

Supporting Information

Acetic Acid Promoted Tandem Cyclization of *in situ* Generated 1,3-Dipoles: Stereoselective Synthesis of Dispiroimidazolidinyl and Dispiropyrrolidinyl Oxindoles with Multiple Chiral Stereocenters

Koorathota Suman and Sathiah Thennarasu*

Organic Chemistry Laboratory, CSIR-Central Leather Research Institute

Adyar, Chennai-600020, India. Fax: (+) 91-44-24911589

E-mail: thennarasu@gmail.com

Contents

¹ H, ¹³ C and DEPT-135 NMR spectra	S2
Single crystal XRD data of 3a and 5a	S61

2. NMR and Mass Spectra of compounds

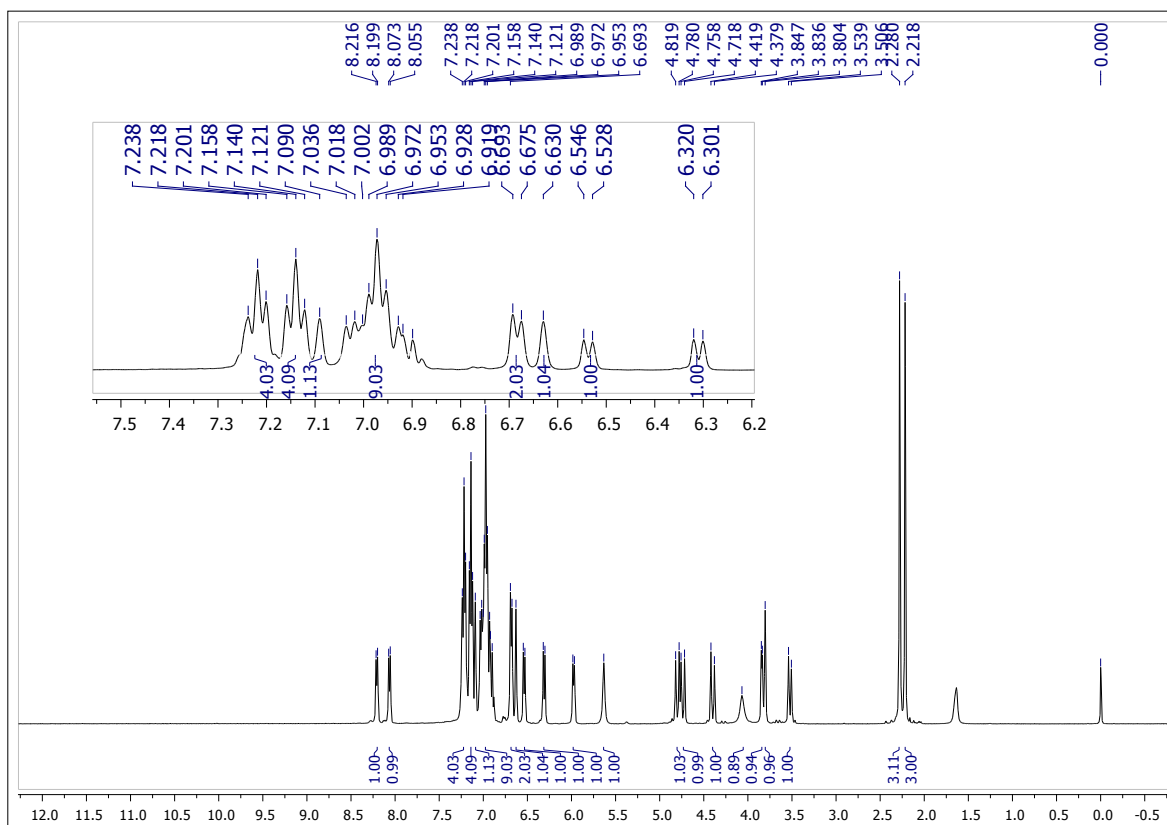


Figure 1. ¹H NMR spectrum of compound 3a

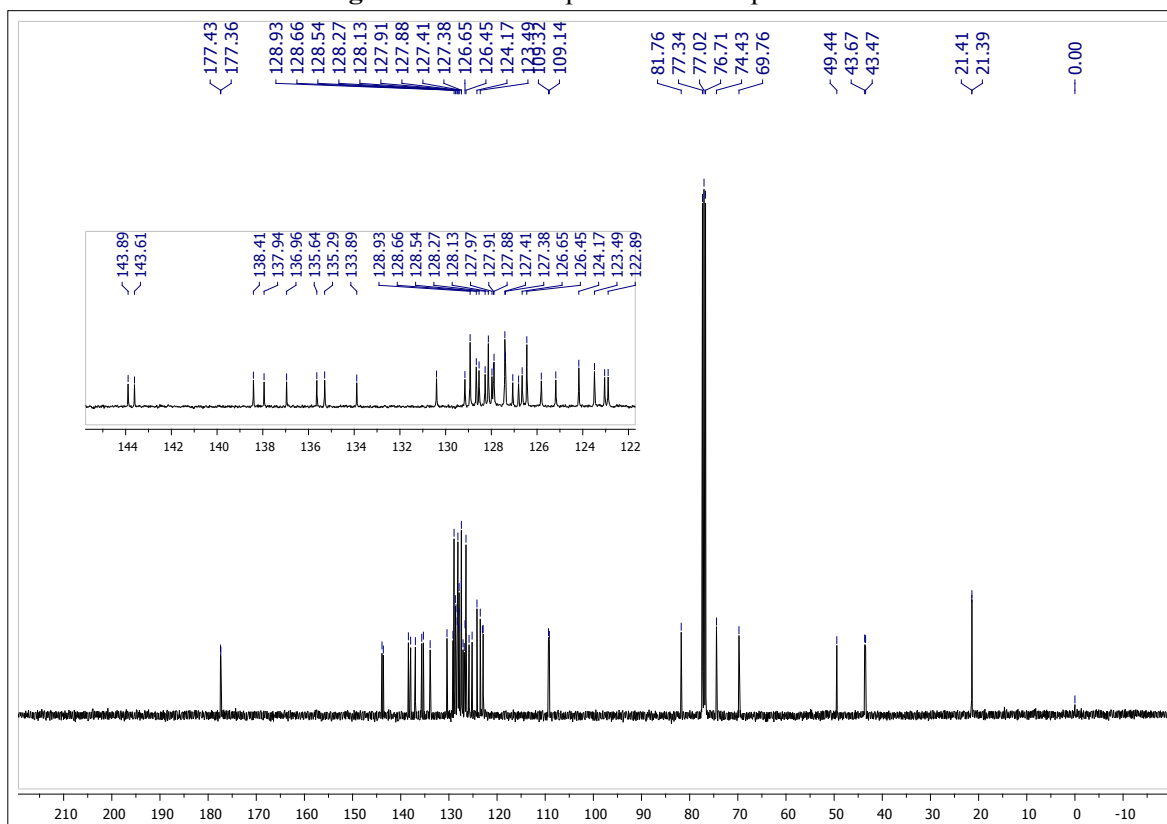


Figure 2. ¹³C NMR spectrum of compound 3a

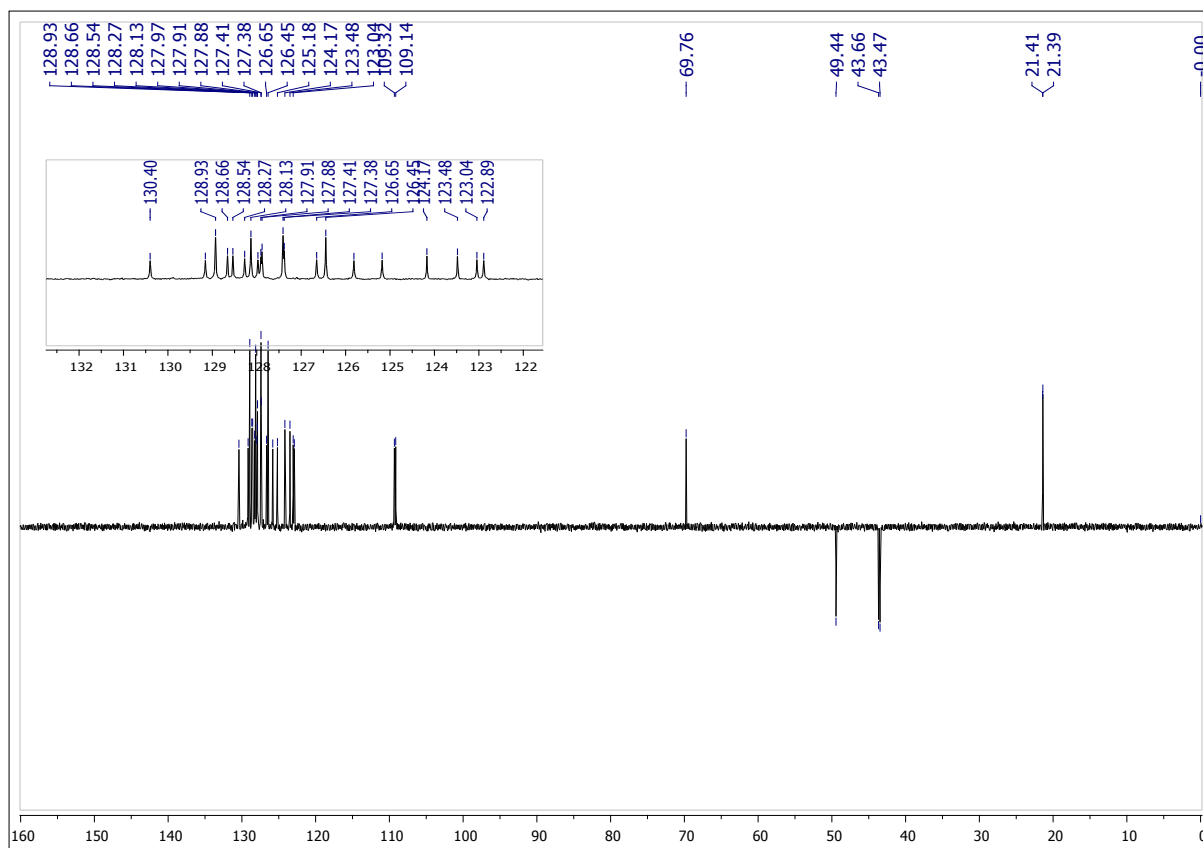


Figure 3. DEPT-135 spectrum of compound 3a

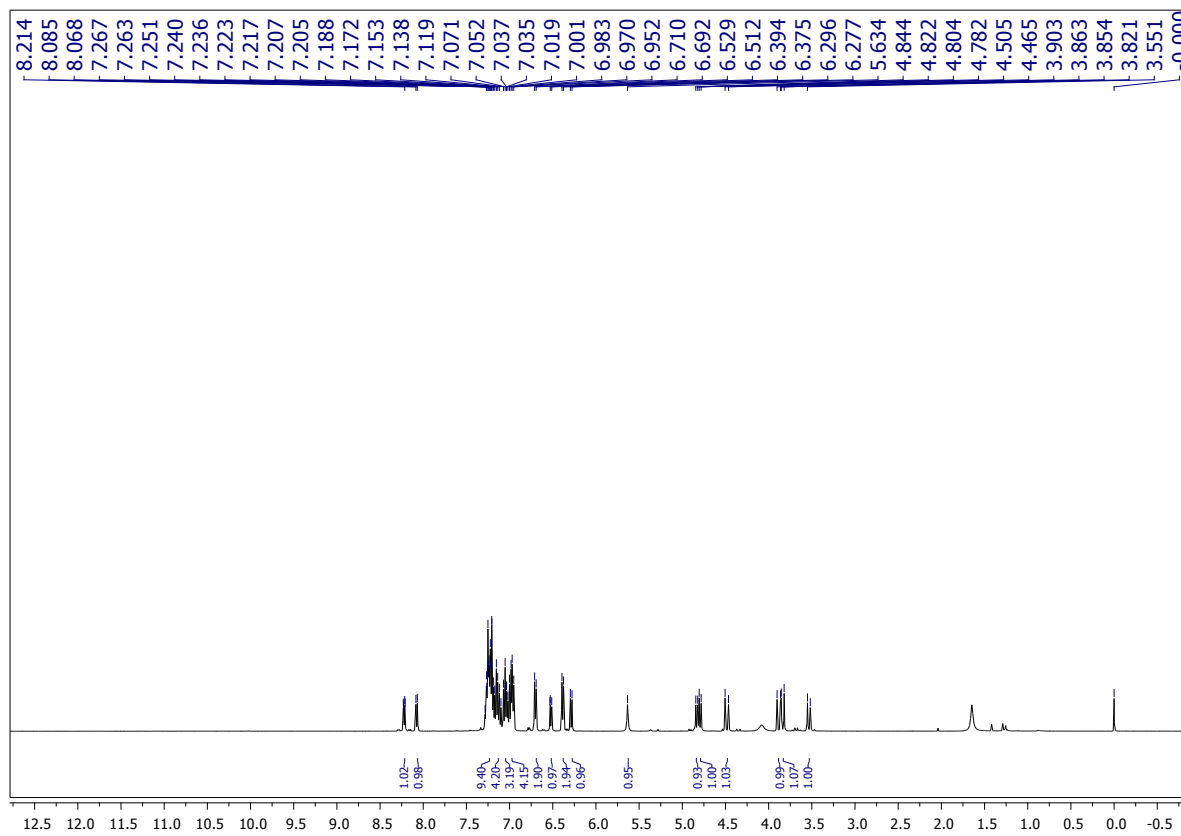


Figure 4. ¹H NMR spectrum of compound 3b

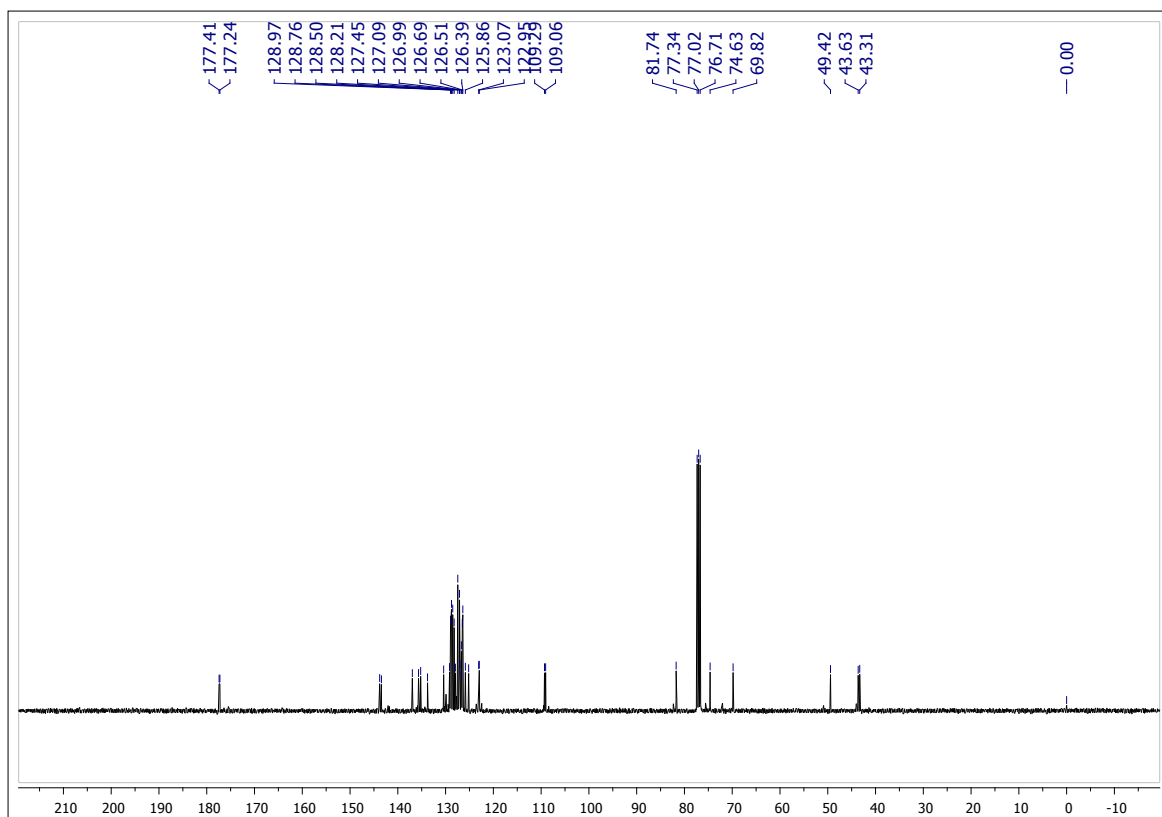


Figure 5. ^{13}C NMR spectrum of compound **3b**

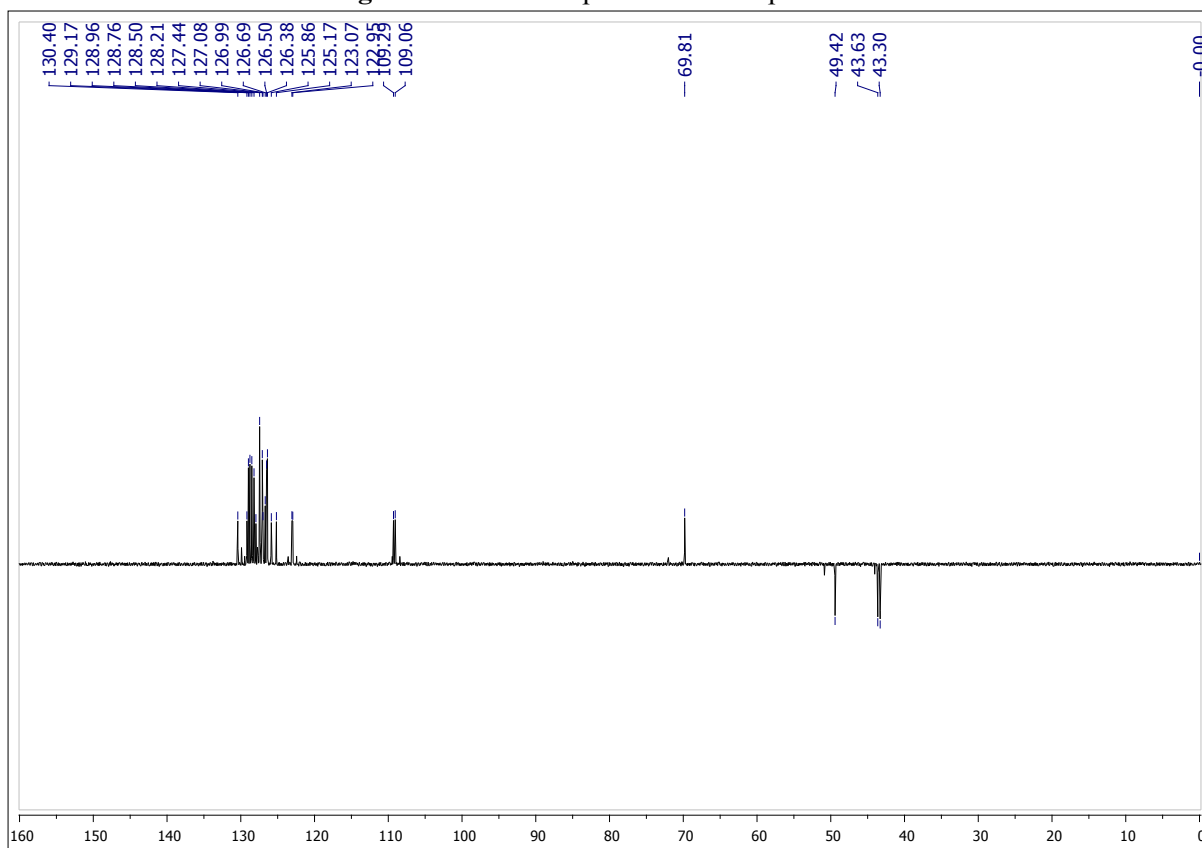


Figure 6. DEPT-135 spectrum of compound **3b**

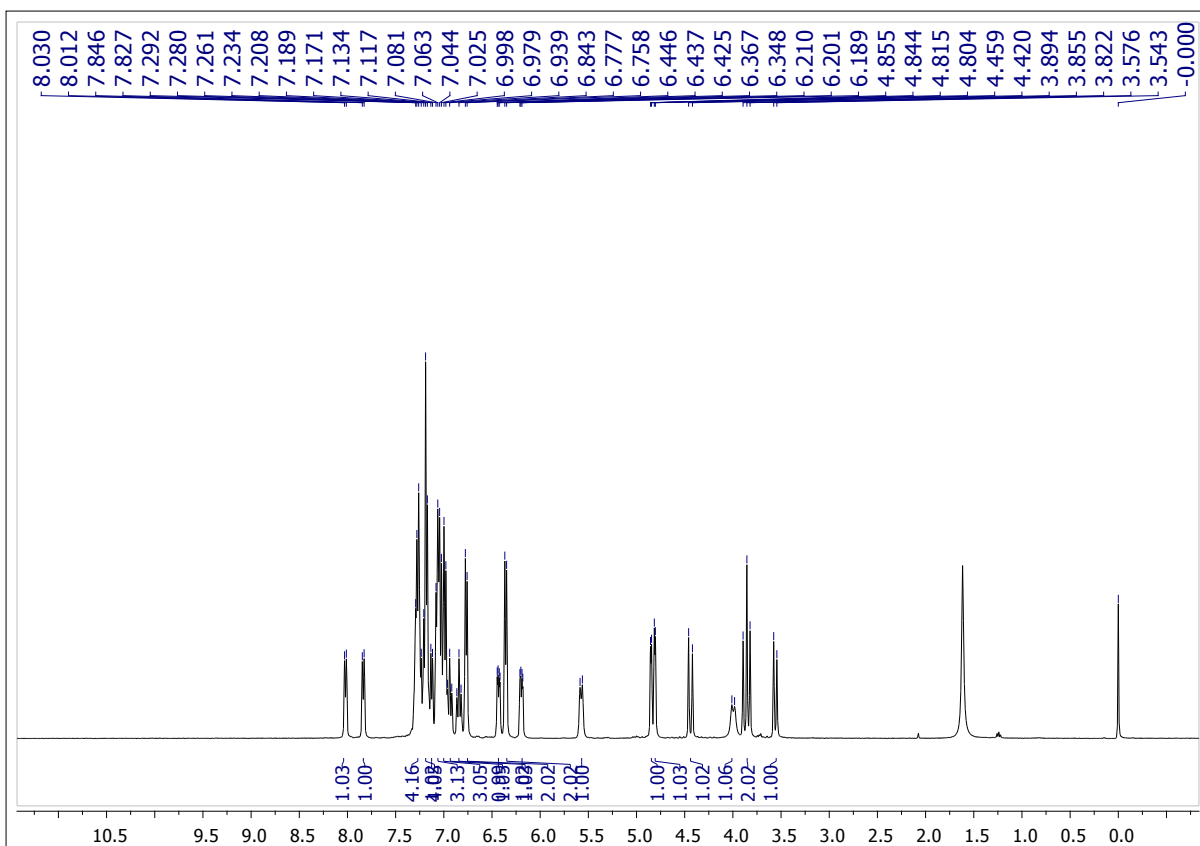


Figure 7. ¹H NMR spectrum of compound 3c

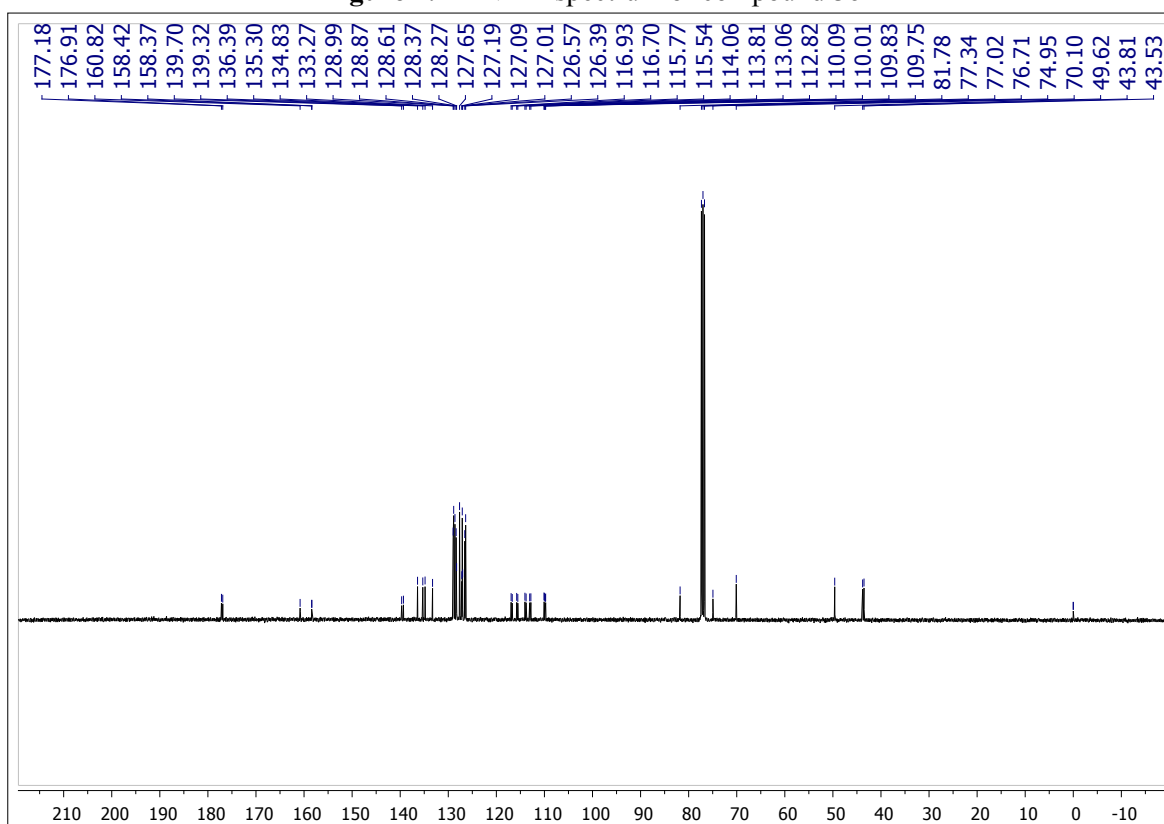


Figure 8. ¹³C NMR spectrum of compound 3c

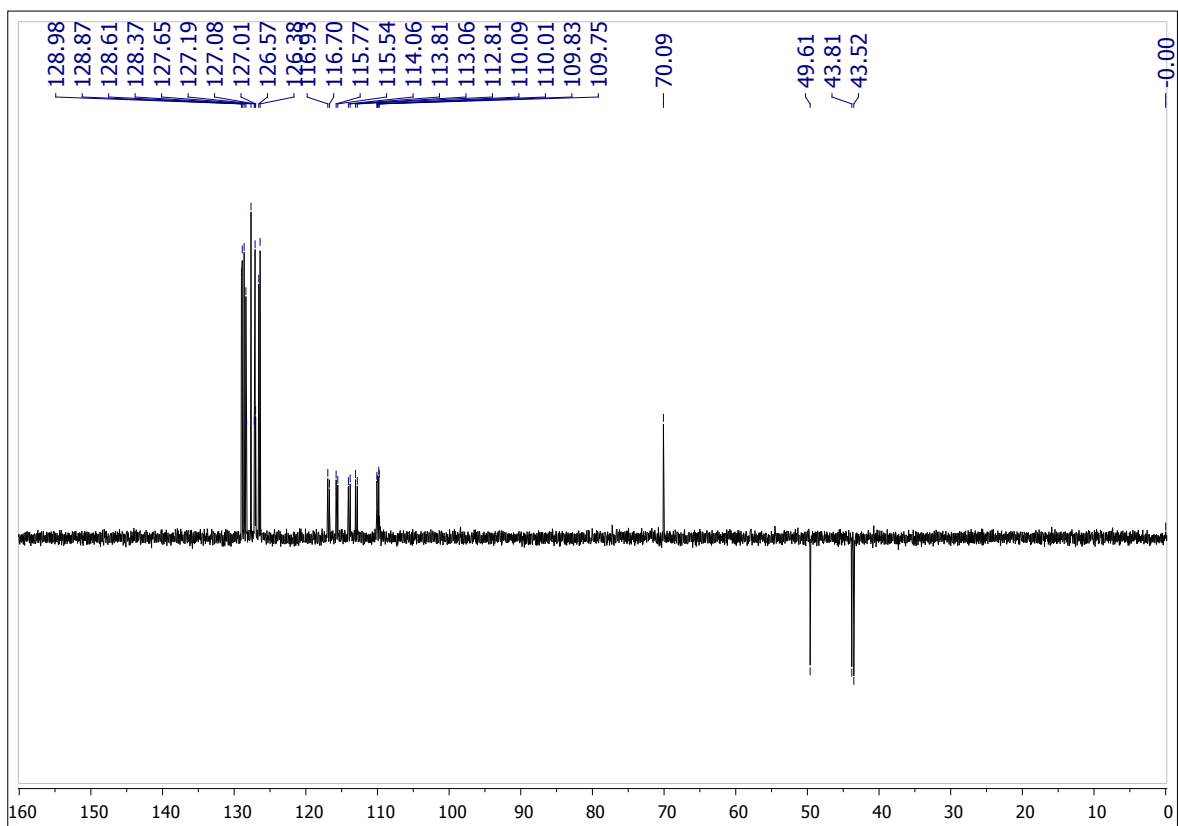


Figure 9. DEPT-135 spectrum of compound 3c

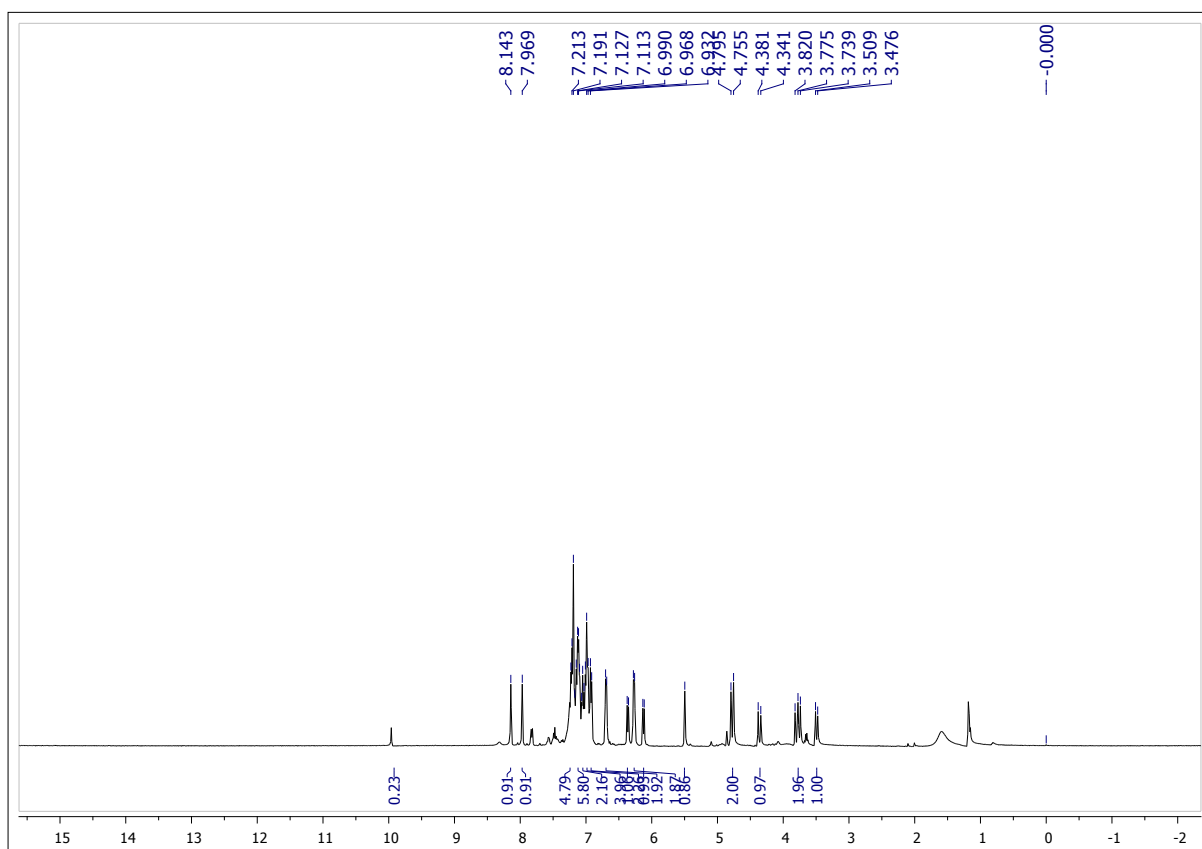


Figure 10. ¹H NMR spectrum of compound 3d

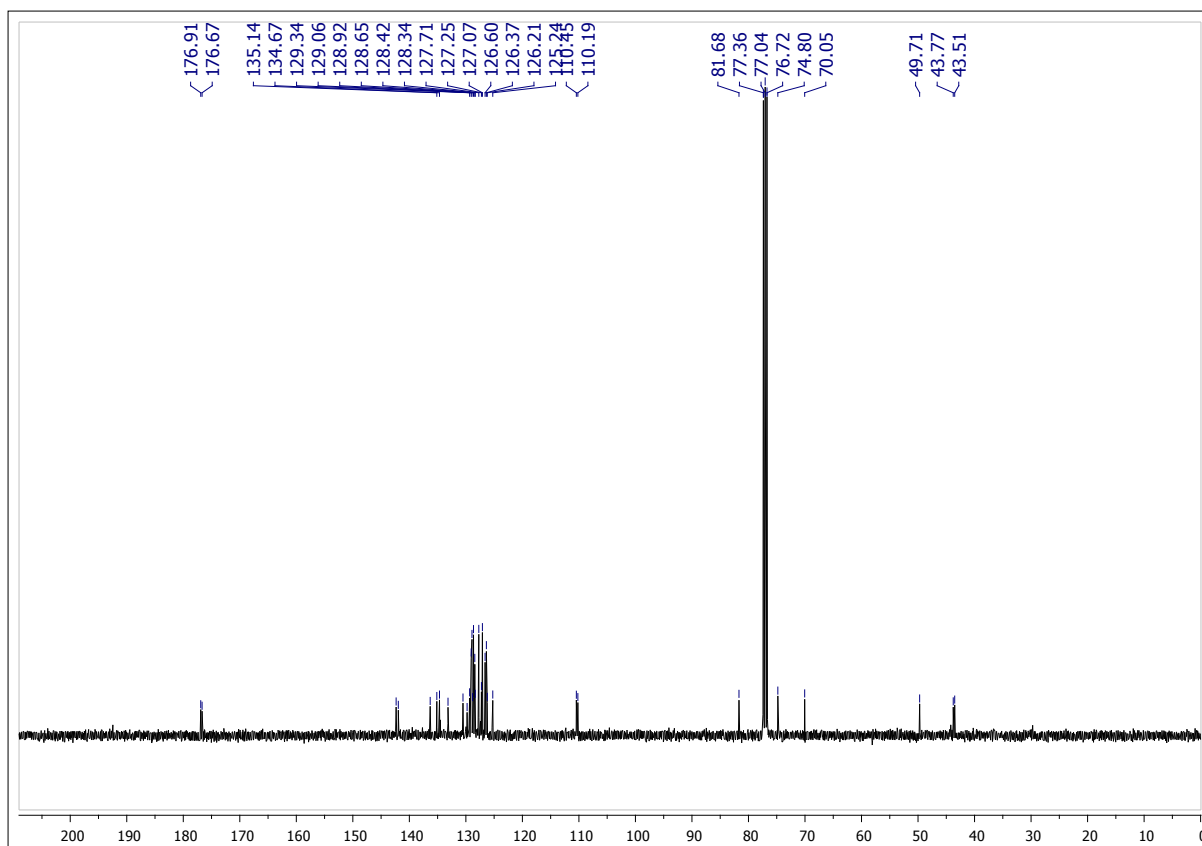


Figure 11. ^{13}C NMR spectrum of compound **3d**

