

Supplementary Materials

Exploration of Indole Alkaloids from Marine Fungus *Pseudallescheria boydii* F44-1 Using an Amino Acid-Directed Strategy

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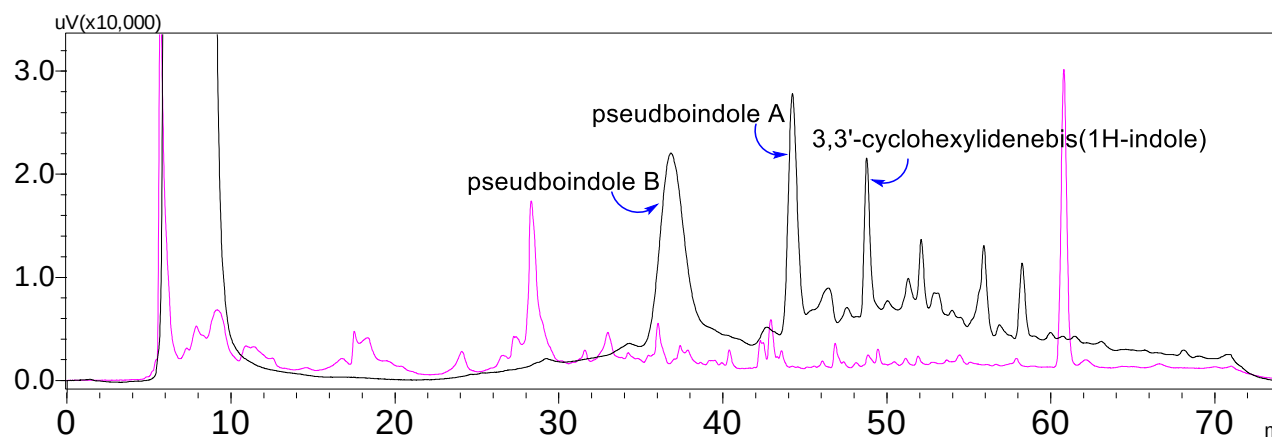
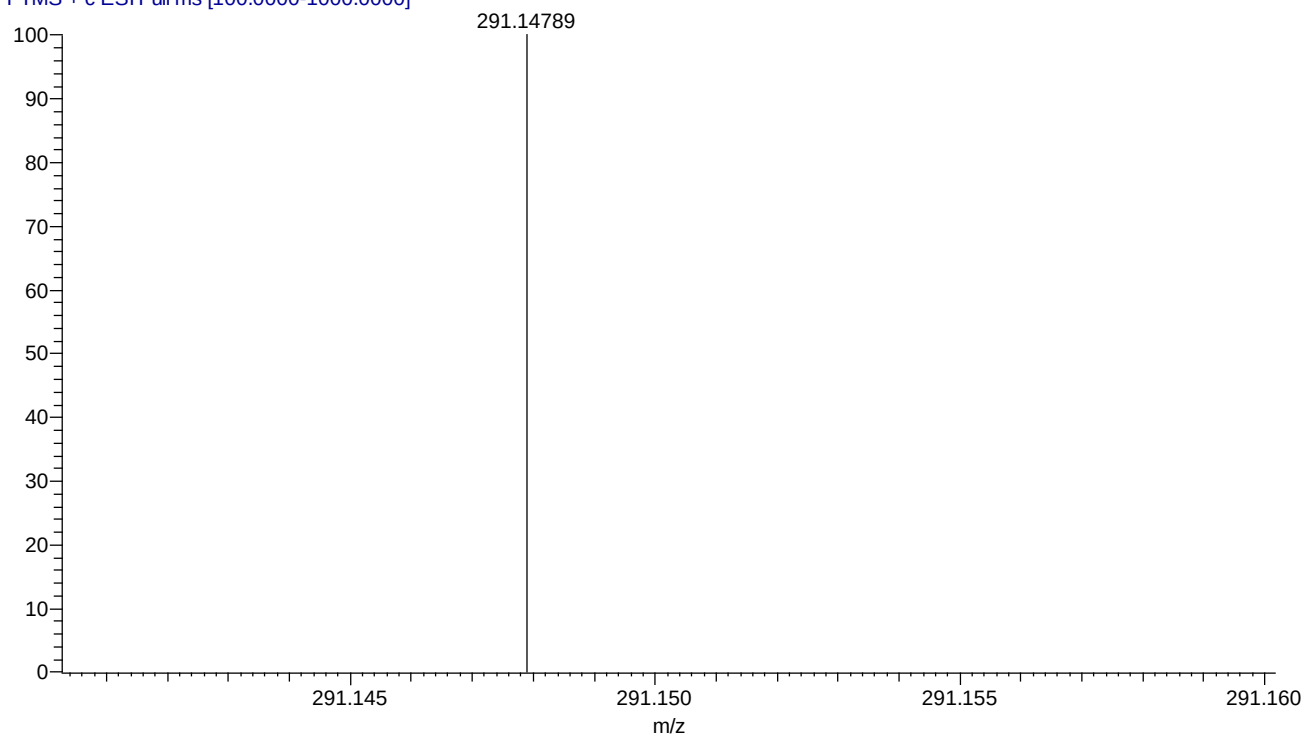


Figure S1. HPLC analysis on the fungal metabolites in different culture media.

HPLC profiles detected at 254 nm of the metabolite extracts of marine fungus *Pseudallescheria boydii* F44-1 cultured in GPY medium (pink line) and GPY medium supplemented with various amino acids (black line). HPLC analysis was used a Shimadzu LC-20AT HPLC pump (Shimadzu Corporation, Nakagyu-ku, Kyoto, Japan) equipped with an SPD-20A dual λ absorbance detector (Shimadzu Corporation, Nakagyu-ku, Kyoto, Japan) and a Shiseido spolar C18 column (4.6 mm I.D. $\times$ 250 mm, 5 μ m) and a step gradient elution with $\text{CH}_3\text{CN}-\text{H}_2\text{O}$. LC time program was listed below:

Time/min	Module	Action	Value/%
0.01	Pumps	H_2O Conc.	30
10.00	Pumps	H_2O Conc.	30
40.00	Pumps	H_2O Conc.	100
60.00	Pumps	H_2O Conc.	100
65.00	Pumps	H_2O Conc.	30
70.00	Pumps	H_2O Conc.	30
75.00	Controller	Stop	

50min #12 RT: 0.03 AV: 1 NL: 3.12E6
T: FTMS + c ESI Full ms [100.0000-1000.0000]



SPECTRUM - simulation:

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
291.14789	291.14919	-4.46	11.5	C19 H19 O N2

Figure S2. HR-(+)ESI-MS spectrum of pseudoboinole A (**1**).

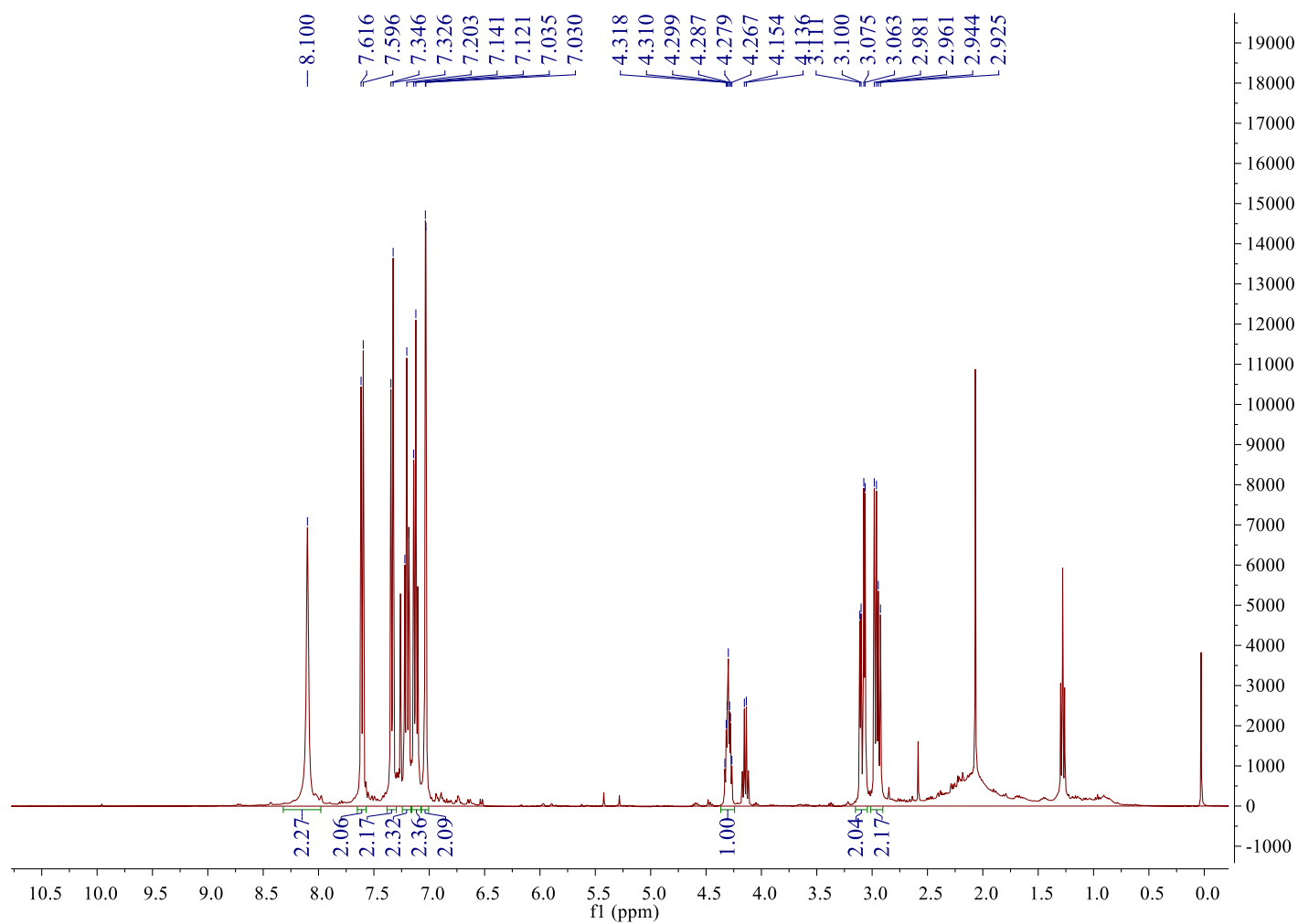


Figure S3. ^1H NMR spectrum of pseudobindole A (**1**) in CDCl_3 (400 MHz).

