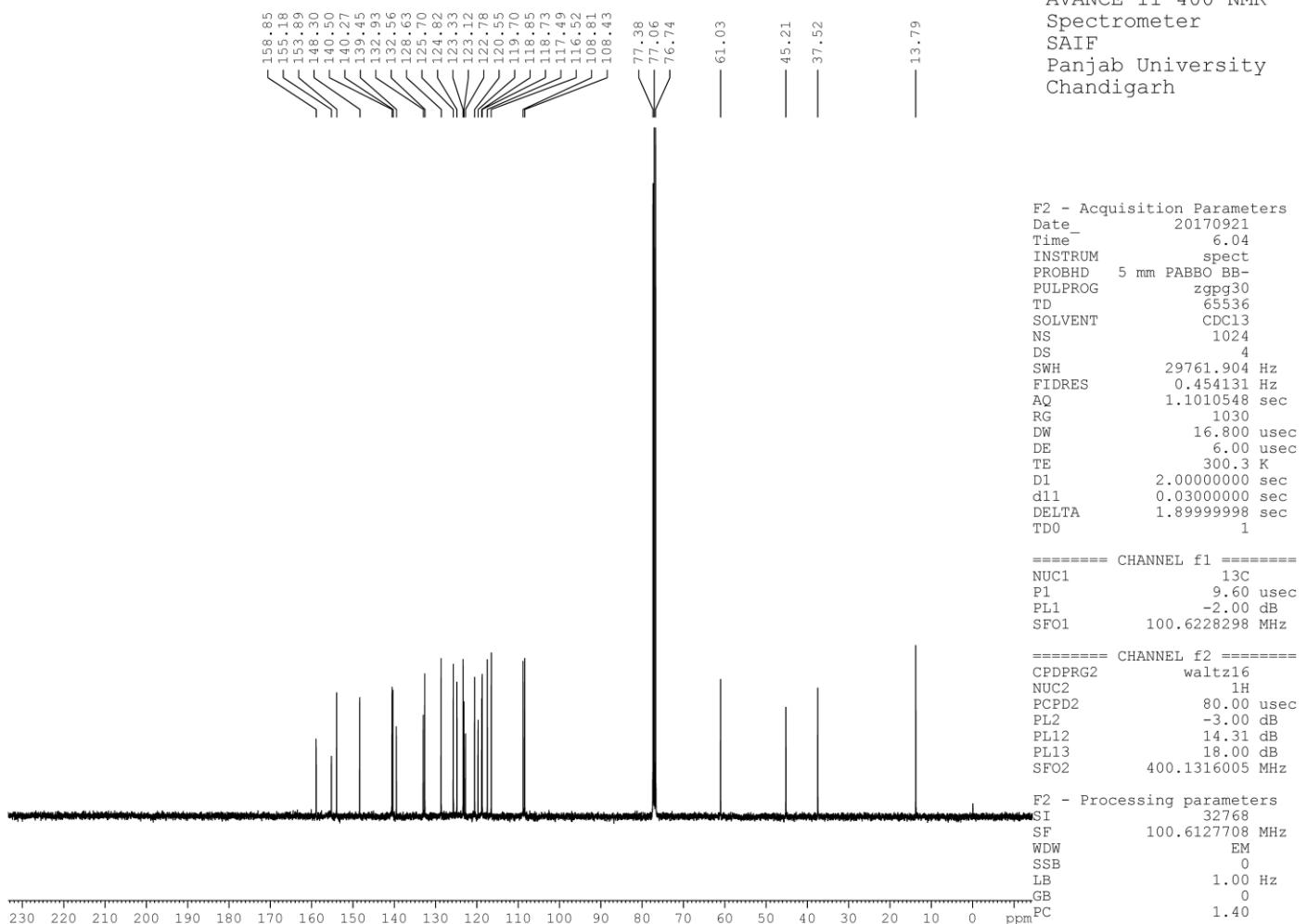


Fig. 17. <sup>13</sup>C NMR spectrum of compound 4a

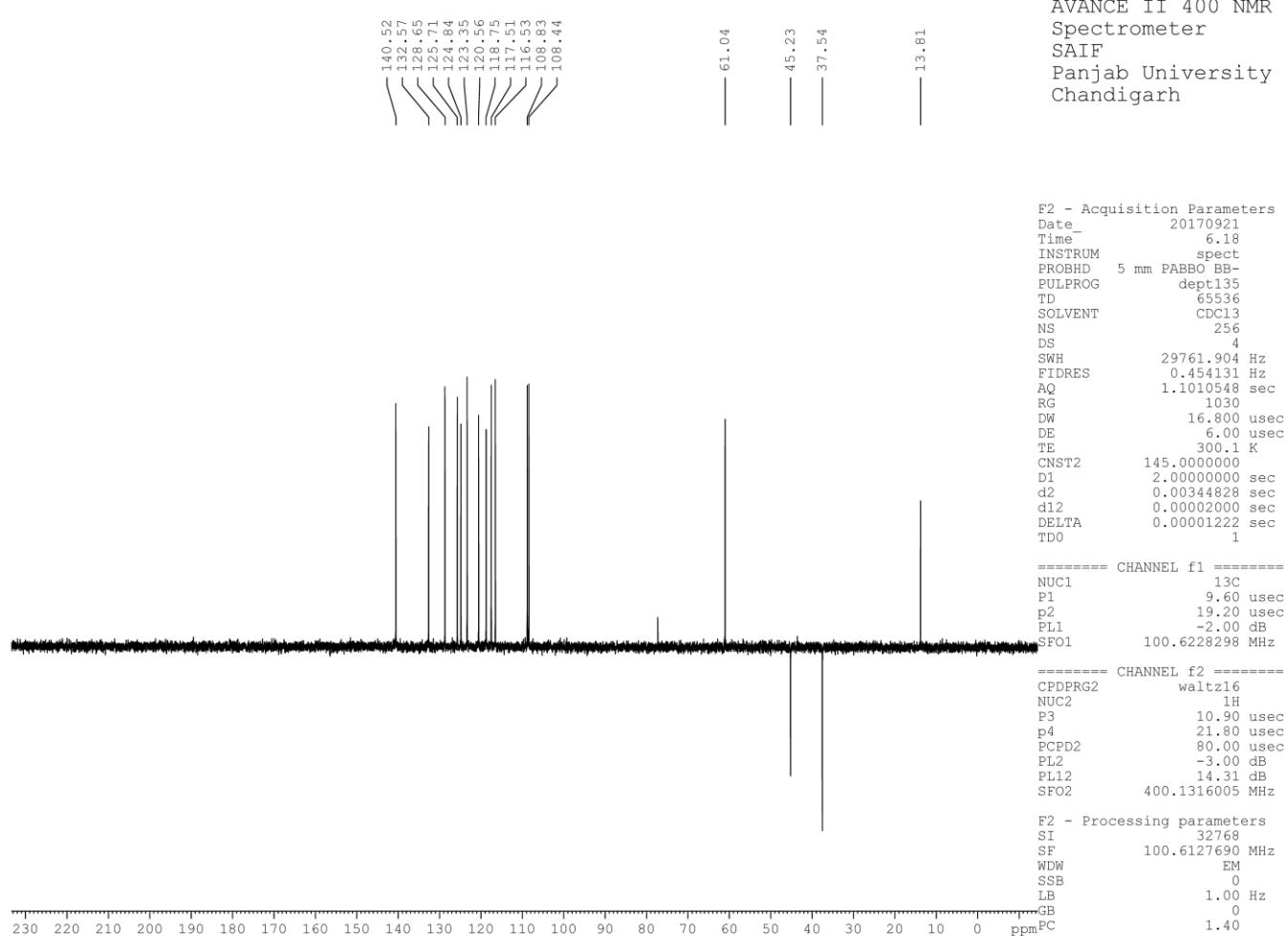


Fig. 18. DEPT-135 spectrum of compound 4a

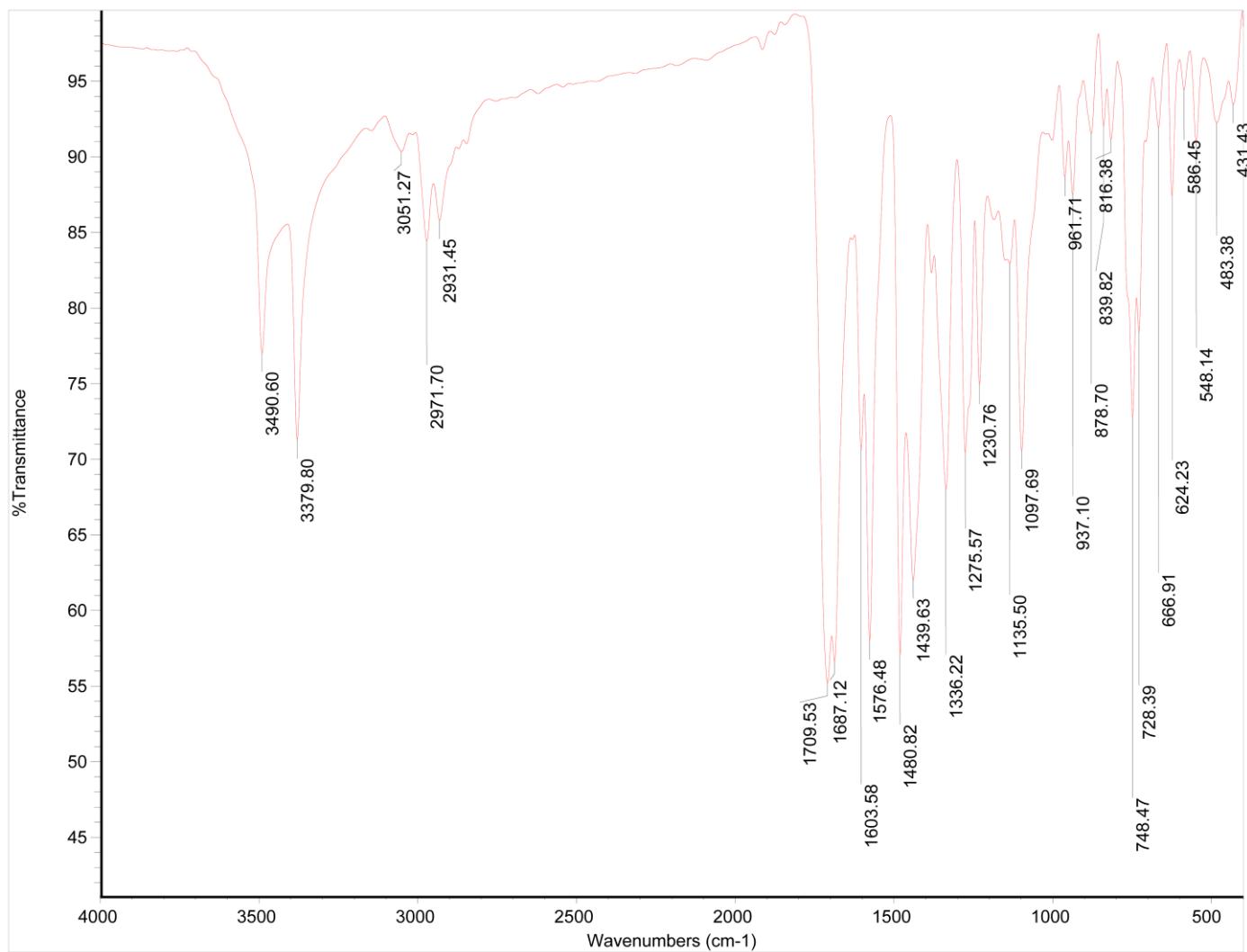


Fig. 19. IR spectrum of compound 4b

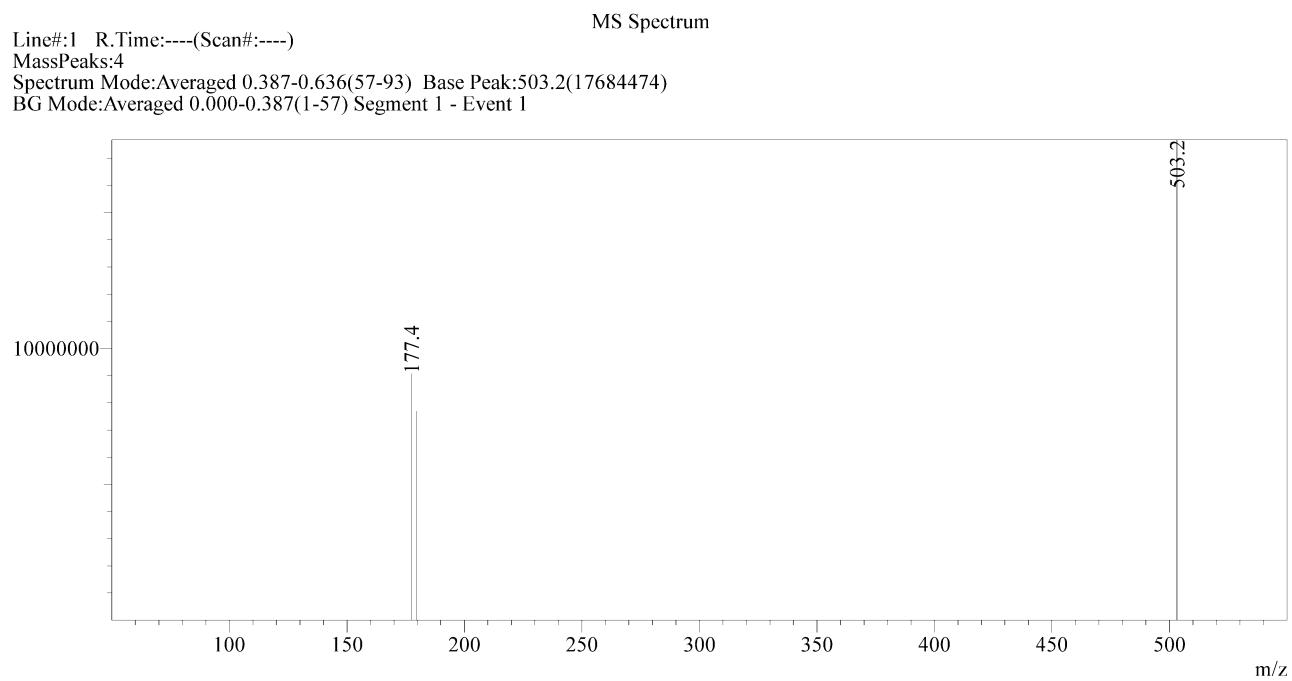


Fig. 20. Mass spectrum of compound 4b

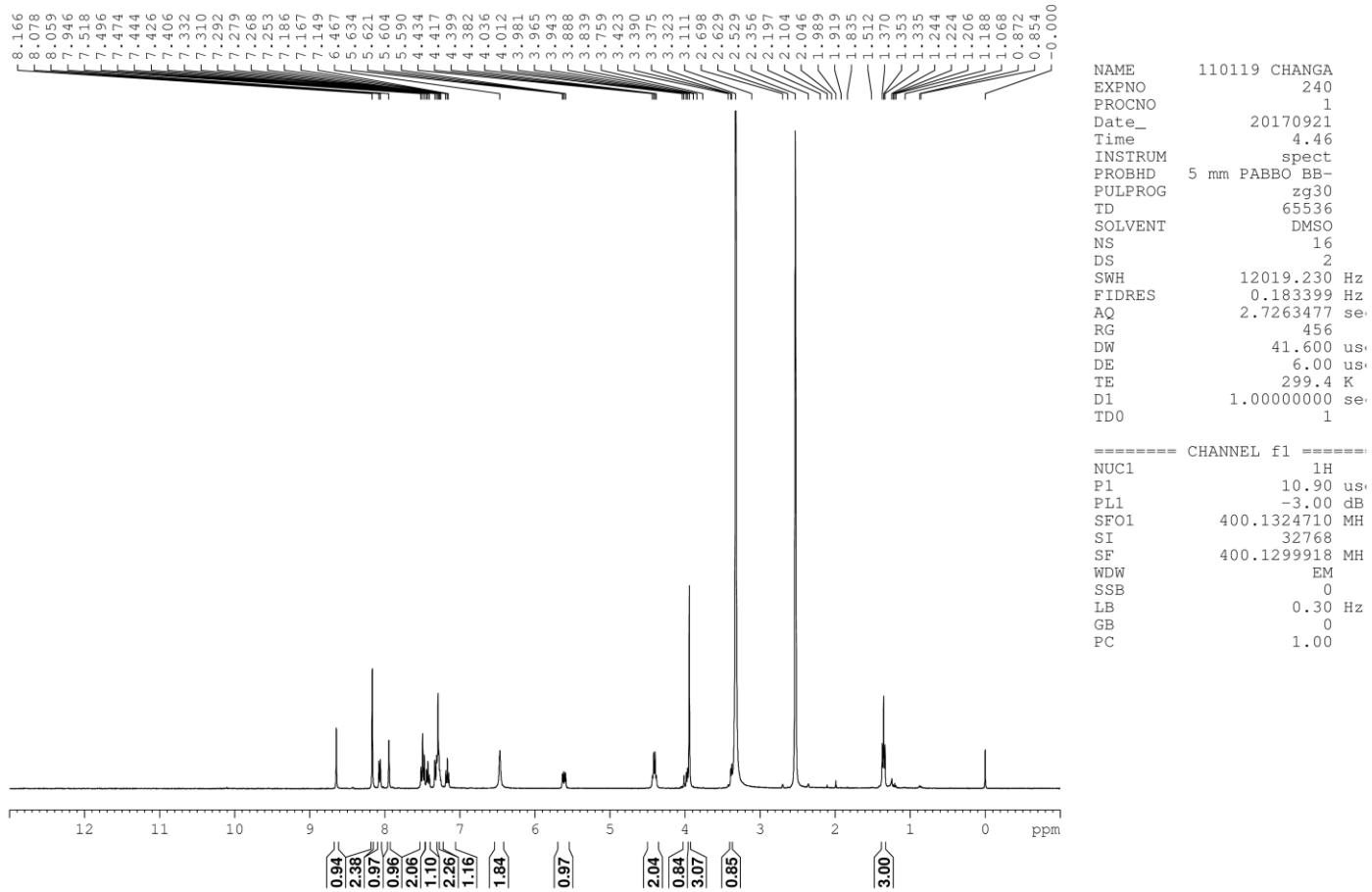


Fig. 21.  $^1\text{H}$  NMR spectrum of compound 4b

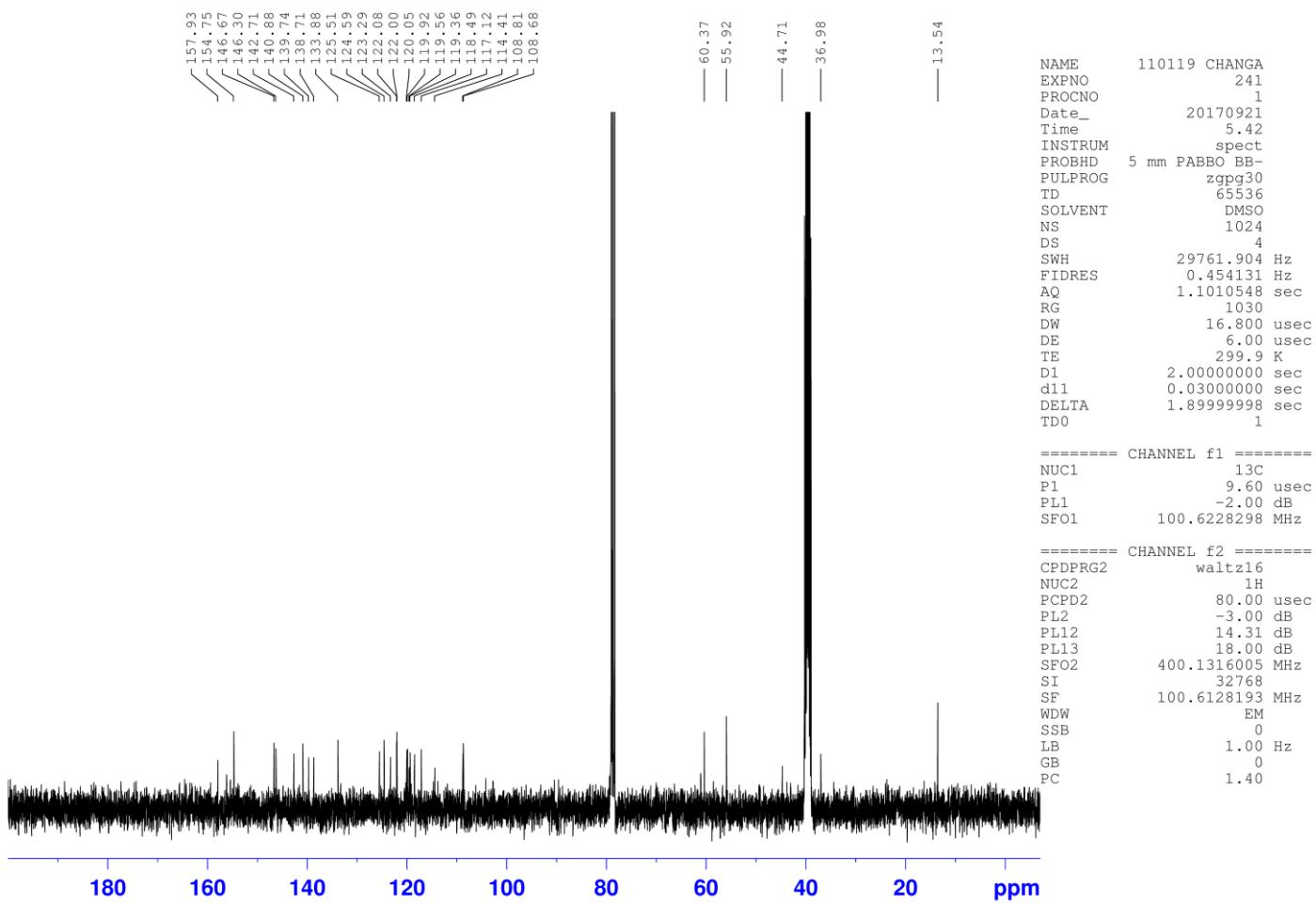


Fig. 22.  $^{13}\text{C}$  NMR spectrum of compound 4b

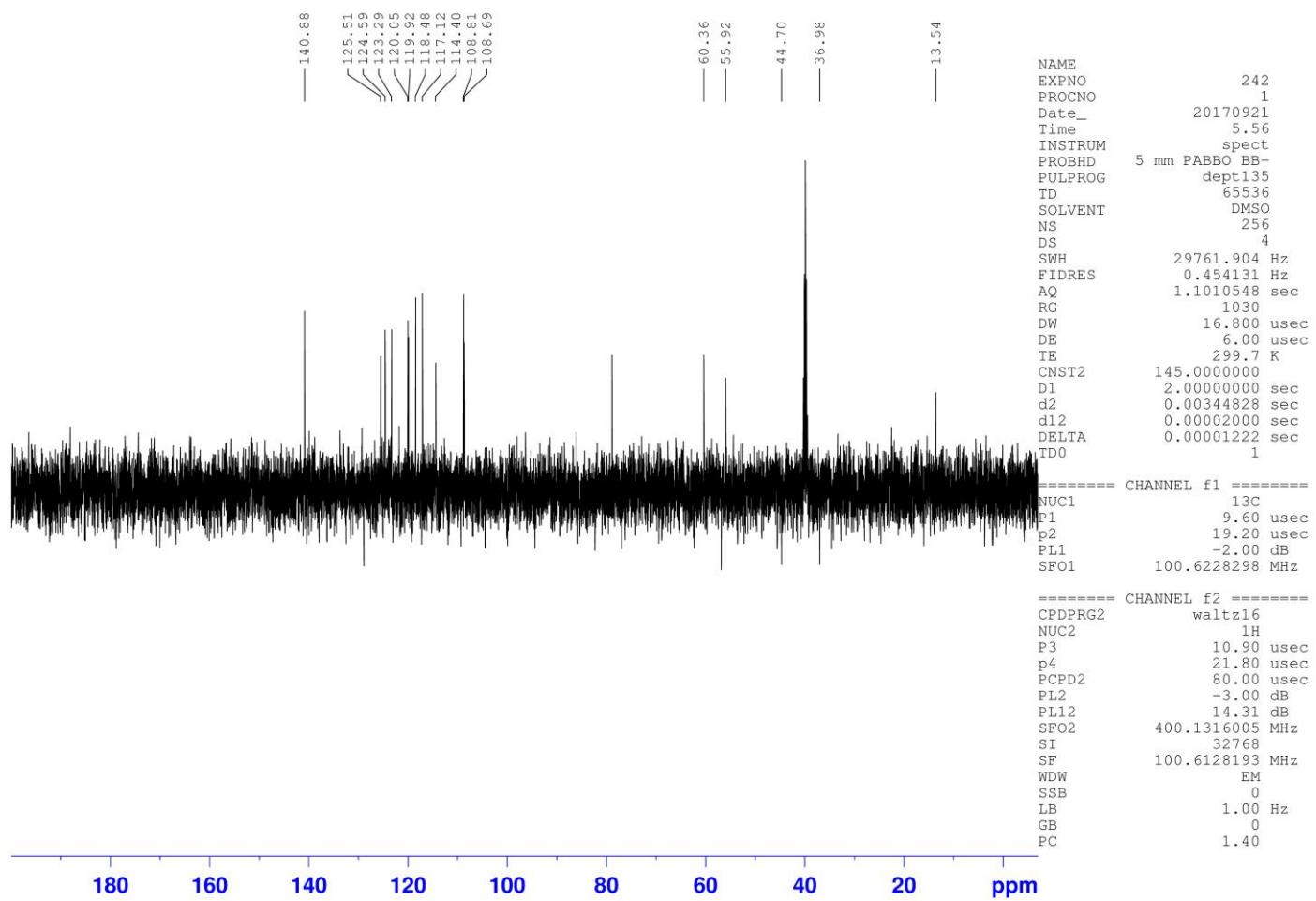


Fig. 23. DEPT-135 spectrum of compound 4b

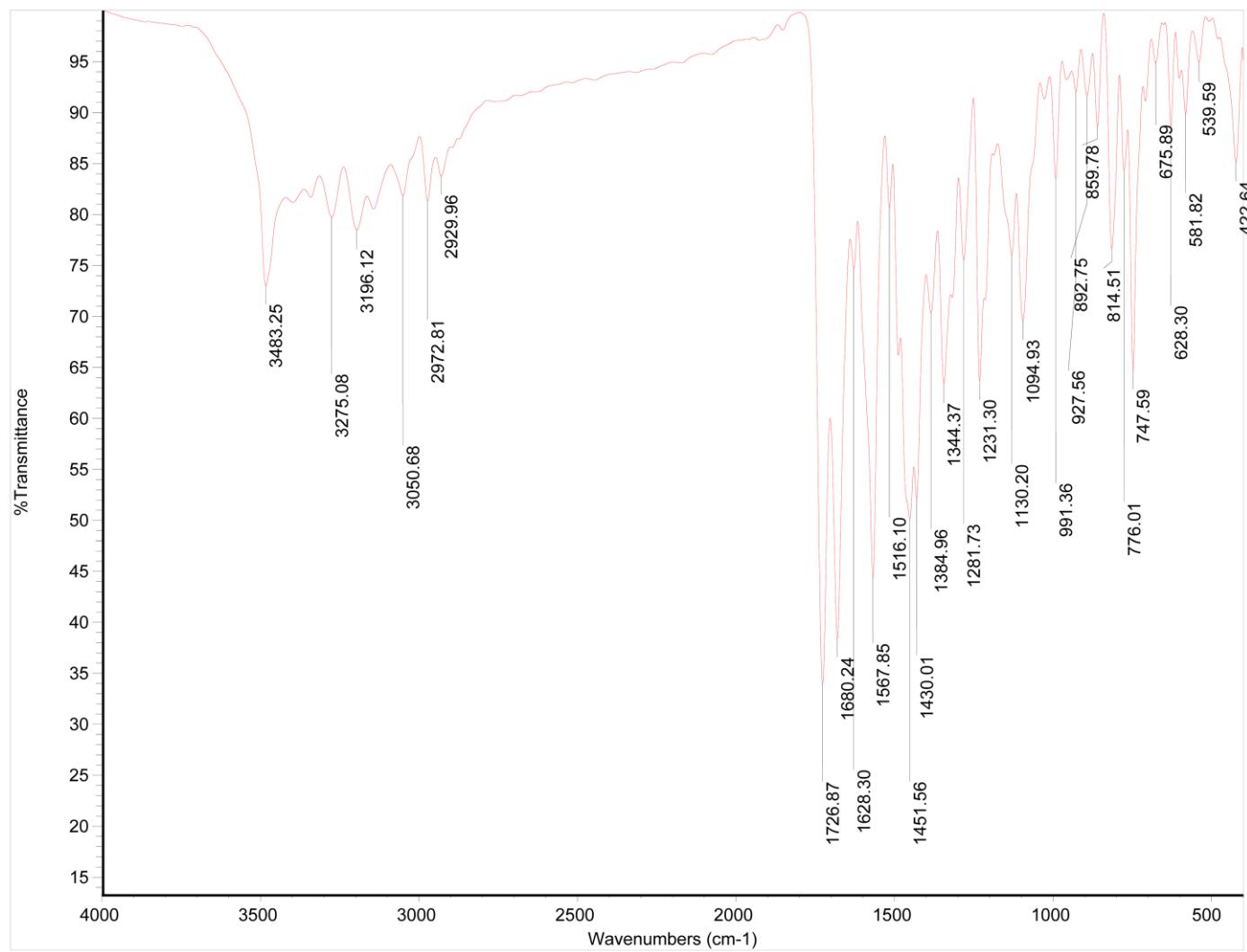


Fig. 24. IR spectrum of compound 4c

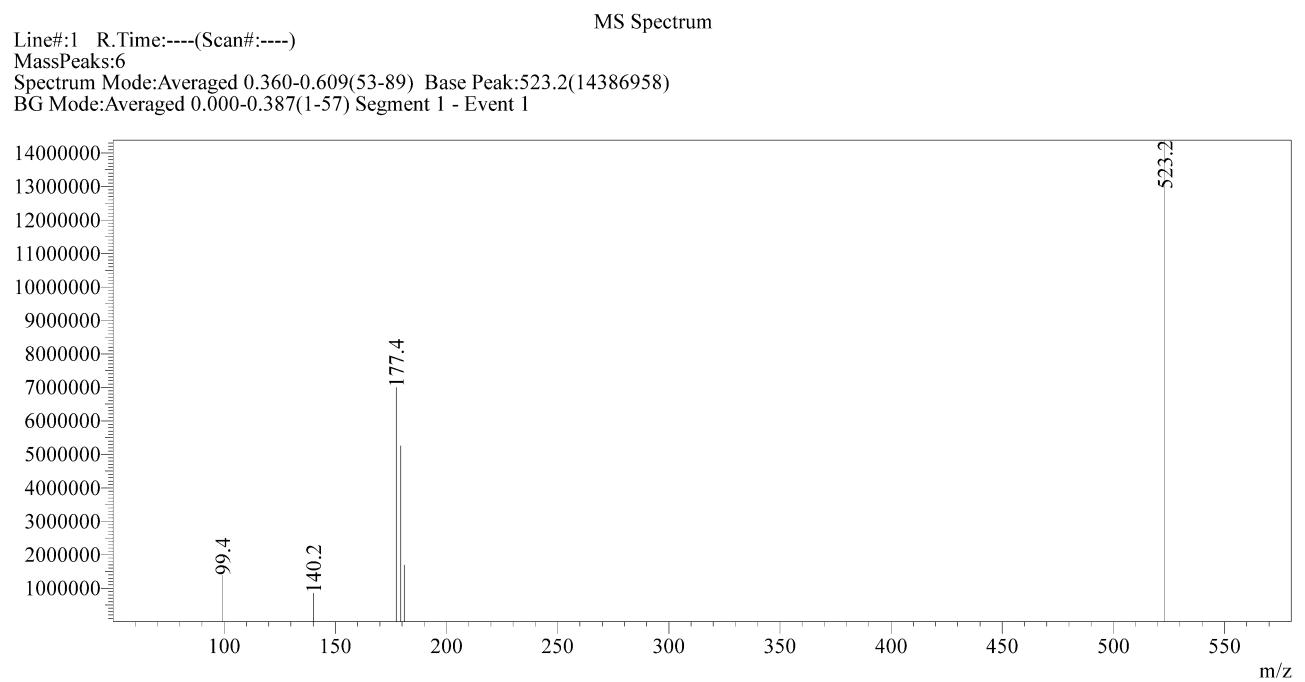


Fig. 25. Mass spectrum of compound 4c

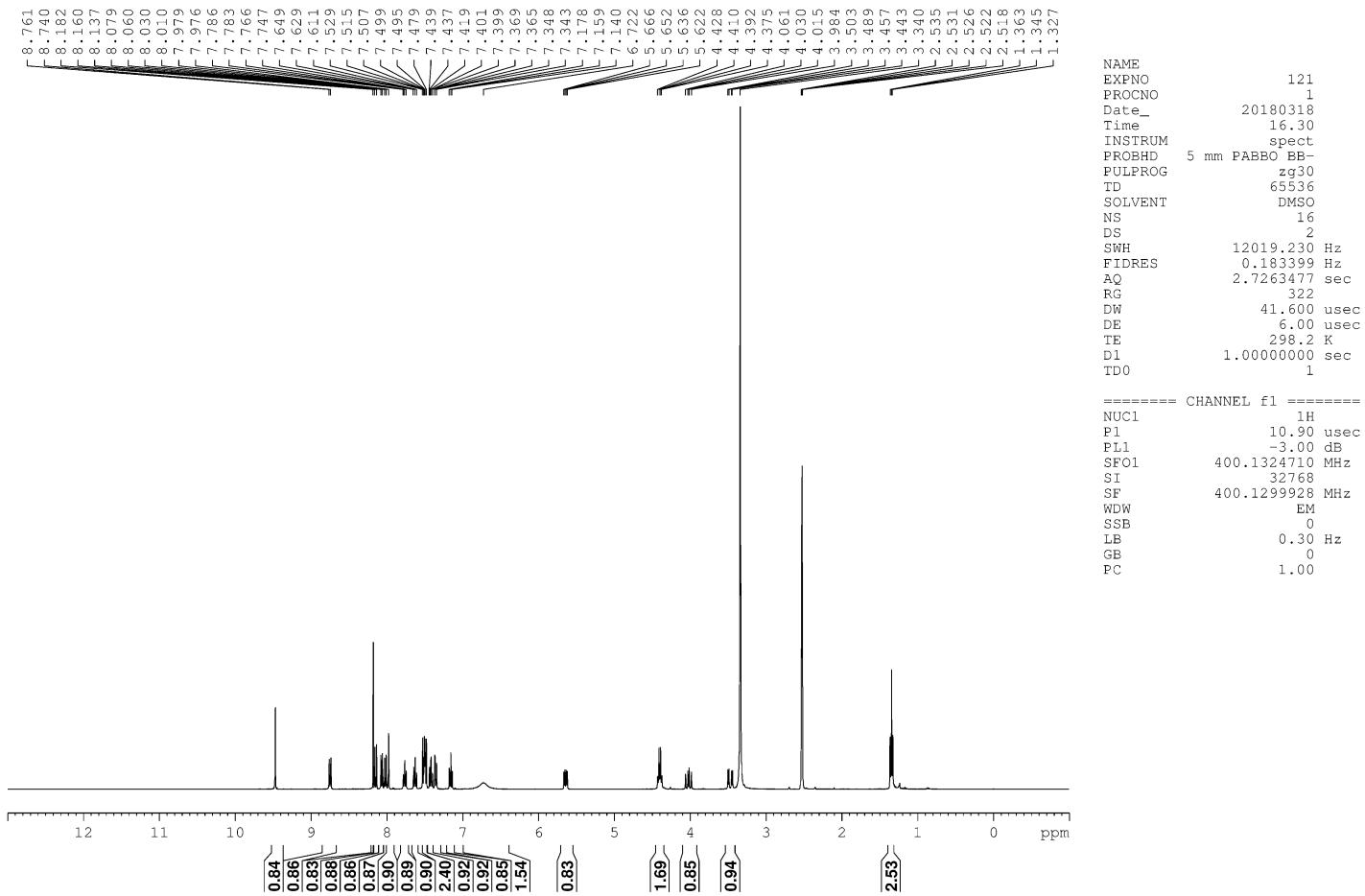


Fig. 26.  $^1\text{H}$  NMR spectrum of compound 4c

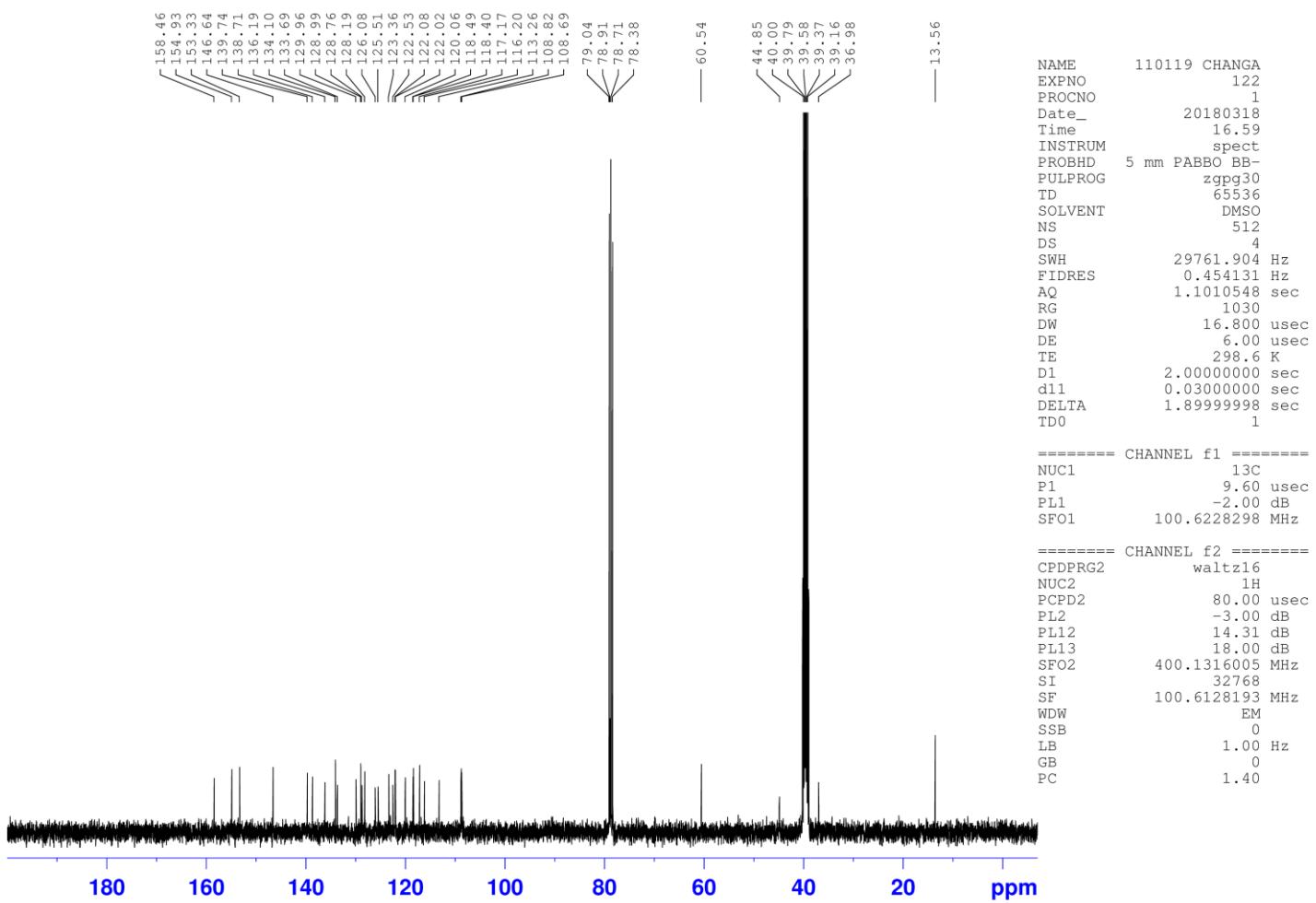


Fig. 27.  $^{13}\text{C}$  NMR spectrum of compound 4c