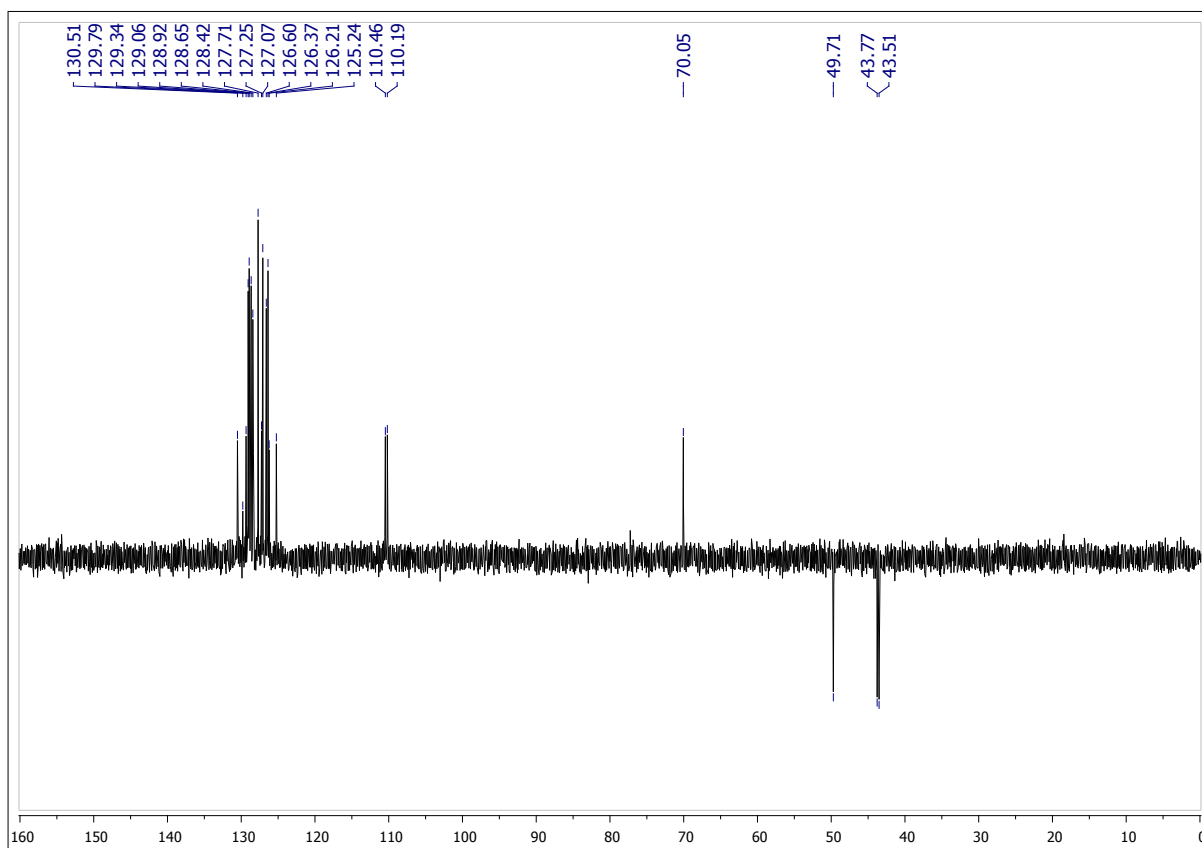


Figure 12. DEPT-135 spectrum of compound **3d**

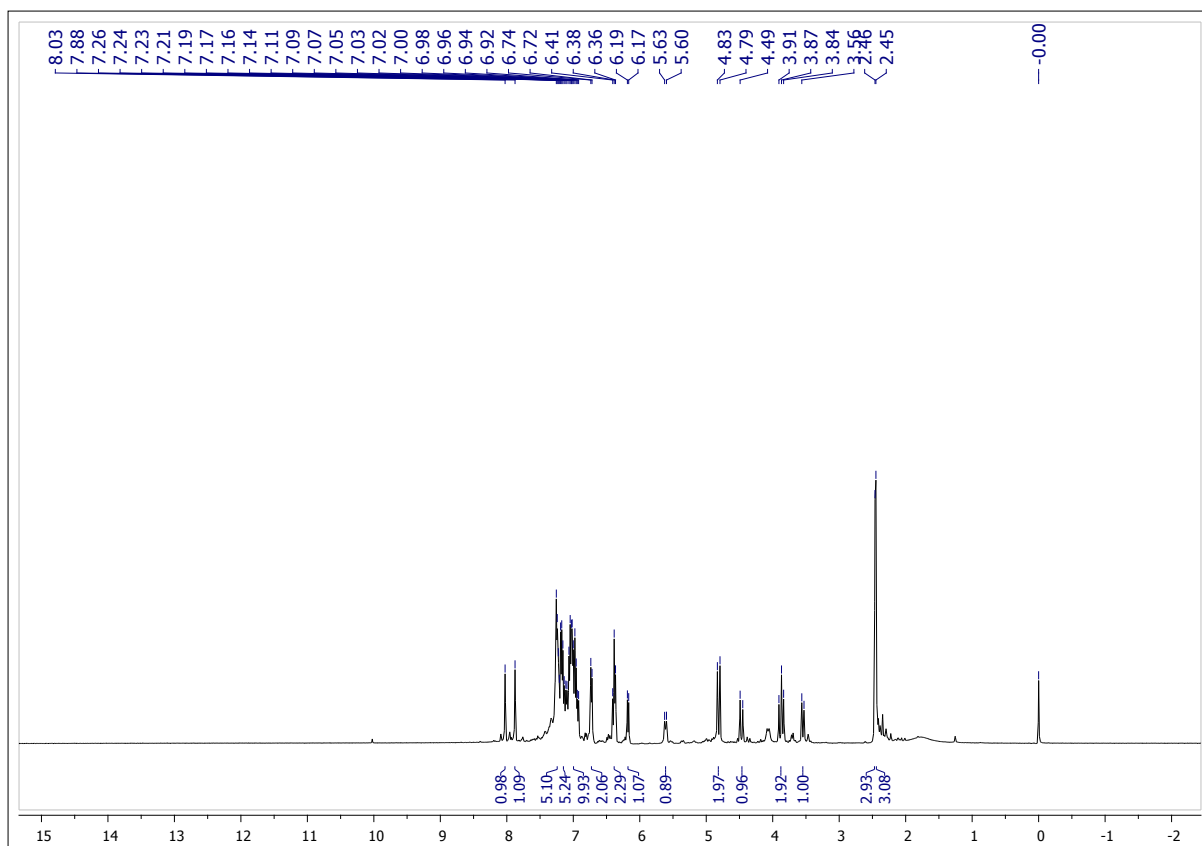


Figure 13. ^1H NMR spectrum of compound **3e**

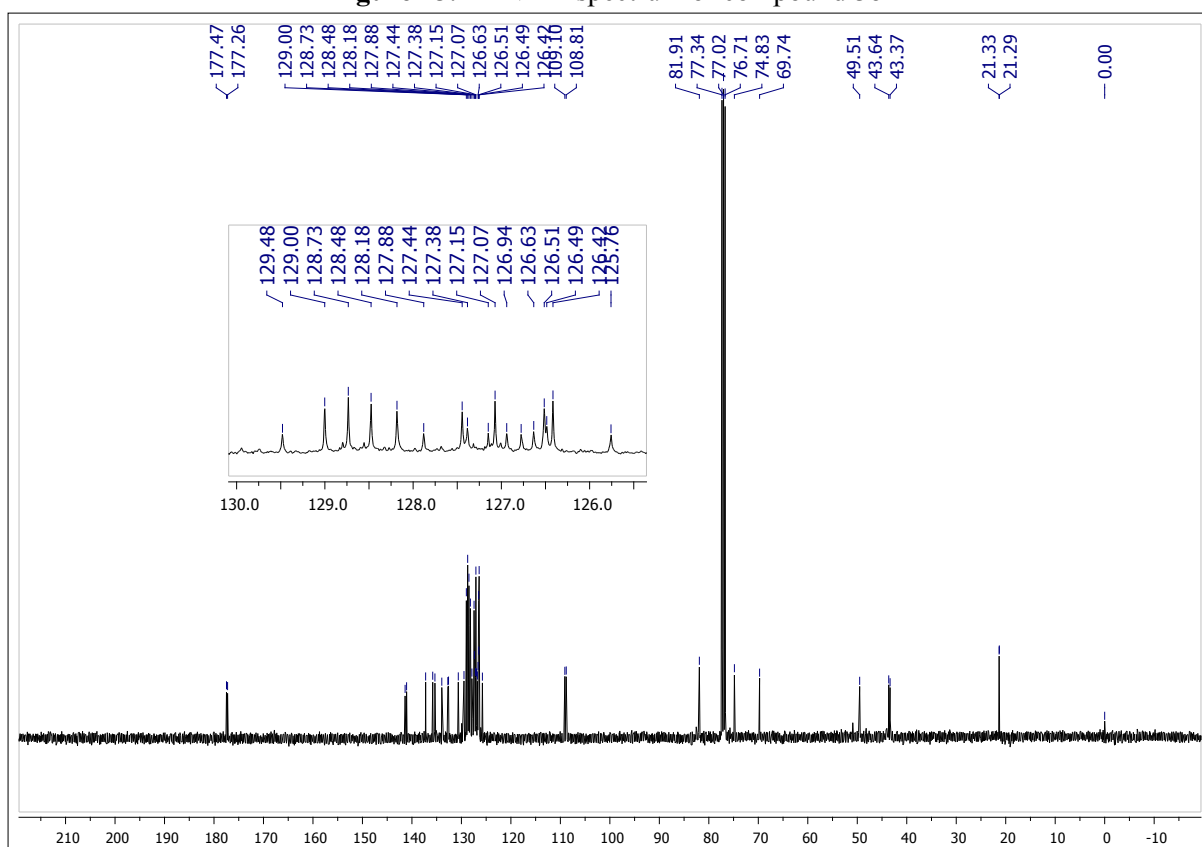


Figure 14. ^{13}C NMR spectrum of compound **3e**

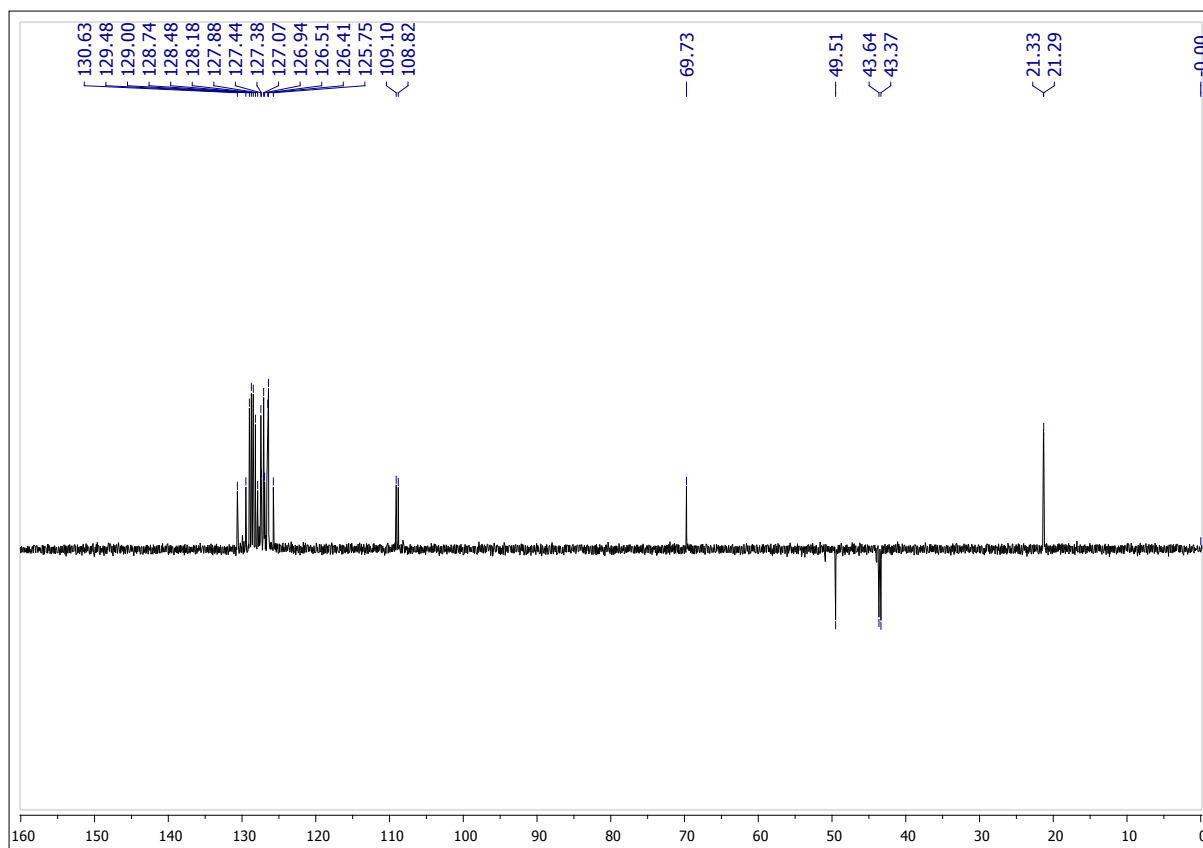


Figure 15. DEPT-135 spectrum of compound 3e

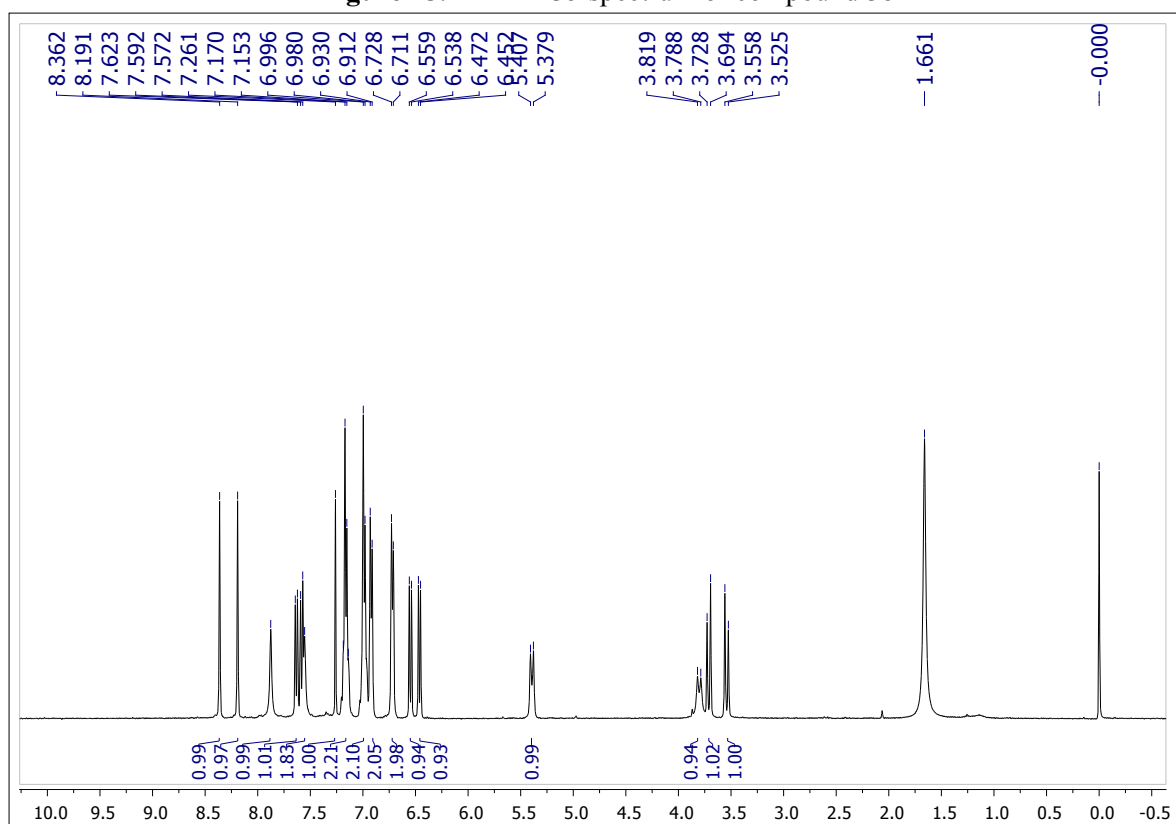


Figure 16: ^1H NMR spectrum of compound 3f

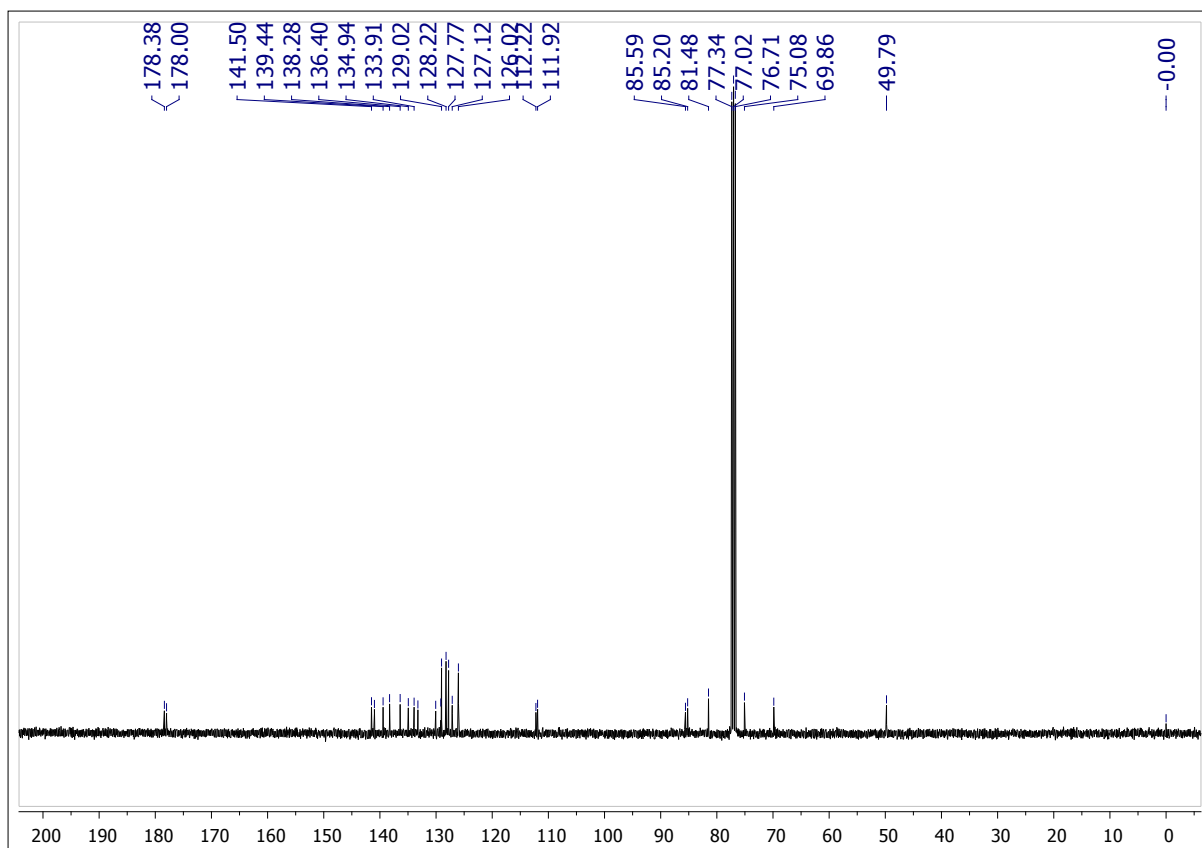


Figure 17. ^{13}C NMR spectrum of compound **3f**

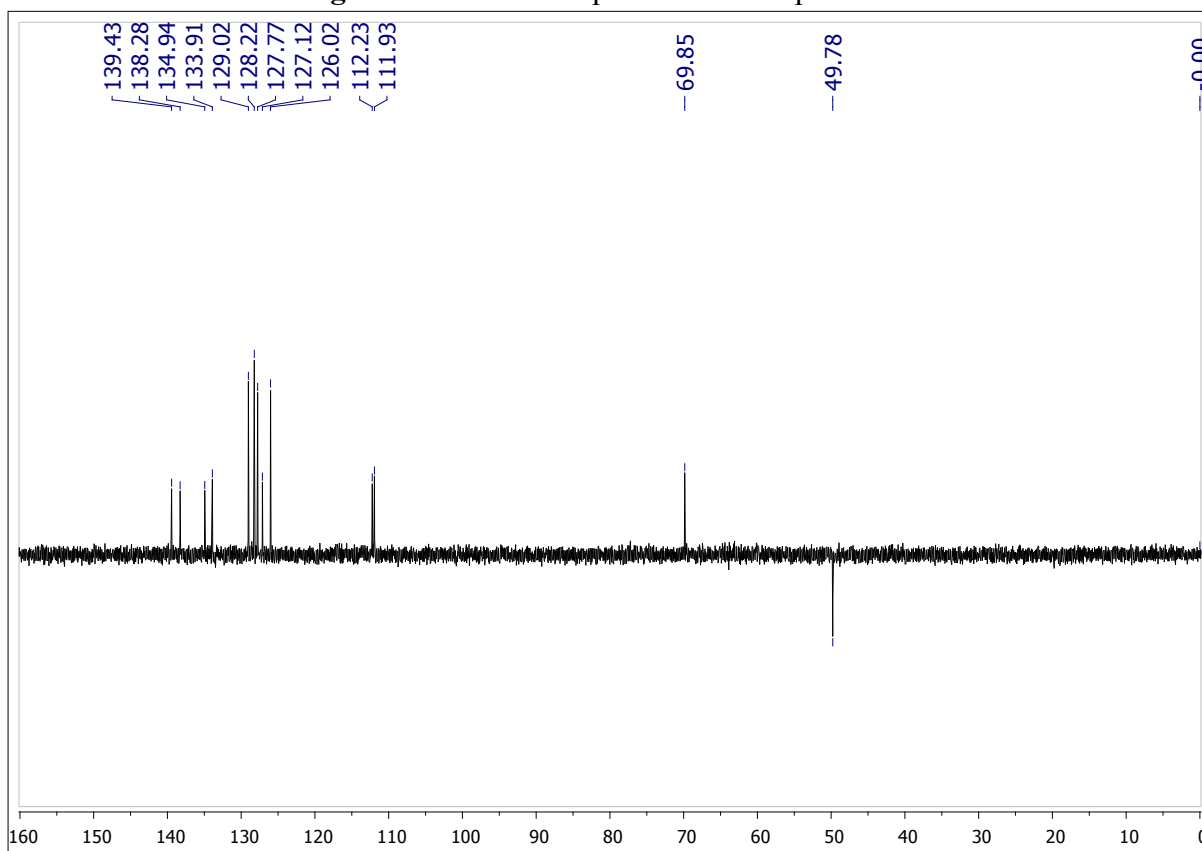


Figure 18. DEPT-135 spectrum of compound **3f**

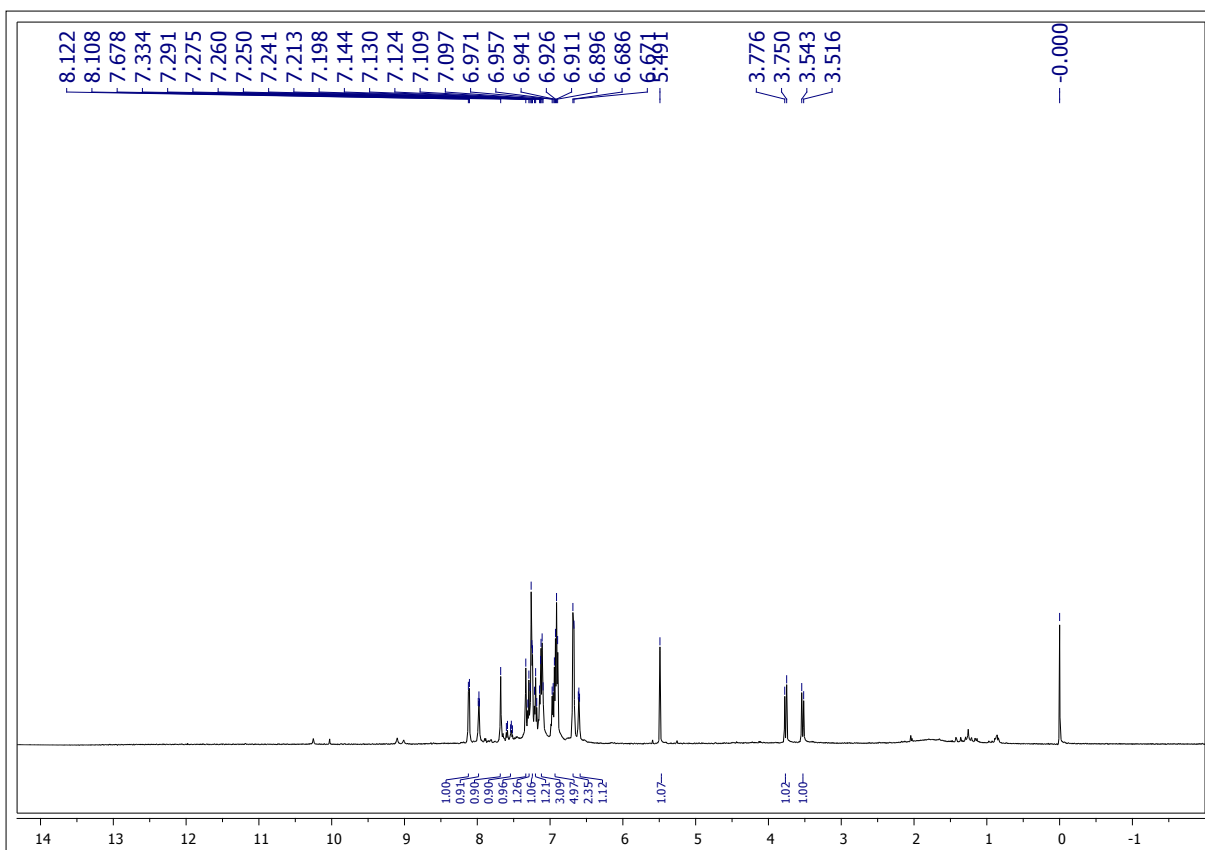


Figure 19. ^1H NMR spectrum of compound **3g**

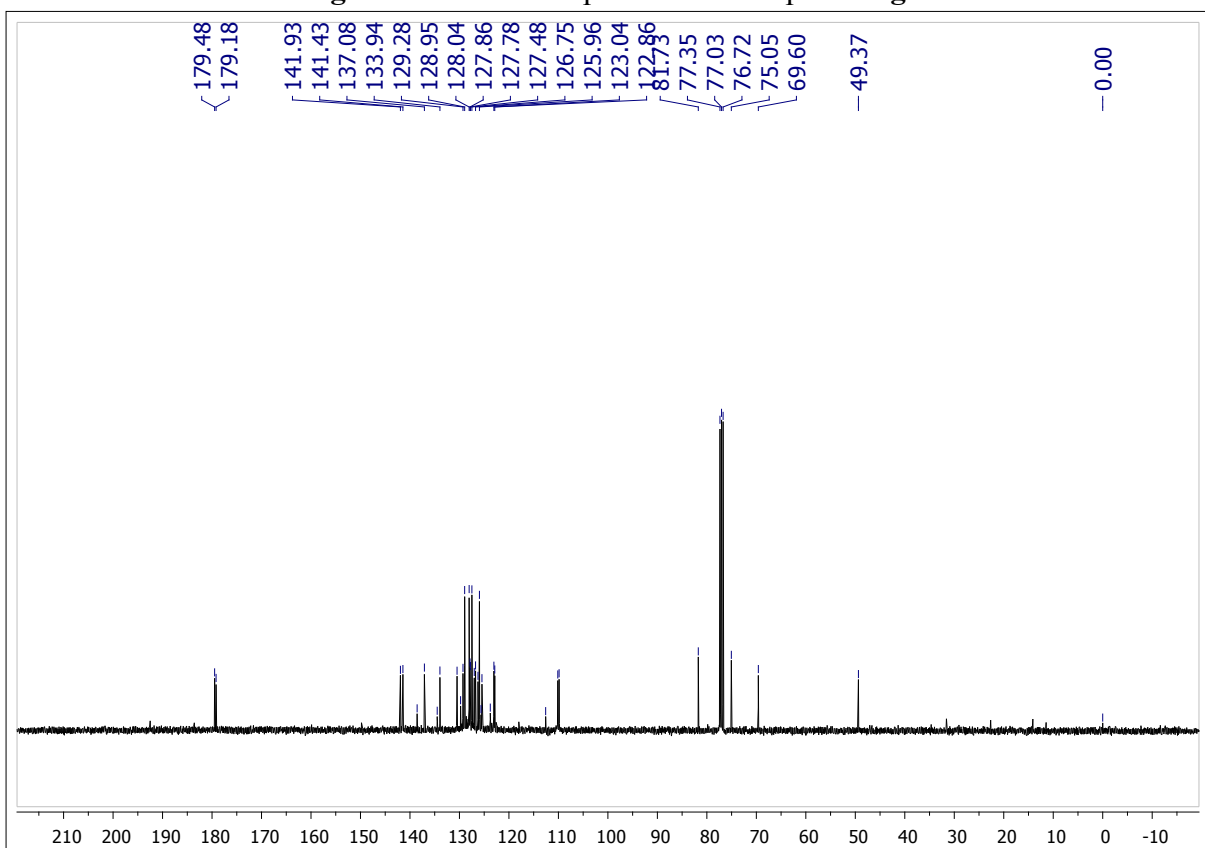


Figure 20. ^{13}C NMR spectrum of compound **3g**

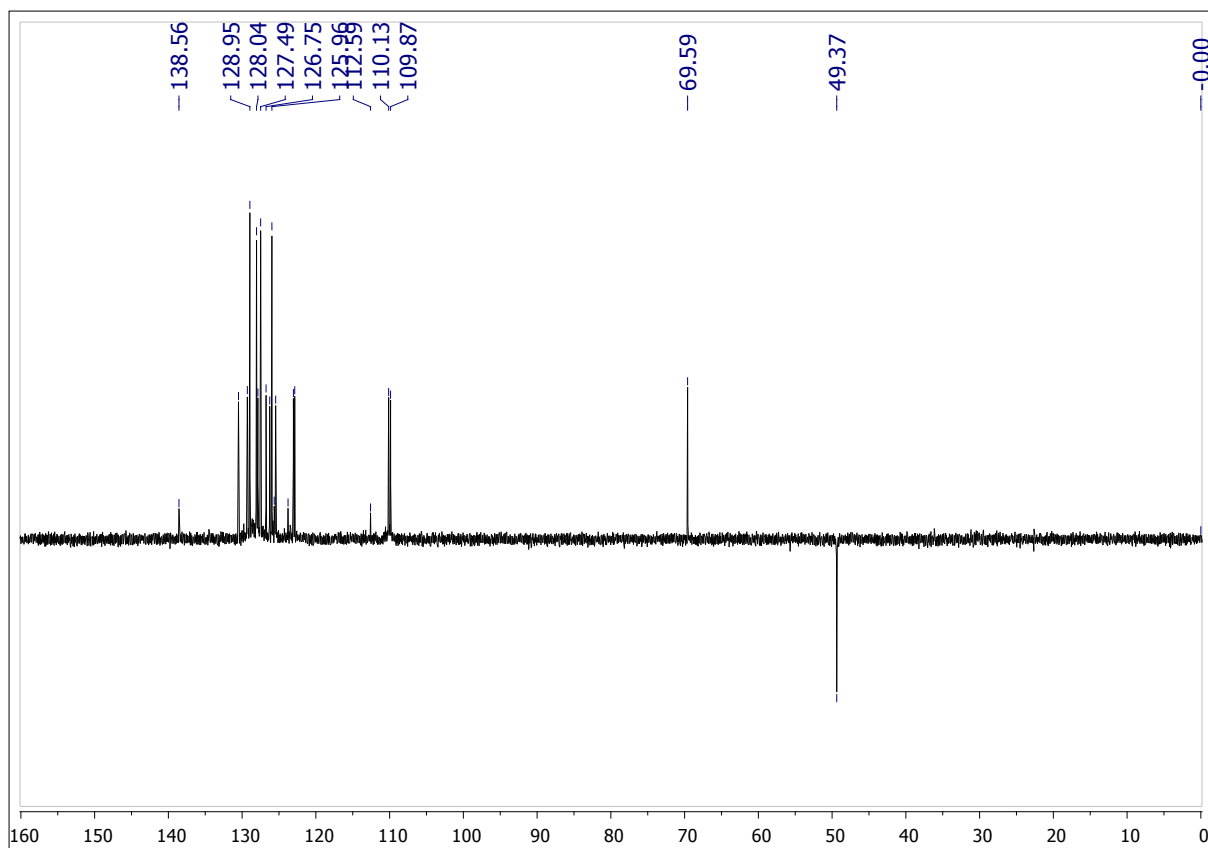


Figure 21. DEPT-135 spectrum of compound 3g

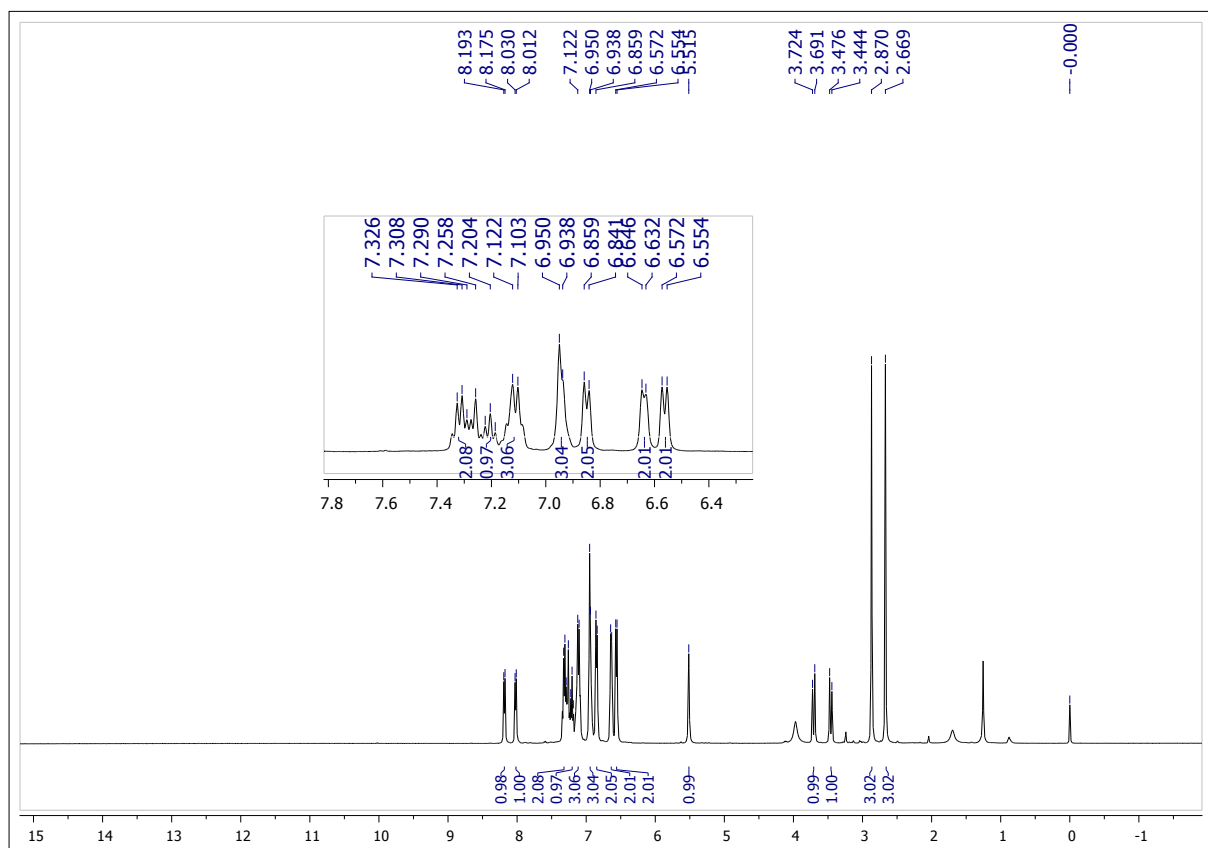


Figure 22. ¹H NMR spectrum of compound 3h

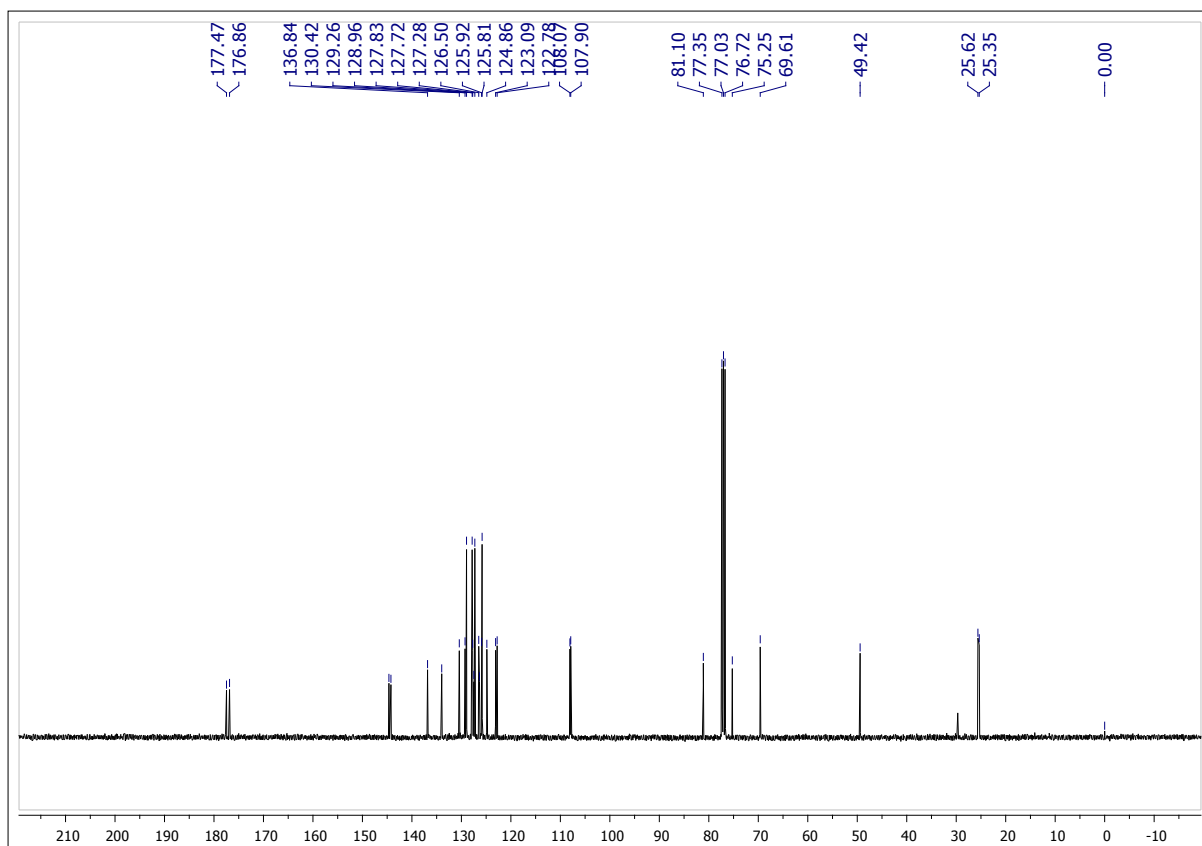


Figure 23. ^{13}C NMR spectrum of compound **3h**

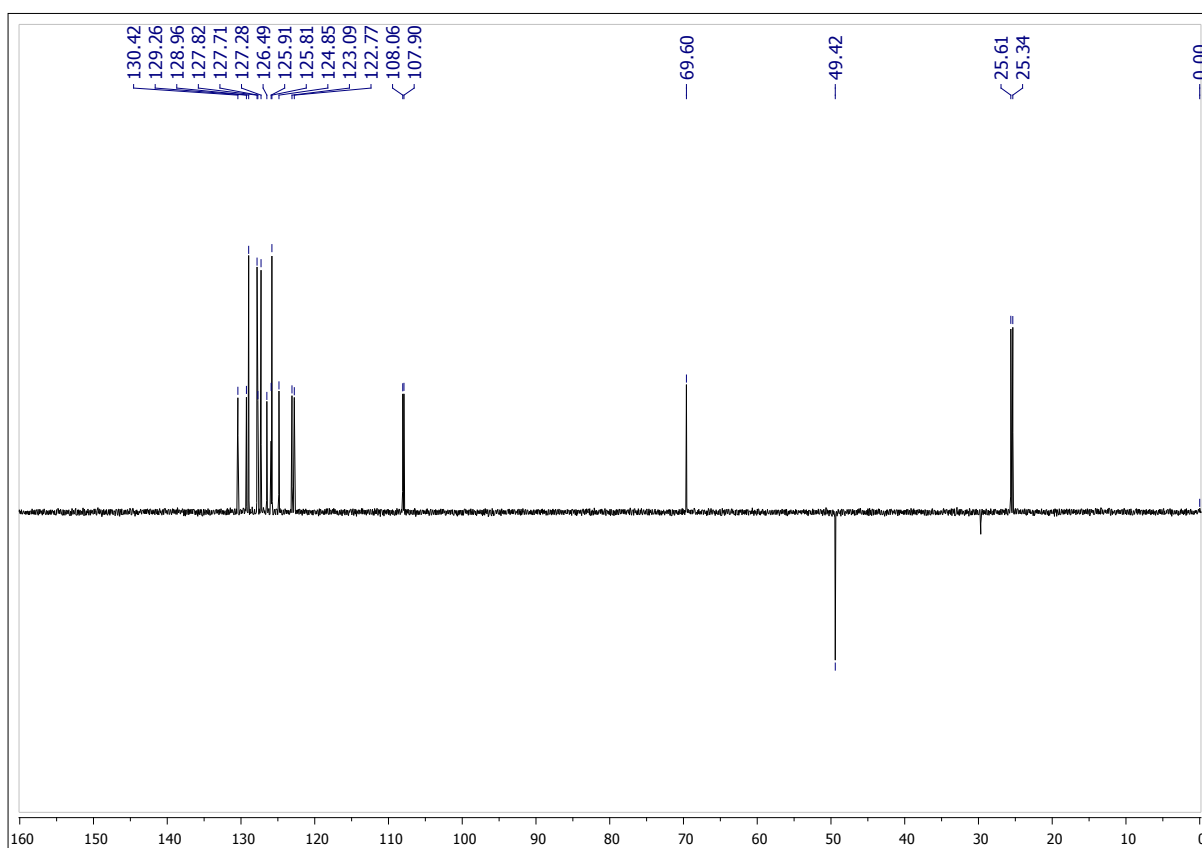


Figure 24. DEPT-135 spectrum of compound **3h**

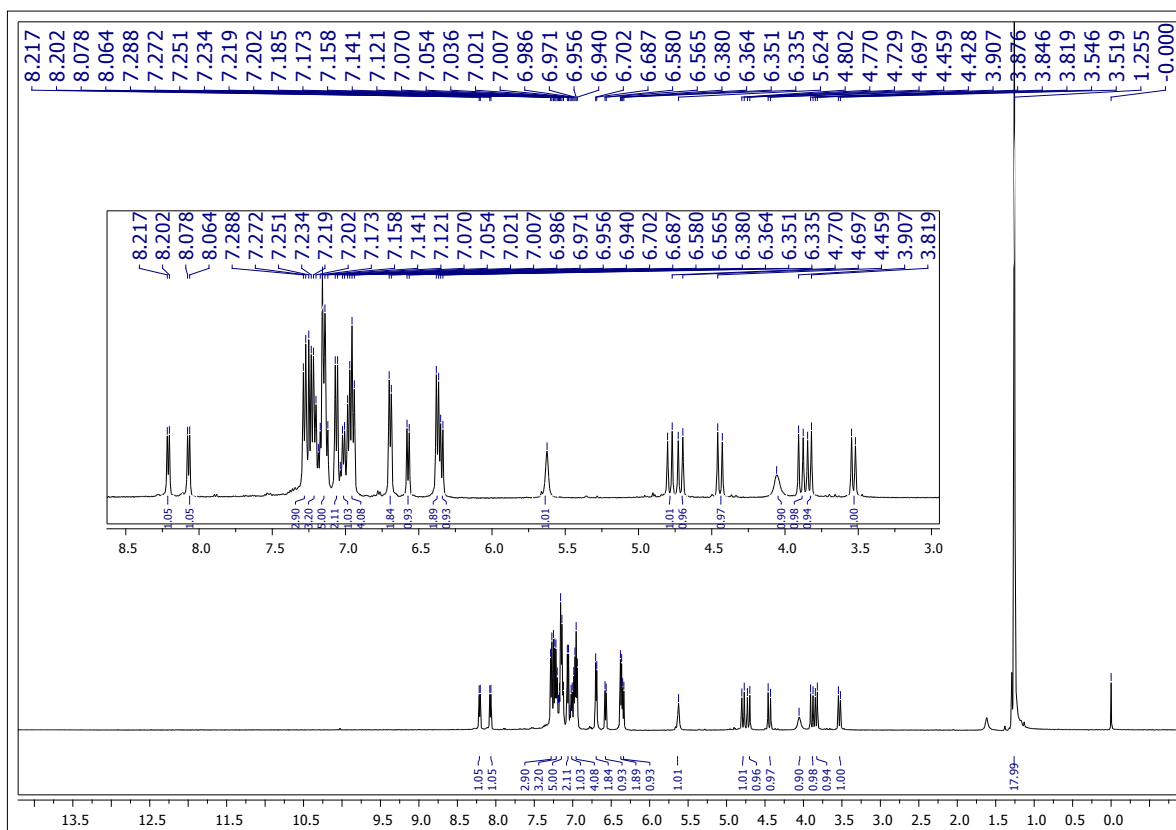


Figure 25. ^1H NMR spectrum of compound **3i**

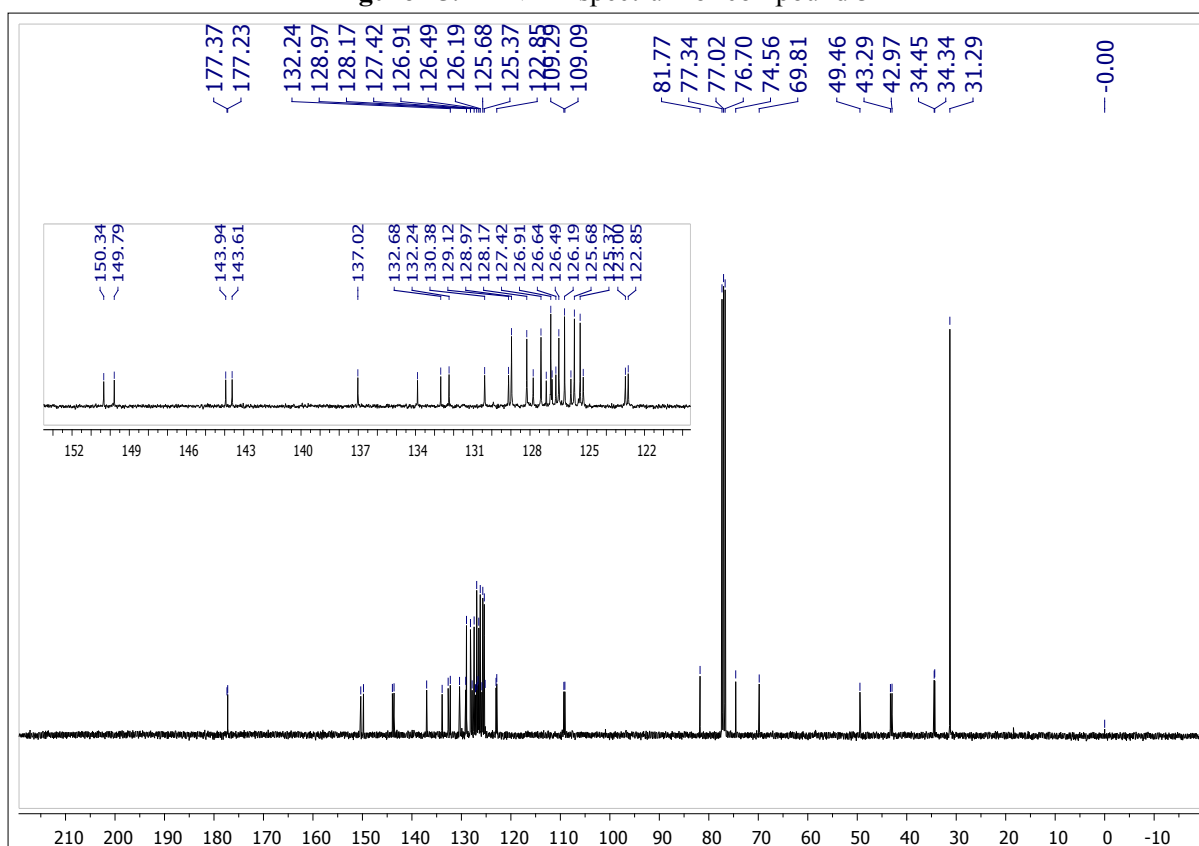


Figure 26. ^{13}C NMR spectrum of compound **3i**

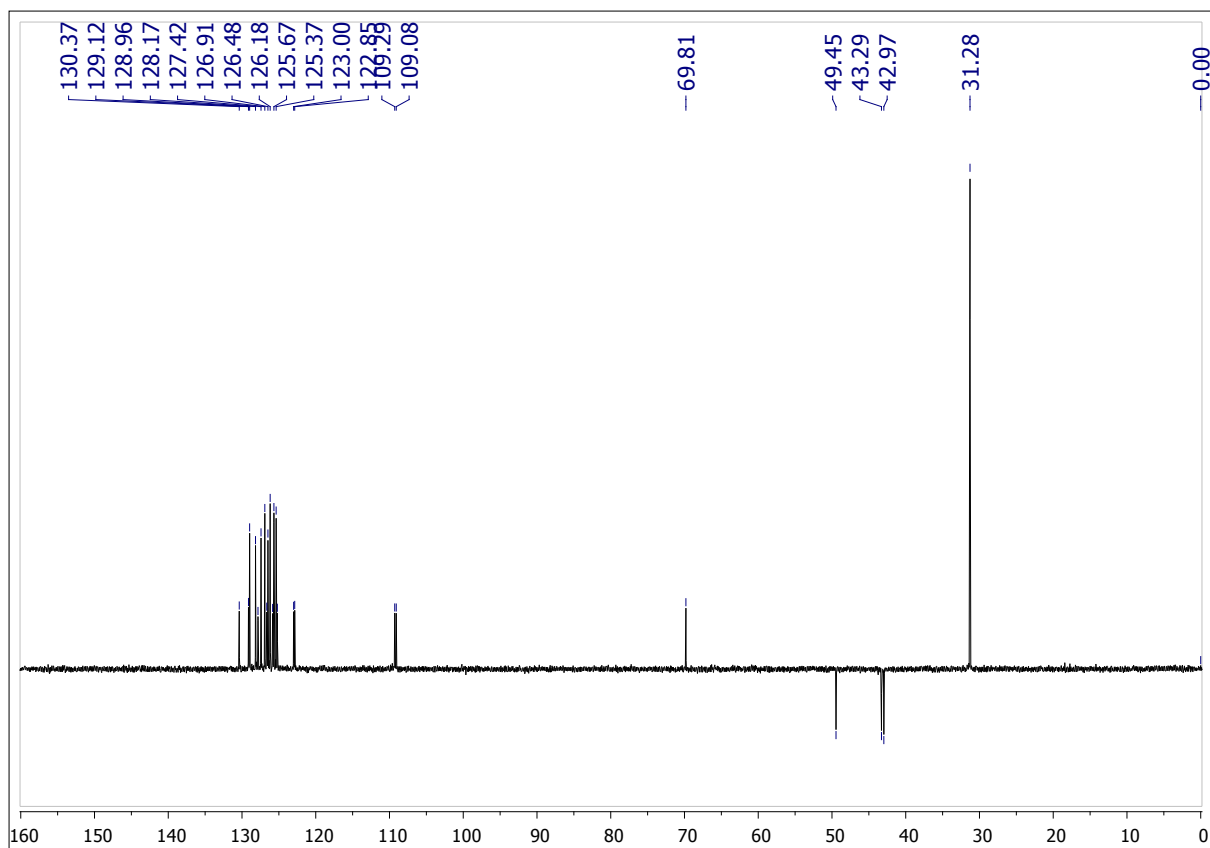


Figure 27. DEPT-135 spectrum of compound **3i**

