

SUPPLEMENTARY INFORMATION

FOR

Azo Derivatives of Monoterpenes as Anti-*Helicobacter pylori* Agents: from the Synthesis to a Structure-Based Target Investigation

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NMR and MS spectra for representative compounds

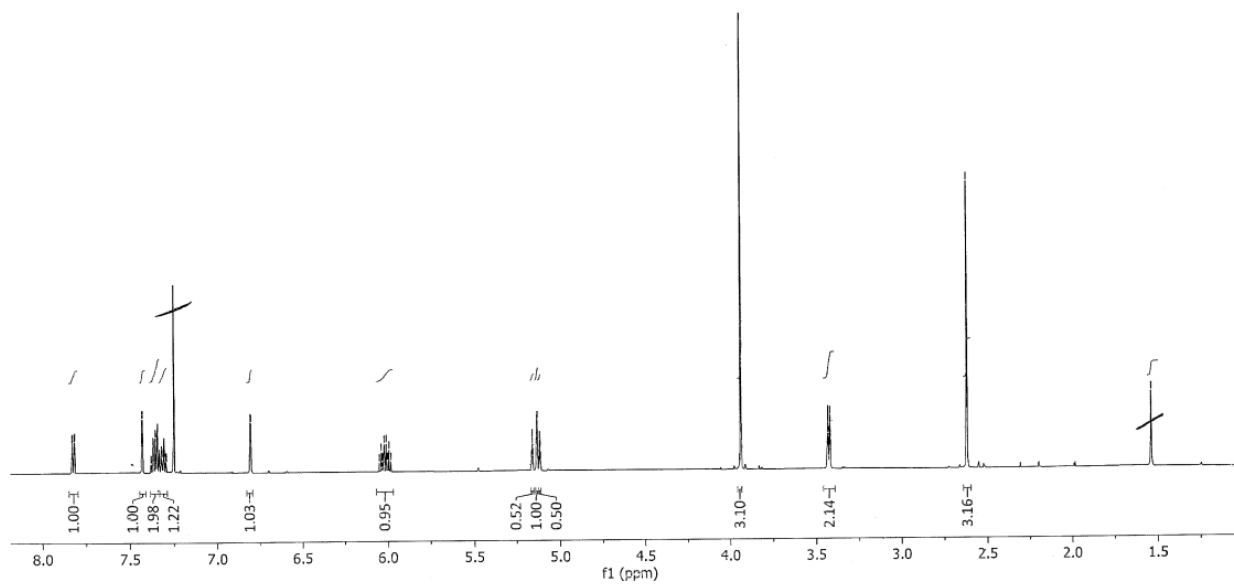


Figure S1. ¹H NMR spectrum of compound **1**.

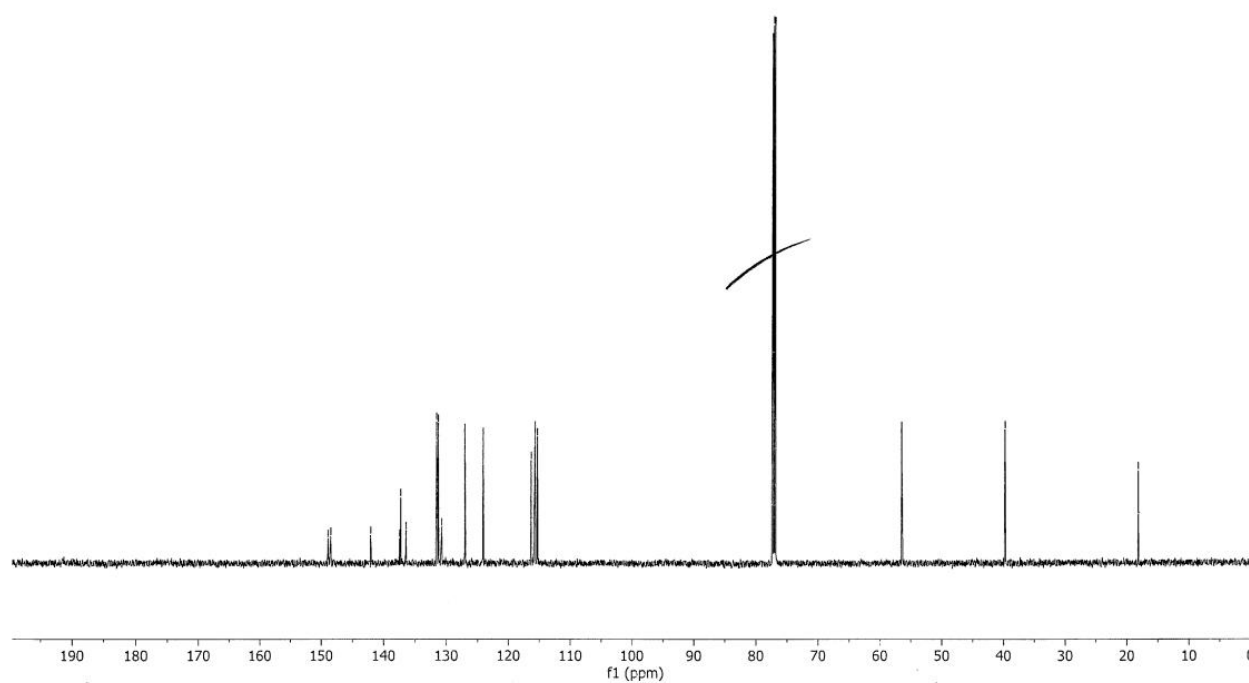


Figure S2. ¹³C NMR spectrum of compound **1**.

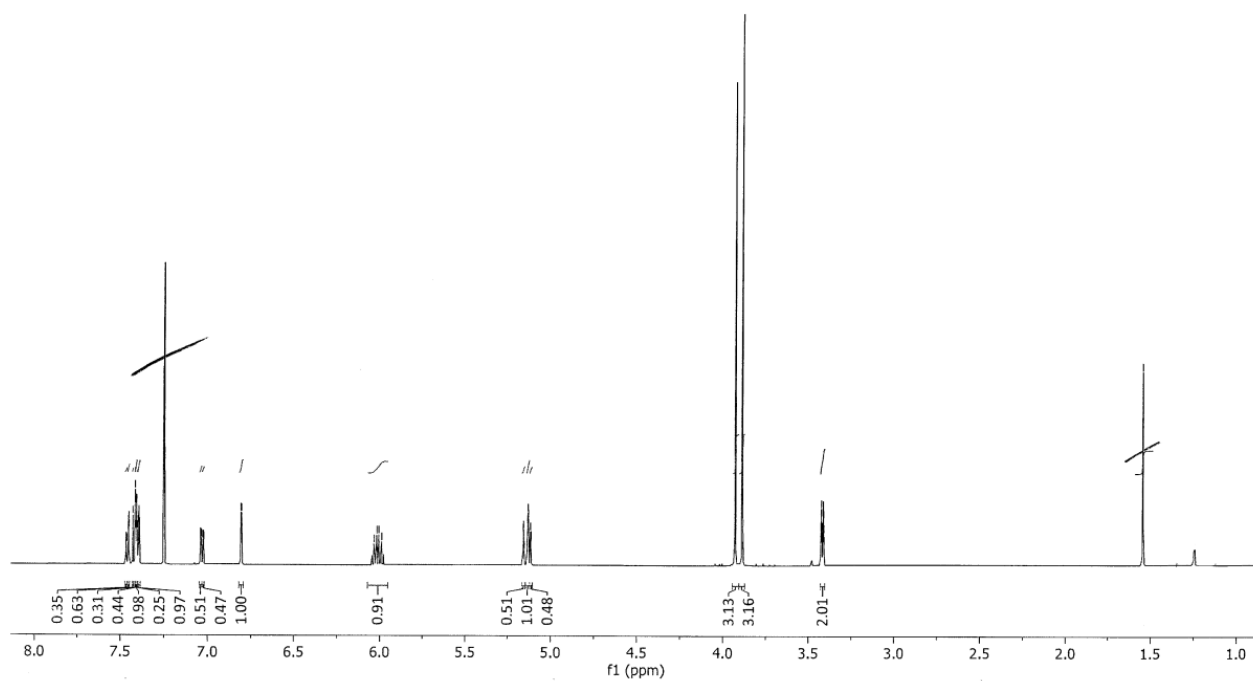


Figure S3. ^1H NMR spectrum of compound **2**.

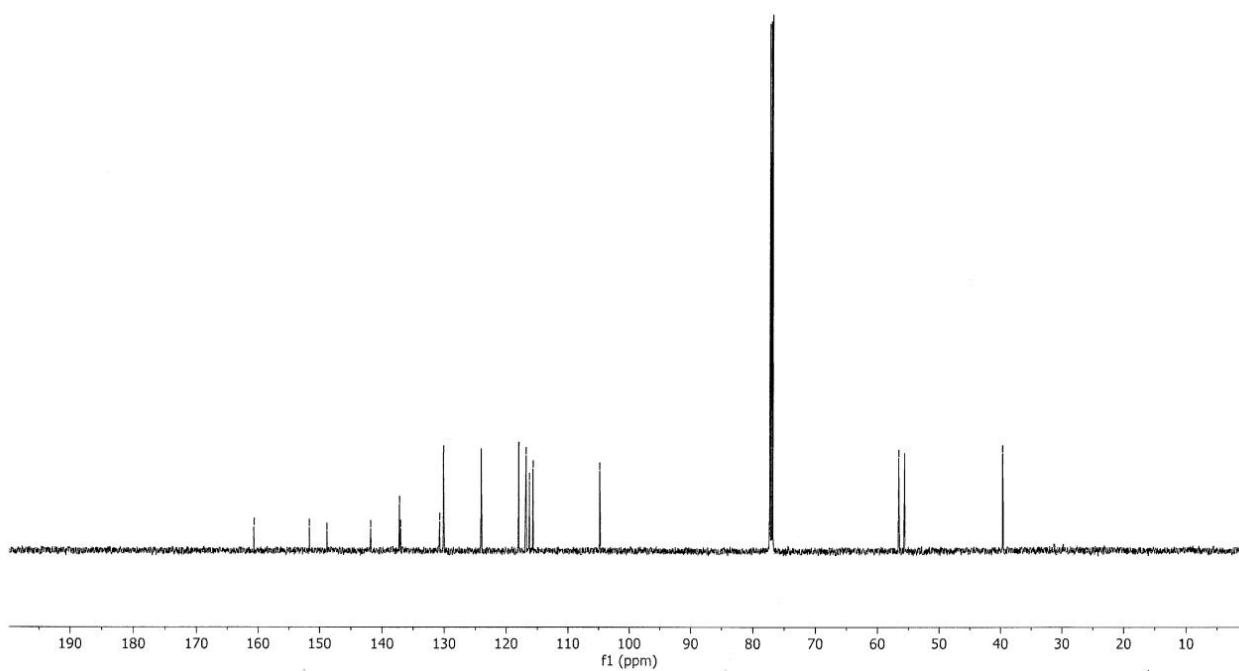


Figure S4. ^{13}C NMR spectrum of compound **2**.

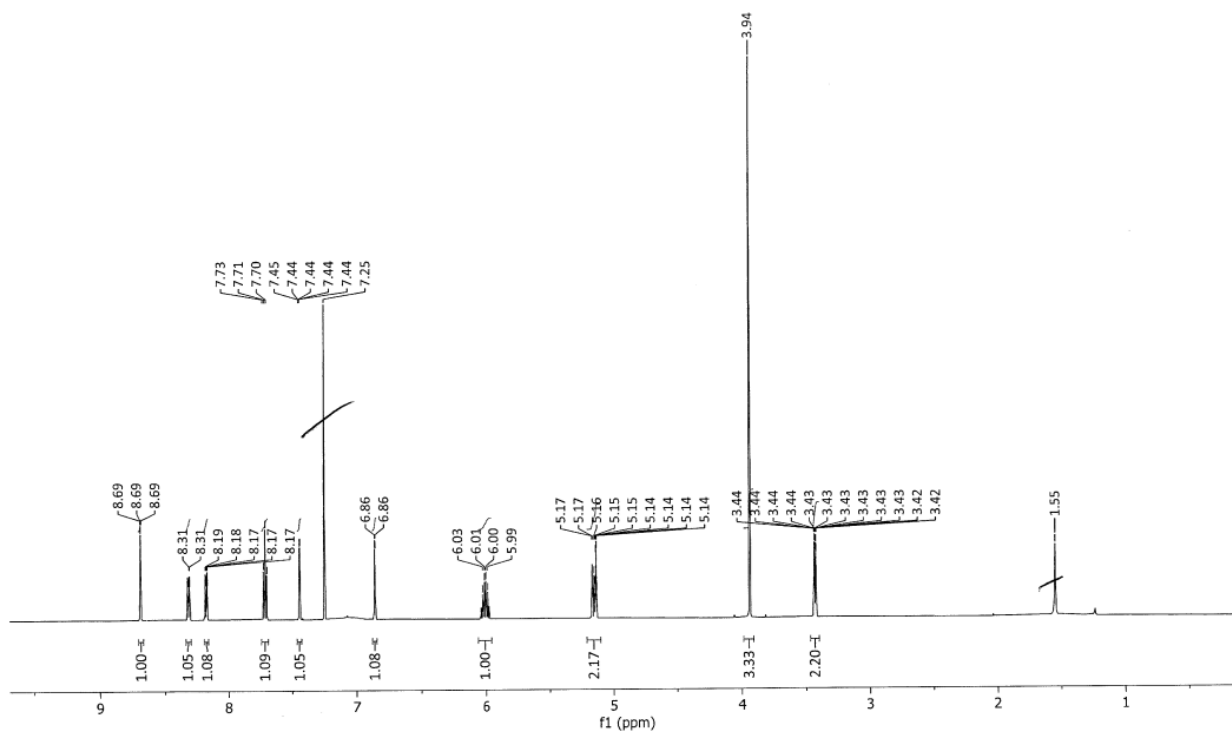


Figure S5. ¹H NMR spectrum of compound 3.

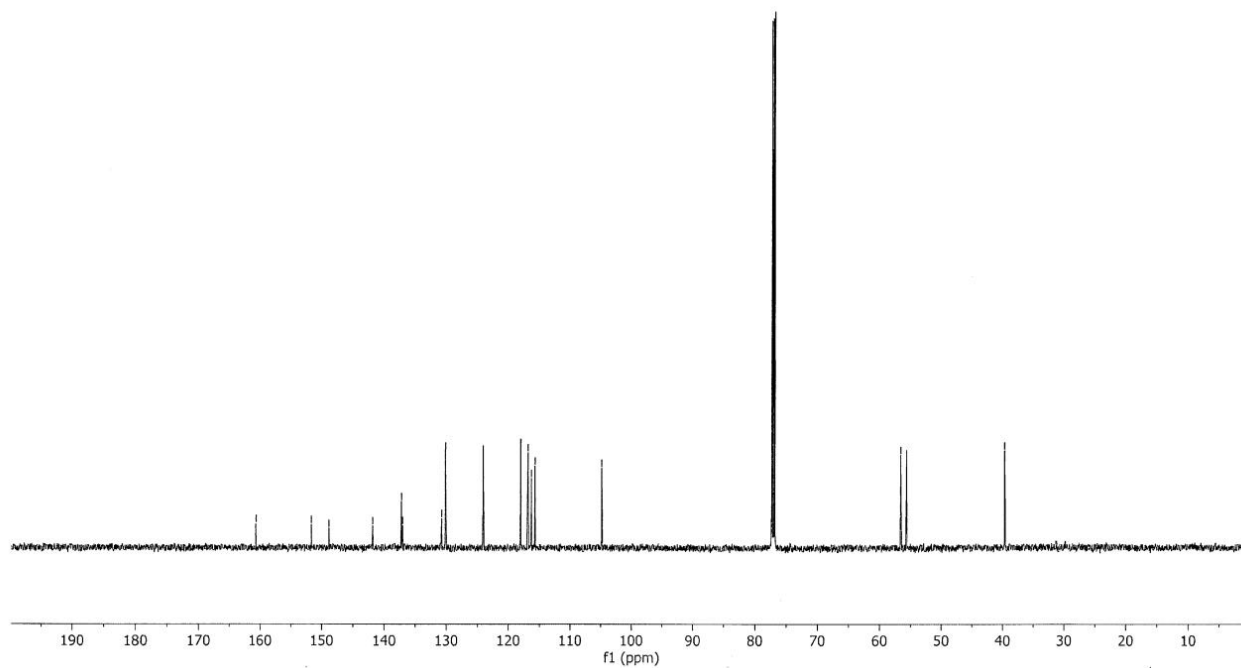
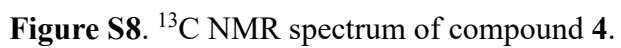


Figure S6. ¹³C NMR spectrum of compound 3.



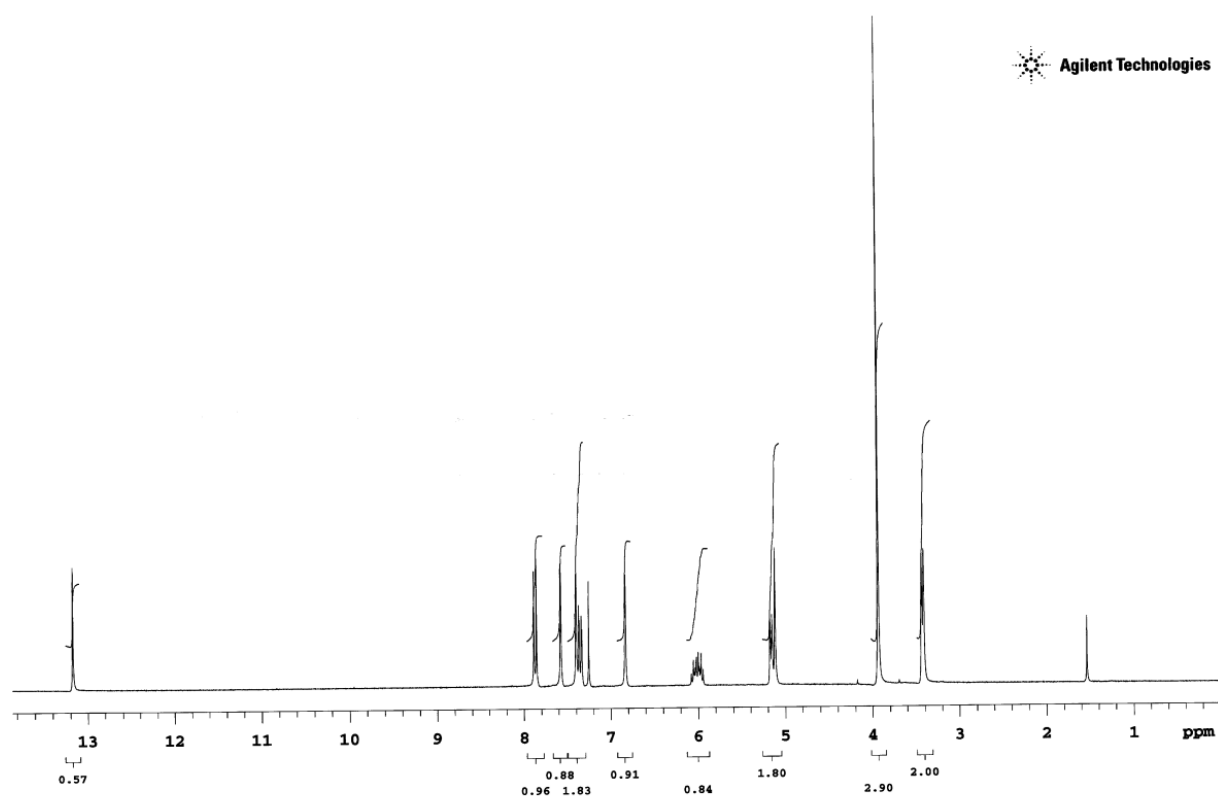


Figure S9. ^1H NMR spectrum of compound **5**.

Gradient Shimming



Sample Name:
E13
Data Collected on:
m300-mercury300
Archive directory:
/export/home/chempack/vnmrsys/data
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (a2pul)
Solvent: cdcl3
Data collected on: Oct 25 2023
Operator: carrador
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.568 sec
Width 18867.9 Hz
1961 repetitions
OBSERVE C13, 75.4847602 MHz
DECOUPLE H1, 300.1991980 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 1 hr, 43 min

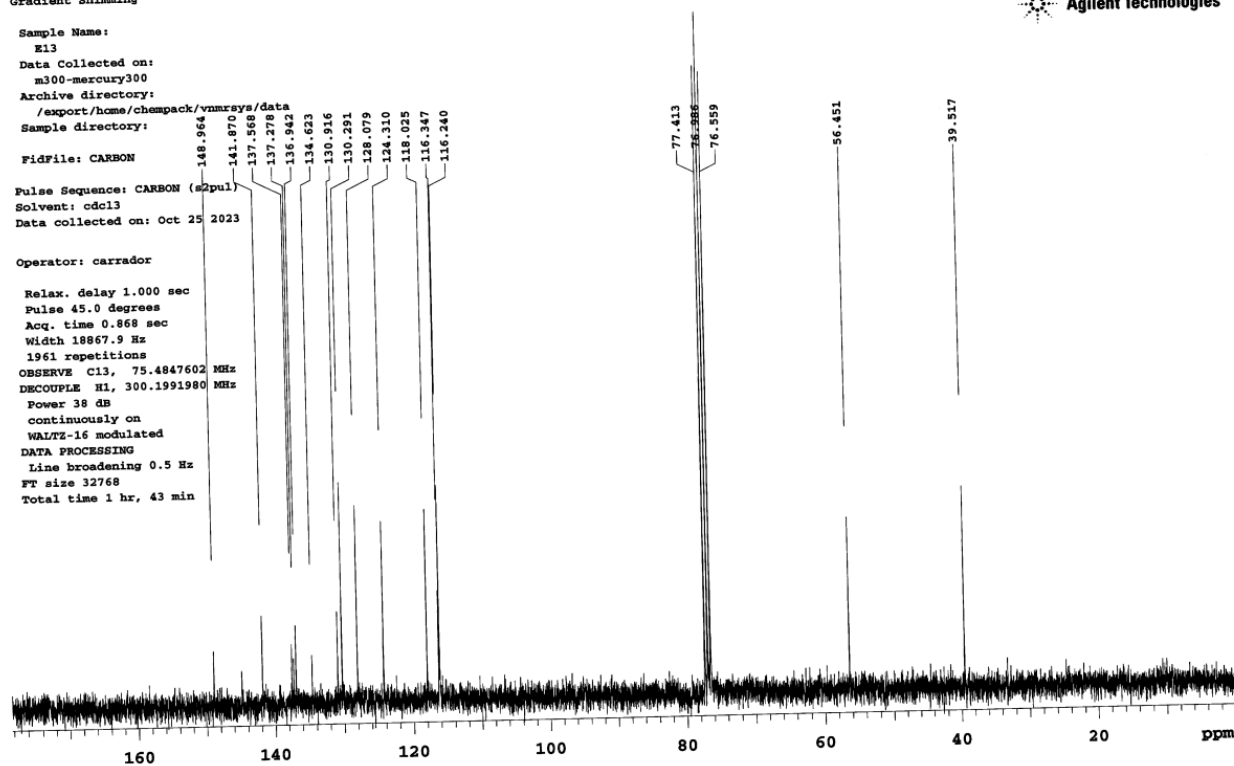


Figure S10. ^{13}C NMR spectrum of compound 5.