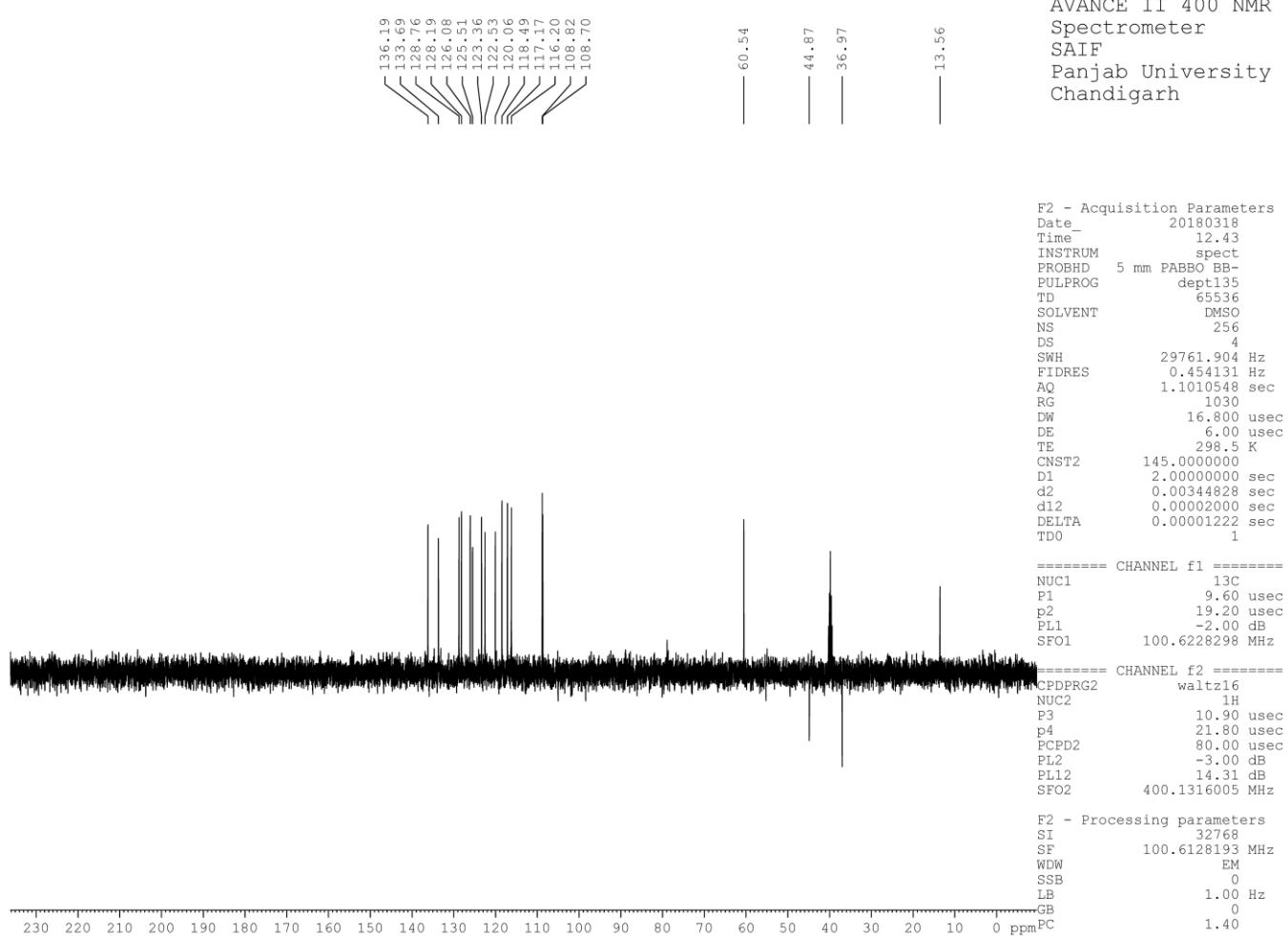


Fig. 28. DEPT-135 spectrum of compound 4c

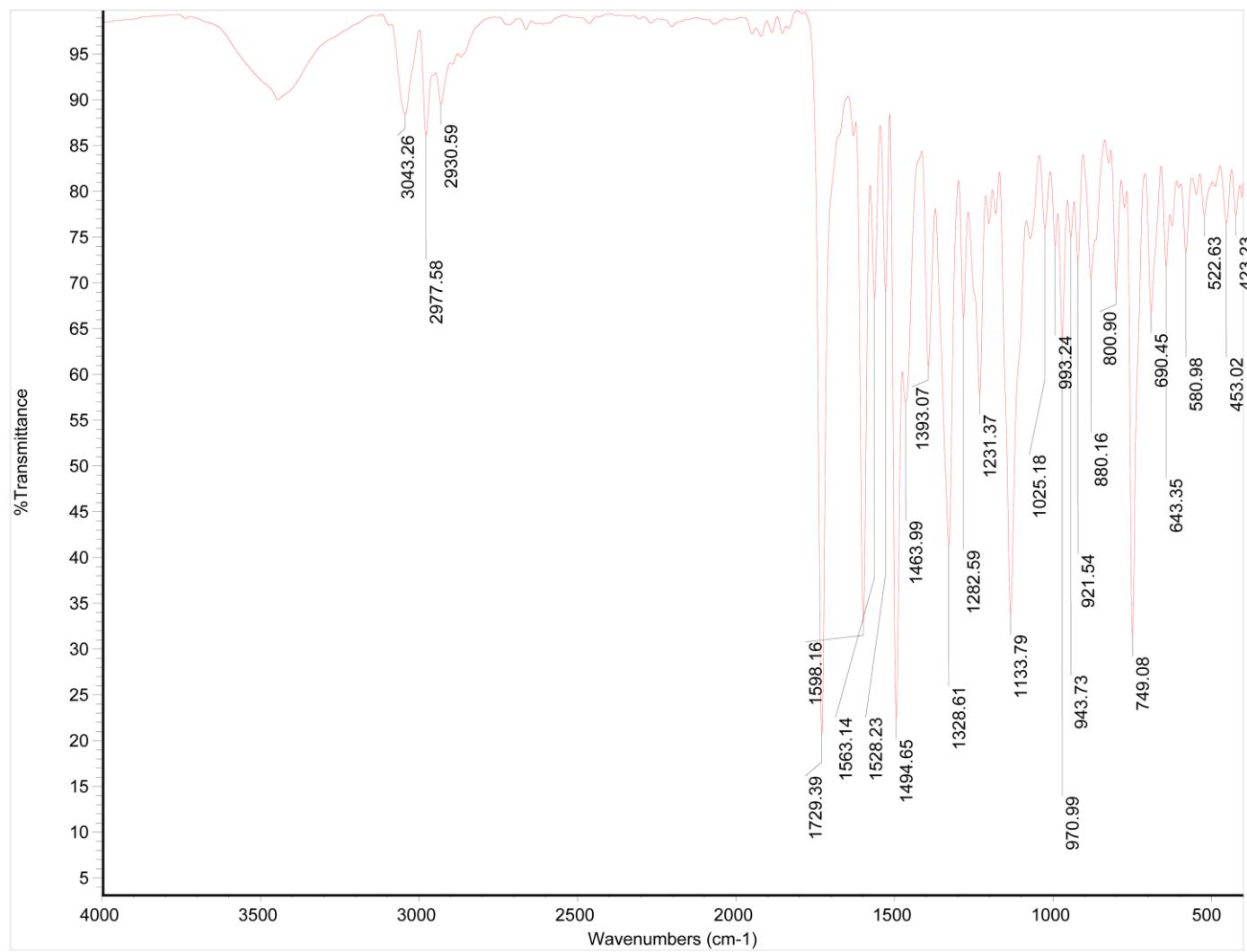


Fig. 29. IR spectrum of compound 5a

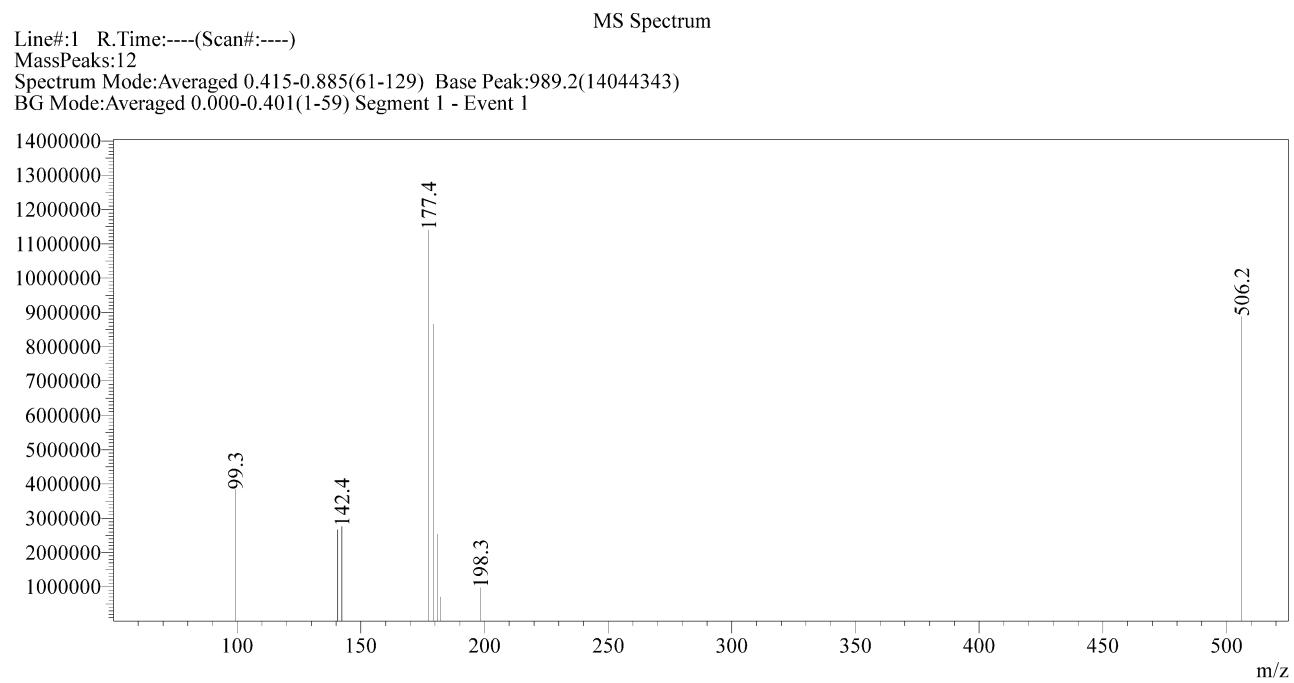


Fig. 30. Mass spectrum of compound 5a

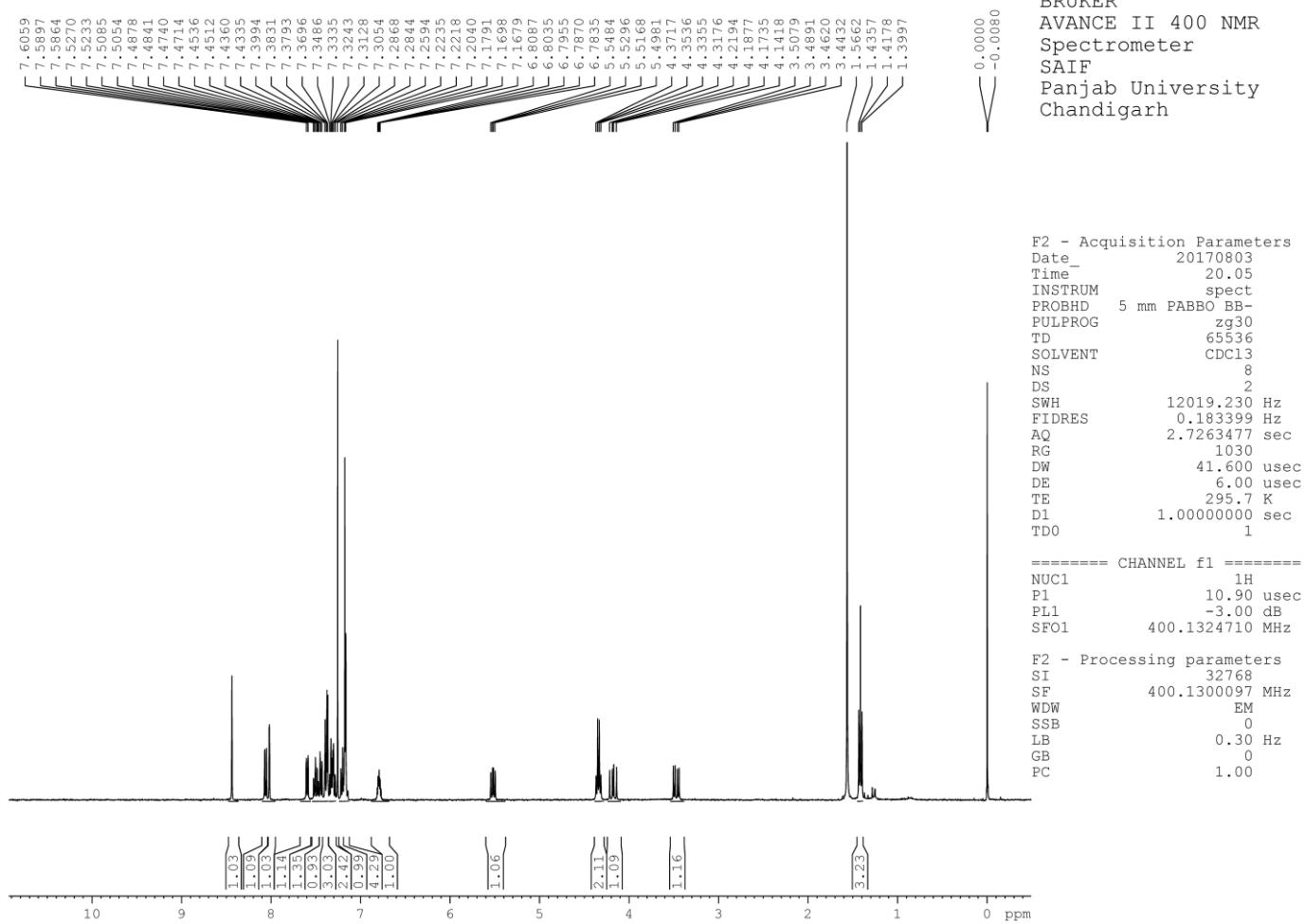


Fig. 31. <sup>1</sup>H NMR spectrum of compound 5a

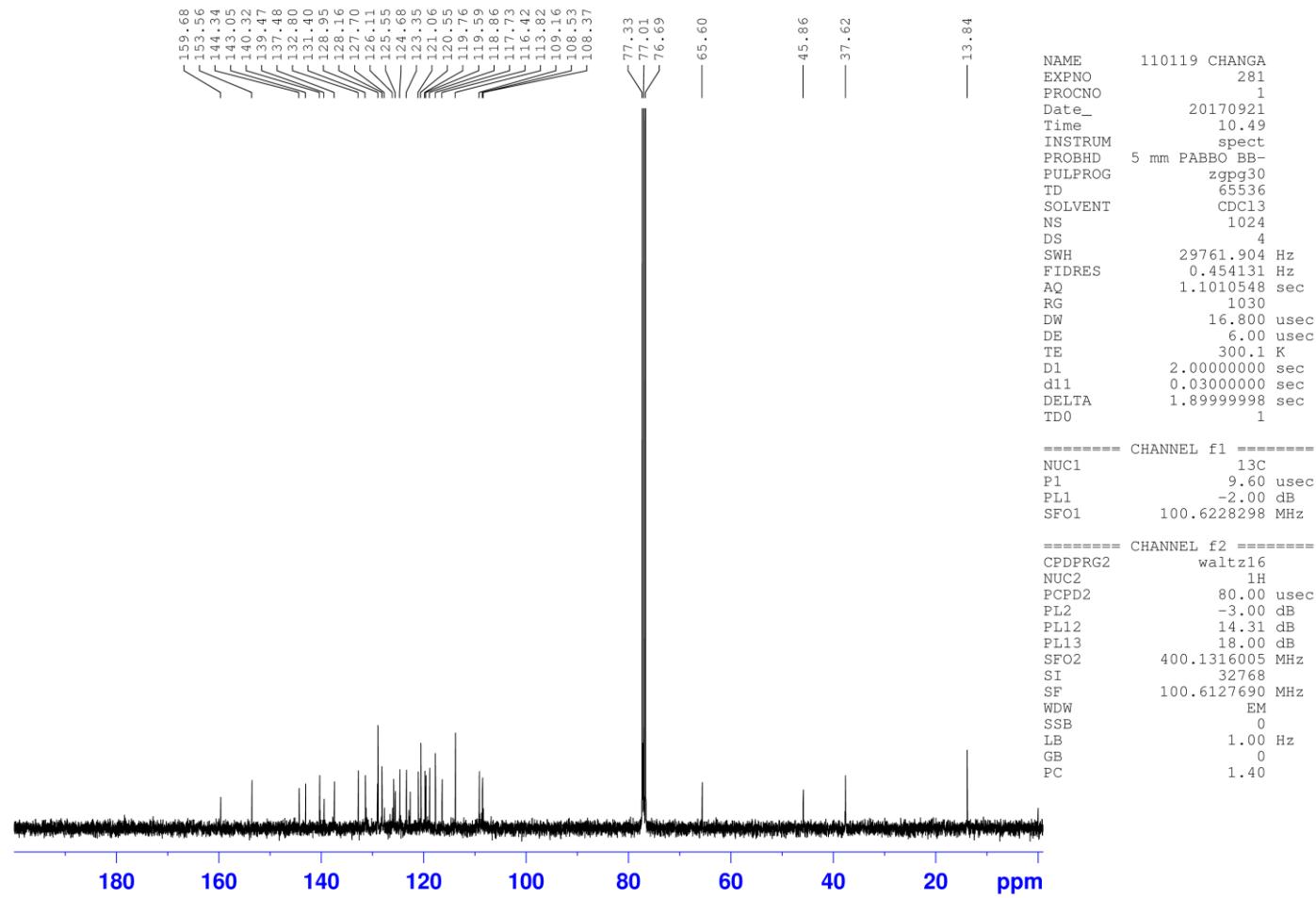


Fig. 32.  $^{13}\text{C}$  NMR spectrum of compound 5a

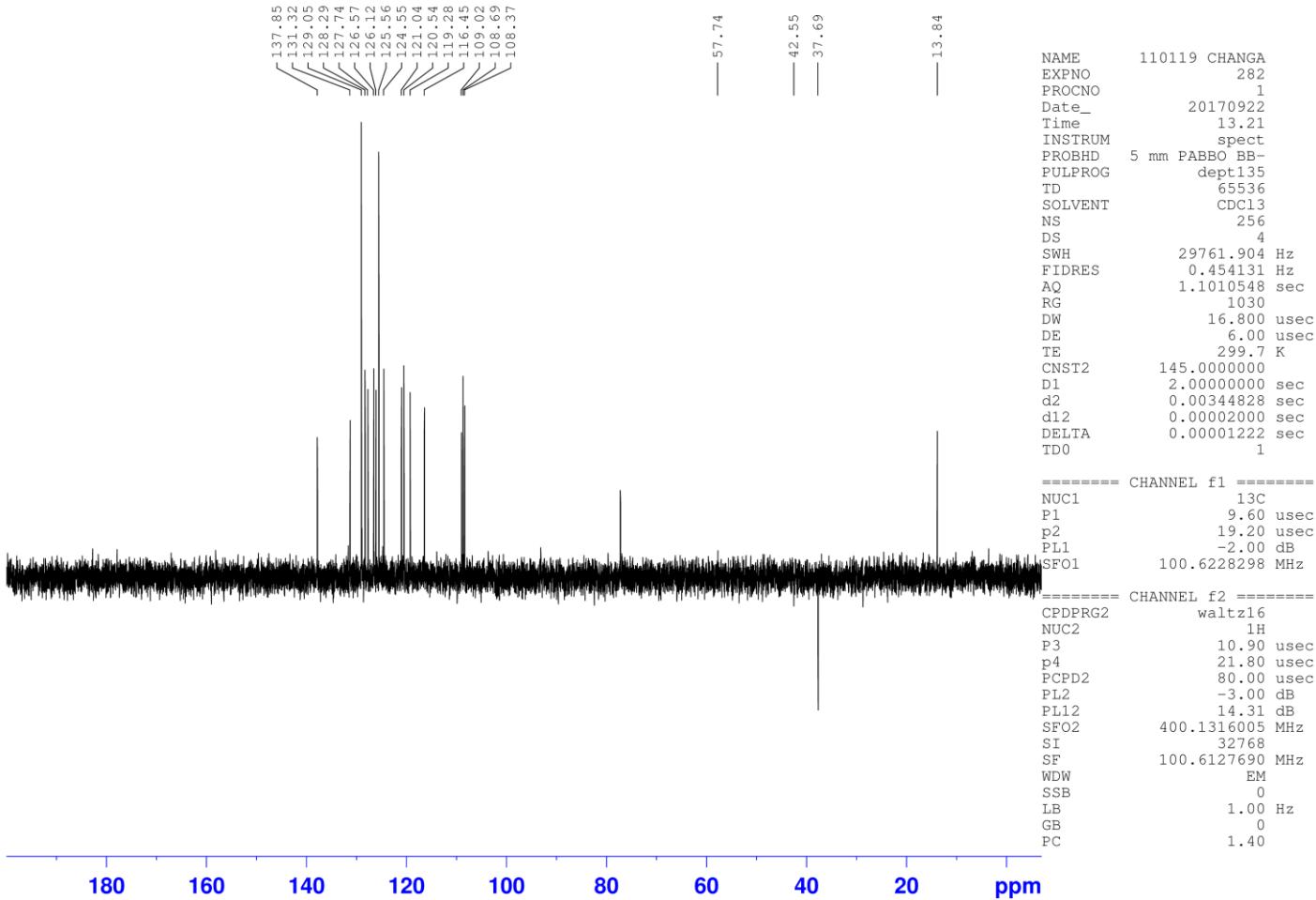


Fig. 33. DEPT-135 spectrum of compound 5a

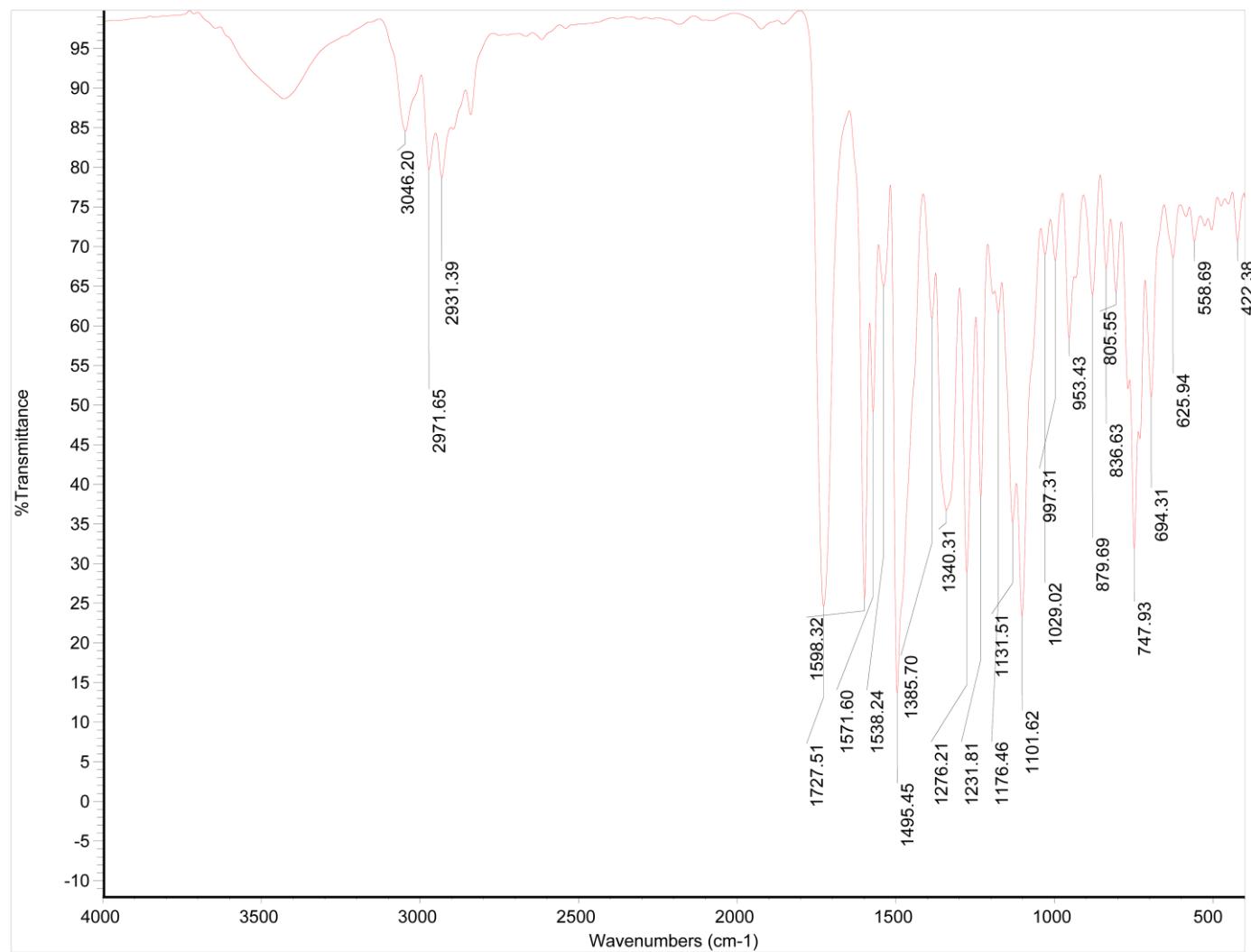


Fig. 34. IR spectrum of compound 5b

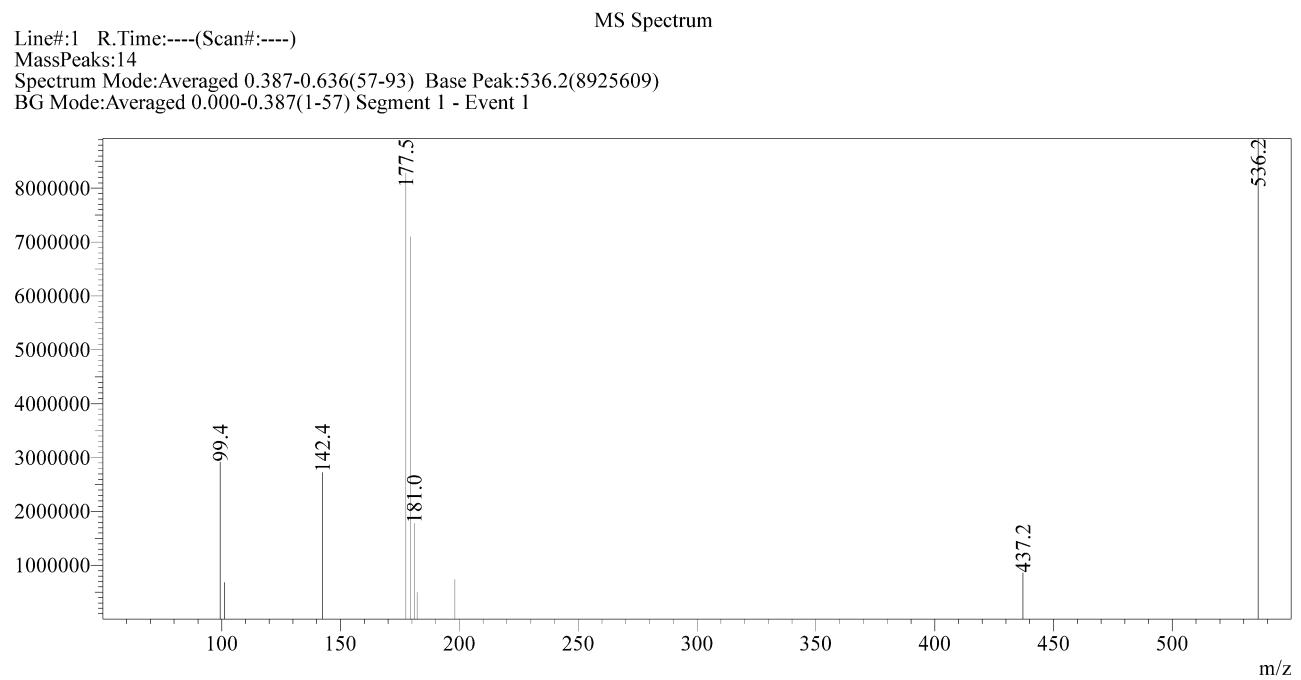


Fig. 35. Mass spectrum of compound 5b

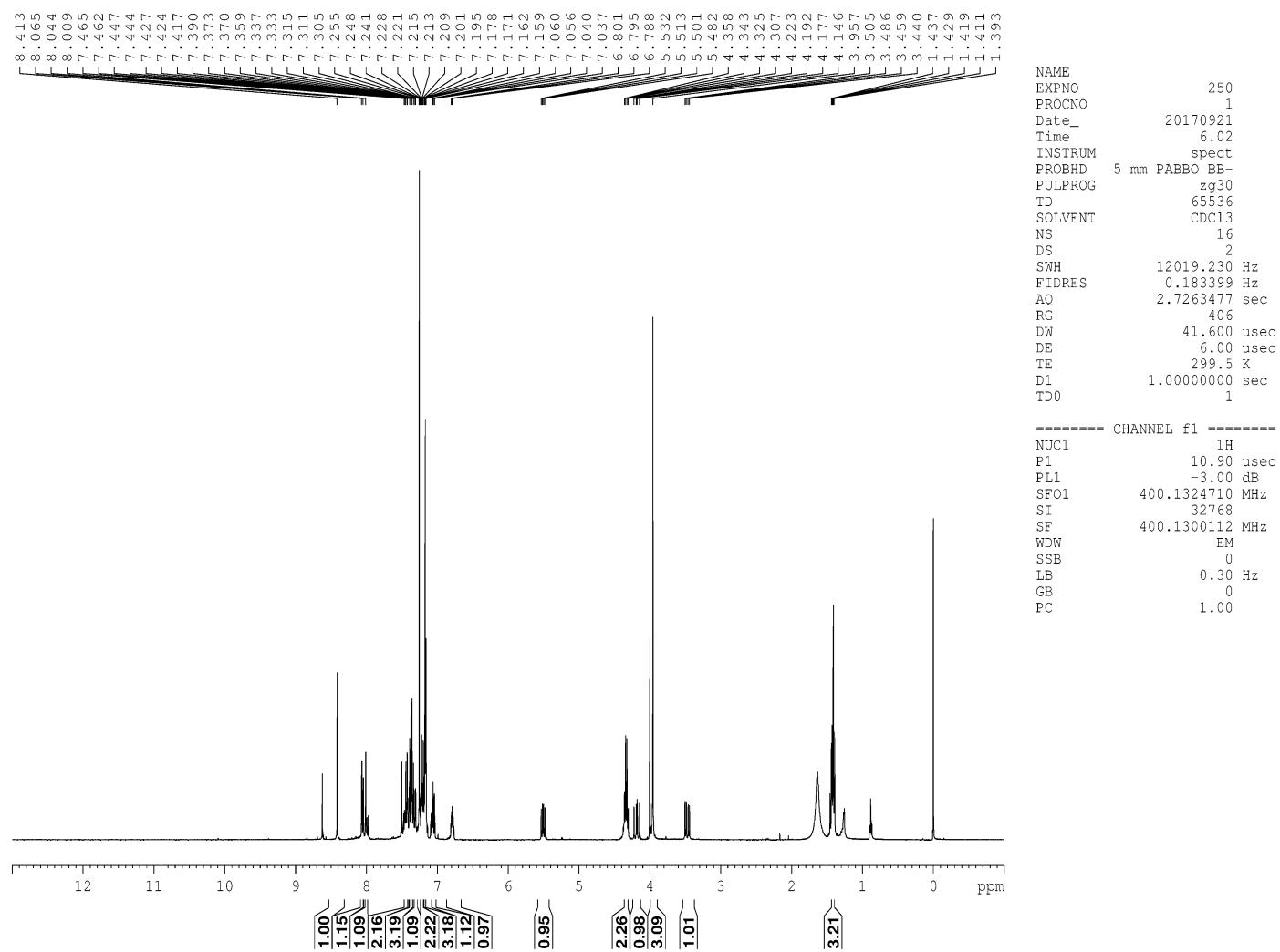


Fig. 36.  $^1\text{H}$  NMR spectrum of compound 5b

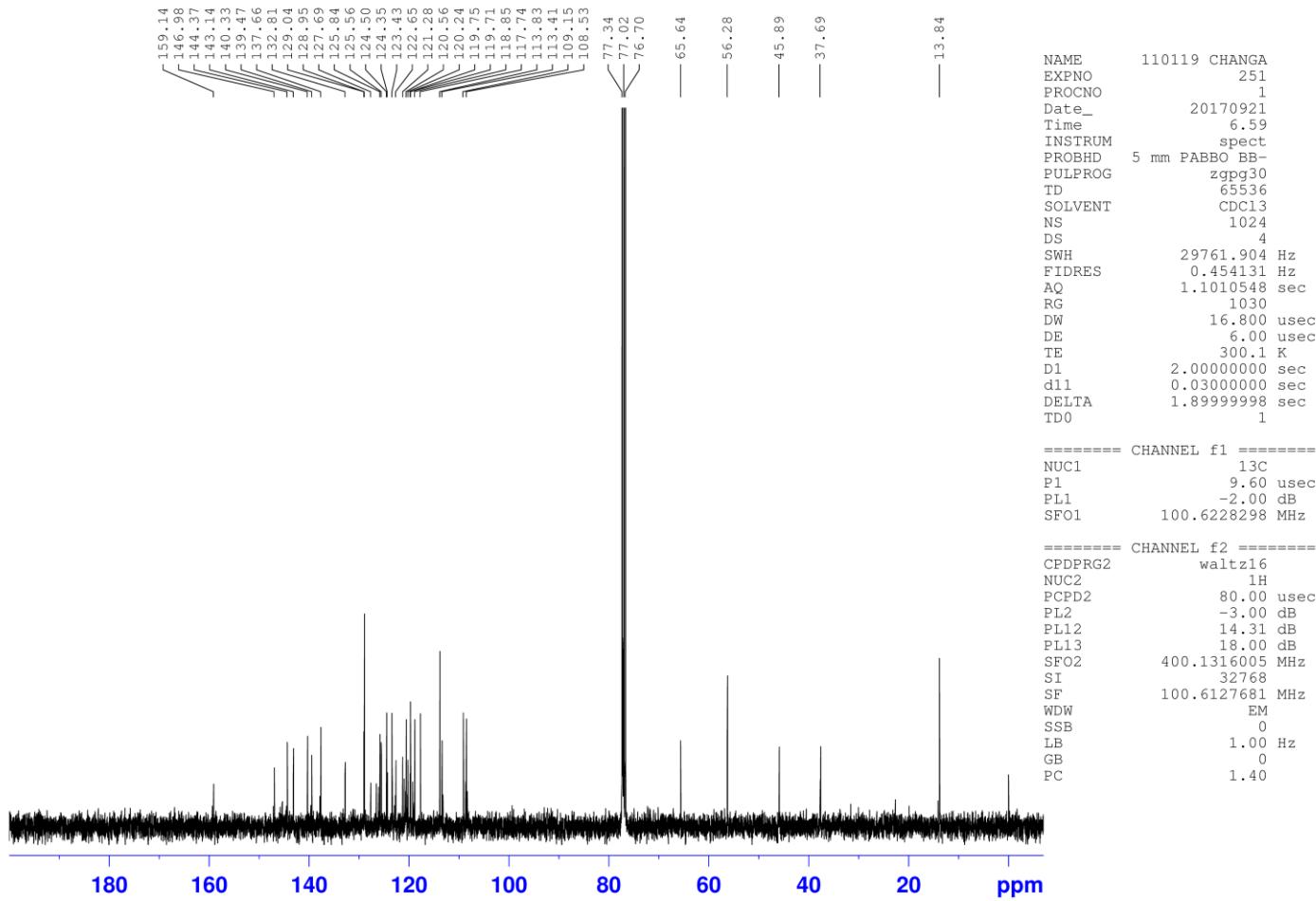


Fig. 37.  $^{13}\text{C}$  NMR spectrum of compound 5b

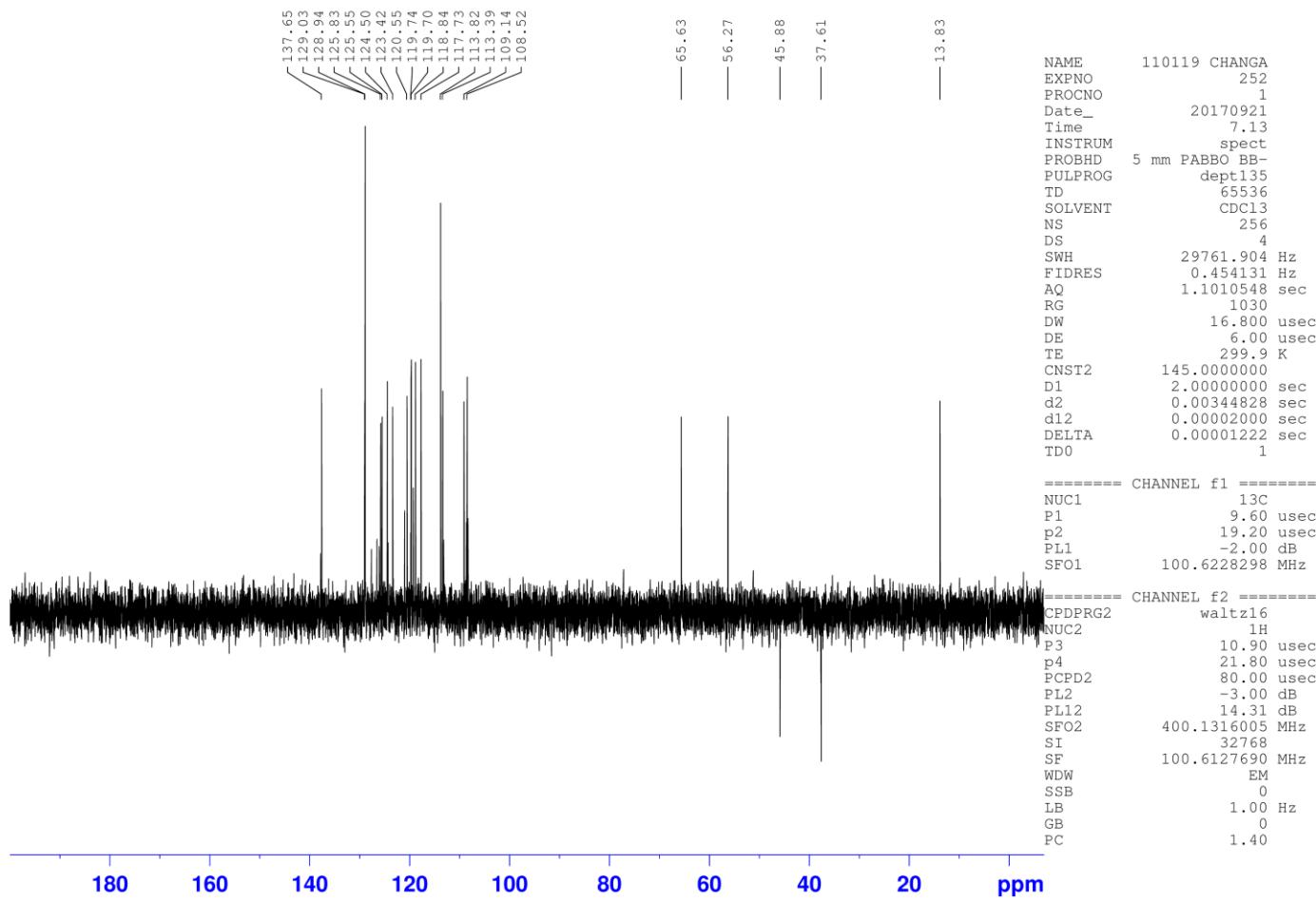


Fig. 38. DEPT-135 spectrum of compound 5b

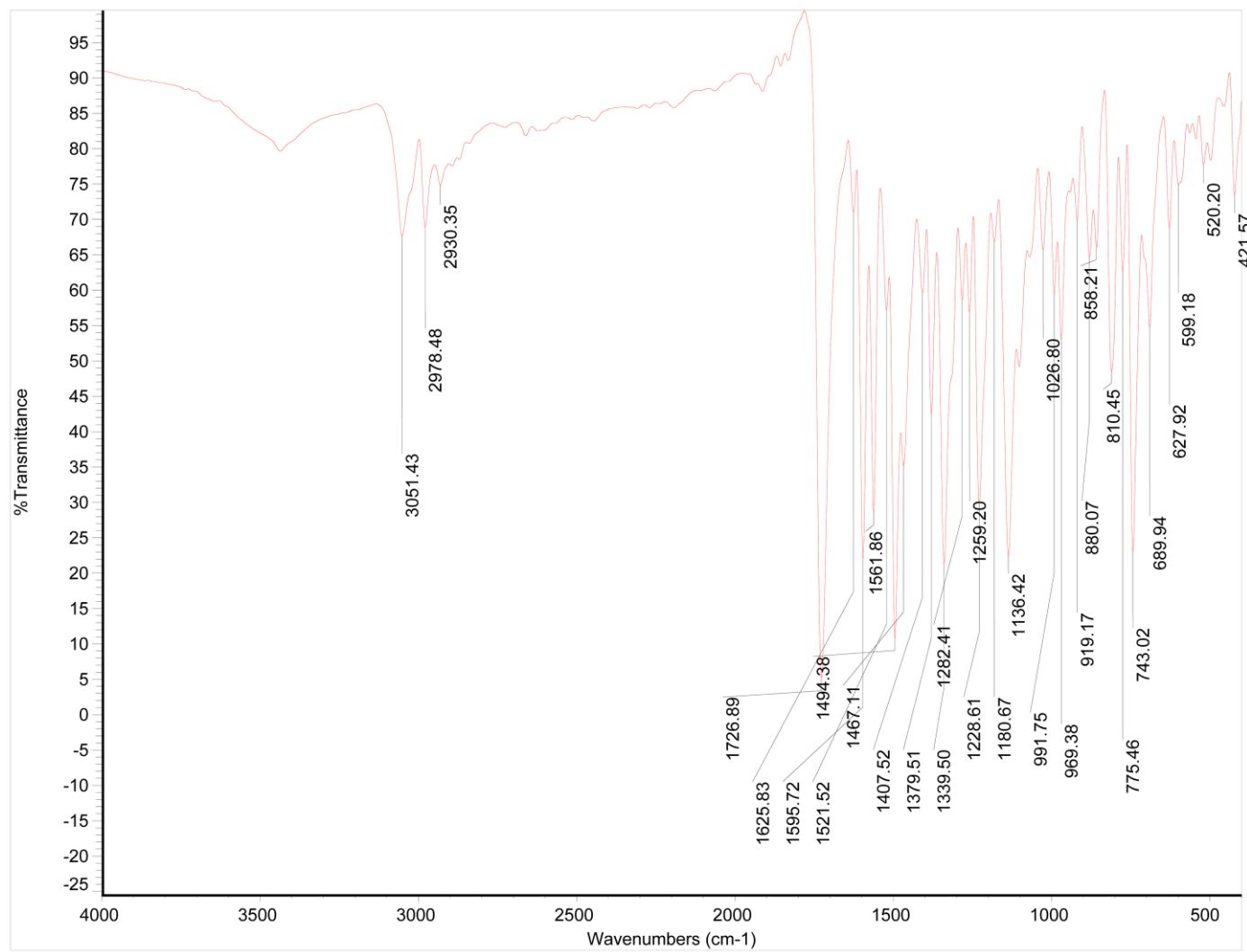