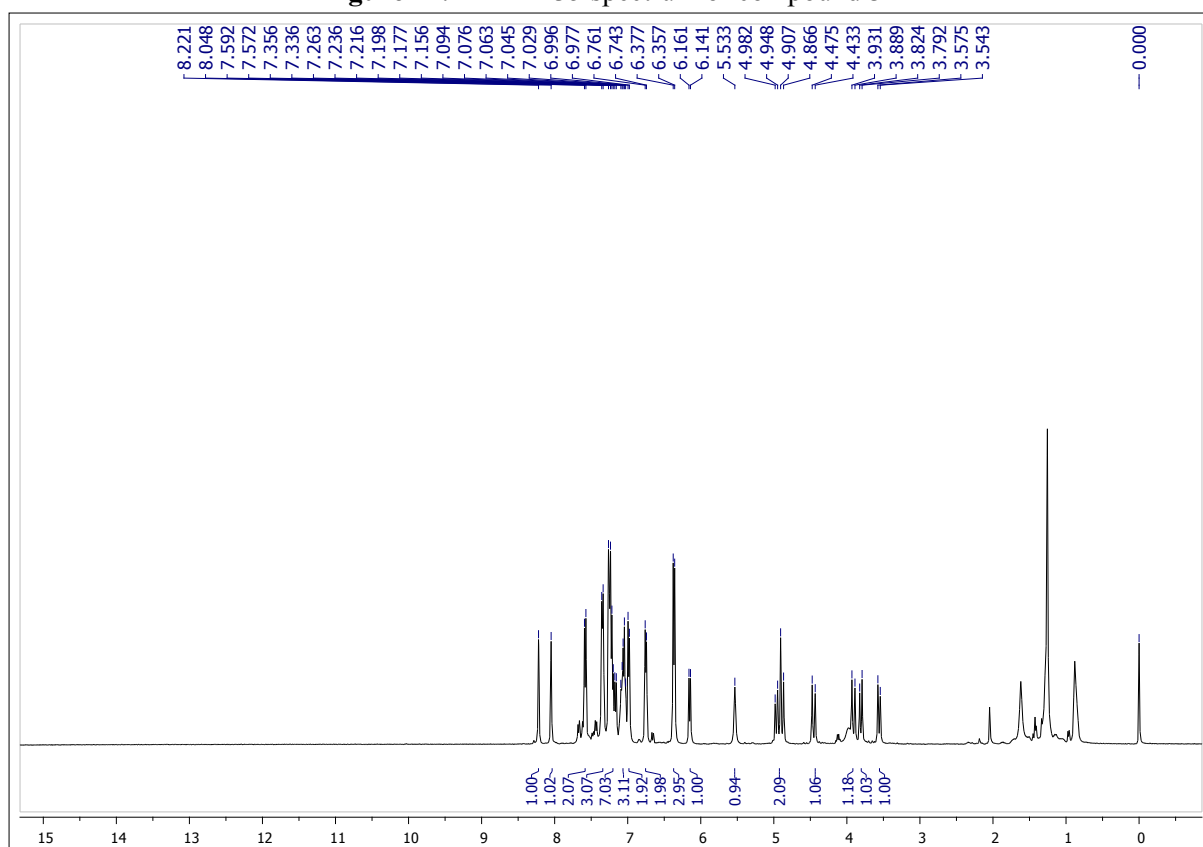


Figure 28. ¹H NMR spectrum of compound **3j**

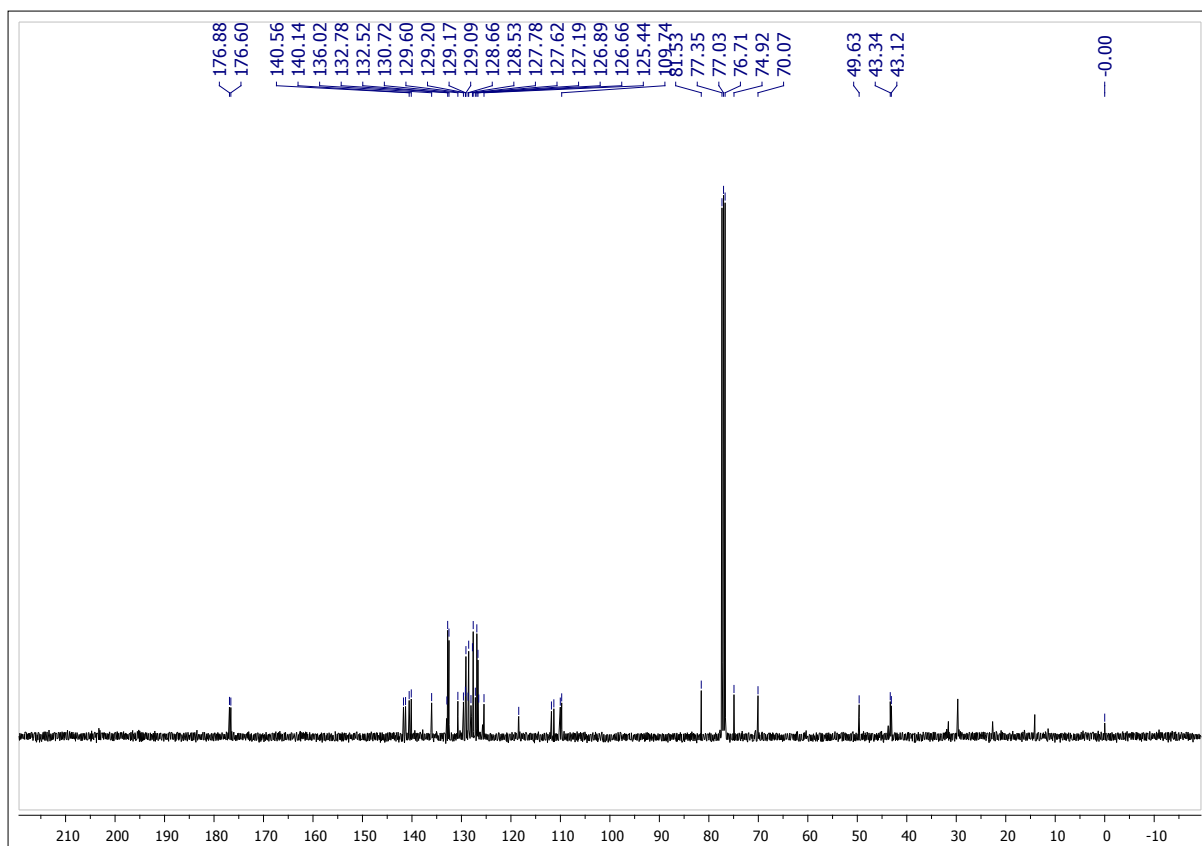


Figure 29. ^{13}C NMR spectrum of compound **3j**

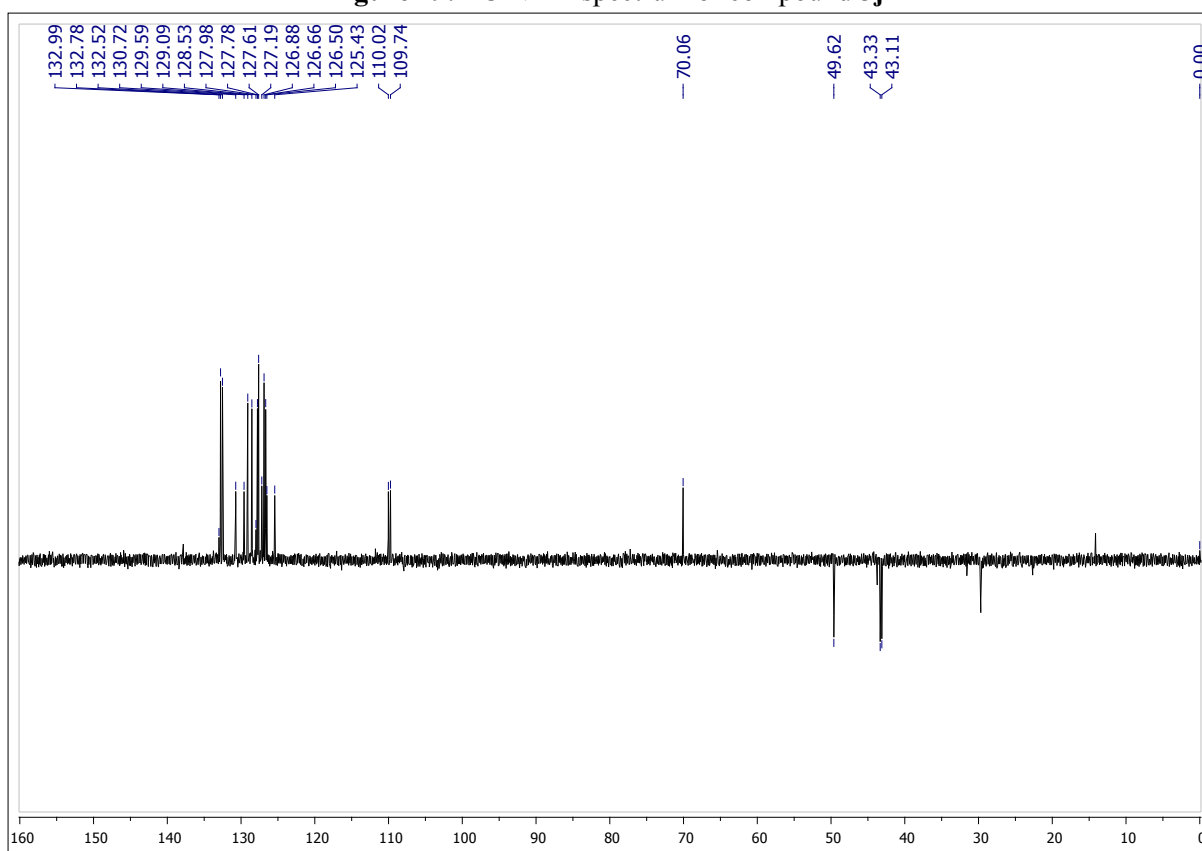


Figure 30. DEPT-135 spectrum of compound **3j**

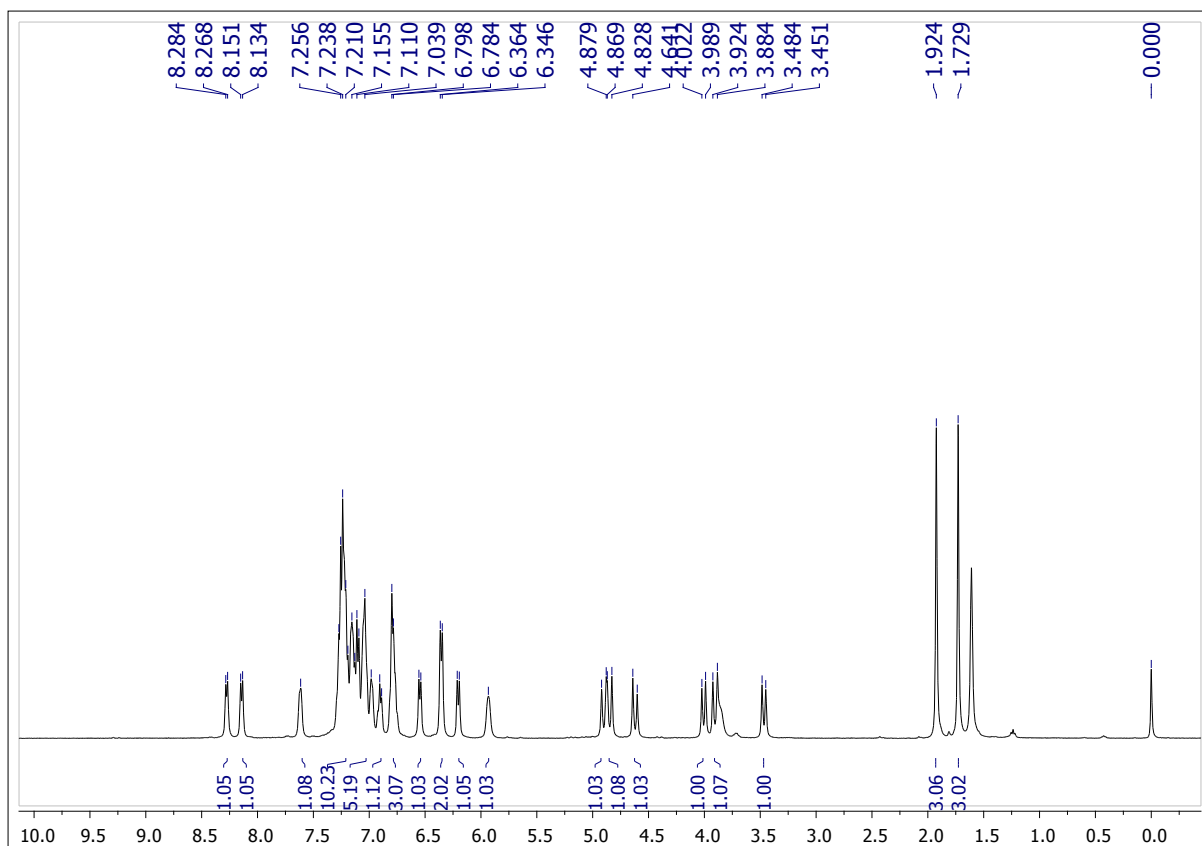


Figure 31. ^1H NMR spectrum of compound **3k**

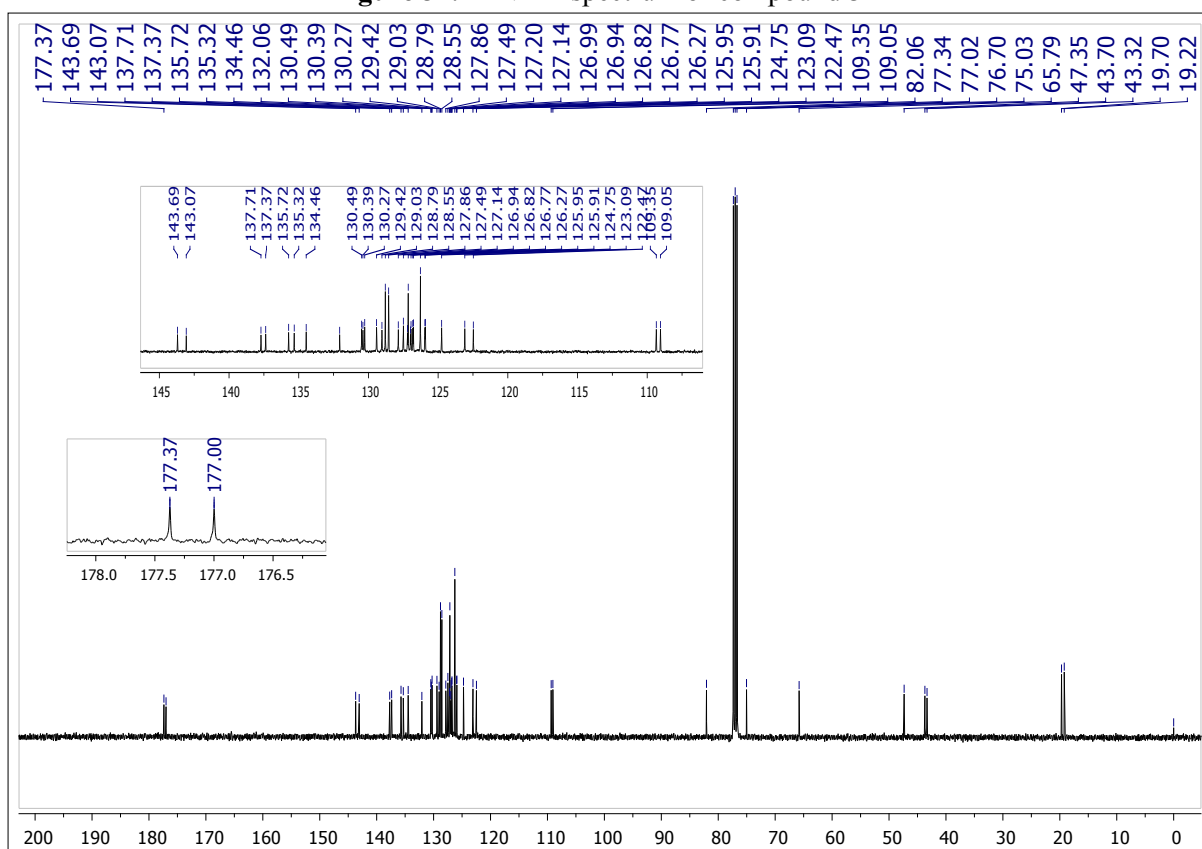


Figure 32. ^{13}C NMR spectrum of compound **3k**

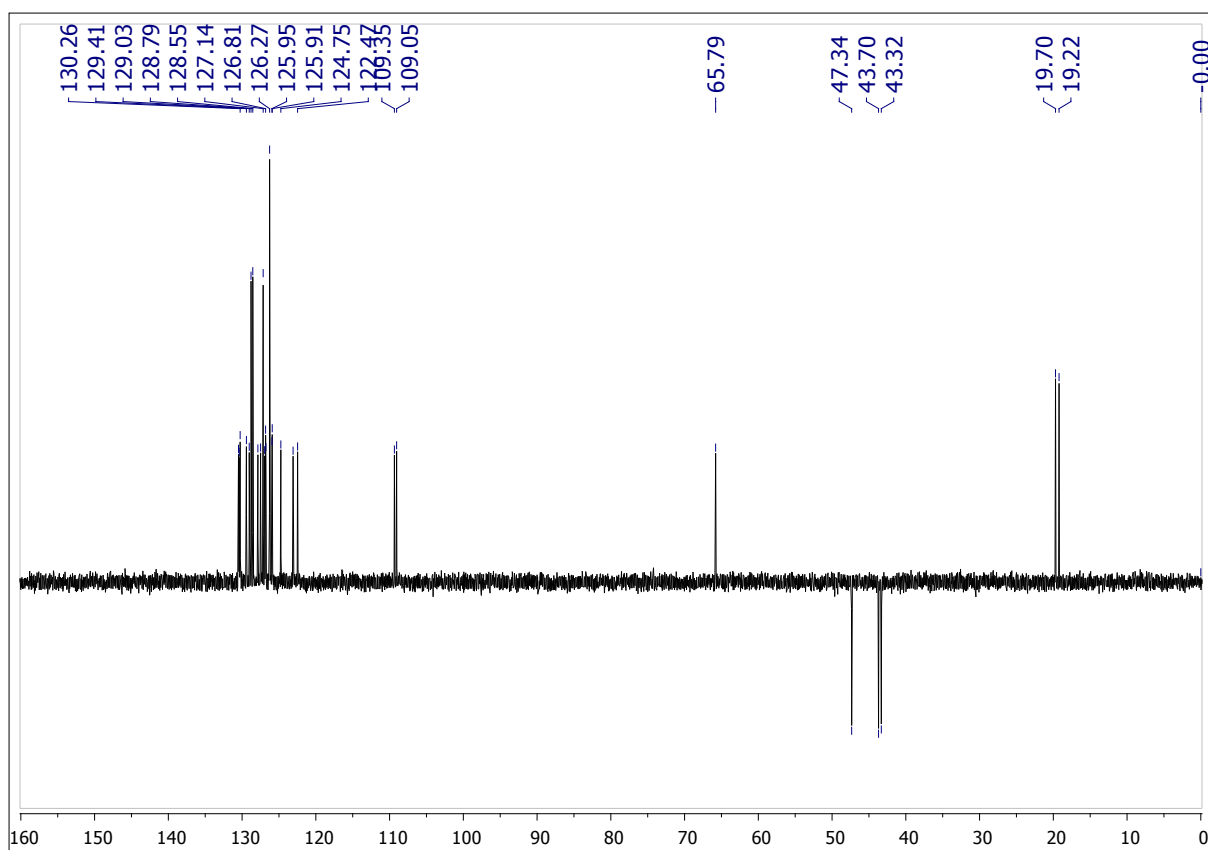


Figure 33. DEPT-135 spectrum of compound 3k

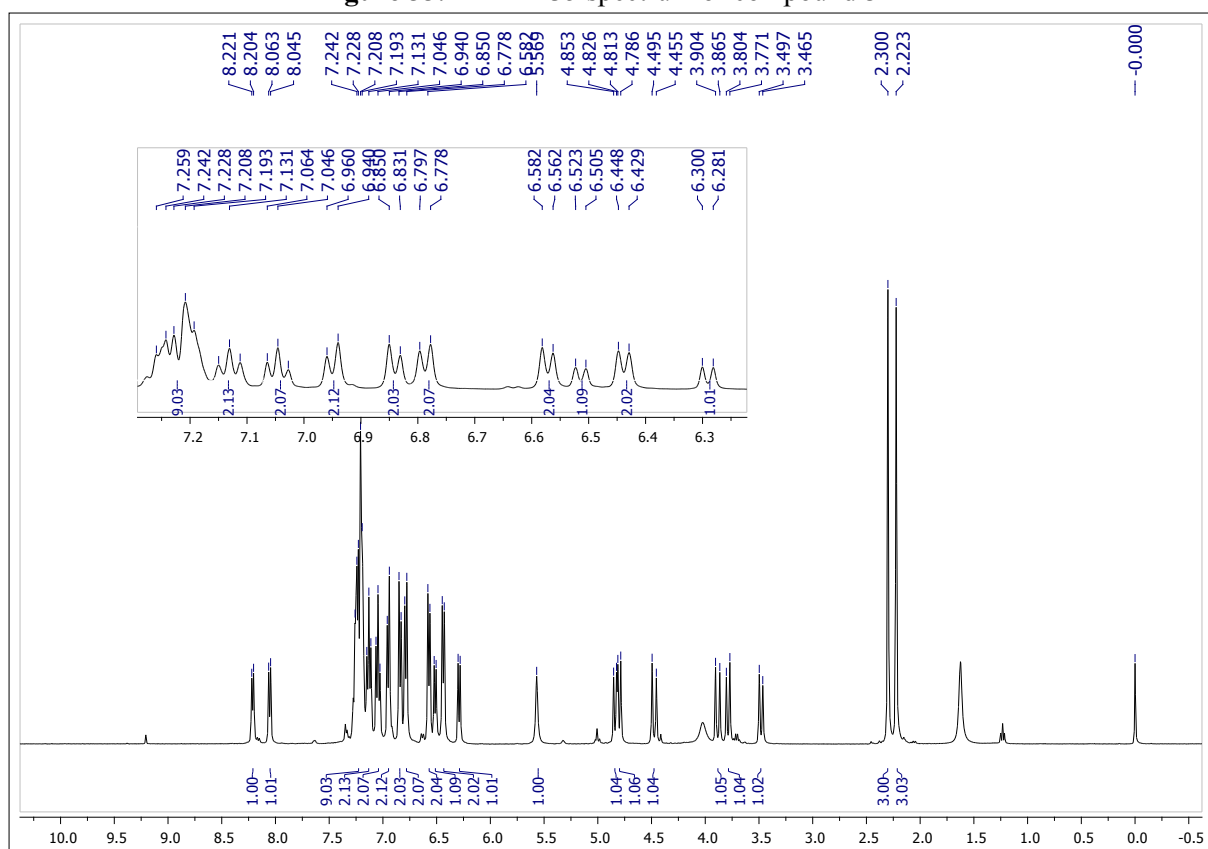


Figure 34. ¹H NMR spectrum of compound 3l

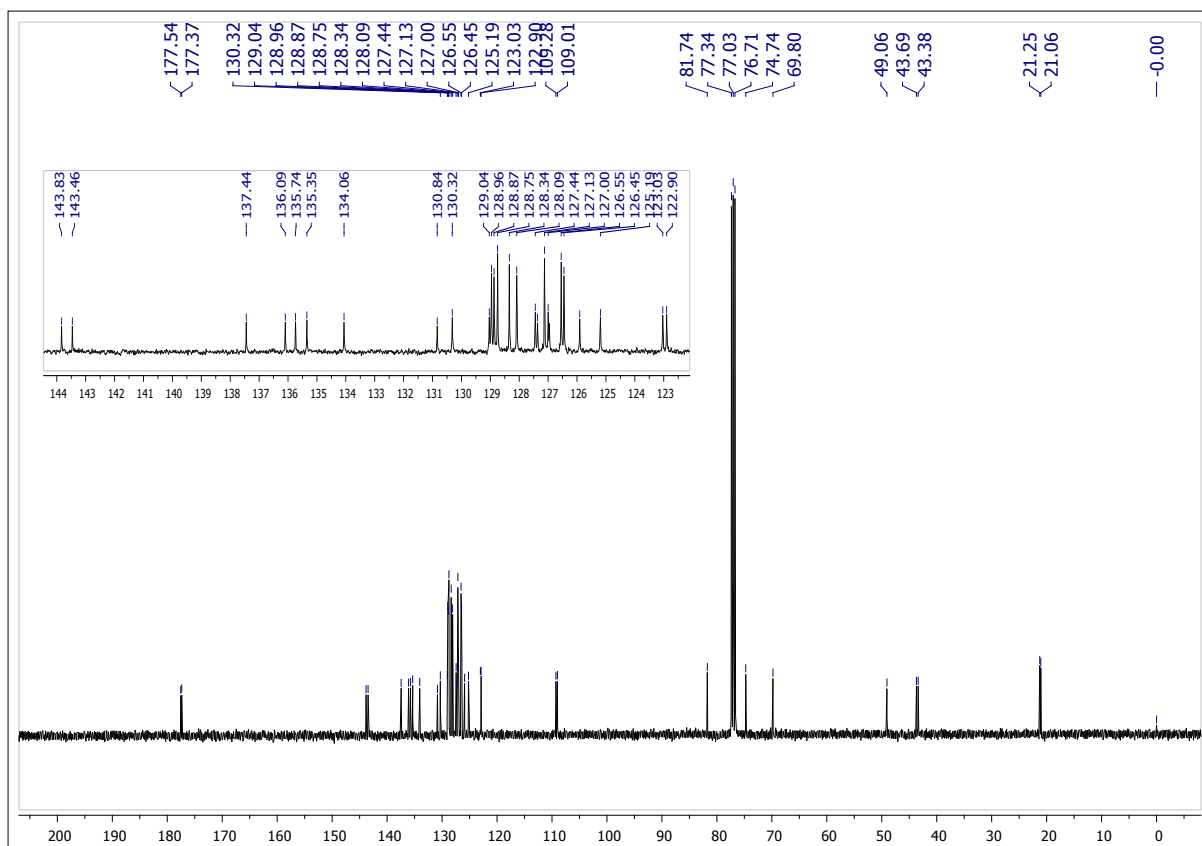


Figure 35. ^{13}C NMR spectrum of compound **31**

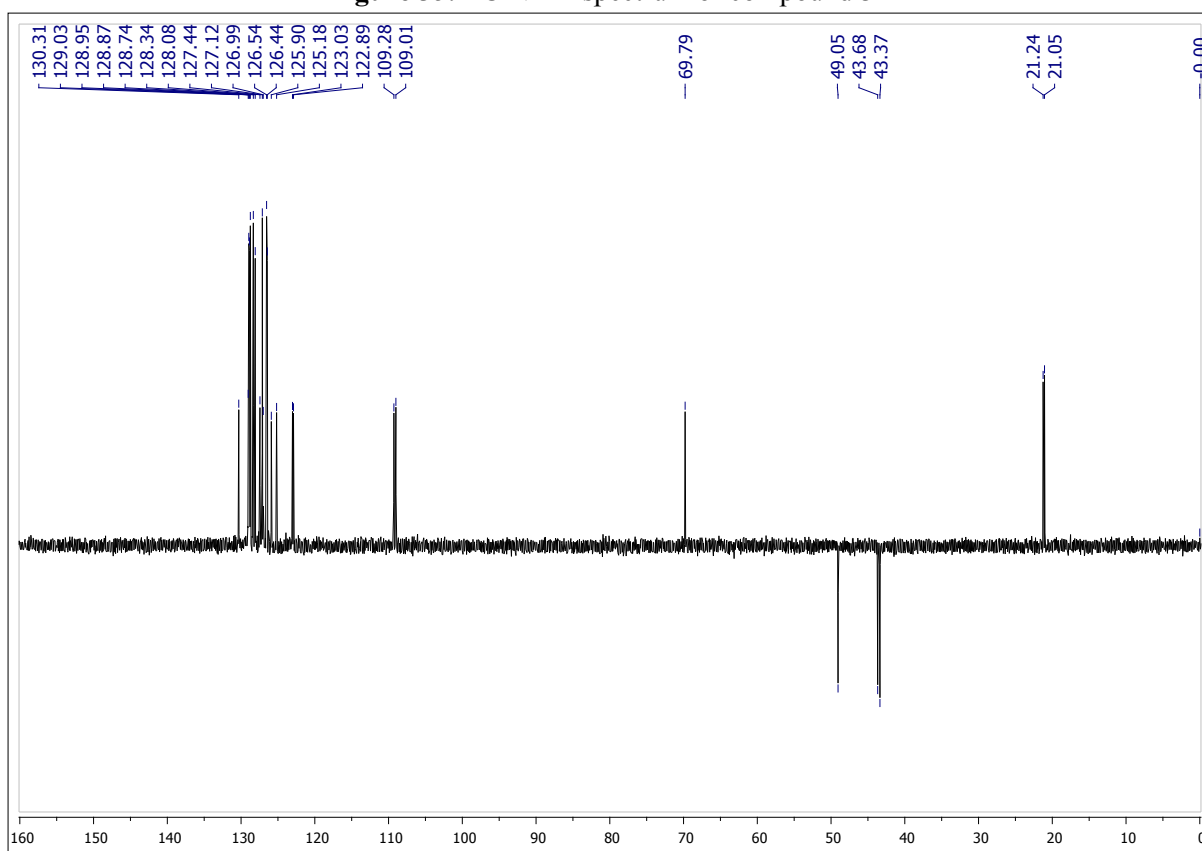


Figure 36. DEPT-135 spectrum of compound **31**

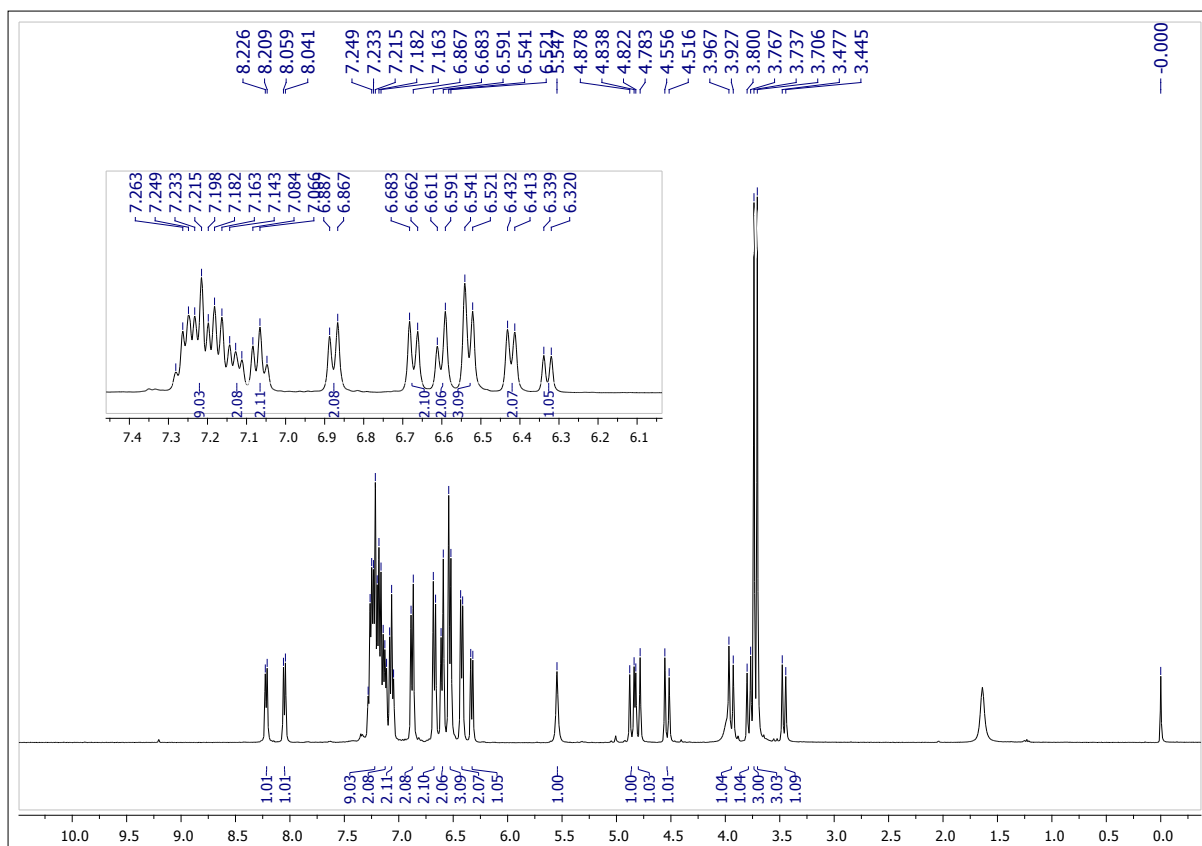


Figure 37. ¹H NMR spectrum of compound 3m

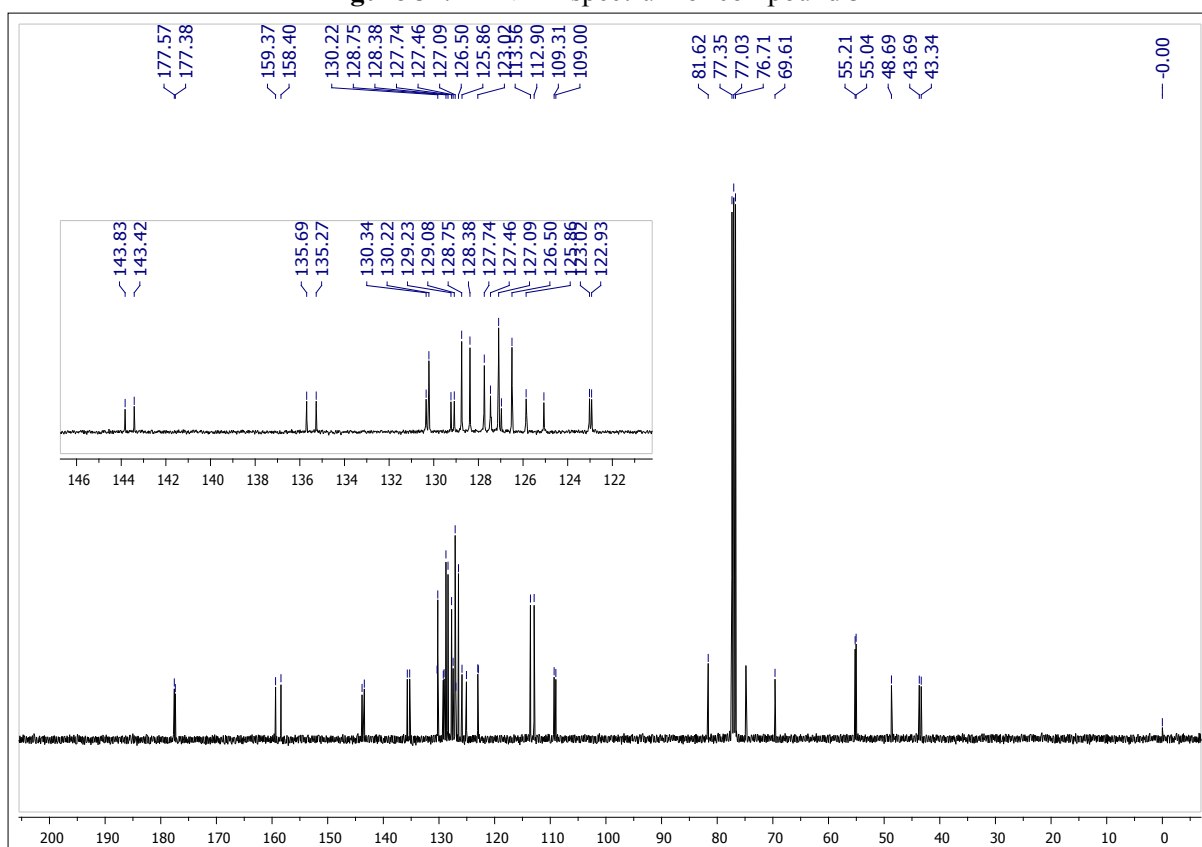


Figure 38. ¹³C NMR spectrum of compound 3m

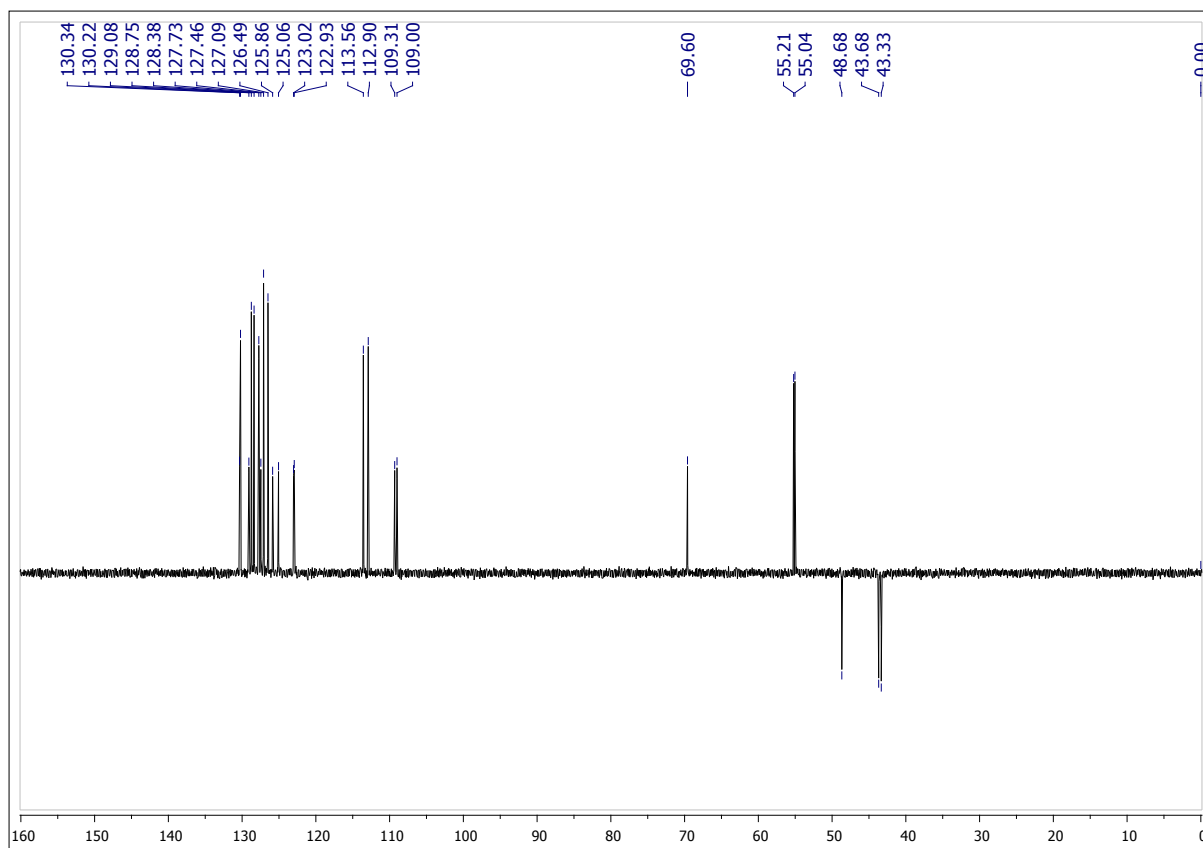


Figure 39. DEPT-135 spectrum of compound 3m

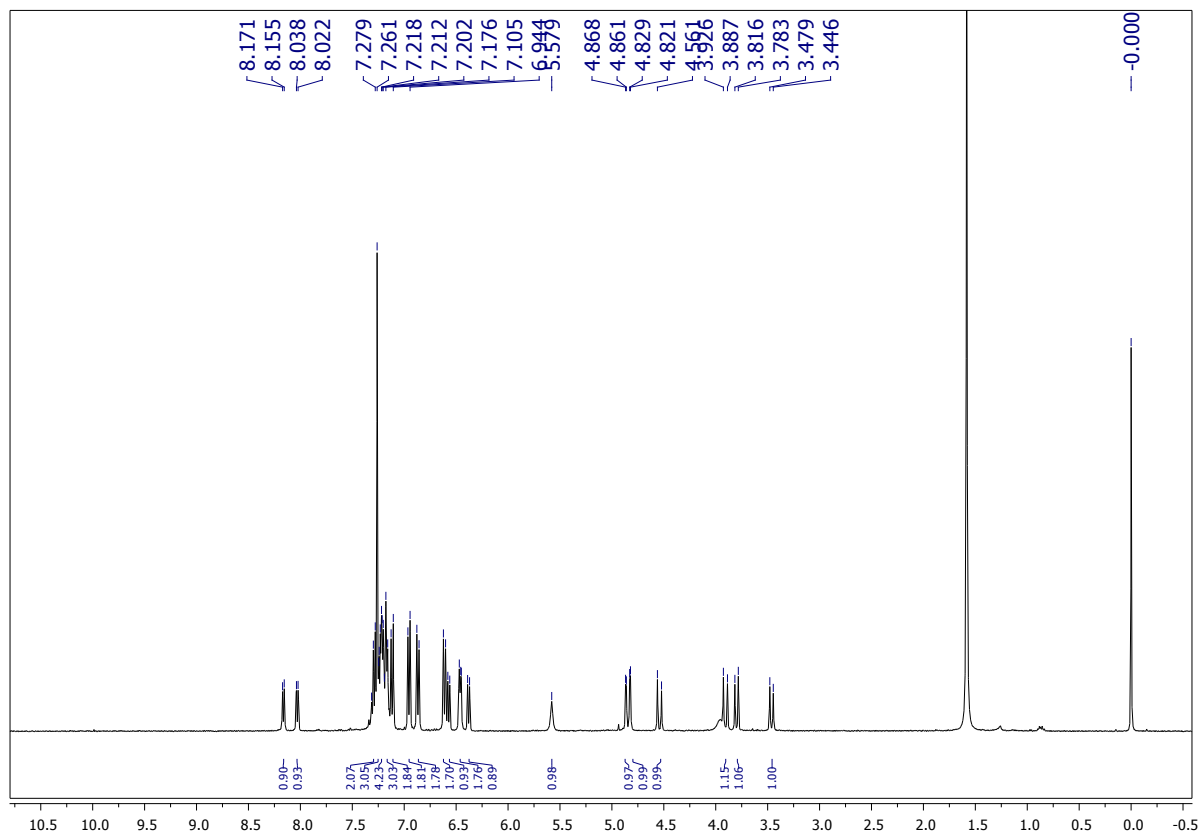


Figure 40. ¹H NMR spectrum of compound 3n

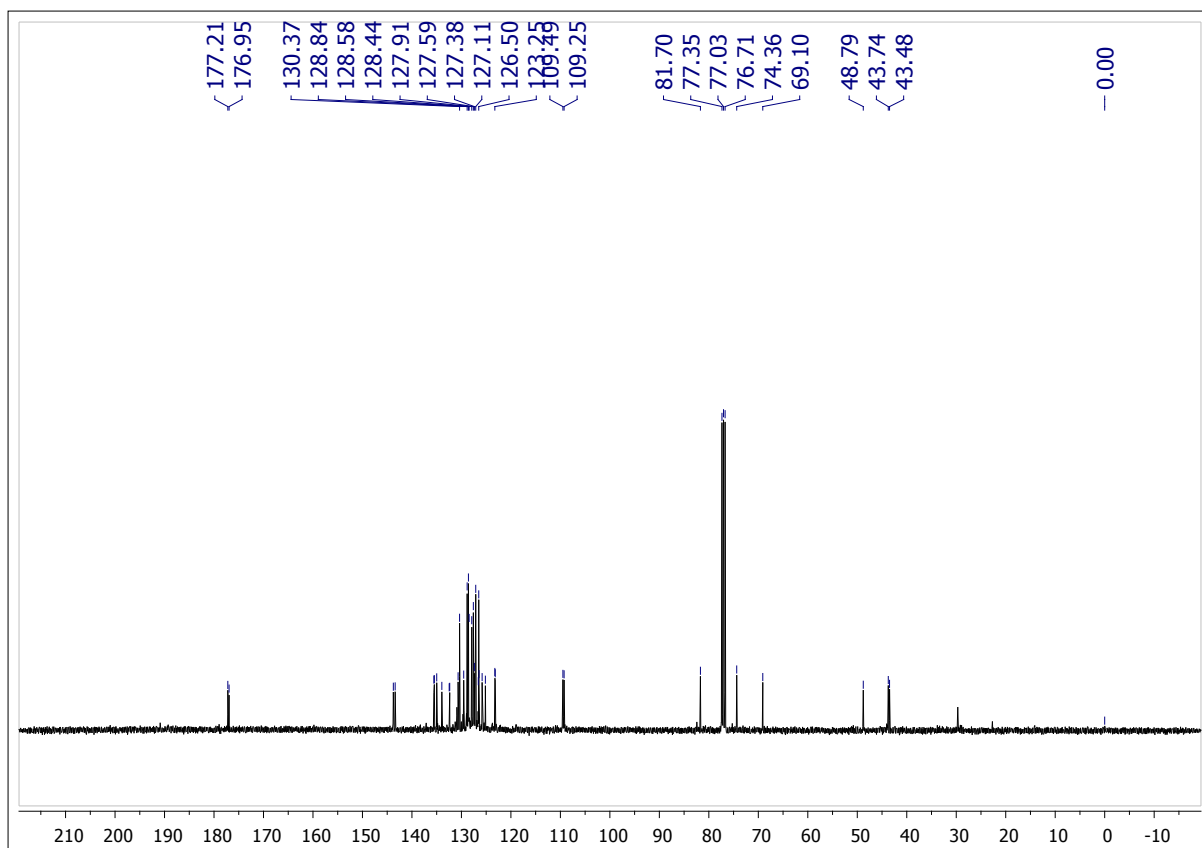


Figure 41. ^{13}C NMR spectrum of compound **3n**

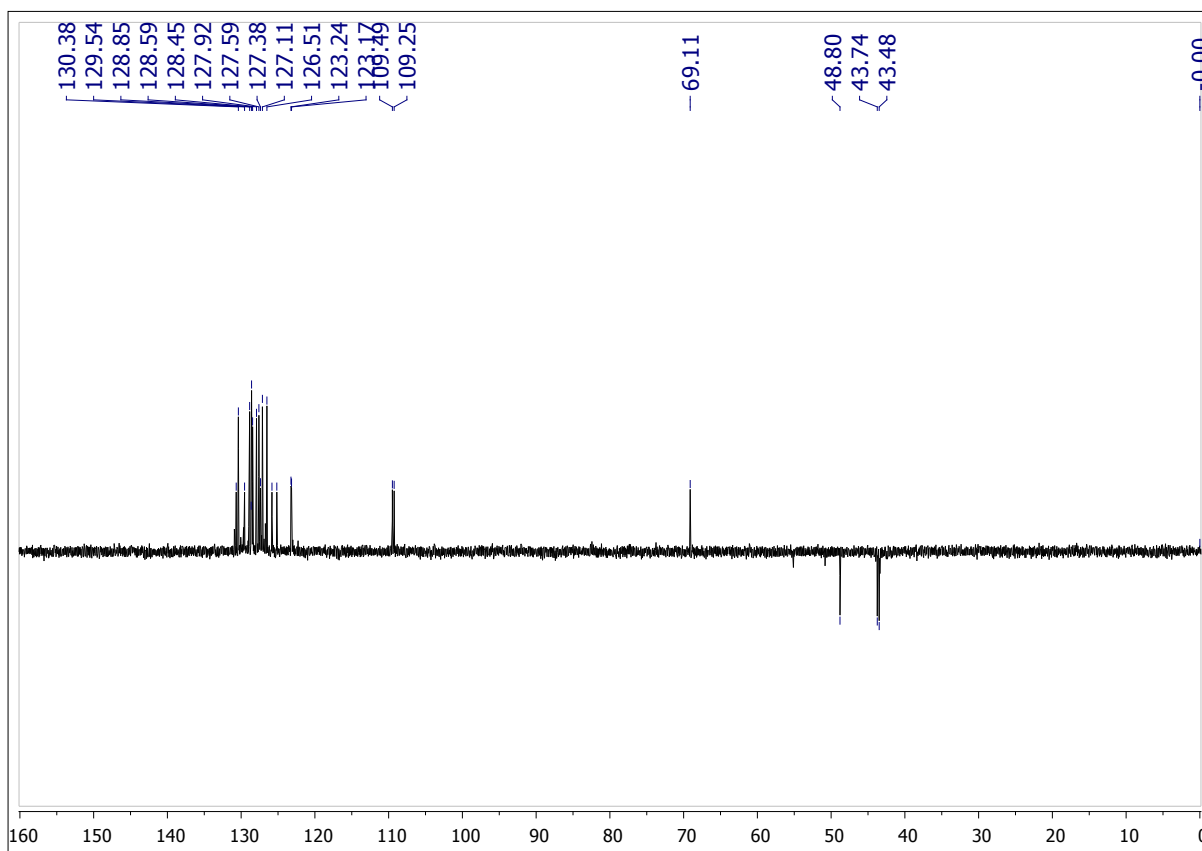


Figure 42. DEPT-135 spectrum of compound **3n**

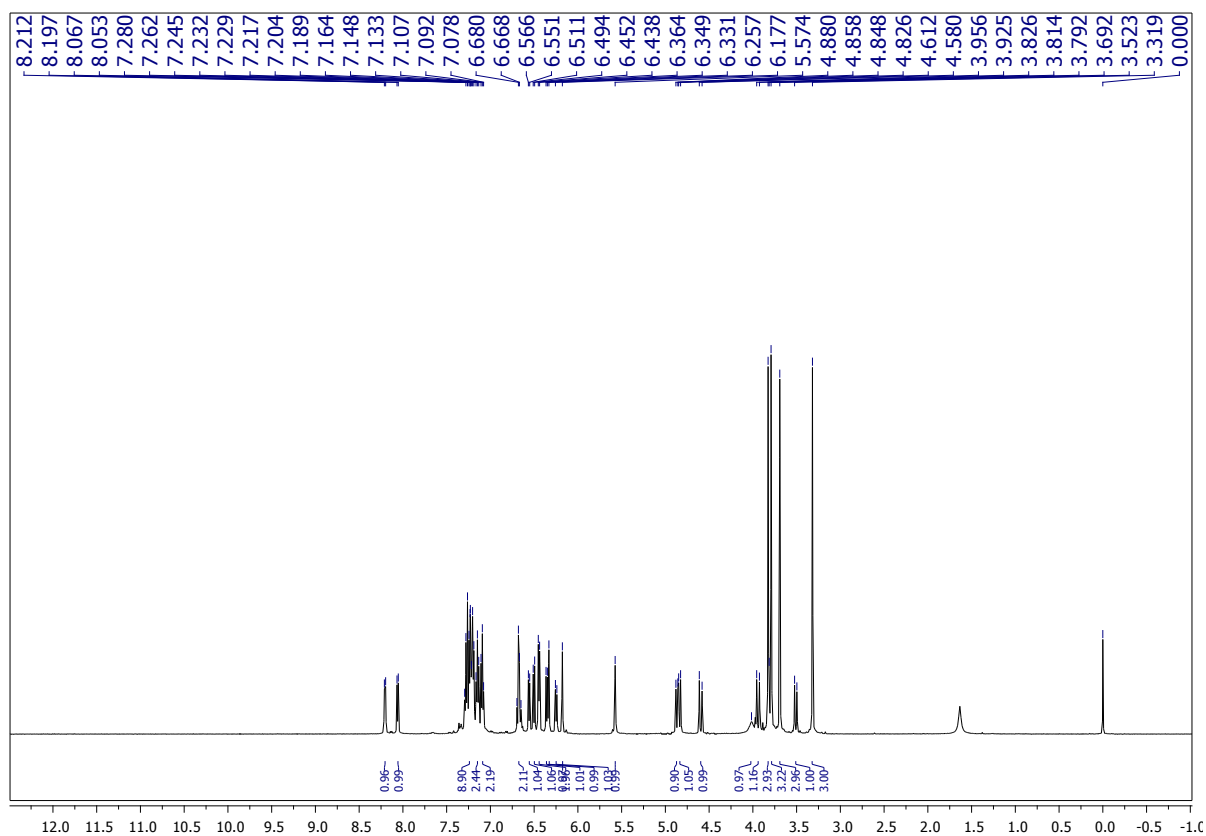


Figure 43. ¹H NMR spectrum of compound 3o

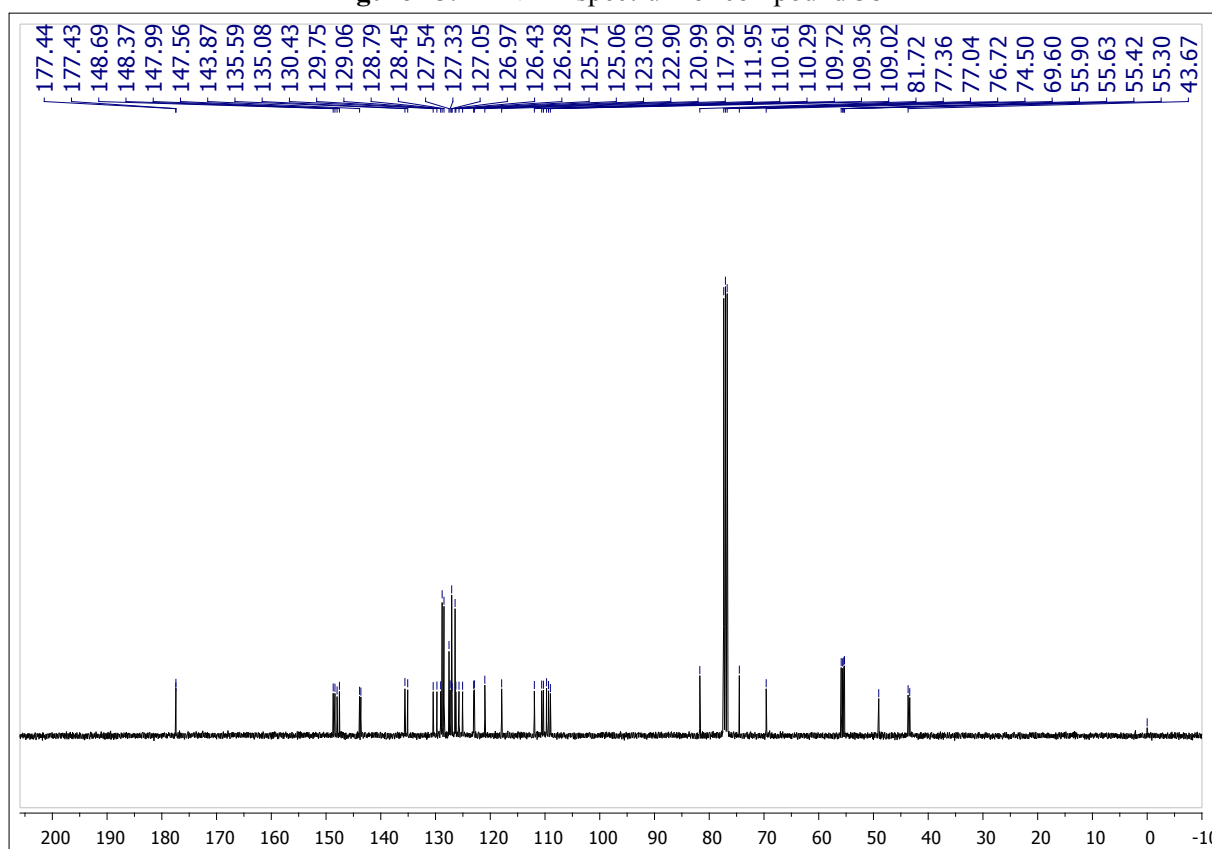


Figure 44. ¹³C NMR spectrum of compound 3o