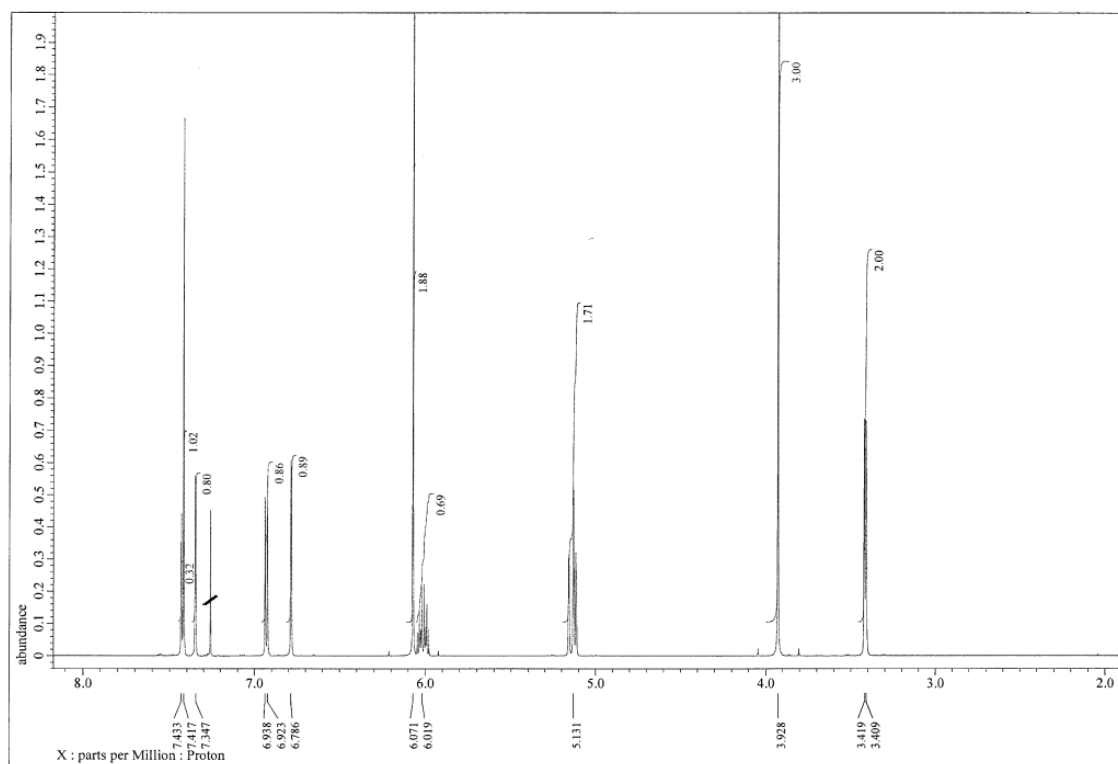


Figure S11. ^1H NMR spectrum of compound 6.

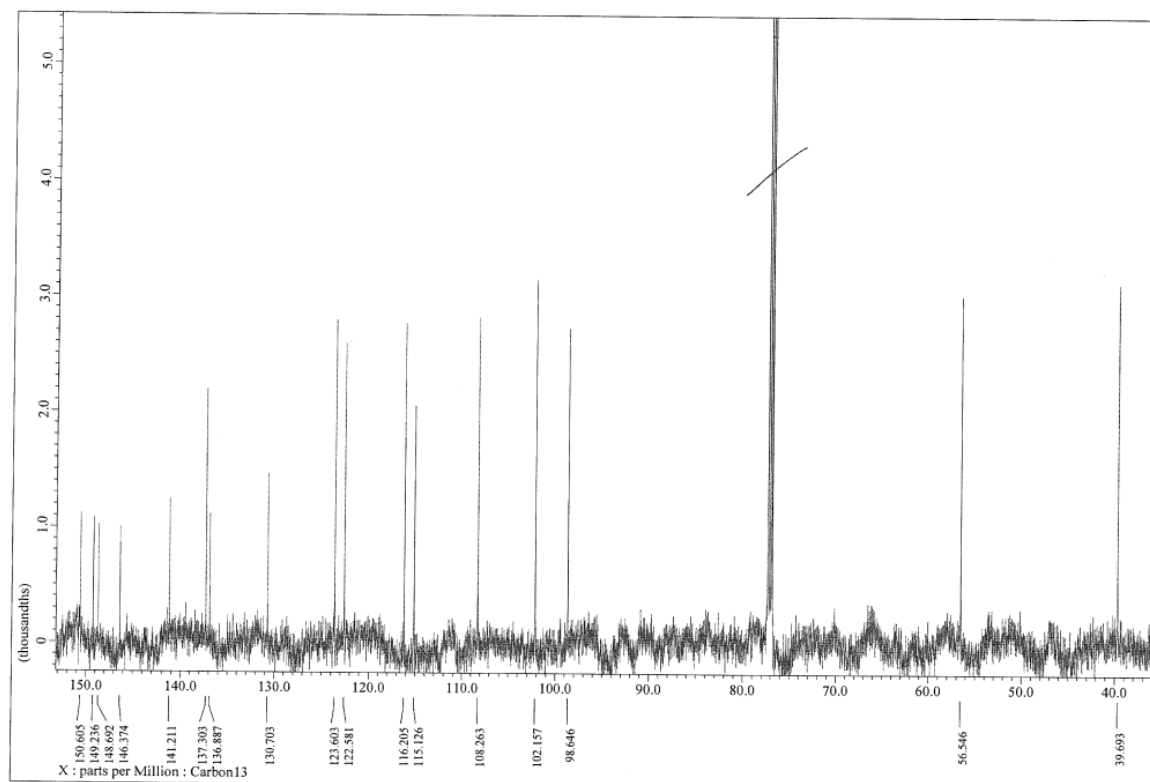


Figure S12. ¹³C NMR spectrum of compound 6.

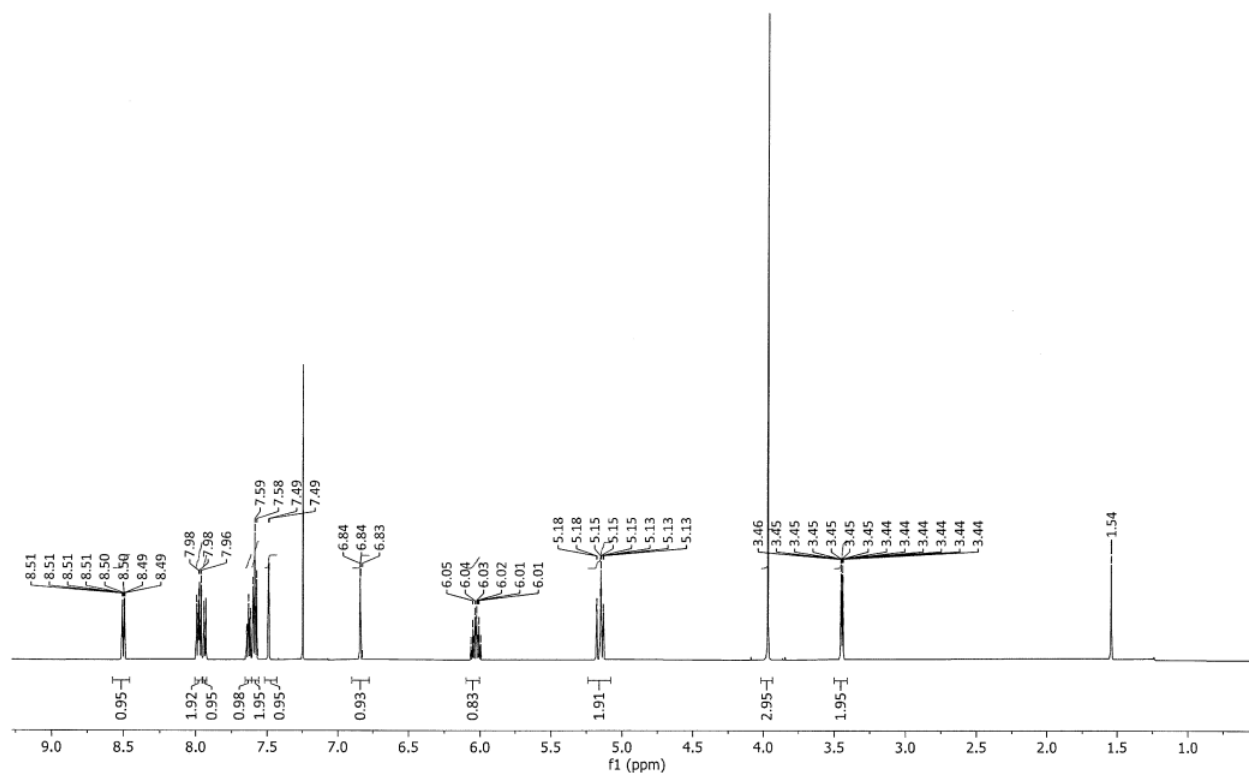


Figure S13. ¹H NMR spectrum of compound 7.

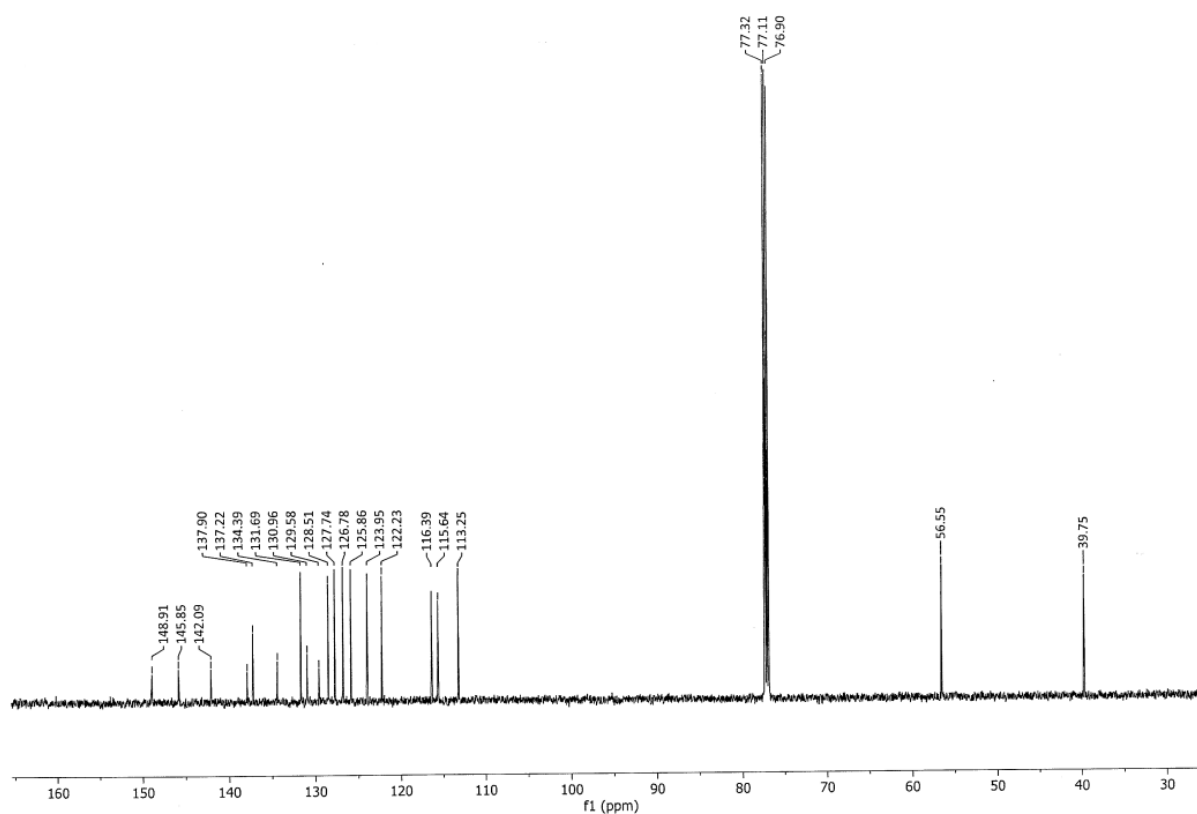


Figure S14. ¹³C NMR spectrum of compound 7.

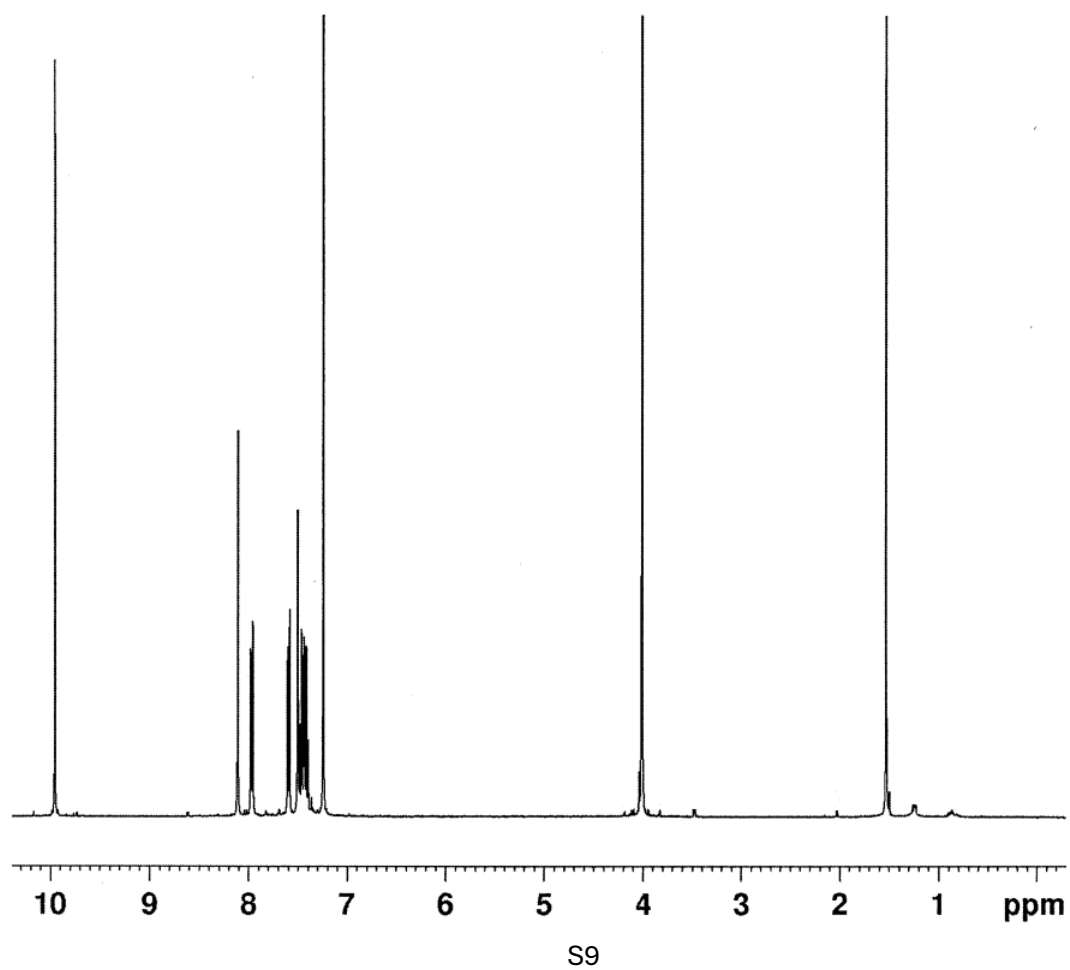


Figure S15. ^1H NMR spectrum of compound 8.

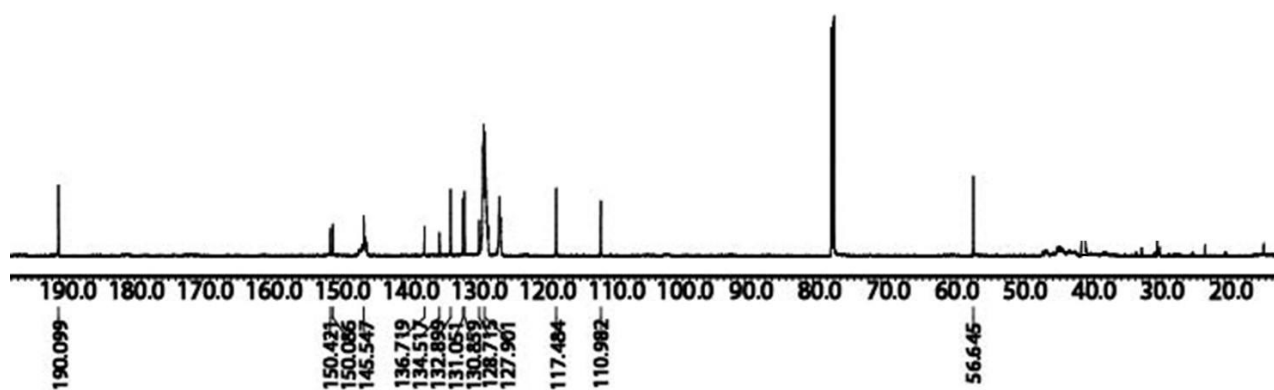


Figure S16. ^{13}C NMR spectrum of compound 8.

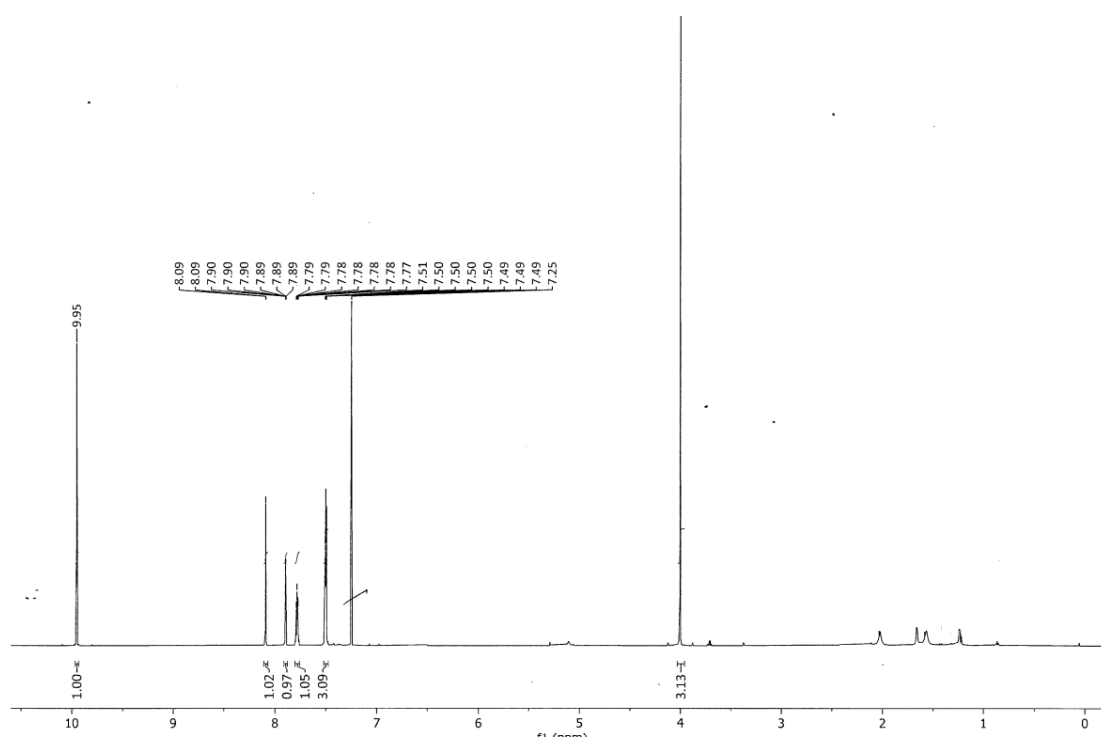


Figure S17. ^1H NMR spectrum of compound 9.

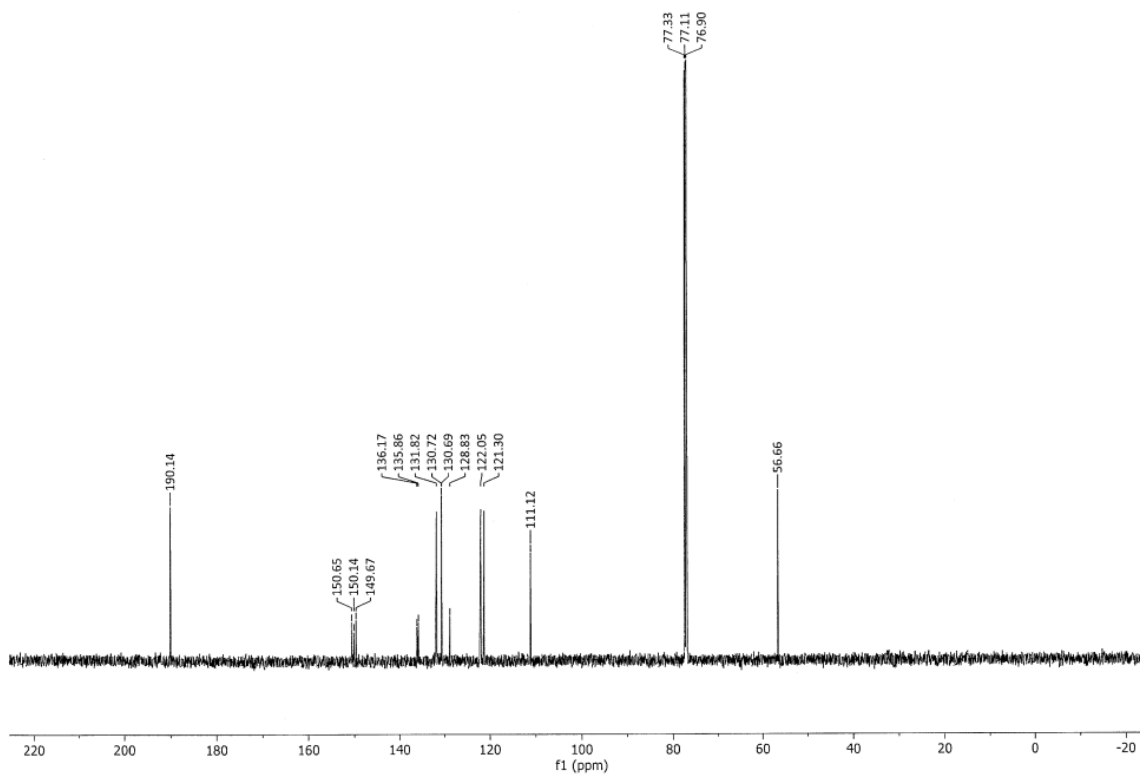
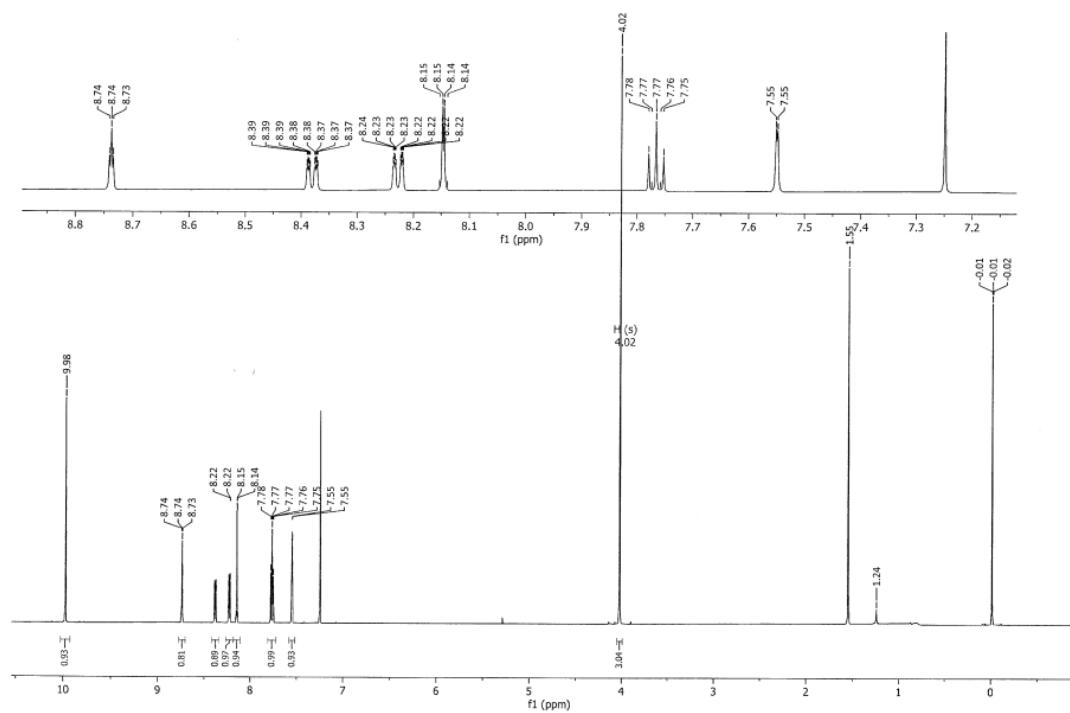


Figure S18. ¹³C NMR spectrum of compound 9.