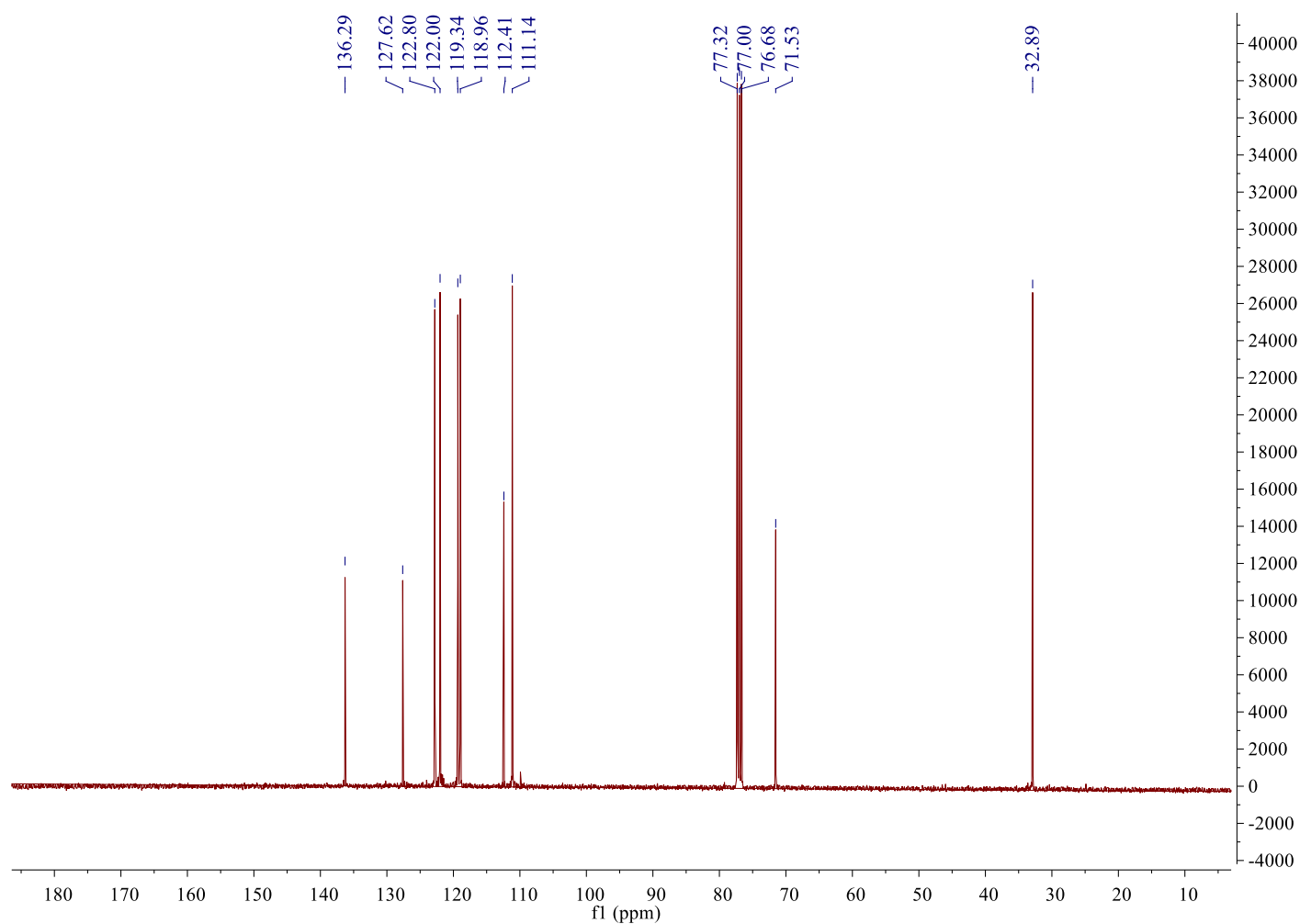


Figure S4. ¹³C NMR spectrum of pseudoboindele A (**1**) in CDCl₃ (100 MHz).

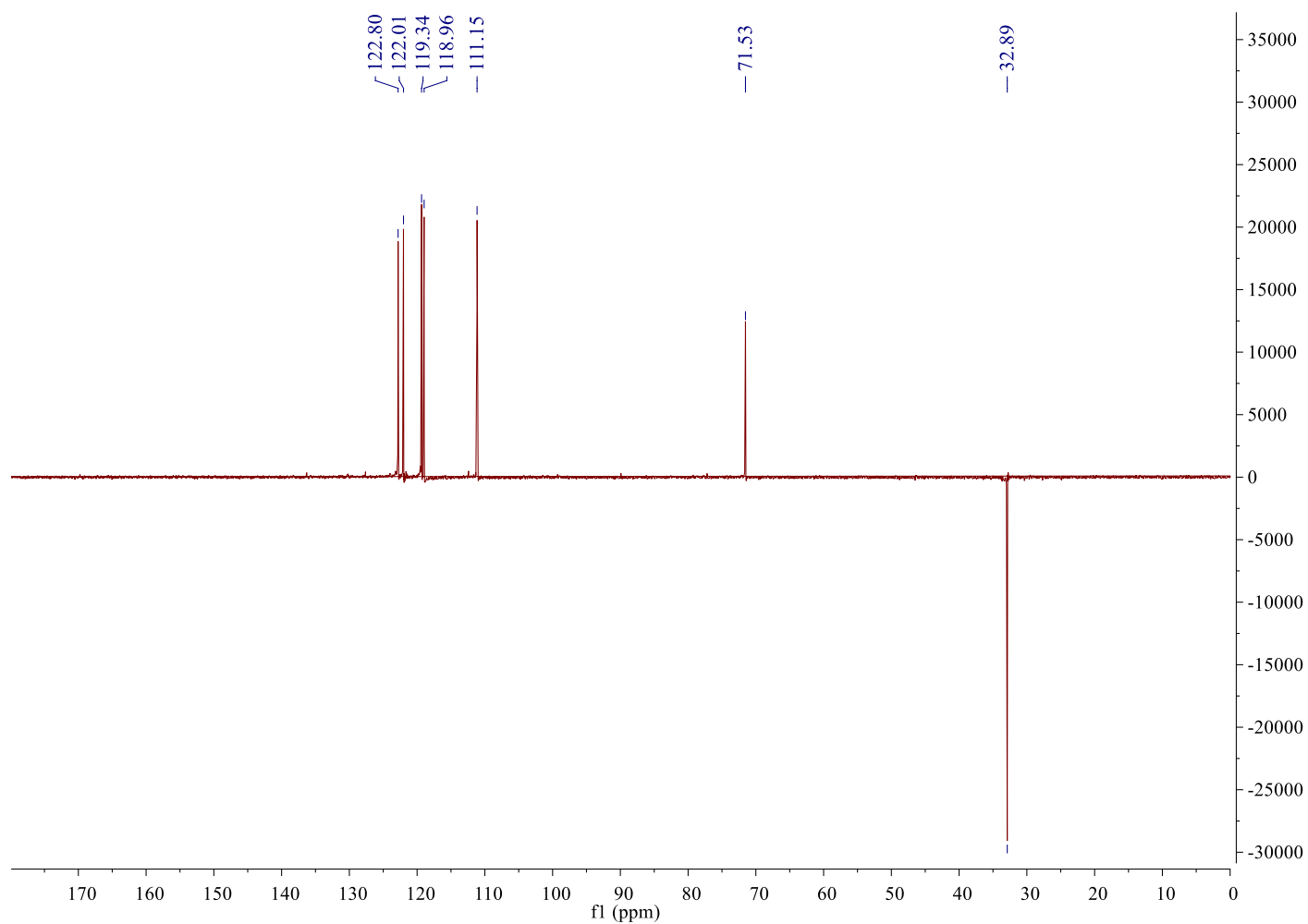


Figure S5. DEPT 135 spectrum of pseudoboindole A (**1**) in CDCl₃ (100 MHz).