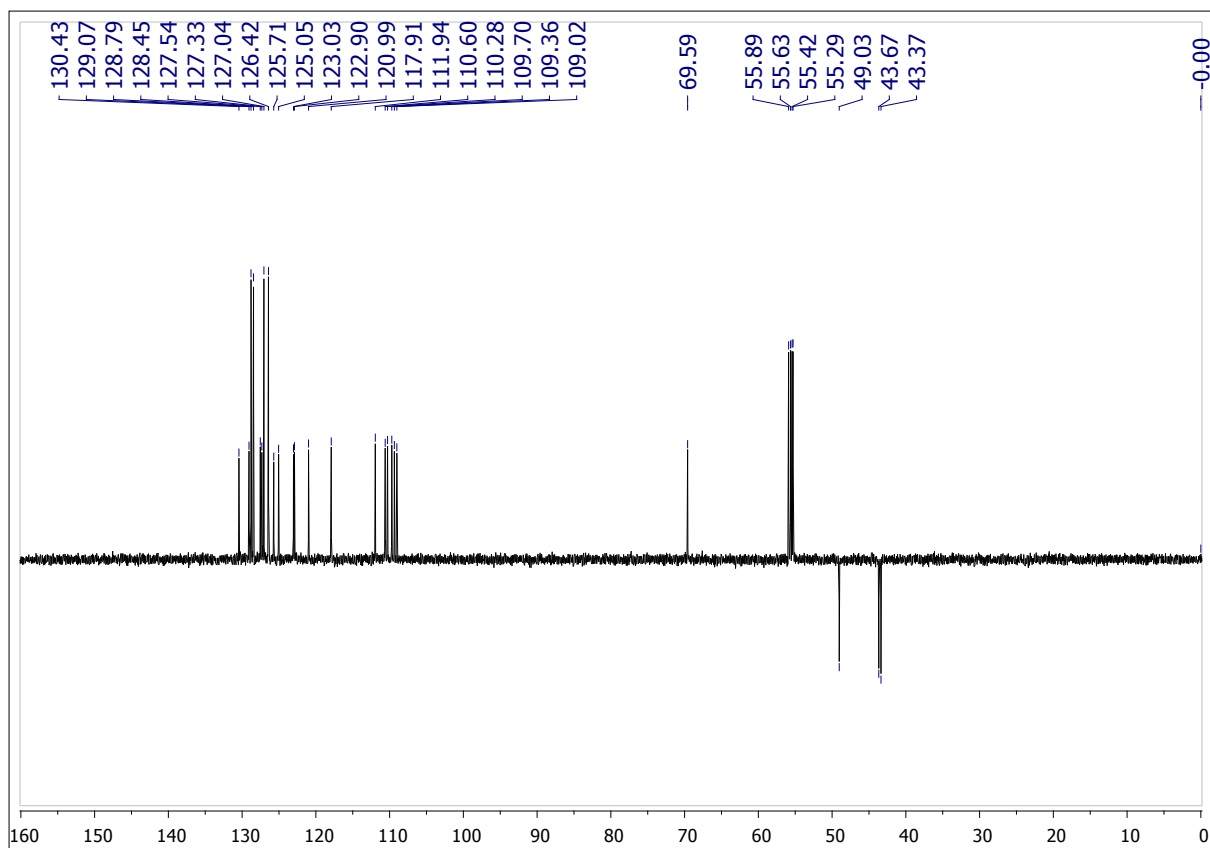


Figure 45. DEPT-135 spectrum of compound **3o**

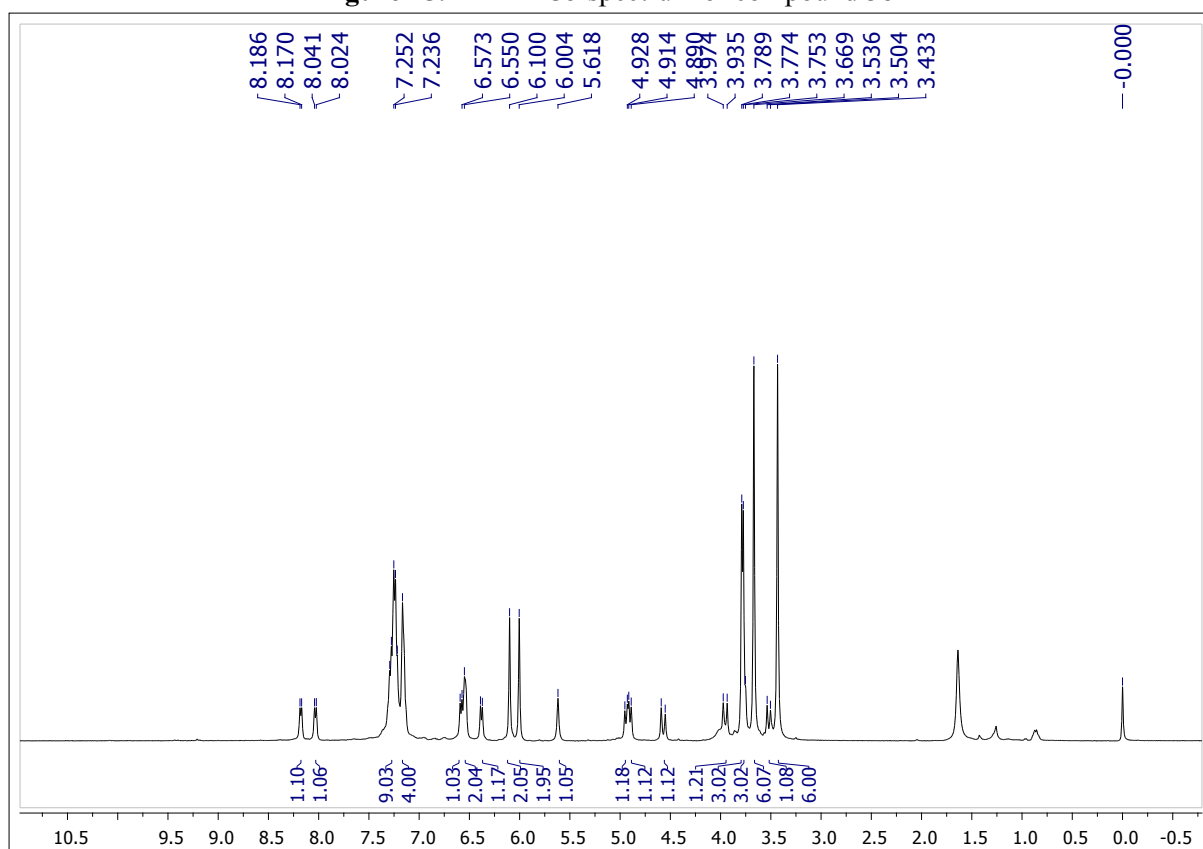


Figure 46. ¹H NMR spectrum of compound **3p**

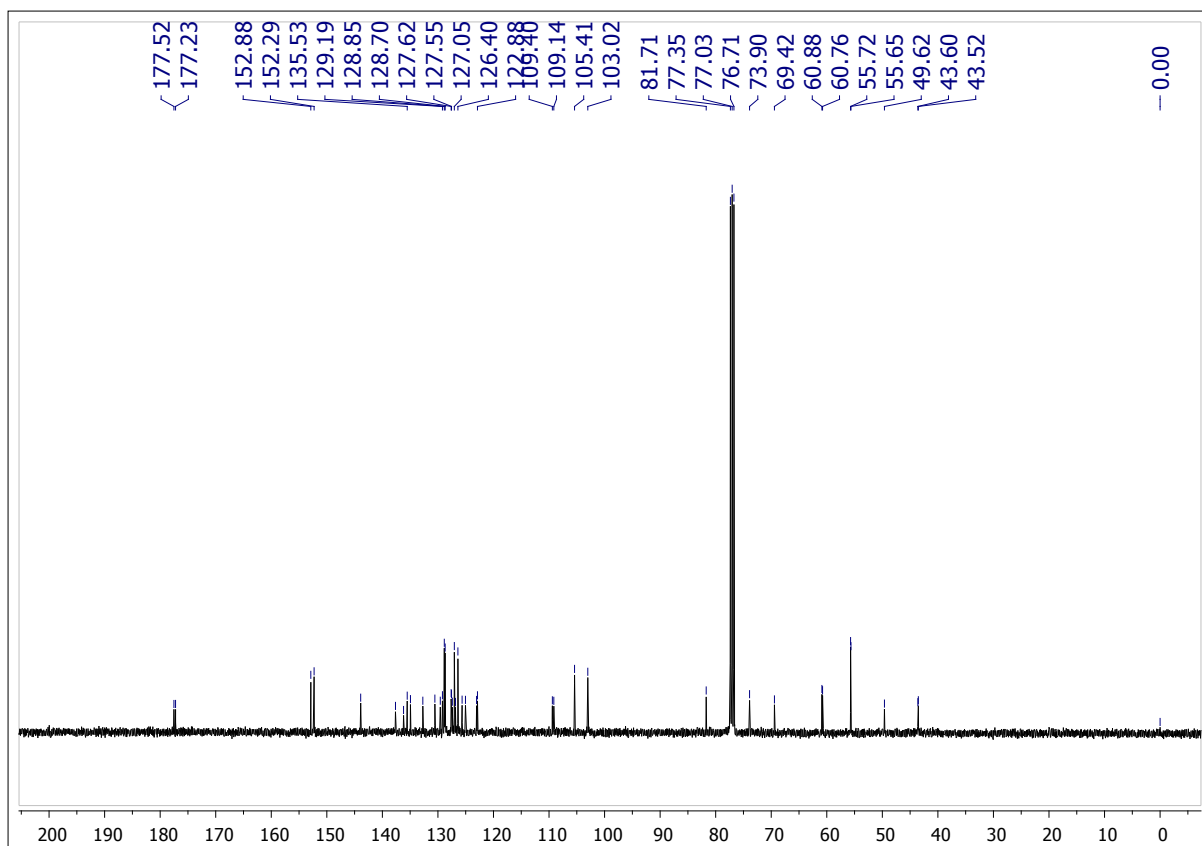


Figure 47. ^{13}C NMR spectrum of compound **3p**

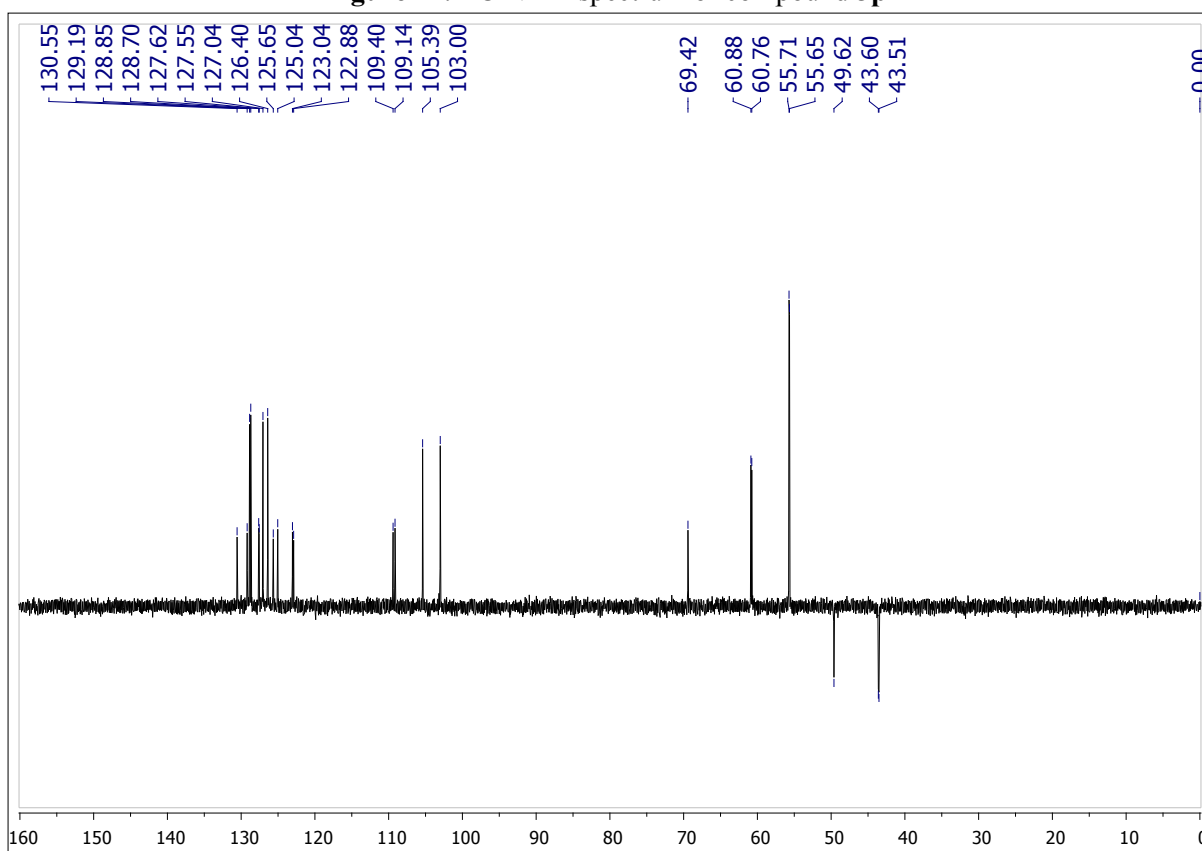


Figure 48. DEPT-135 spectrum of compound **3p**

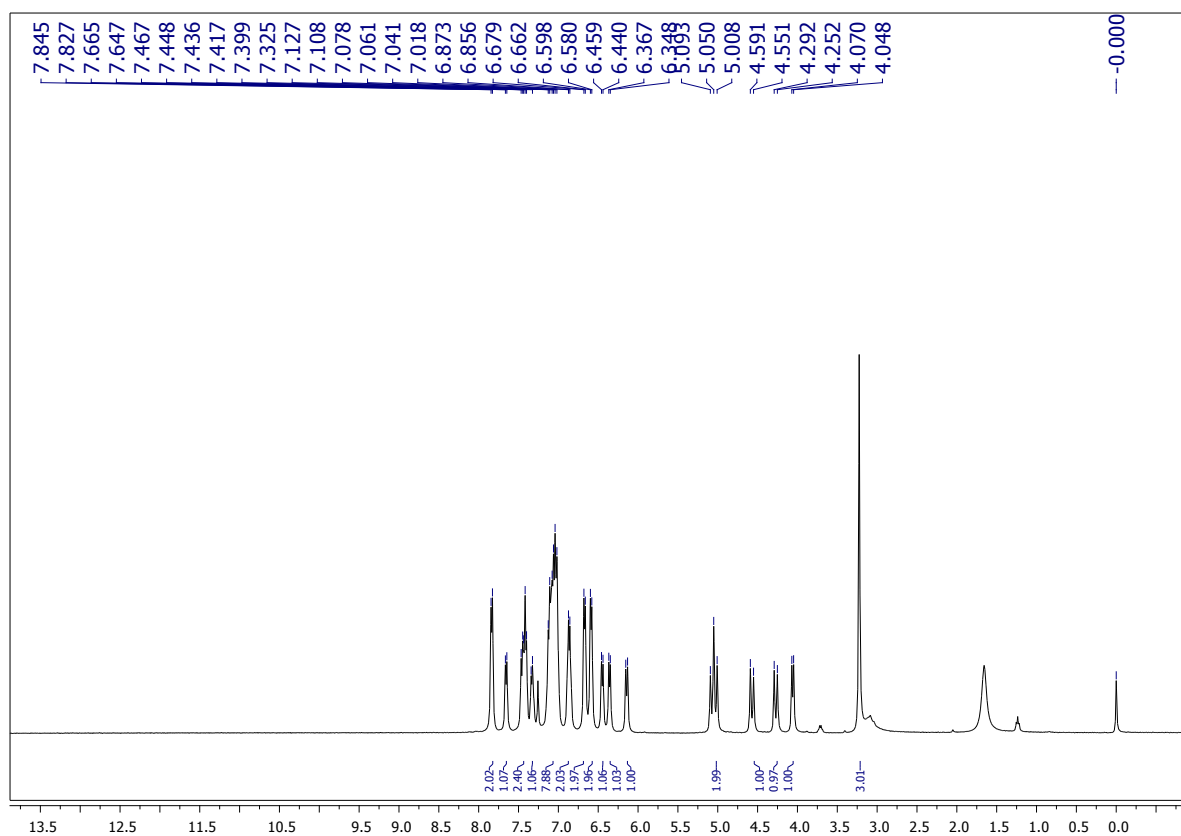


Figure 49. ^1H NMR spectrum of compound **5a**

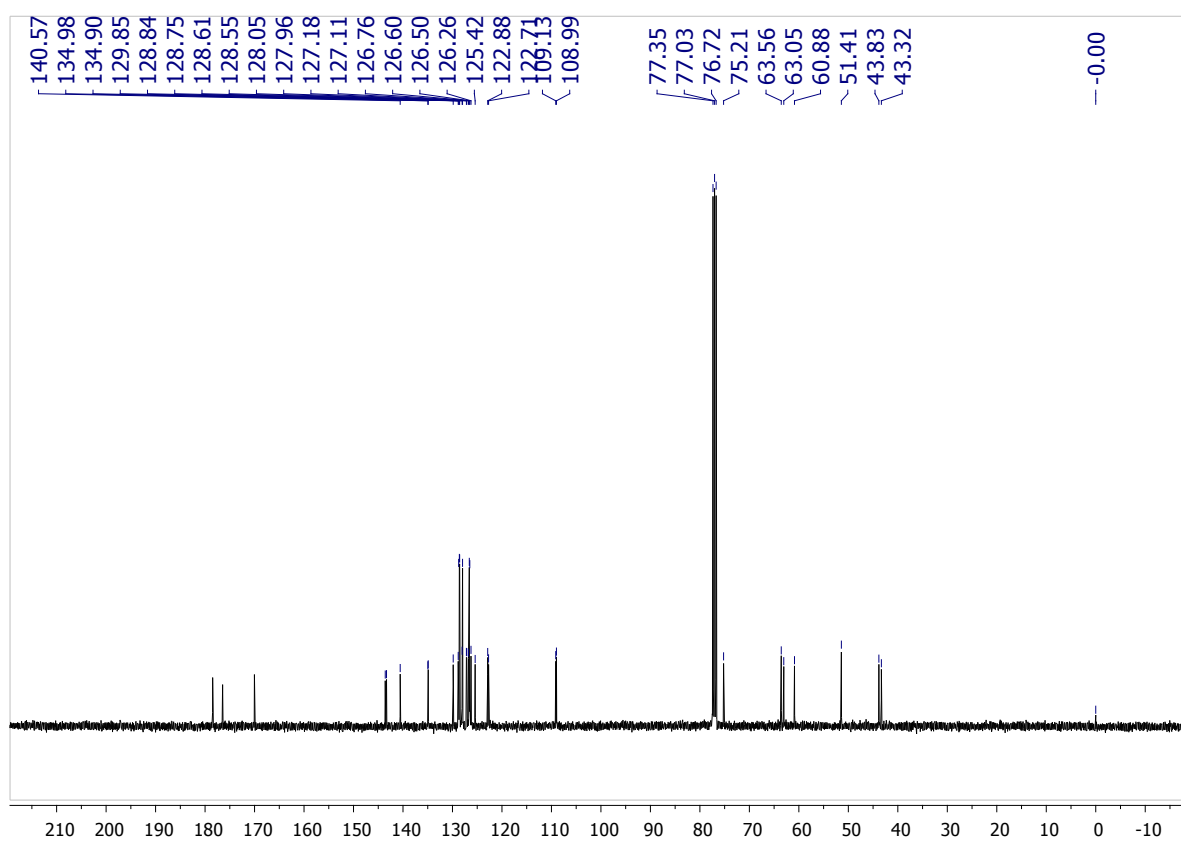


Figure 50. ^{13}C NMR spectrum of compound **5b**

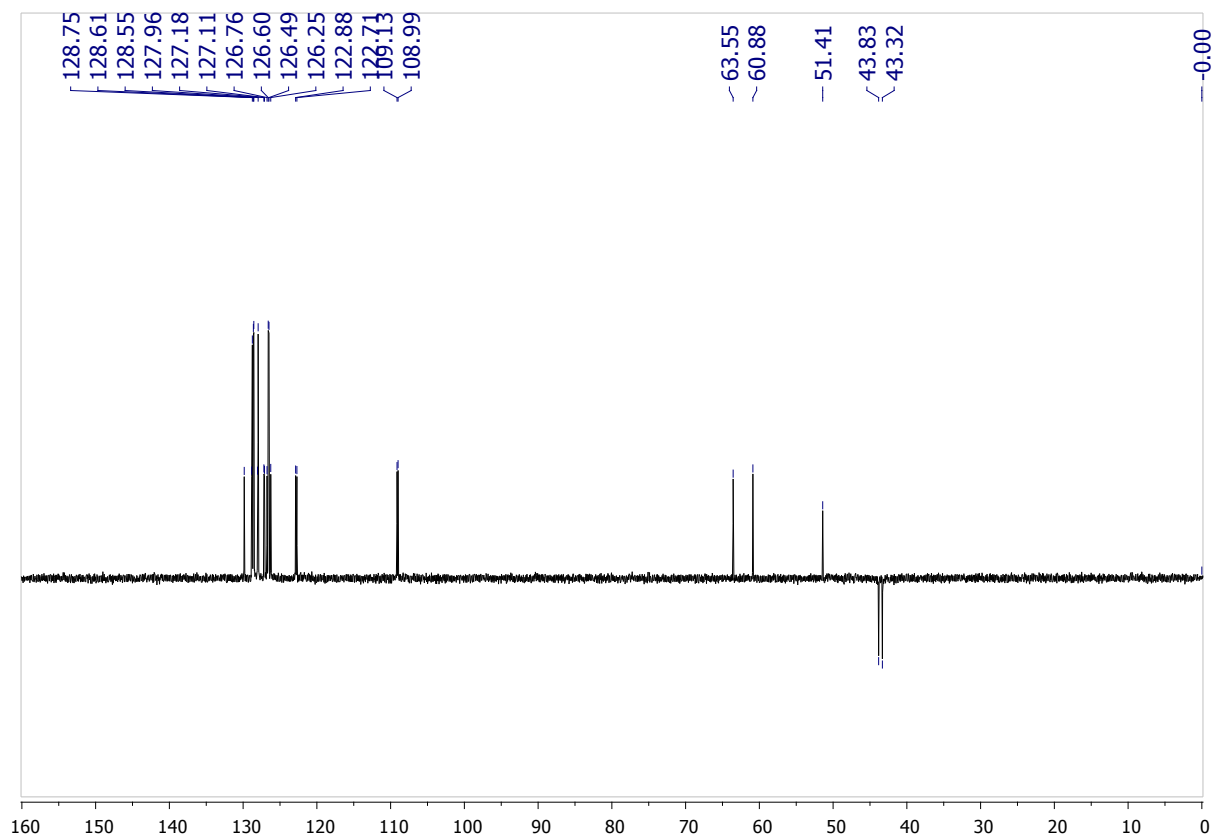


Figure 51. DEPT-135 spectrum of compound 5a

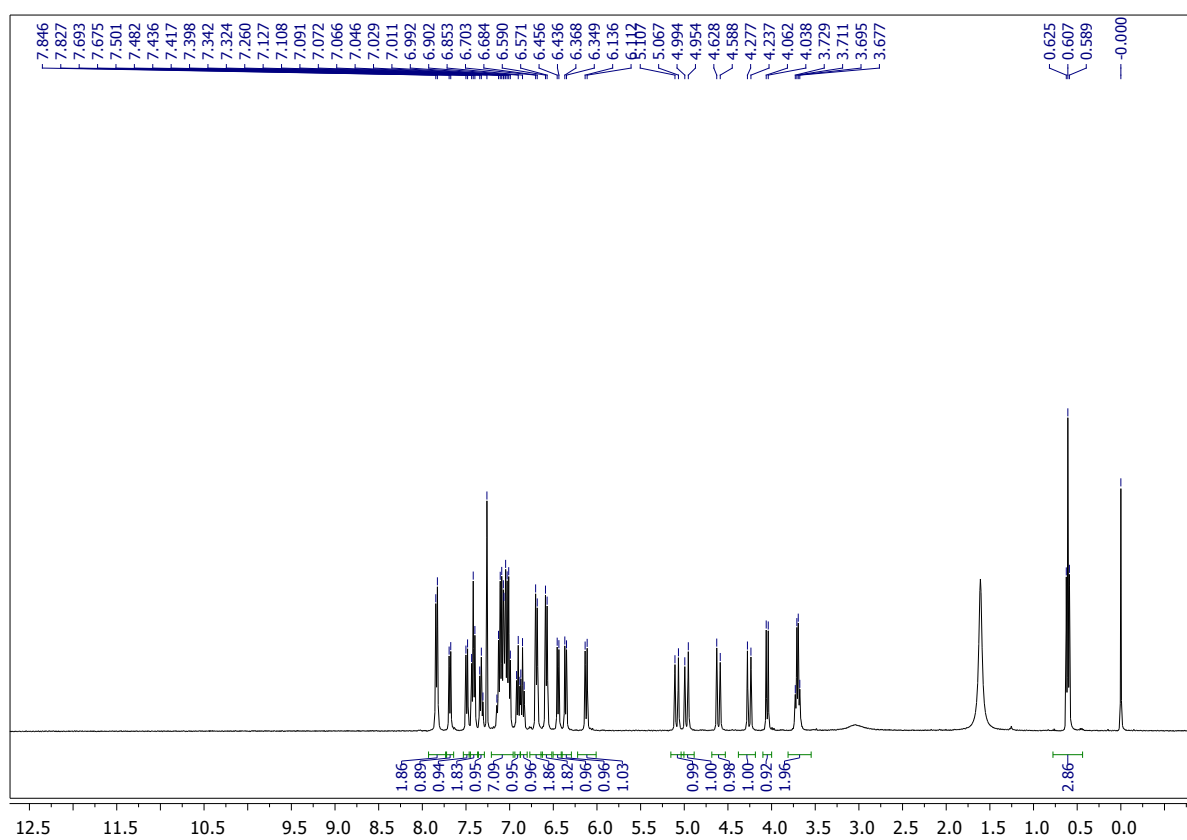


Figure 52. ¹H NMR spectrum of compound 5b

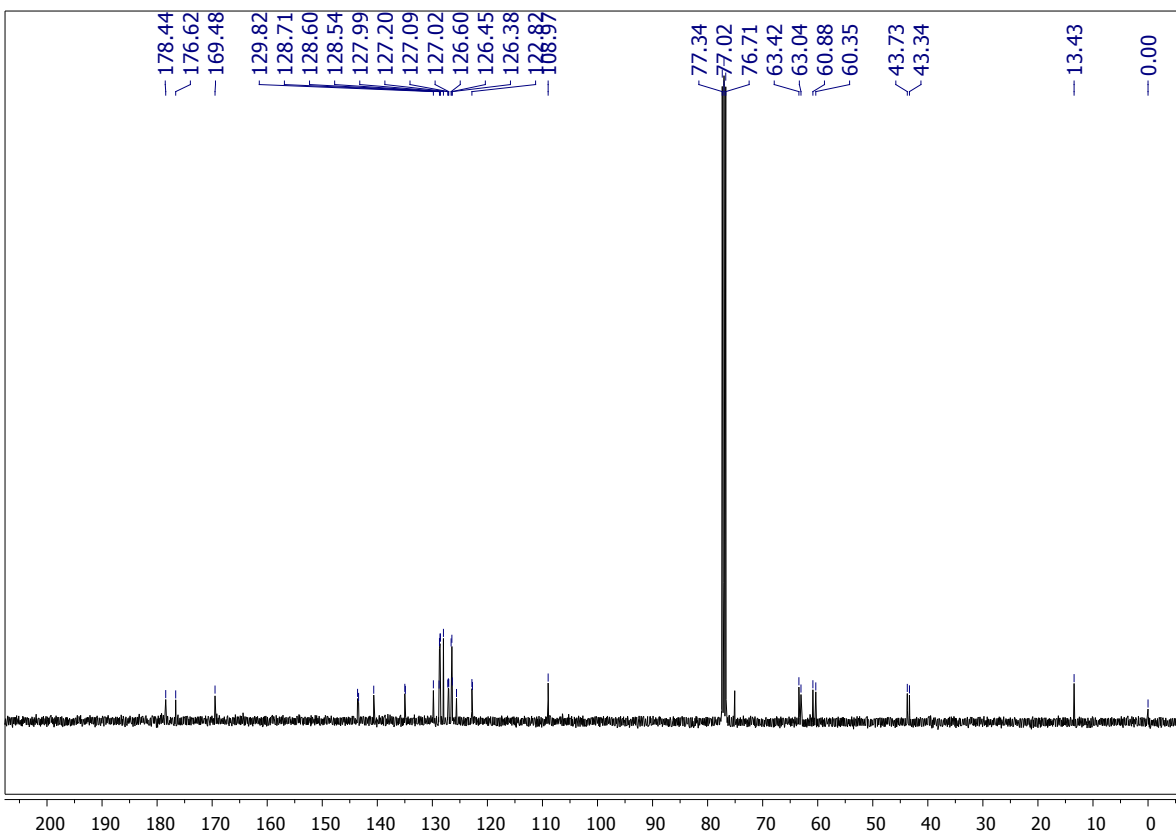


Figure 53. ^{13}C NMR spectrum of compound **5b**

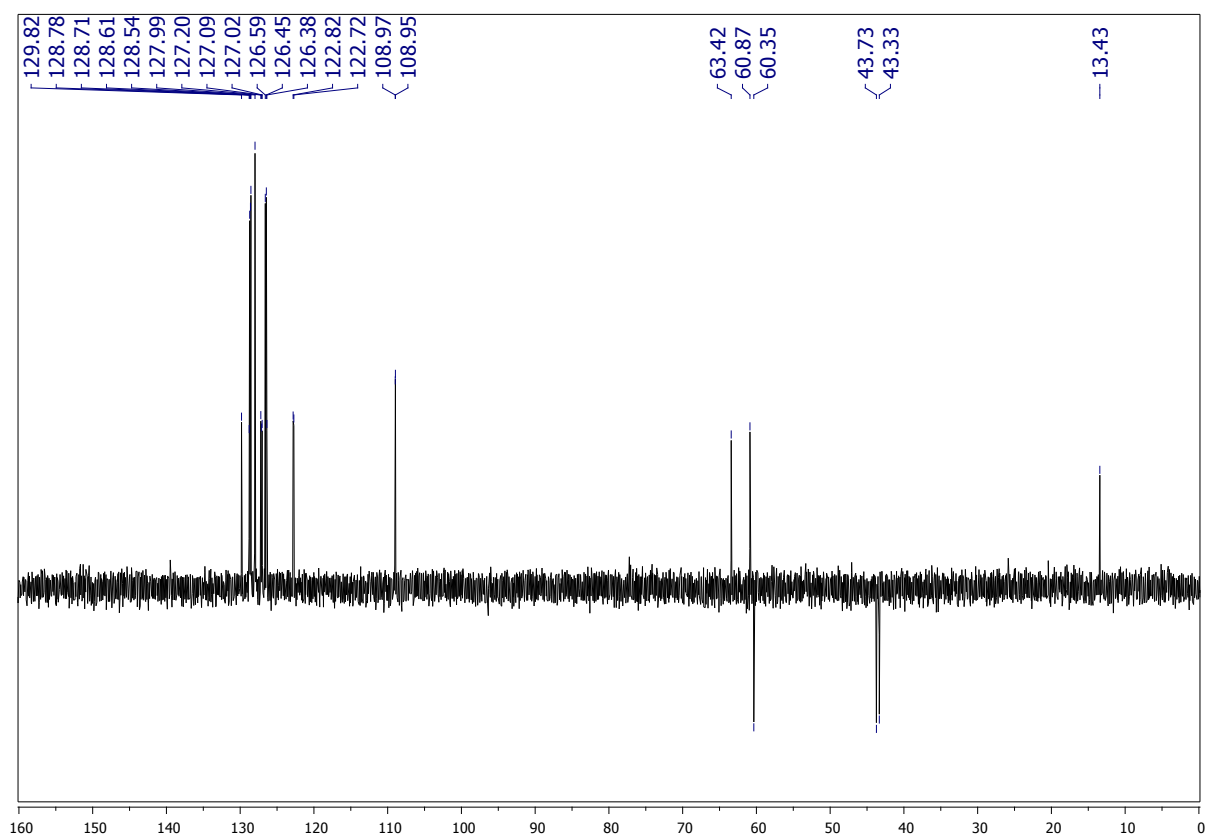


Figure 54. DEPT-135 spectrum of compound **5b**

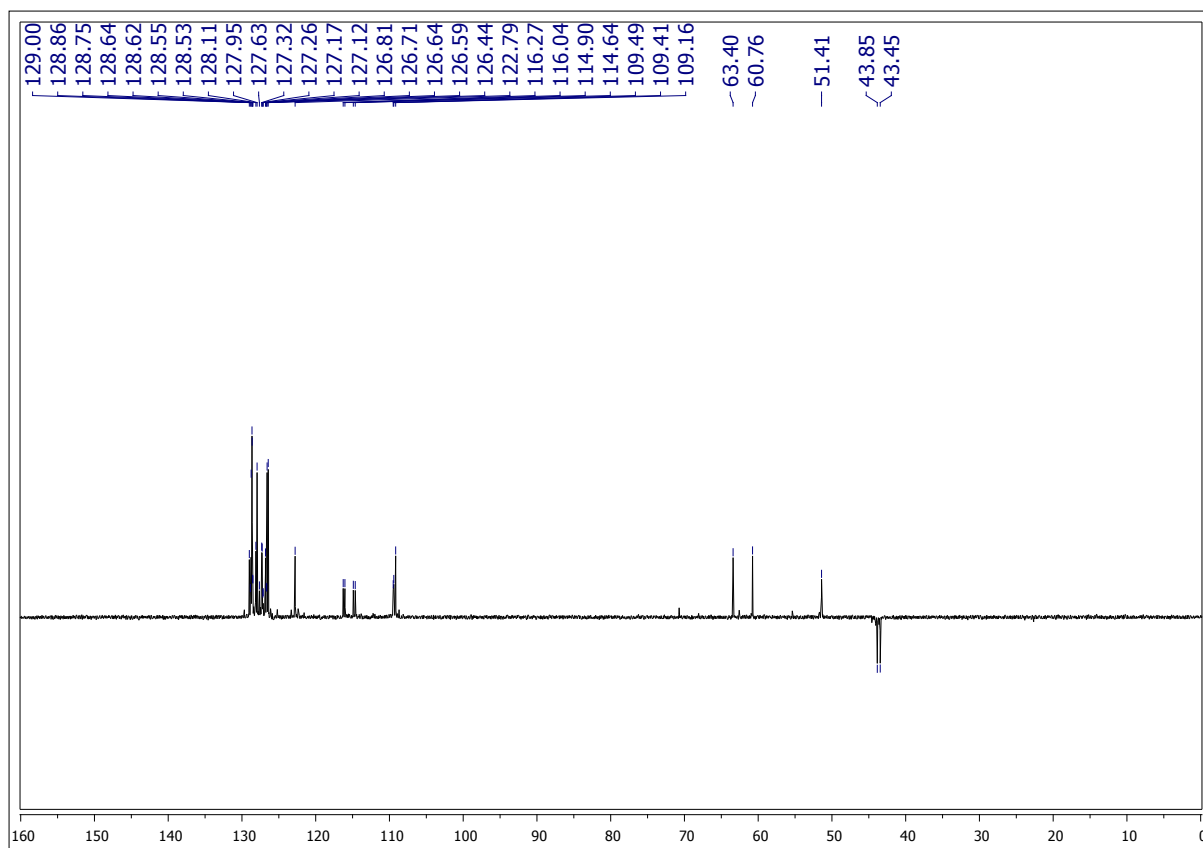


Figure 57. DEPT-135 spectrum of compound 5c

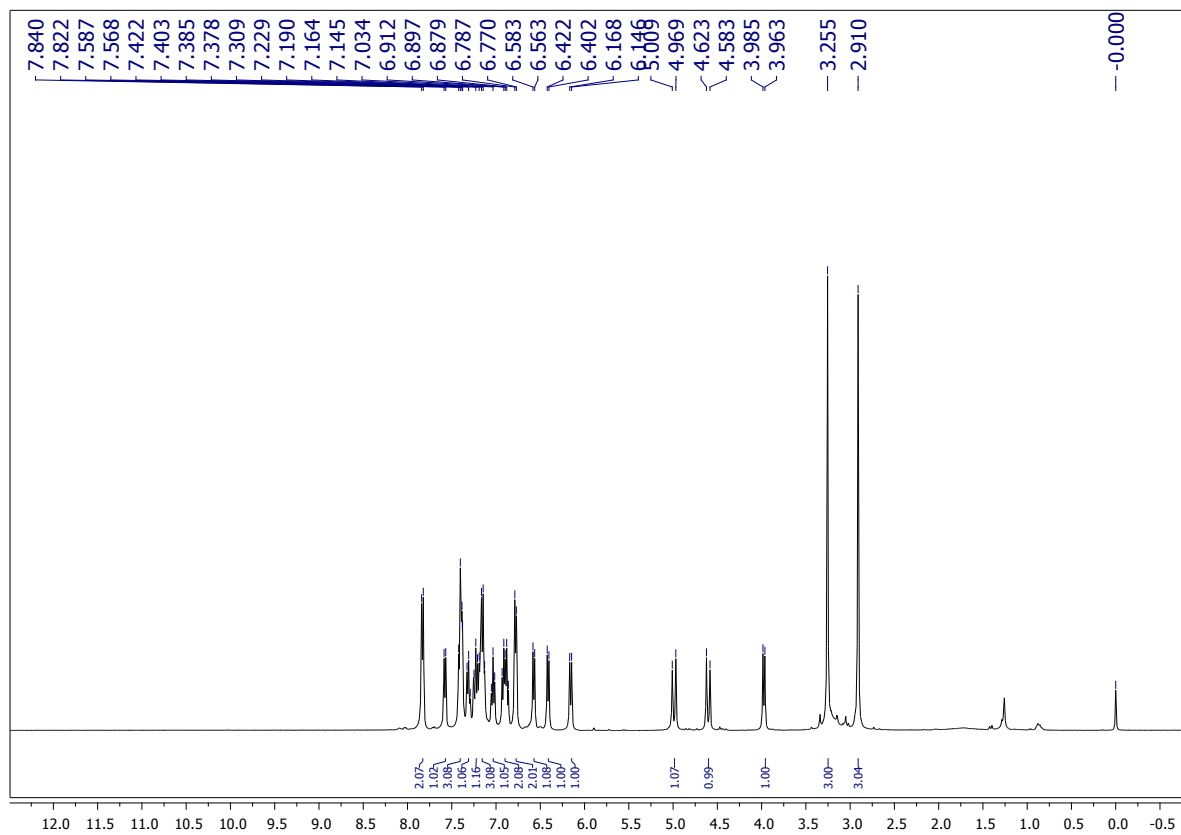


Figure 58. ¹H NMR spectrum of compound 5d

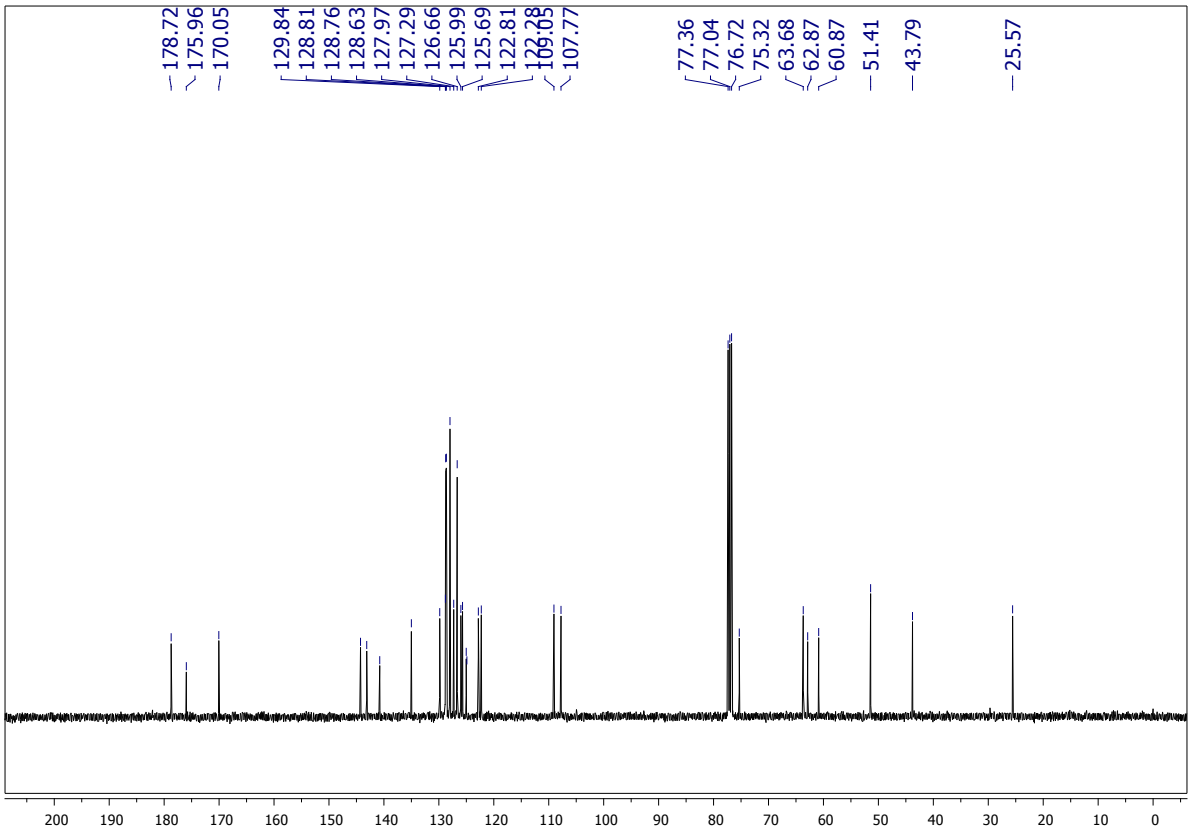


Figure 59. ^{13}C NMR spectrum of compound **5d**

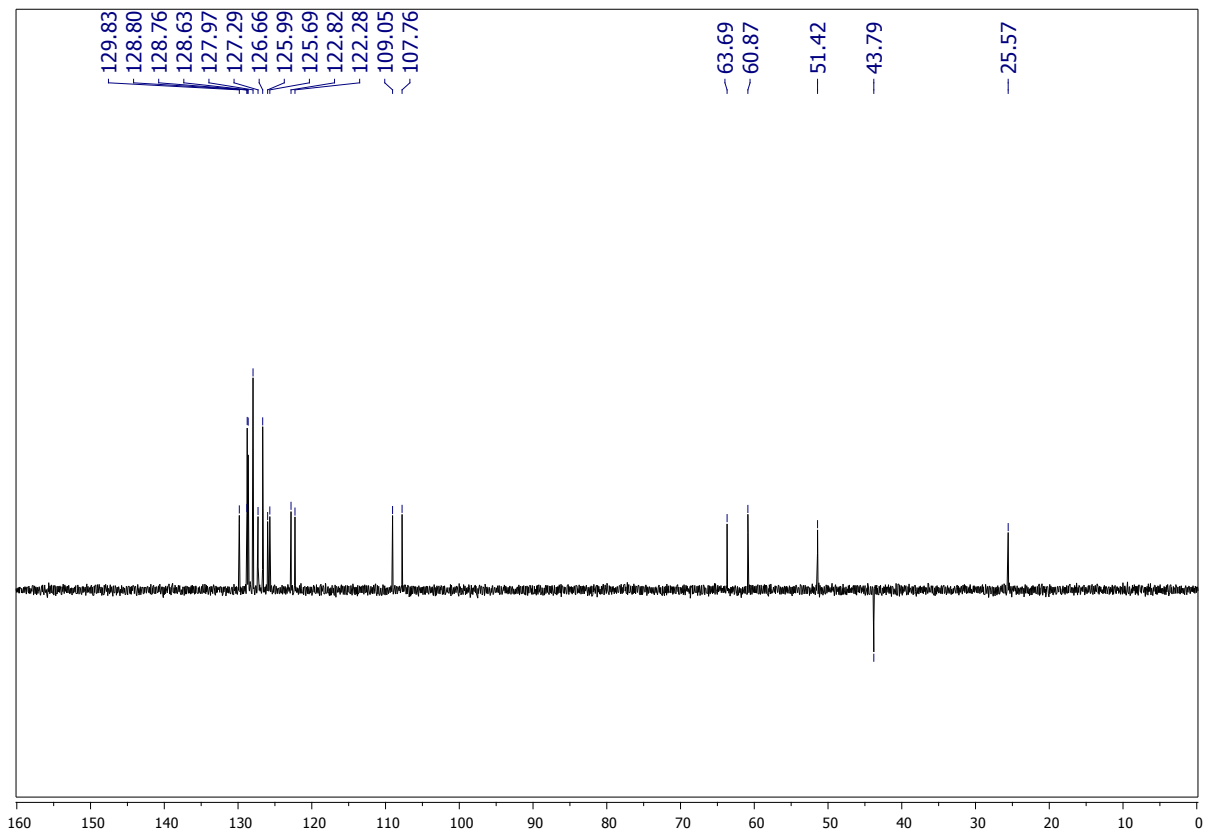


Figure 60. DEPT-135 spectrum of compound **5d**

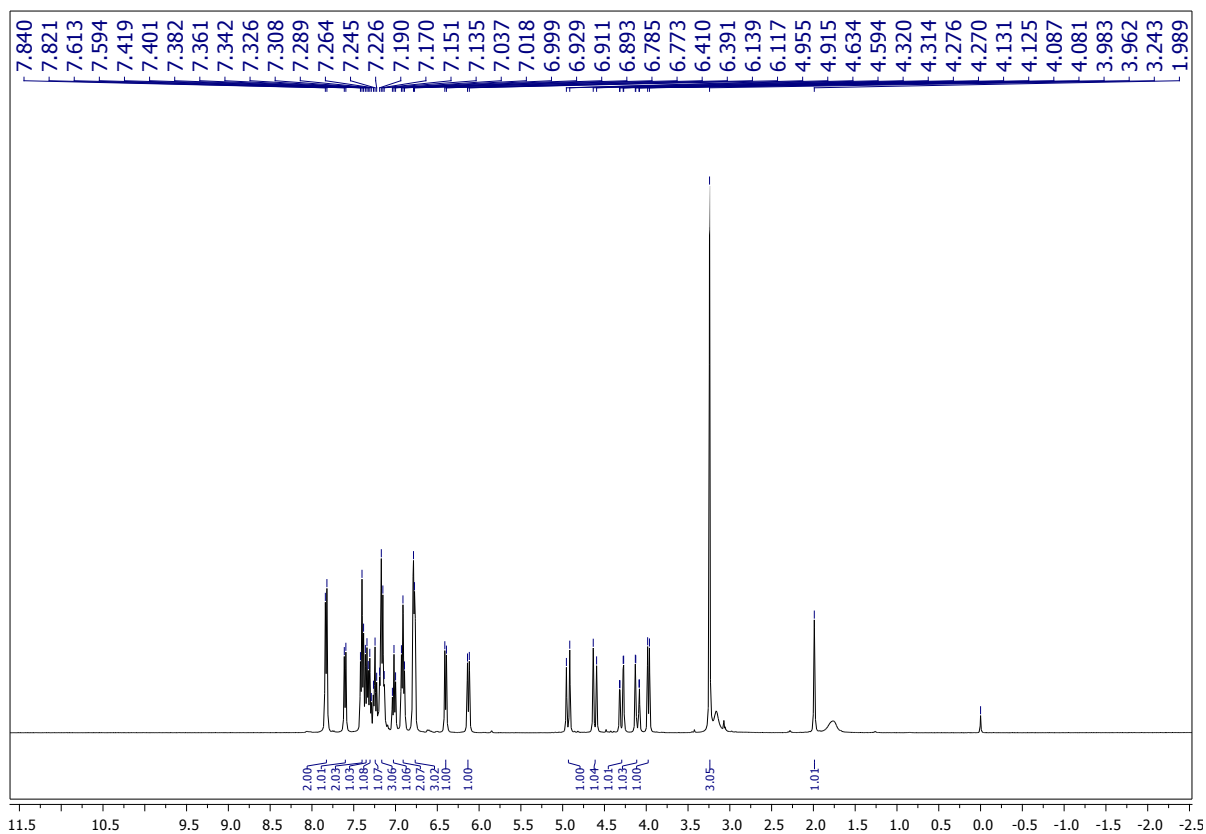


Figure 61. ^1H NMR spectrum of compound **5e**

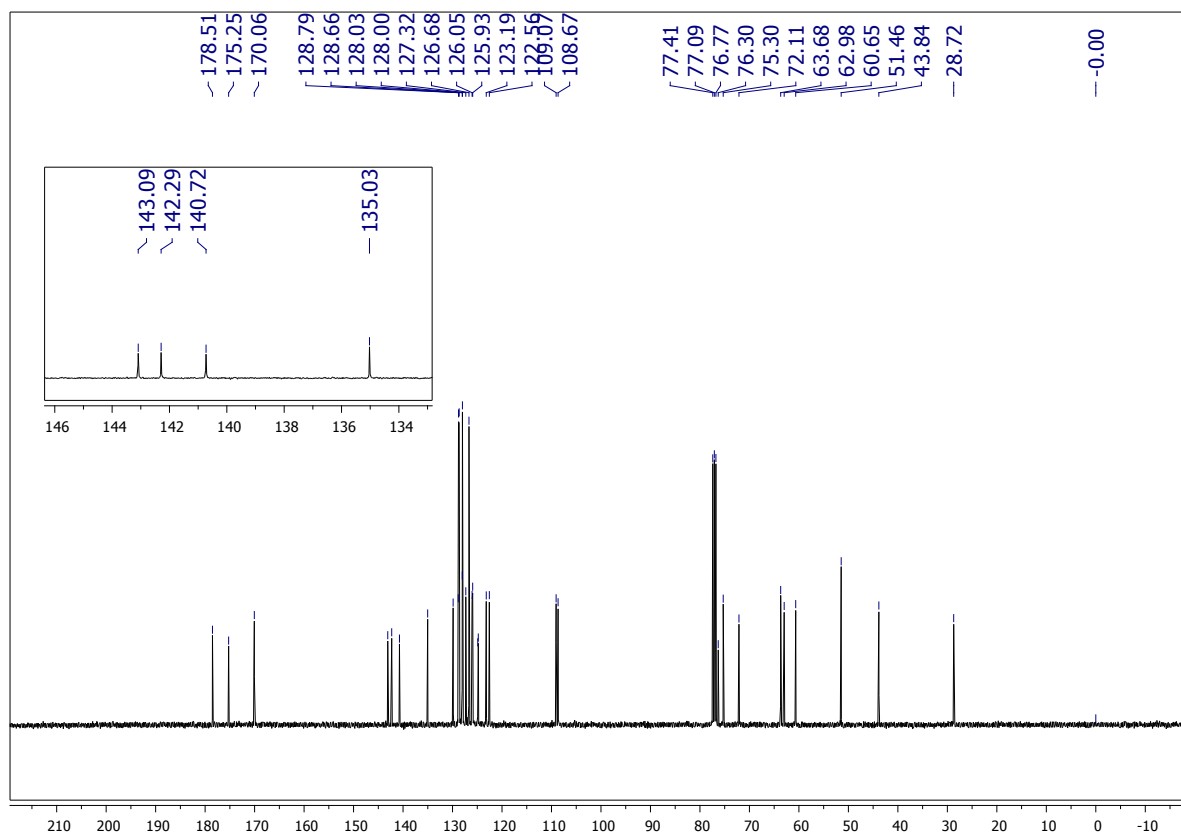


Figure 62. ^{13}C NMR spectrum of compound **5e**