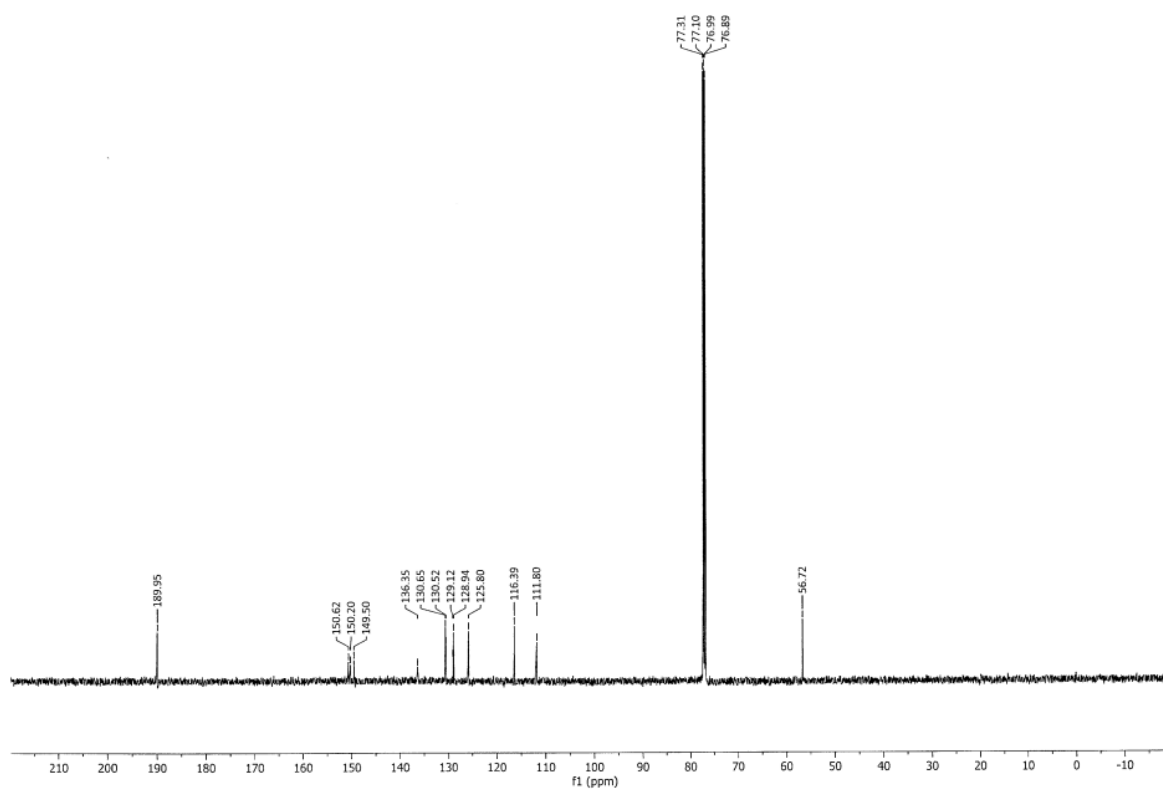


Figure S20. ¹³C NMR spectrum of compound 10.

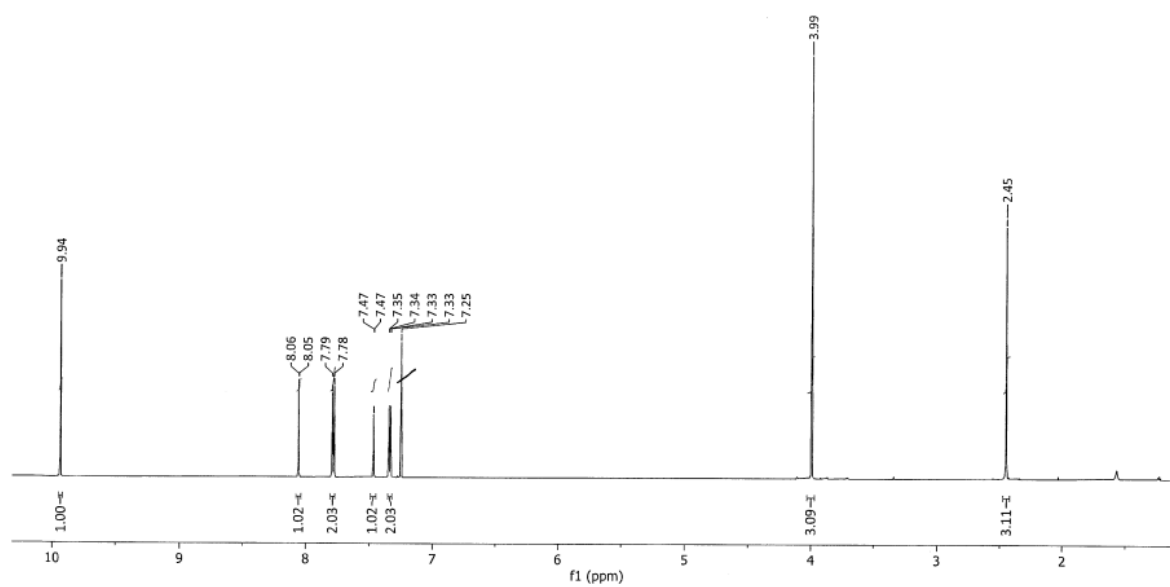


Figure S21. ¹H NMR spectrum of compound 11.

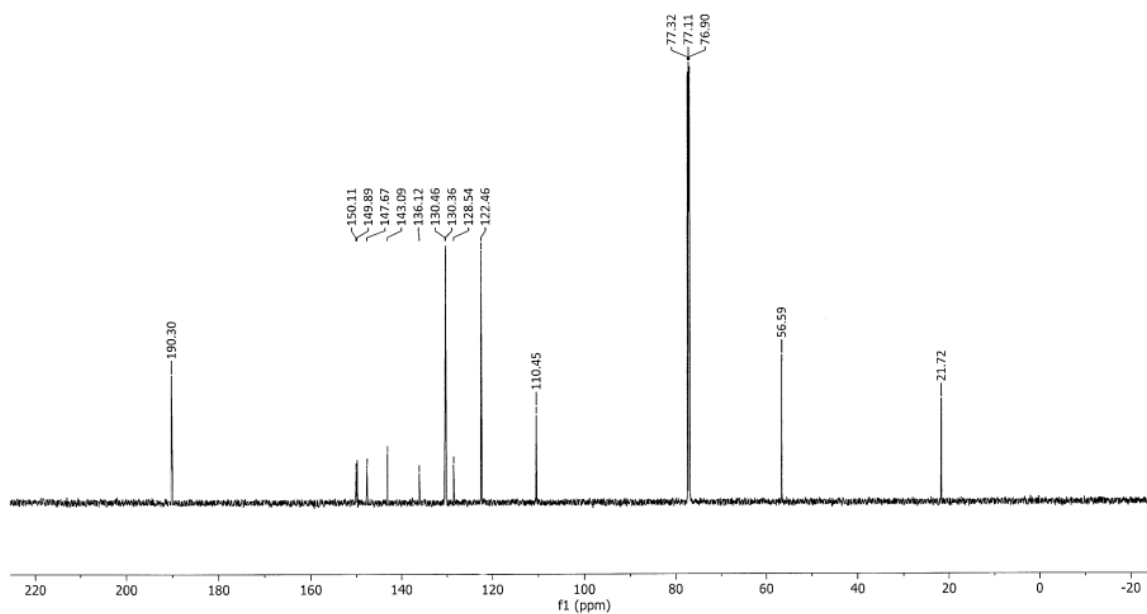


Figure S22. ^{13}C NMR spectrum of compound 11.

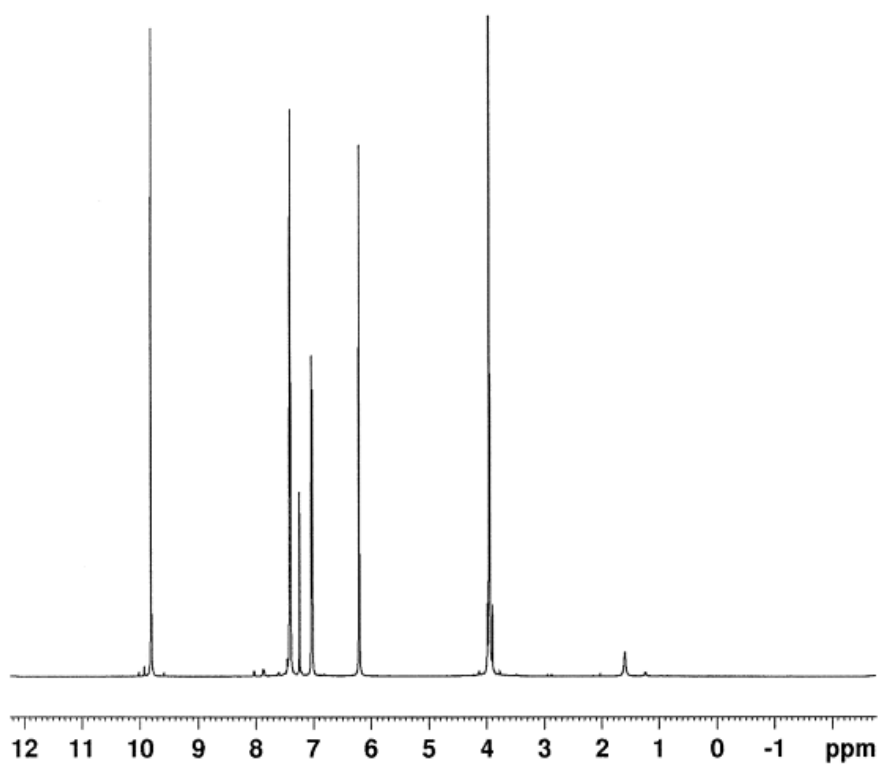


Figure S23. ^1H NMR spectrum of compound **12**.

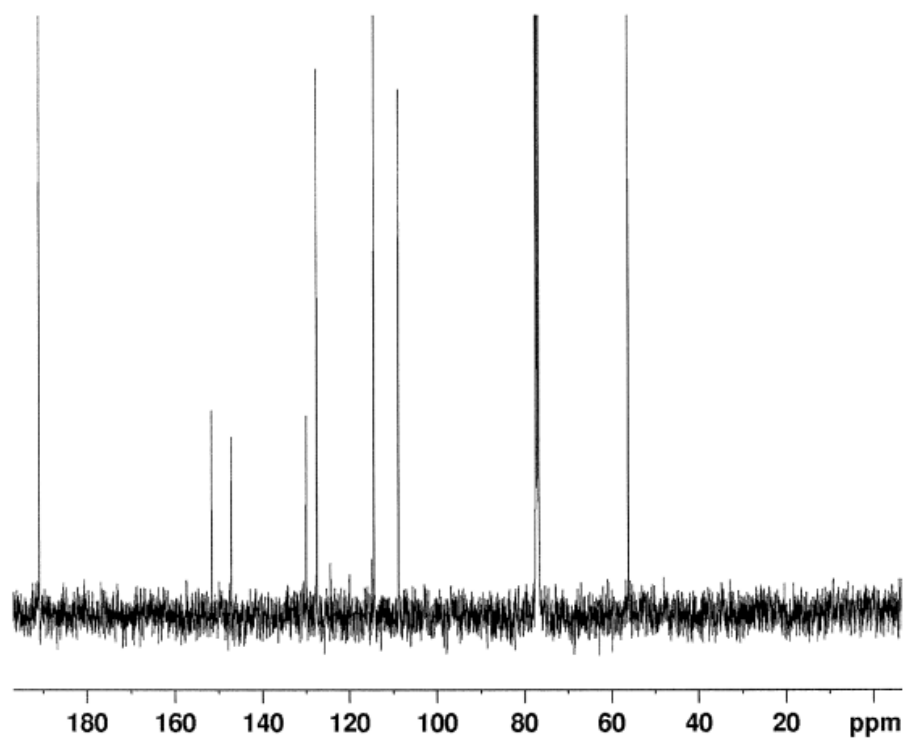


Figure S24. ^{13}C NMR spectrum of compound **12**.

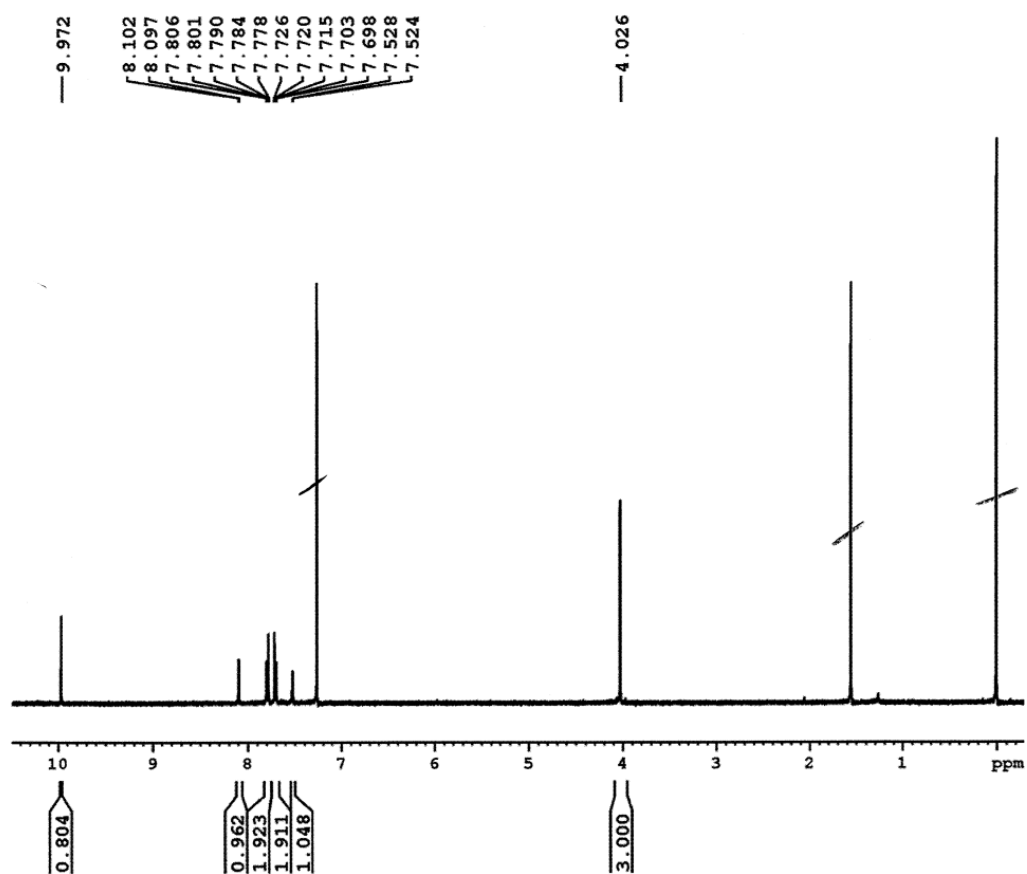


Figure S25. ^1H NMR spectrum of compound 13.

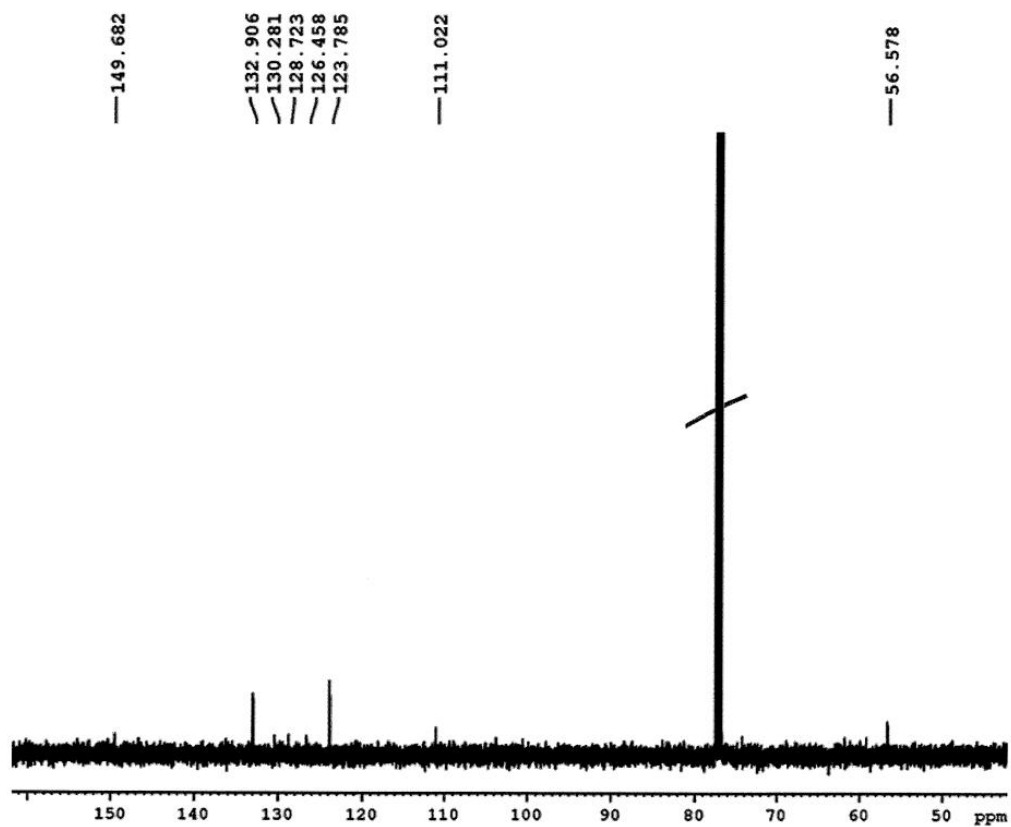


Figure S26. ^{13}C NMR spectrum of compound 13.

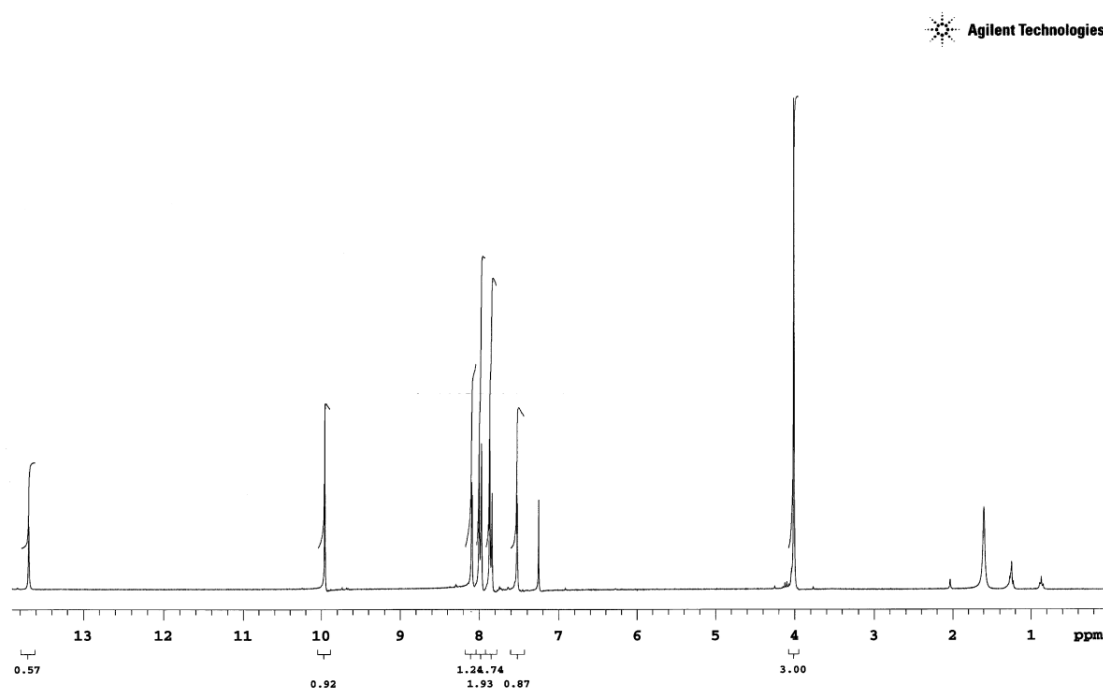


Figure S27. ^1H NMR spectrum of compound 14.

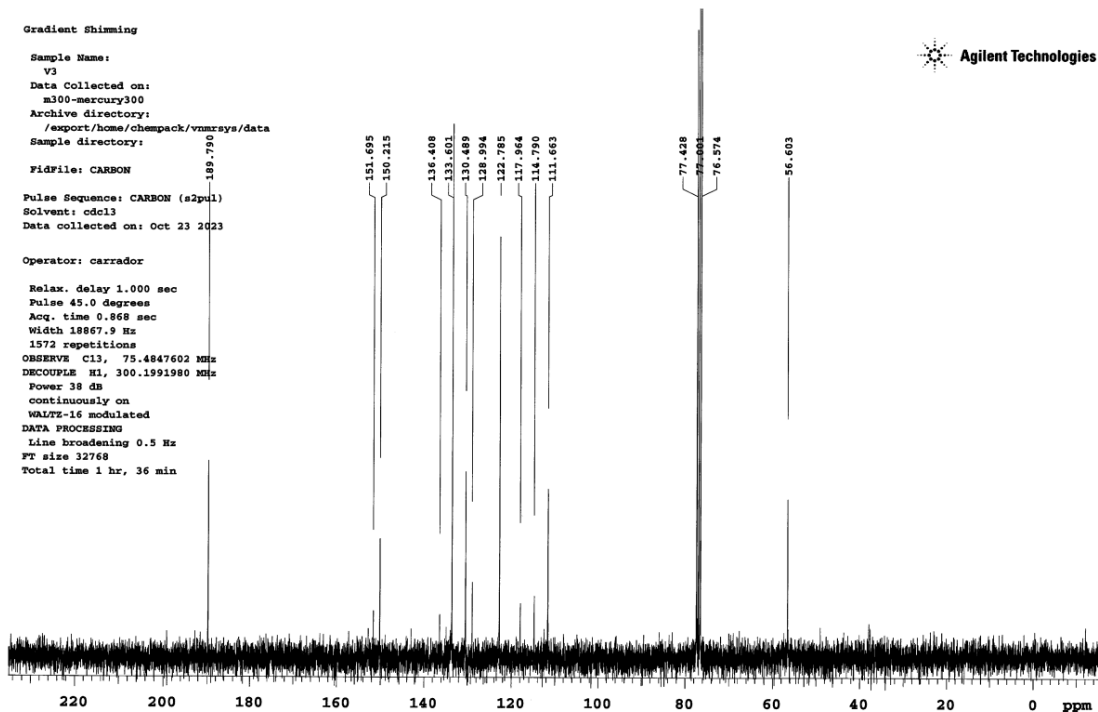


Figure S28. ^{13}C NMR spectrum of compound 14.

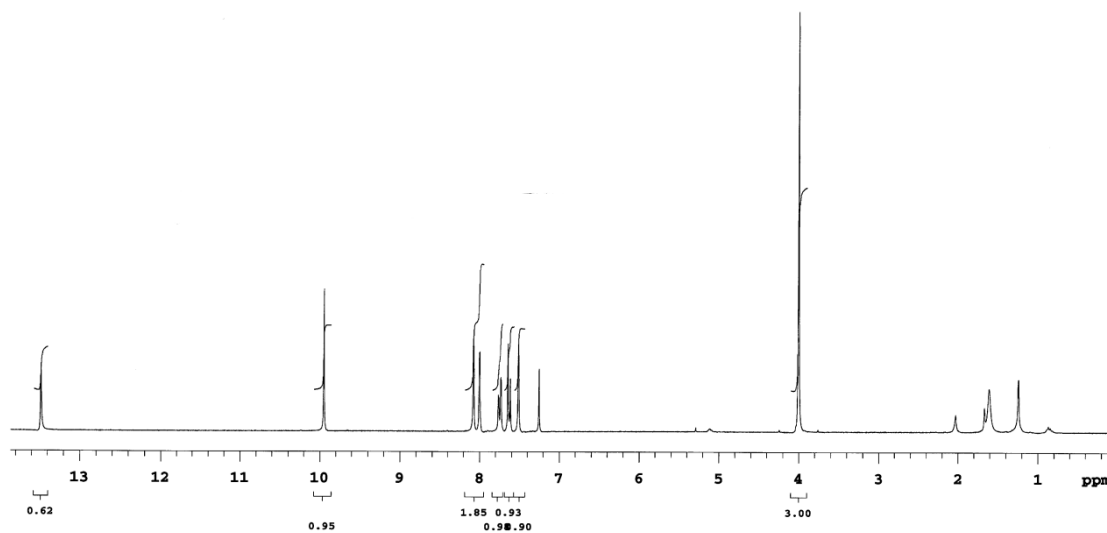


Figure S29. ^1H NMR spectrum of compound 15.