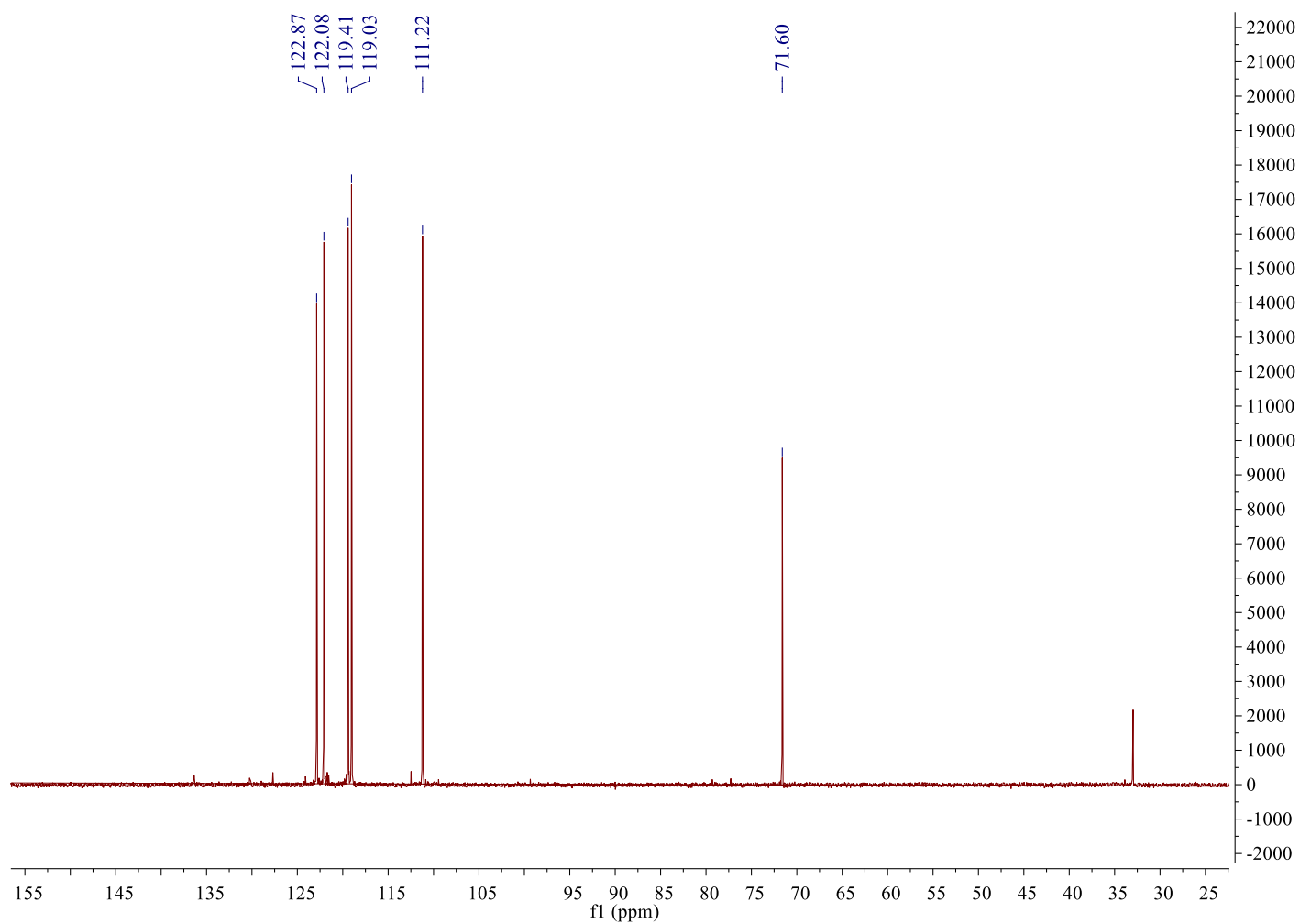


Figure S6. DEPT 90 spectrum of pseudoboinole A (**1**) in CDCl₃ (100 MHz).

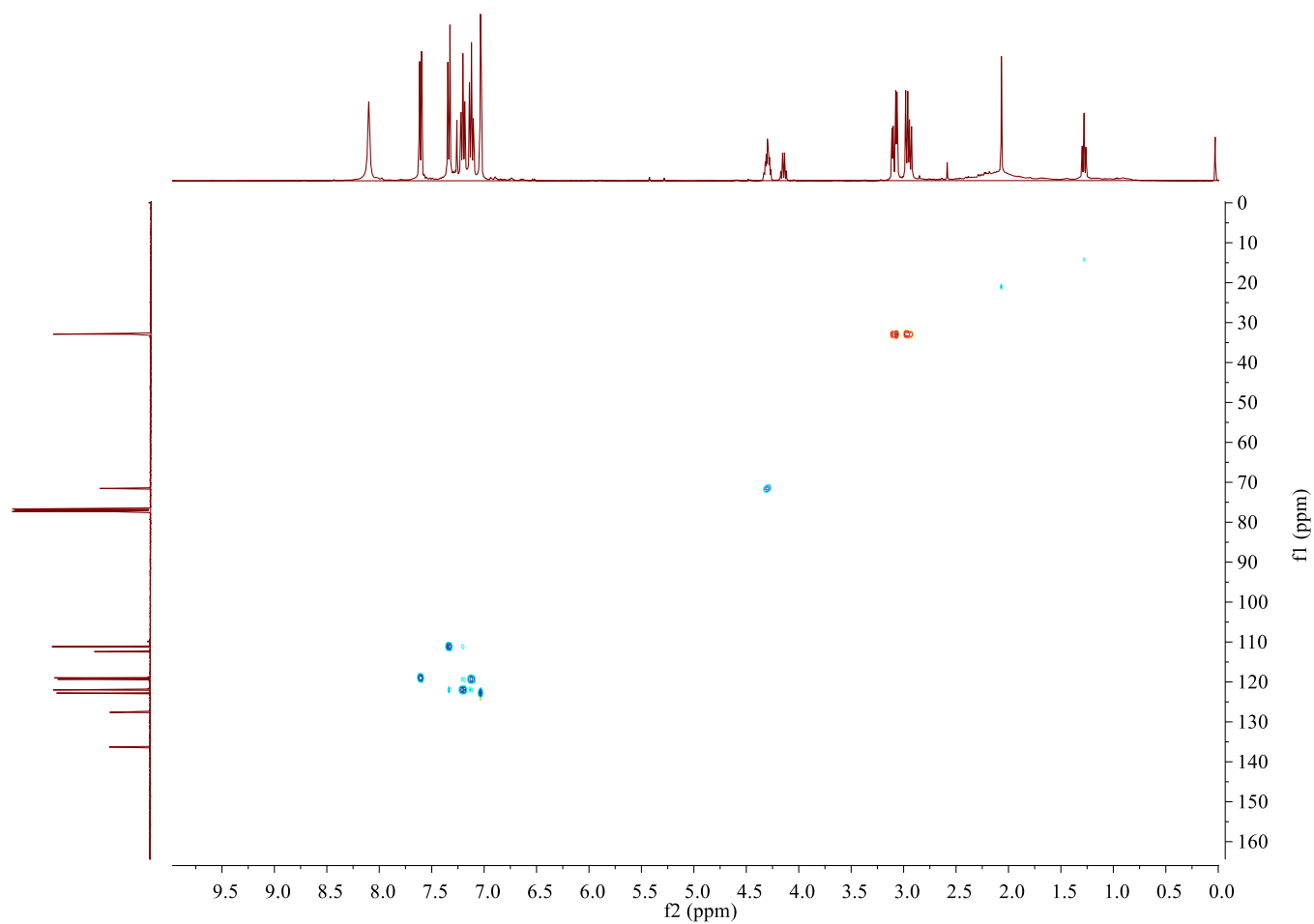


Figure S7. HMQC spectrum of pseudobindole A (**1**) in CDCl_3 .

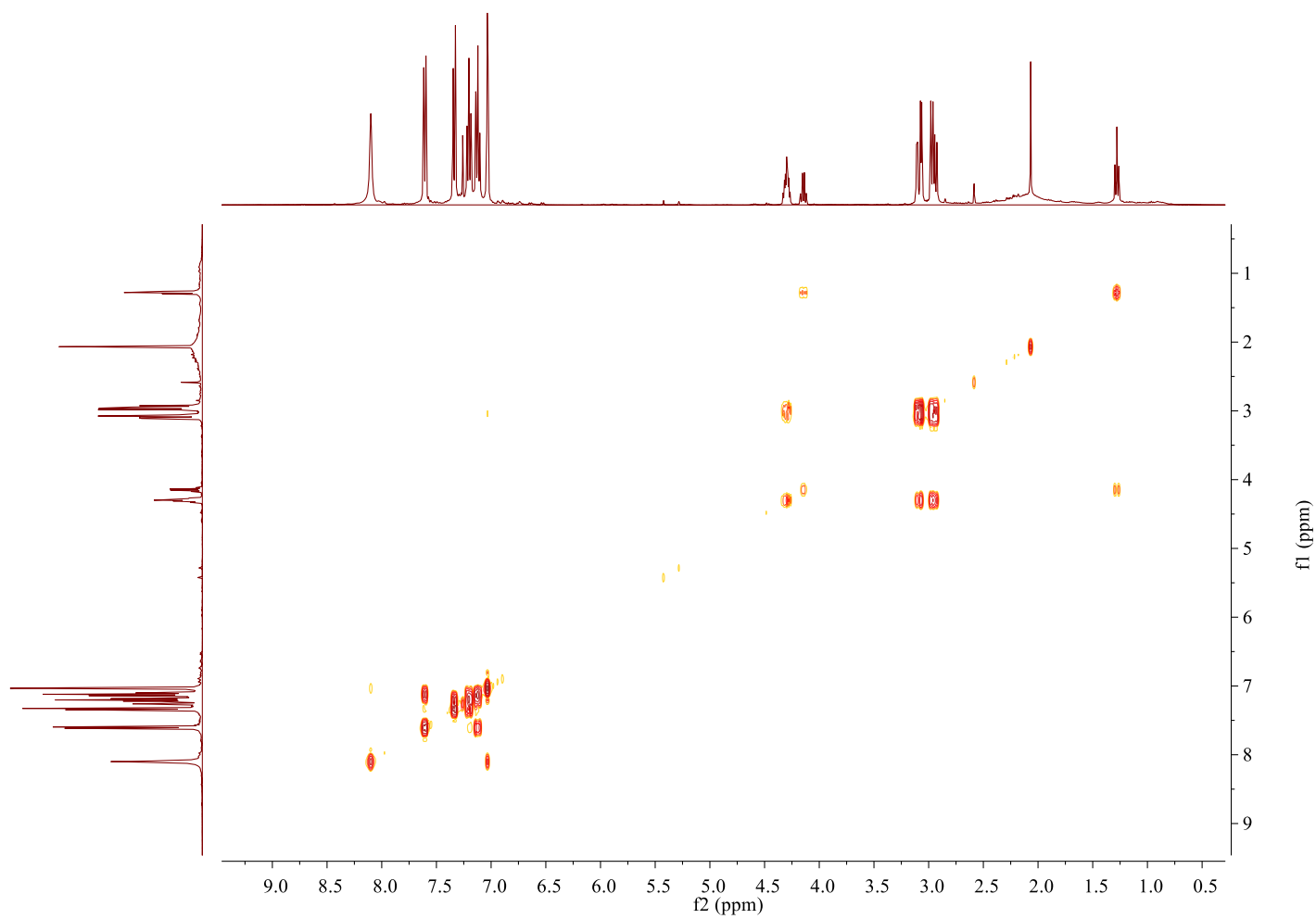


Figure S8. ^1H - ^1H COSY spectrum of pseudobindole A (**1**) in CDCl_3 .