Fig. 39. IR spectrum of compound 5c

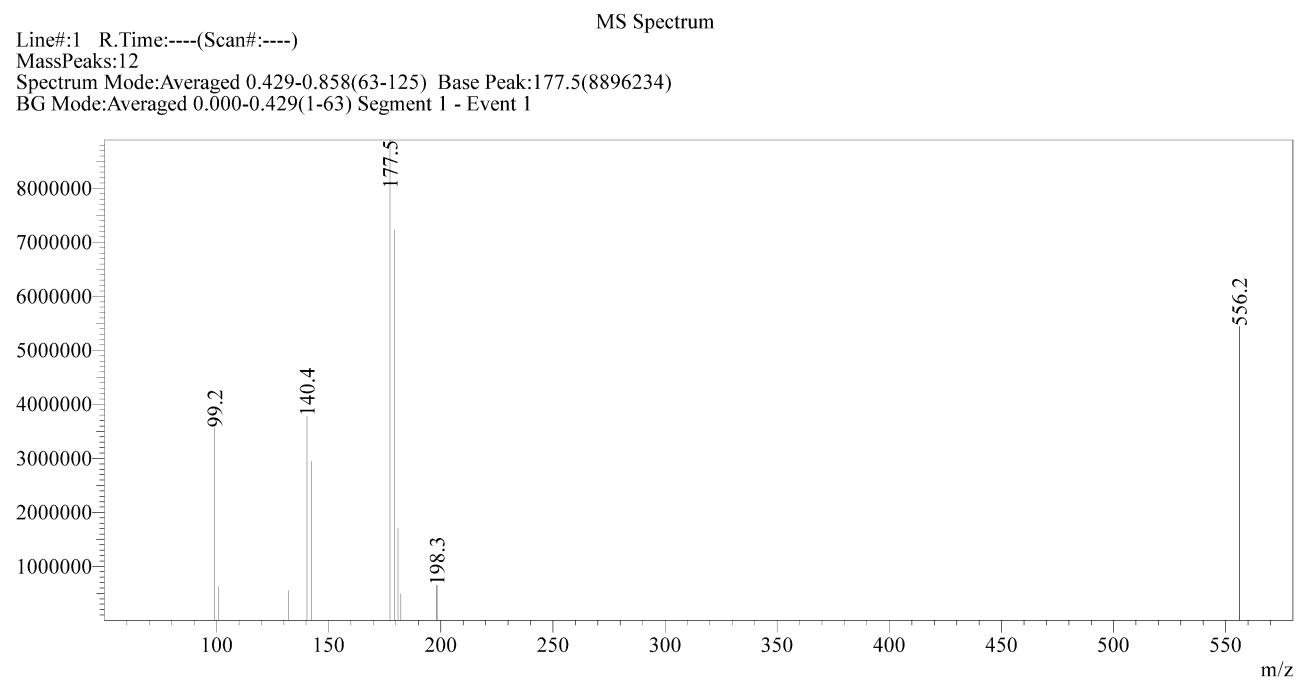


Fig. 40. Mass spectrum of compound 5c

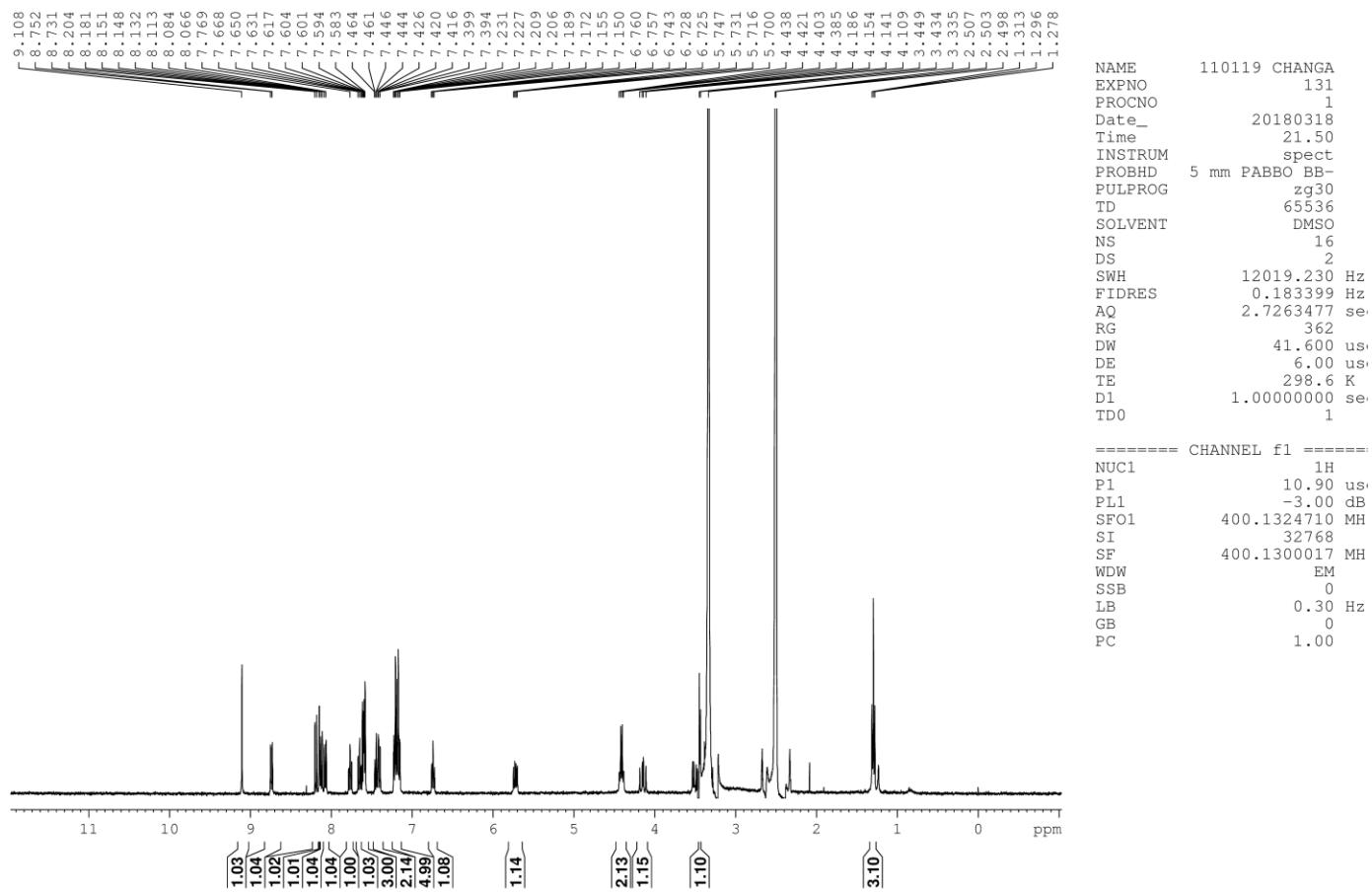


Fig. 41.  $^1\text{H}$  NMR spectrum of compound 5c

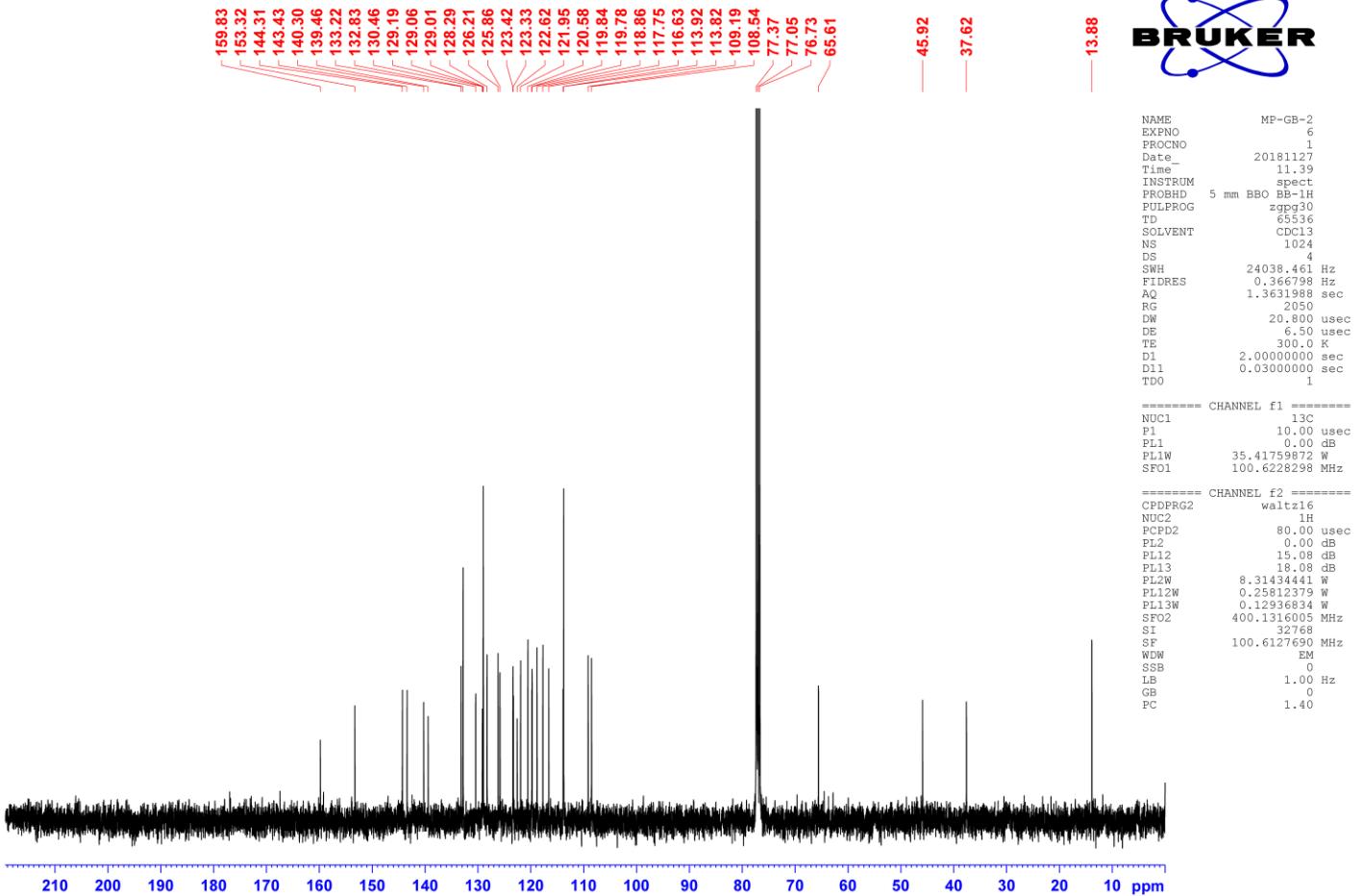


Fig. 42.  $^{13}\text{C}$  NMR spectrum of compound 5c

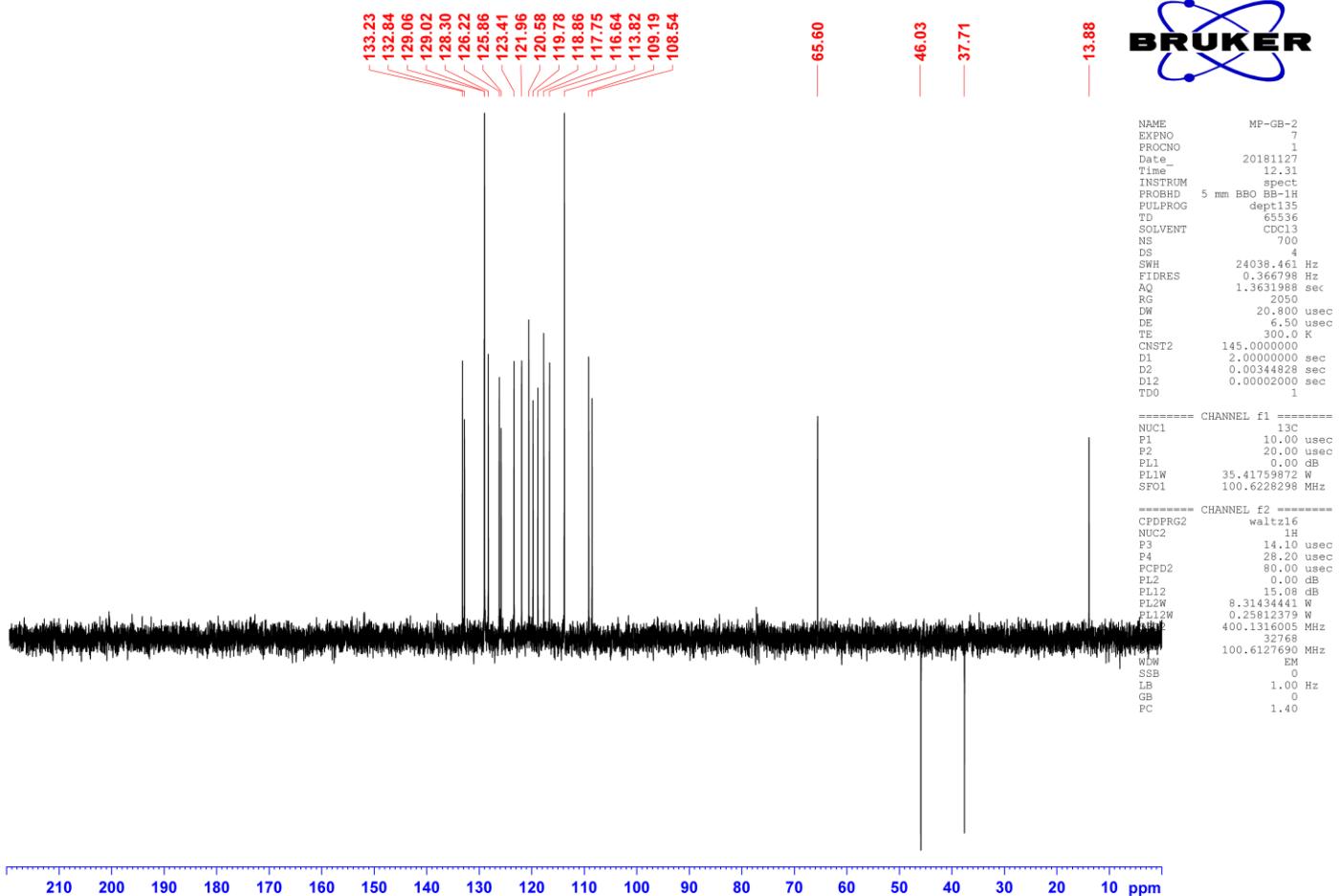


Fig. 43. DEPT-135 spectrum of compound 5c

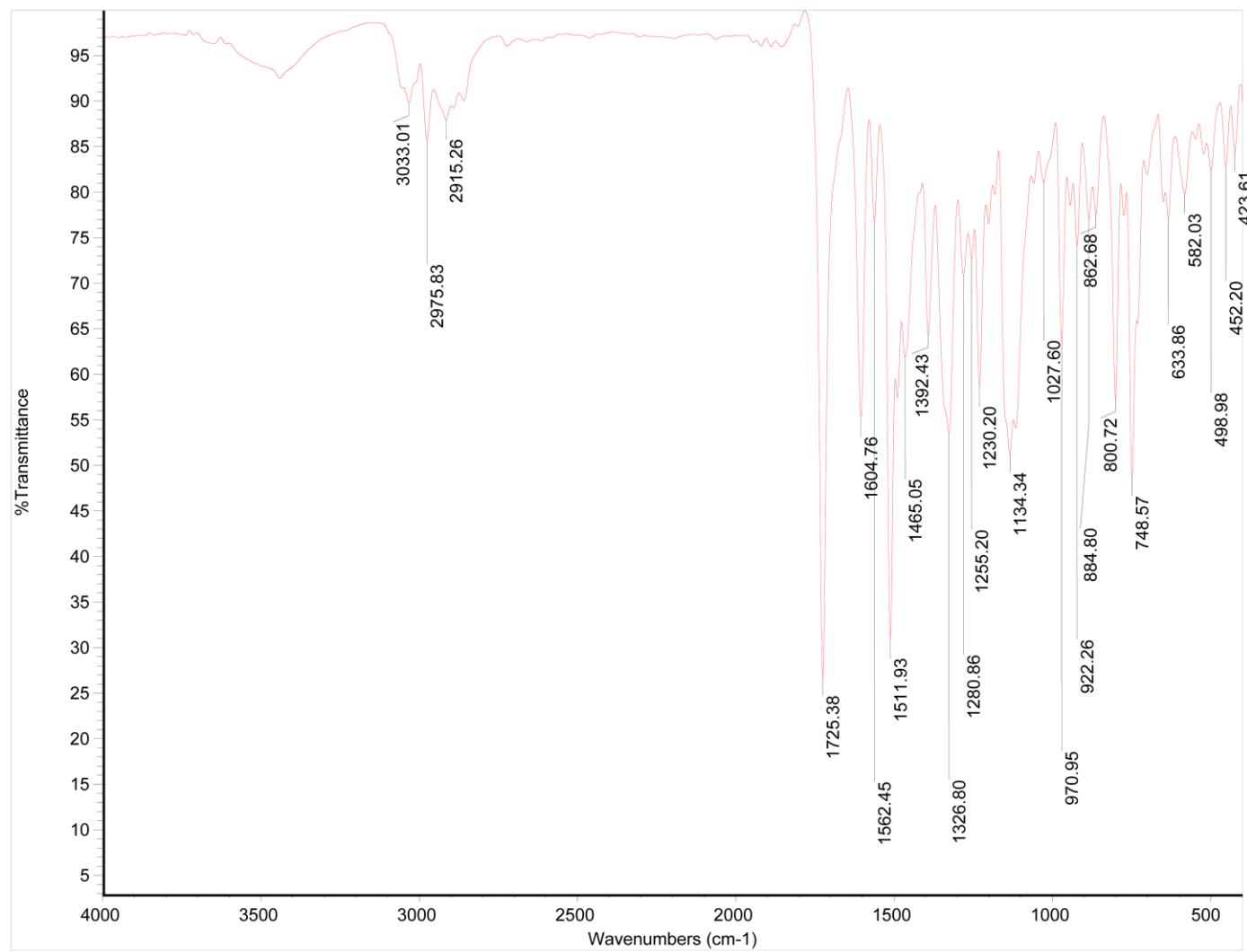


Fig. 44. IR spectrum of compound 6a

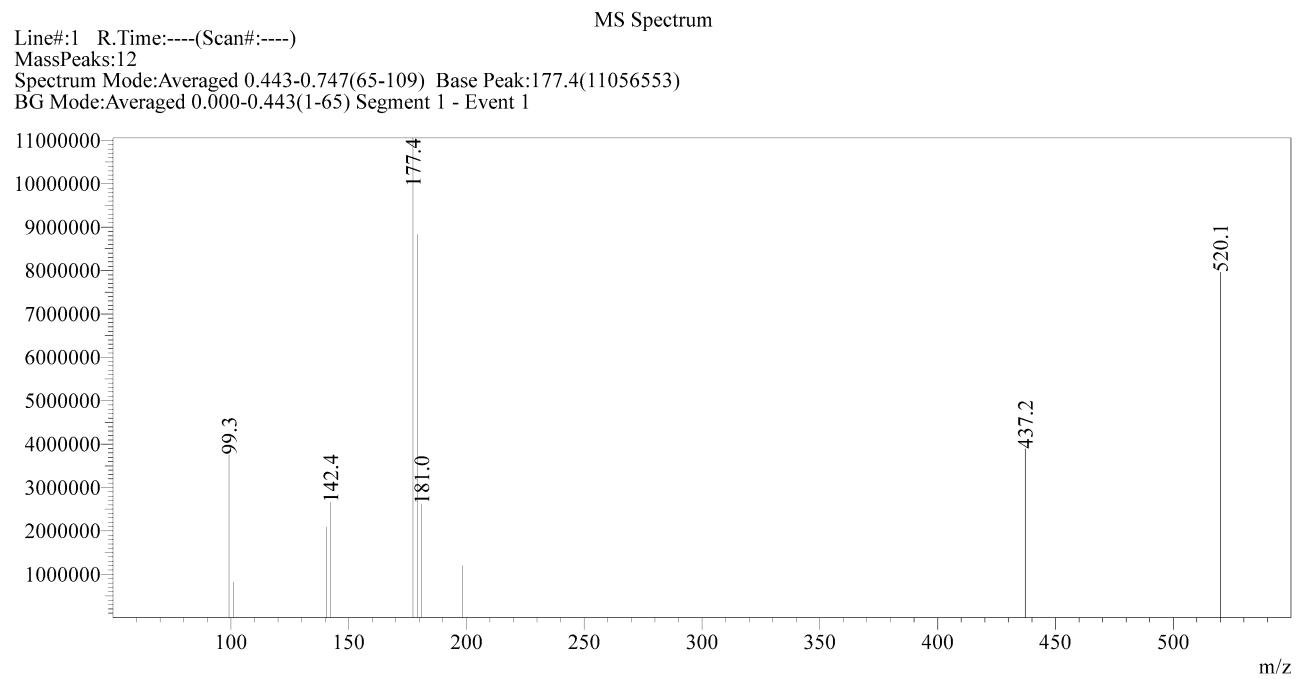


Fig. 45. Mass spectrum of compound 6a

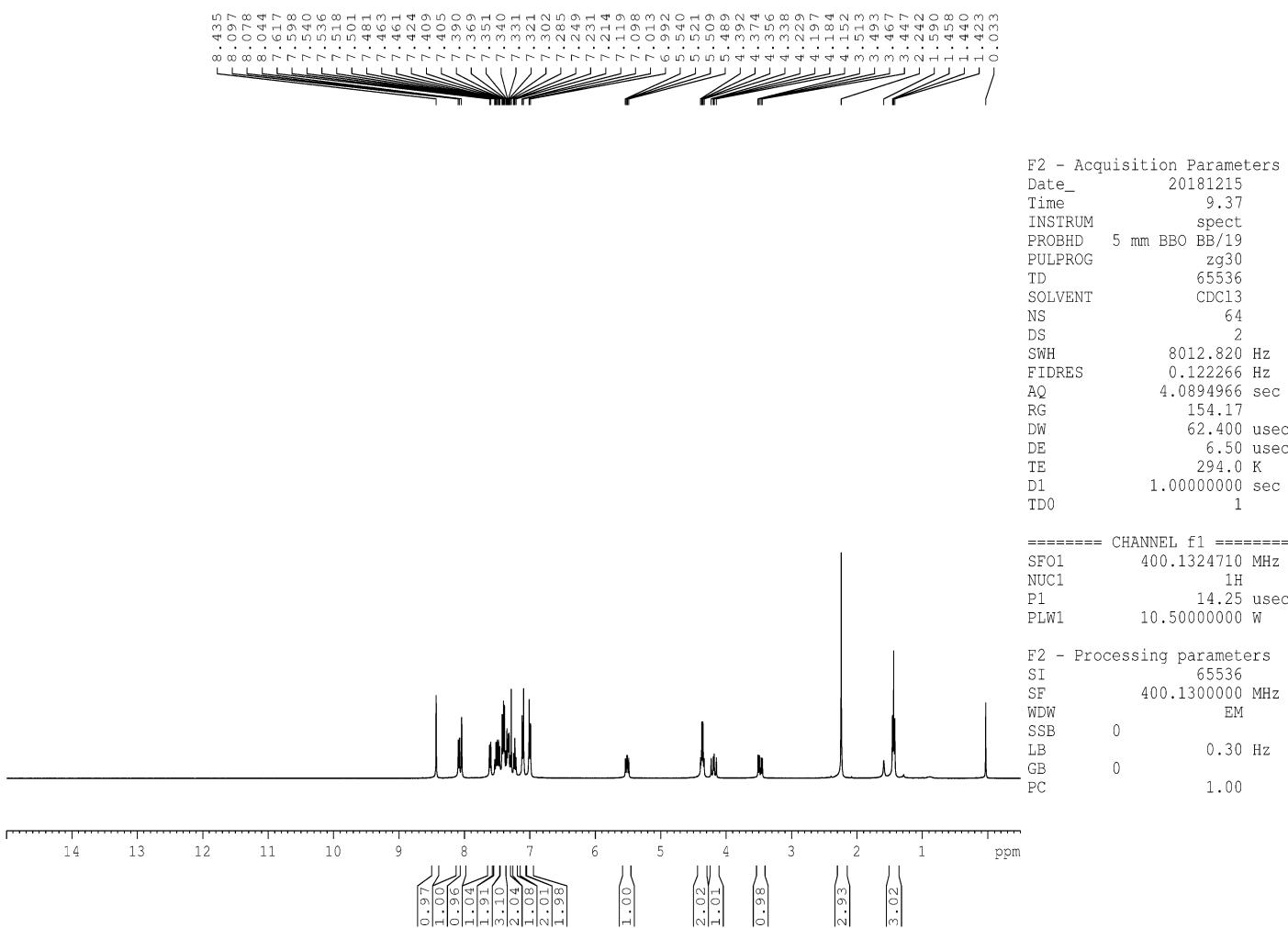


Fig. 46. <sup>1</sup>H NMR spectrum of compound 6a

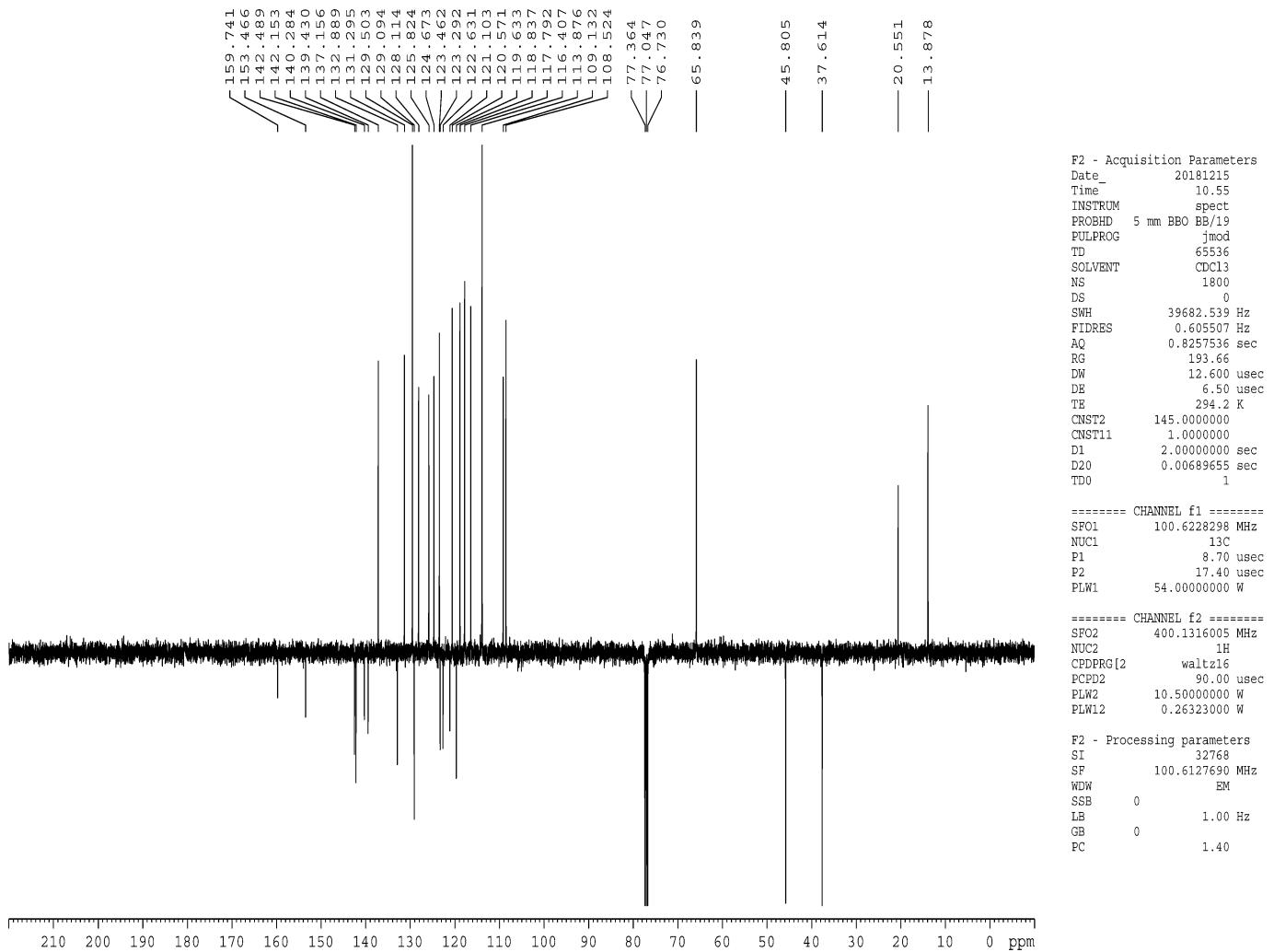


Fig. 47. APT spectrum of compound 6a

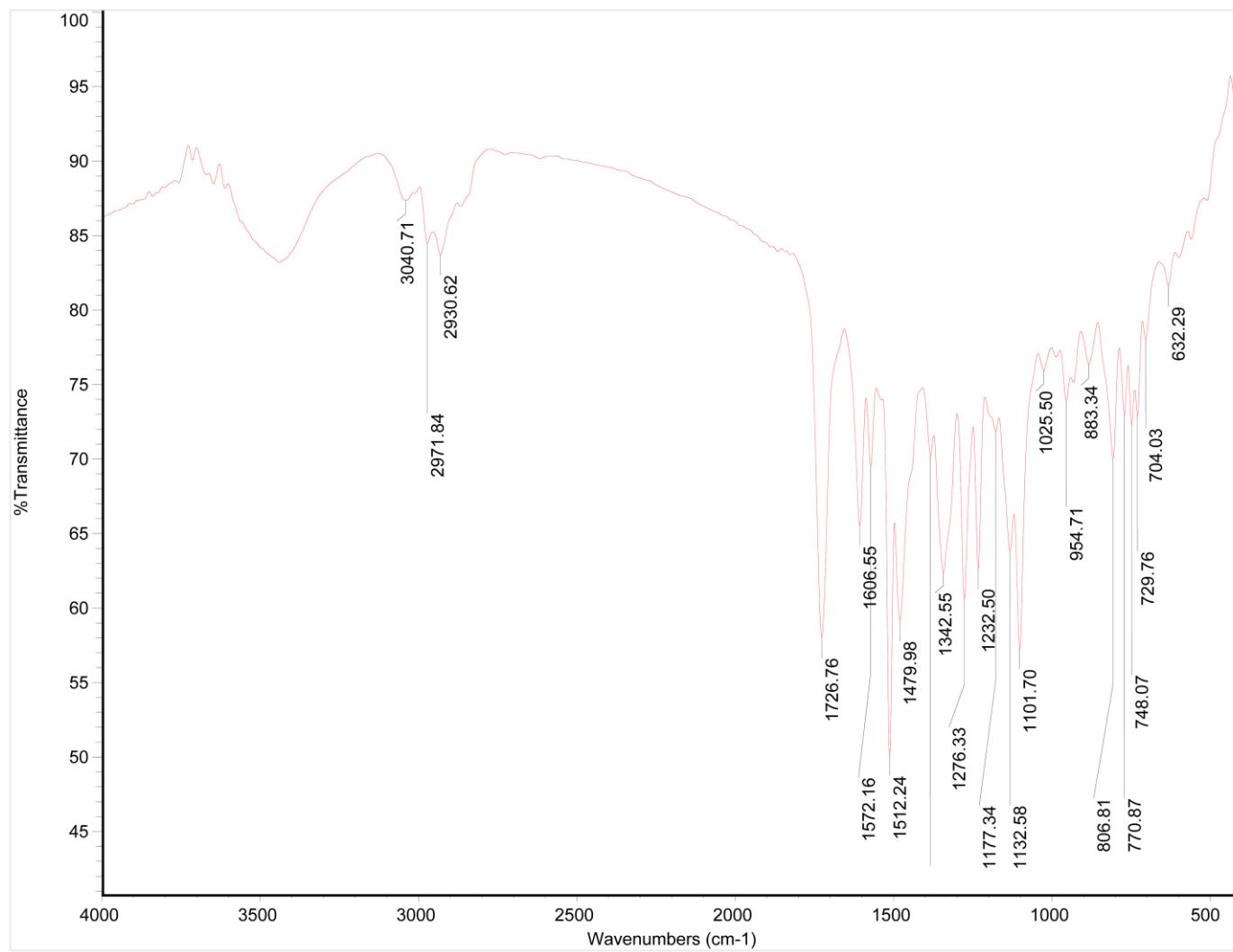


Fig. 48. IR spectrum of compound 6b

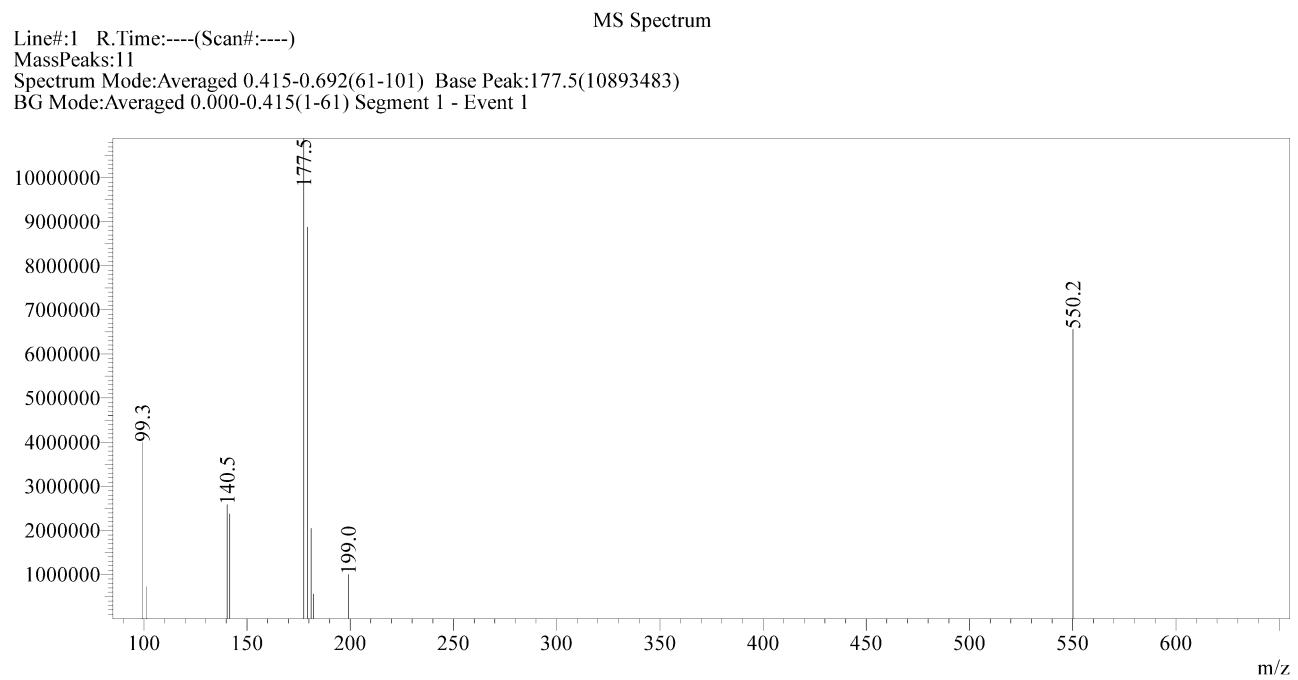


Fig. 49. Mass spectrum of compound 6b

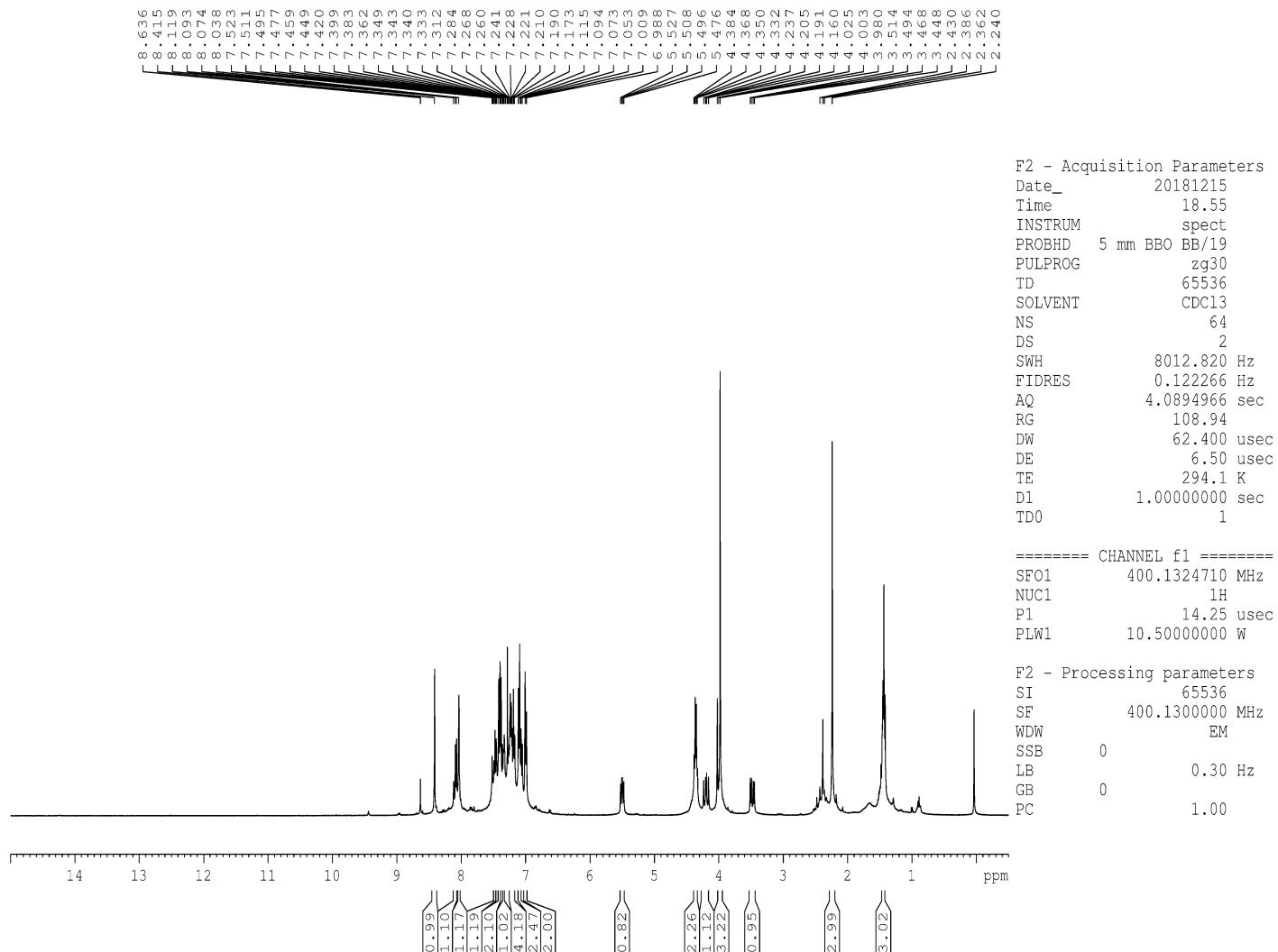


Fig. 50.  $^1\text{H}$  NMR spectrum of compound 6b