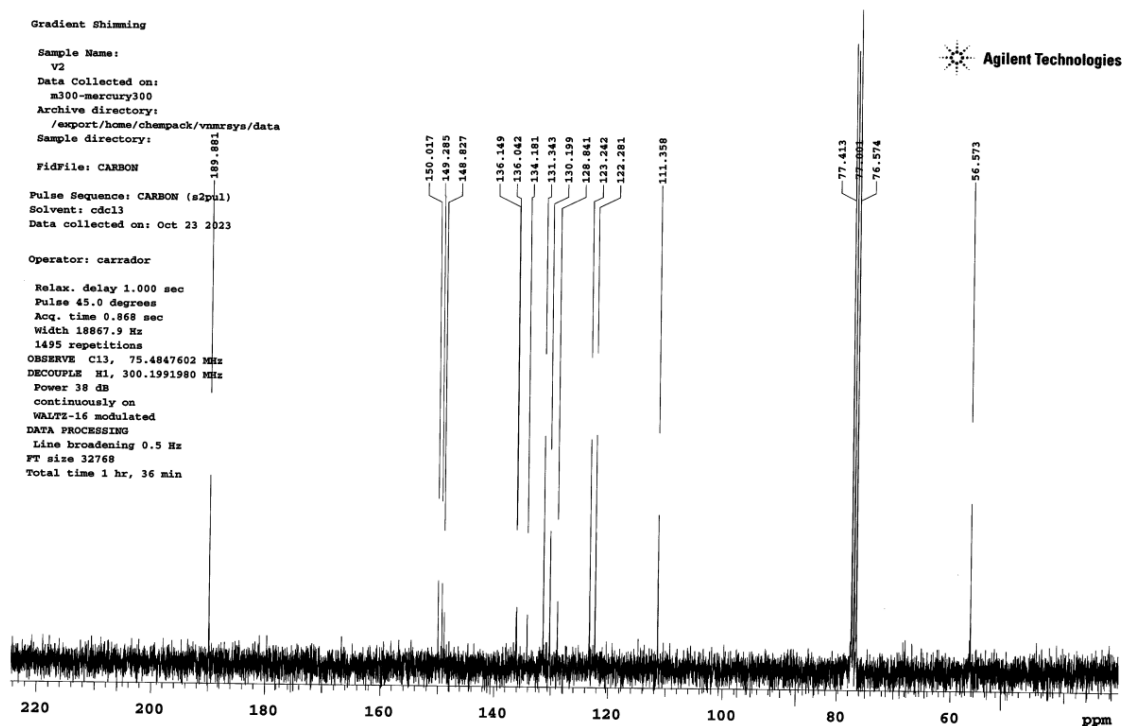


Figure S30. ^{13}C NMR spectrum of compound 15.

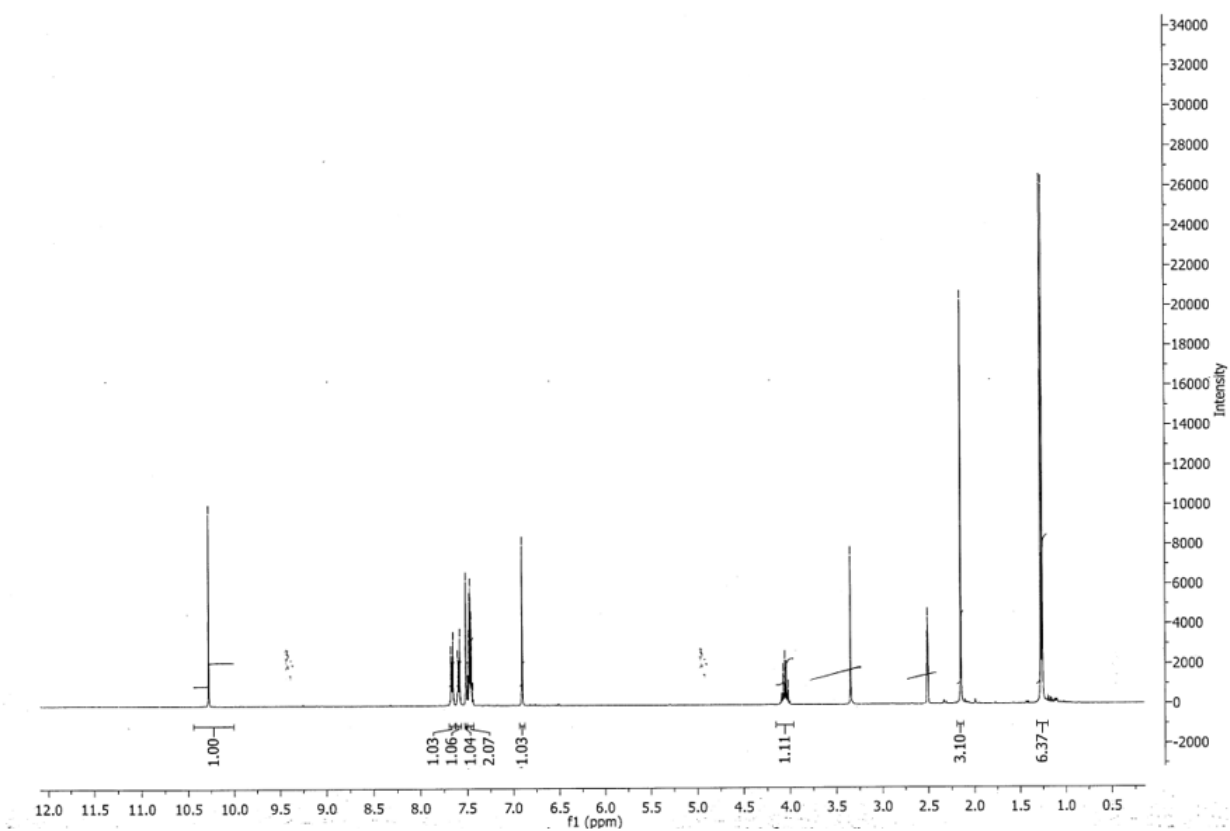


Figure S31. ¹H NMR spectrum of compound 16.

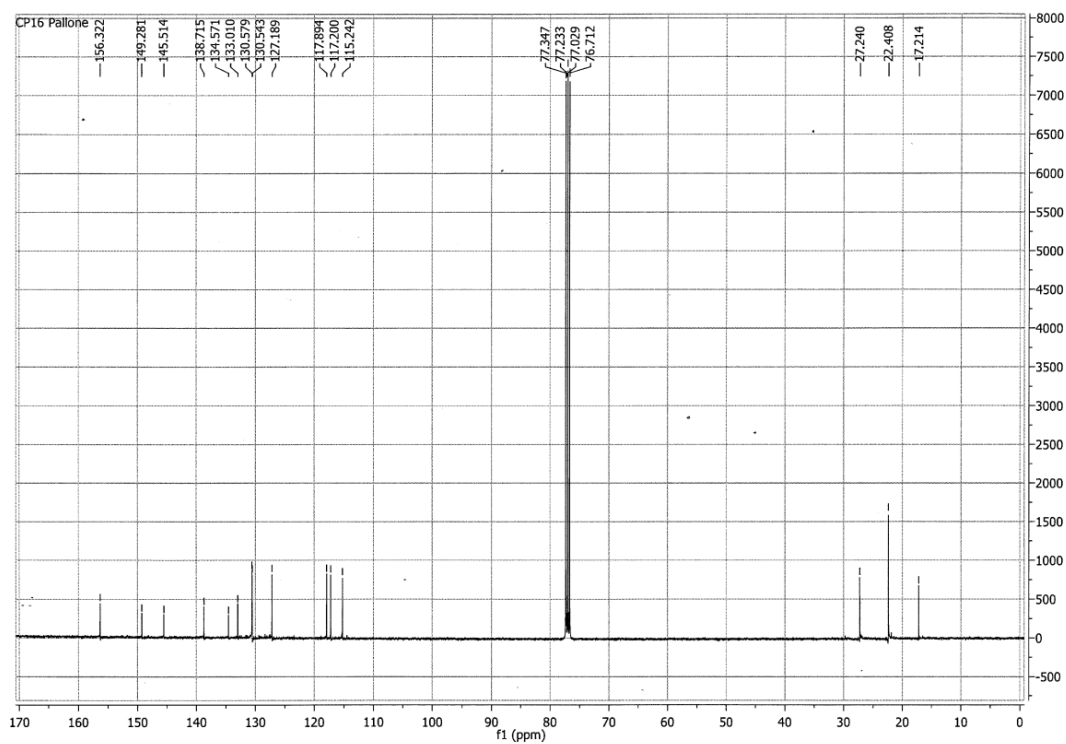


Figure S32. ¹³C NMR spectrum of compound 16.

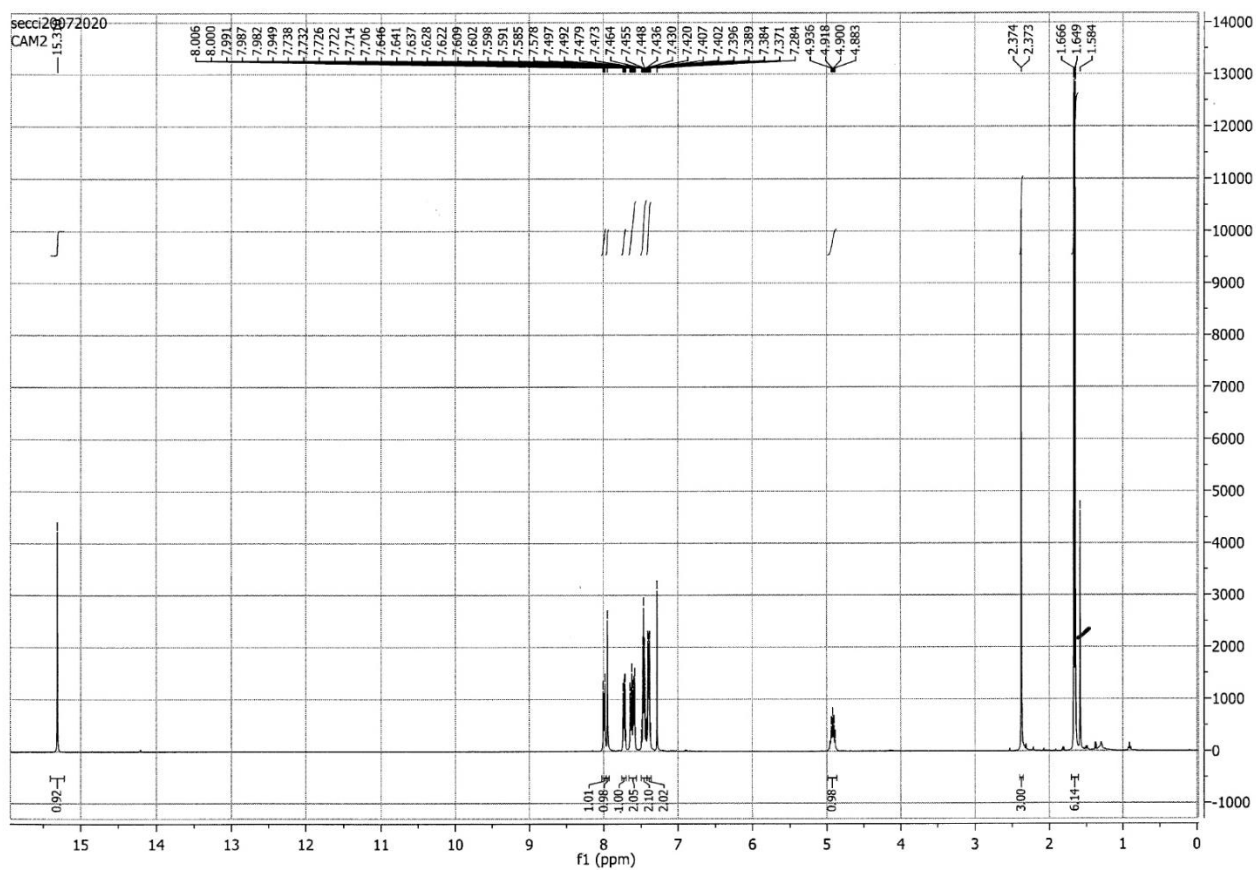


Figure S33. ^1H NMR spectrum of compound 17.

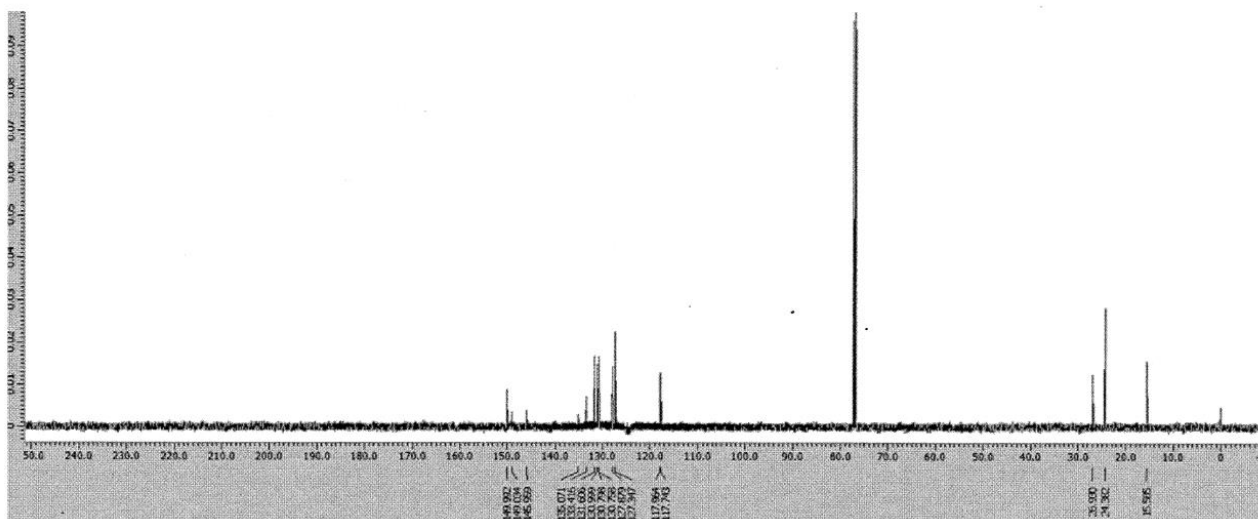


Figure S34. ^{13}C NMR spectrum of compound 17.

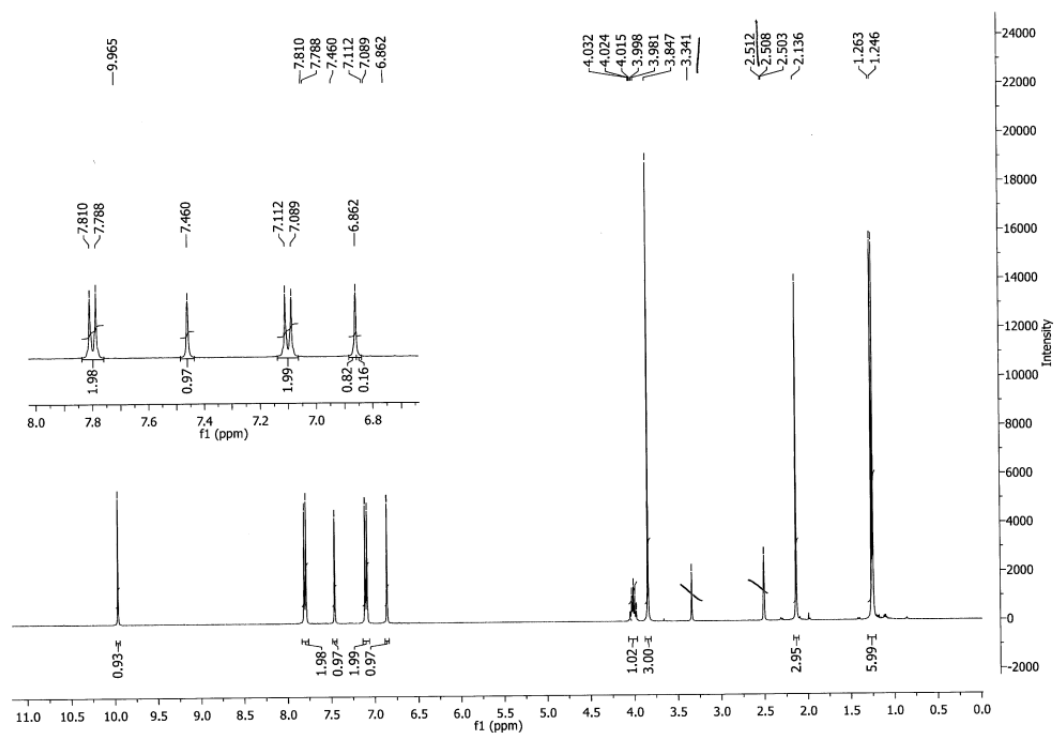


Figure S35. ¹H NMR spectrum of compound **18**.

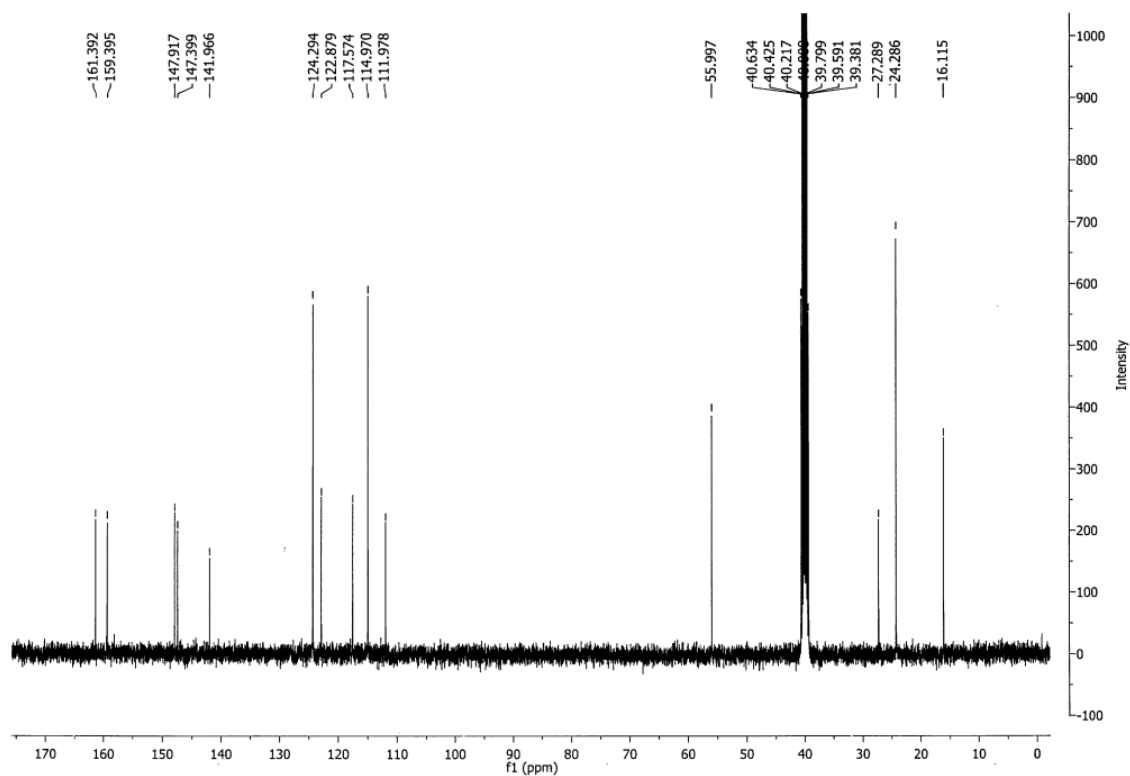


Figure S36. ¹³C NMR spectrum of compound **18**.

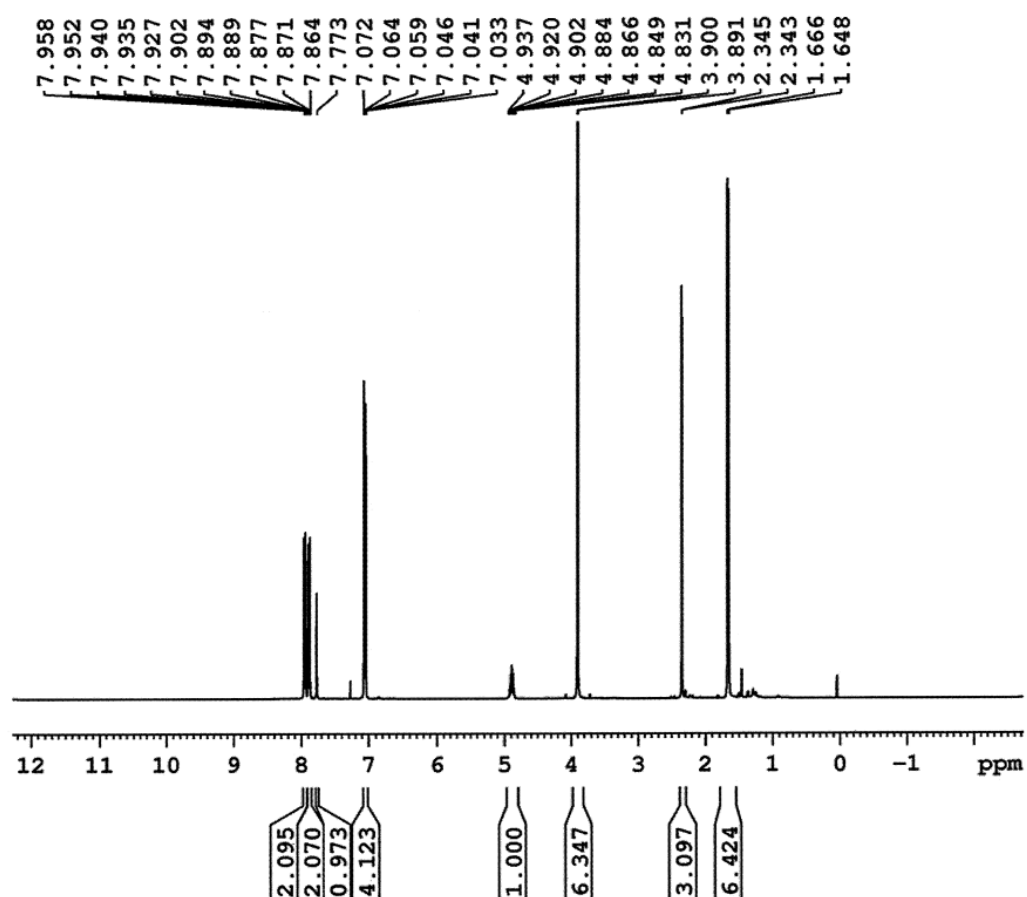


Figure S37. ¹H NMR spectrum of compound 19.

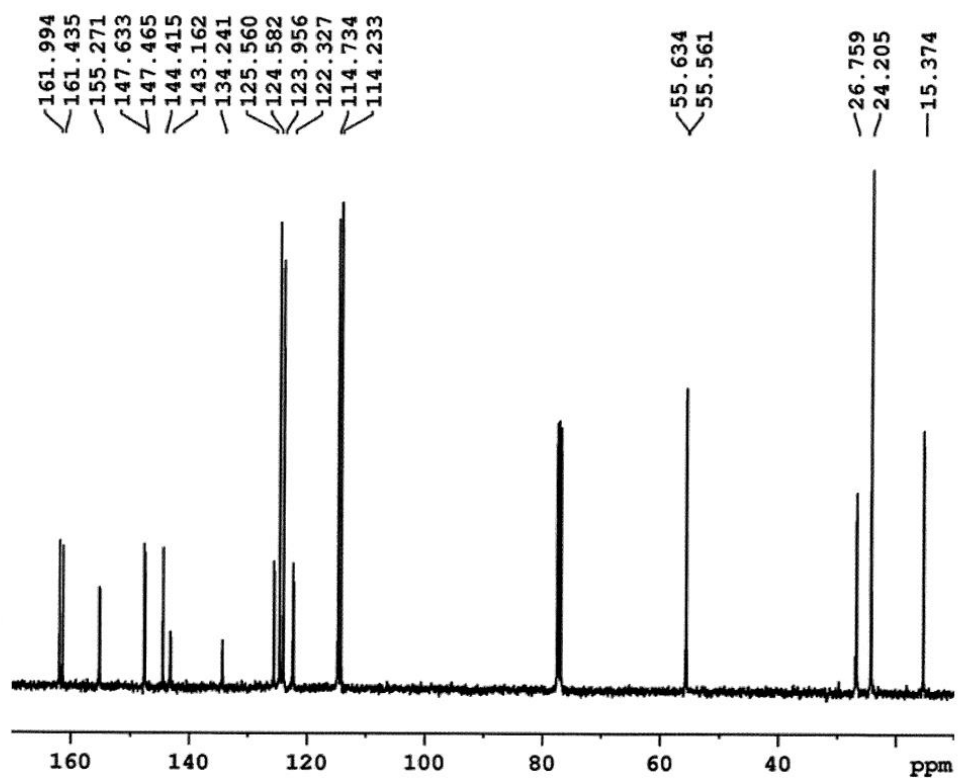


Figure S38. ^{13}C NMR spectrum of compound **19**.