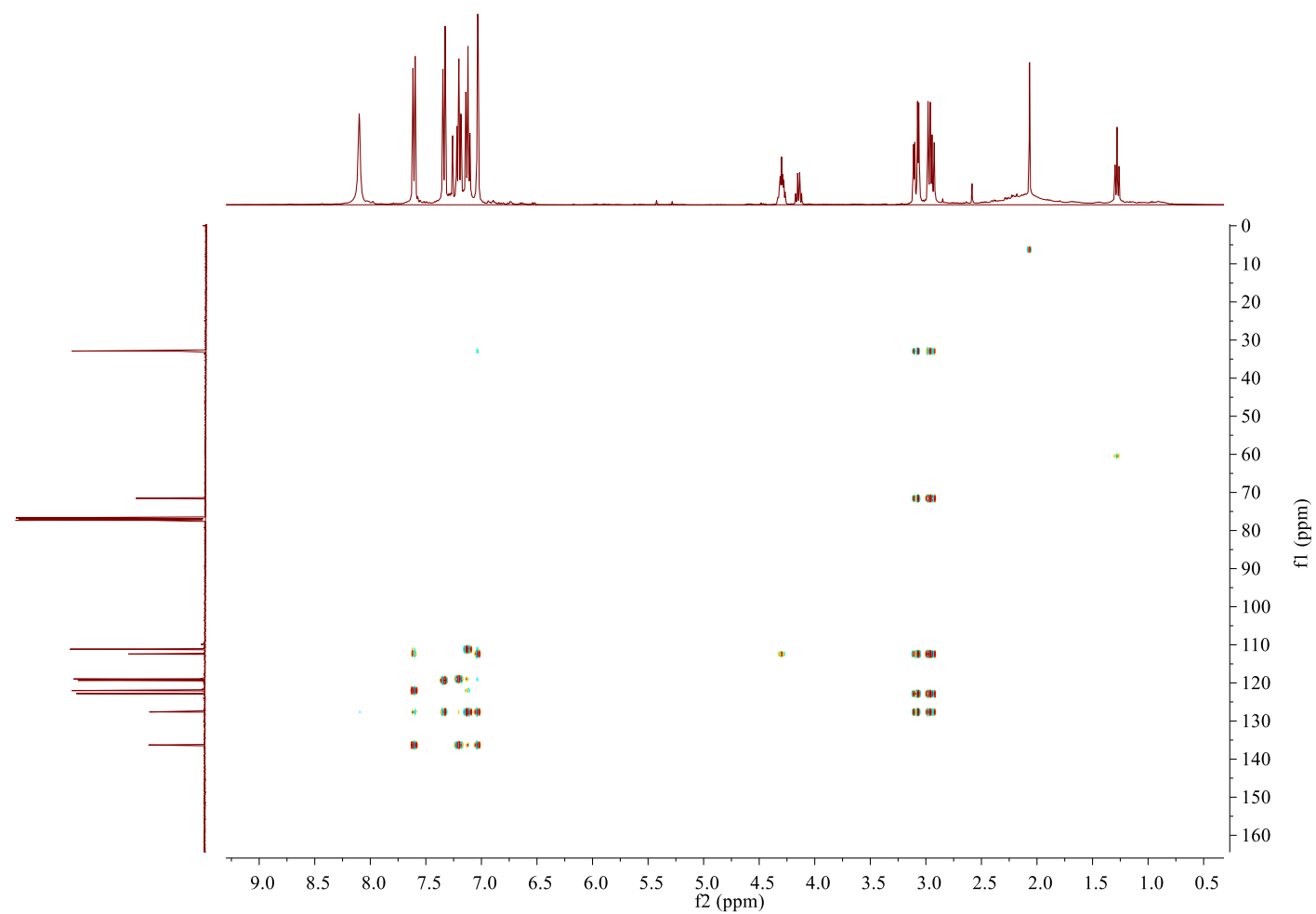


Figure S9. HMBC spectrum of pseudobindole A (**1**) in CDCl₃.

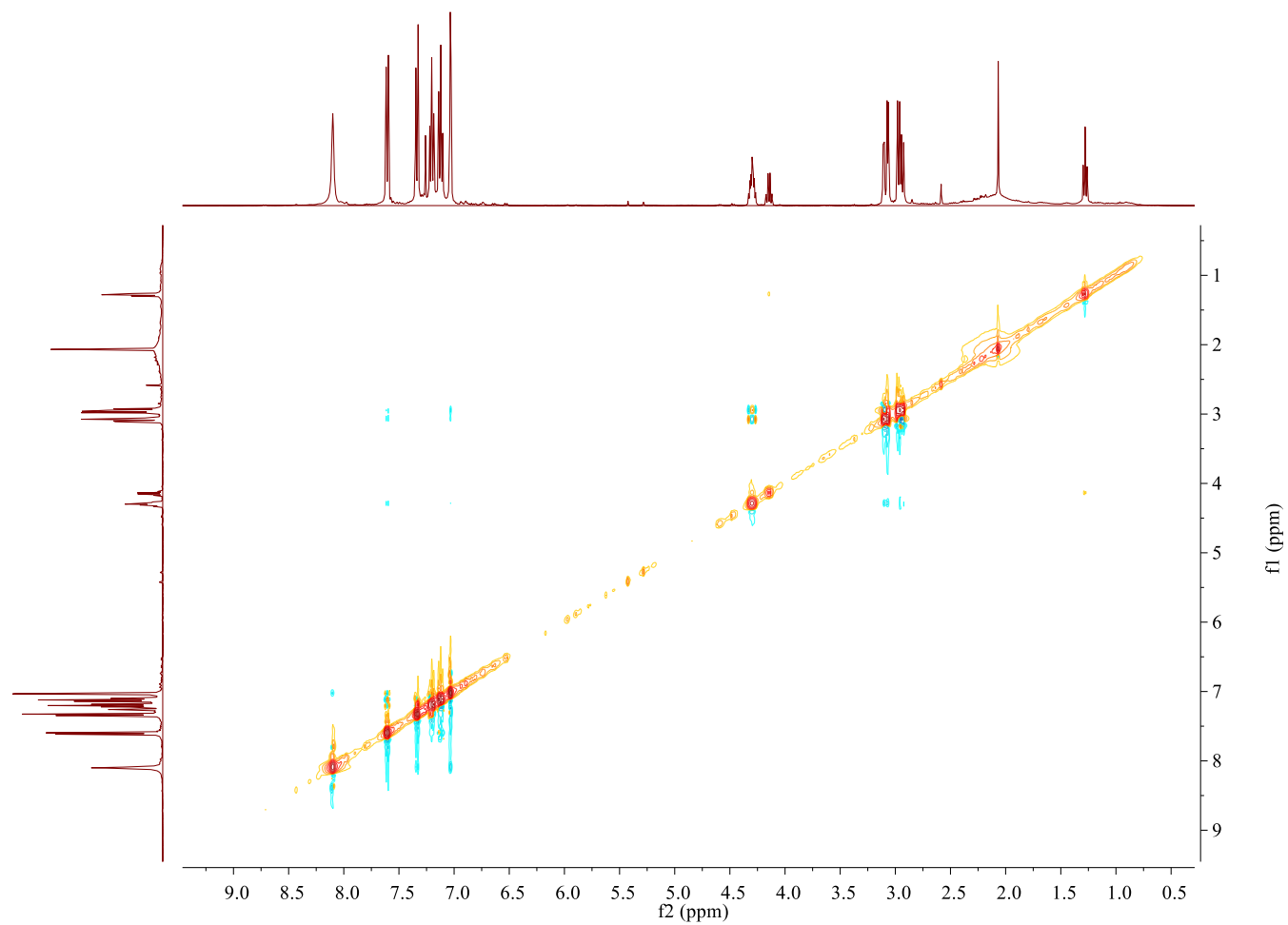
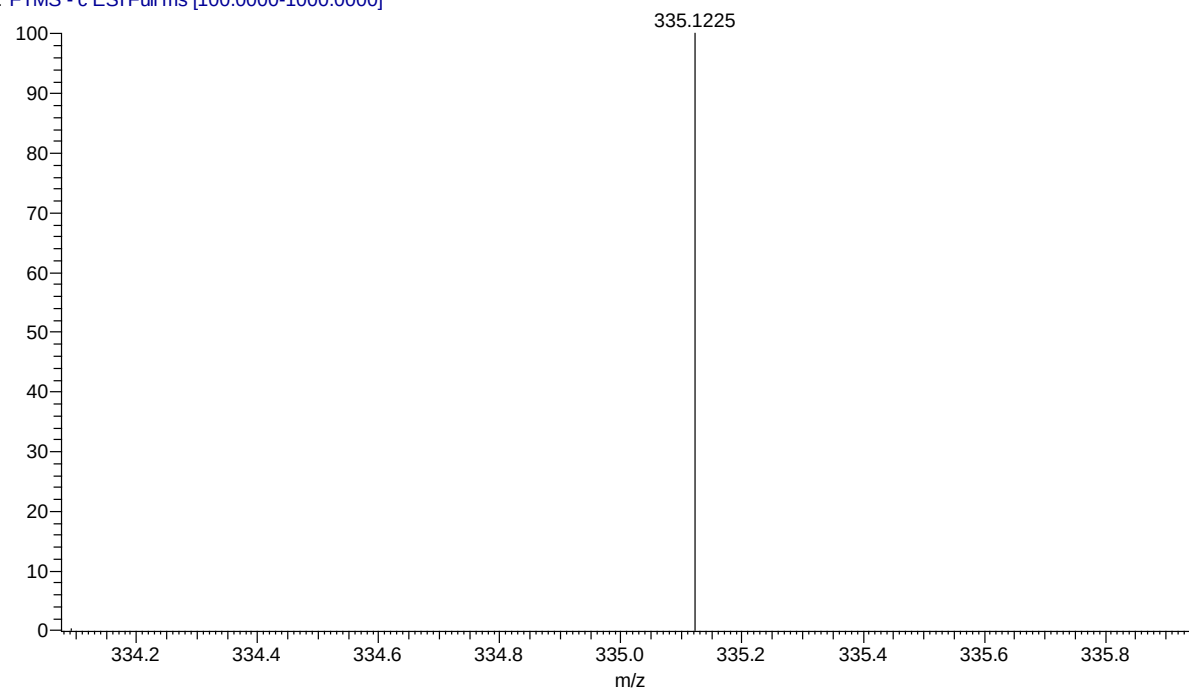


Figure S10. NOESY spectrum of pseudobindole A (**1**) in CDCl₃.