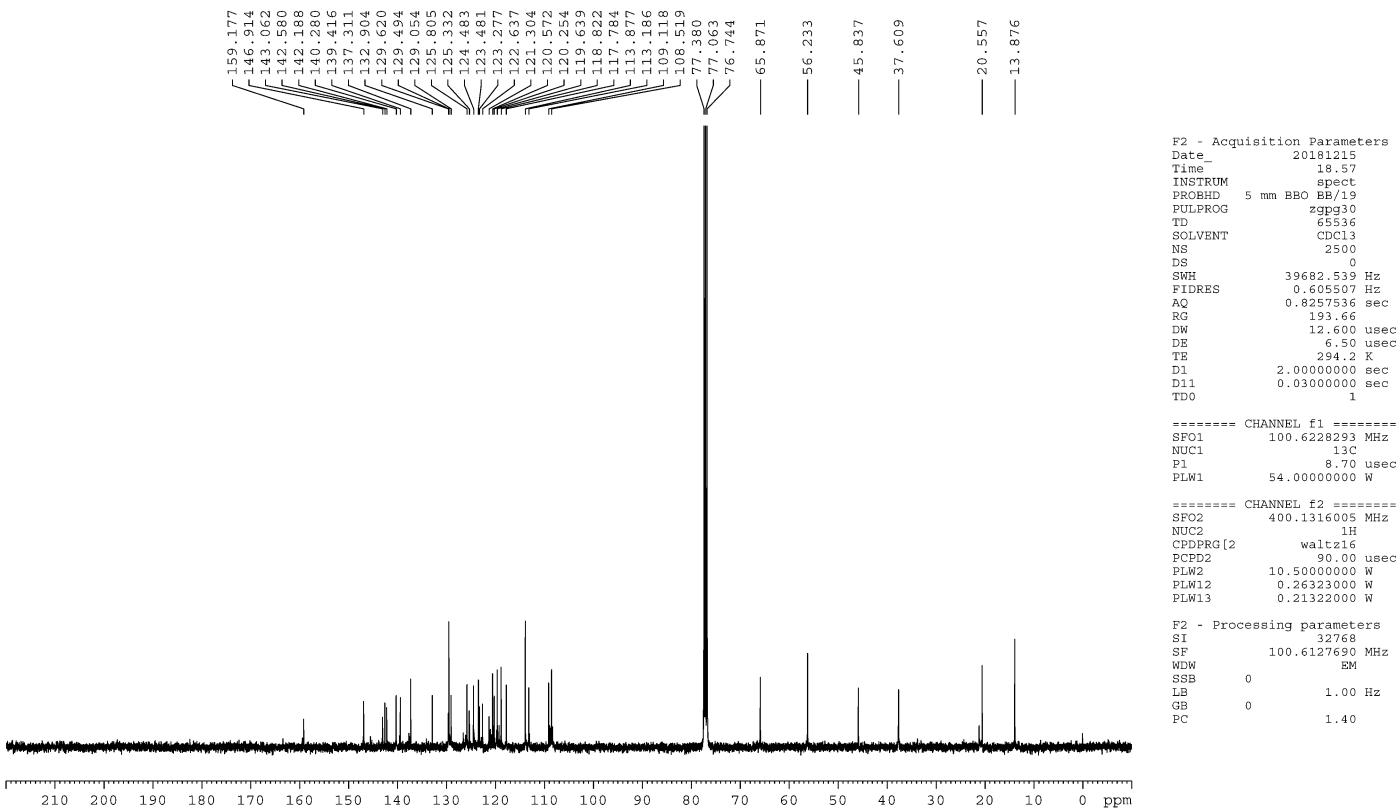


Fig. 51. <sup>13</sup>C NMR spectrum of compound 6b

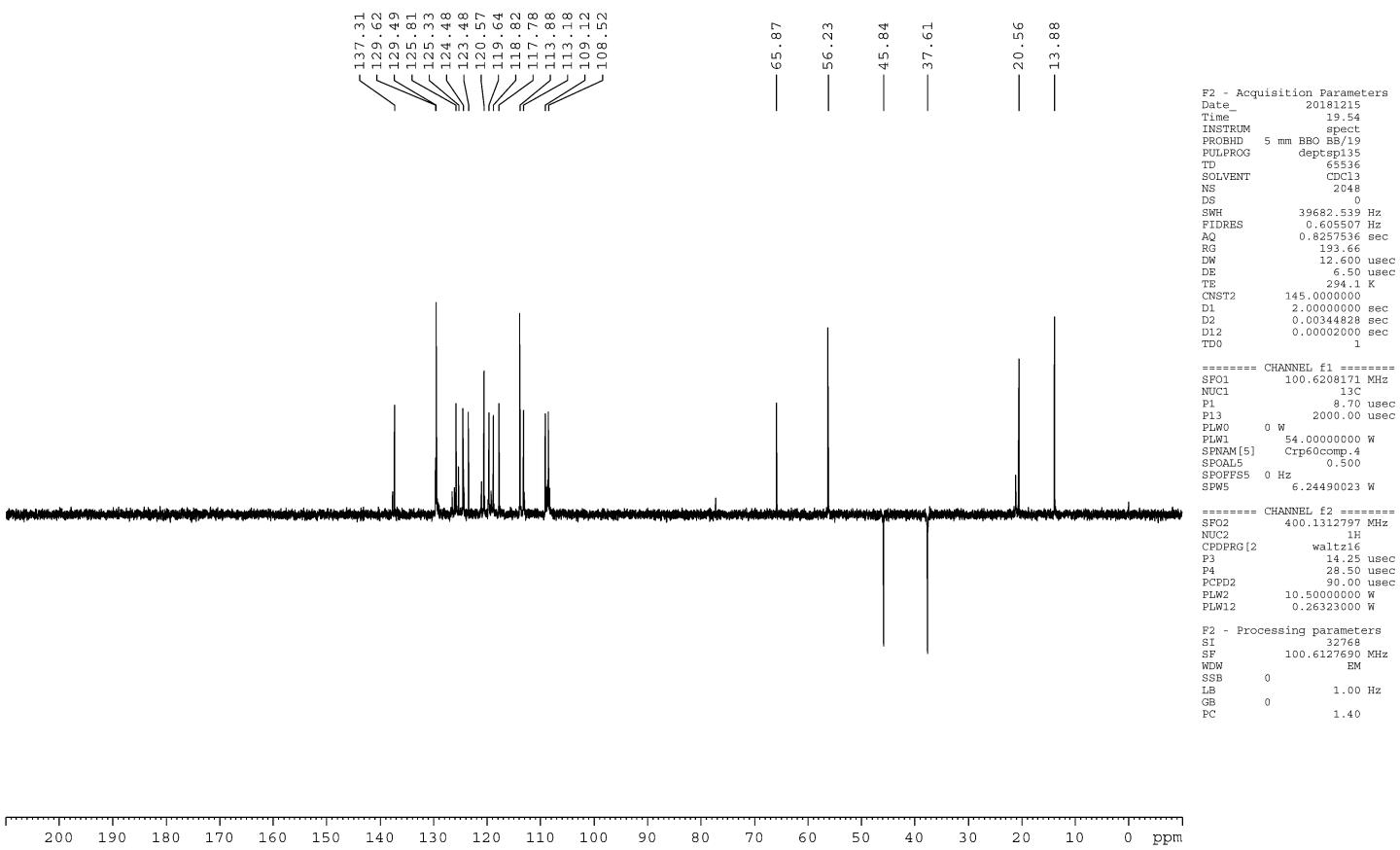


Fig. 52. DEPT-135 spectrum of compound 6b

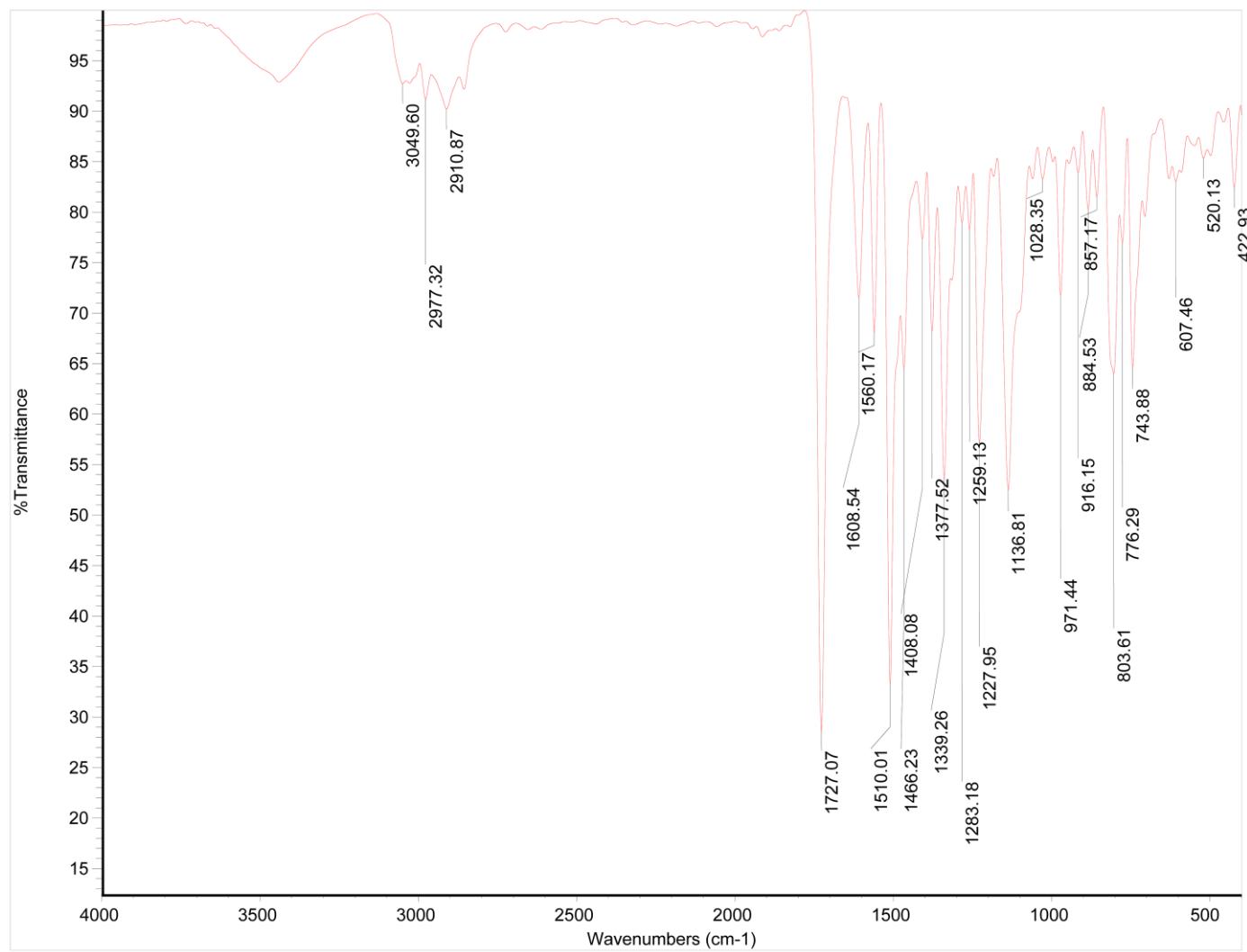


Fig. 53. IR spectrum of compound 6c

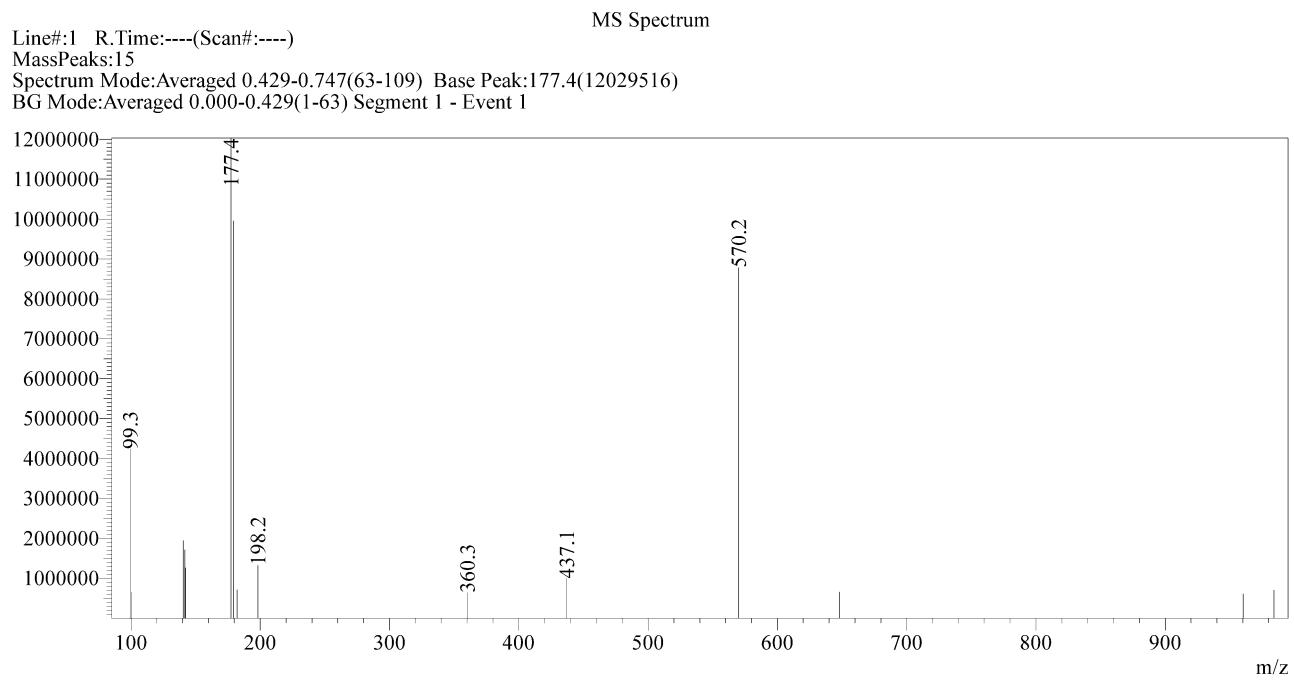


Fig. 54. Mass spectrum of compound 6c

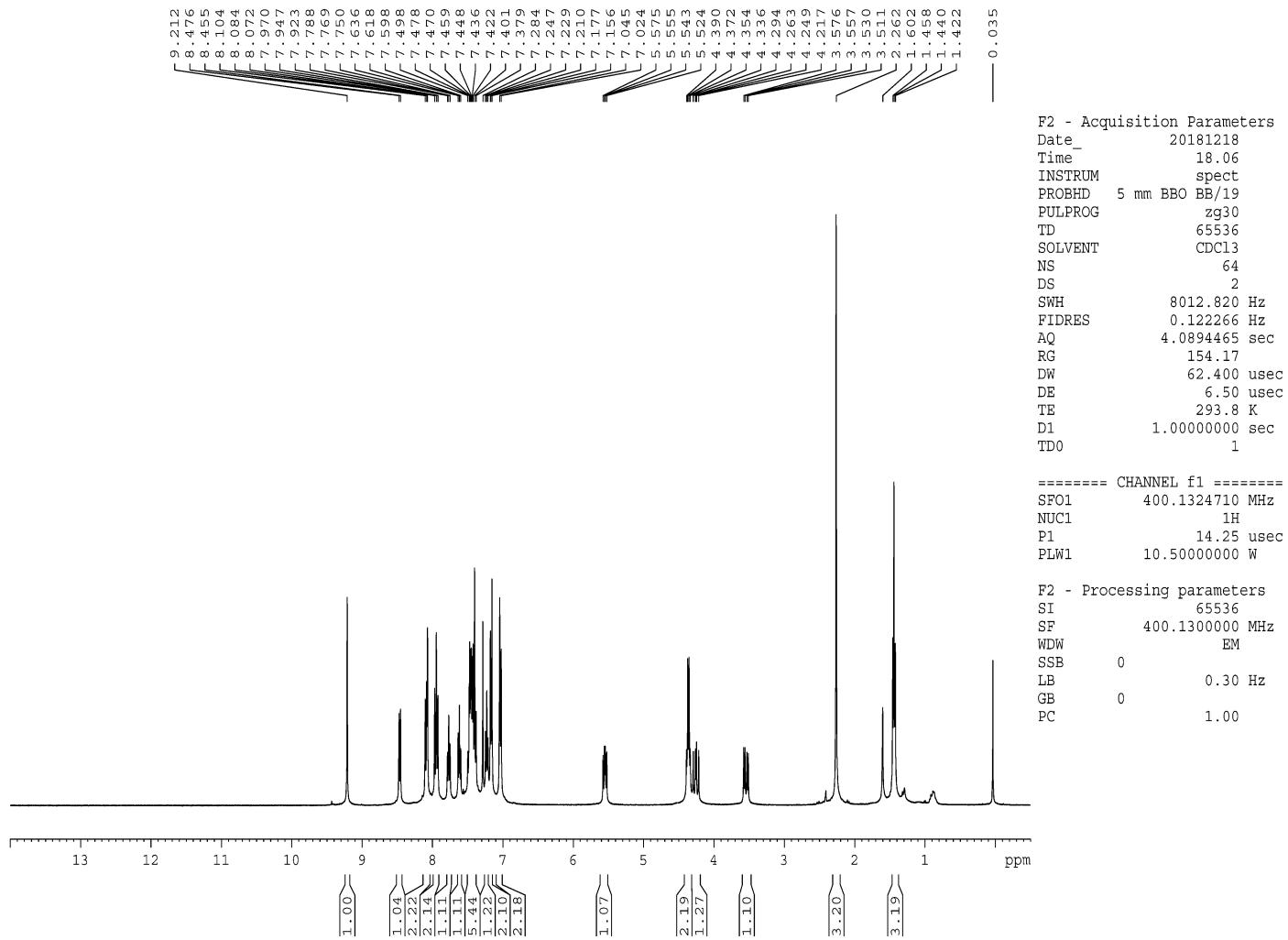


Fig. 55. <sup>1</sup>H NMR spectrum of compound 6c

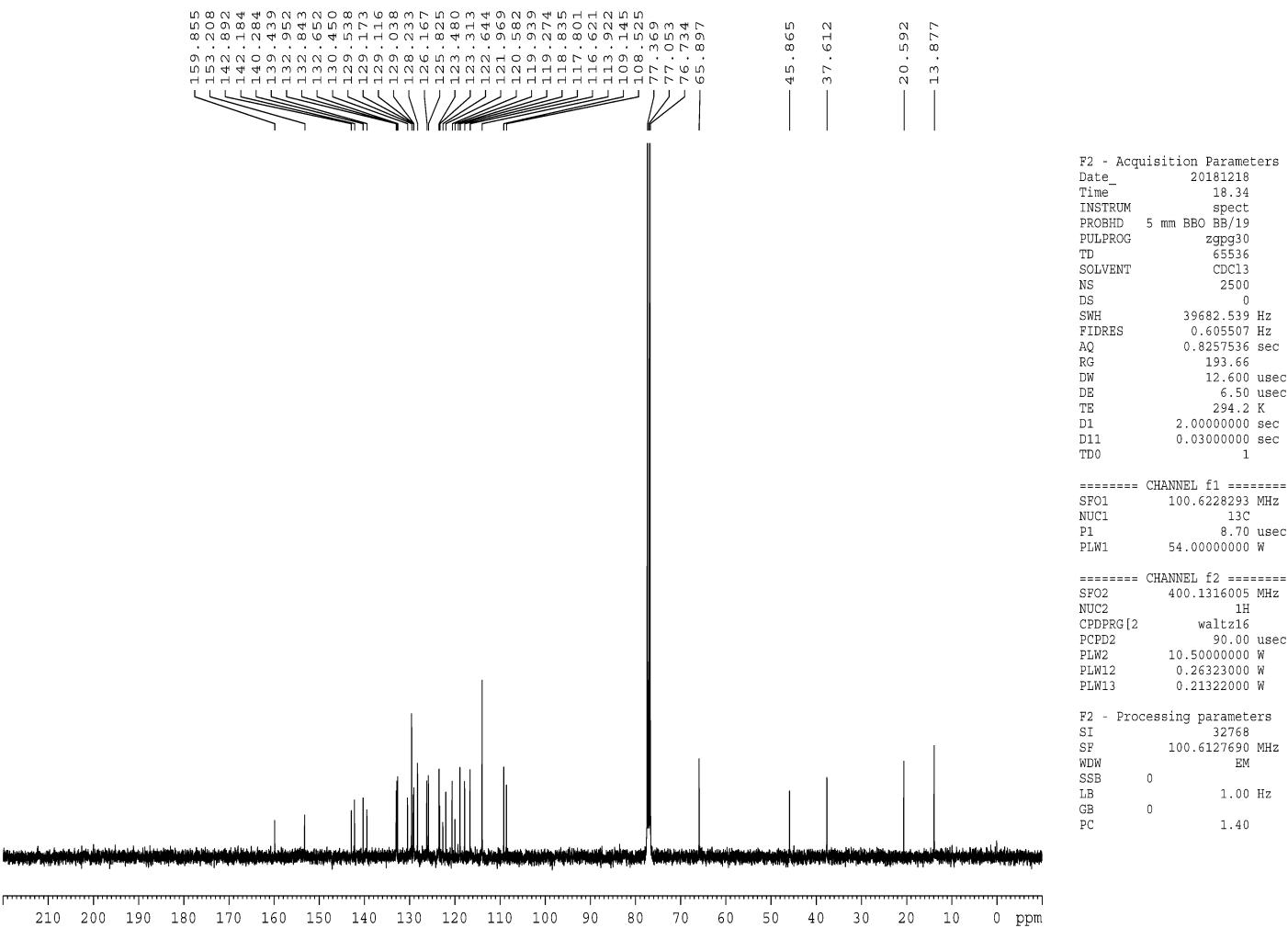


Fig. 56. <sup>13</sup>C NMR spectrum of compound 6c

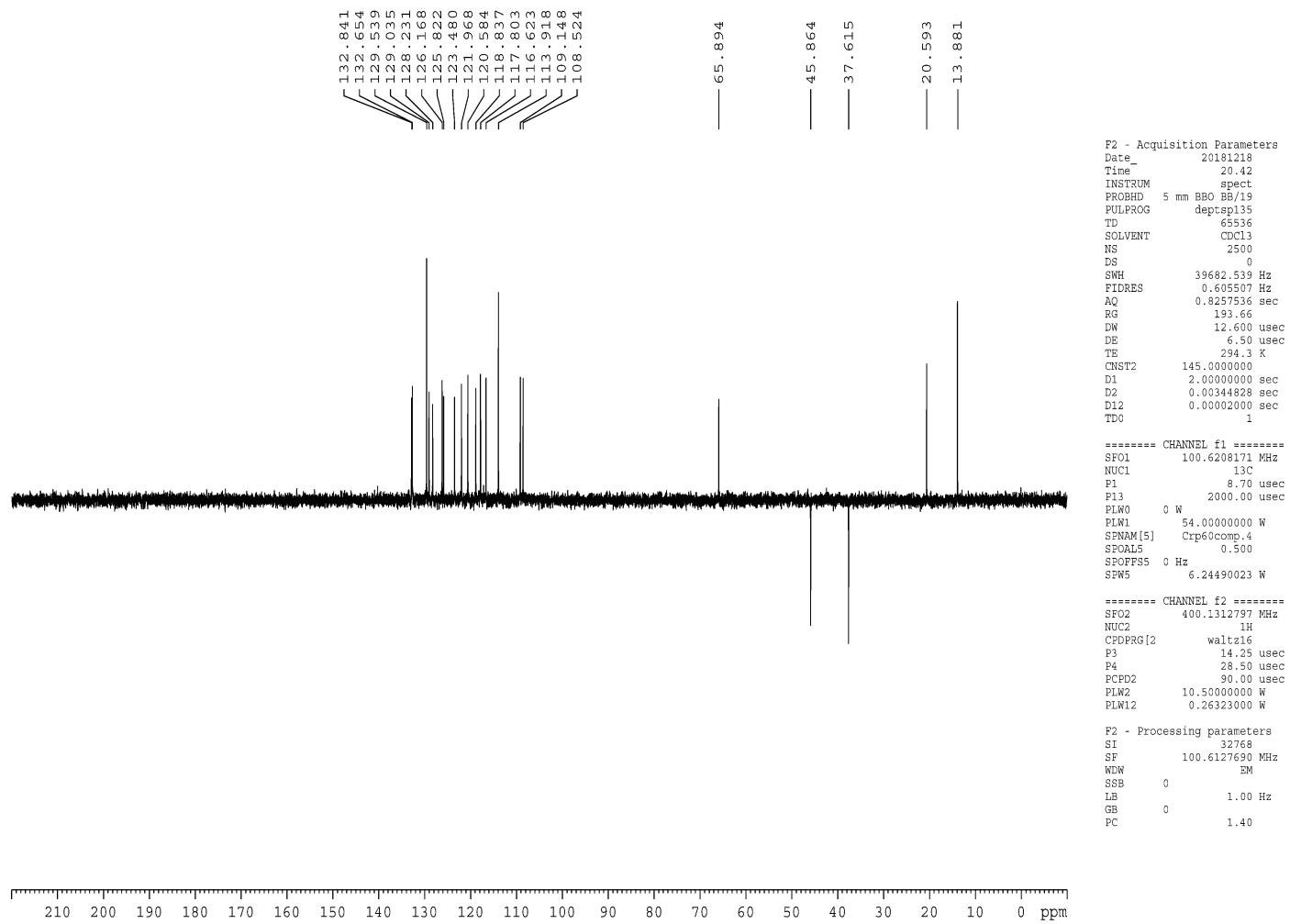


Fig. 57. DEPT-135 spectrum of compound 6c

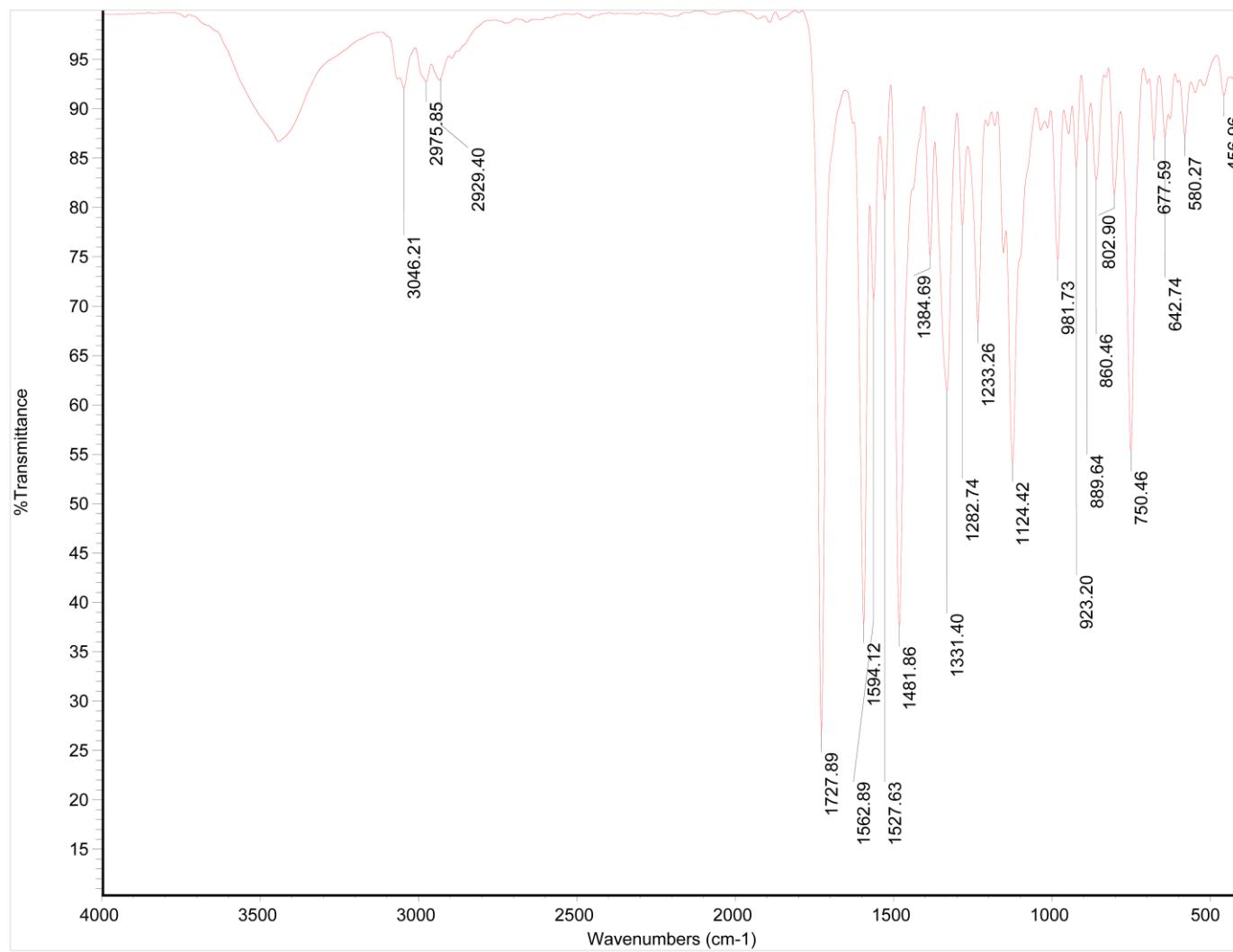


Fig. 58. IR spectrum of compound 7a

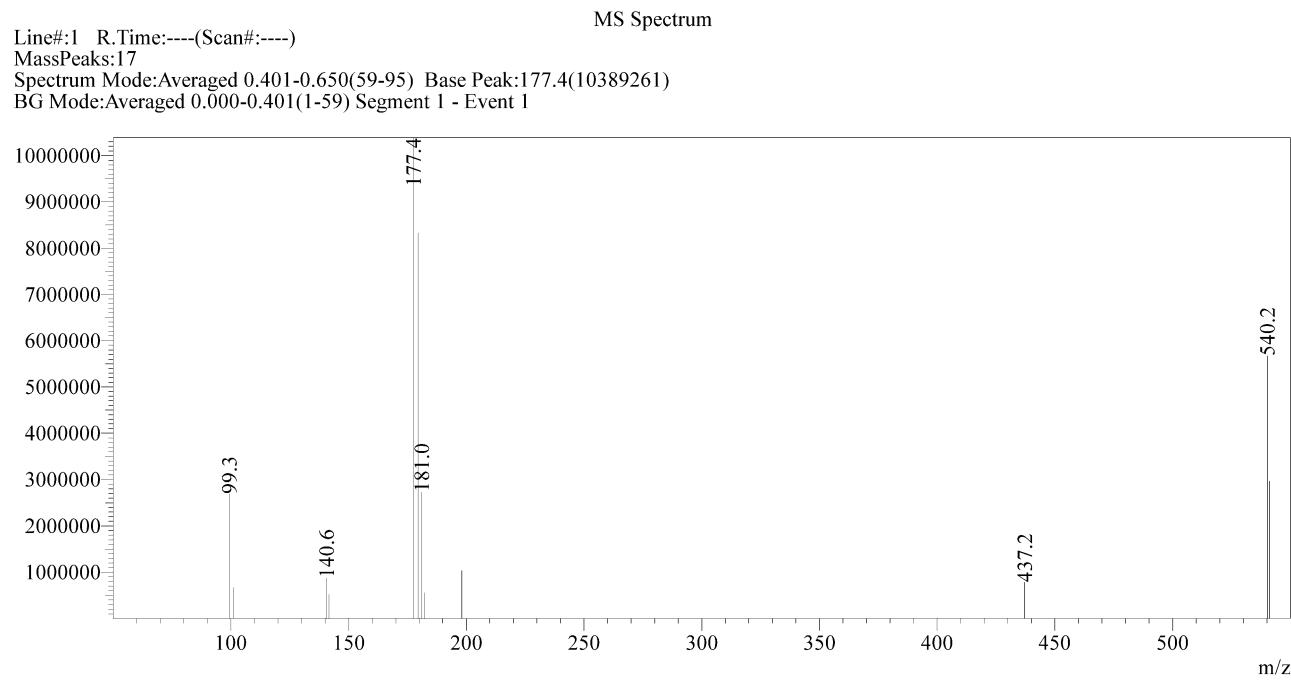


Fig. 59. Mass spectrum of compound 7a

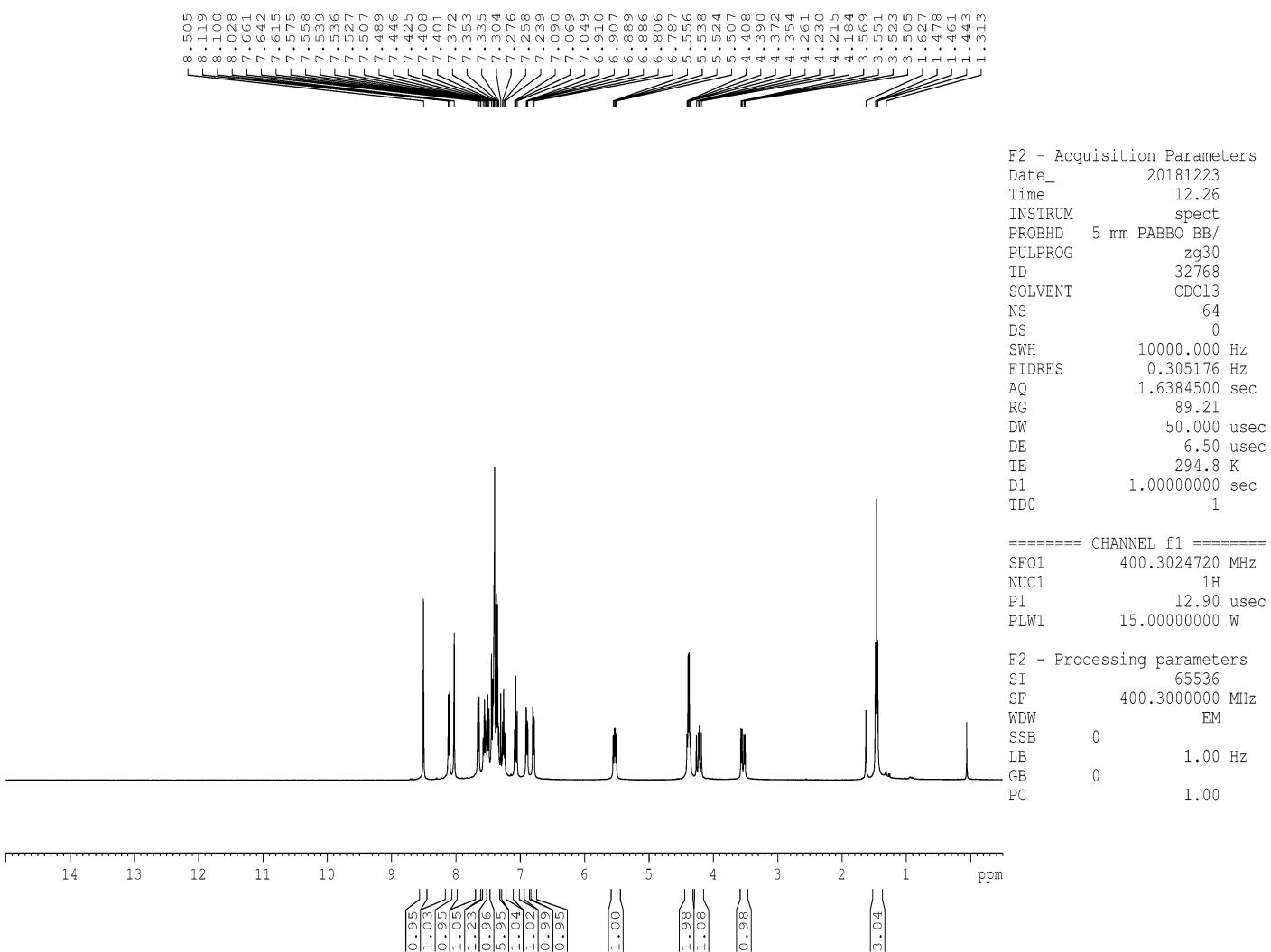


Fig. 60.  $^1\text{H}$  NMR spectrum of compound 7a

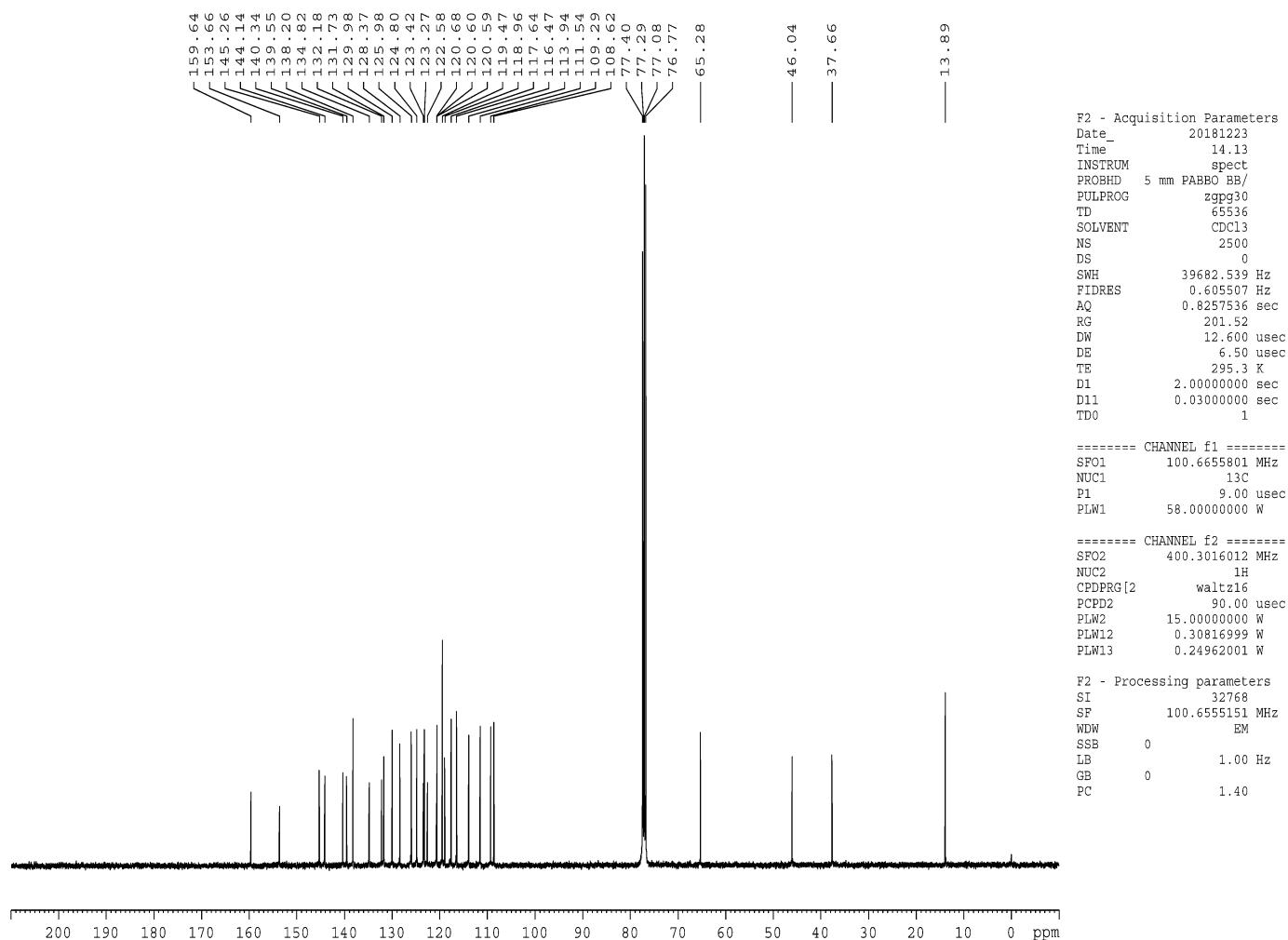


Fig. 61. <sup>13</sup>C NMR spectrum of compound 7a

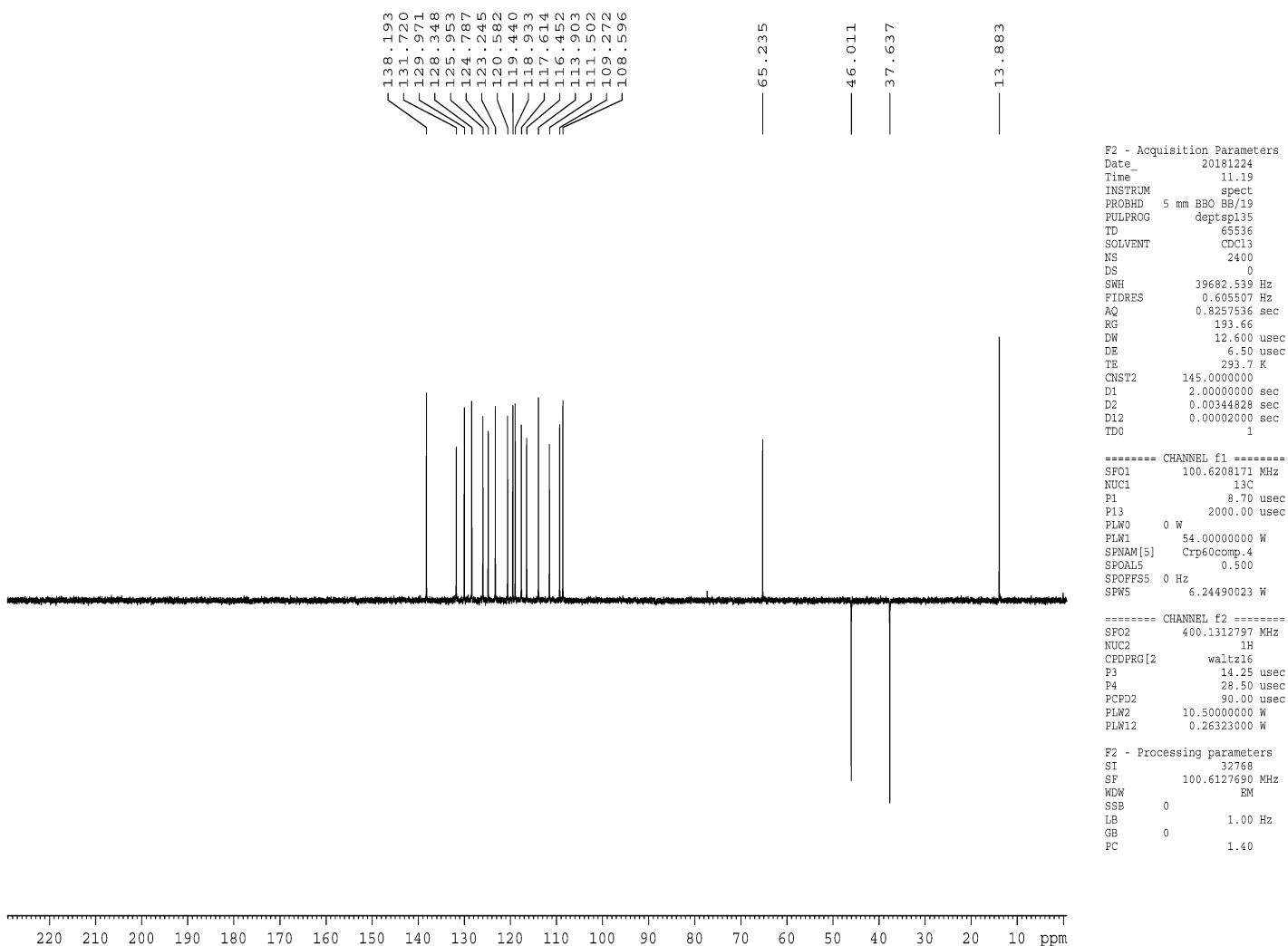