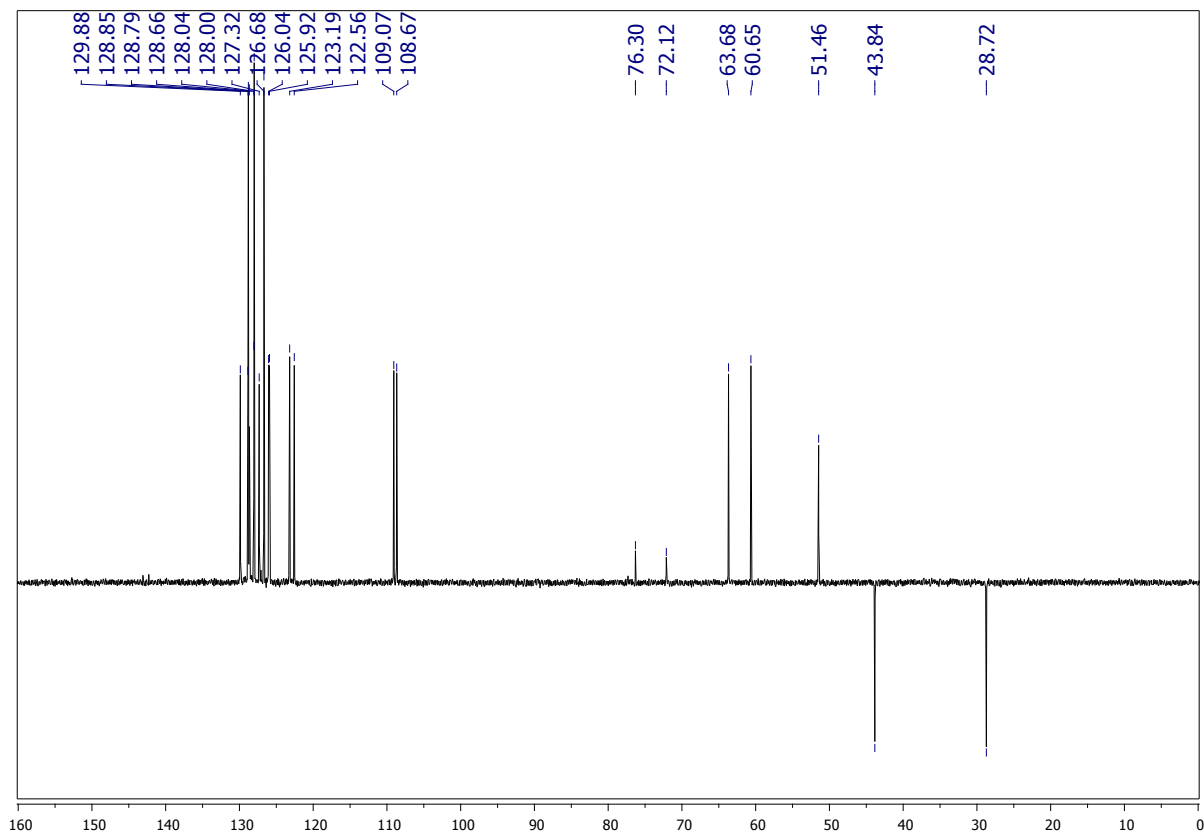


Figure 63. DEPT-135 spectrum of compound 5e

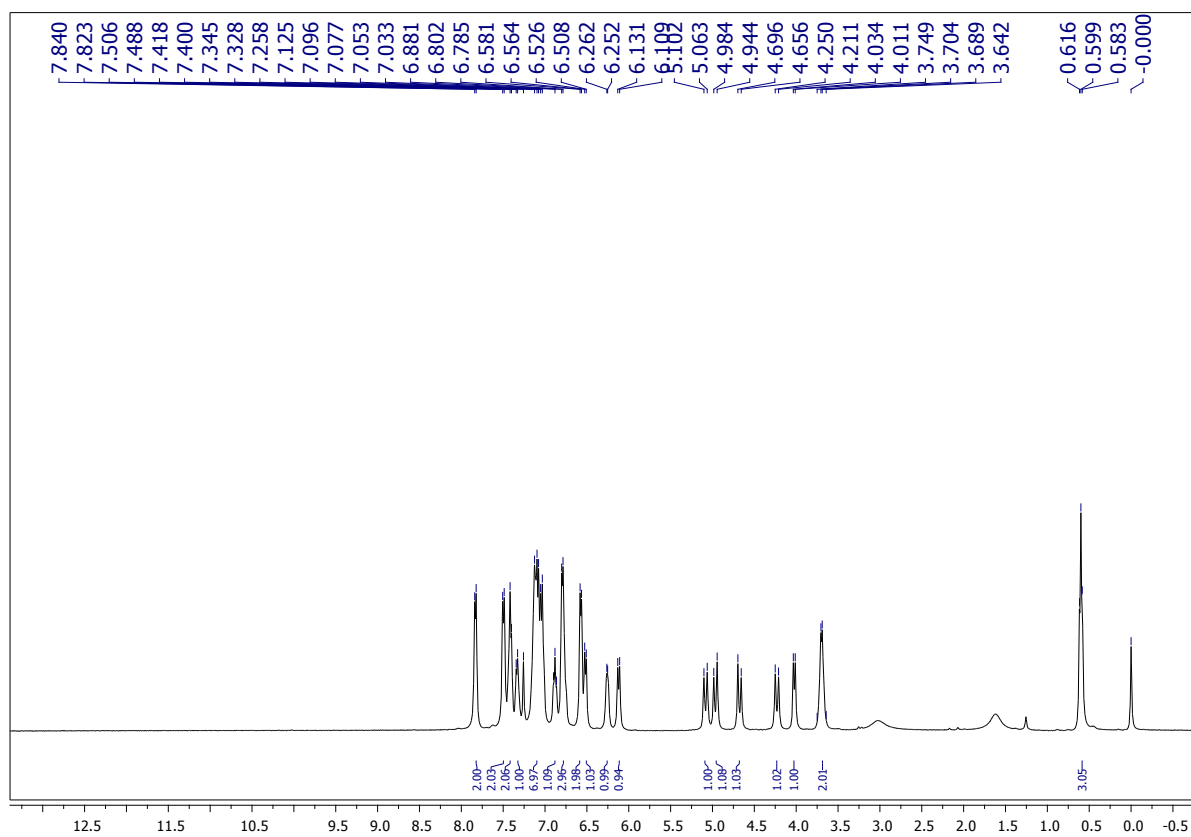


Figure 64. ¹H NMR spectrum of compound 5f

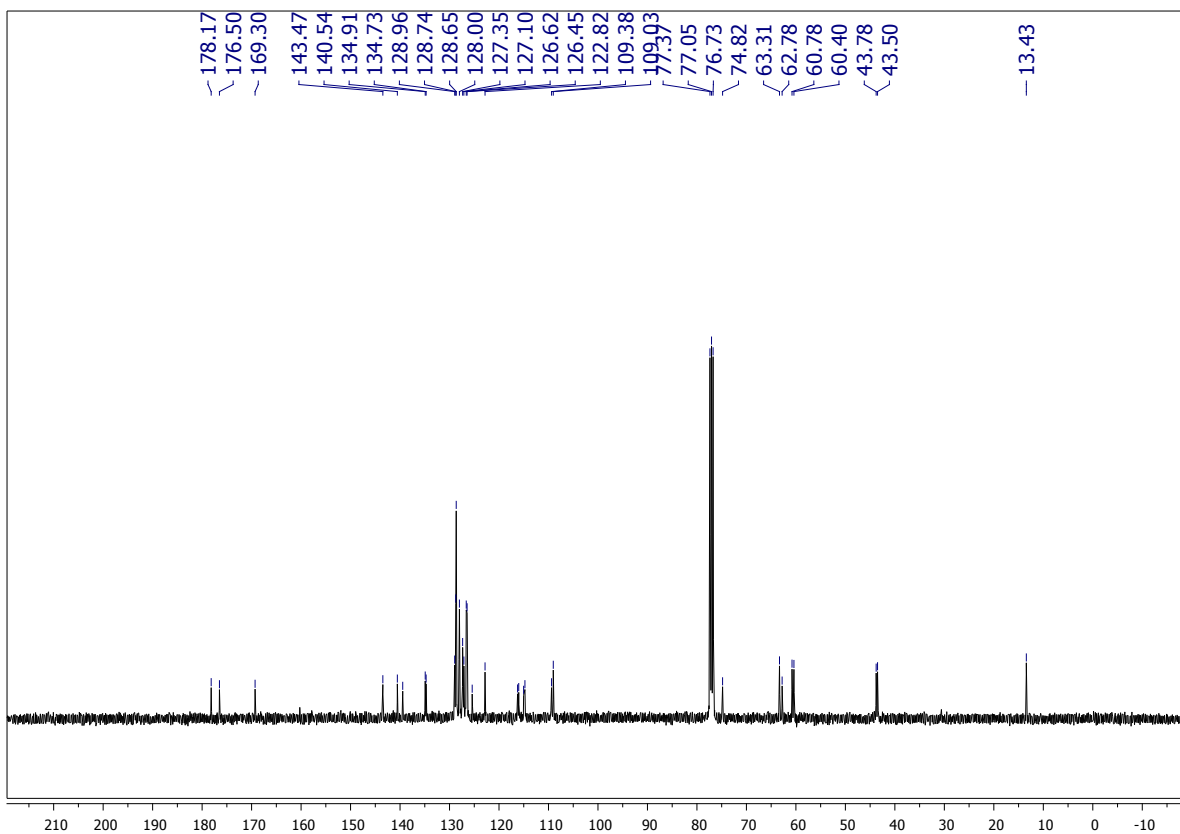


Figure 65. ^{13}C NMR spectrum of compound **5f**

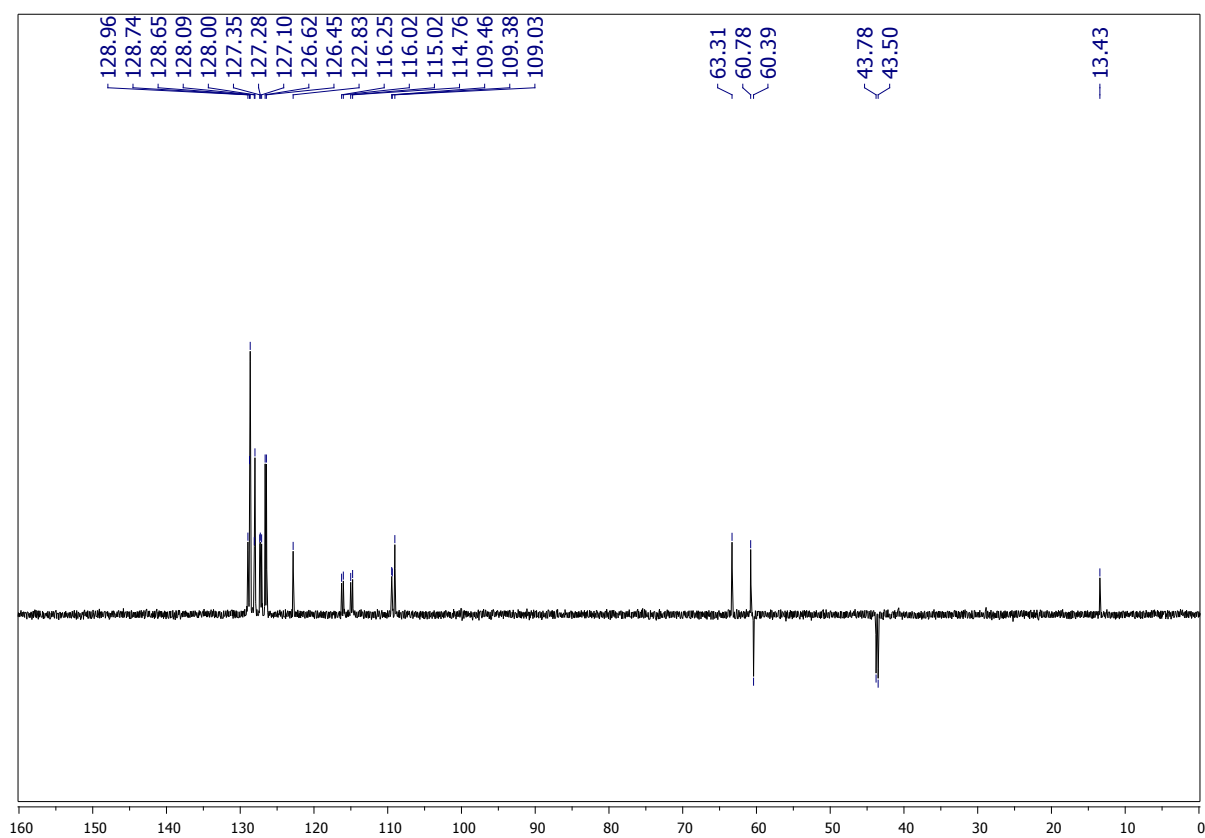


Figure 66. DEPT-135 spectrum of compound **5f**

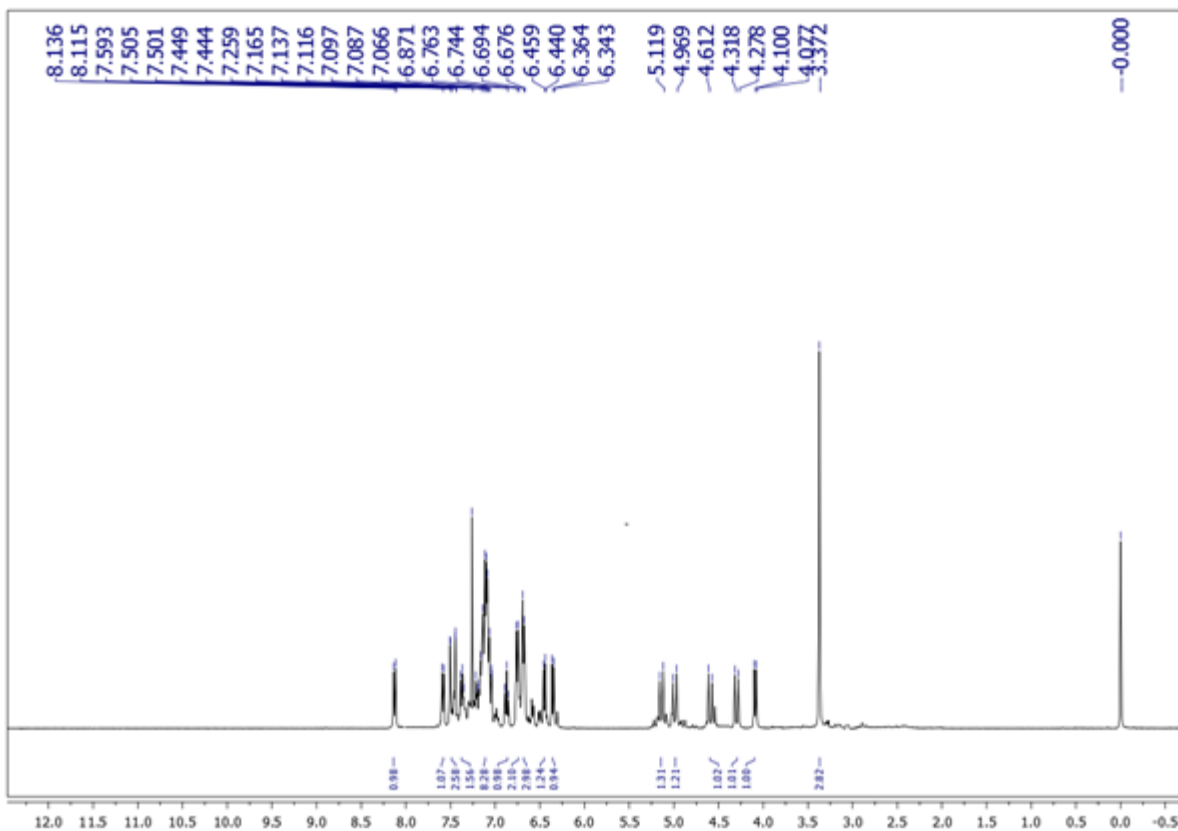


Figure 67. ^1H NMR spectrum of compound **5g**

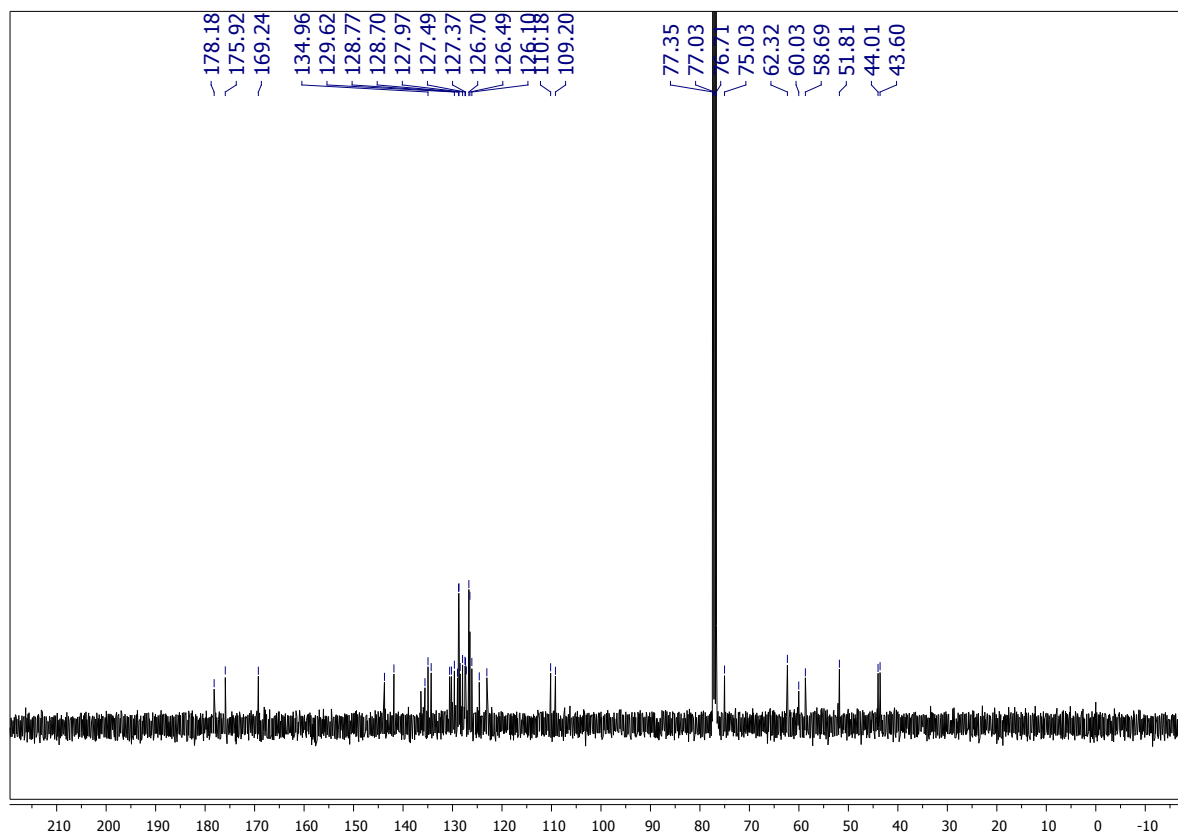


Figure 68. ^{13}C NMR spectrum of compound **5g**

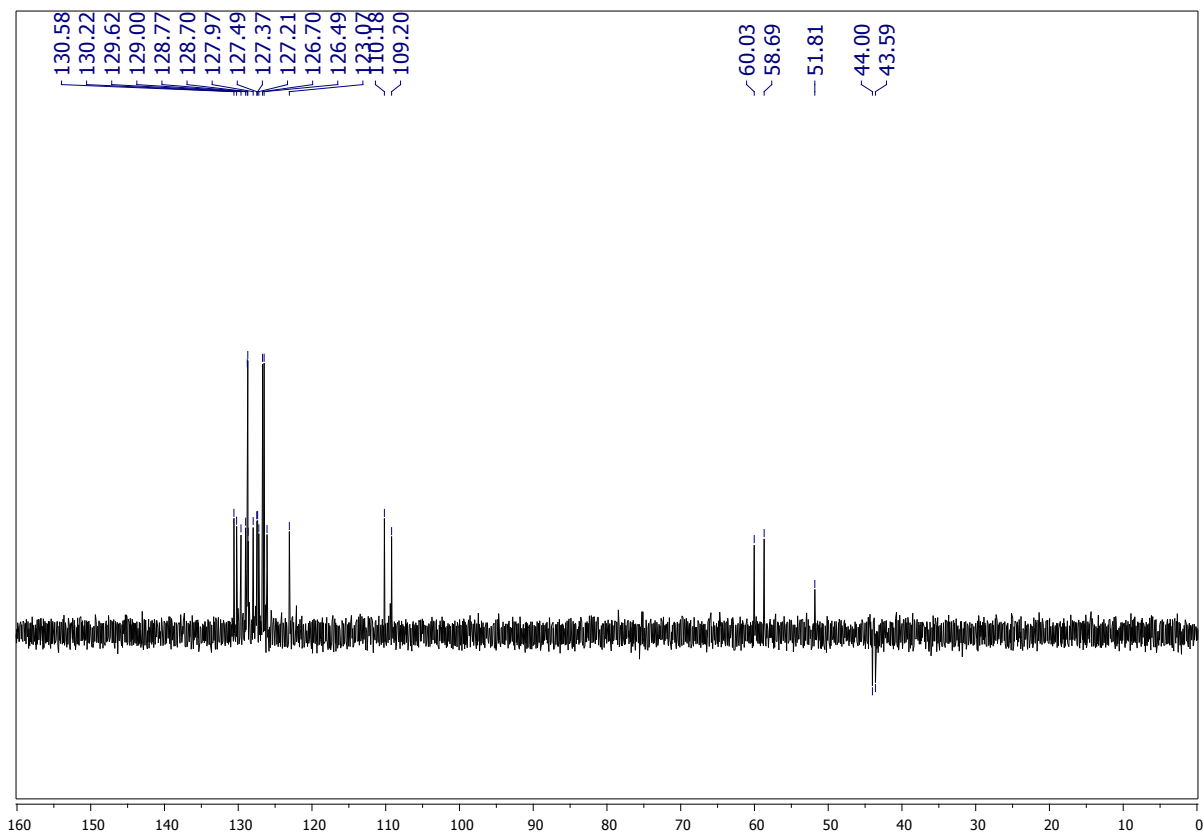


Figure 69. DEPT-135 spectrum of compound 5g

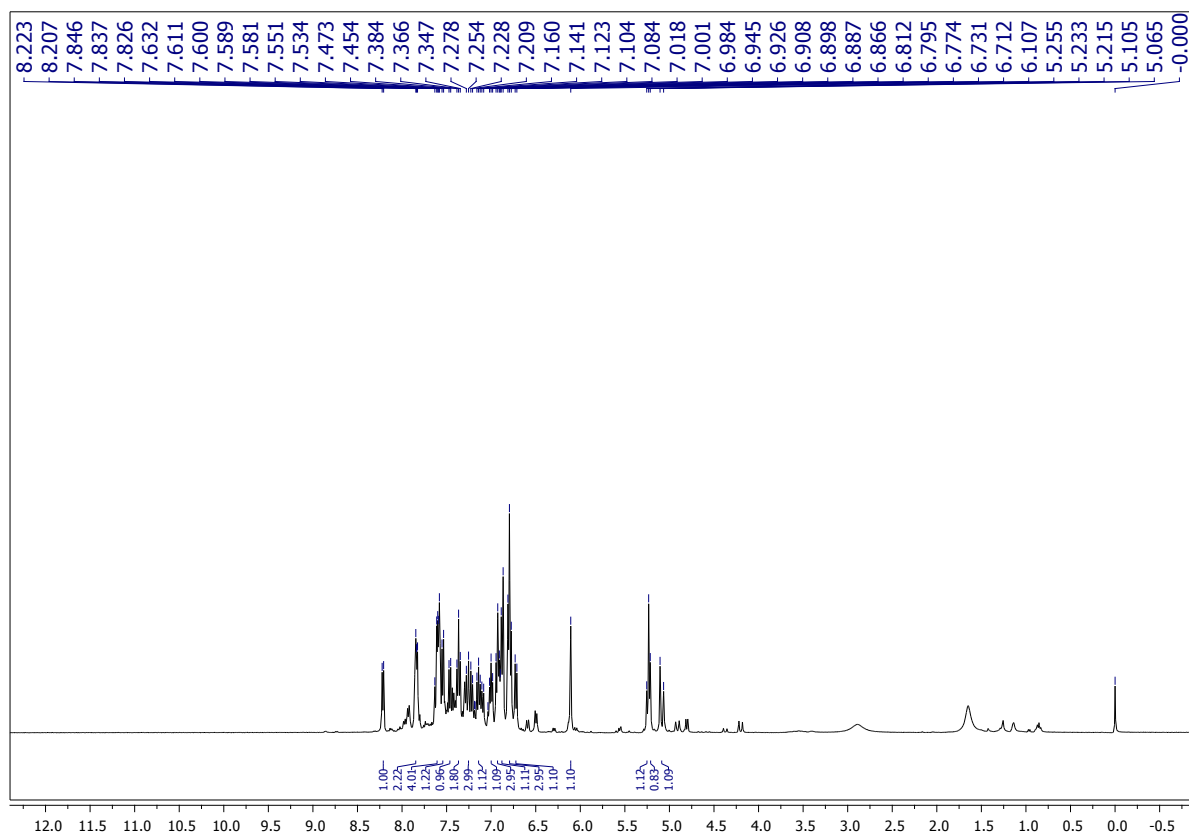


Figure 70. ¹H NMR spectrum of compound 7a

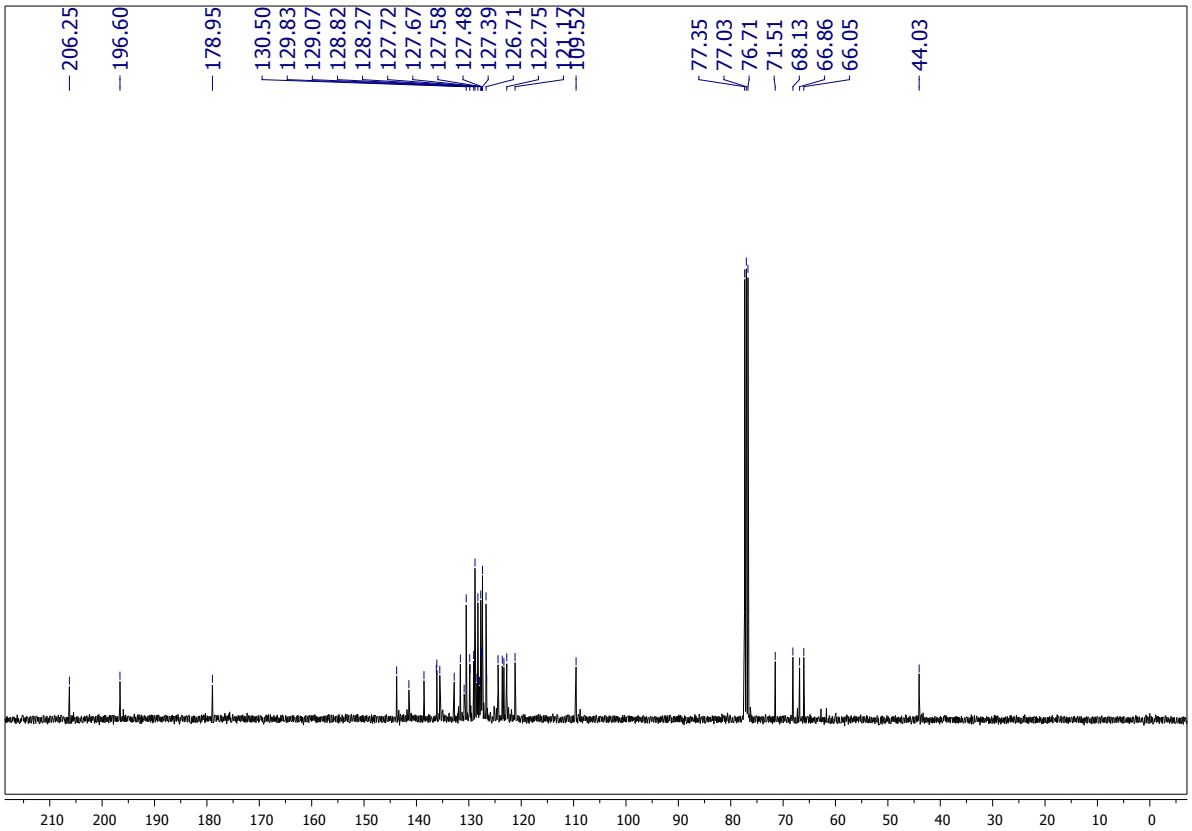


Figure 71. ^{13}C NMR spectrum of compound 7a

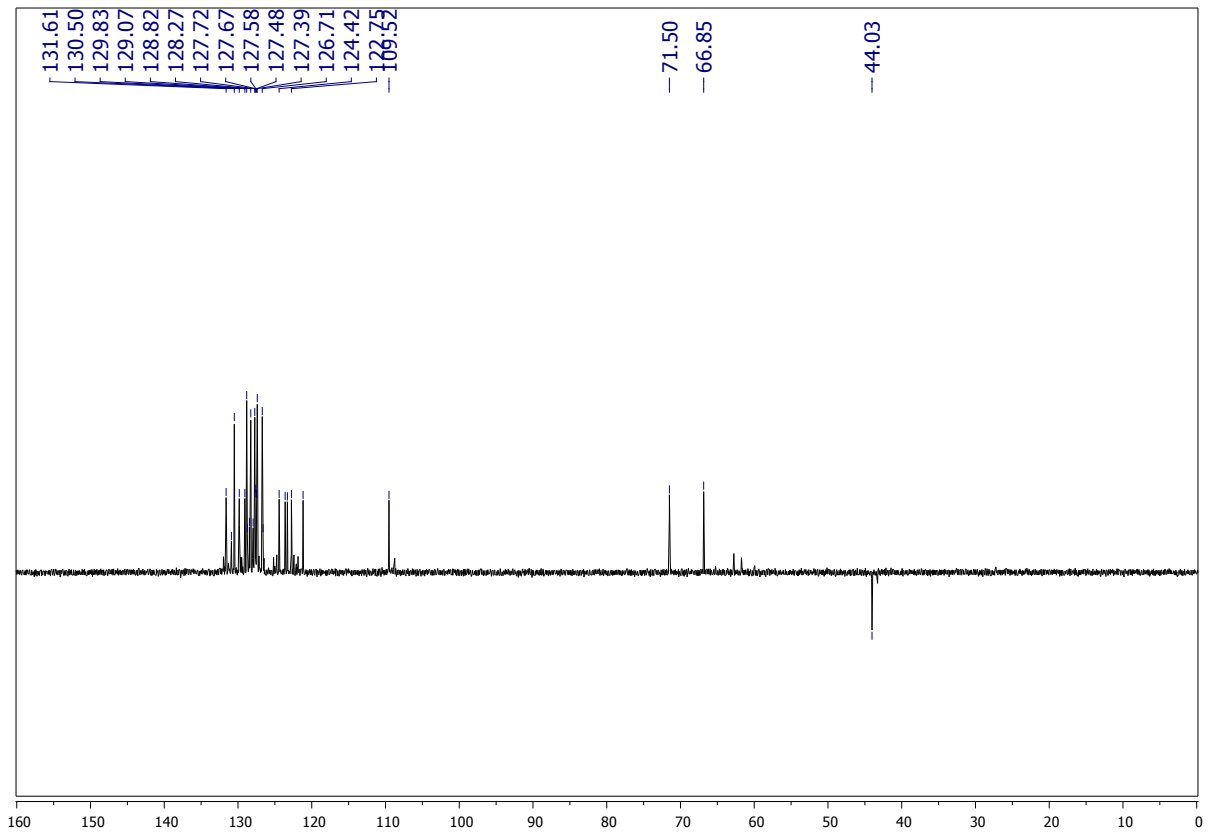


Figure 72. DEPT-135 spectrum of compound 7a

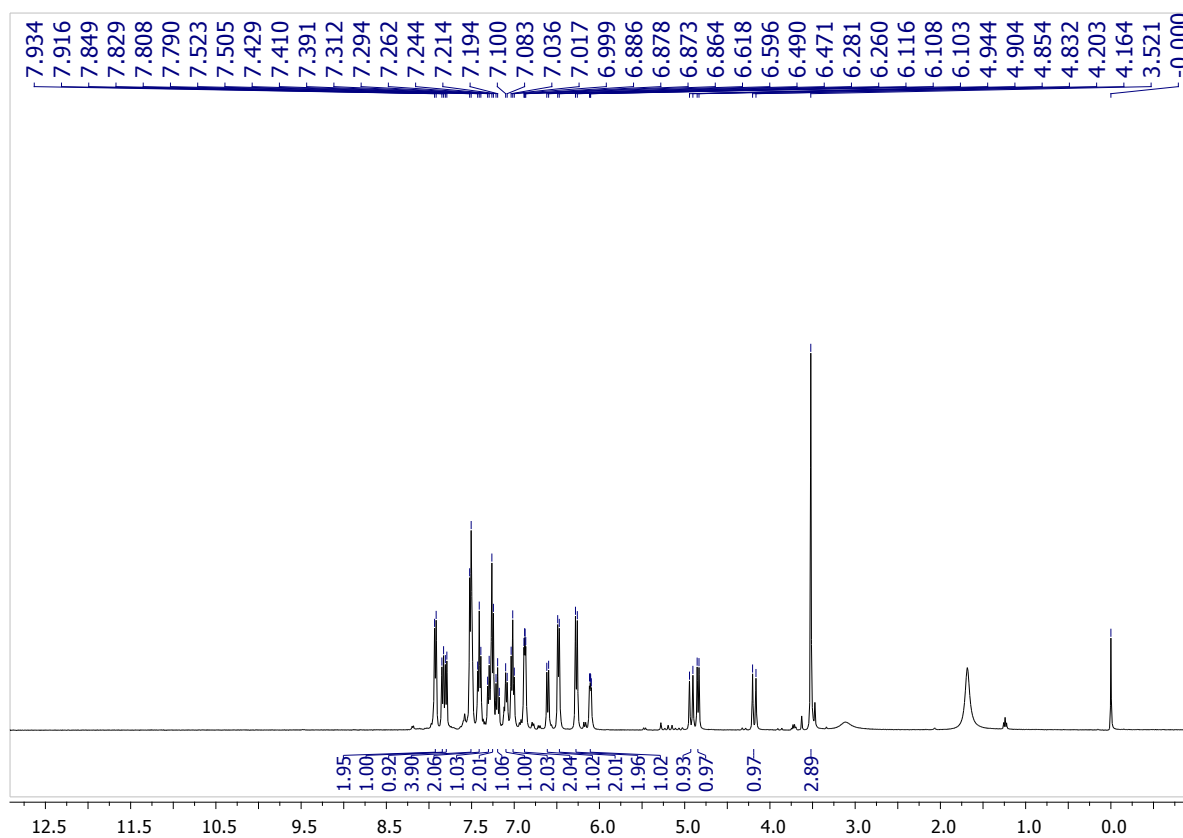


Figure 73. ^1H NMR spectrum of compound **7b**

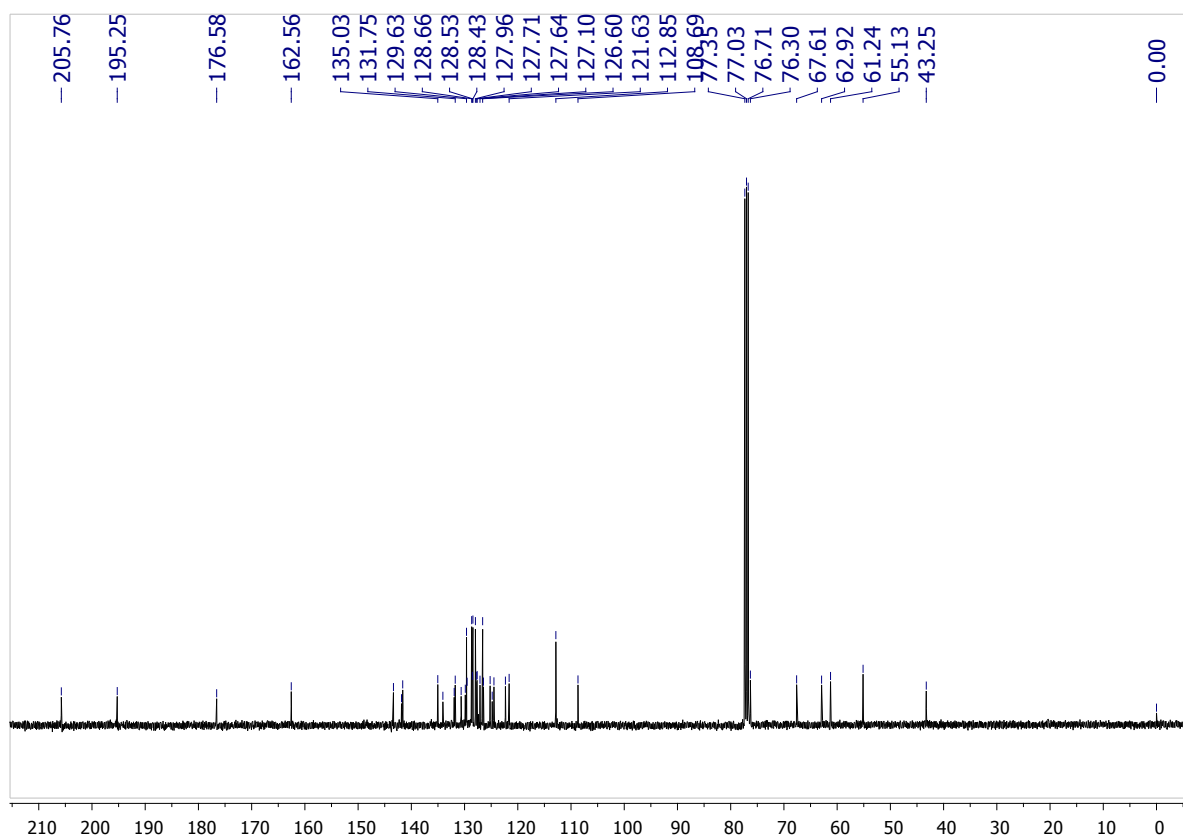


Figure 74. ^{13}C NMR spectrum of compound **7b**

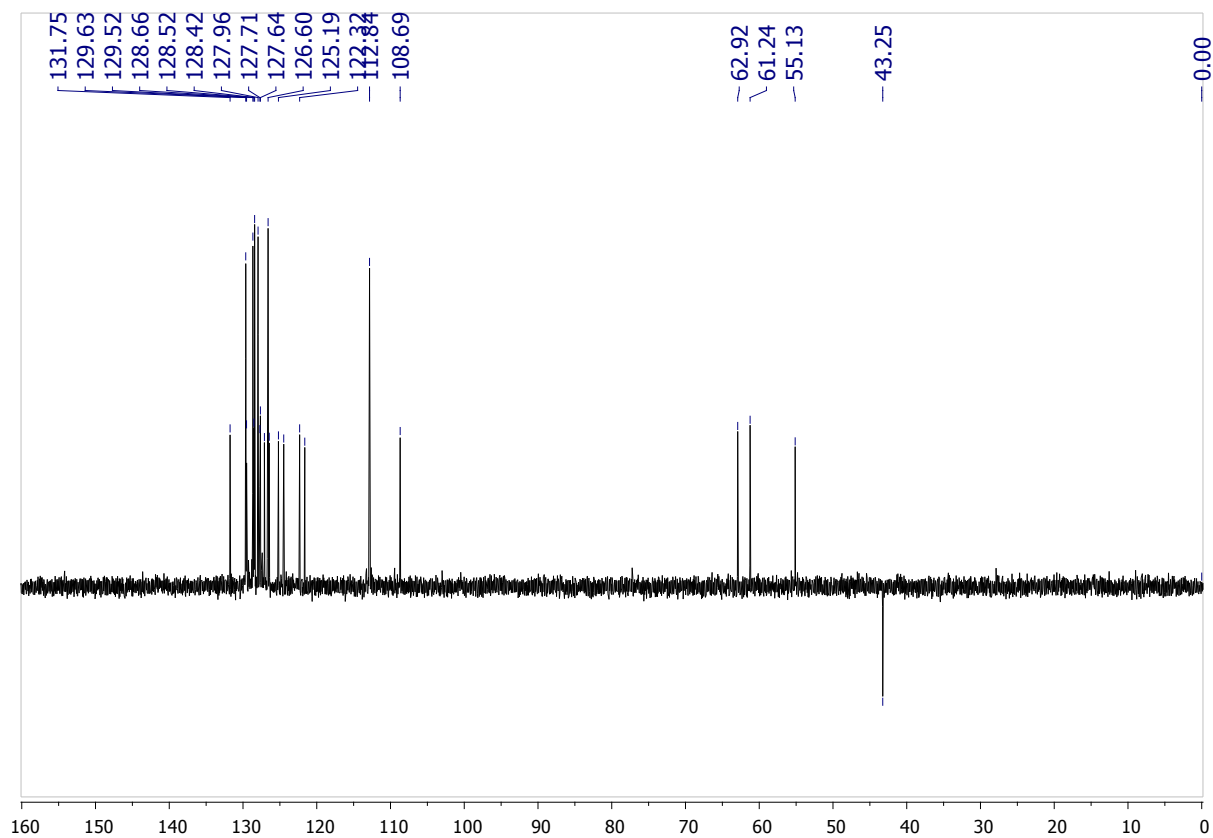


Figure 75. DEPT-135 spectrum of compound 7b

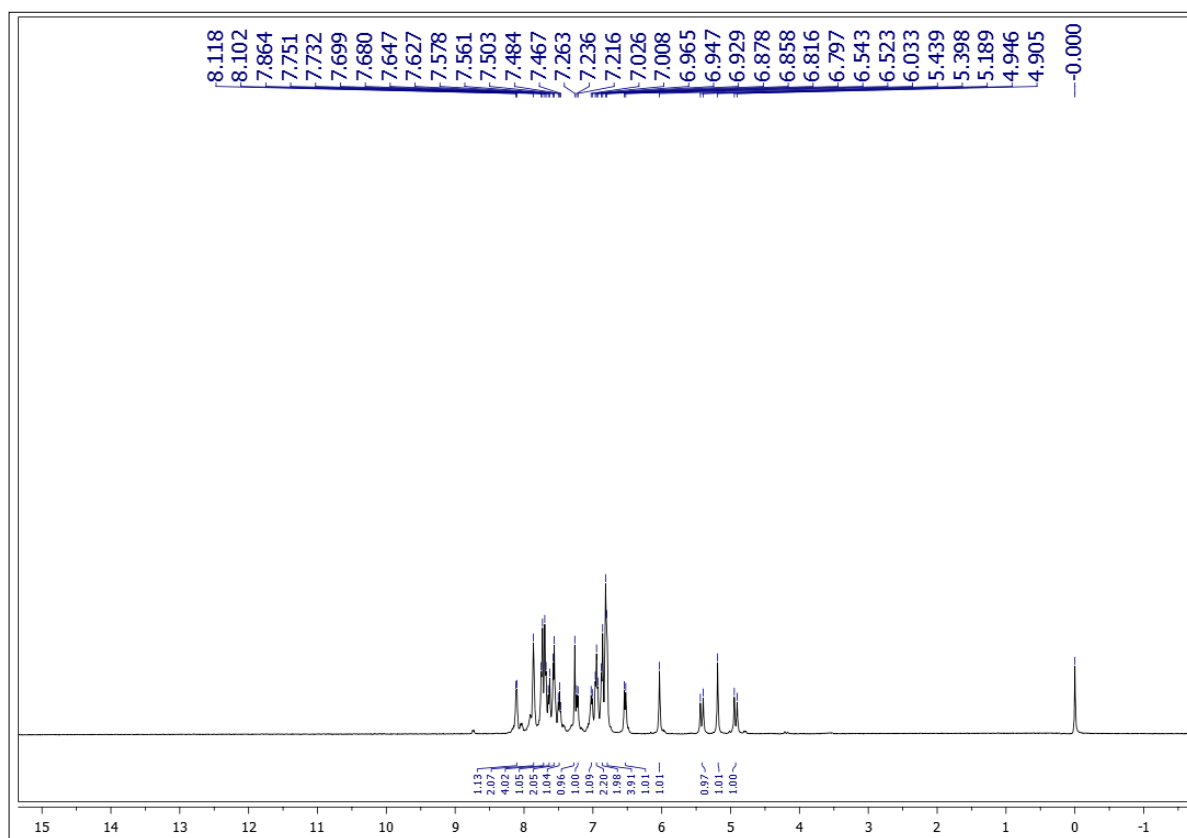


Figure 76. ¹H NMR spectrum of compound 7c

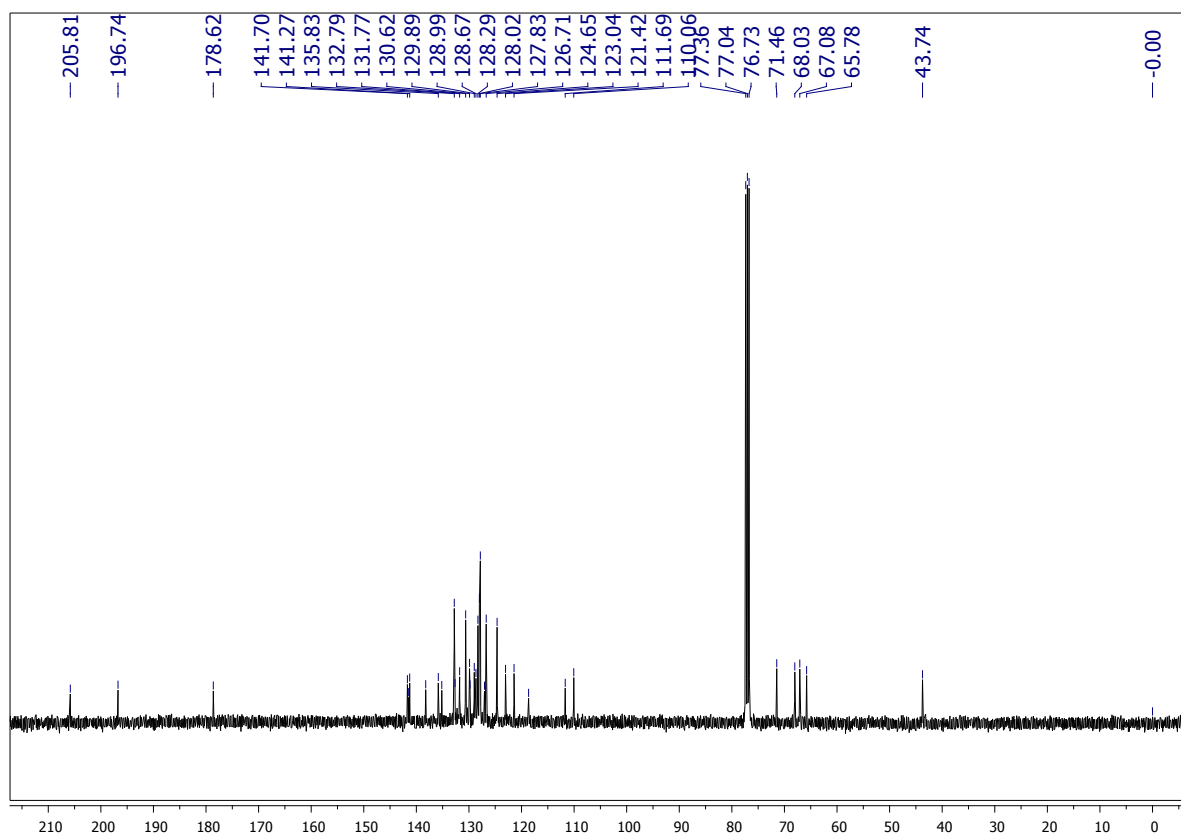


Figure 77. ^{13}C NMR spectrum of compound **7c**

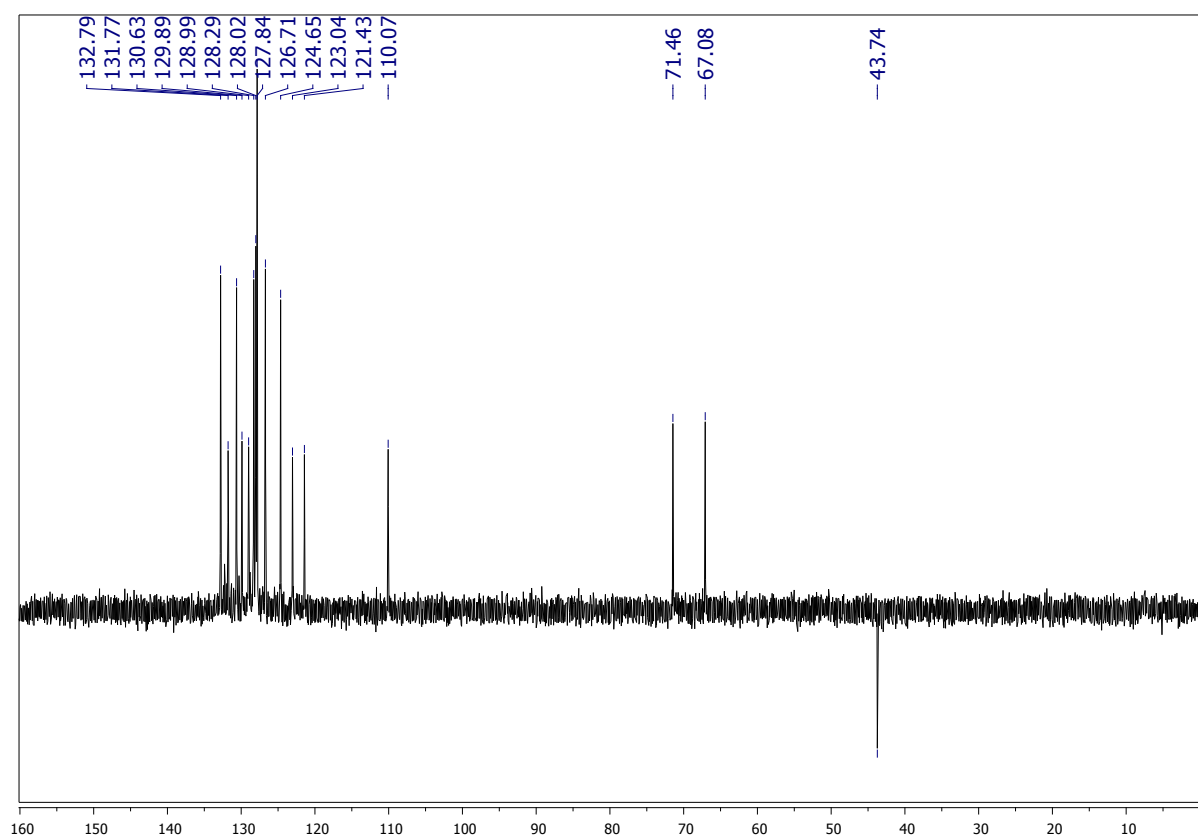


Figure 78. DEPT-135 spectrum of compound **7c**

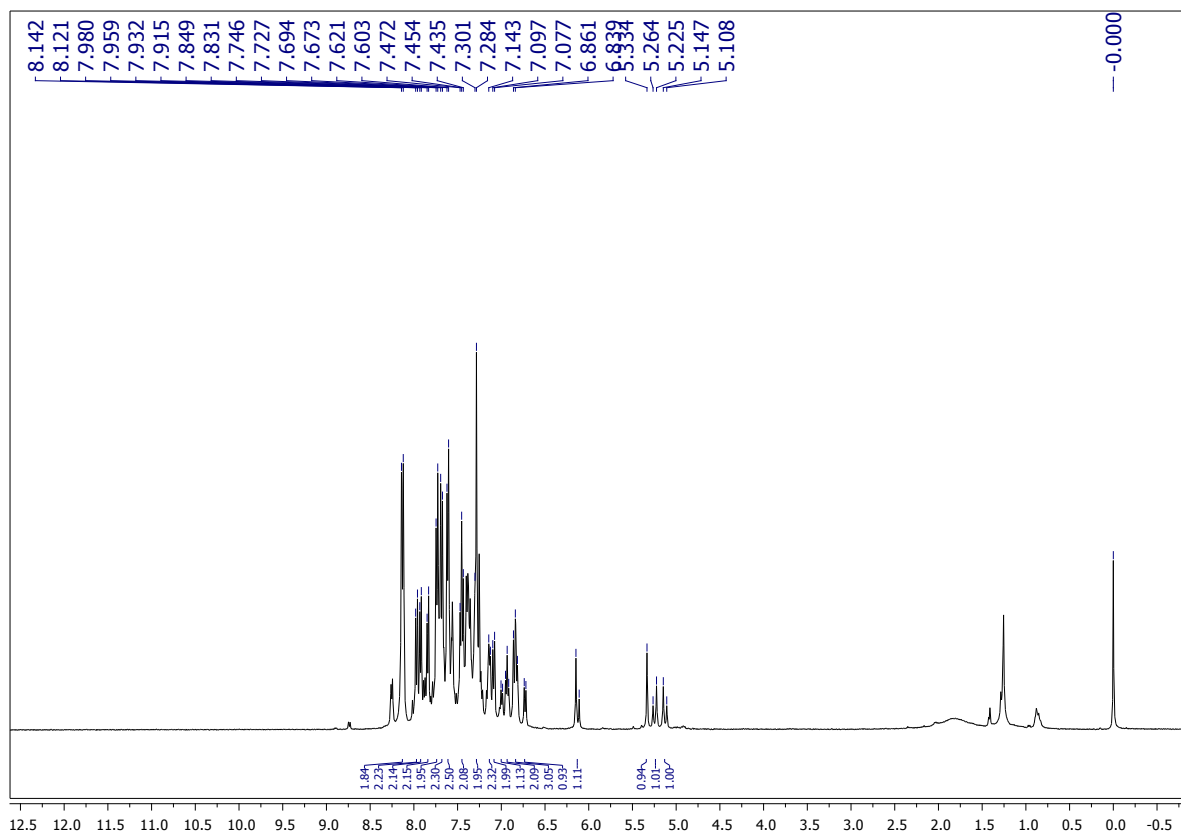


Figure 79. ^1H NMR spectrum of compound **7d**