SO-17010A0134-3 171011180839 #6 RT: 0.05 AV: 1 NL: 4.69E6
T: FTMS - c ESI Full ms [100.0000-1000.0000]



SPECTRUM - simulation:

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
335.1225	335.1224	0.52	12.5	C20 H19 O N2 S

Figure S11. HR-(-)ESI-MS spectrum of pseudboindole B (2).

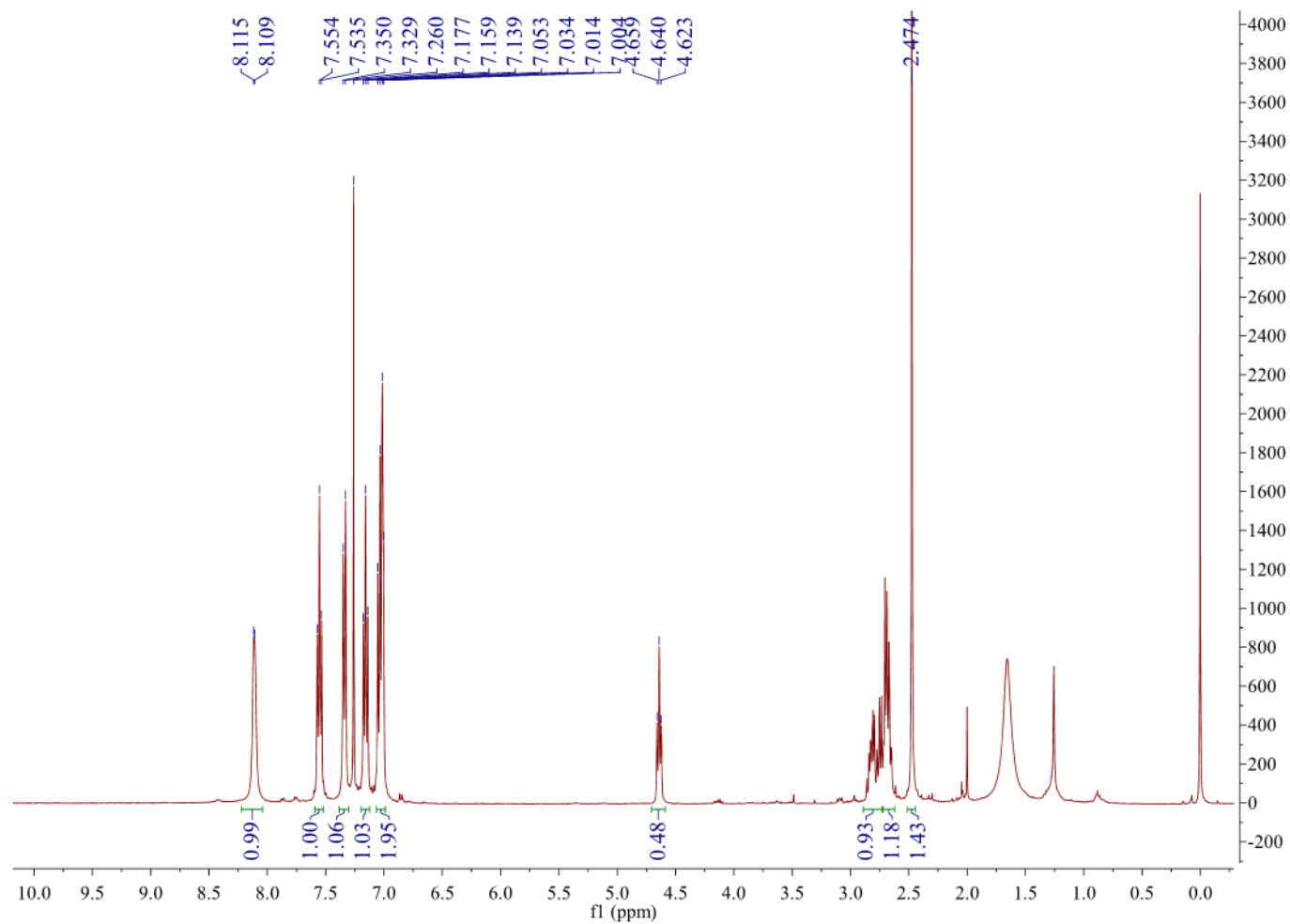


Figure S12. ^1H NMR spectrum of pseudobindole B (**2**) in CDCl_3 (400 MHz).

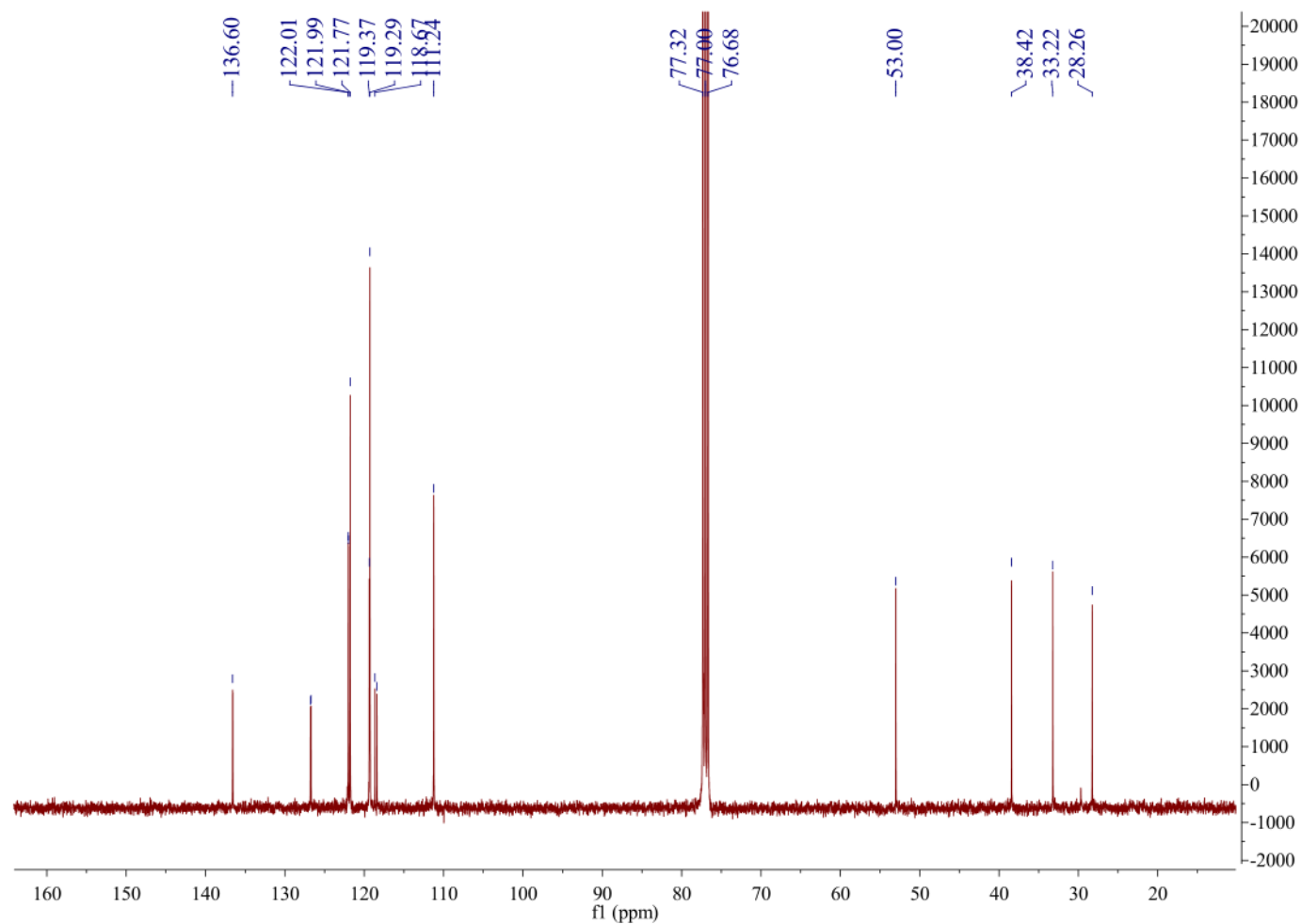


Figure S13. ^{13}C NMR spectrum of pseudobindole B (2) in CDCl_3 (100 MHz).