Fig. 62. DEPT-135 spectrum of compound 7a

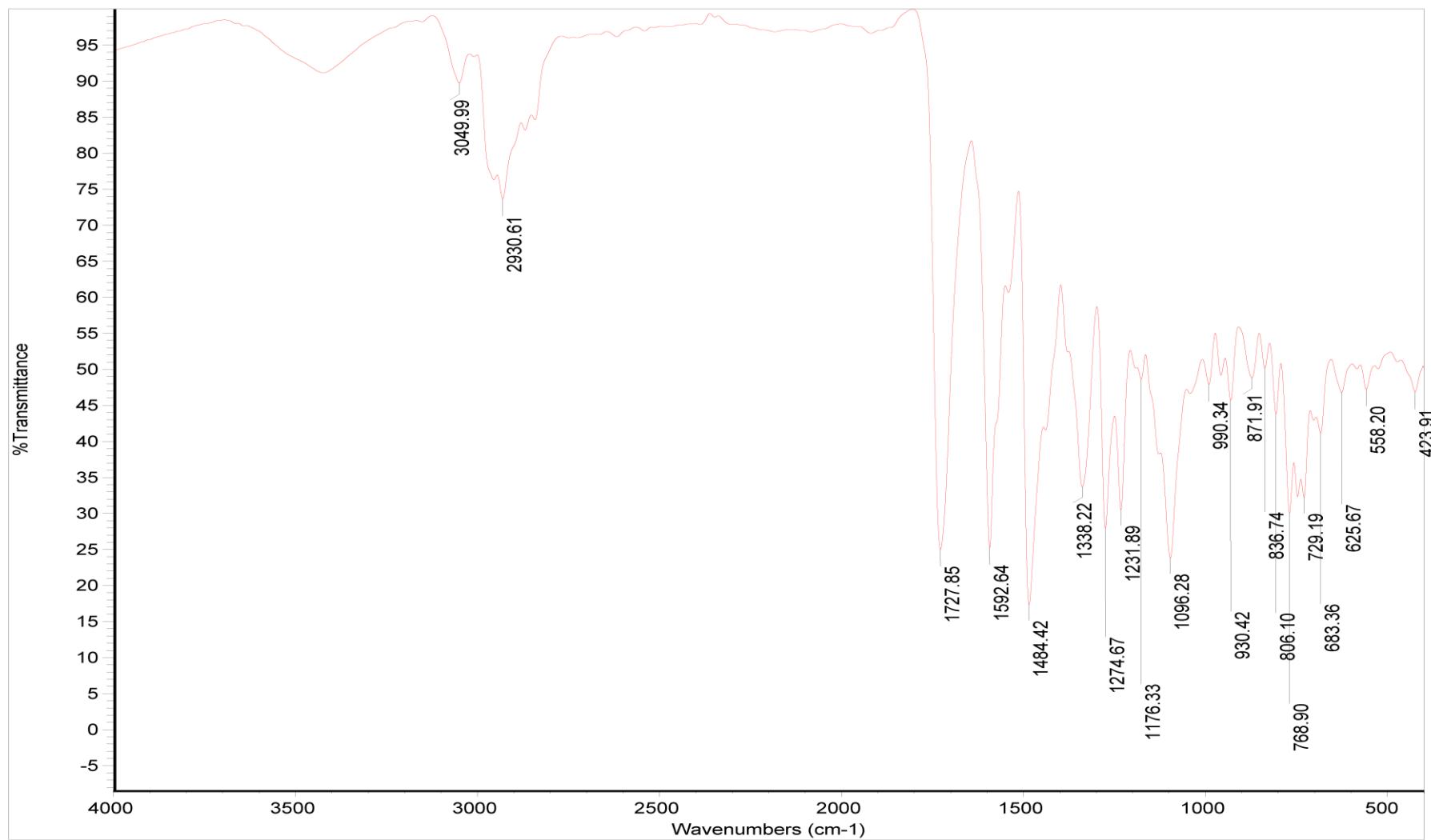


Fig. 63. IR spectrum of compound 7b

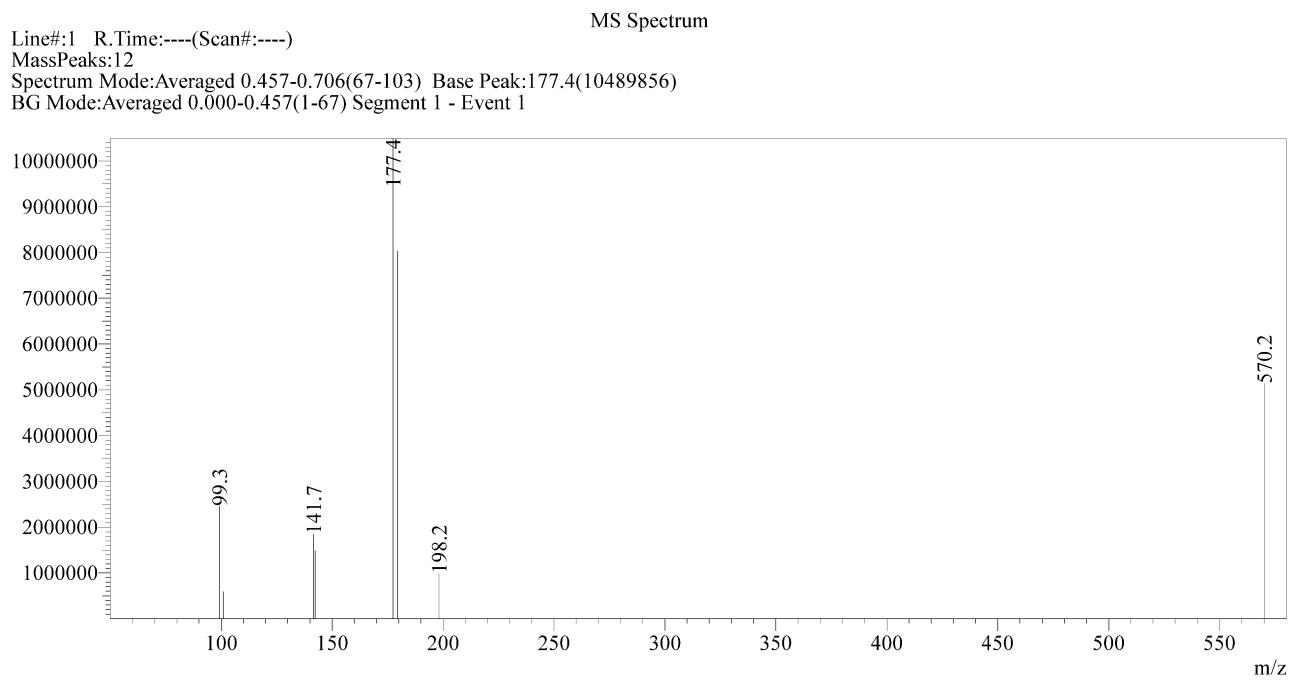


Fig. 64. Mass spectrum of compound 7b

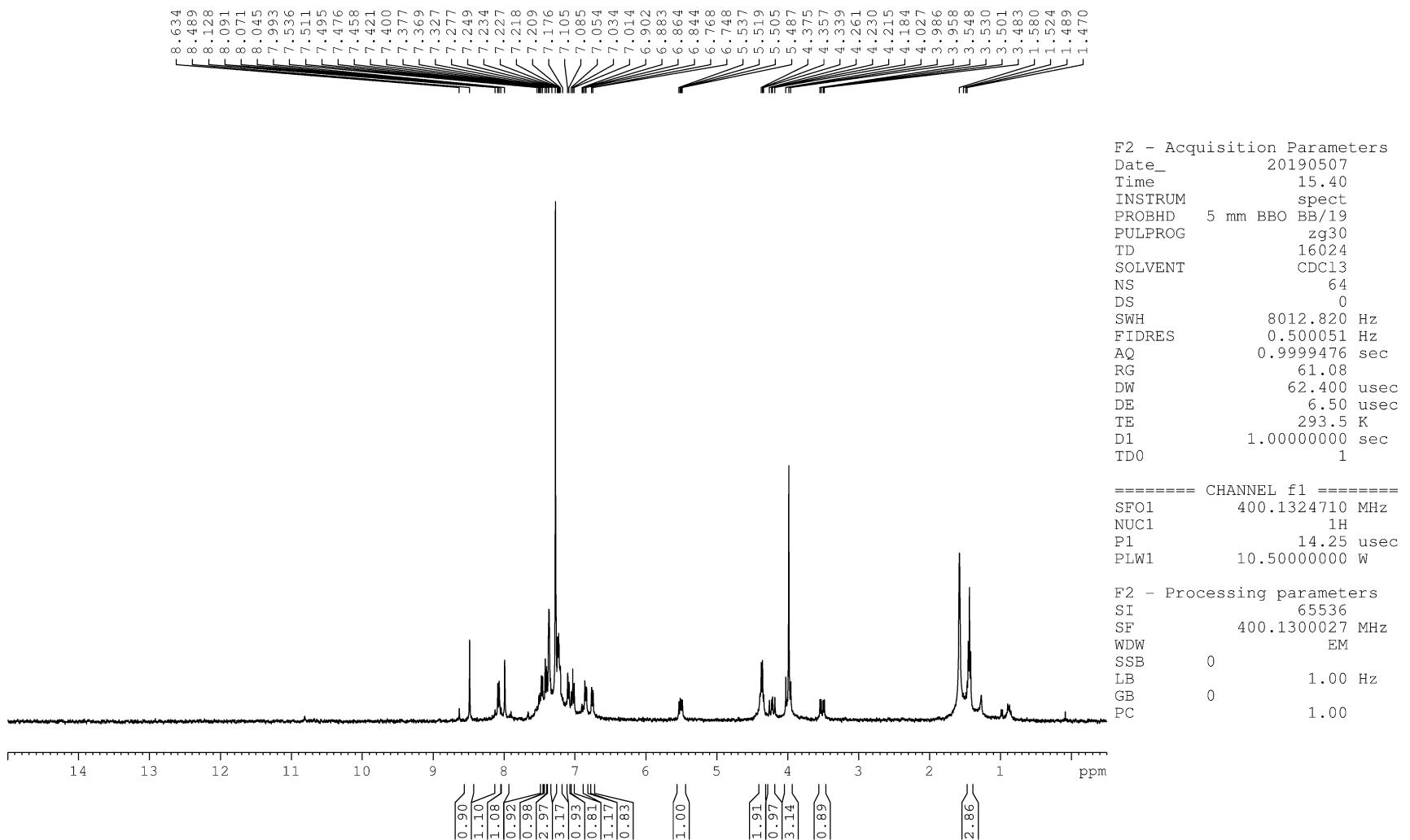


Fig. 65.  $^1\text{H}$  NMR spectrum of compound 7b

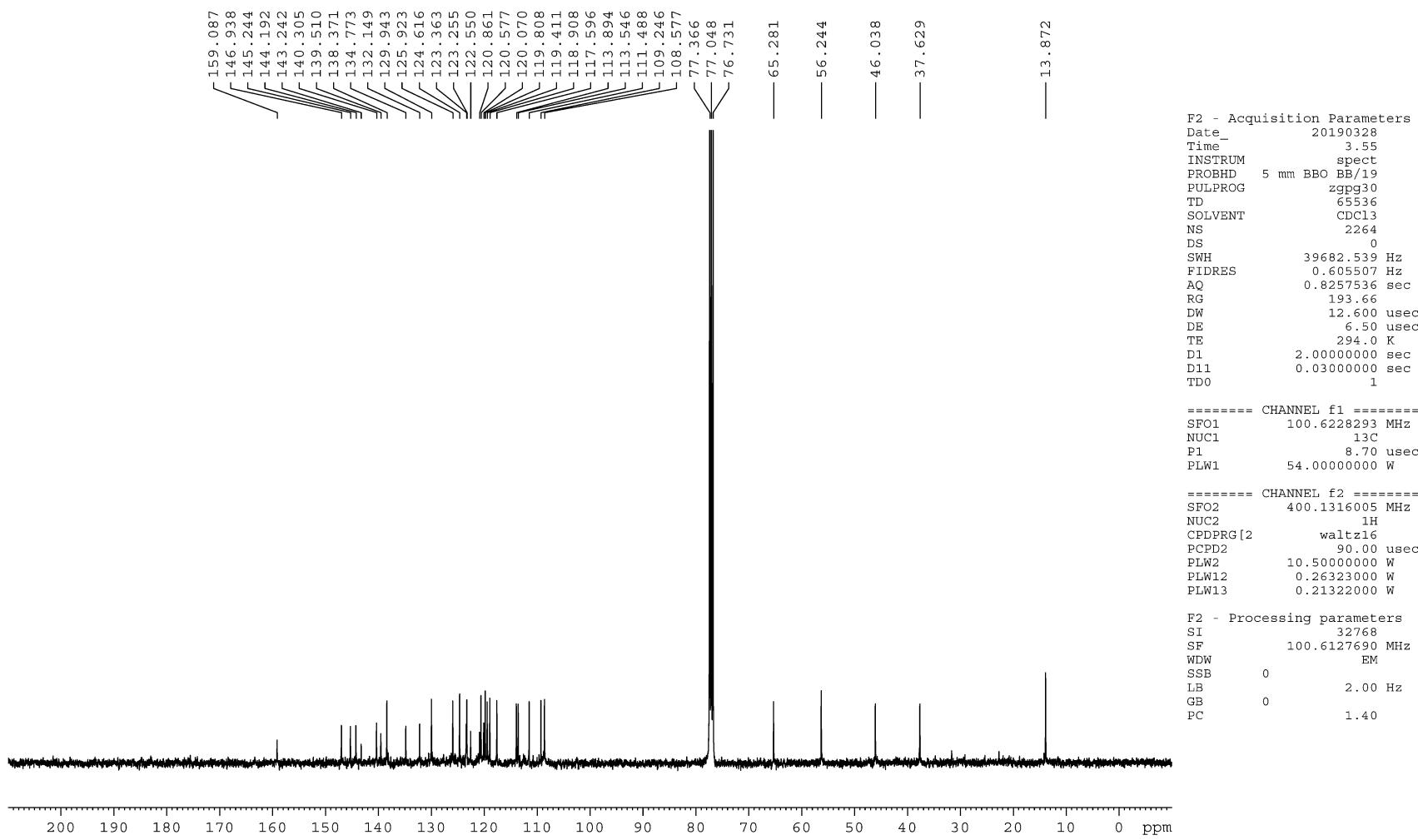


Fig. 66. <sup>13</sup>C NMR spectrum of compound 7b

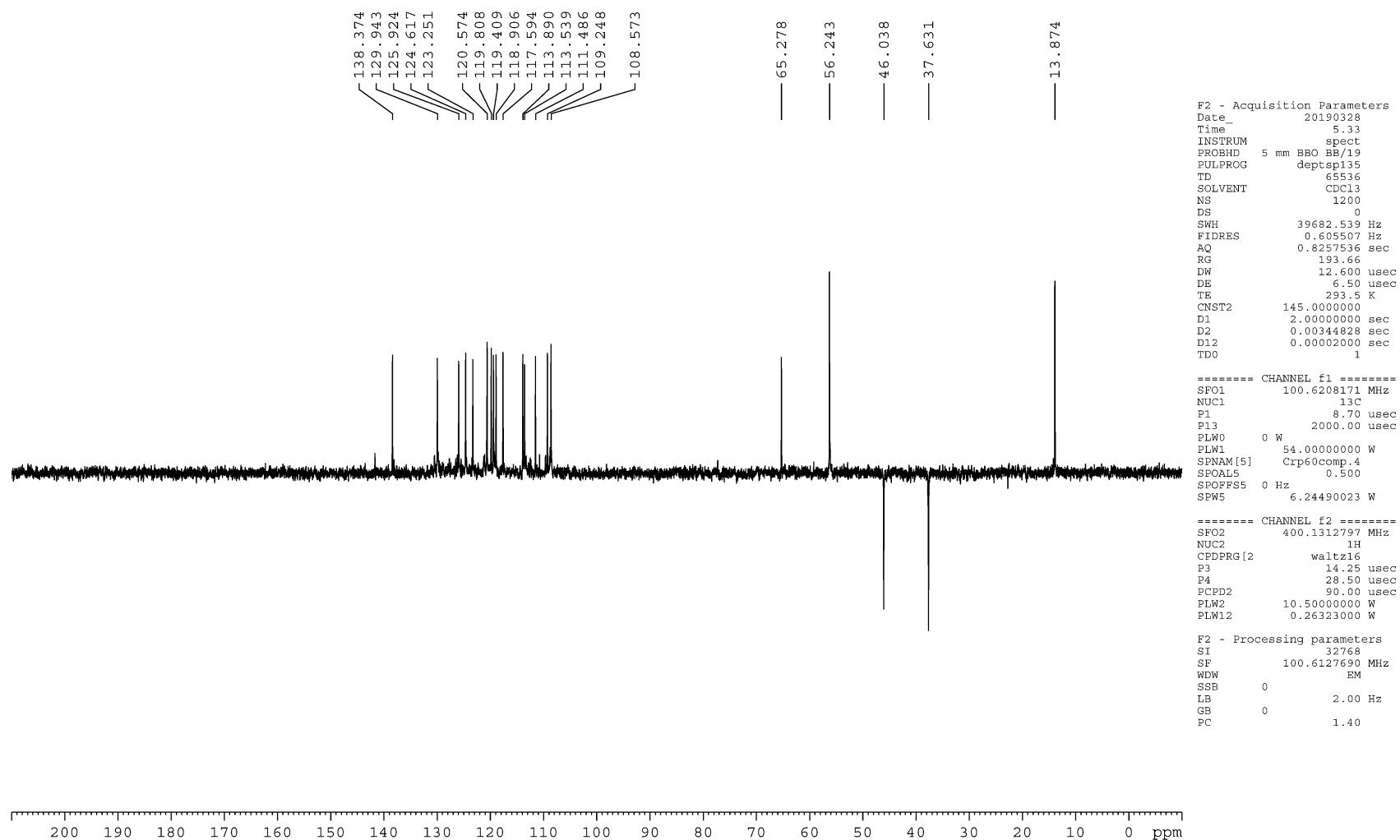


Fig. 67. DEPT-135 spectrum of compound 7b

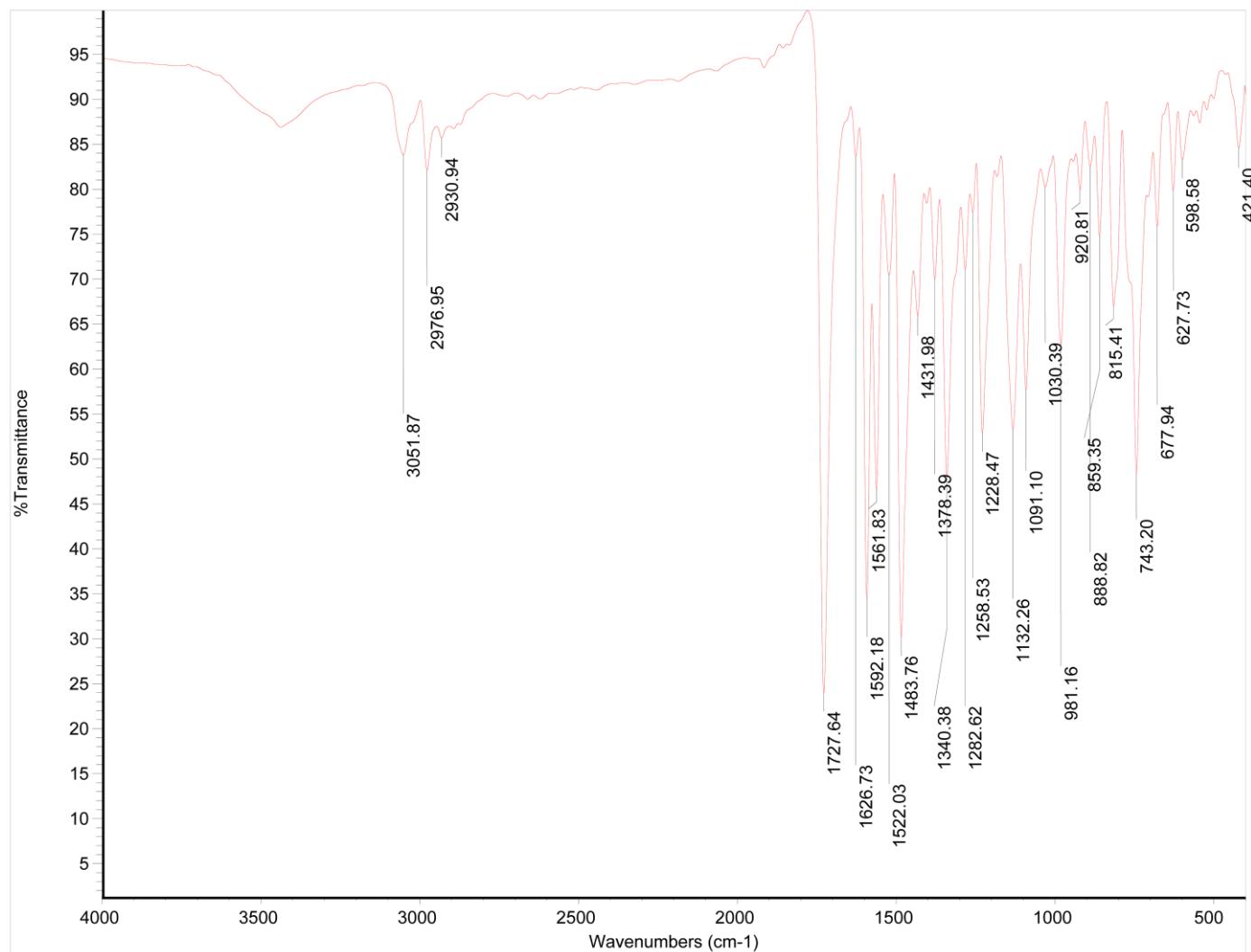


Fig. 68. IR spectrum of compound 7c

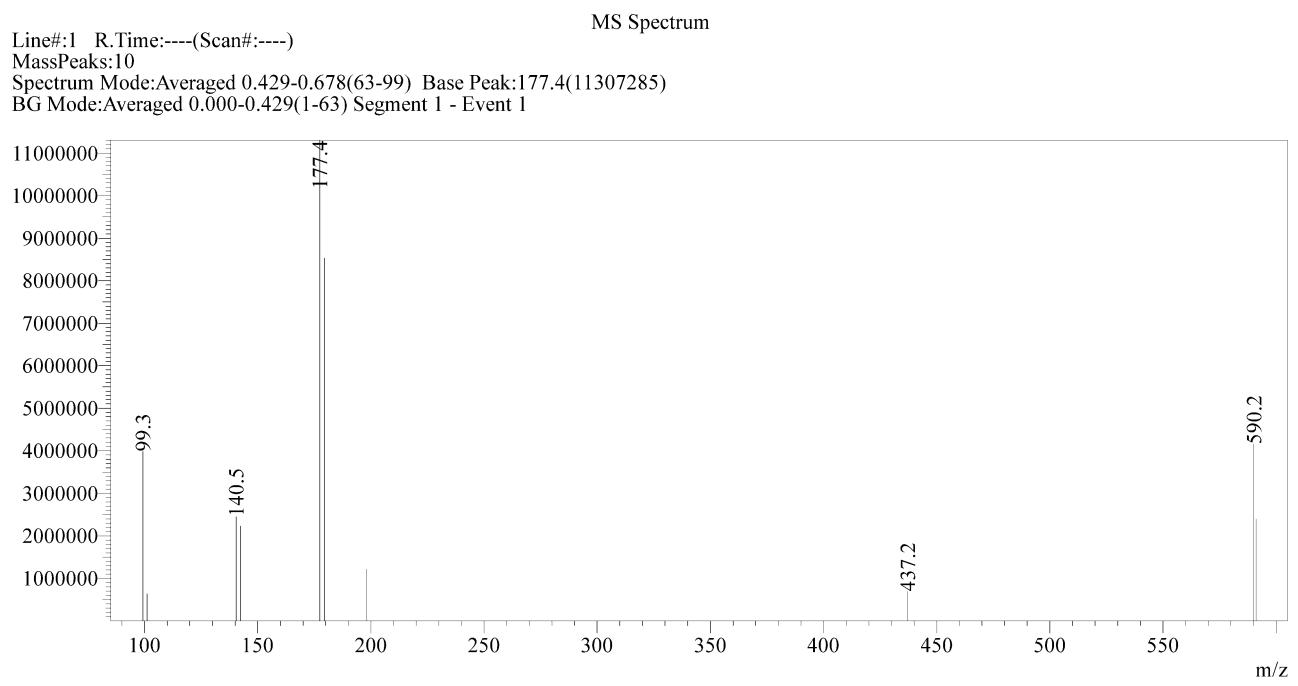


Fig. 69. Mass spectrum of compound 7c

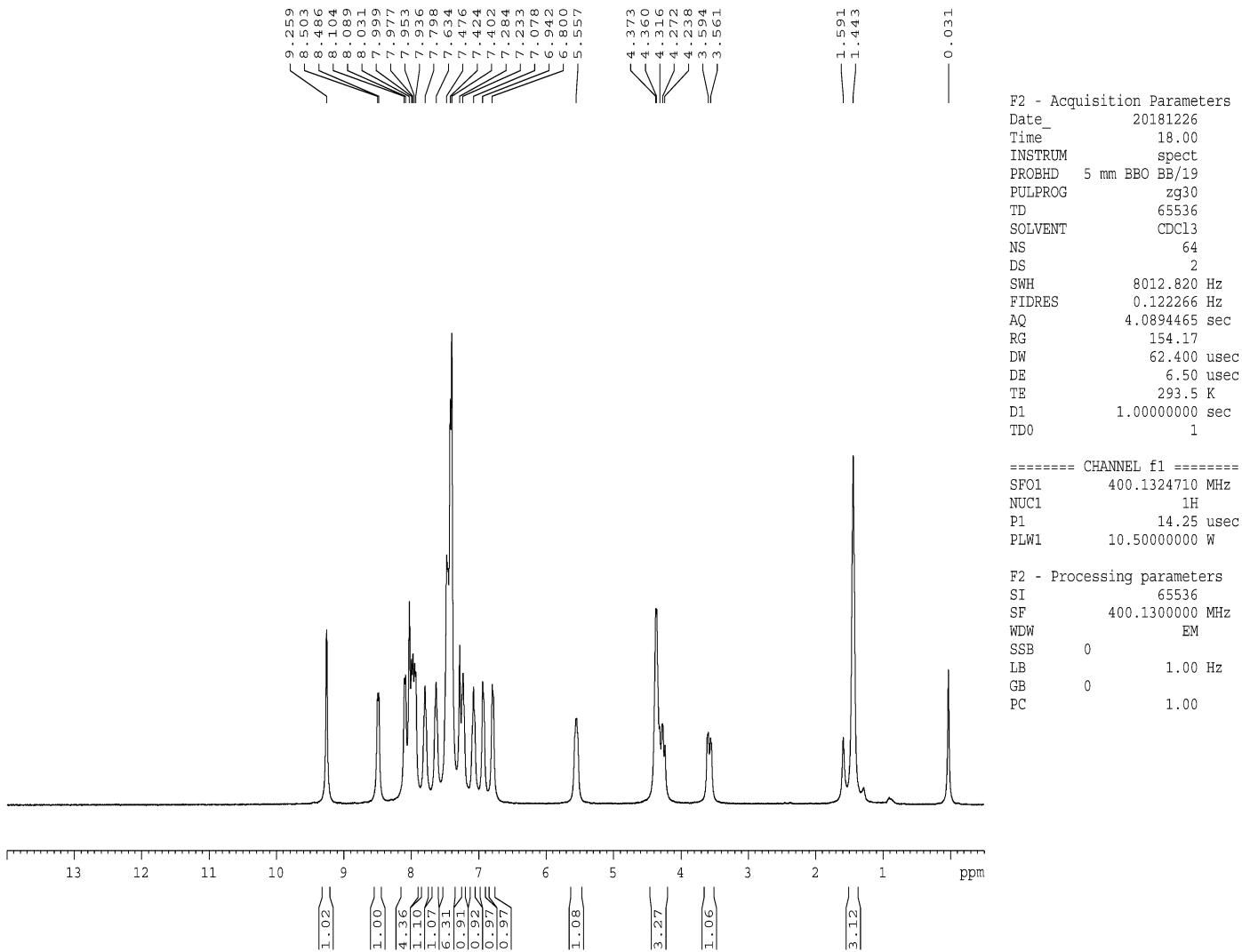


Fig. 70. <sup>1</sup>H NMR spectrum of compound 7c

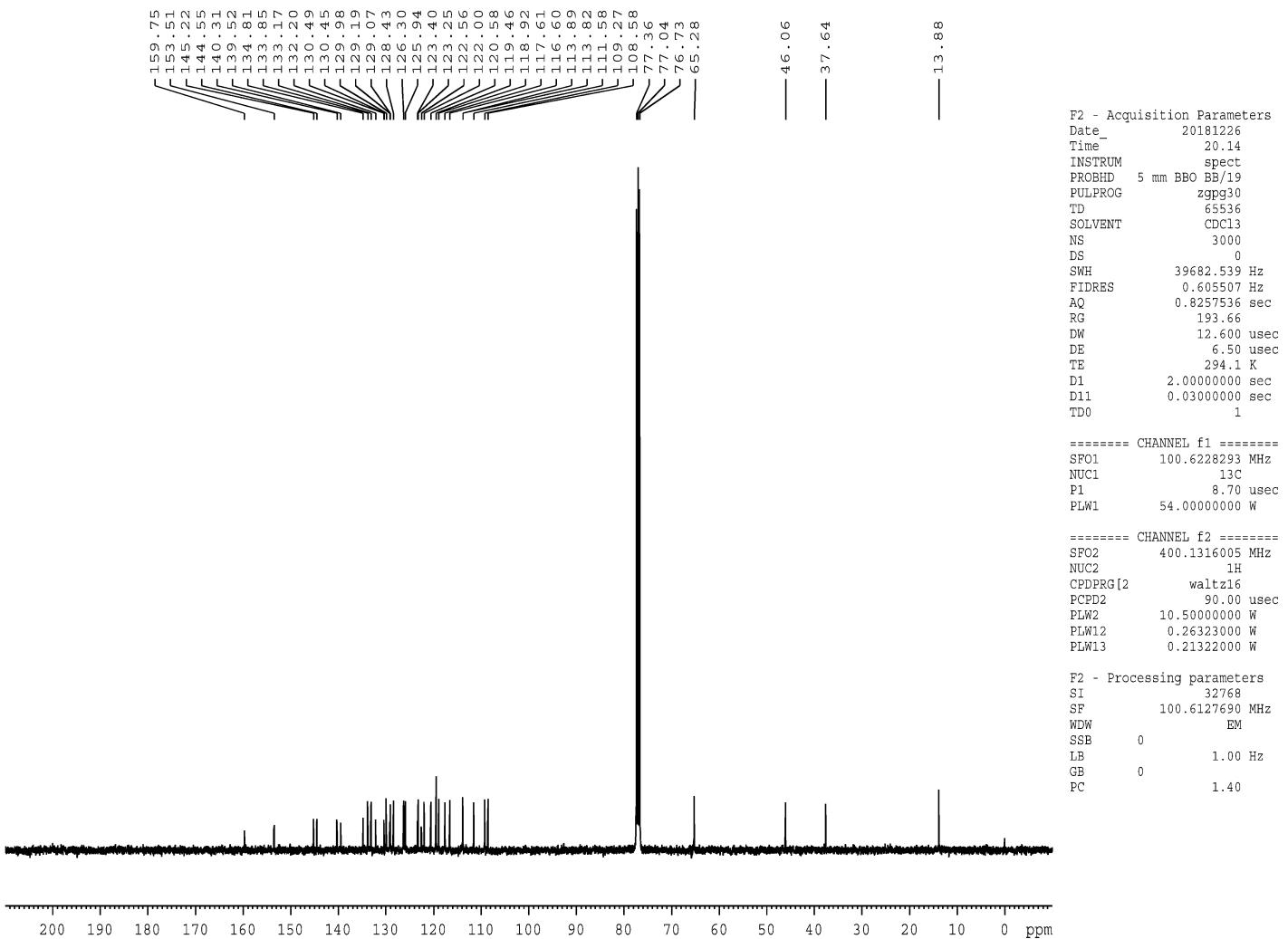


Fig. 71. <sup>13</sup>C NMR spectrum of compound 7c

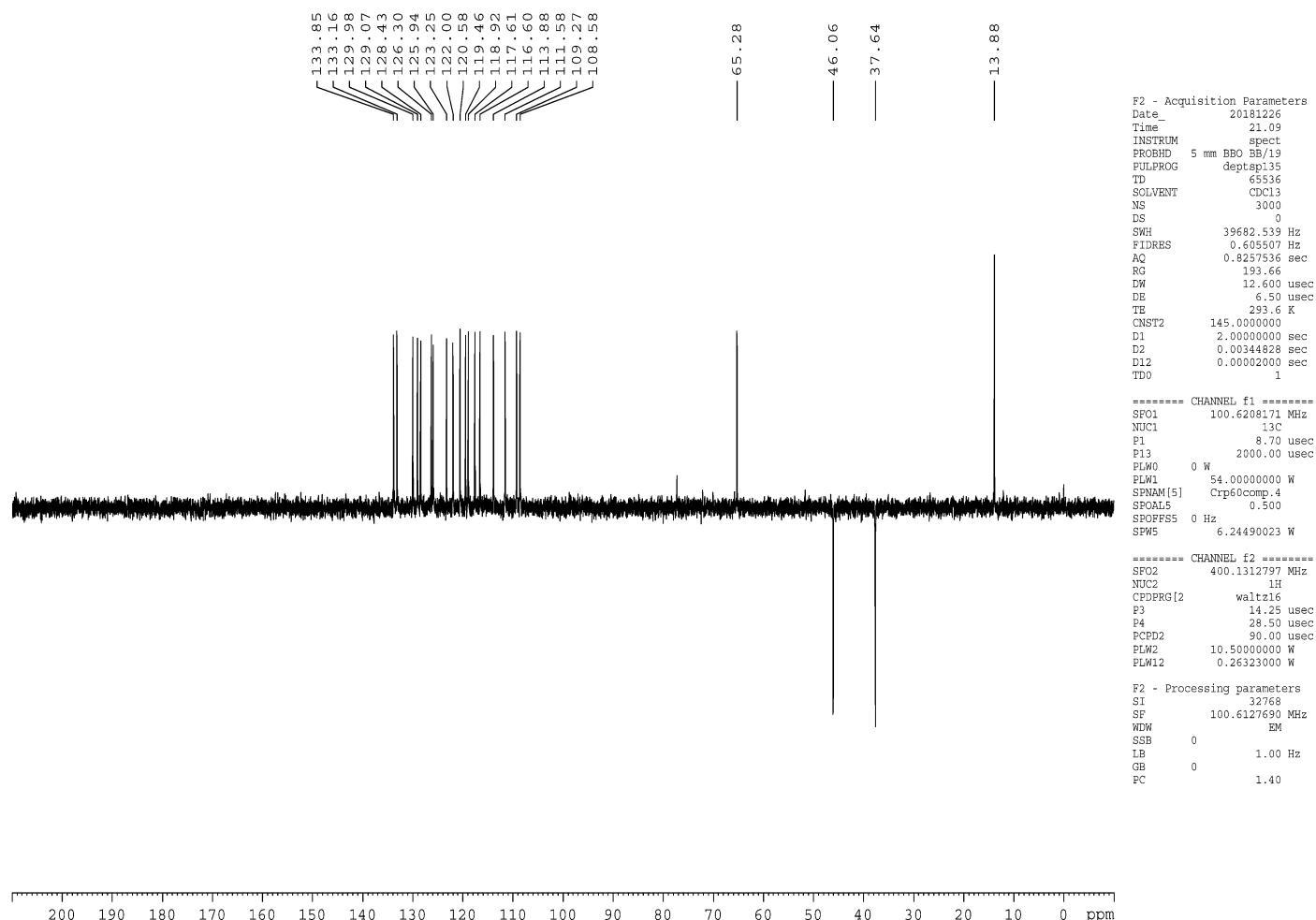


Fig. 72. DEPT-135 spectrum of compound 7c

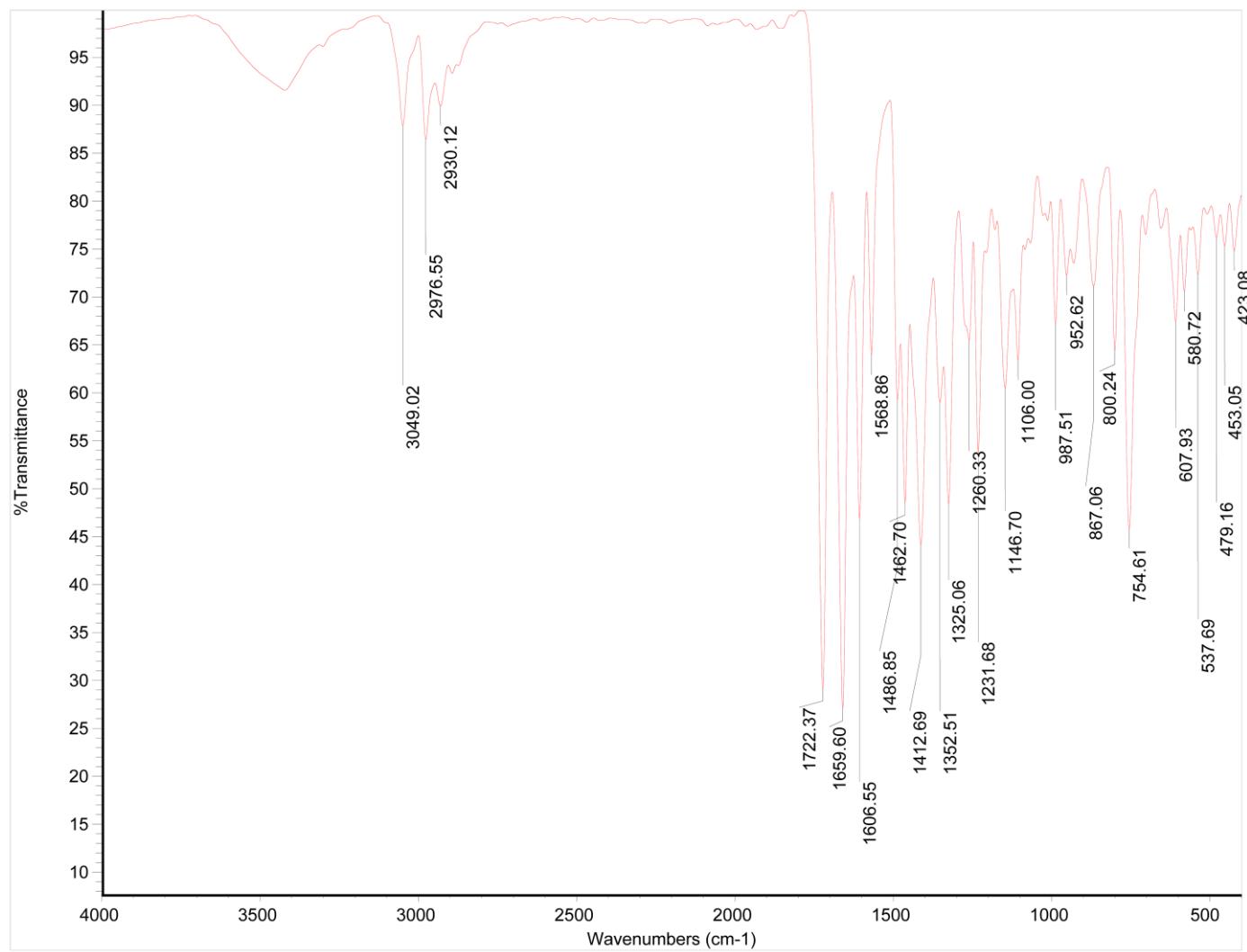


Fig. 73. IR spectrum of compound 8a