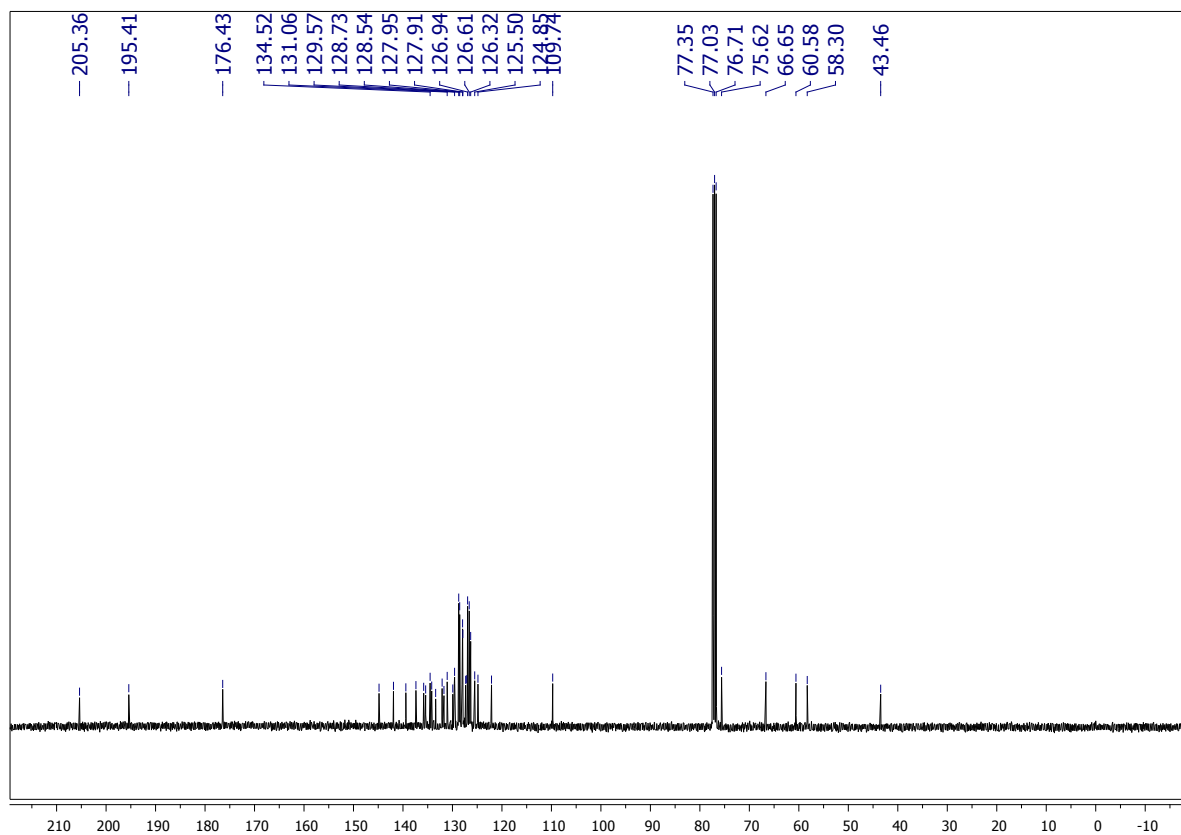


Figure 80. ^{13}C NMR spectrum of compound **7d**

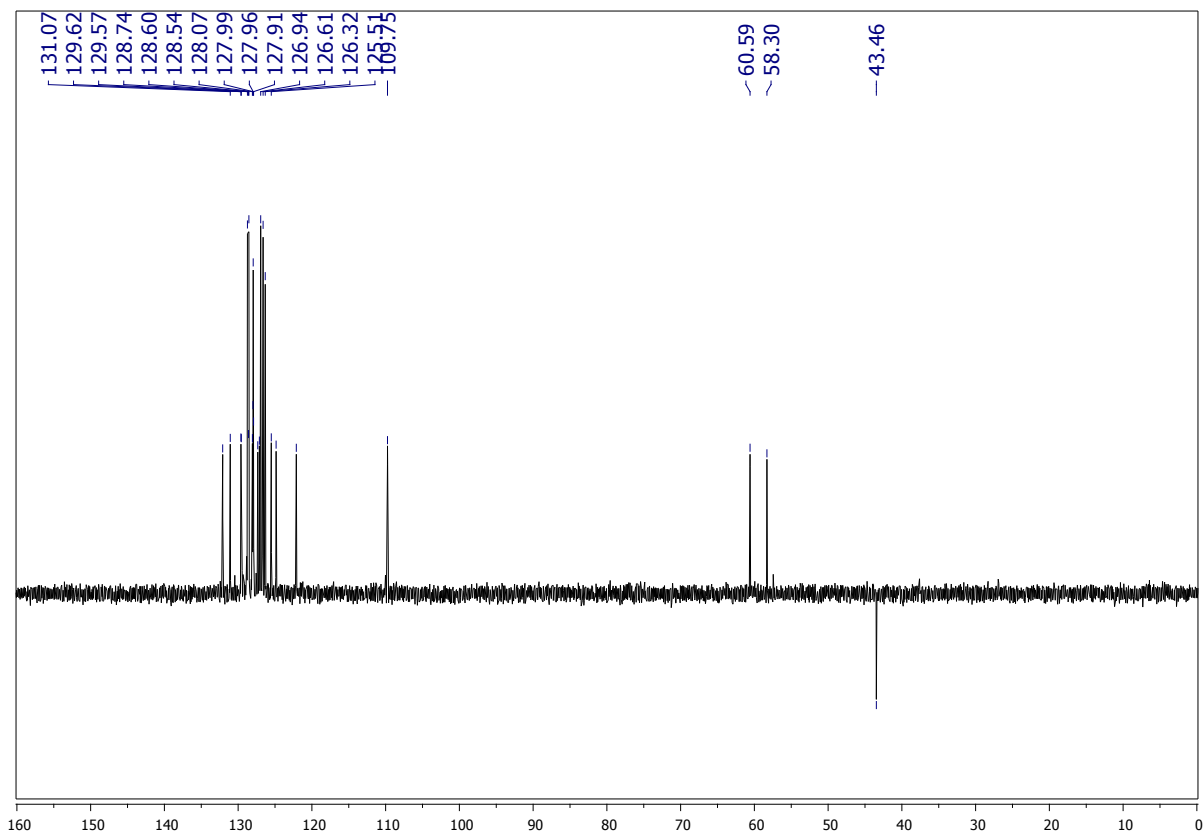


Figure 81. DEPT-135 spectrum of compound 7d

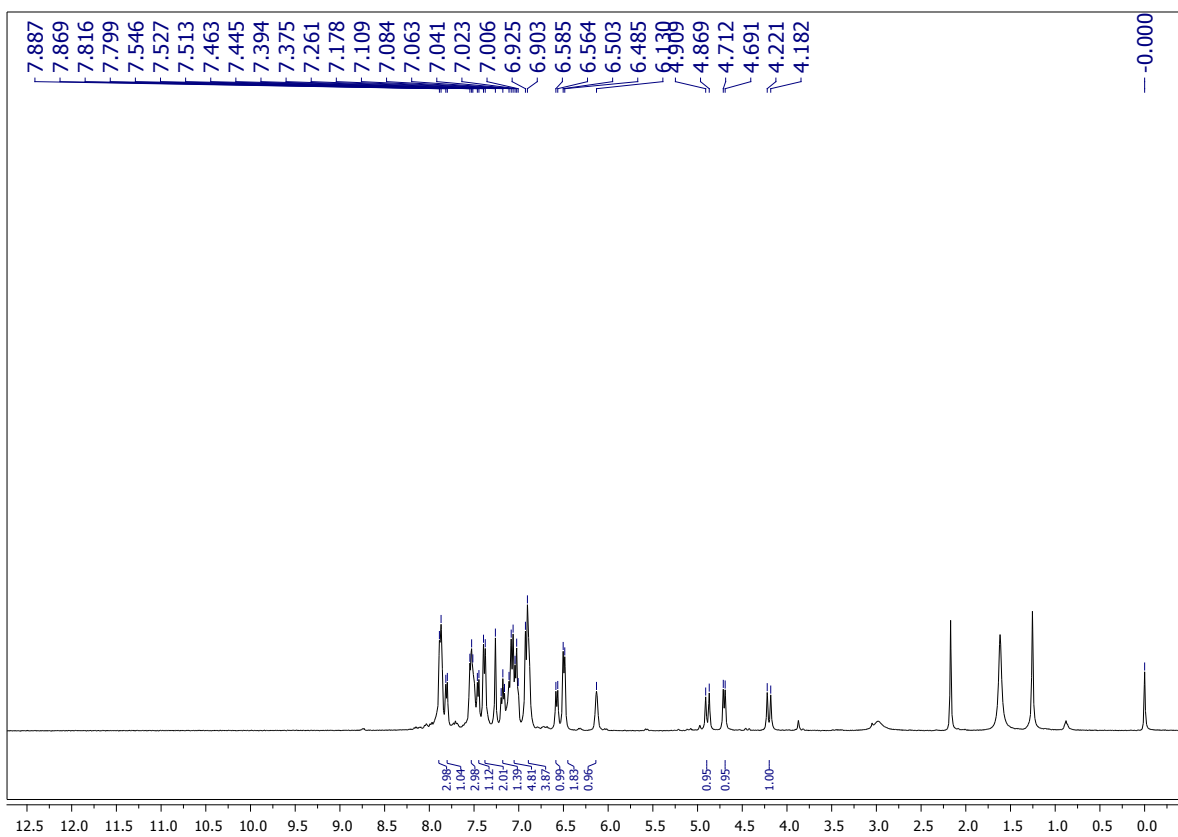


Figure 82. ¹H NMR spectrum of compound 7e

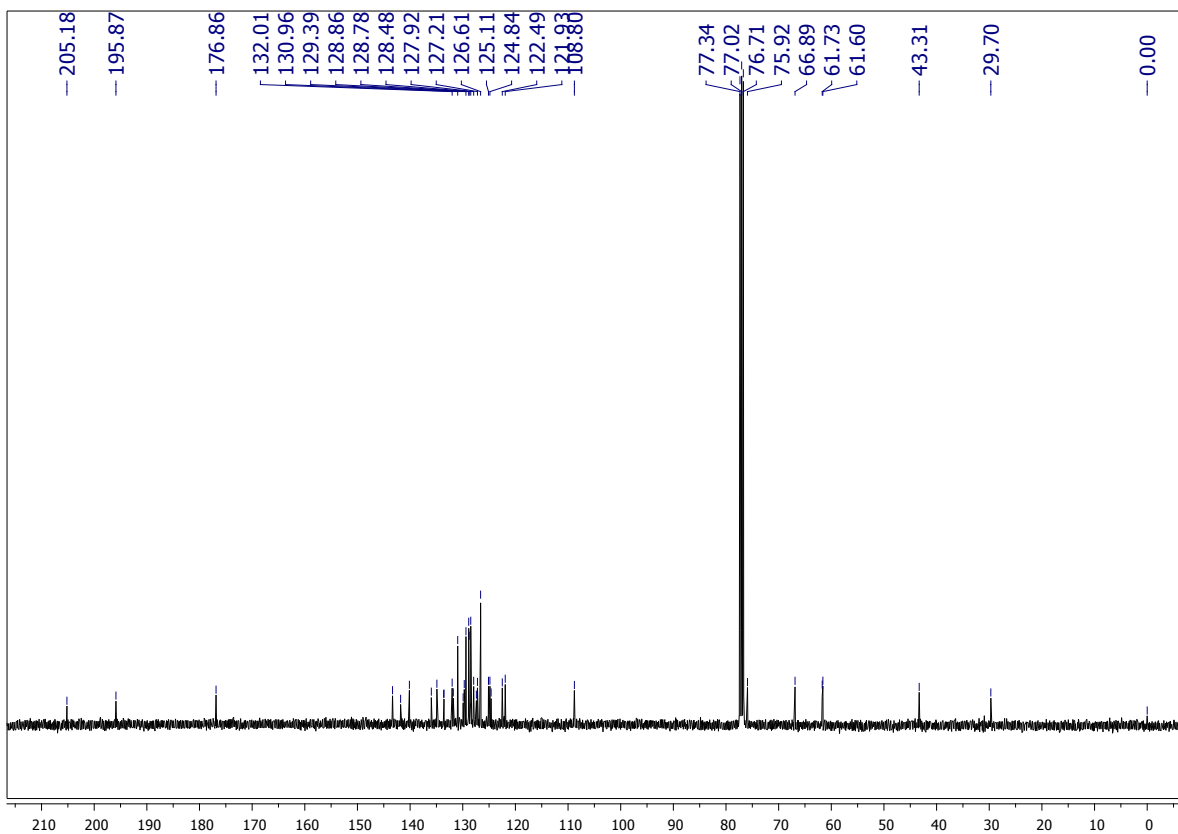


Figure 83. ^{13}C NMR spectrum of compound **7e**

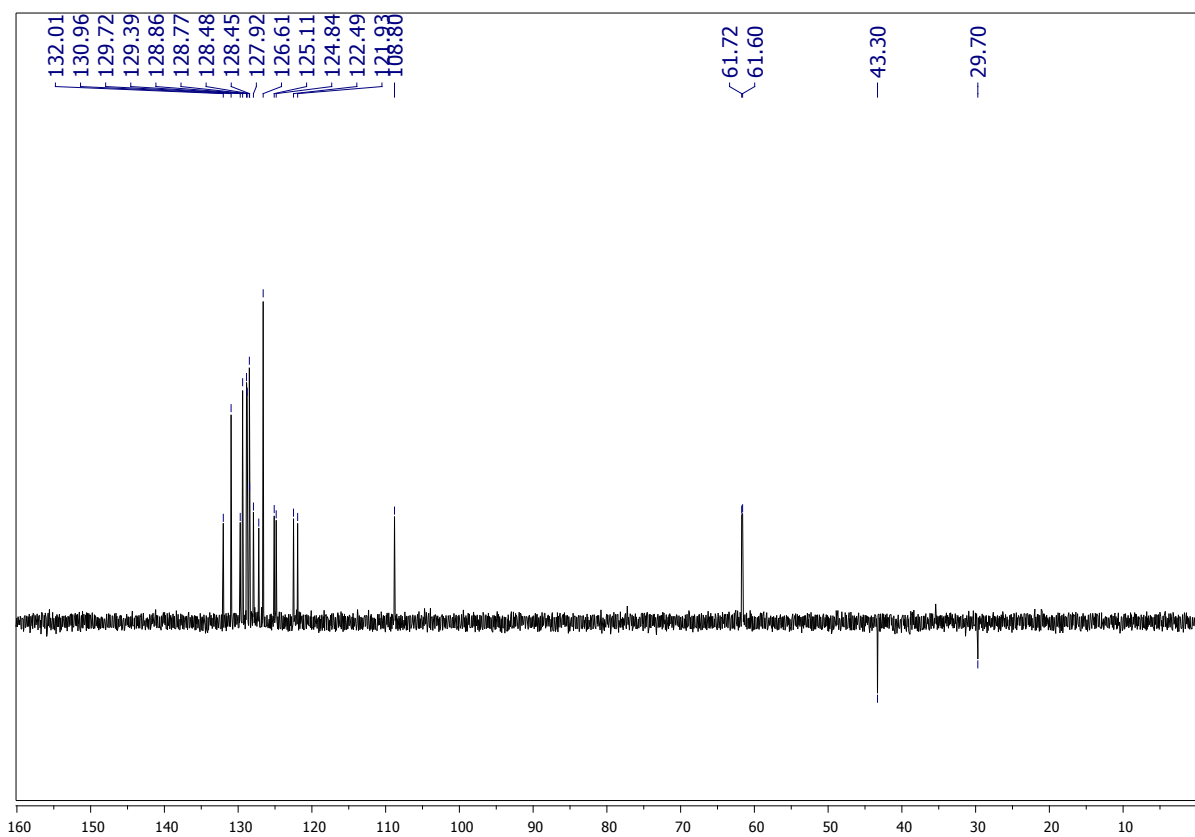


Figure 84. DEPT-135 spectrum of compound **7e**

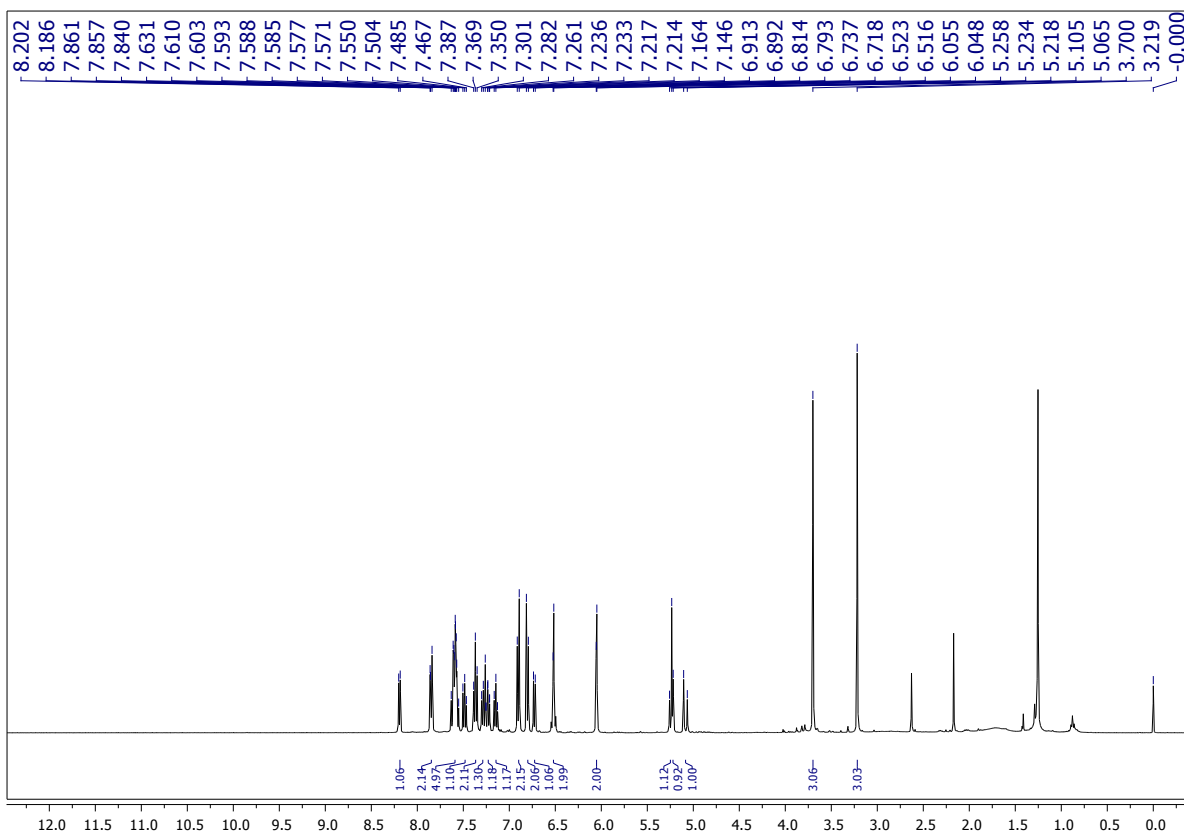


Figure 85. ^1H NMR spectrum of compound **7f**

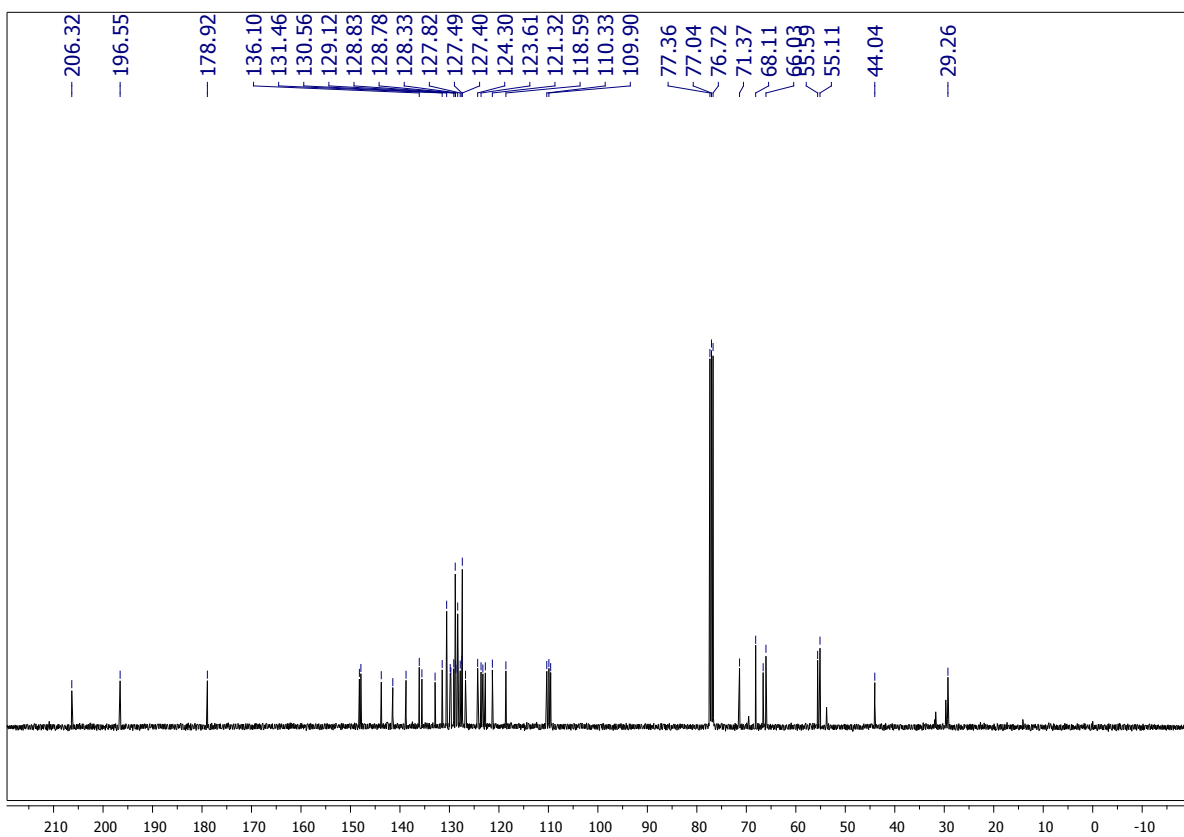


Figure 86. ^{13}C NMR spectrum of compound **7f**

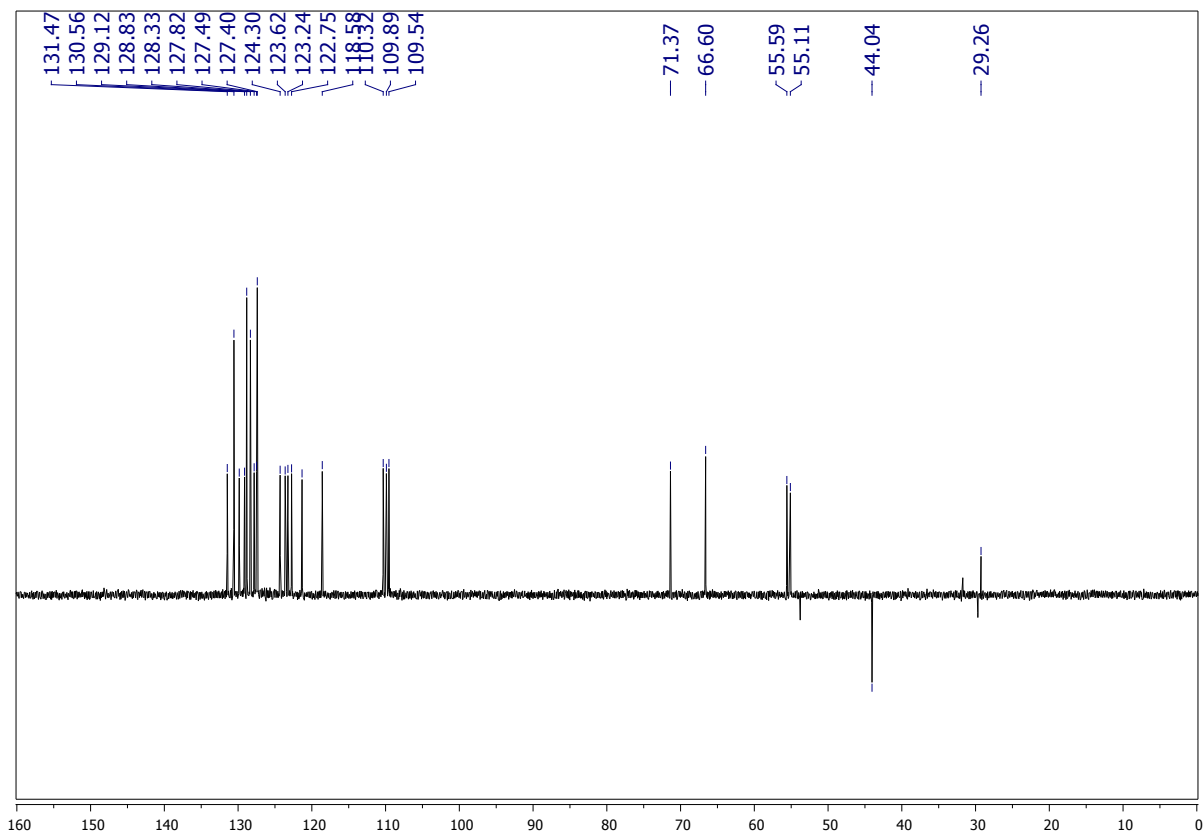


Figure 87. DEPT-135 spectrum of compound 7f

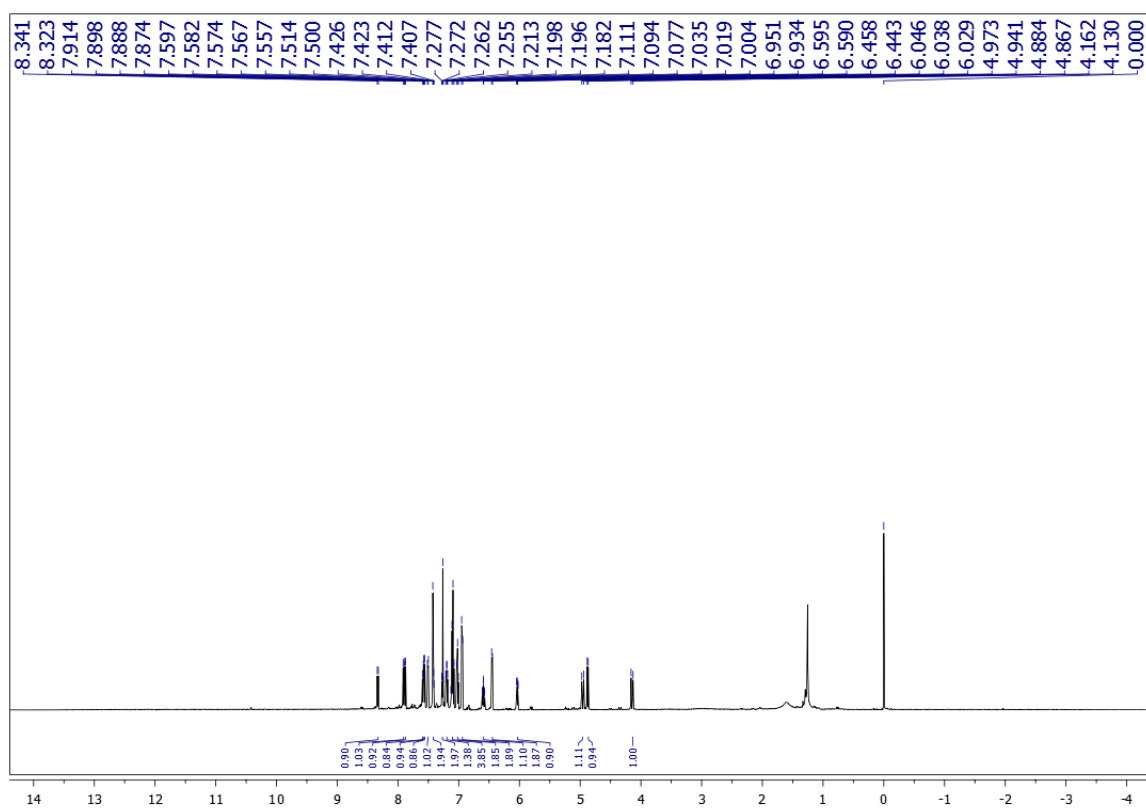


Figure 88. ¹H NMR spectrum of compound 7g

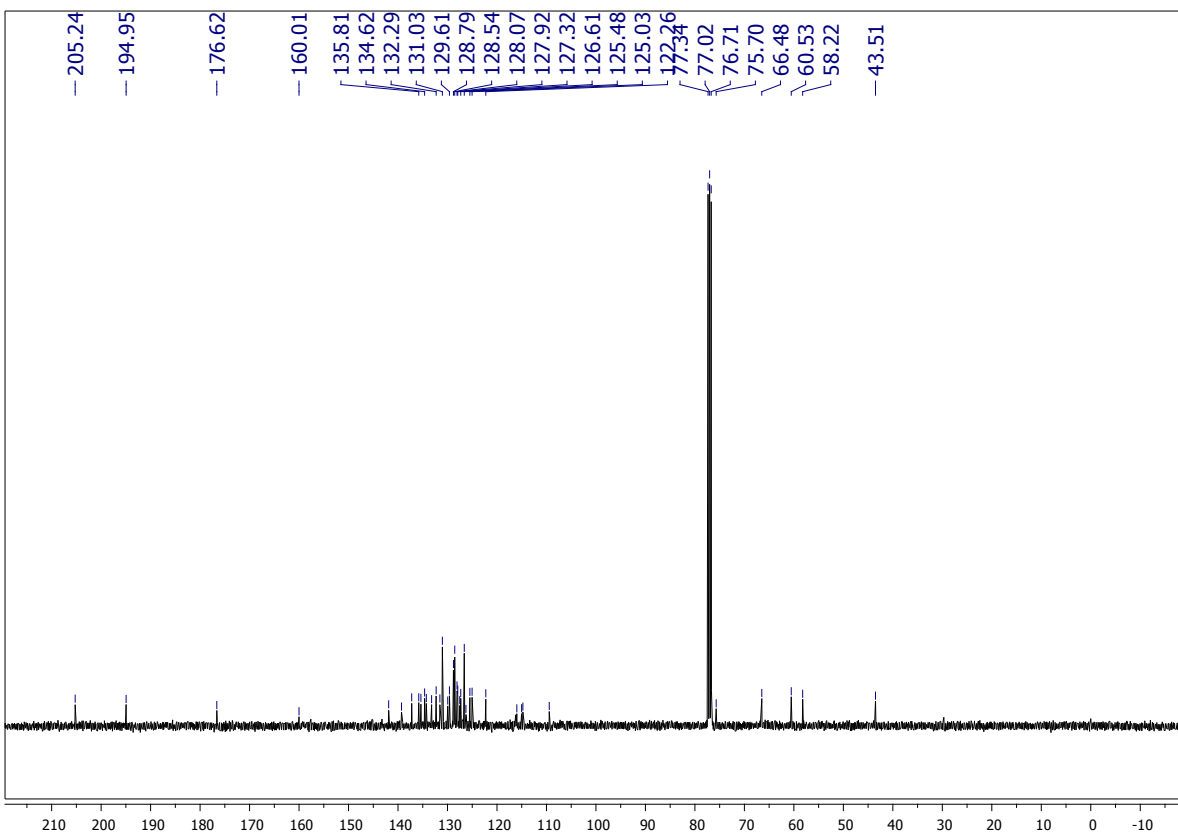


Figure 89. ^{13}C NMR spectrum of compound **7g**

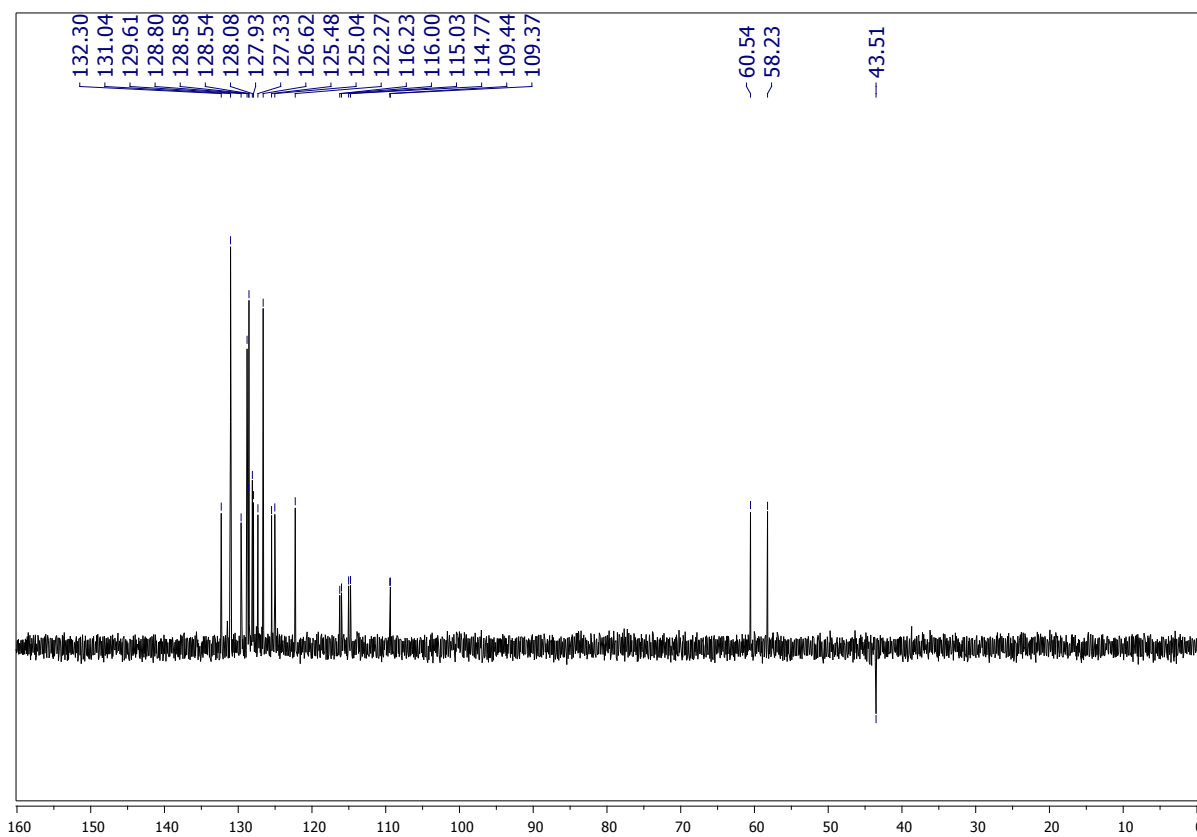


Figure 90. DEPT-135 spectrum of compound **7g**

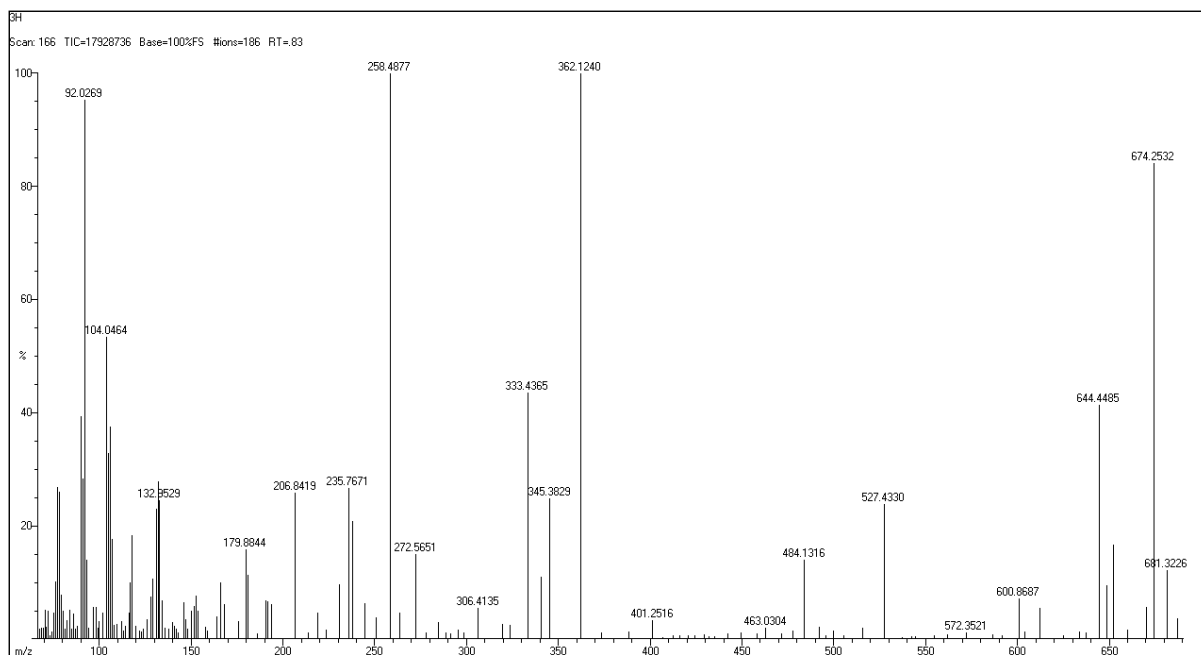


Figure 91. Mass spectrum of **3a**

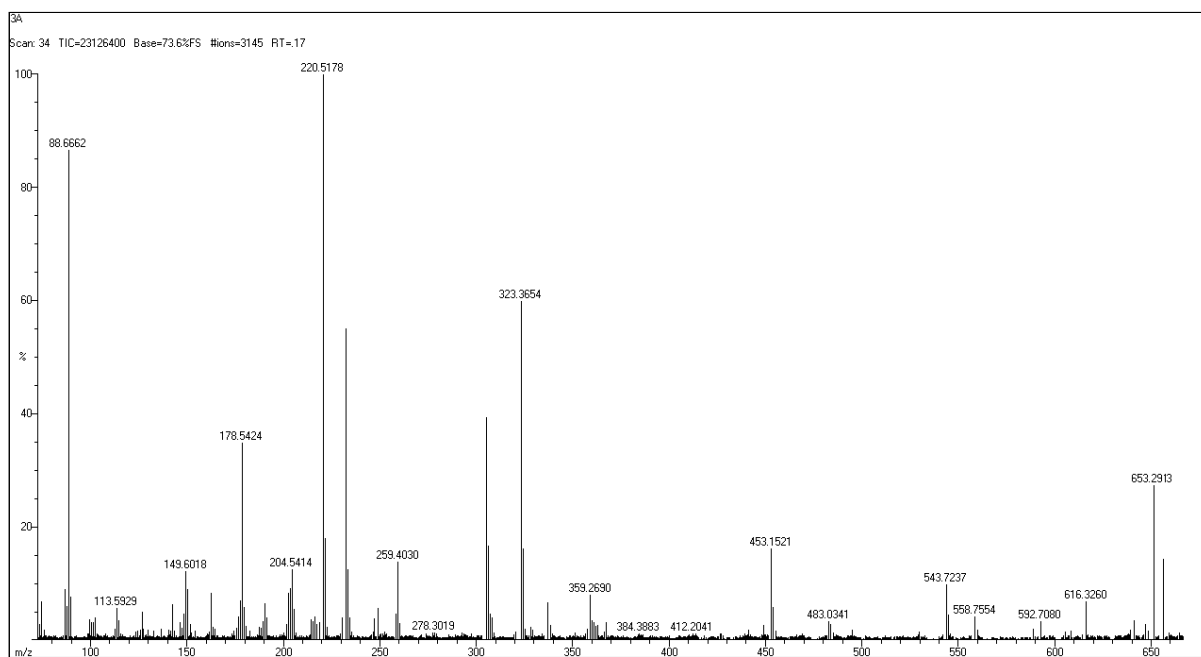


Figure 92. Mass spectrum of **3b**

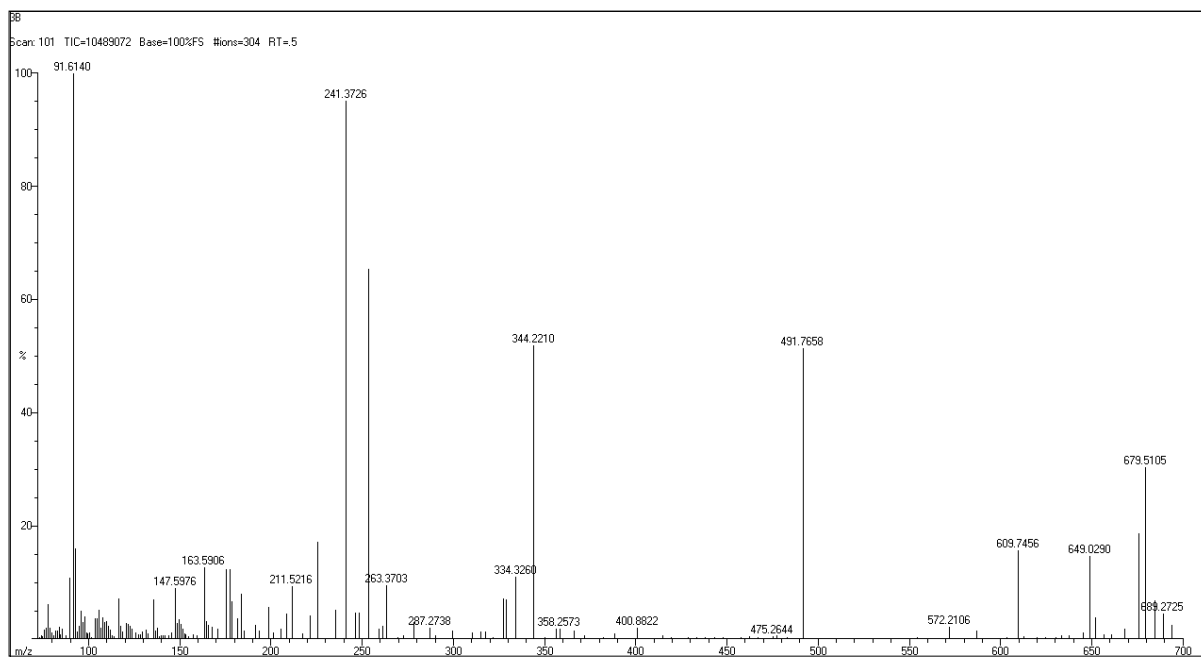


Figure 93. Mass spectrum of **3c**

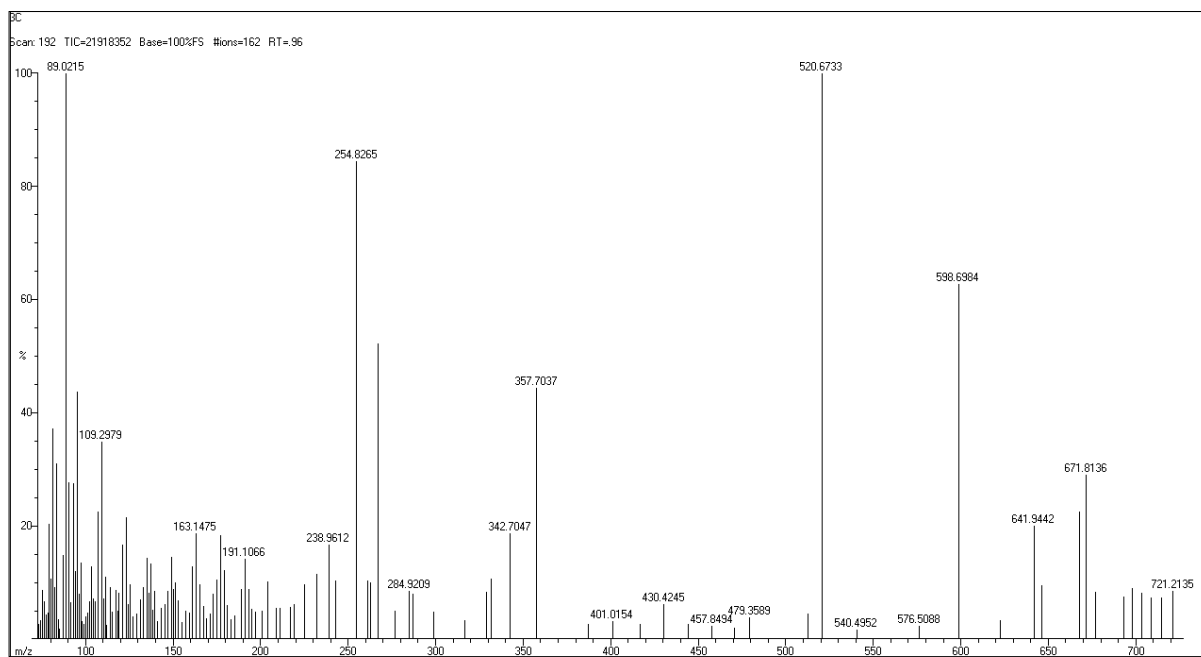


Figure 94. Mass spectrum of **3d**

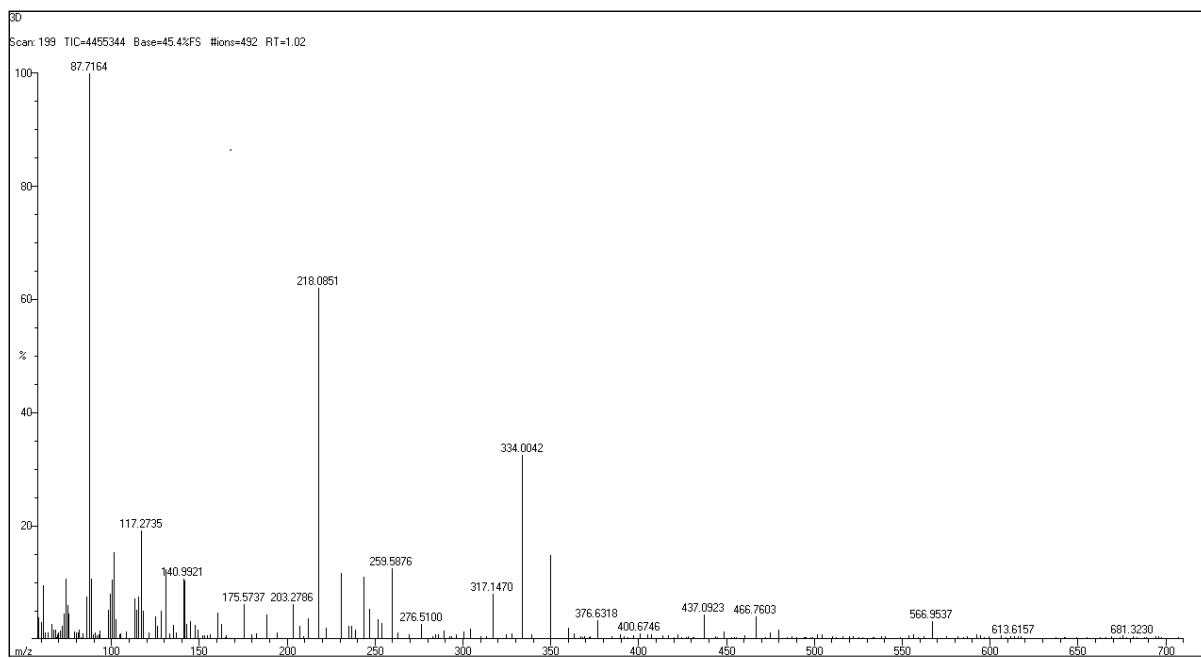


Figure 95. Mass spectrum of **3e**

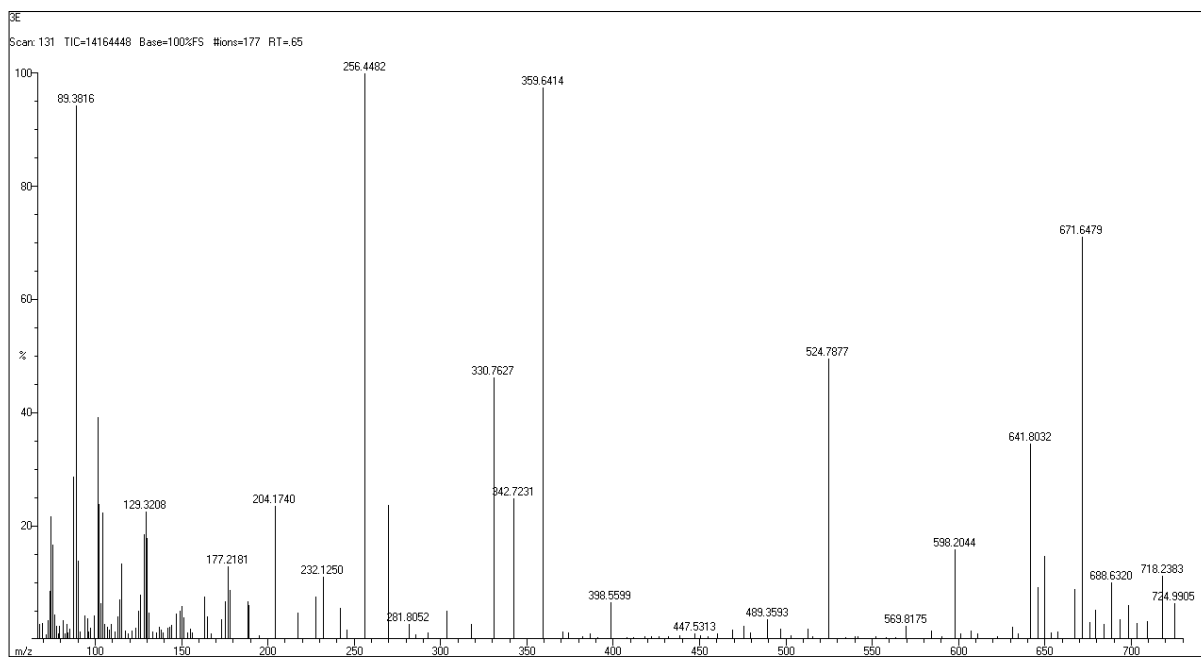


Figure 96. Mass spectrum of **3f**