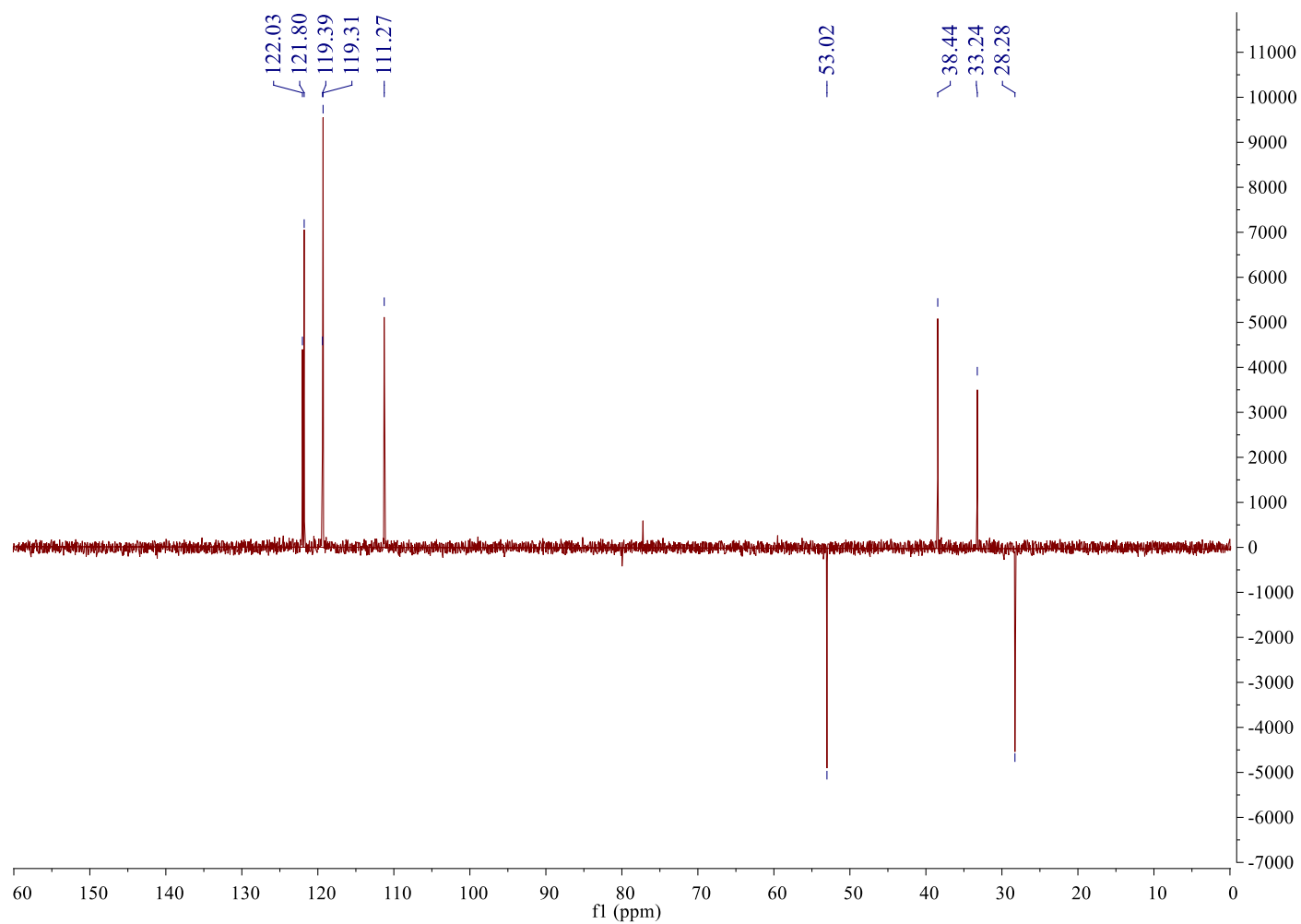


Figure S14. DEPT 135 spectrum of pseudobindole B (2) in CDCl₃ (100 MHz).

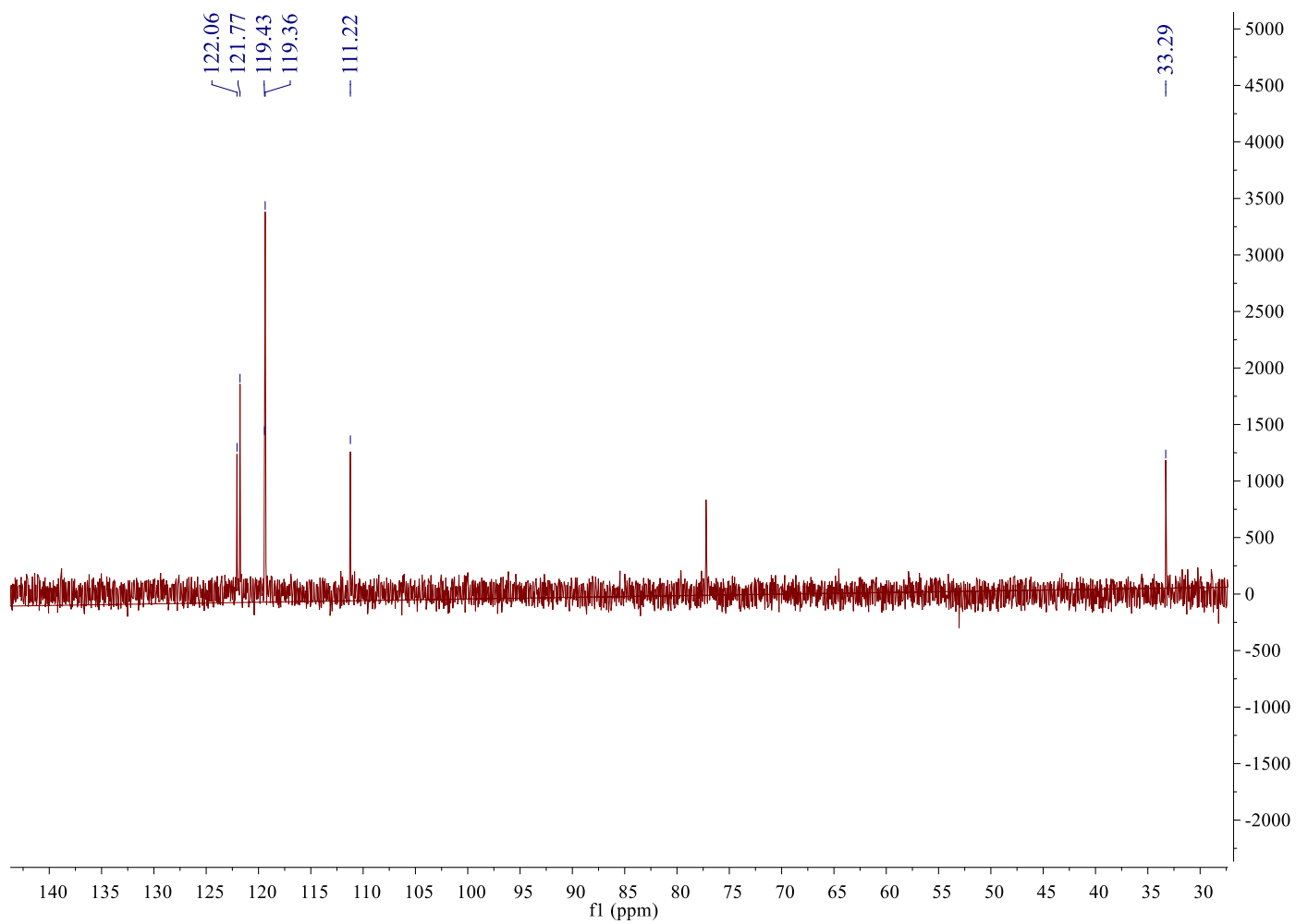


Figure S15. DEPT 90 spectrum of pseudobindole B (**2**) in CDCl₃ (100 MHz).

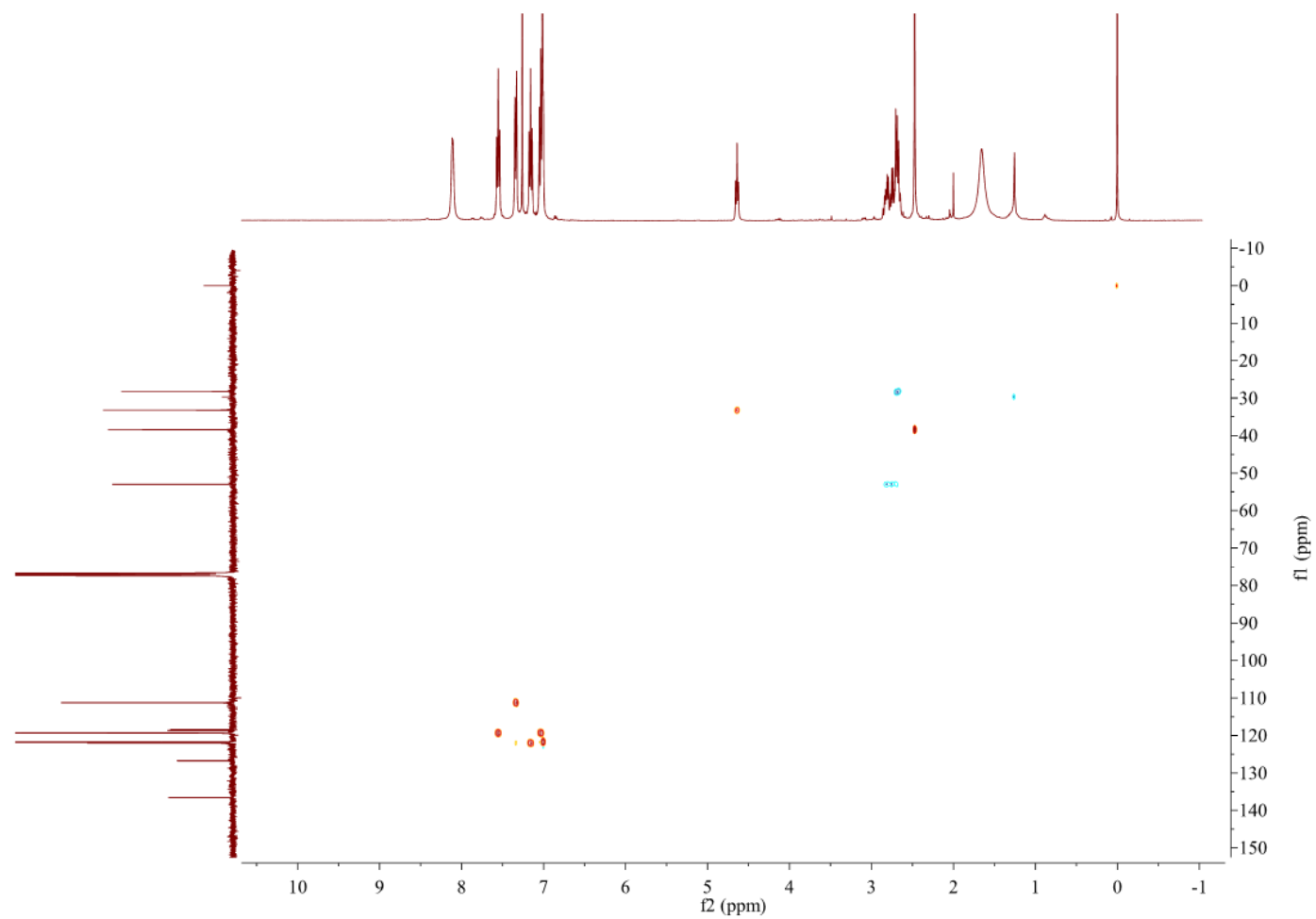


Figure S16. HMQC spectrum of pseudobindole B (**2**) in CDCl_3 .