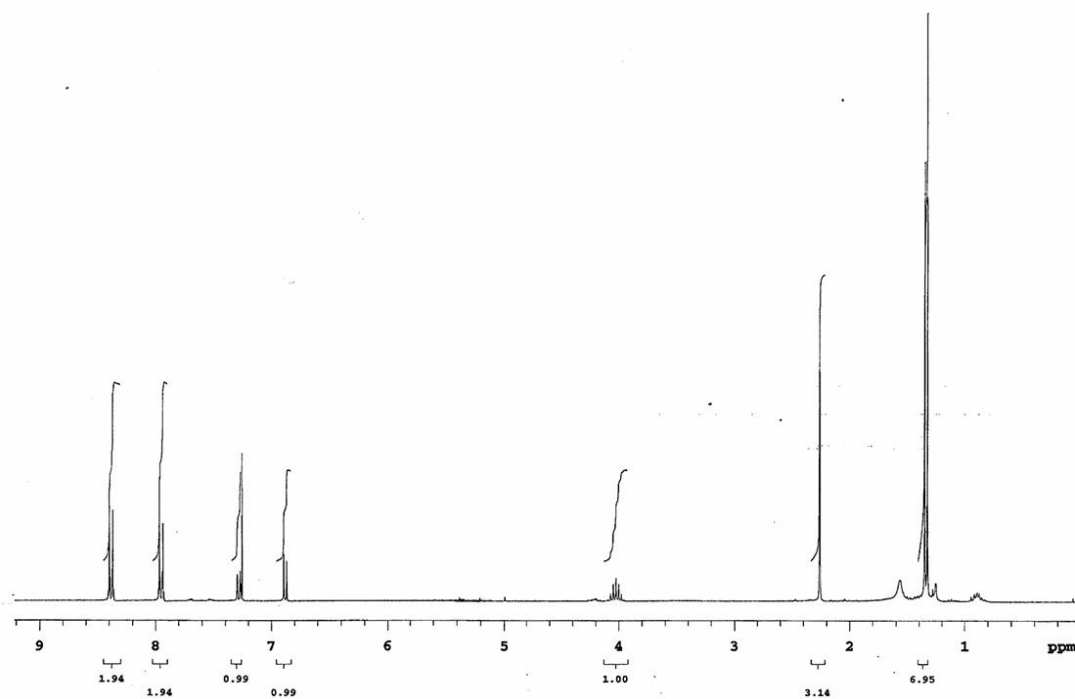


Figure S39. ^1H NMR spectrum of compound **20**.

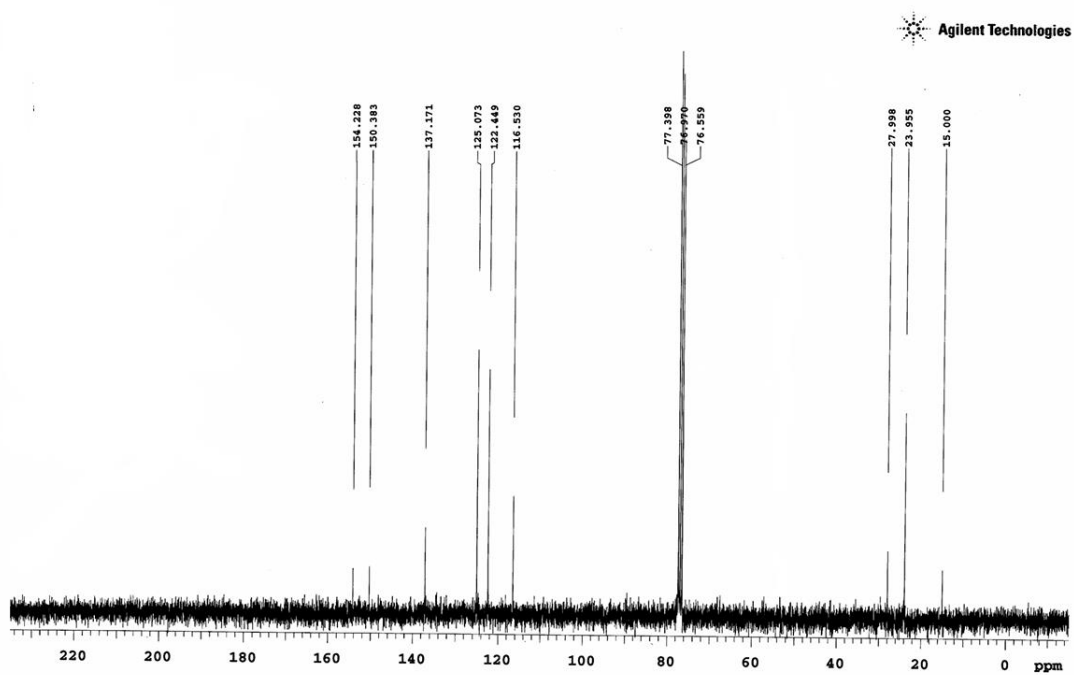


Figure S40. ^{13}C NMR spectrum of compound **20**.

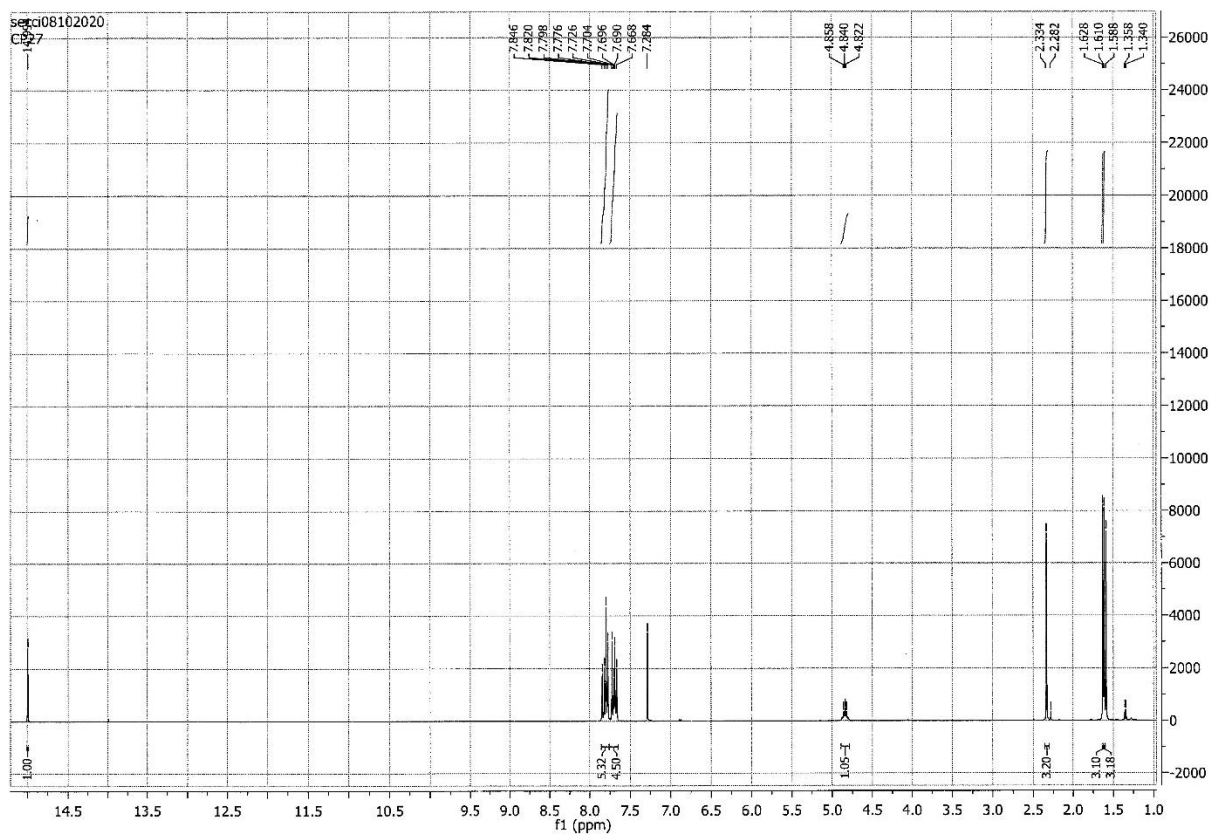


Figure S41. ^1H NMR spectrum of compound **21**.

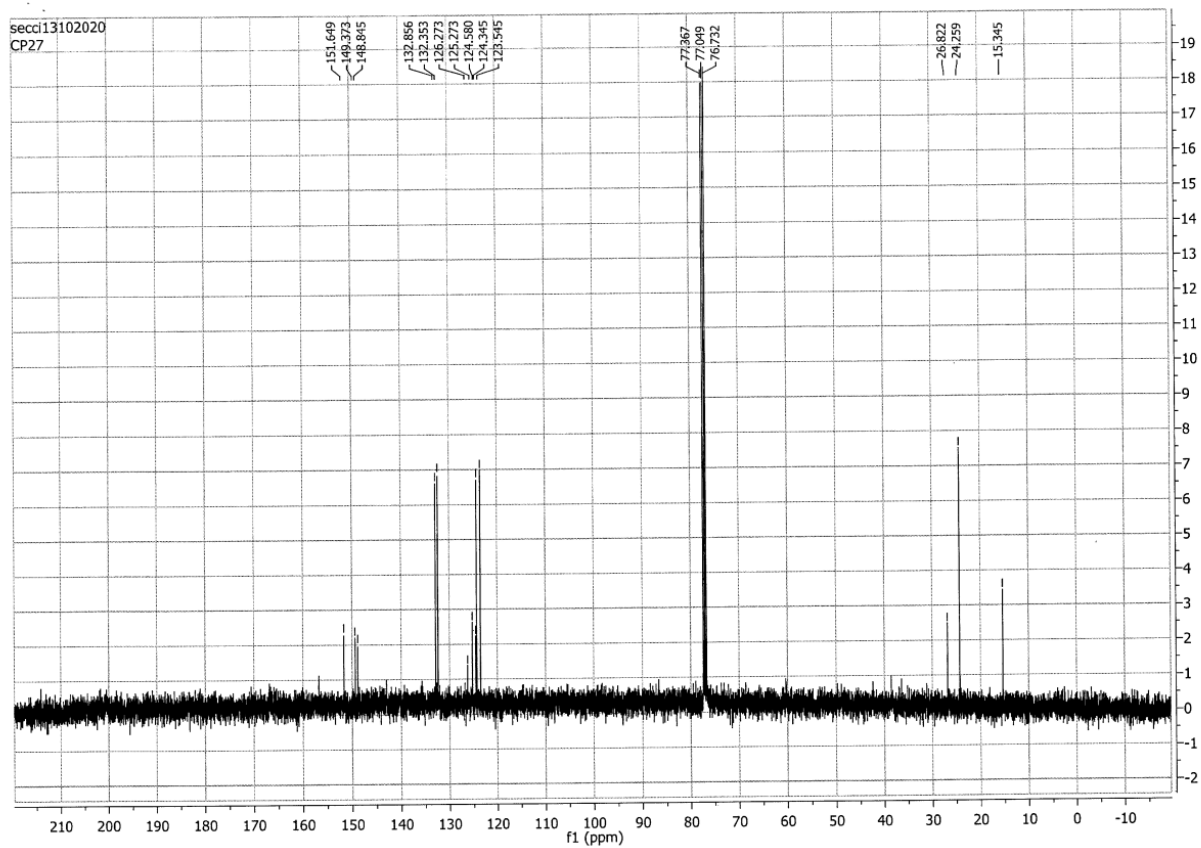


Figure S42. ^{13}C NMR spectrum of compound 21.

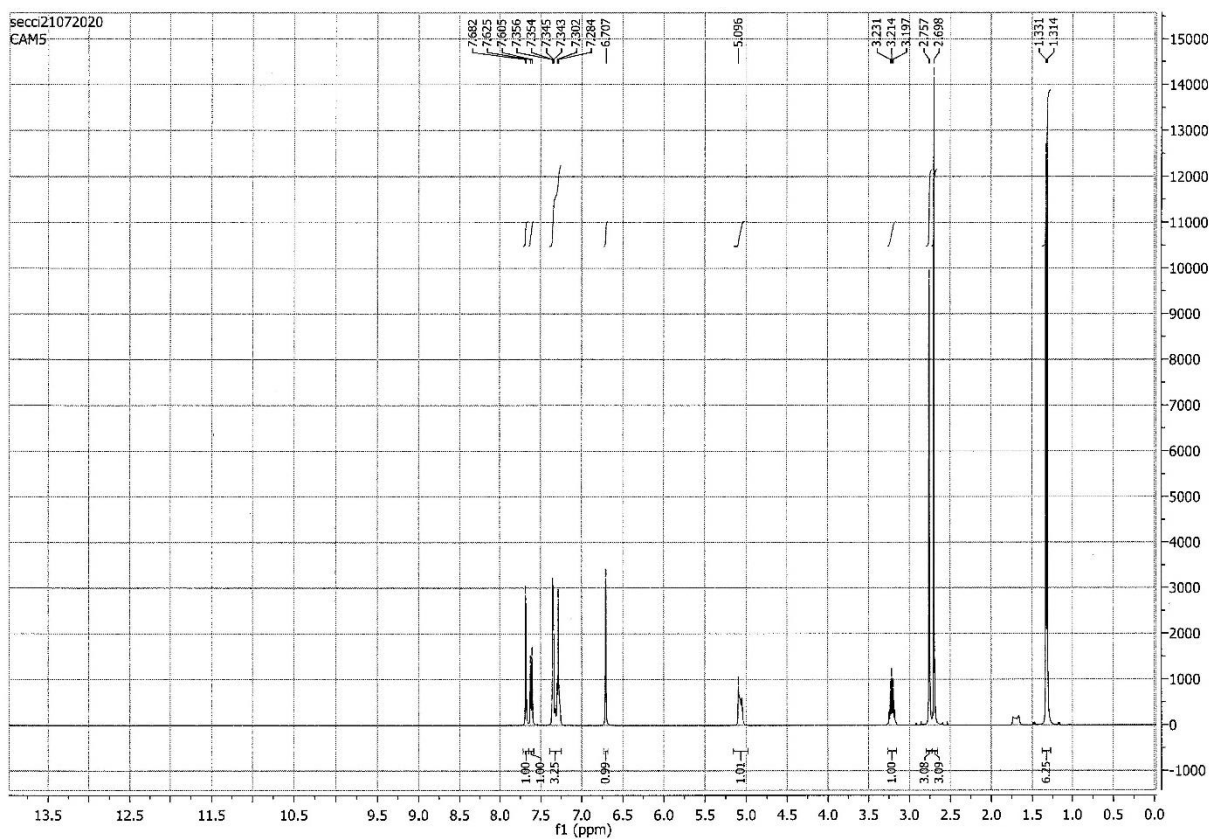


Figure S43. ^1H NMR spectrum of compound 22.

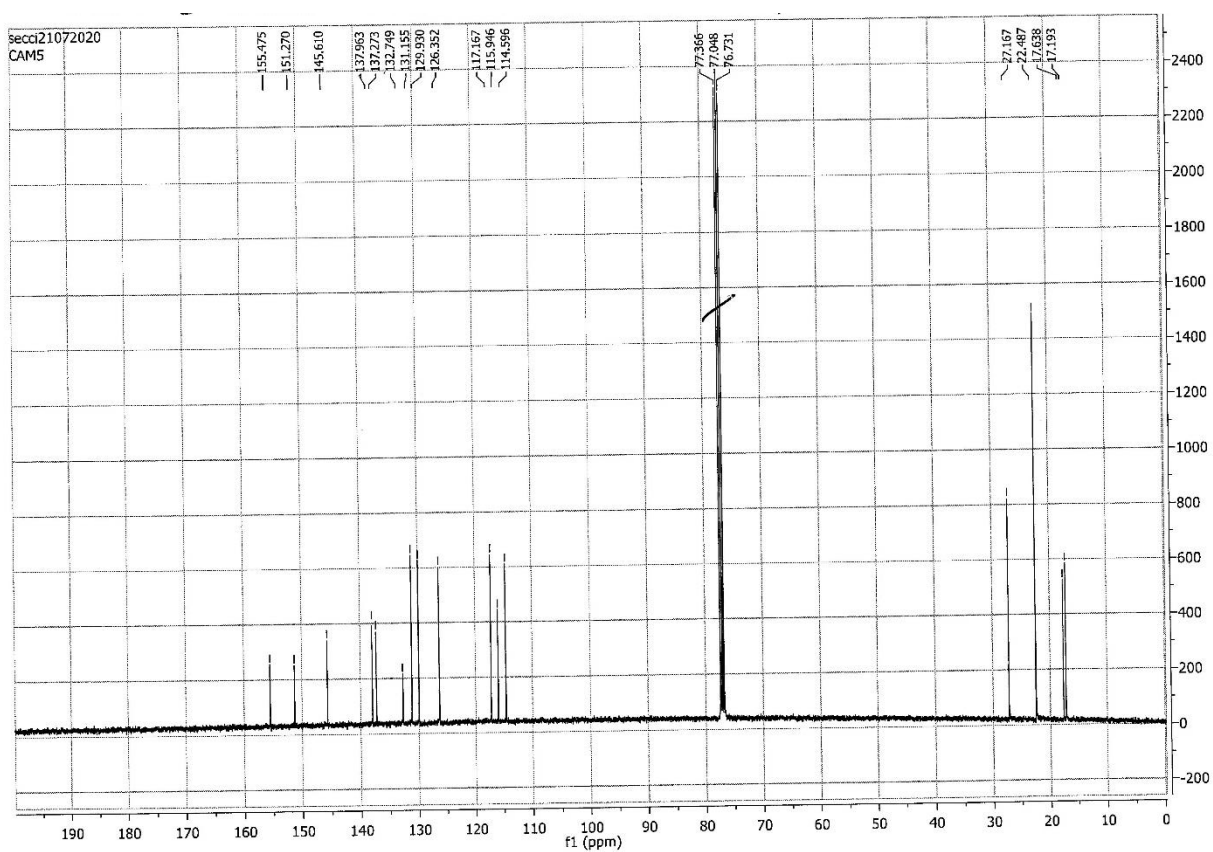


Figure S44. ^{13}C NMR spectrum of compound 22.

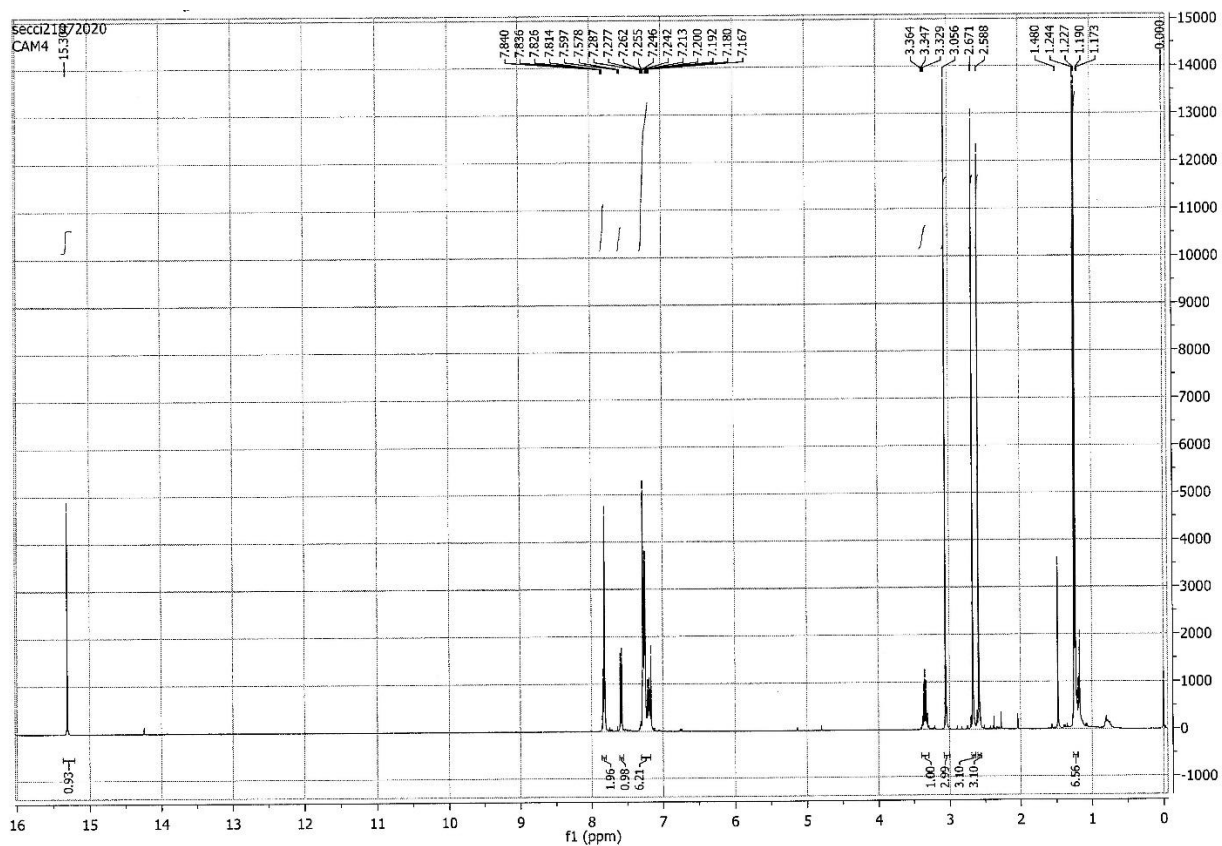


Figure S45. ^1H NMR spectrum of compound 23.

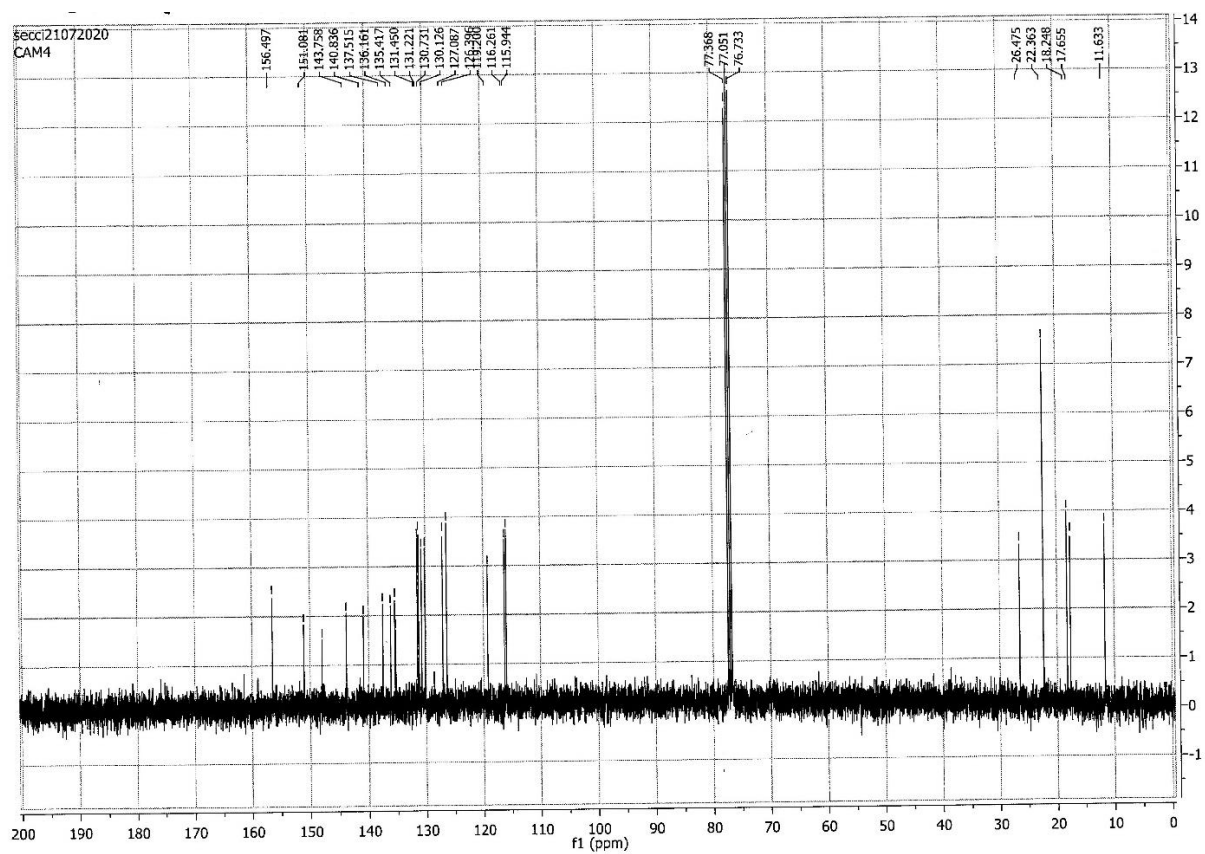


Figure S46. ^{13}C NMR spectrum of compound **23**.