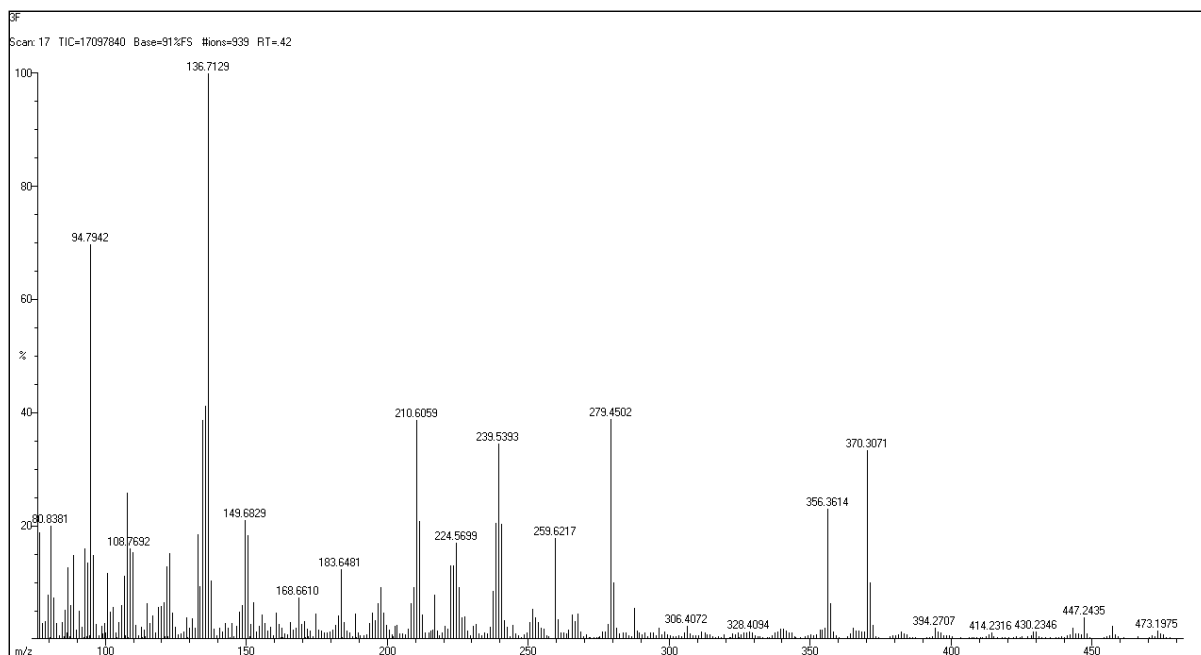


Figure 97. Mass spectrum of **3g**

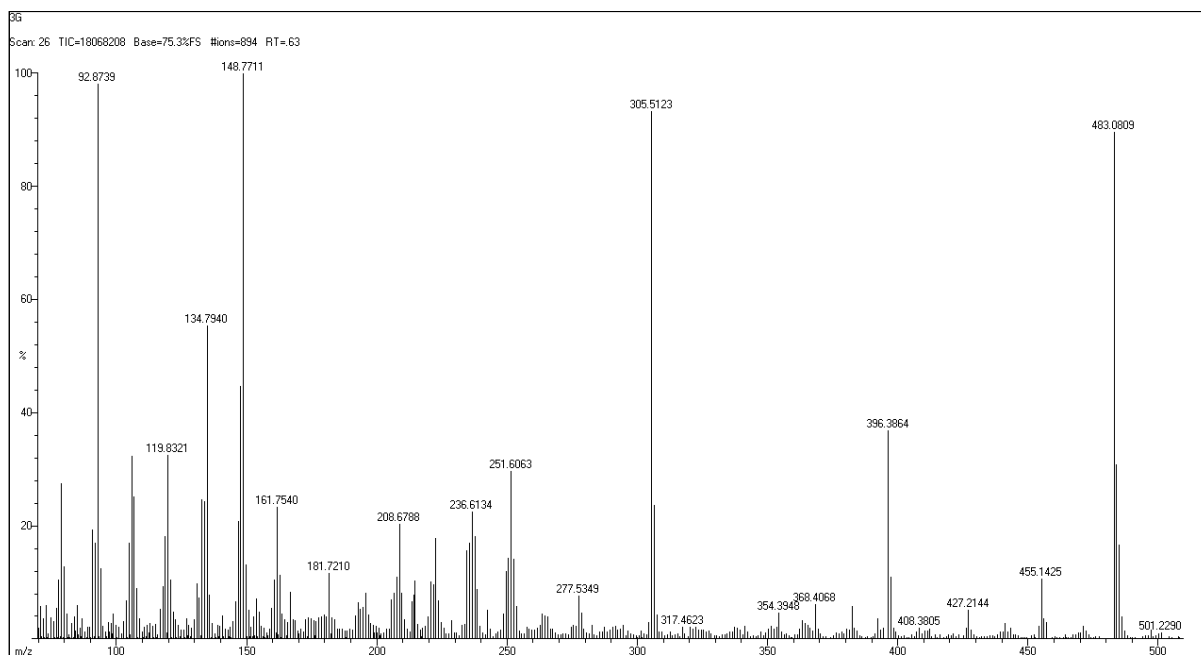


Figure 98. Mass spectrum of **3h**

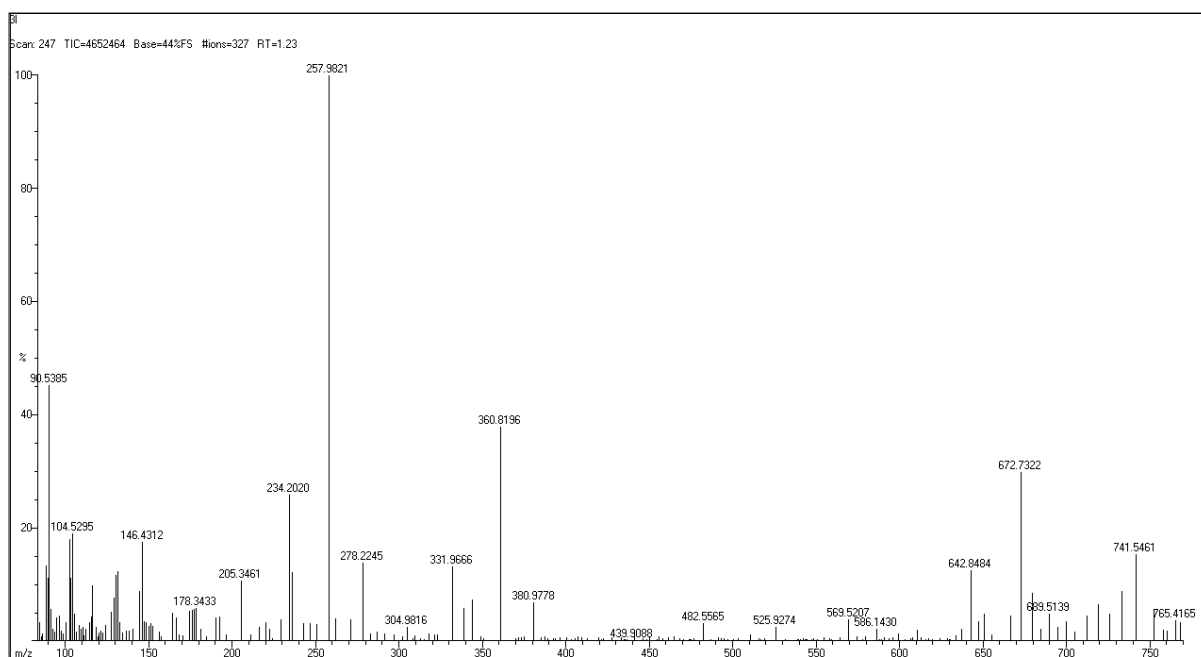


Figure 99. Mass spectrum of **3i**

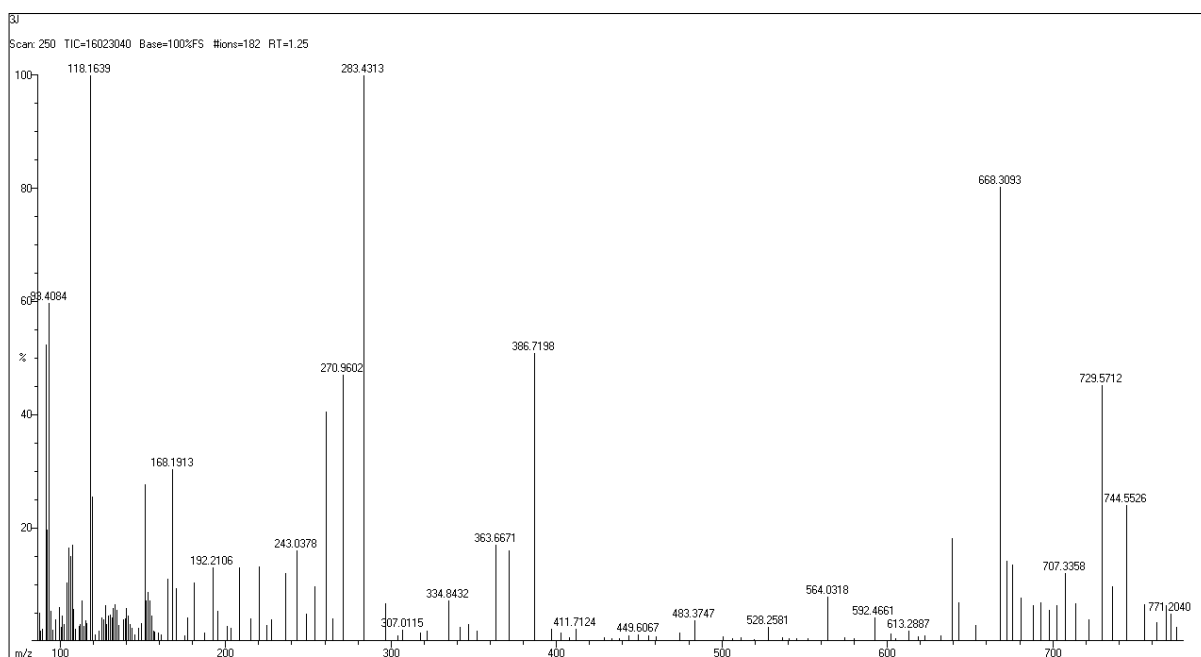


Figure 100. Mass spectrum of **3j**

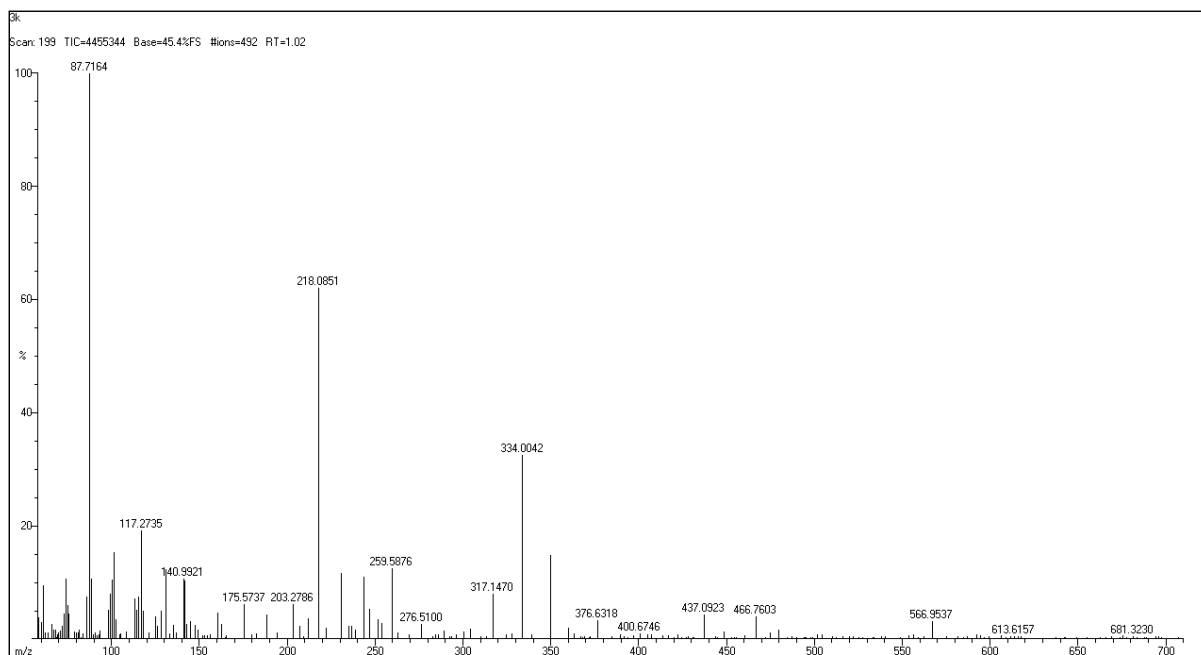


Figure 101. Mass spectrum of **3k**

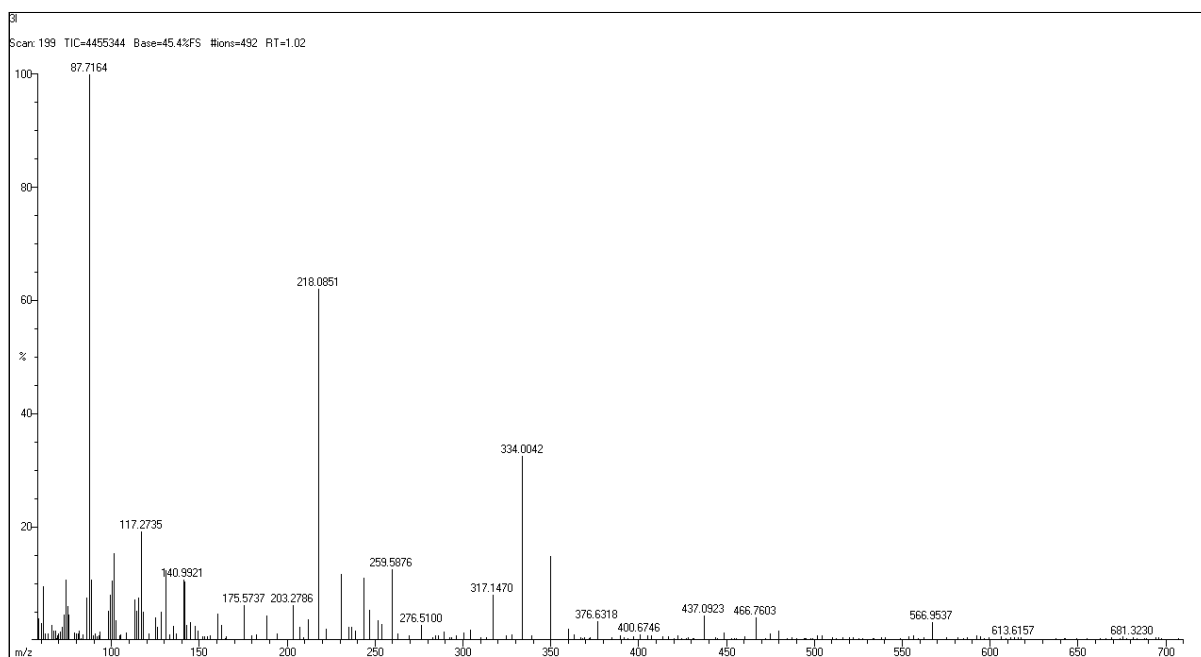


Figure 102. Mass spectrum of **3l**

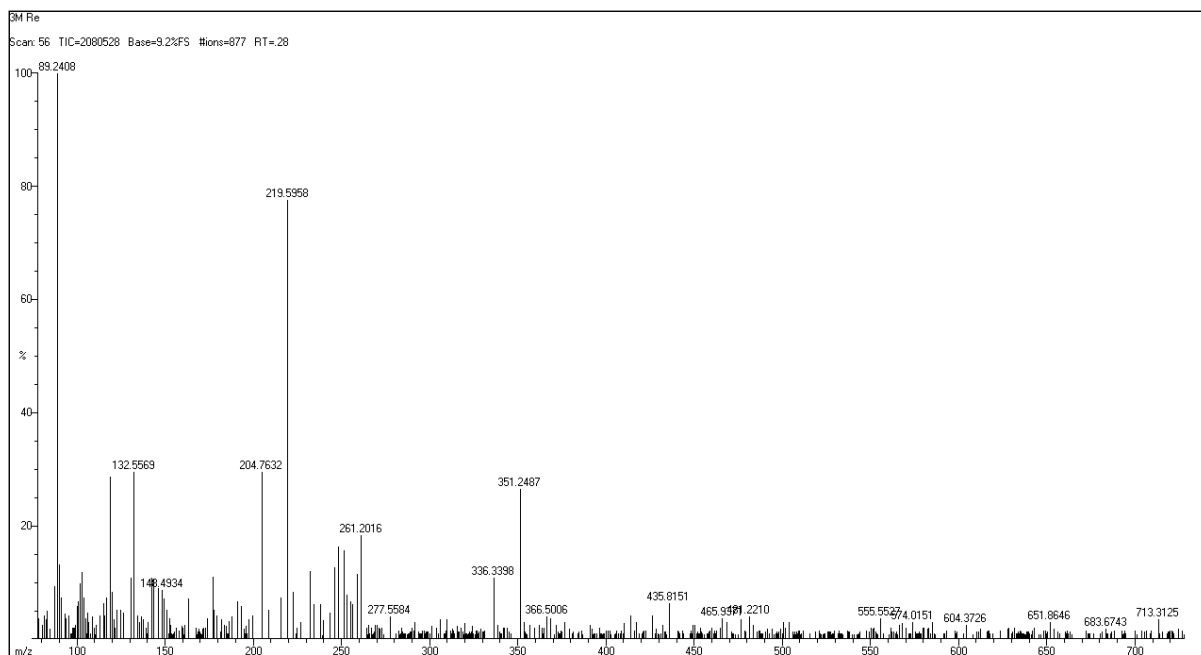


Figure 103. Mass spectrum of 3m

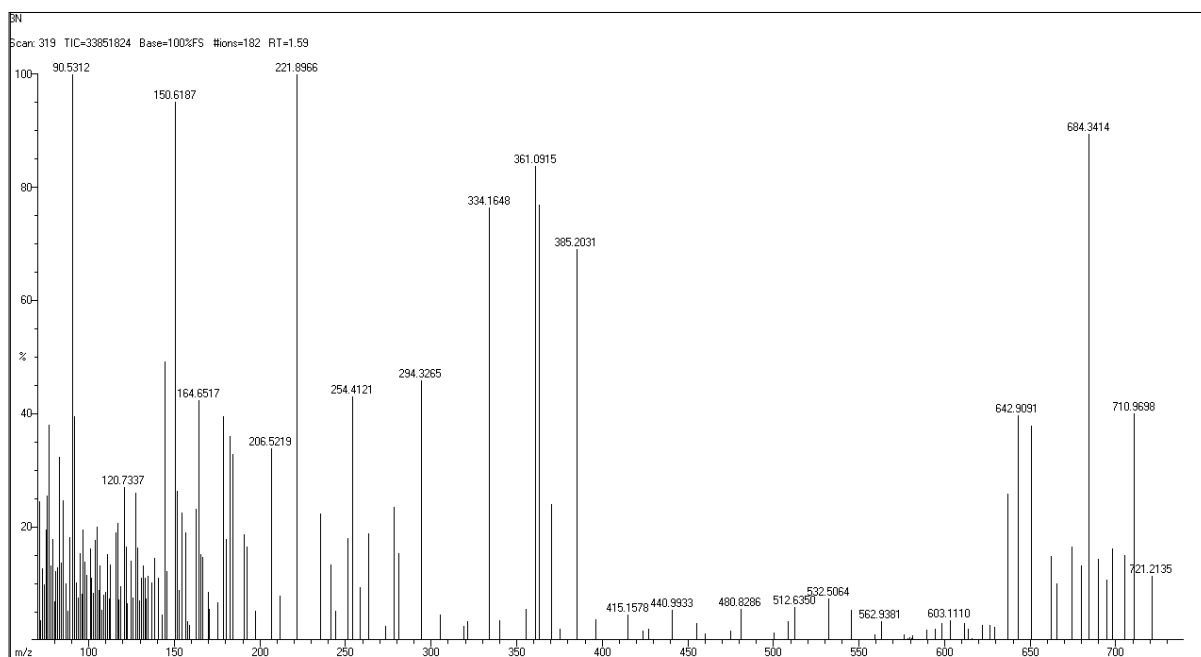


Figure 104. Mass spectrum of 3n

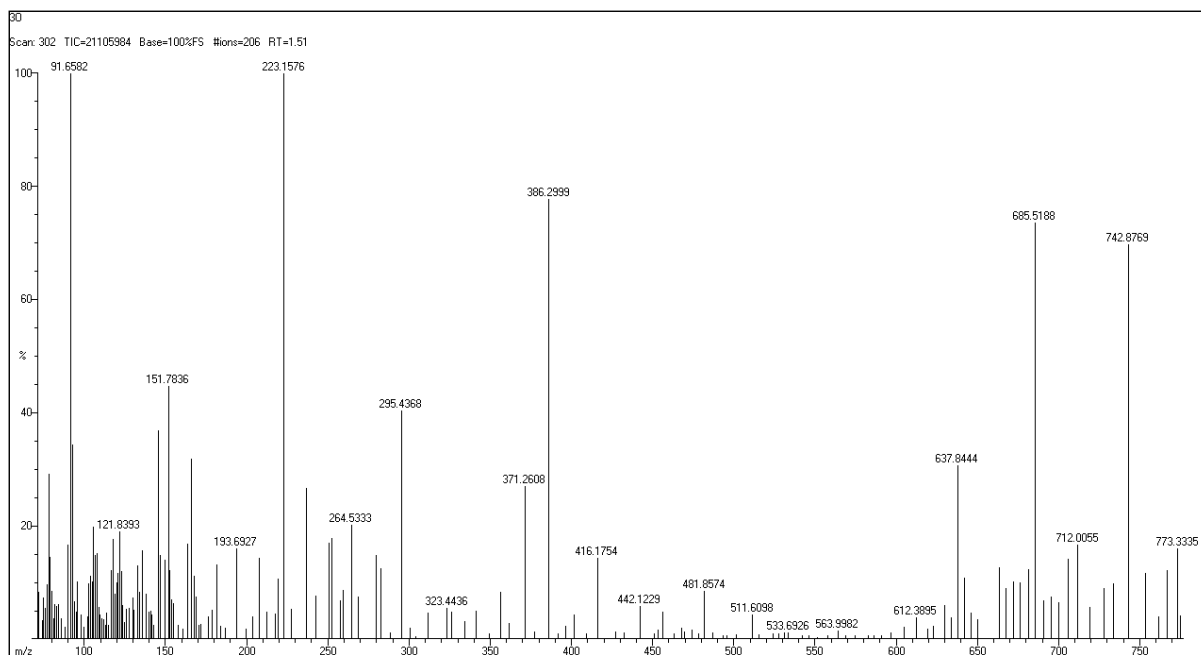


Figure 105. Mass spectrum of **3o**

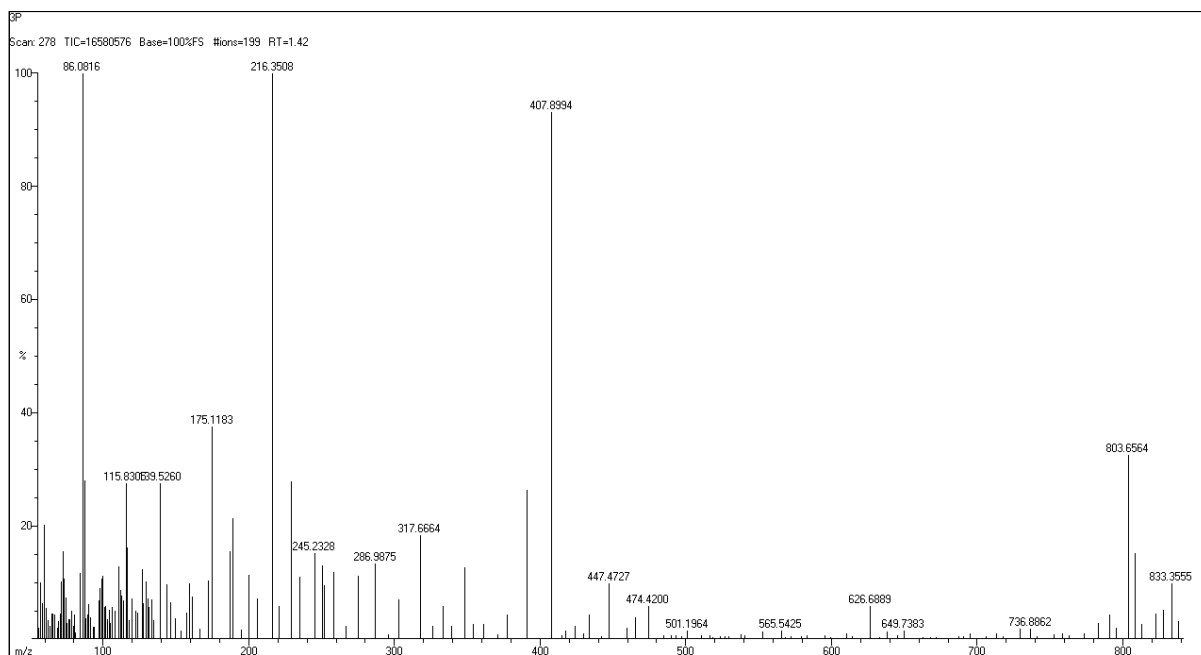


Figure 106. Mass spectrum of **3p**

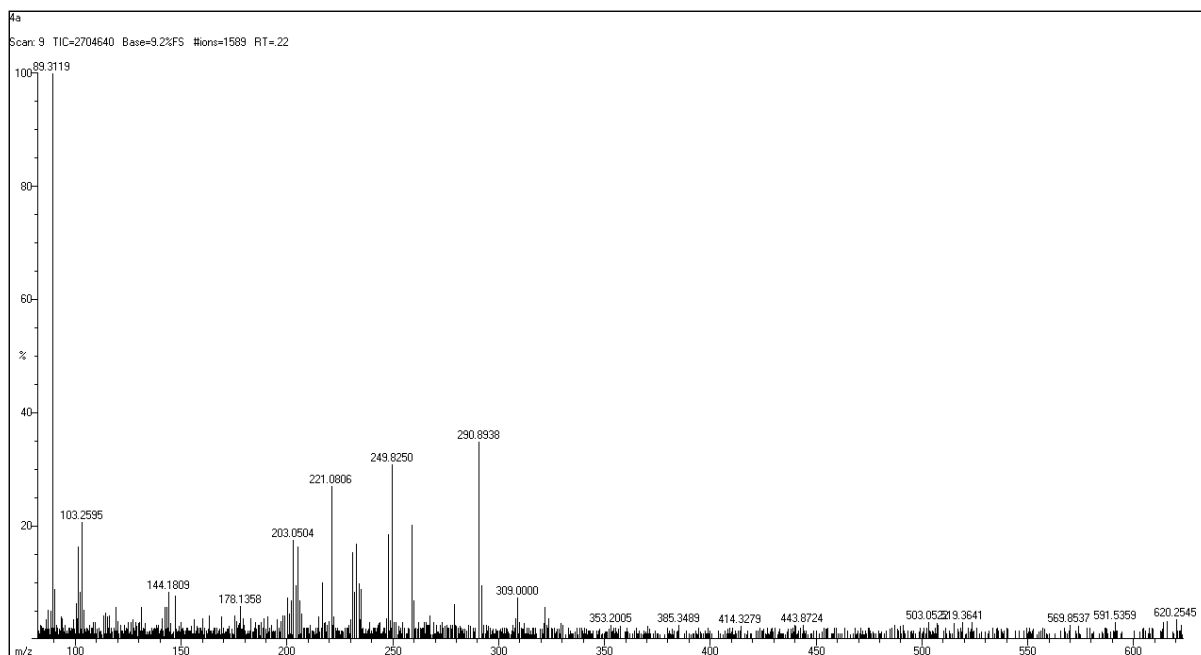


Figure 107. Mass spectrum of **5a**

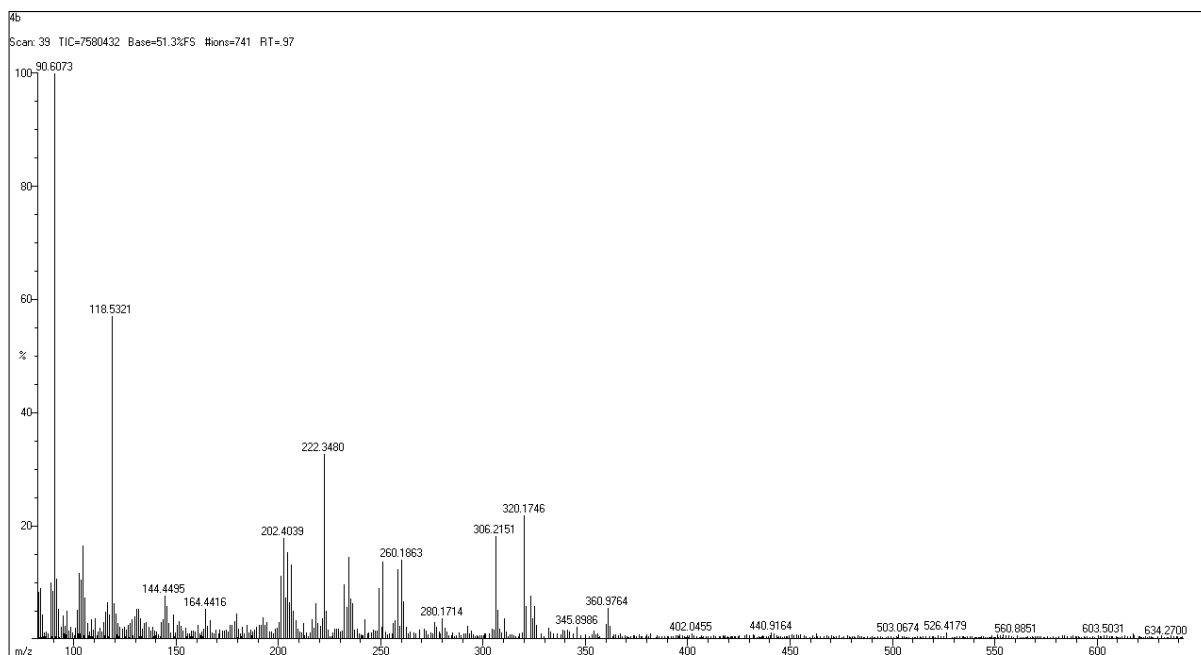


Figure 108. Mass spectrum of **5b**

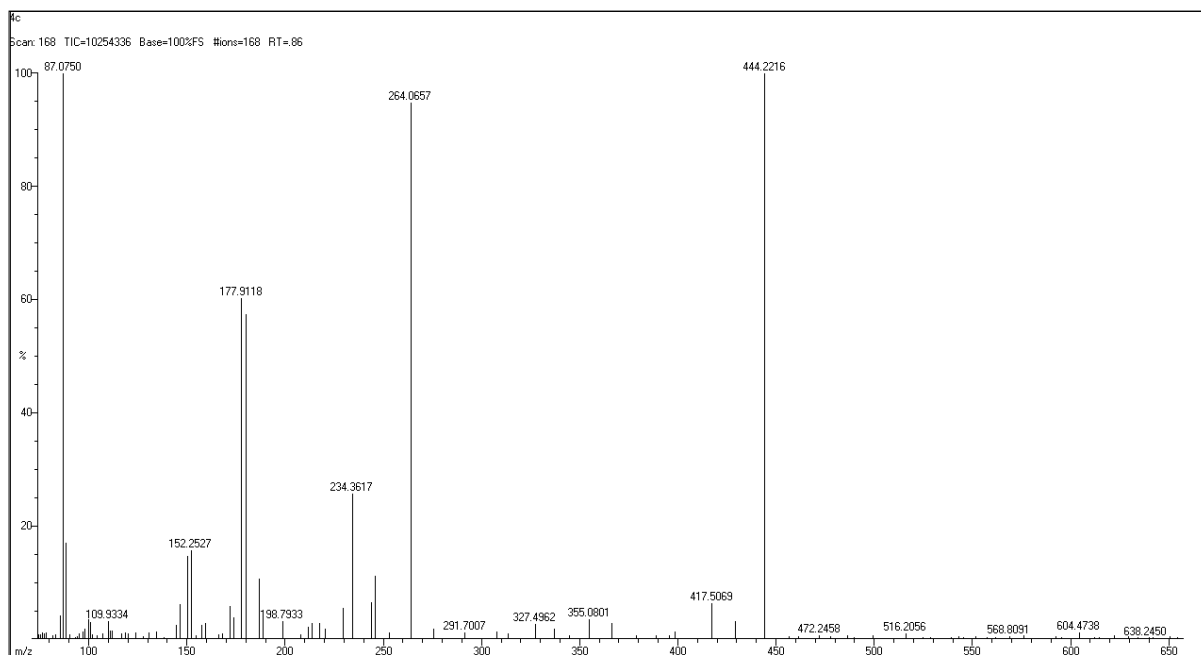


Figure 109. Mass spectrum of 5c

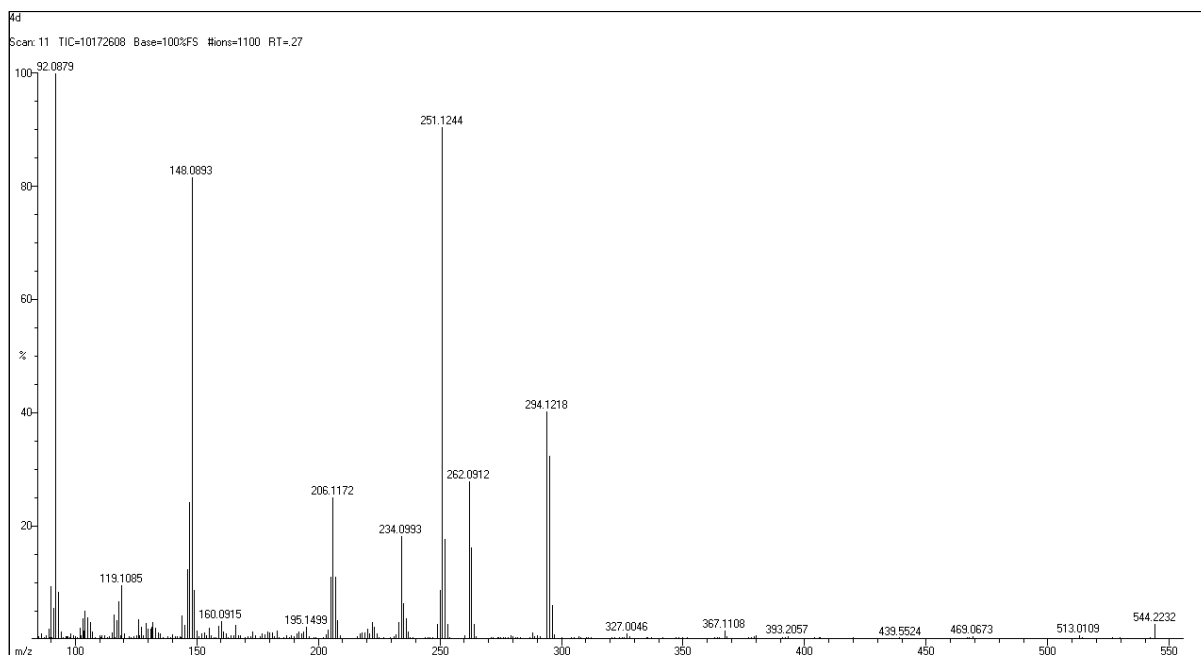


Figure 110. Mass spectrum of 5d

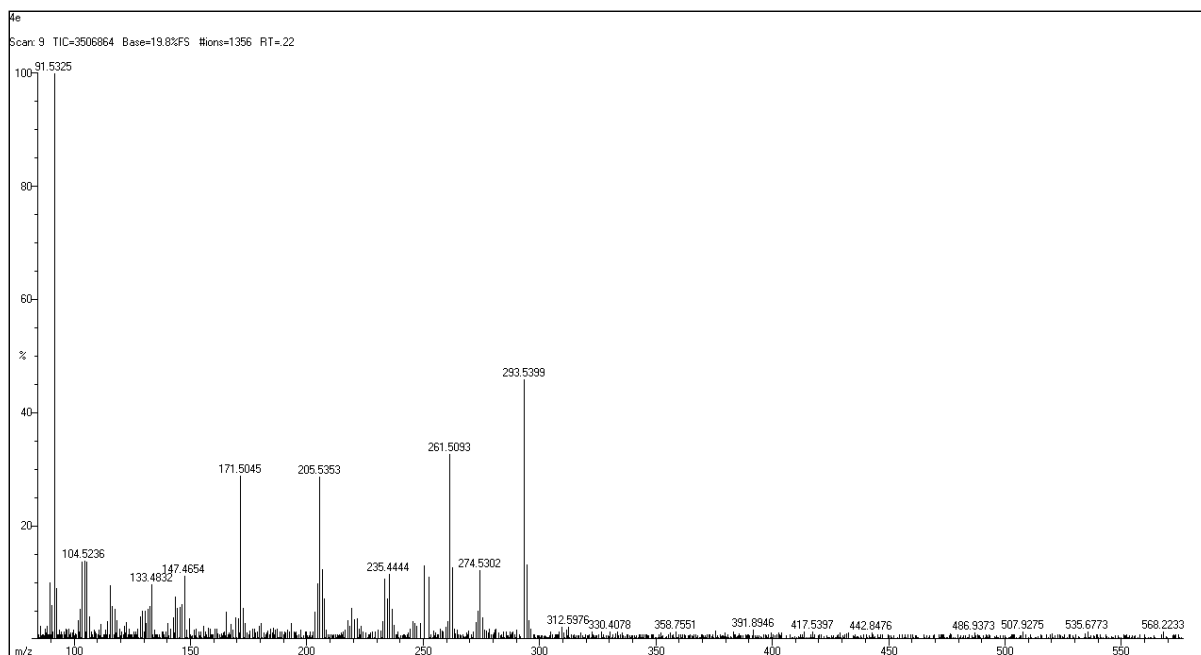


Figure 111. Mass spectrum of 5e

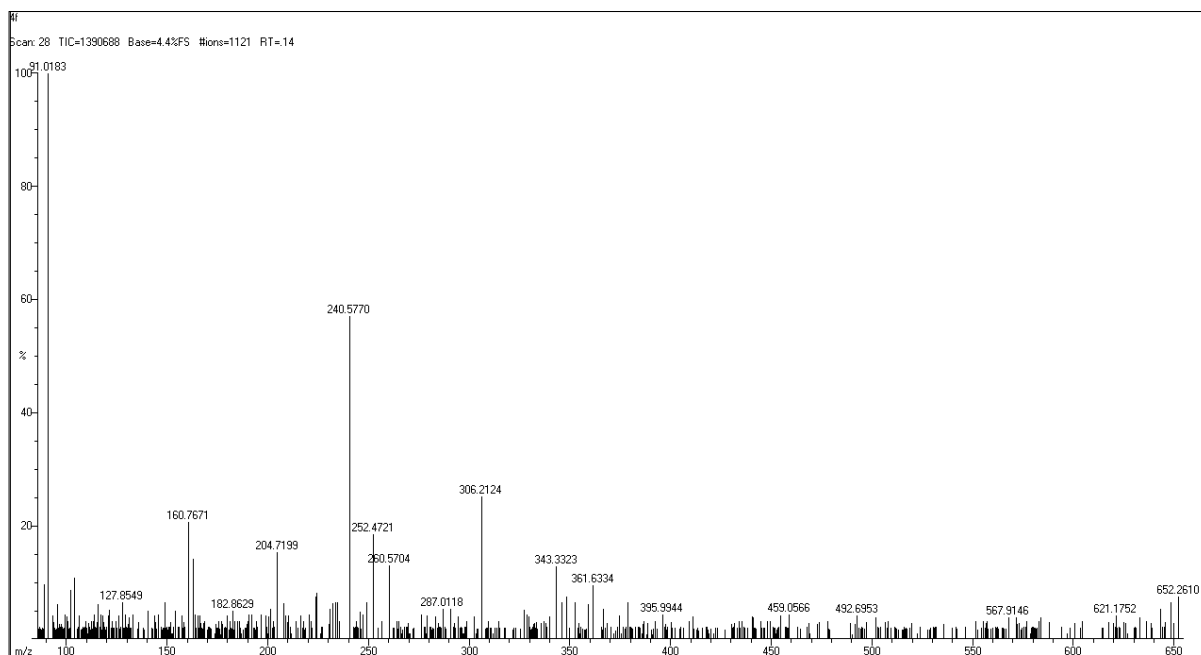


Figure 112. Mass spectrum of 5f

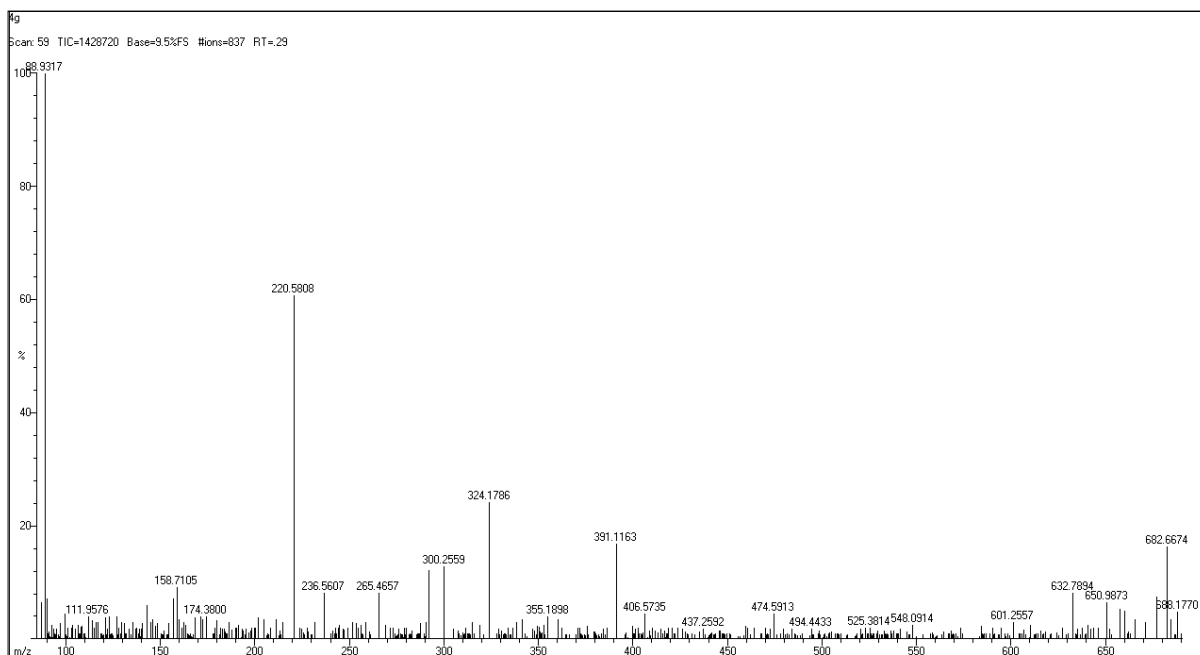


Figure 113. Mass spectrum of 5g

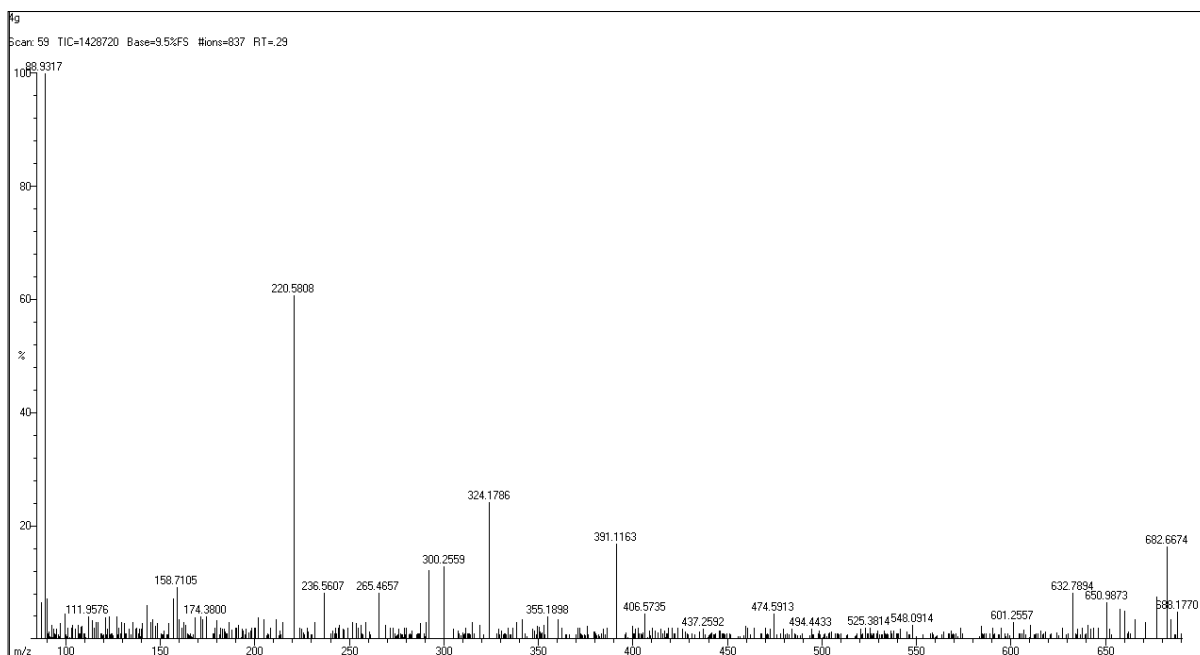


Figure 114. Mass spectrum of 7a

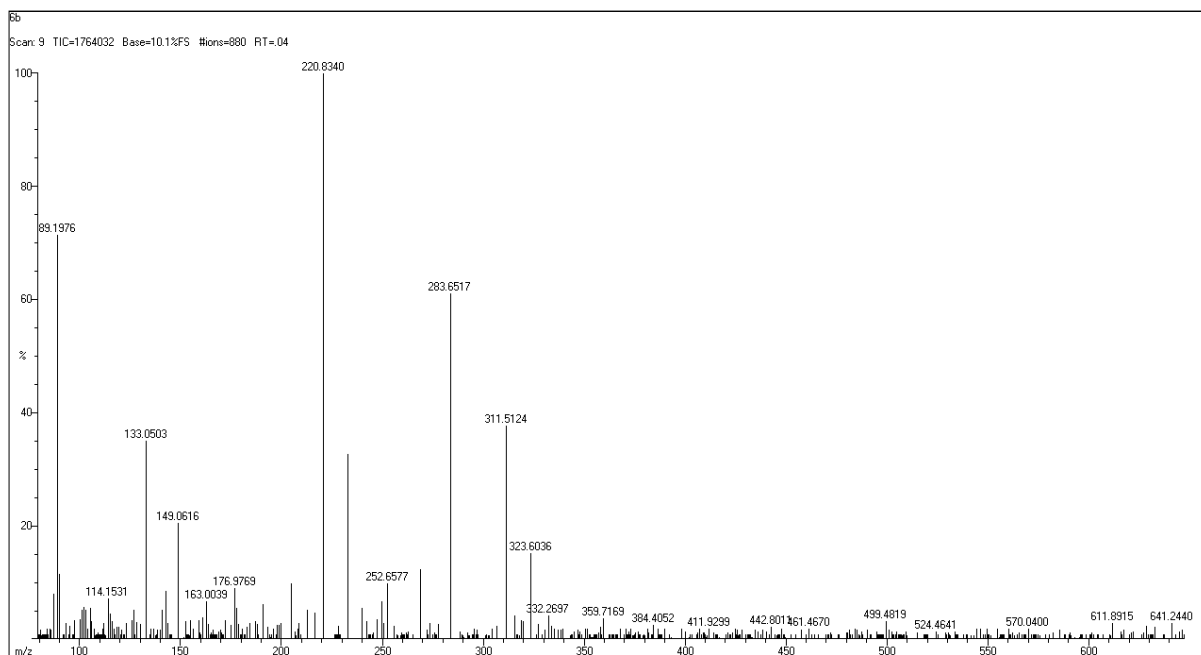


Figure 115. Mass spectrum of 7b