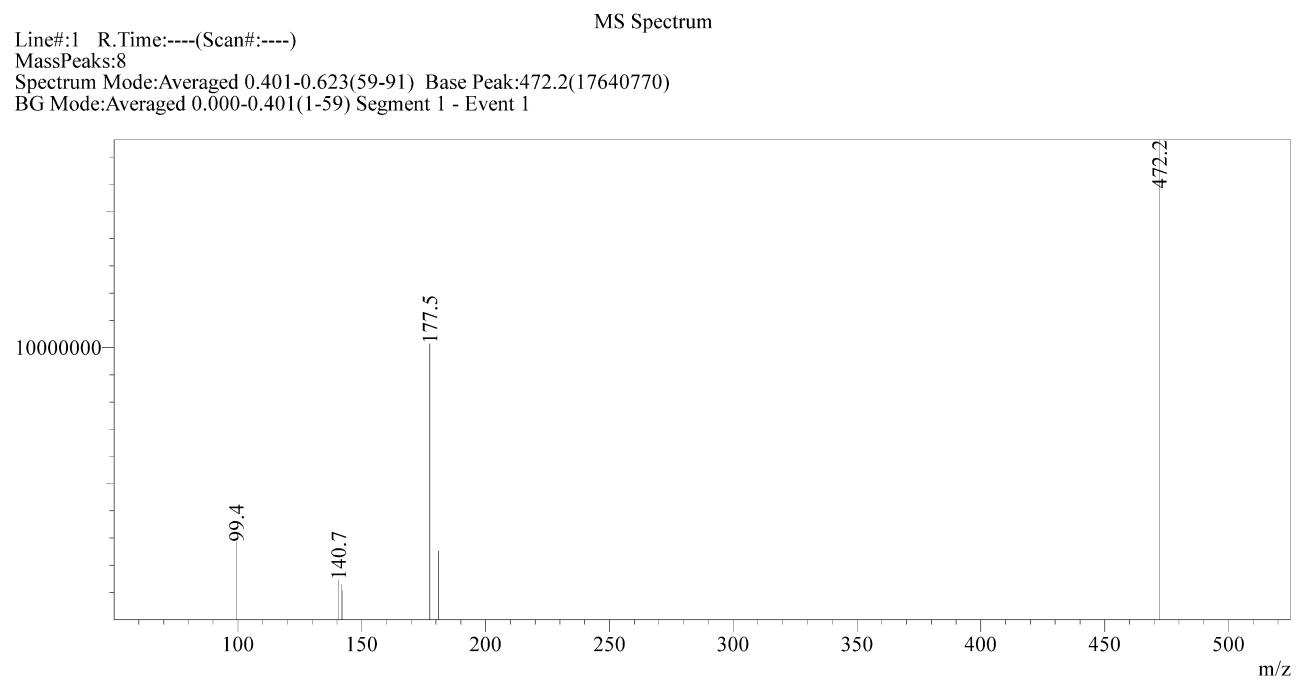


Fig. 74. Mass spectrum of compound 8a

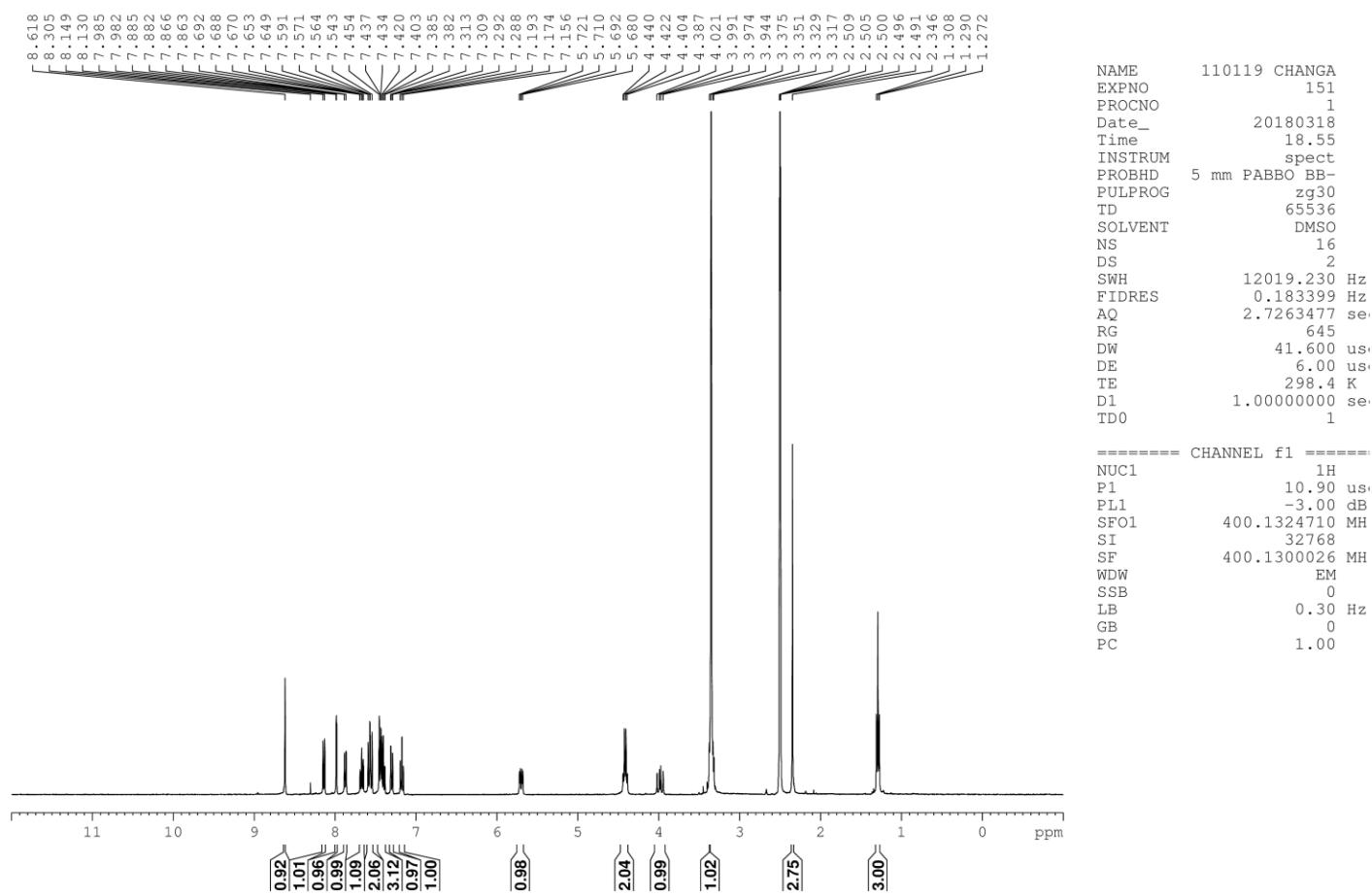


Fig. 75.  $^1\text{H}$  NMR spectrum of compound 8a

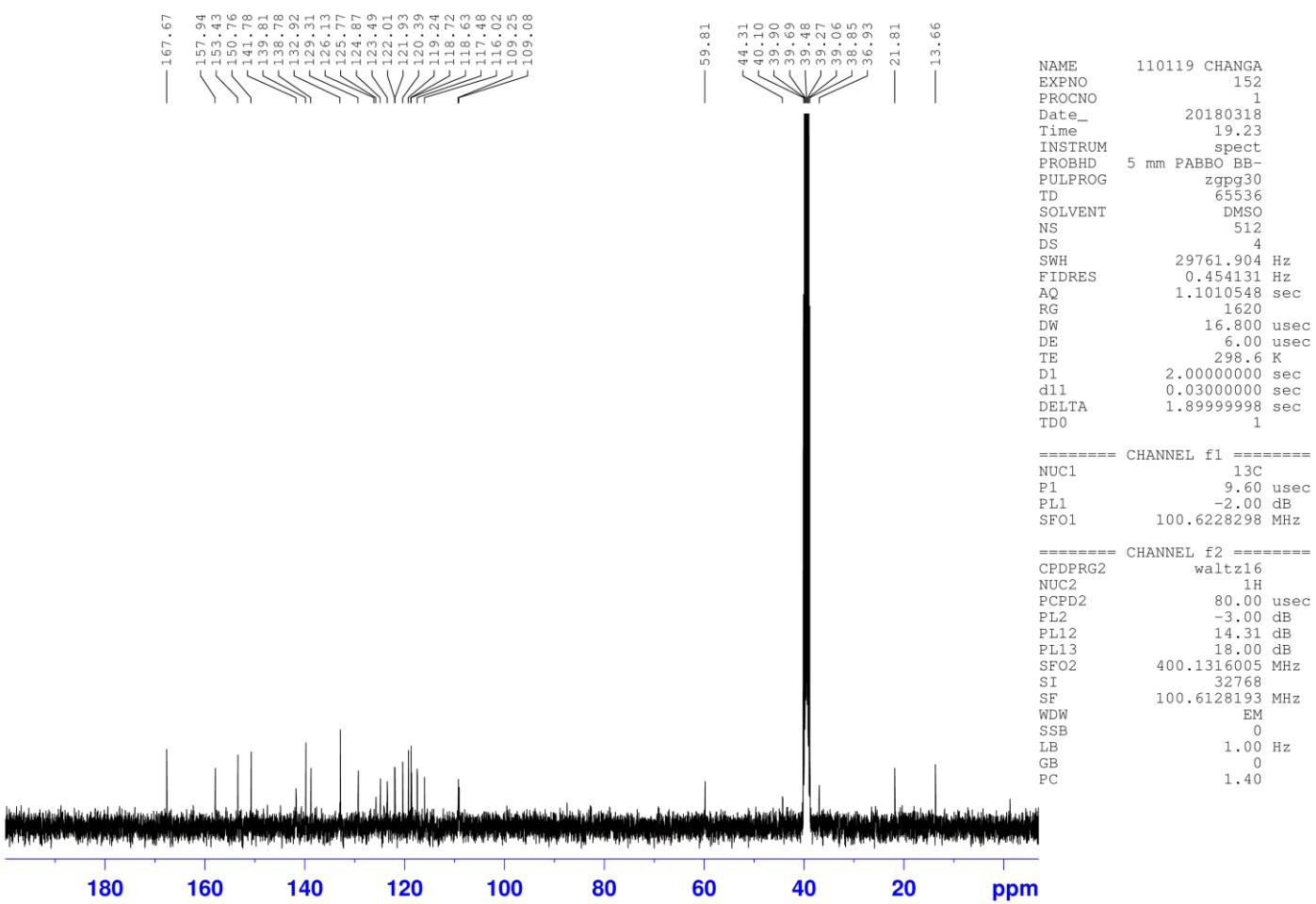


Fig. 76.  $^{13}\text{C}$  NMR spectrum of compound 8a

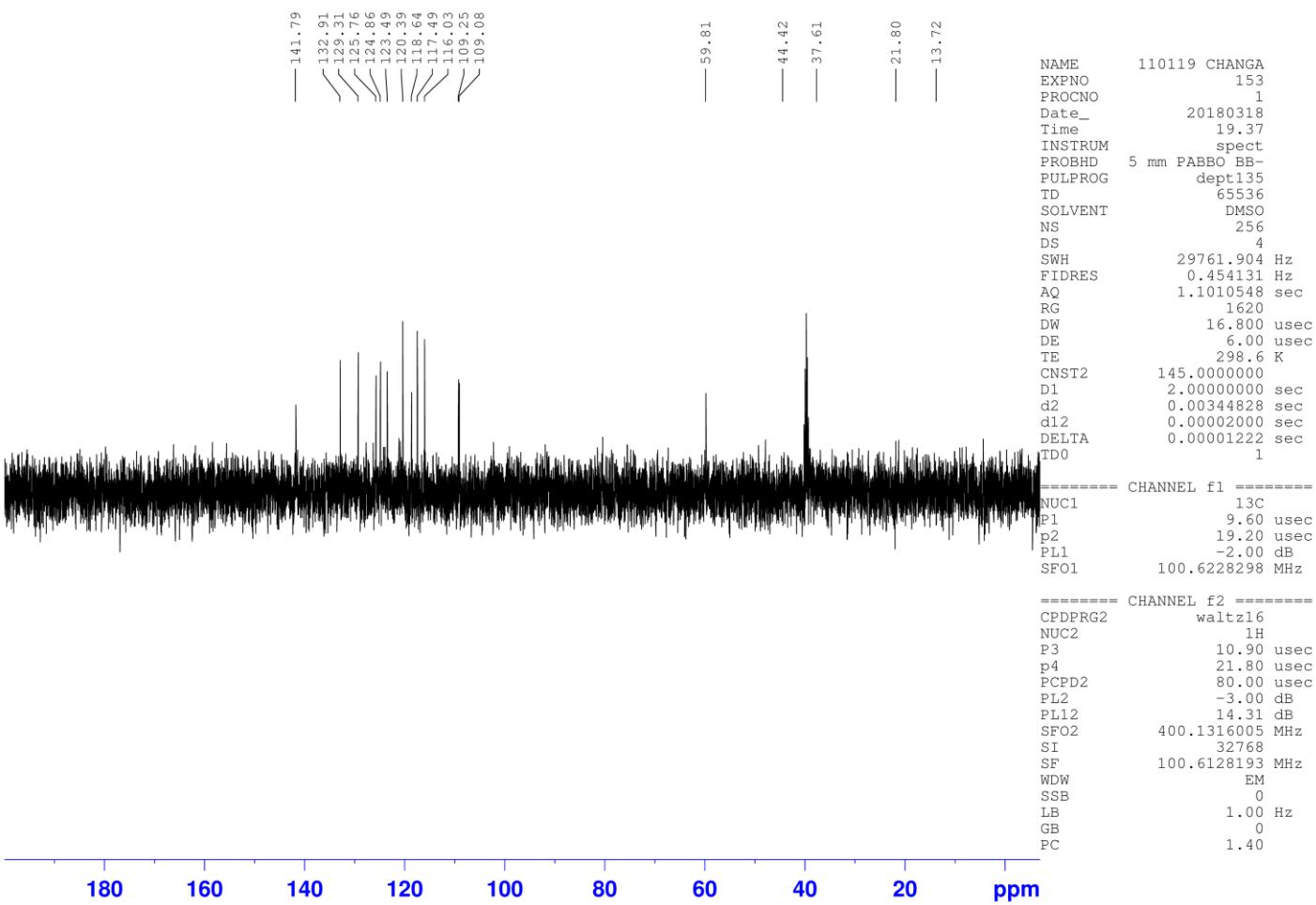


Fig. 77. DEPT-135 spectrum of compound 8a

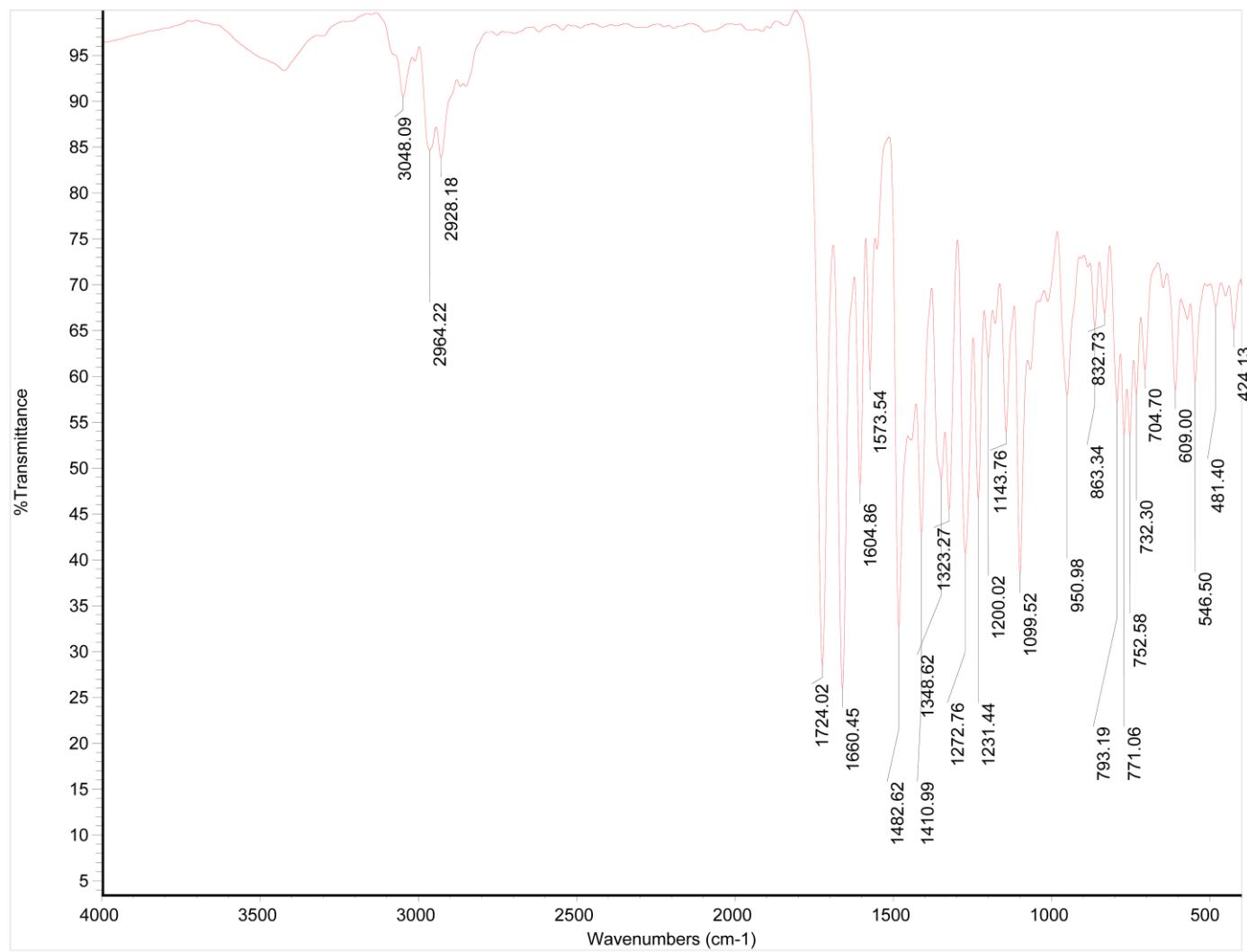


Fig. 78. IR spectrum of compound 8b

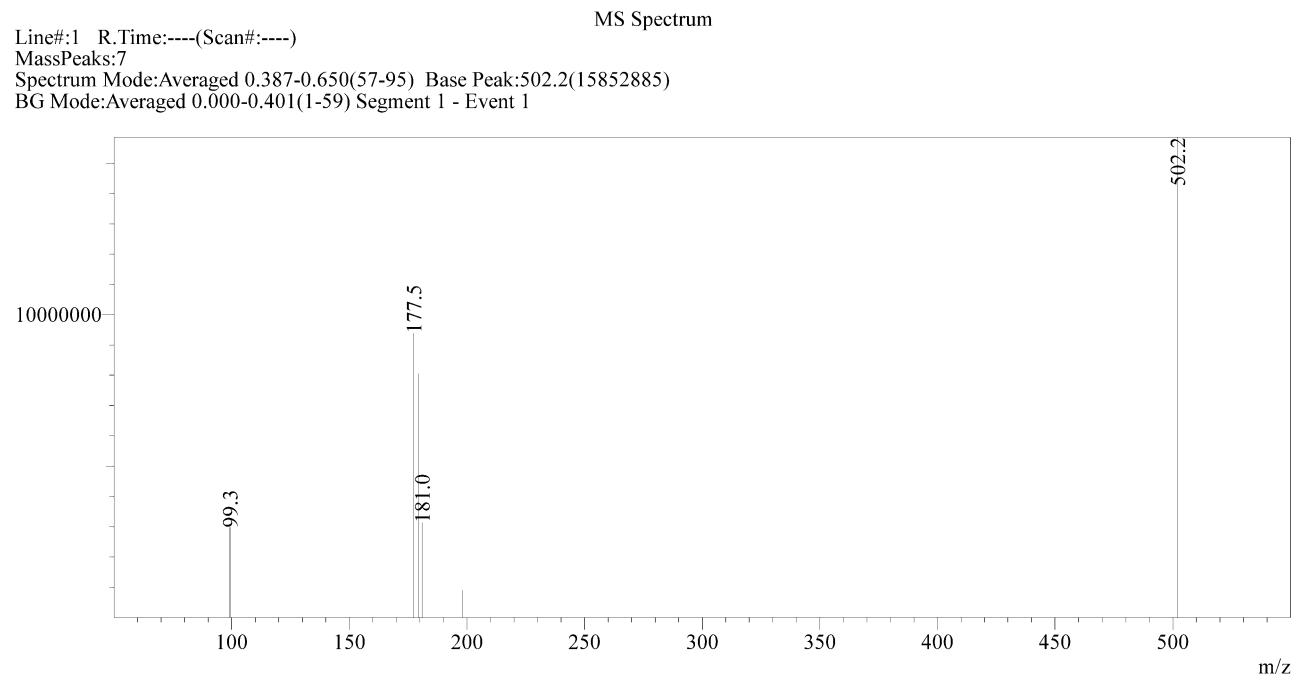


Fig. 79. Mass spectrum of compound 8b

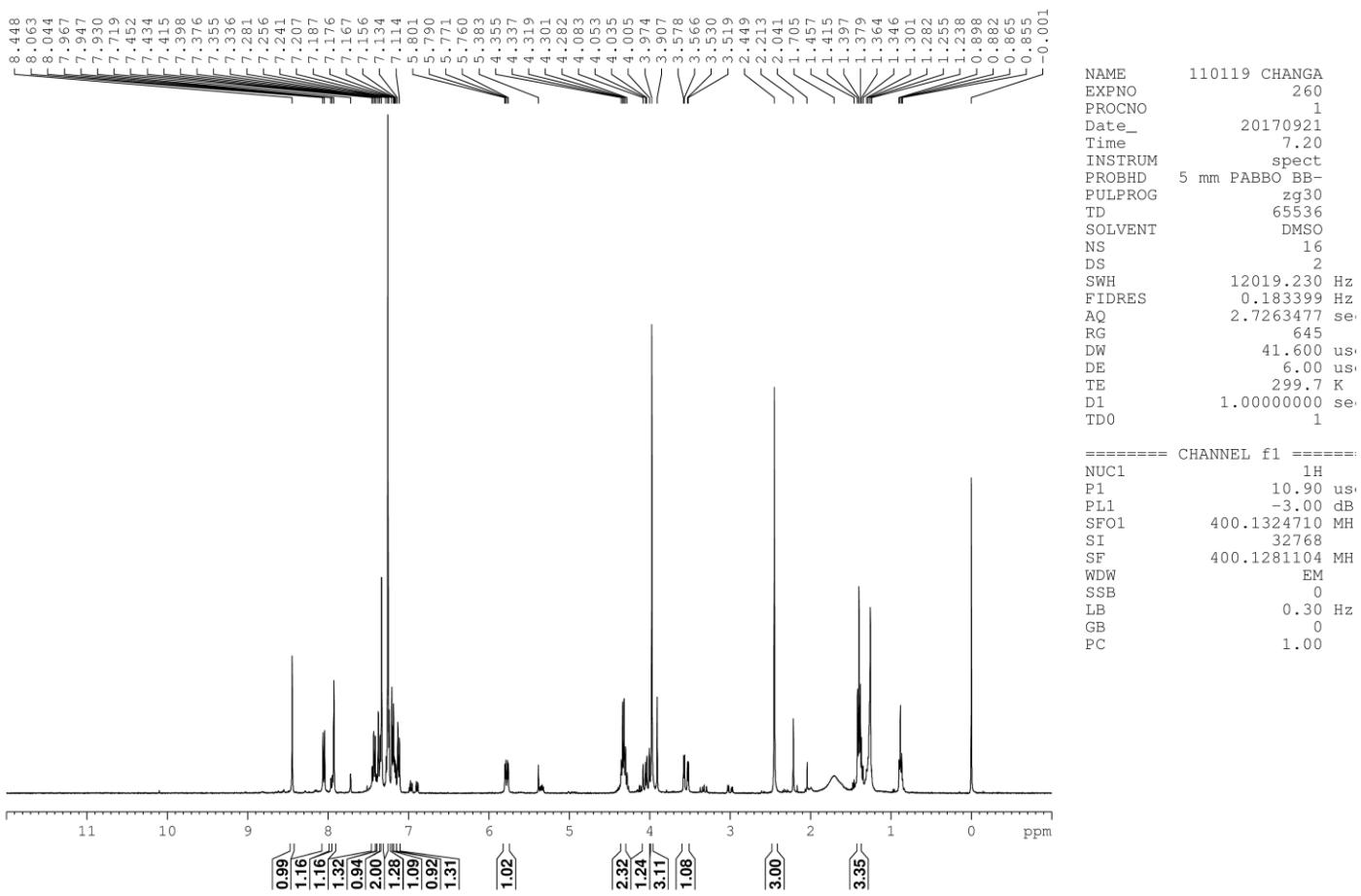


Fig. 80.  $^1\text{H}$  NMR spectrum of compound 8b

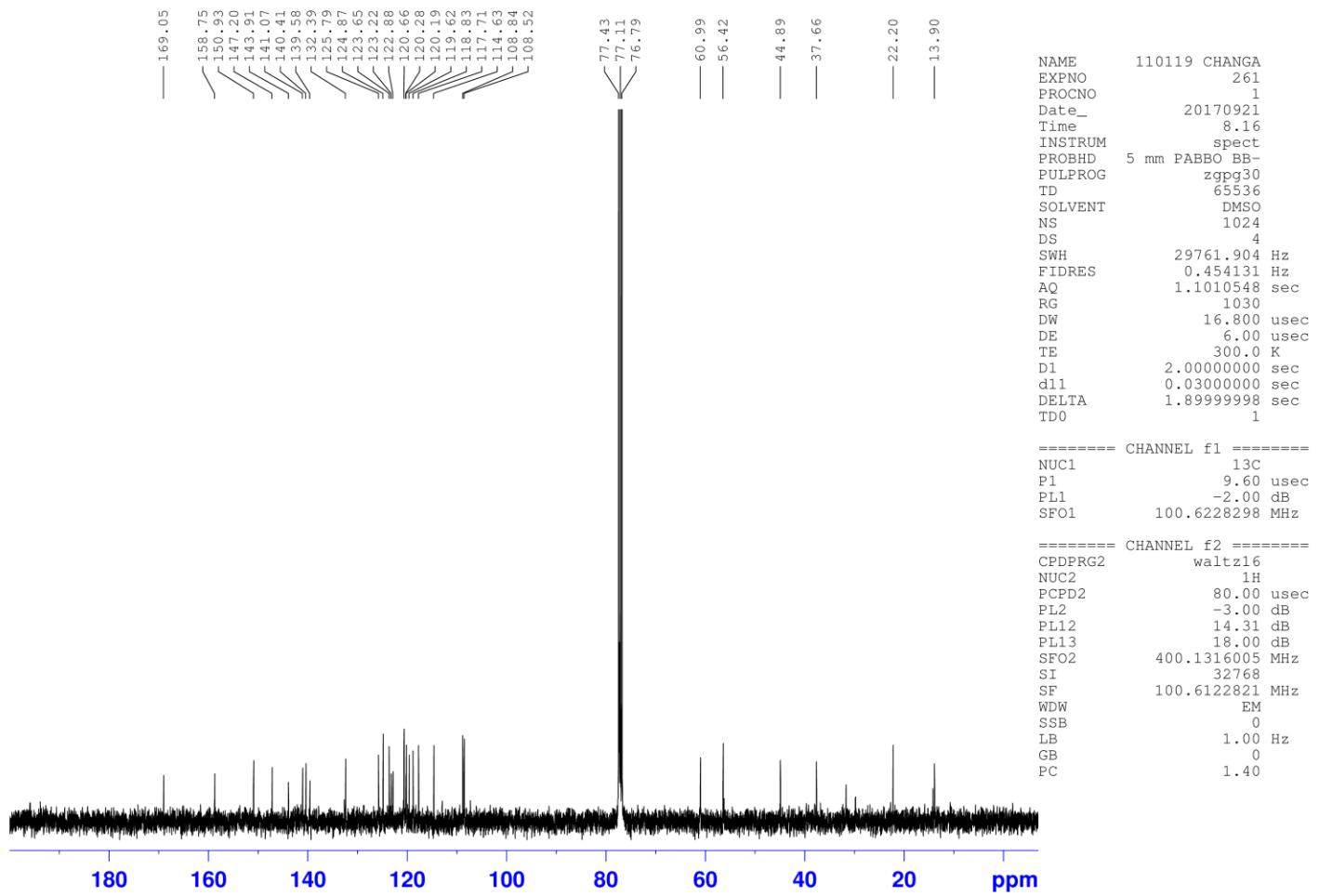


Fig. 81.  $^{13}\text{C}$  NMR spectrum of compound 8b

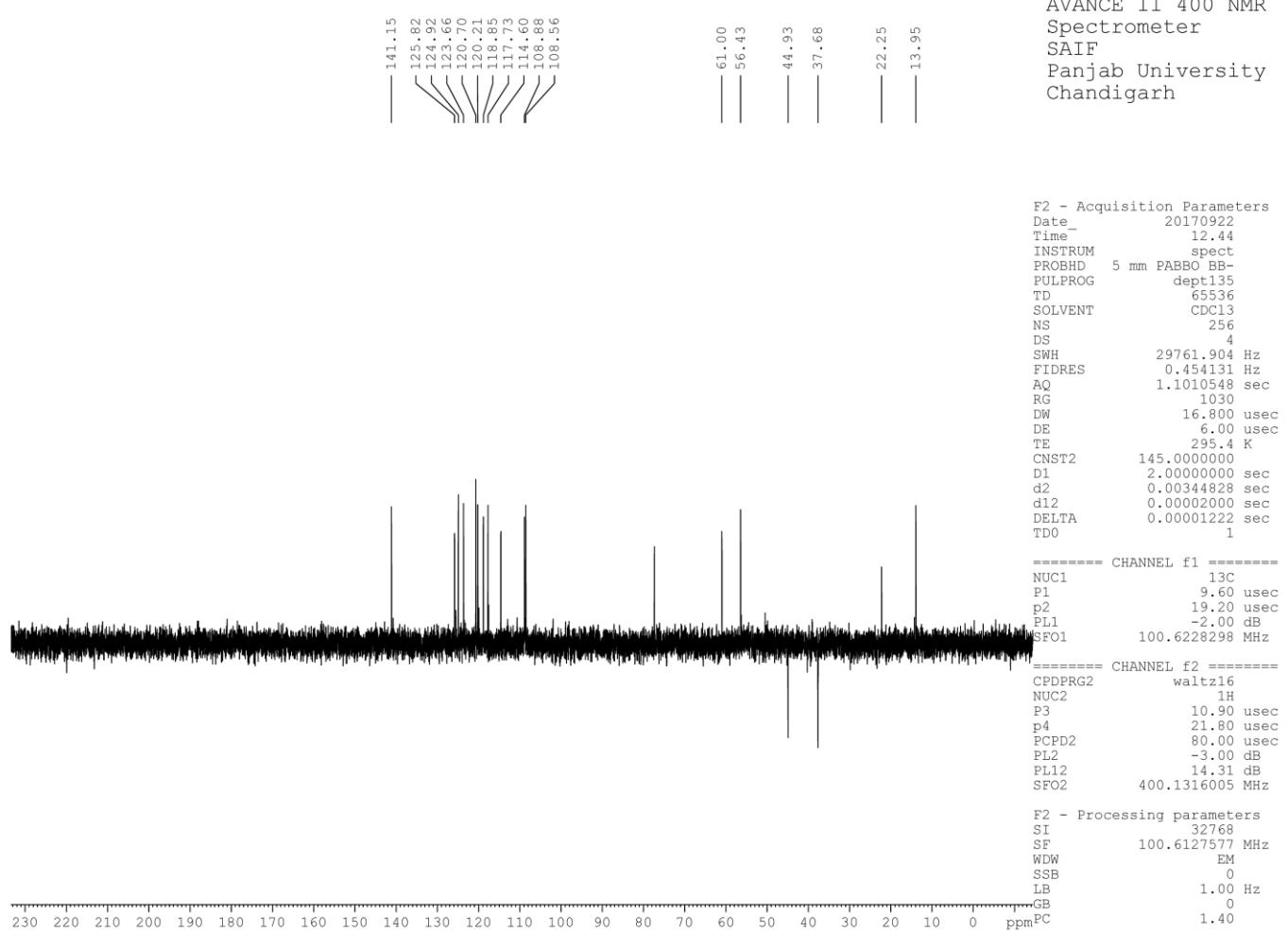


Fig. 82. DEPT-135 spectrum of compound 8b

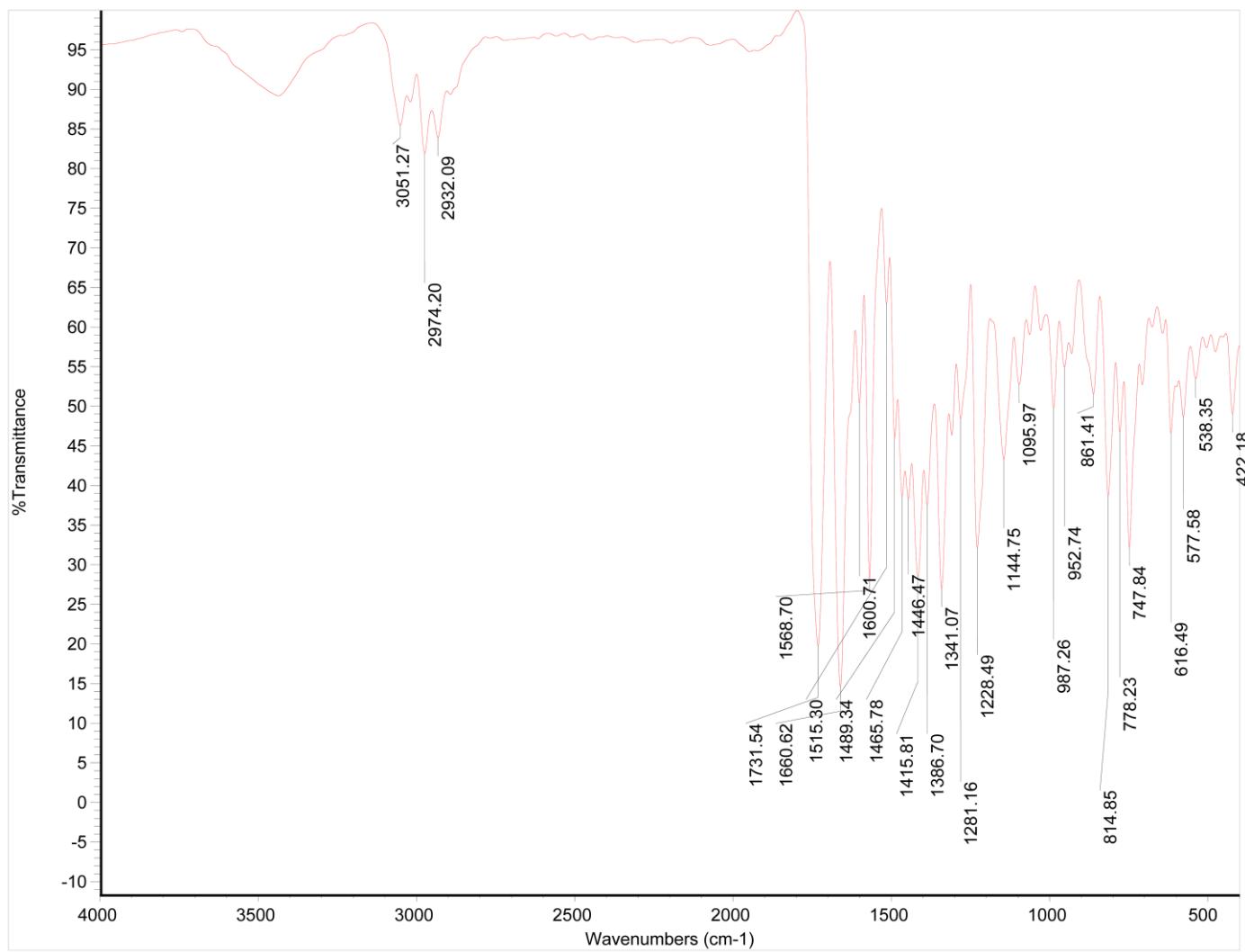


Fig. 83. IR spectrum of compound 8c

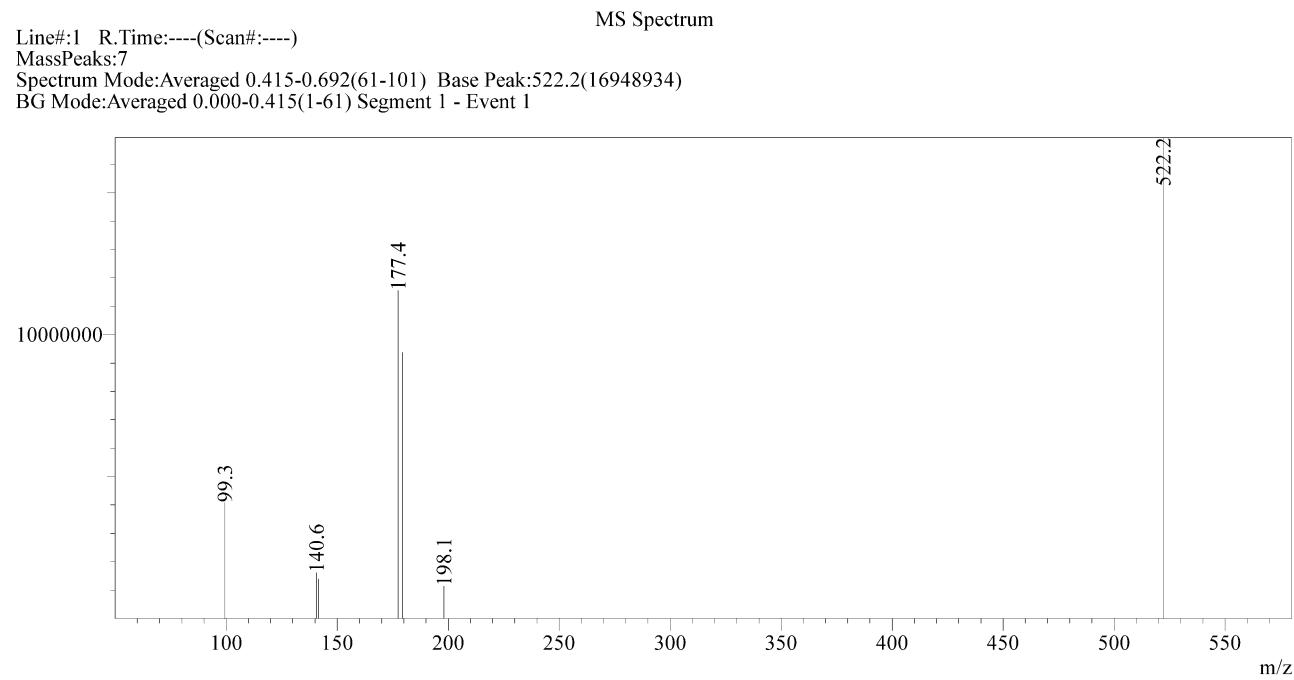
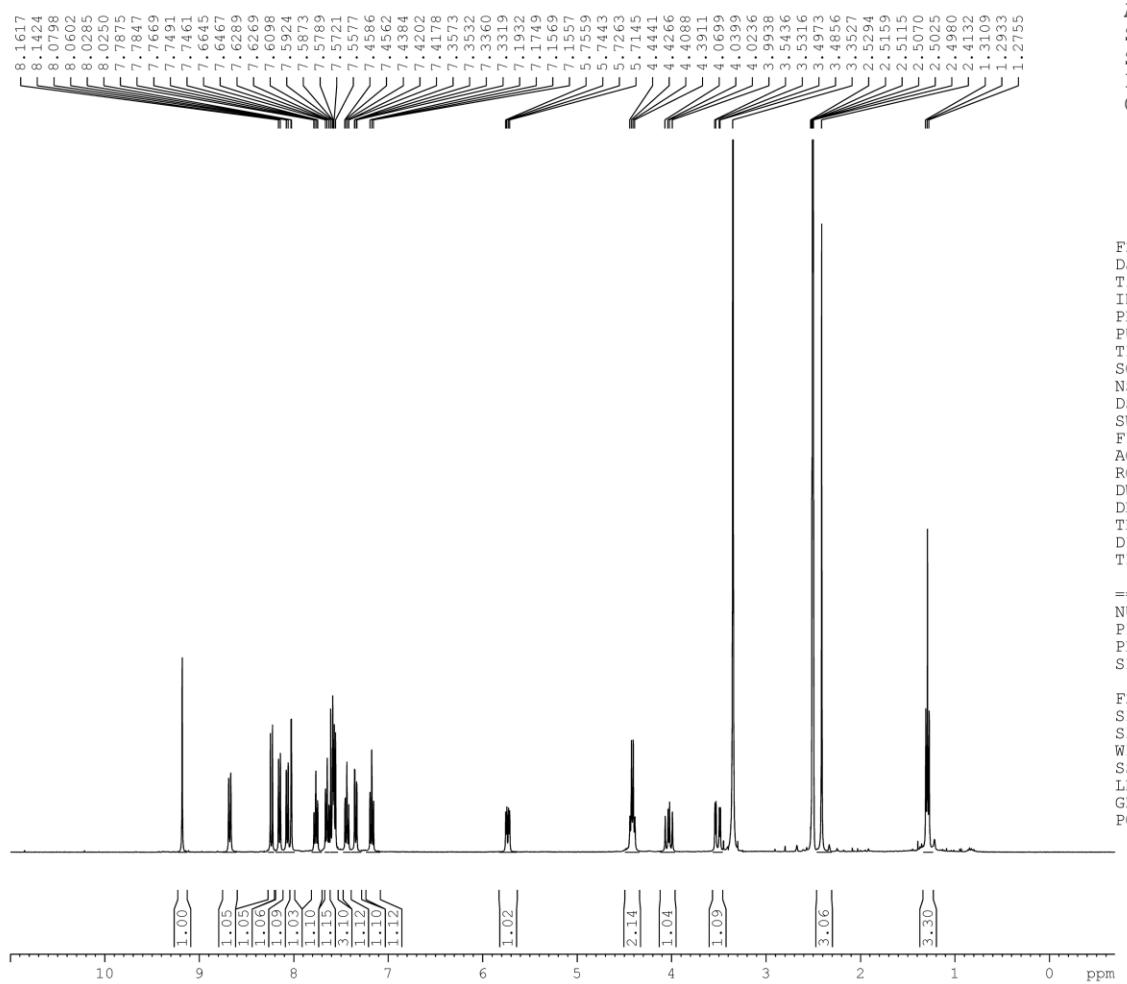