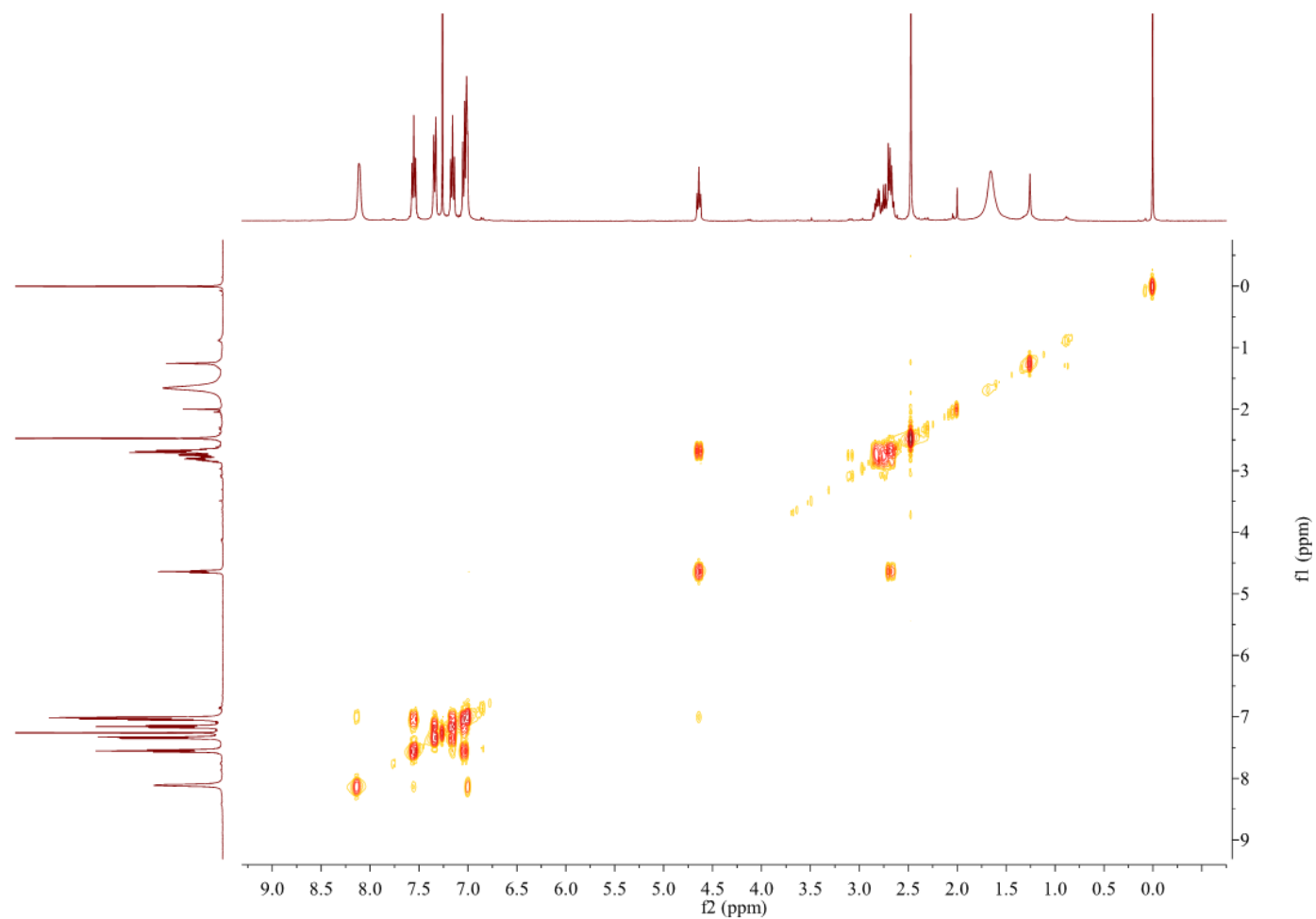


Figure S17. ^1H - ^1H COSY spectrum of pseudobindole B (**2**) in CDCl_3 .

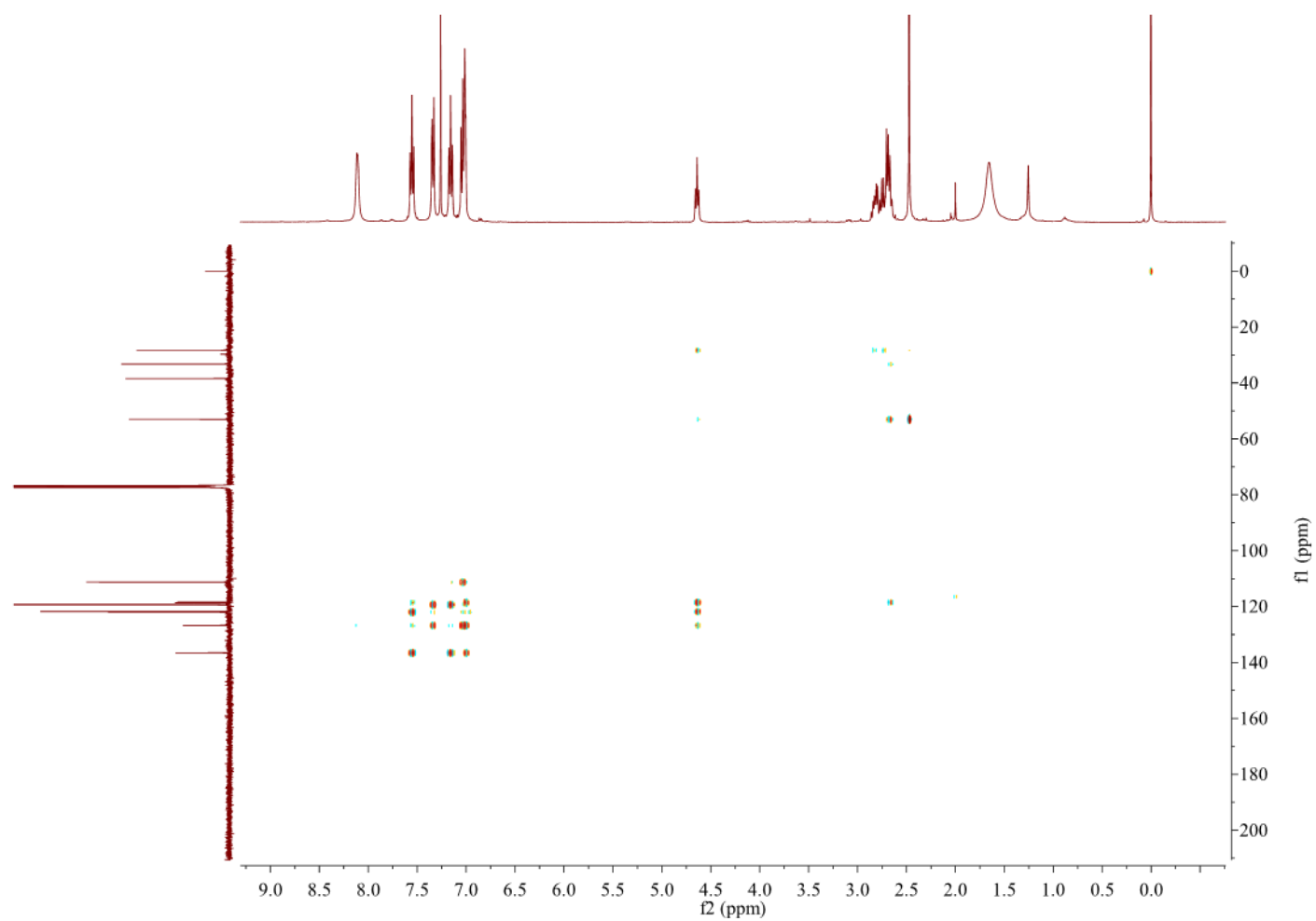


Figure S18. HMBC spectrum of pseudobindole B (**2**) in CDCl₃.