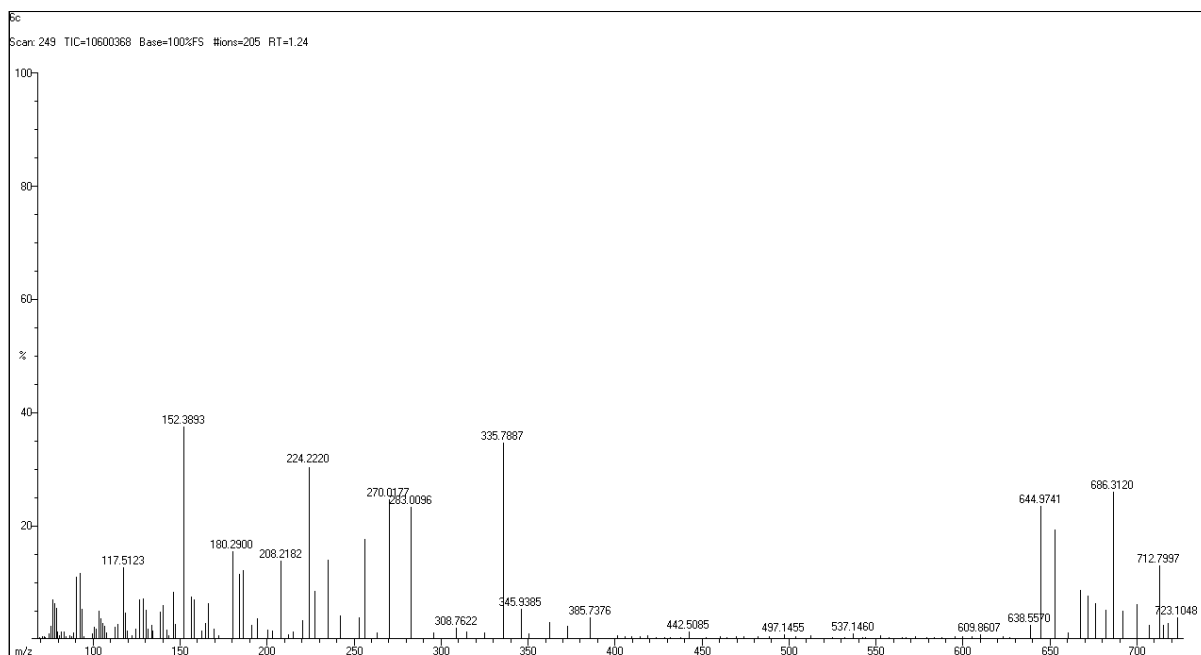


Figure 116. Mass spectrum of 7c

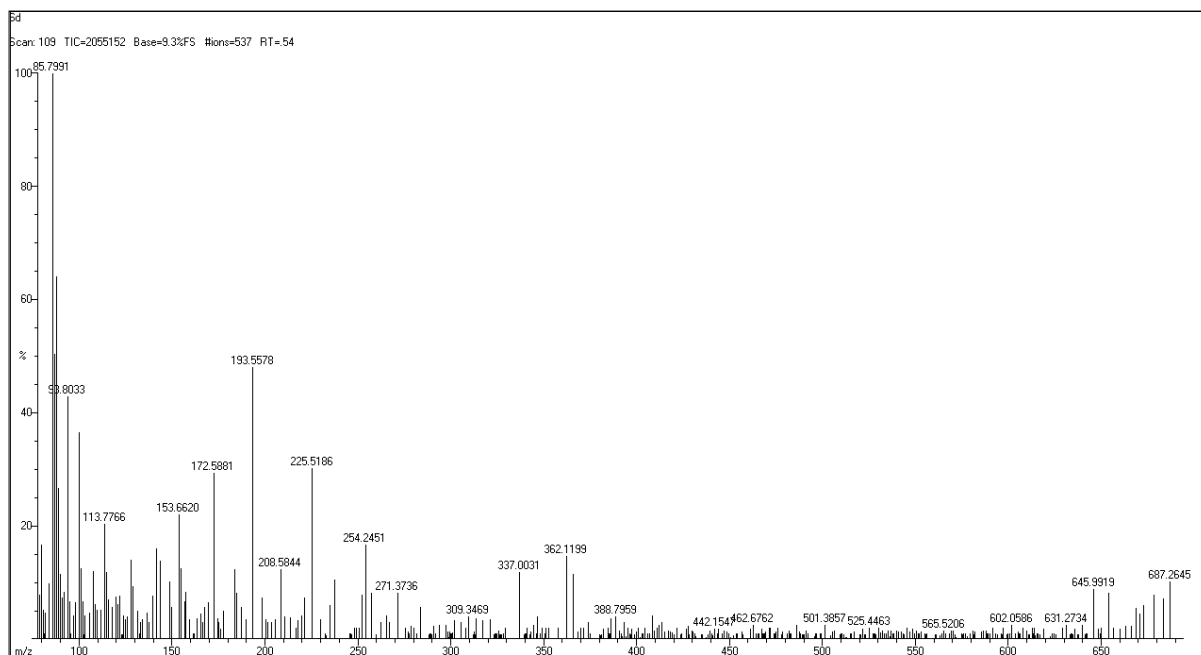


Figure 117. Mass spectrum of 7d

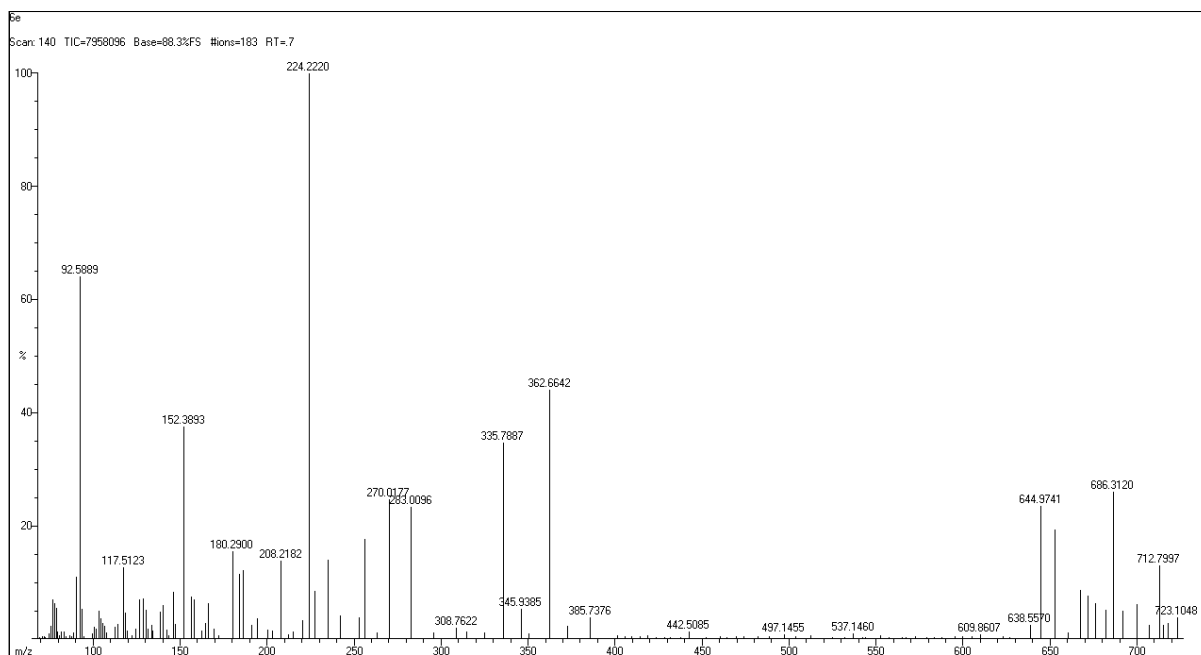


Figure 118. Mass spectrum of 7e

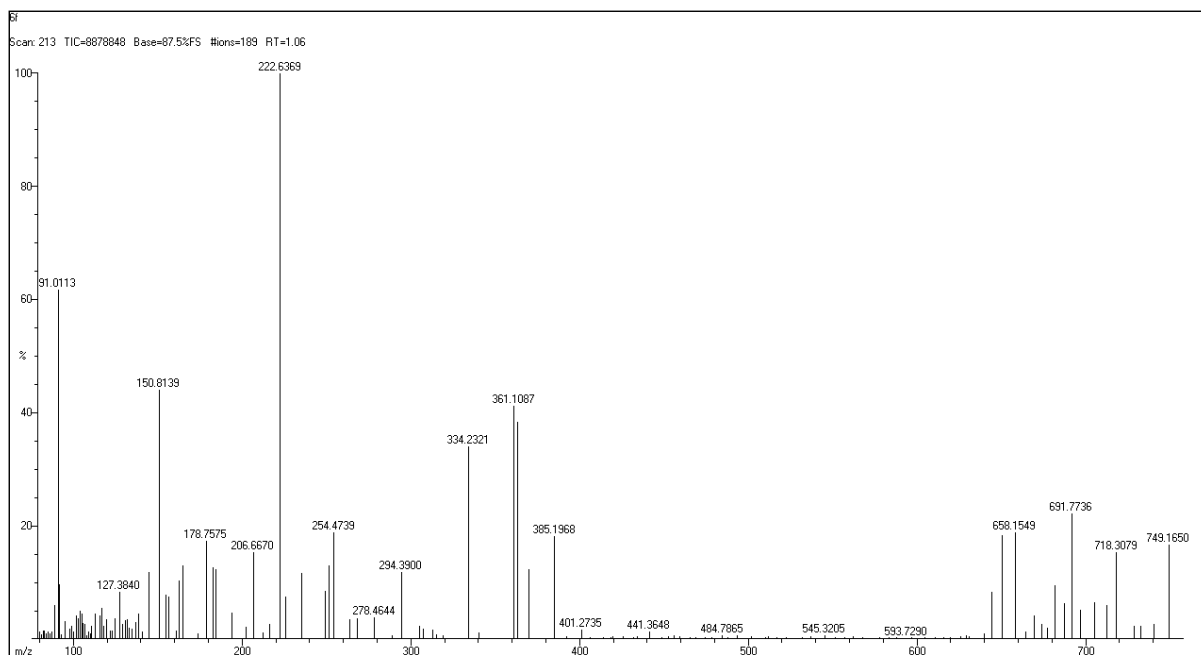


Figure 119. Mass spectrum of **7f**

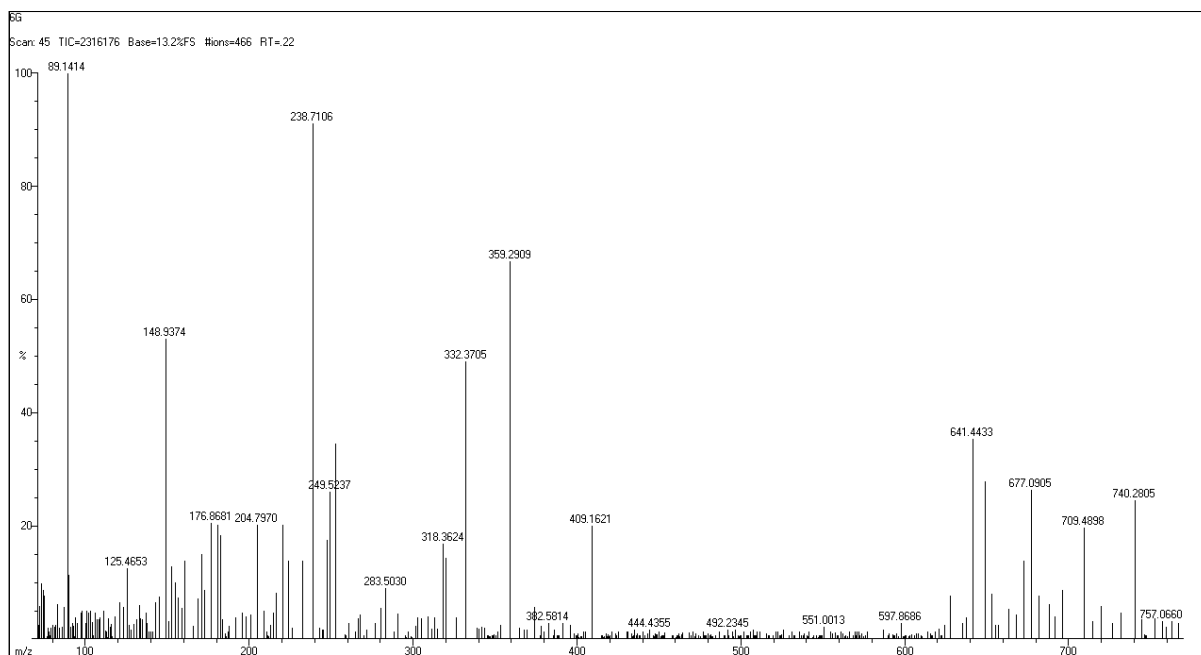
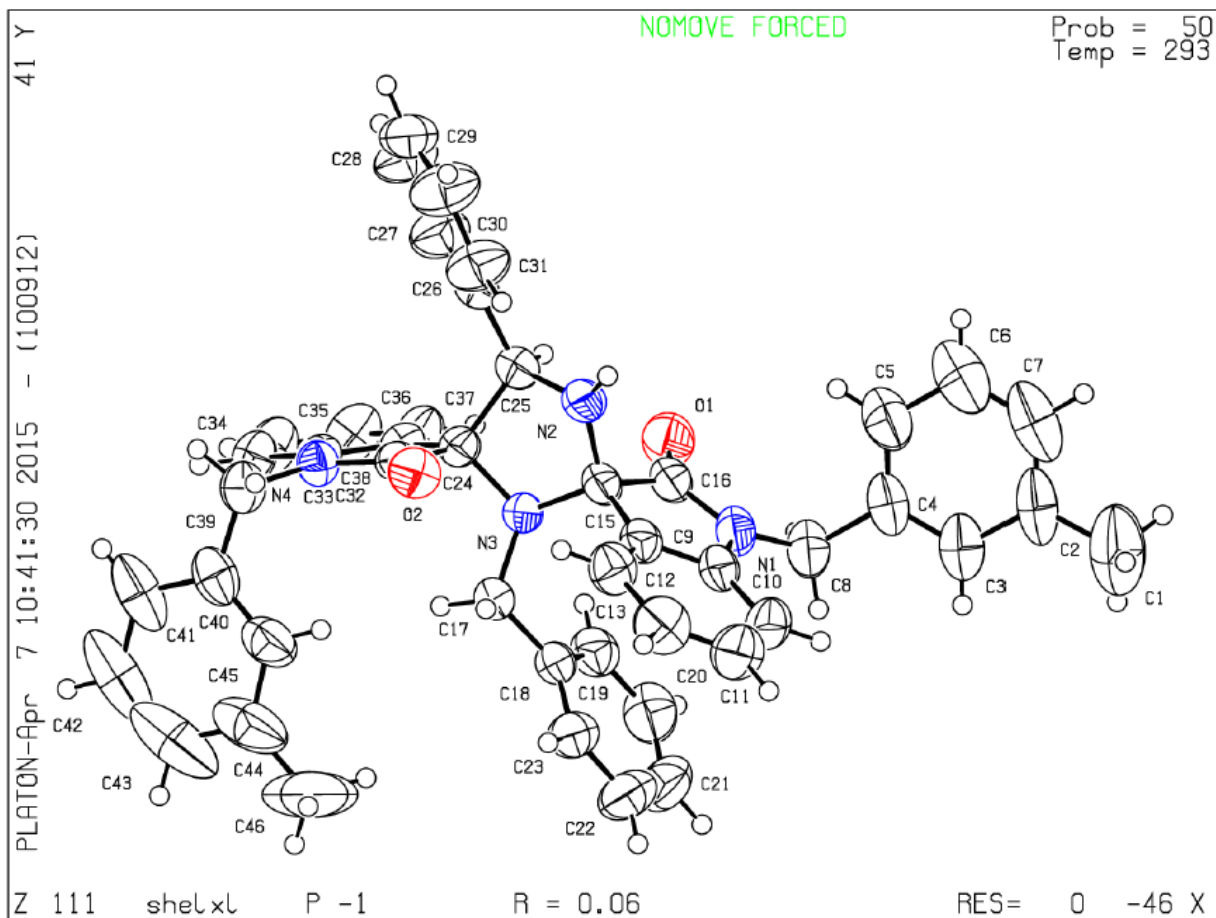


Figure 120. Mass spectrum of **7g**

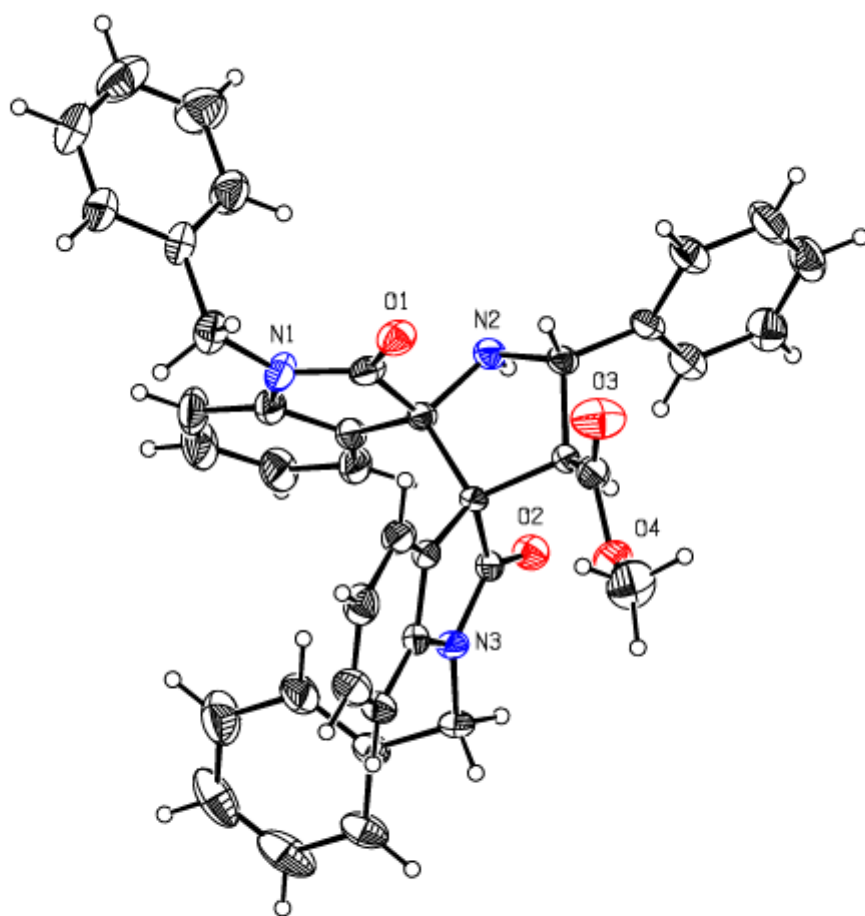


ORTEP diagram of compound 3a

Single crystal XRD data of 5a

Table 2. Crystal data and structure refinement for 5a

Identification code	5a
Empirical formula	C40 H33 N3 O4
Formula weight	619.69
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2/n
Unit cell dimensions	a = 22.523(2) Å alpha = 90 deg. b = 8.9345(7) Å beta = 105.100(3) deg. c = 32.983(3) Å gamma = 90 deg
Volume	6408.2(10) Å ³
Z, Calculated density	8, 1.285 Mg/m ³
Absorption coefficient	0.084 mm ⁻¹
F(000)	2608
Crystal size	0.250 x 0.220 x 0.150 mm
Theta range for data collection	0.987 to 23.481 deg.
Limiting indices	-24<=h<=25, -9<=k<=9, -36<=l<=34
Reflections collected / unique	22466 / 22466 [R(int) = ?]
Completeness to theta = 23.481	97.6 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	22466 / 0 / 859
Goodness-of-fit on F ²	1.062
Final R indices [I>2sigma(I)]	R1 = 0.0757, wR2 = 0.2041
R indices (all data)	R1 = 0.1188, wR2 = 0.2449
Extinction coefficient	0.0008(3)
Largest diff. peak and hole	0.274 and -0.280 e.Å ⁻³



ORTEP diagram of compound 5a