Fig. 84. Mass spectrum of compound 8c



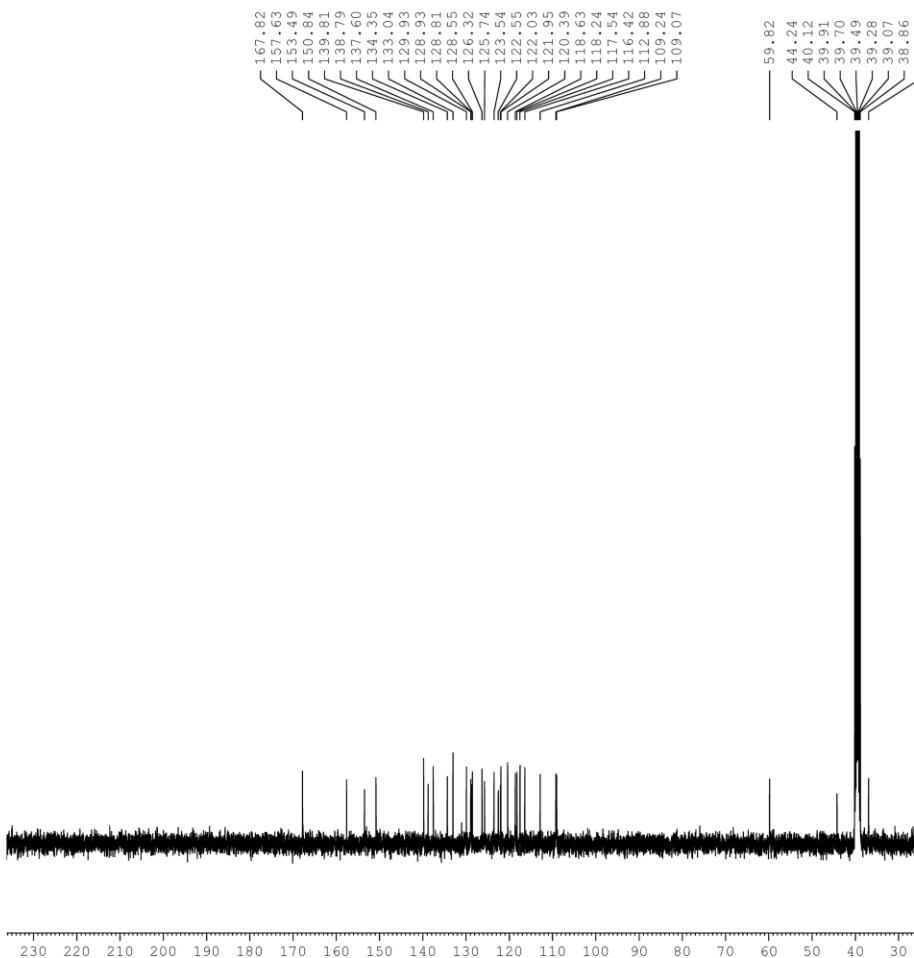
BRUKER  
AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

F2 - Acquisition Parameters  
 Date\_ 20180318  
 Time\_ 13.36  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 12019.230 Hz  
 FIDRES 0.183399 Hz  
 AQ 2.7263477 sec  
 RG 287  
 DW 41.600 usec  
 DE 6.00 usec  
 TE 298.4 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 ======  
 NUC1 1H  
 P1 10.90 usec  
 PL1 -3.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Fig. 85.  $^1\text{H}$  NMR spectrum of compound 8c



BRUKER  
AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

F2 - Acquisition Parameters  
 Date\_ 20180318  
 Time 14.05  
 INSTRUM spect  
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 512  
 DS 4  
 SWH 29761.904 Hz  
 FIDRES 0.454131 Hz  
 AQ 1.1010548 sec  
 RG 1030  
 DW 16.800 usec  
 DE 6.00 usec  
 TE 298.8 K  
 D1 2.0000000 sec  
 d11 0.03000000 sec  
 DELTA 1.8999999 sec  
 TDO 1

===== CHANNEL f1 ======