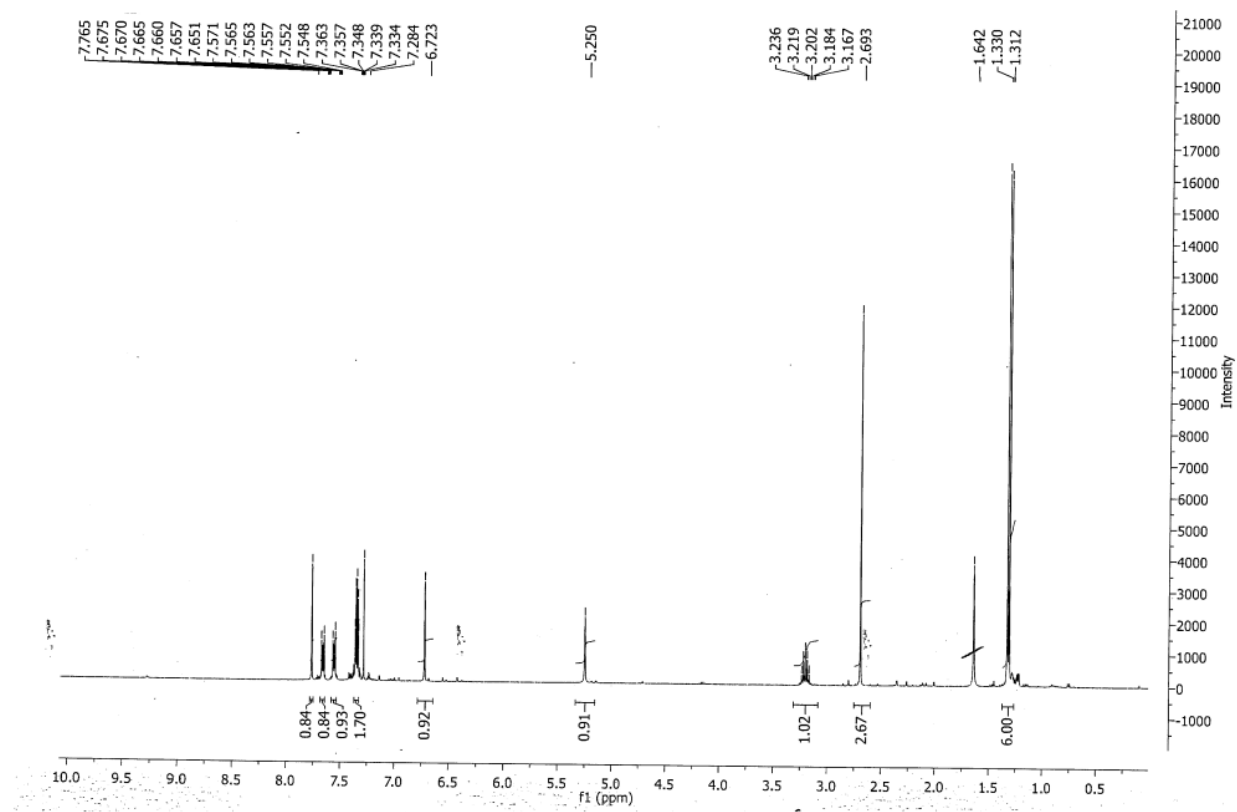


Figure S47. ^1H NMR spectrum of compound **24**.

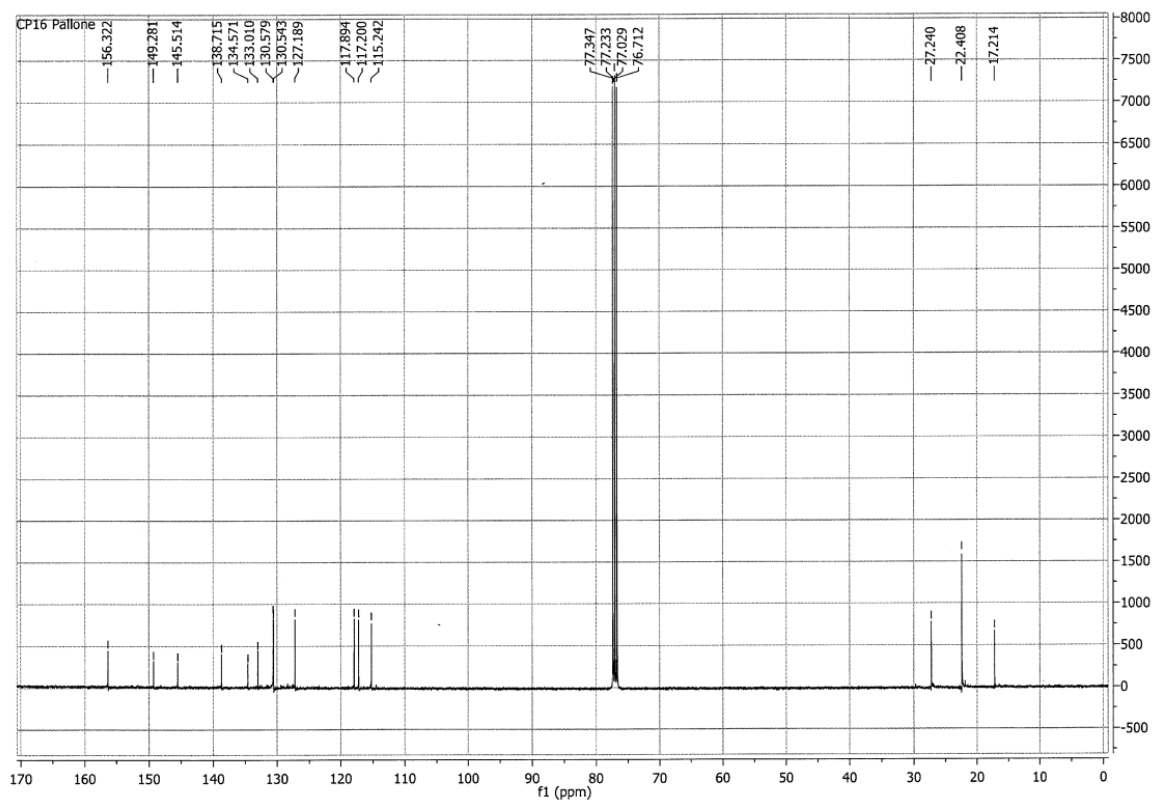


Figure S48. ^{13}C NMR spectrum of compound **24**.

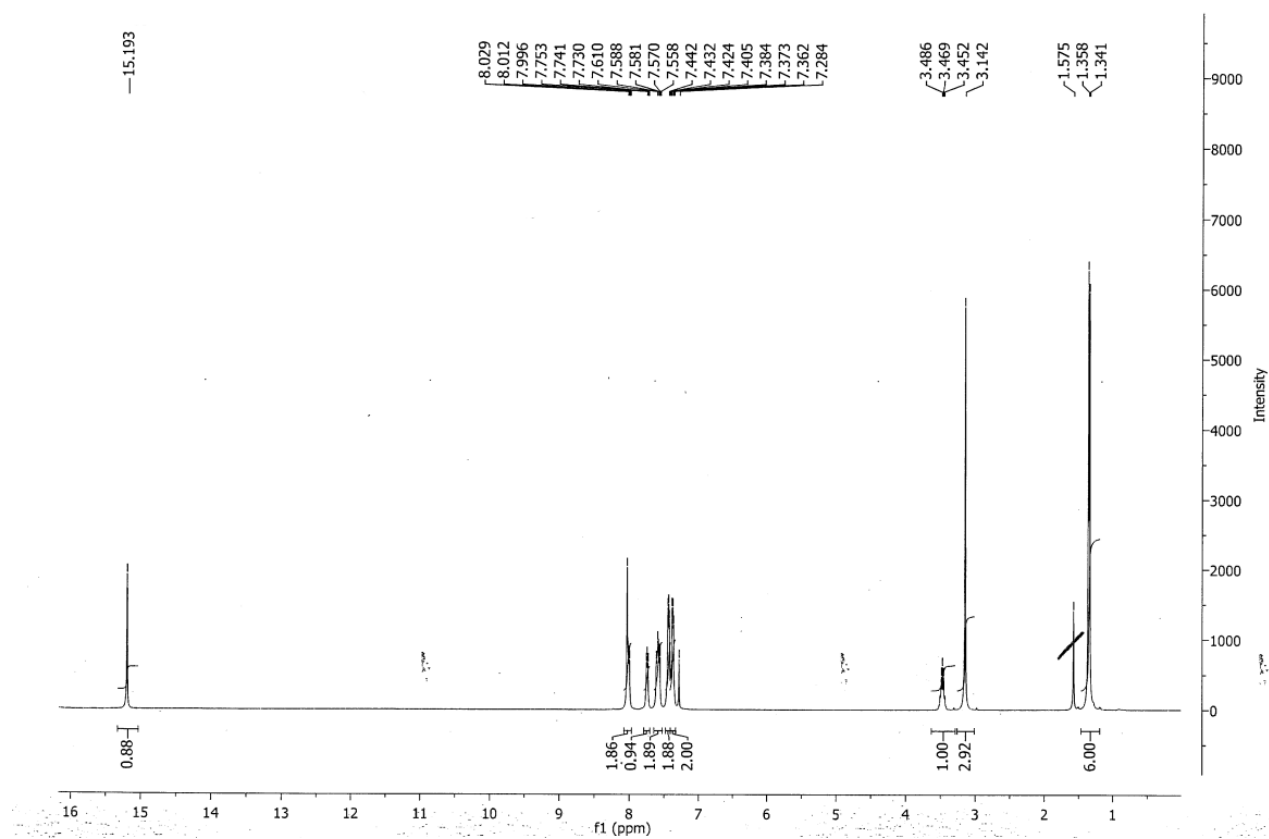


Figure S49. ^1H NMR spectrum of compound **25**.

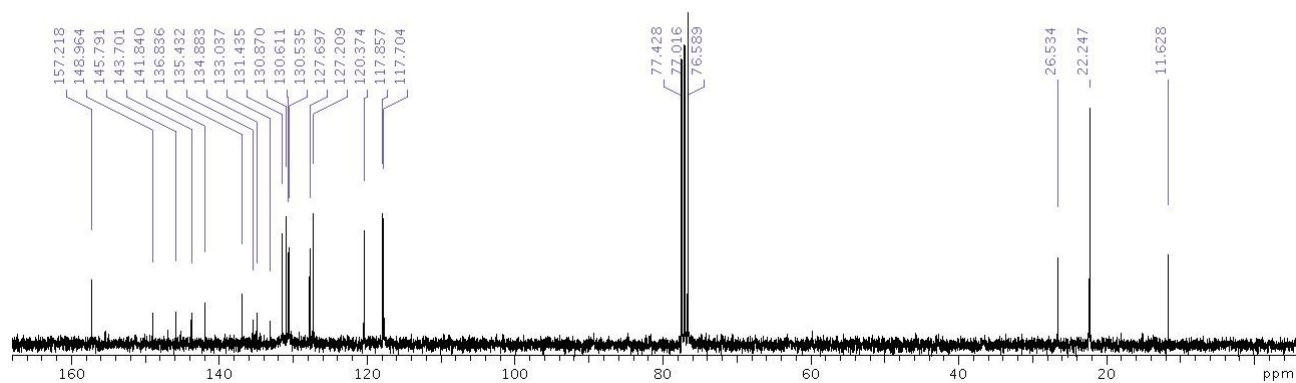


Figure S50. ^1H NMR spectrum of compound **25**.

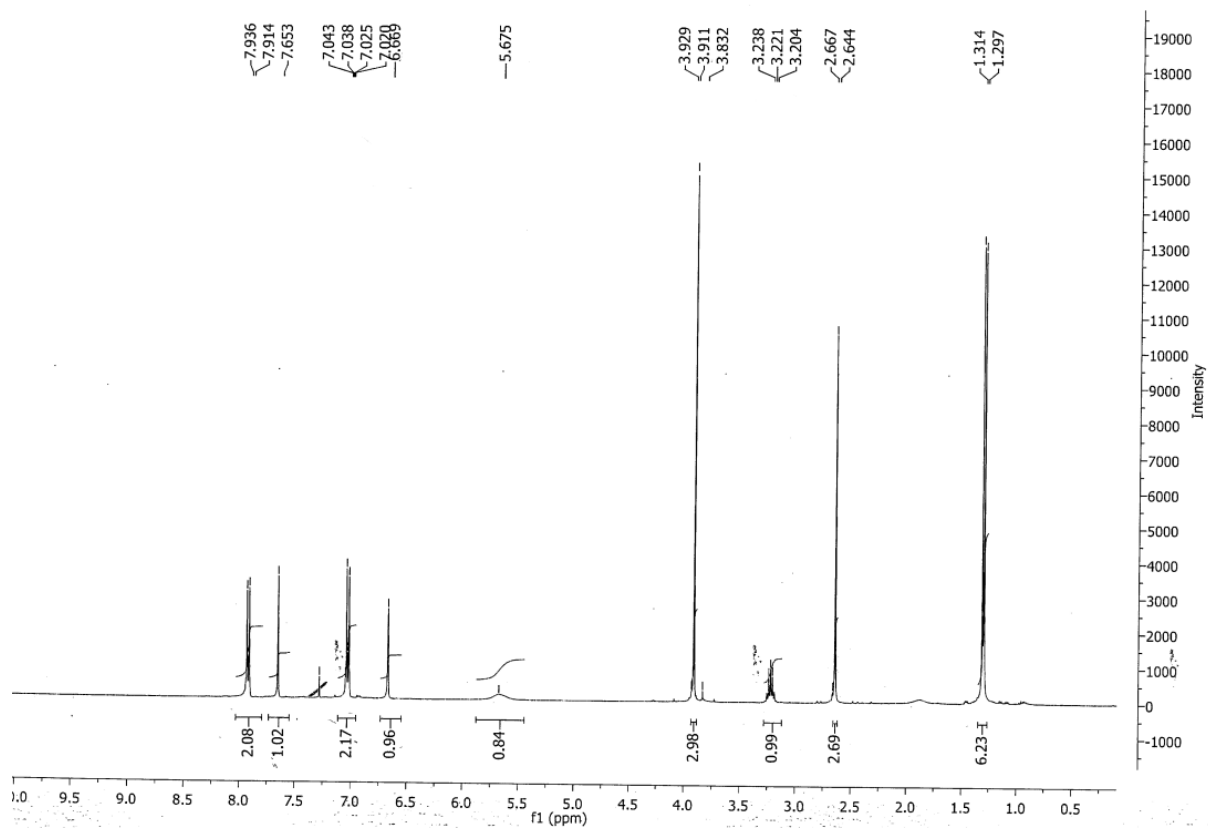


Figure S51. ^1H NMR spectrum of compound **26**.

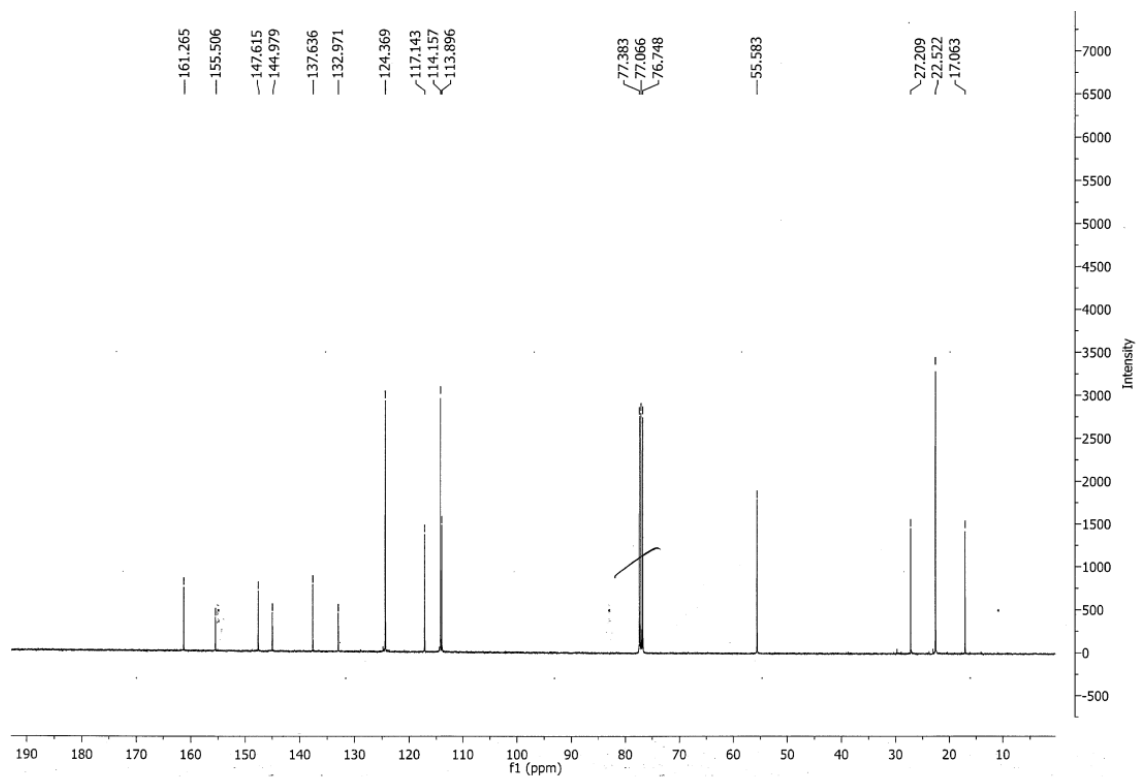


Figure S52. ^{13}C NMR spectrum of compound **26**.

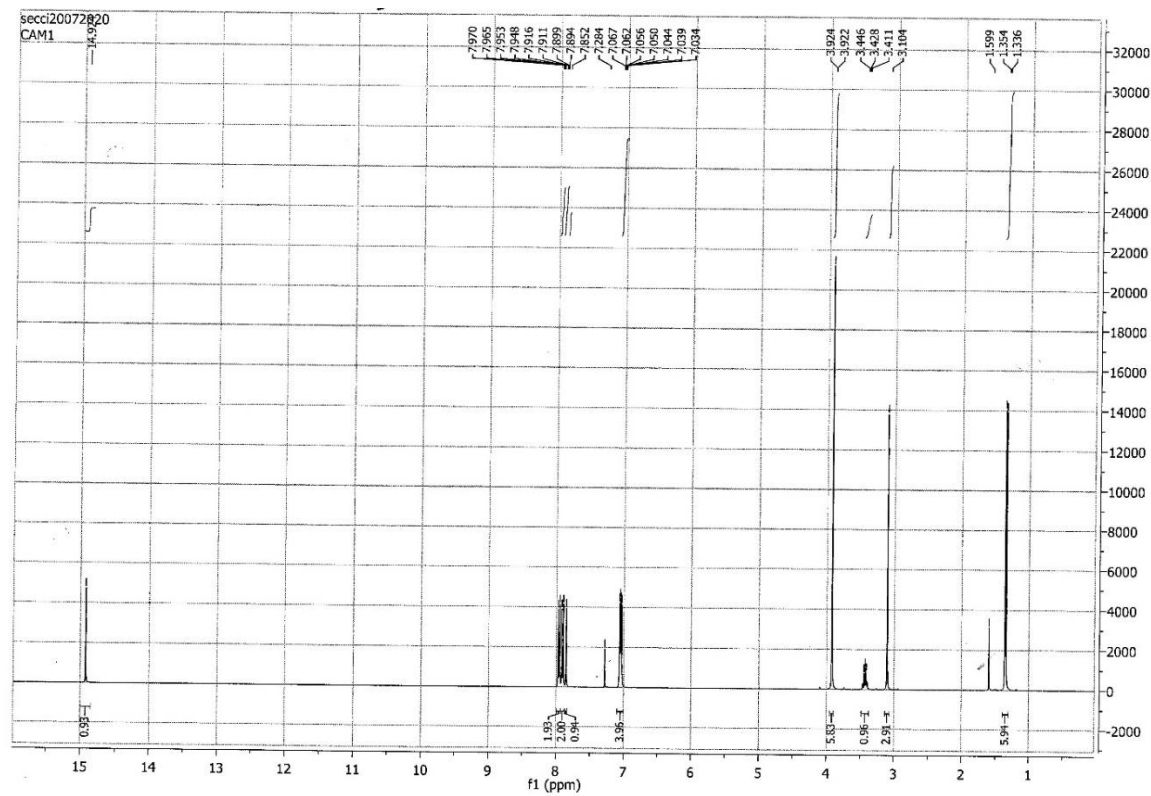


Figure S53. ^1H NMR spectrum of compound **27**.

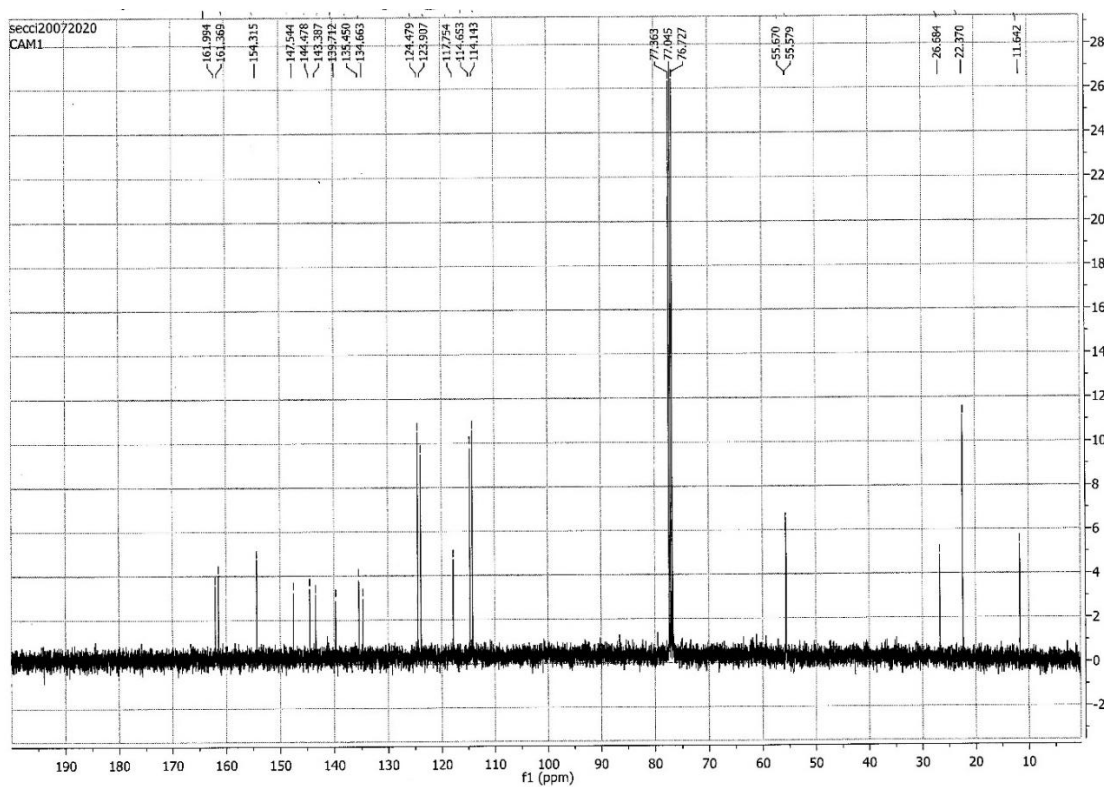


Figure S54. ^1H NMR spectrum of compound **27**.

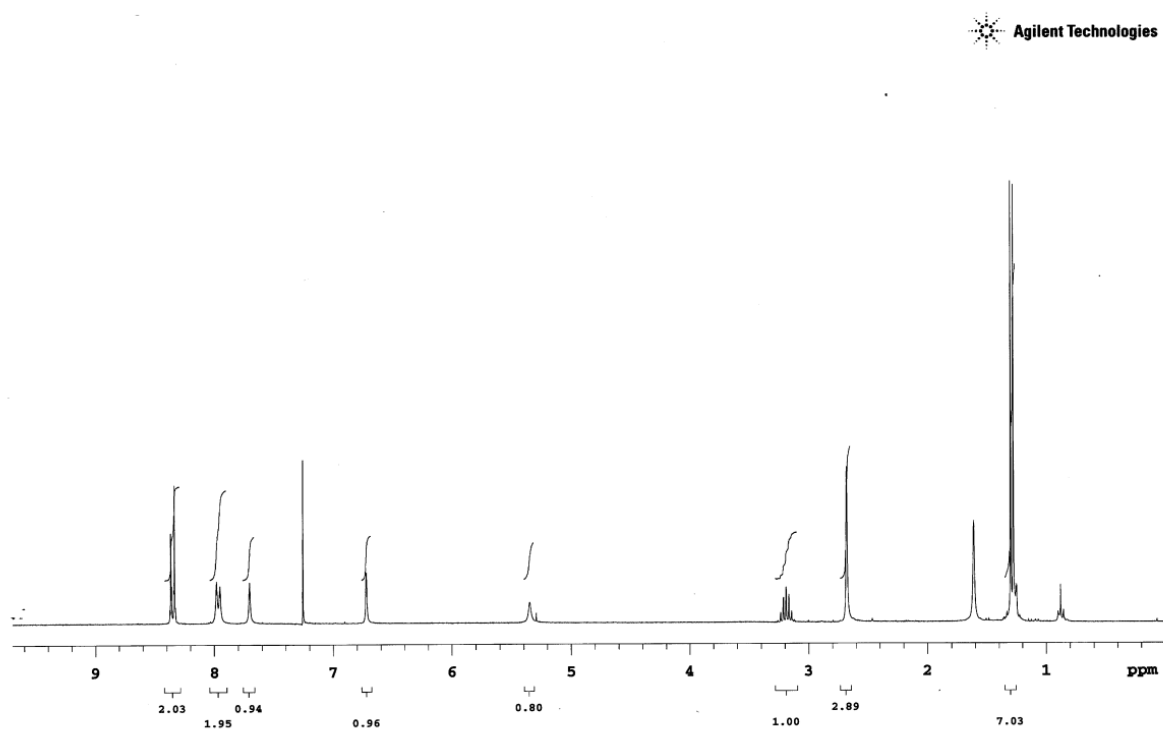


Figure S55. ^1H NMR spectrum of compound **28**.

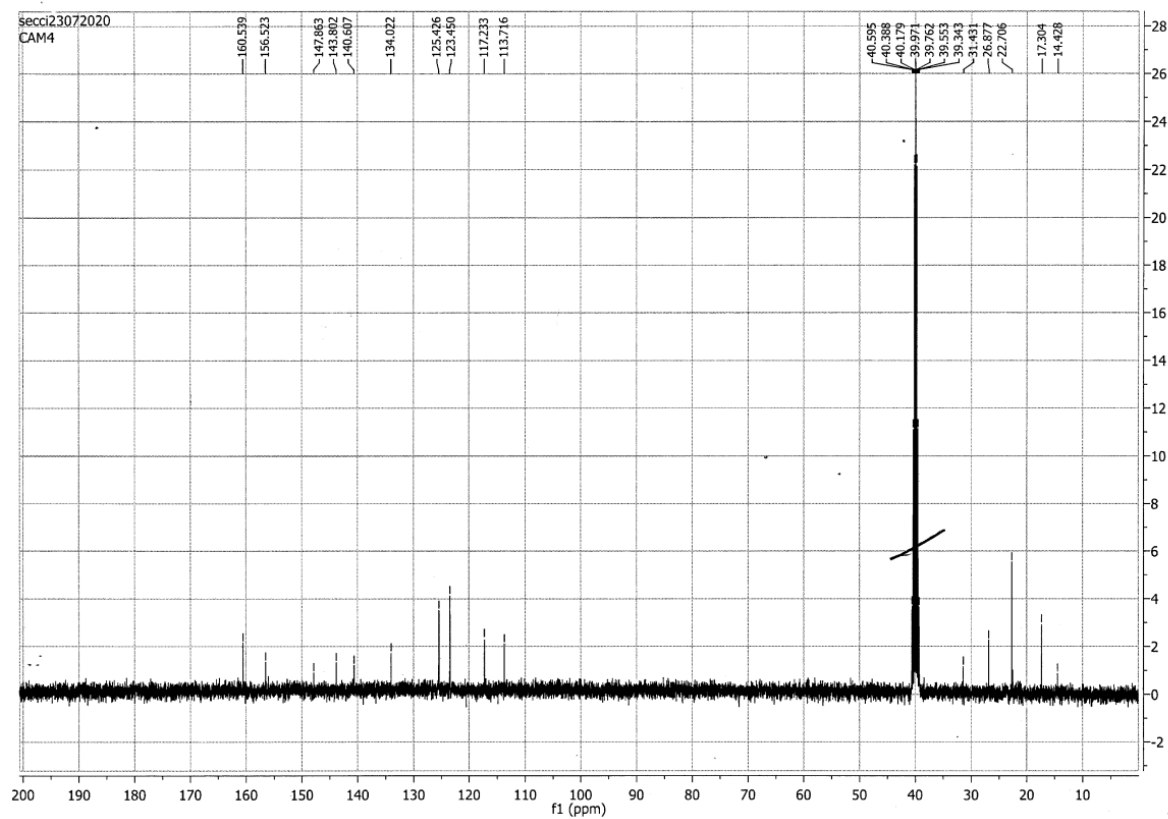


Figure S56. ^{13}C NMR spectrum of compound **28**.

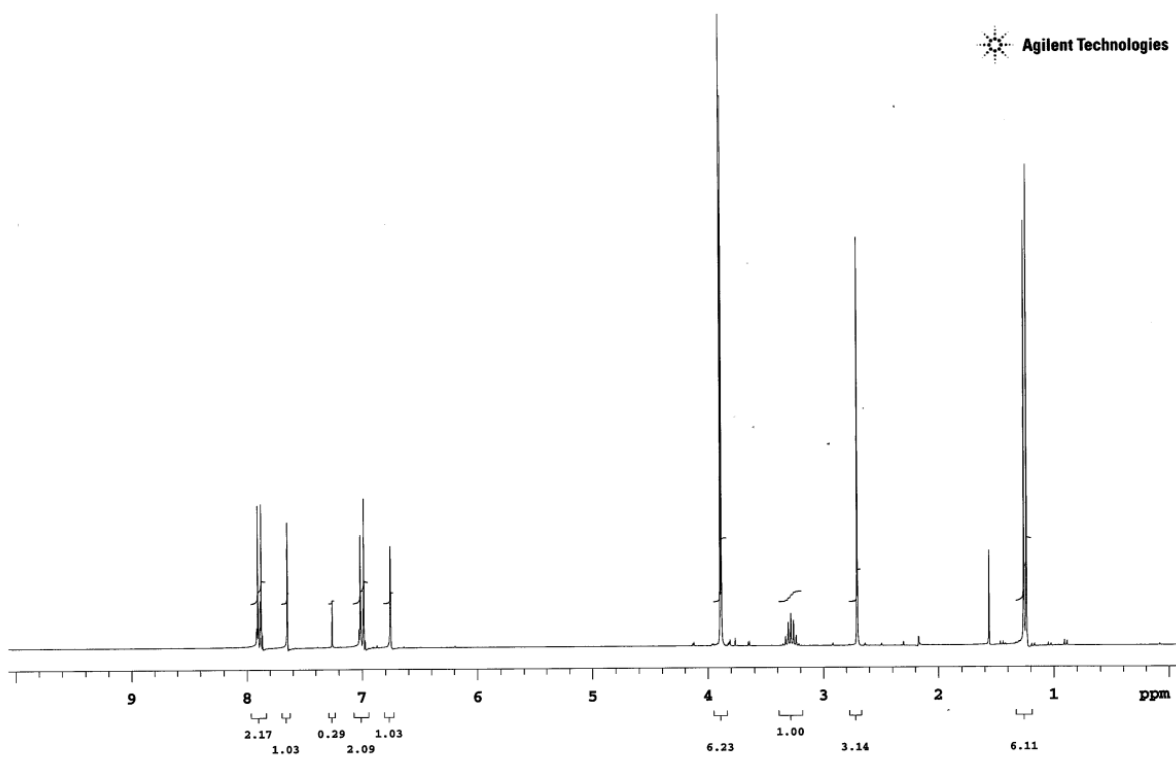


Figure S57. ^1H NMR spectrum of compound 29.

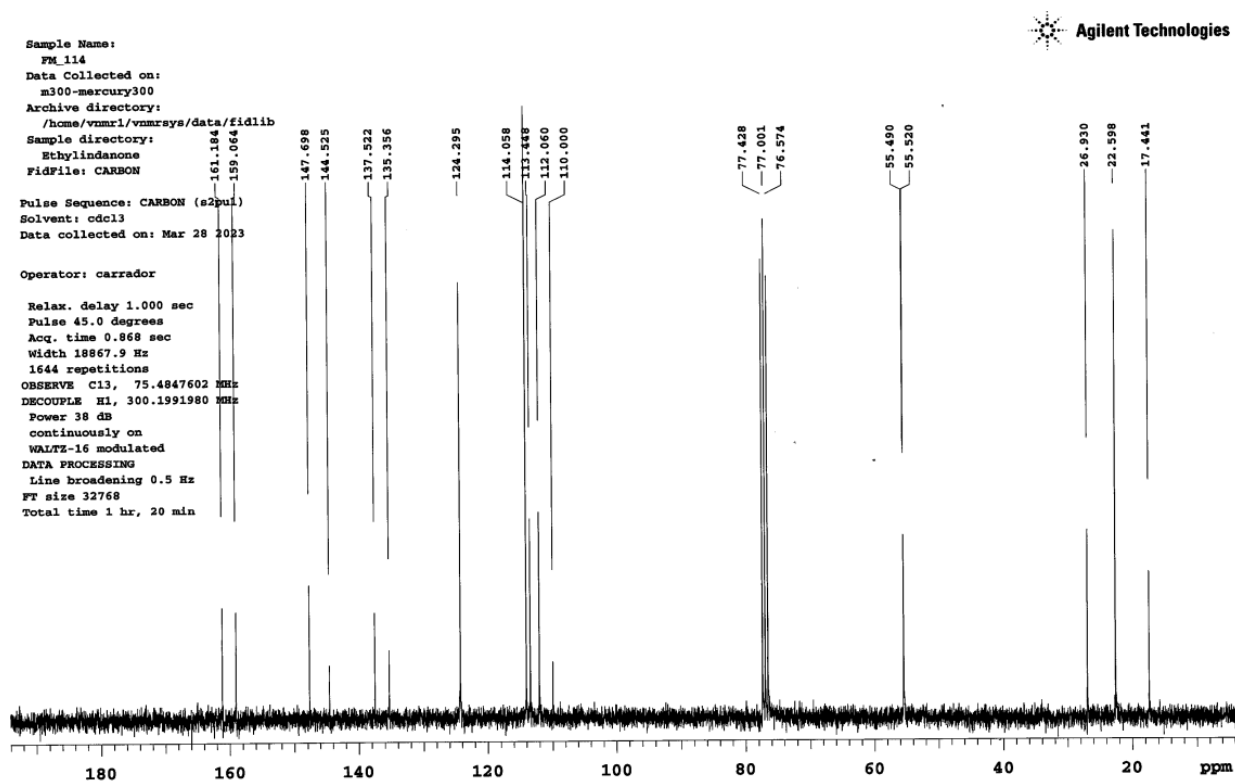


Figure S58. ^{13}C NMR spectrum of compound 29.

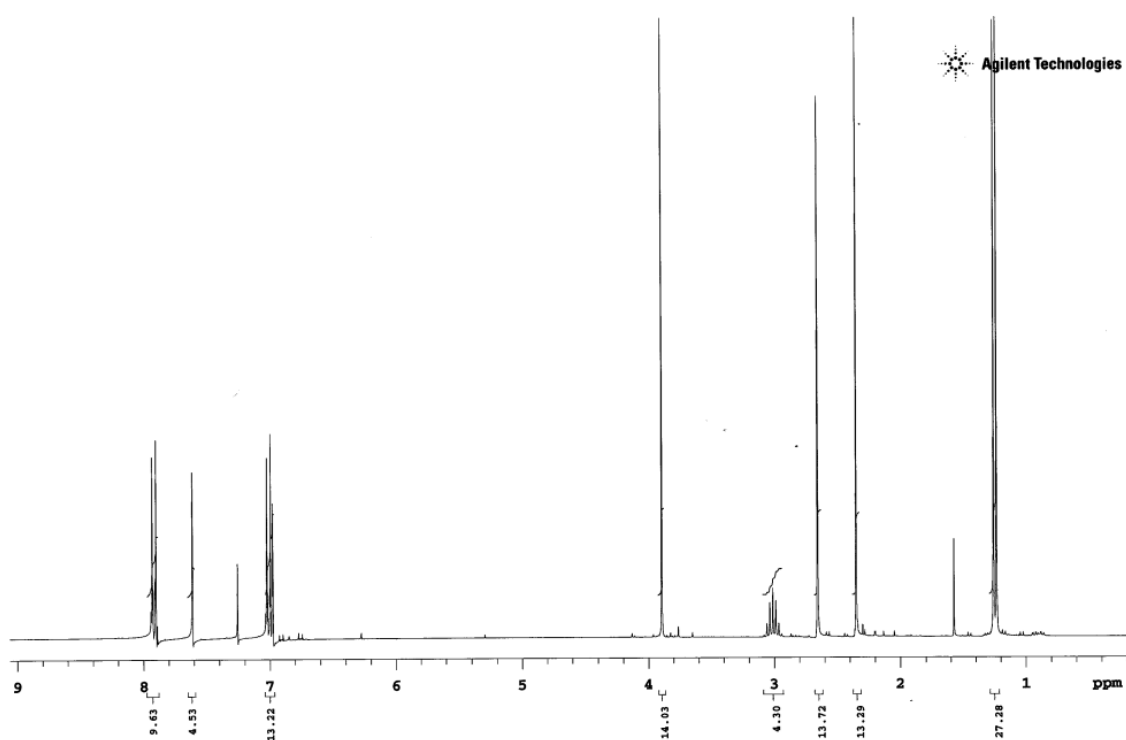


Figure S59. ^1H NMR spectrum of compound **30**.

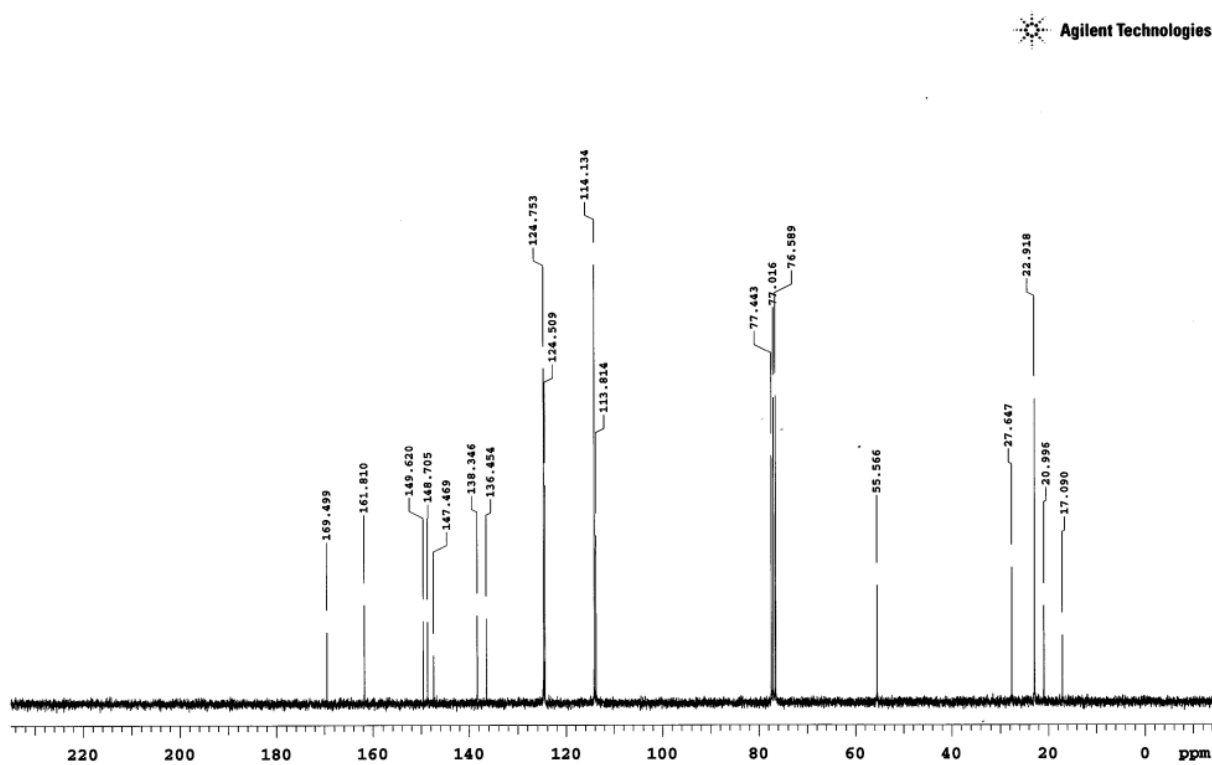


Figure S60. ^{13}C NMR spectrum of compound **30**.

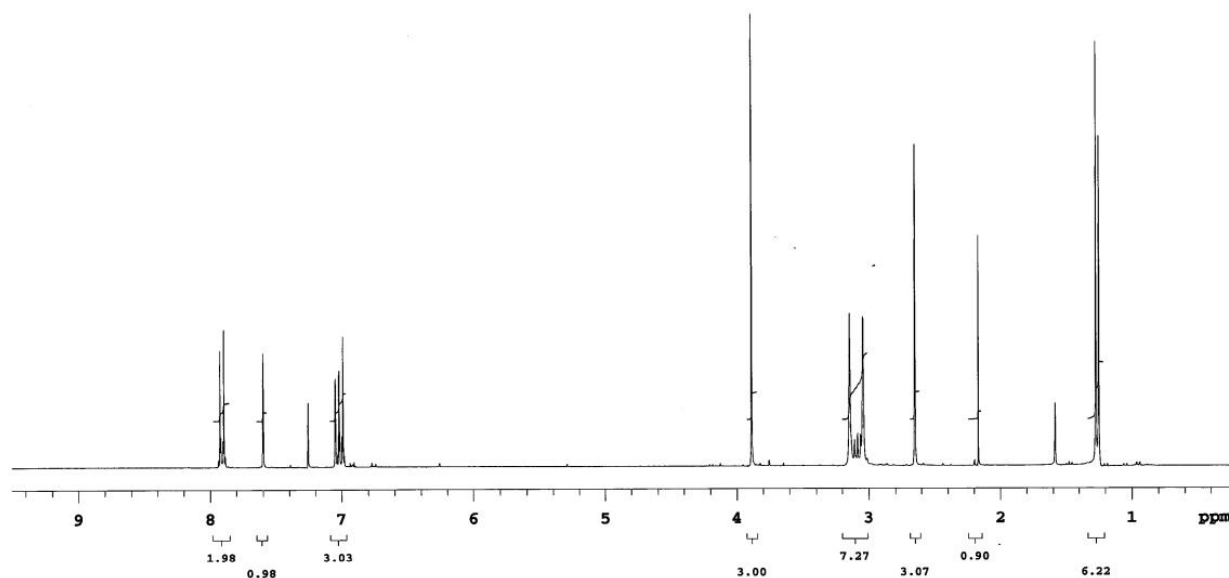


Figure S61. ^1H NMR spectrum of compound 31.

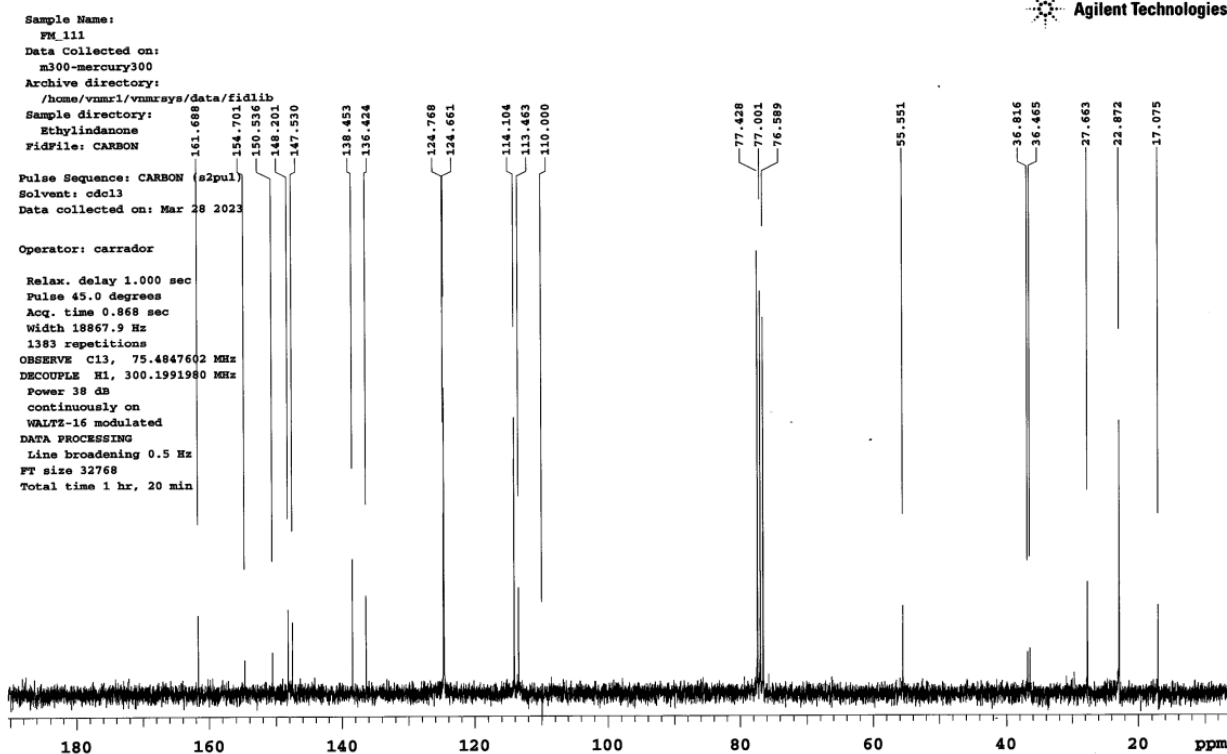


Figure S62. ^{13}C NMR spectrum of compound 31.

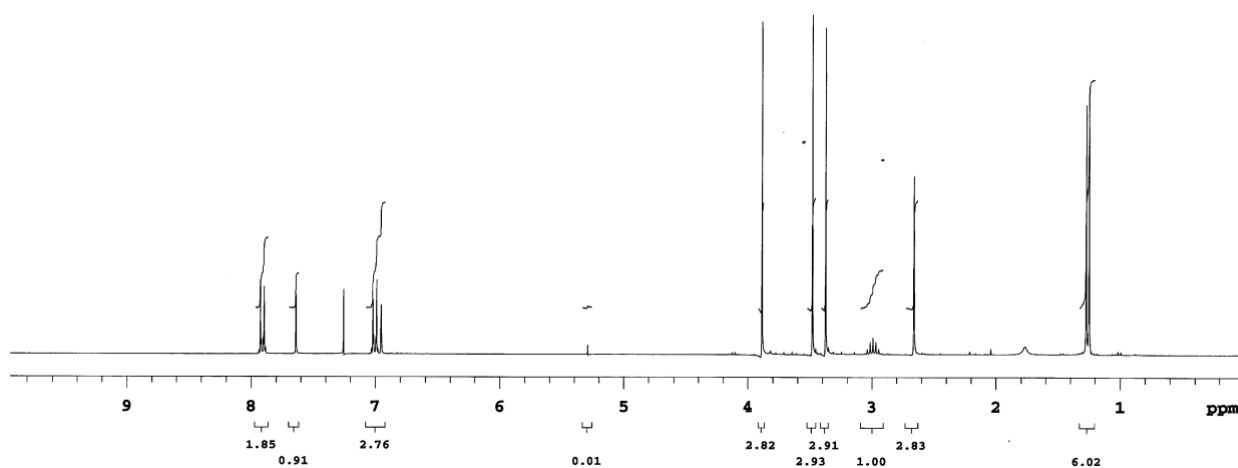


Figure S63. ^1H NMR spectrum of compound 32.