NUC1 13C  
 P1 9.60 usec  
 PL1 -2.00 dB  
 SFO1 100.6228298 MHz

===== CHANNEL f2 ======

CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -3.00 dB  
 PL12 14.31 dB  
 PL13 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6128193 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

Fig. 86.  $^{13}\text{C}$  NMR spectrum of compound 8c

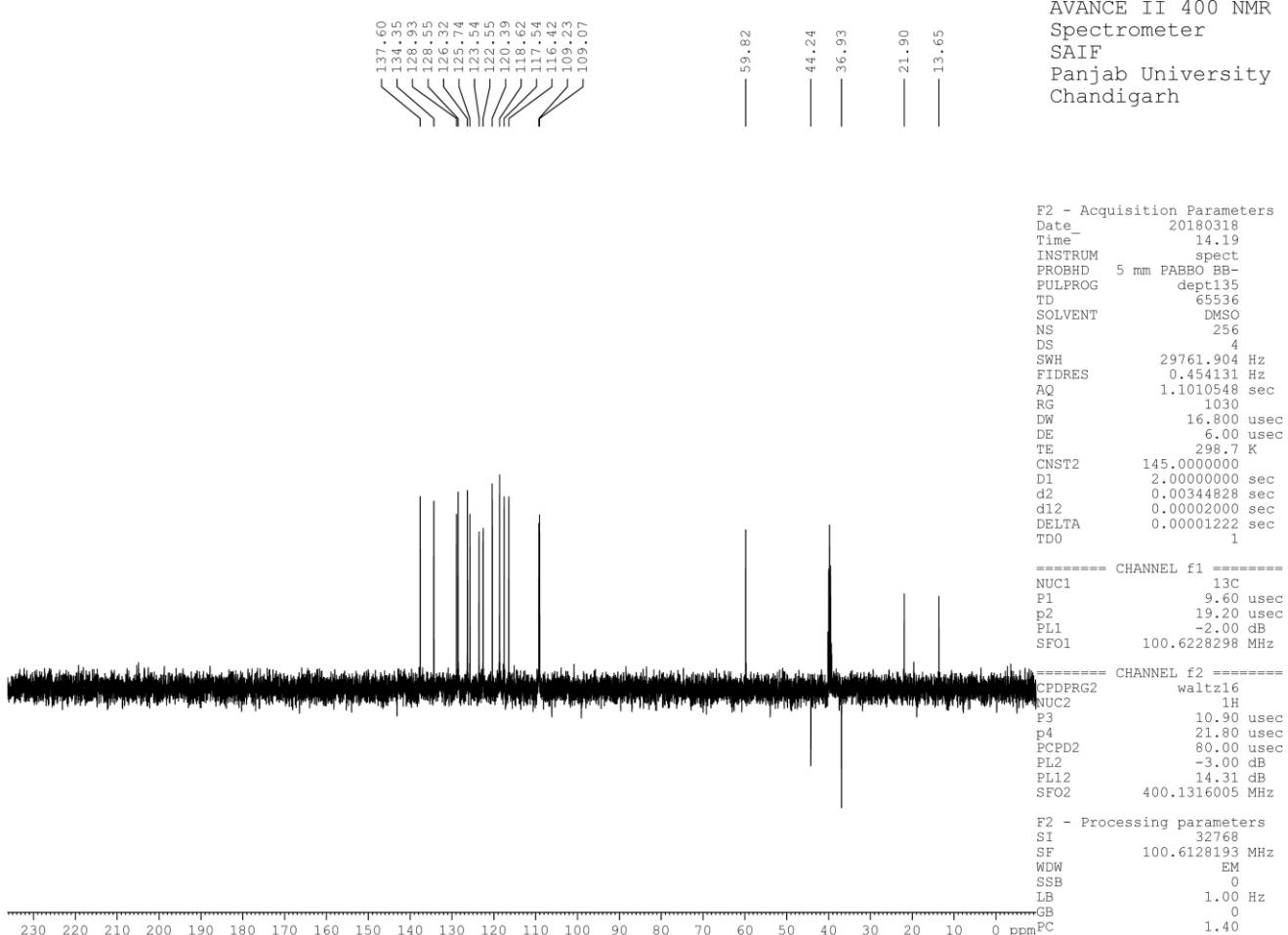


Fig. 87. DEPT-135 spectrum of compound 8c

Note: Some of the synthesized compounds identified with equivalent protons and carbons atoms in their structures. Either DMSO or CDCl<sub>3</sub> used for the solvation of compounds in NMR. In some cases for better resolution of signals, mixture of DMSO and CDCl<sub>3</sub> used that is visible in spectra. Some tiny aliphatic signals visible in some of the spectra which were due to solvent trapped during column chromatography purification, those compounds were further purified to remove trapped solvent for utilization of their further application purpose.