Gradient Shimming

Sample Name: FM125
 Data Collected on: m300-mercury300
 Archive directory: /export/home/chempack/vnmrsys/data
 Sample directory:
 FidFile: FM125.C13
 Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Jun 9 2023
 Operator: carrador
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 1620 repetitions
 OBSERVE C13, 75.4847602 MHz
 DECOUPLE H1, 300.1991980 MHz
 Power 38 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 1 hr, 36 min

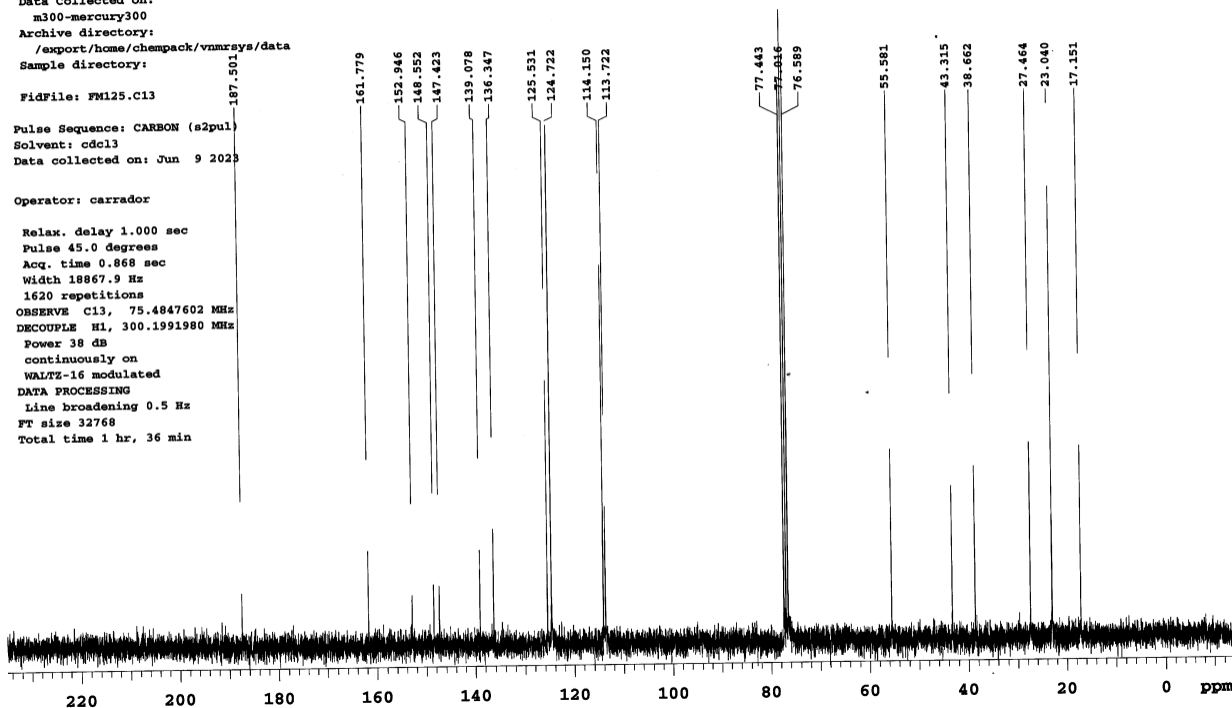


Figure S64. ^{13}C NMR spectrum of compound 32.

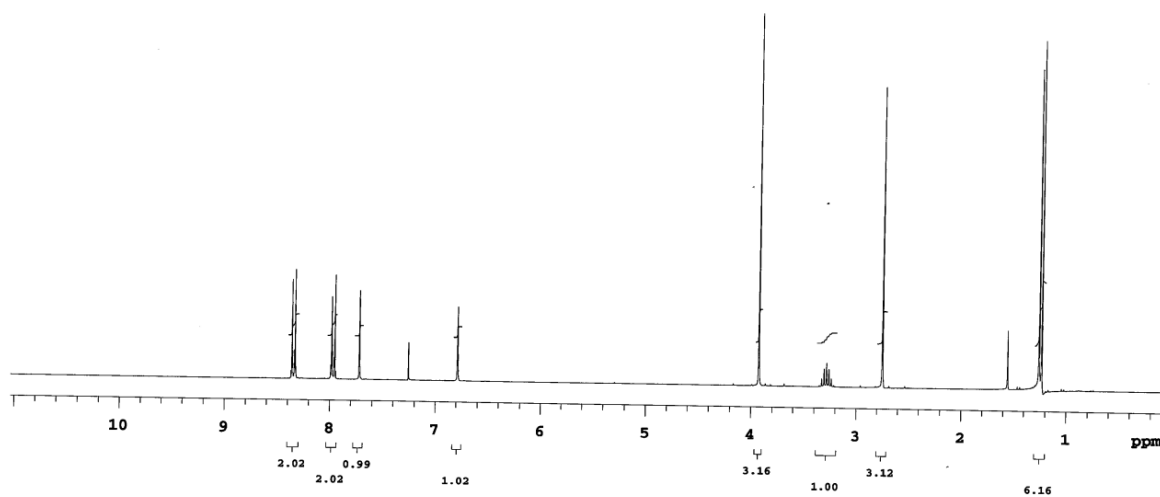


Figure S65. ¹H NMR spectrum of compound 33.

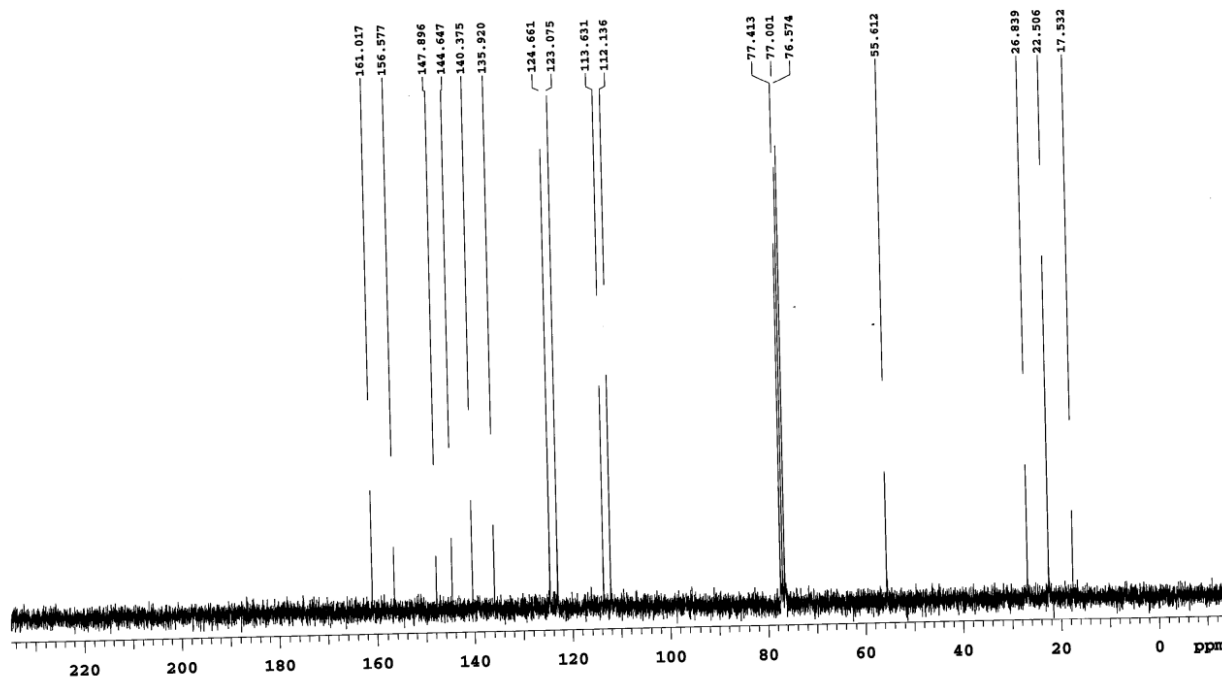


Figure S66. ¹³C NMR spectrum of compound 33.

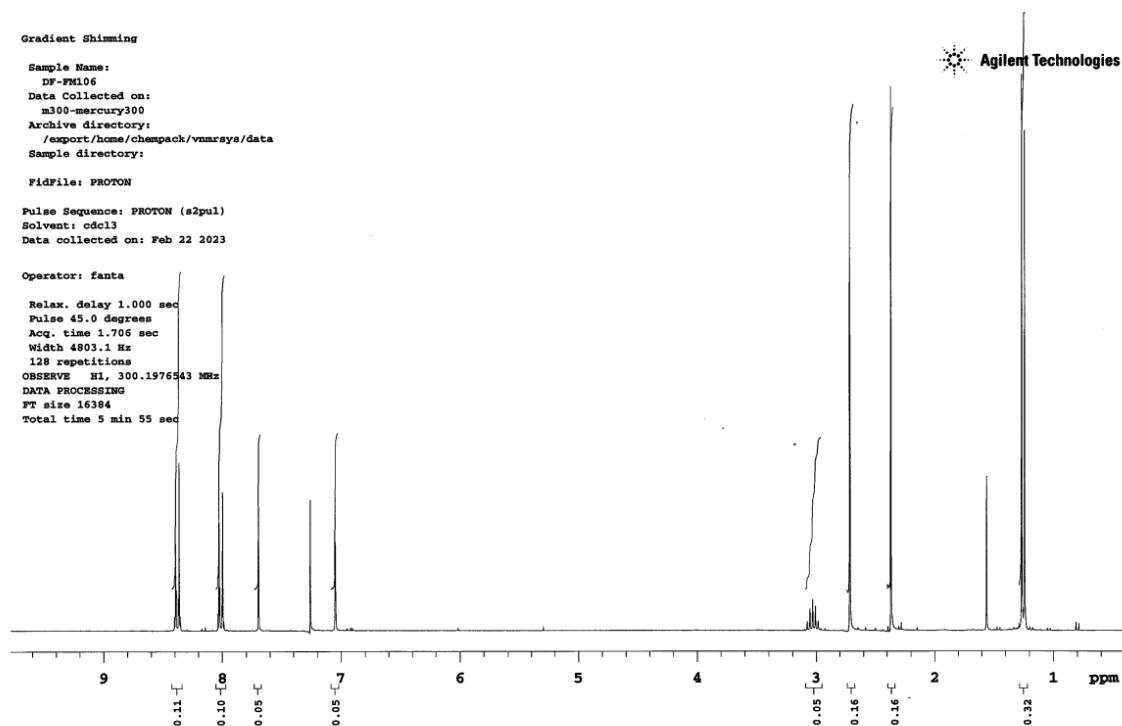


Figure S67. ^1H NMR spectrum of compound **34**.

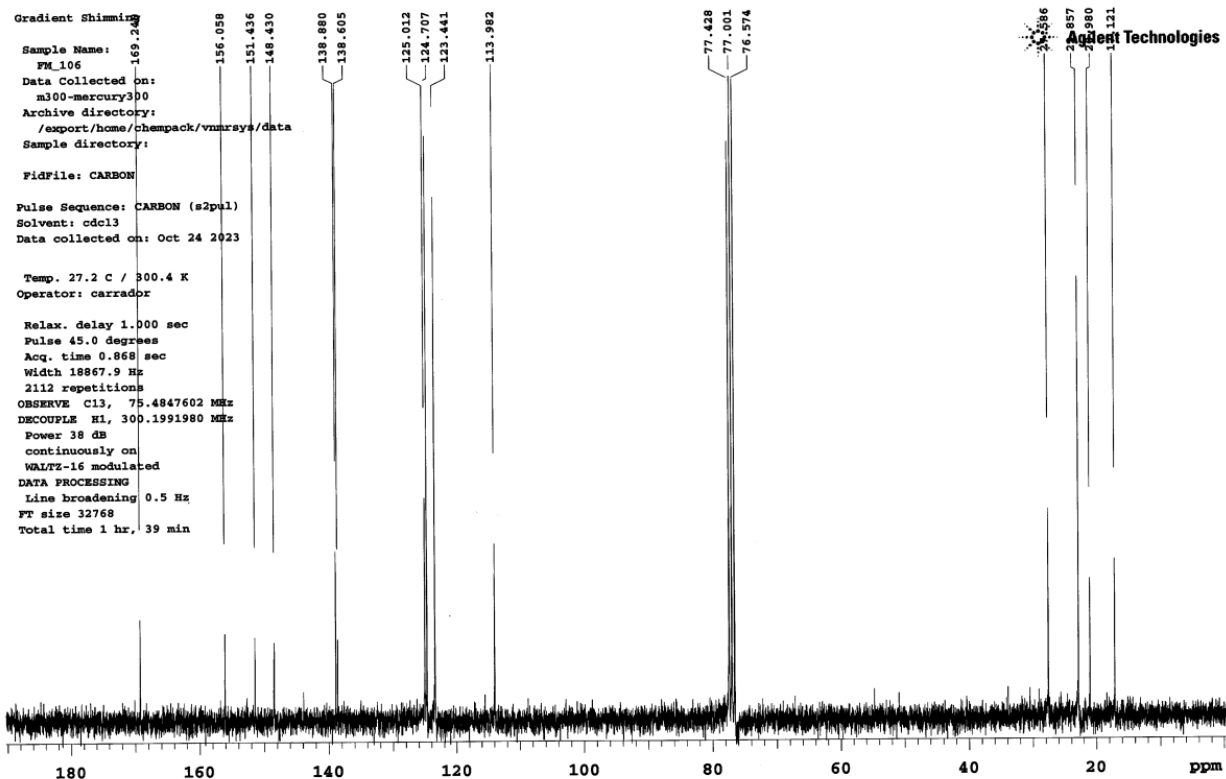


Figure S68. ^{13}C NMR spectrum of compound **34**.

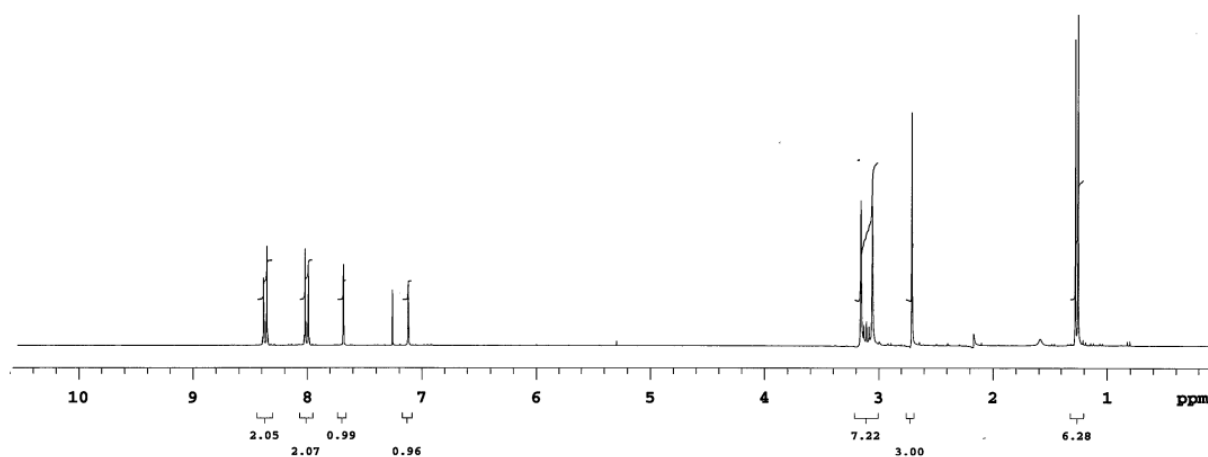


Figure S69. ¹H NMR spectrum of compound 35.

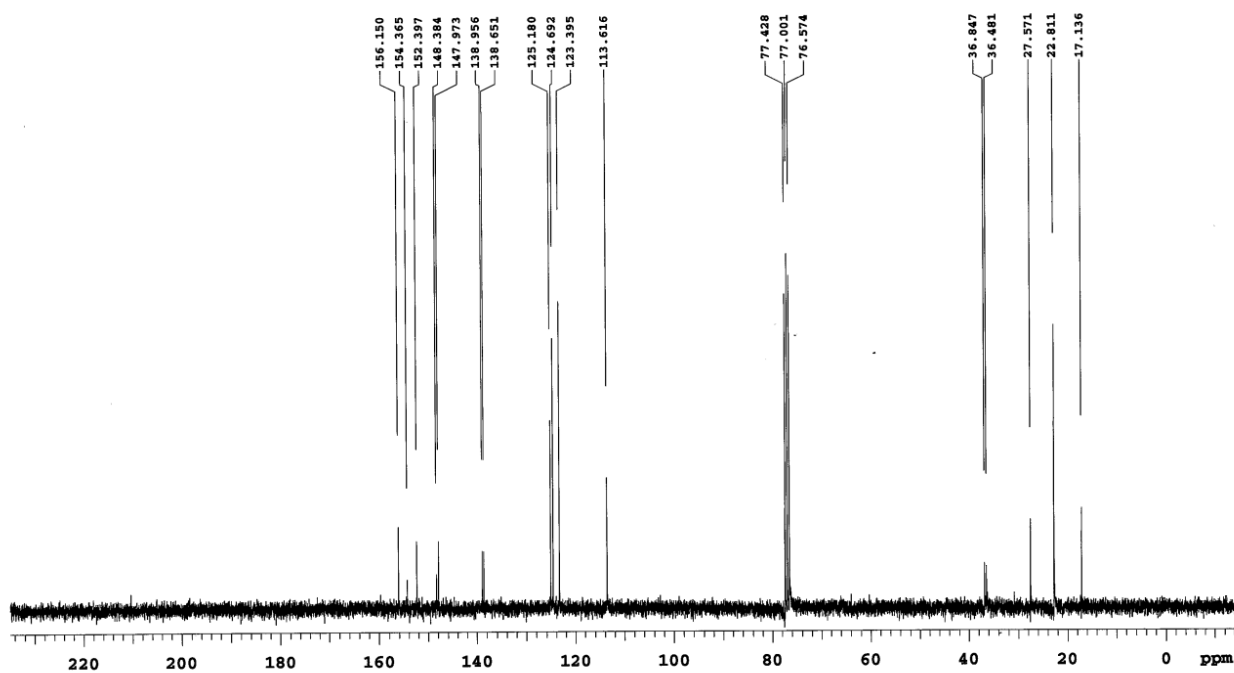


Figure S70. ^{13}C NMR spectrum of compound **35**.

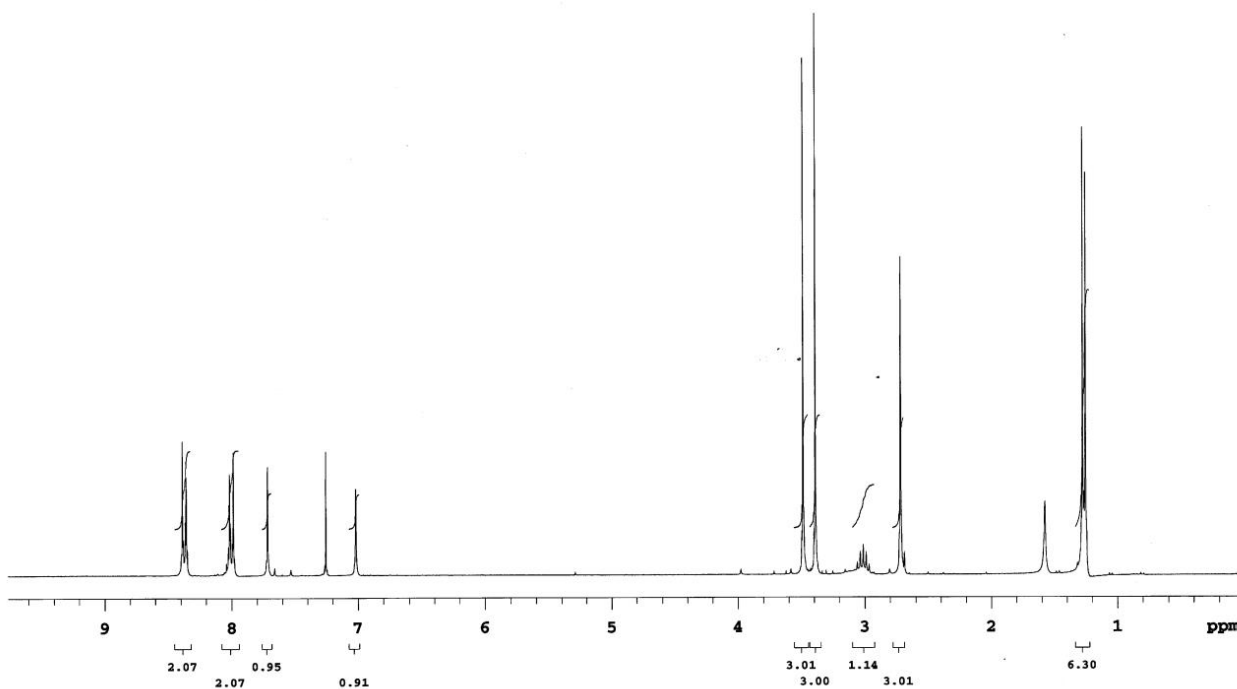


Figure S71. ^1H NMR spectrum of compound **36**.

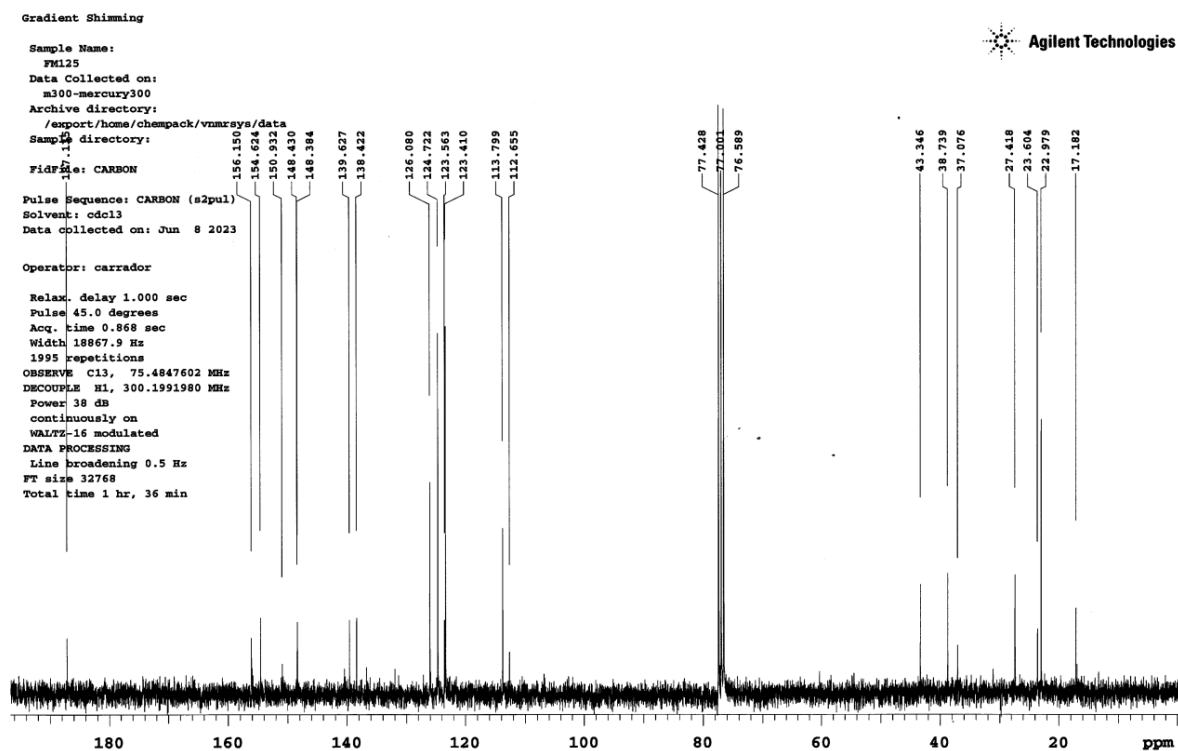


Figure S72. ^{13}C NMR spectrum of compound **36**.