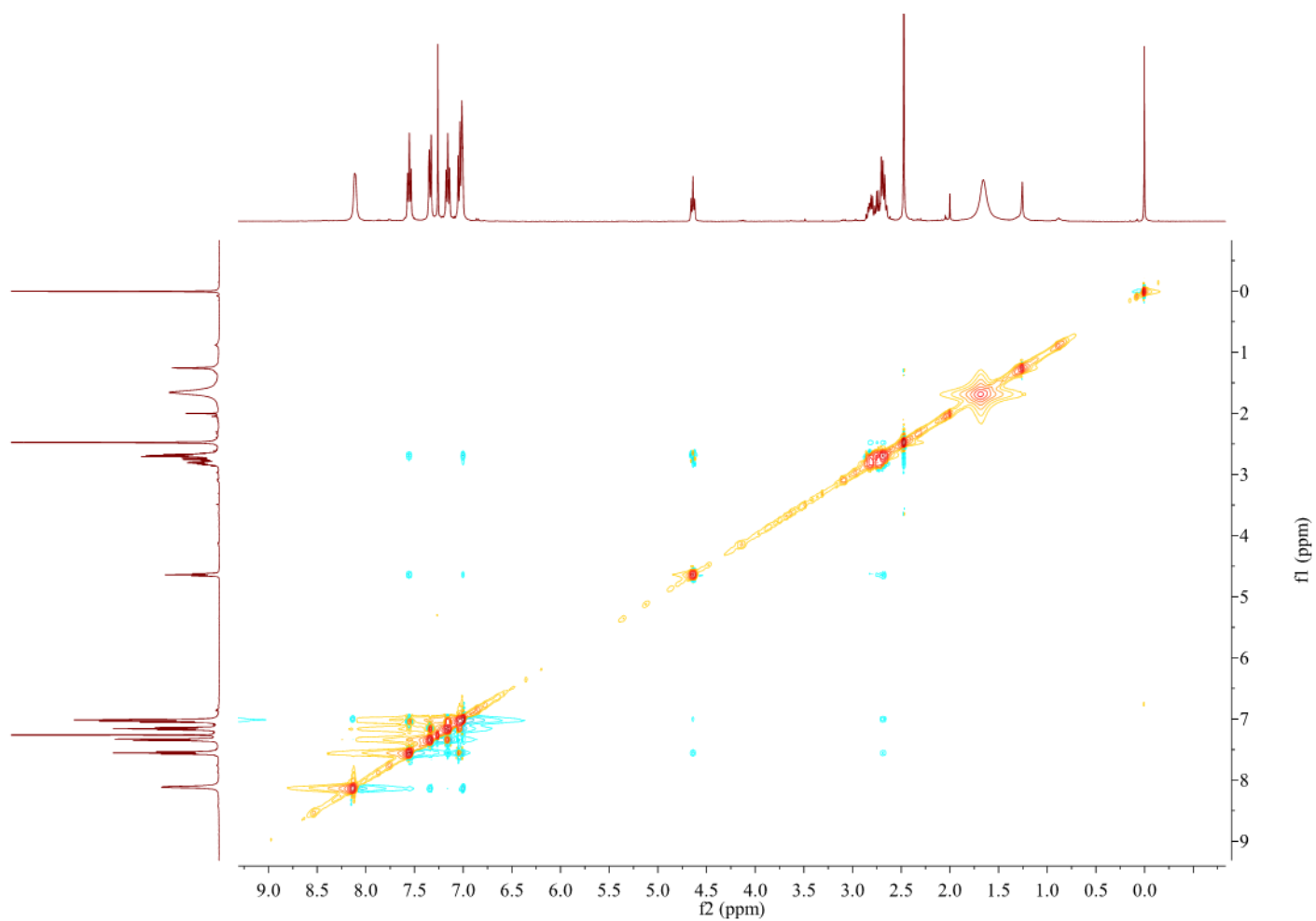
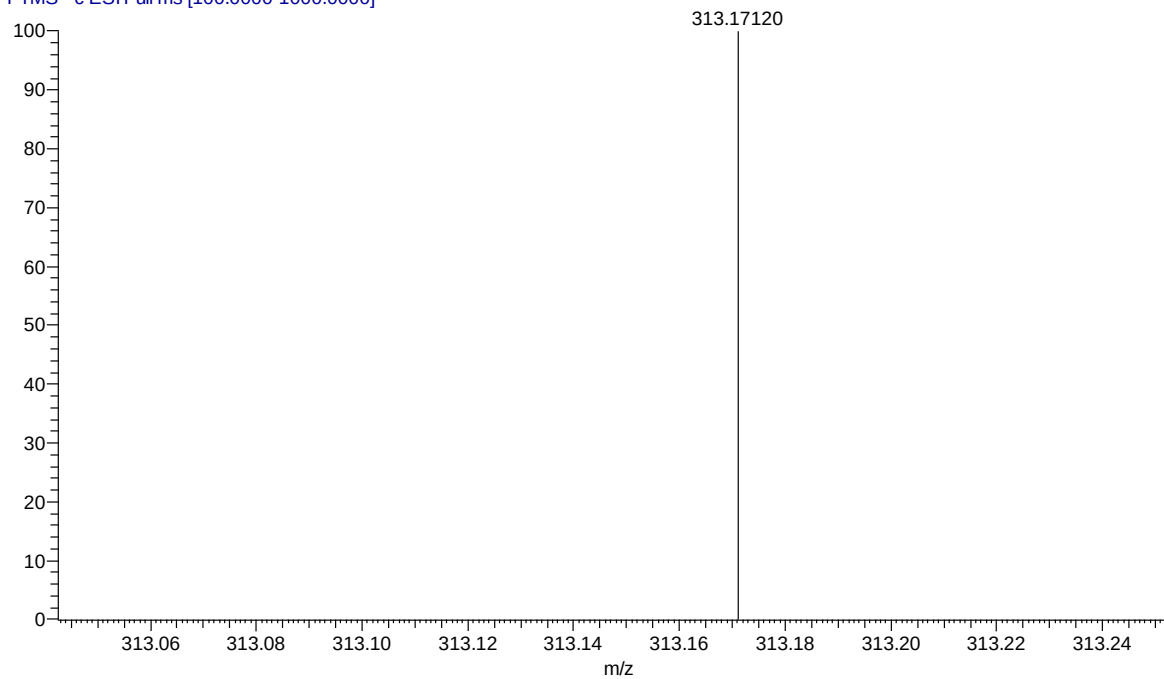


Figure S19. NOESY spectrum of pseudoboindole B (2) in CDCl₃.

(-) 舍CI-1712a0322-1 #9 RT: 0.09 AV: 1 NL: 7.28E6
T: FTMS - c ESI Full ms [100.0000-1000.0000]



SPECTRUM - simulation:

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
313.17120	313.17102	0.57	13.5	C22 H21 N2

Figure S20. HR-(-)ESI-MS spectrum of 3,3'-cyclohexylidenebis(1*H*-indole) (**3**).

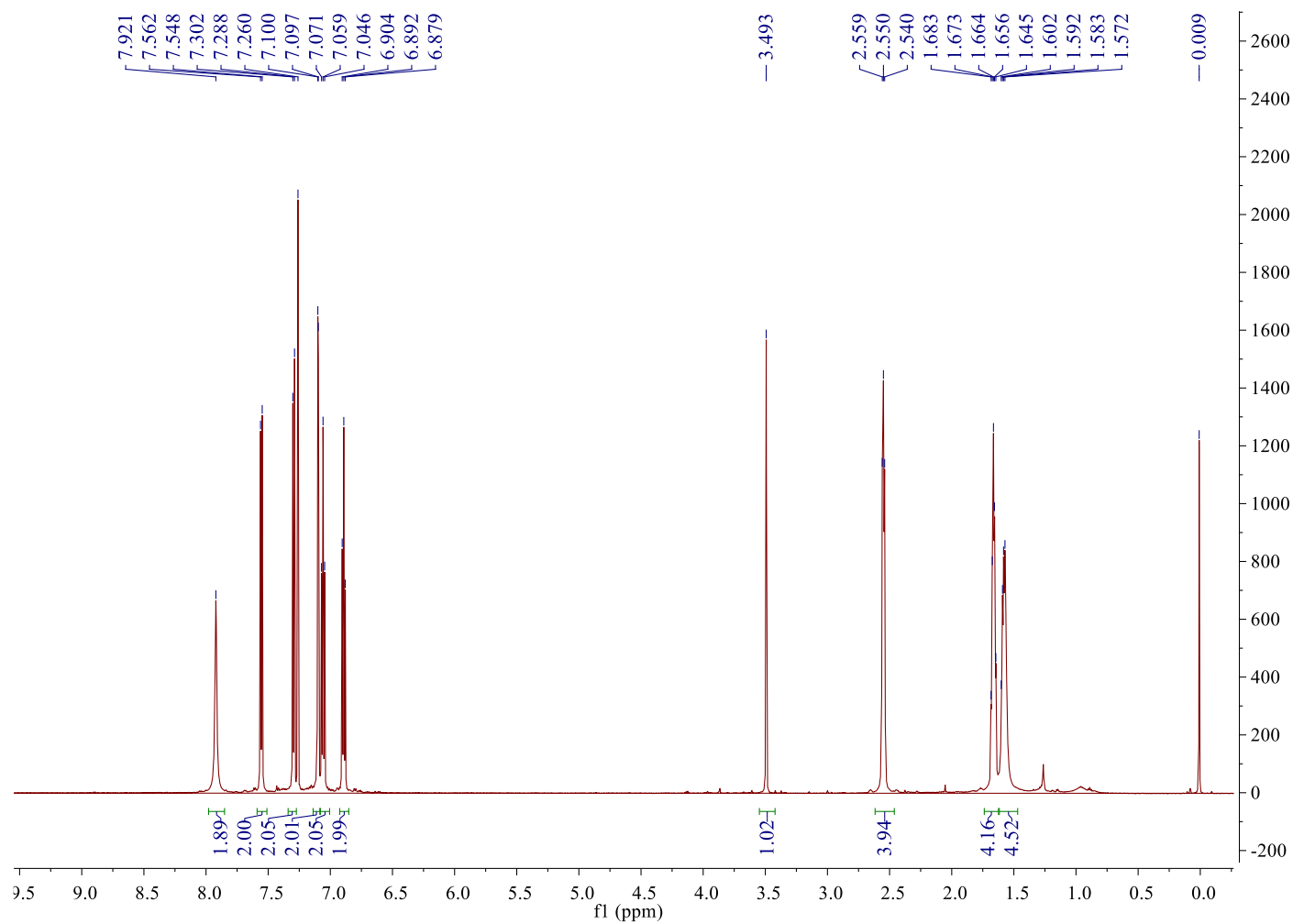


Figure S21. ¹H NMR spectrum of 3,3'-cyclohexylidenebis(1H-indole) (**3**) in CDCl₃ (600 MHz).

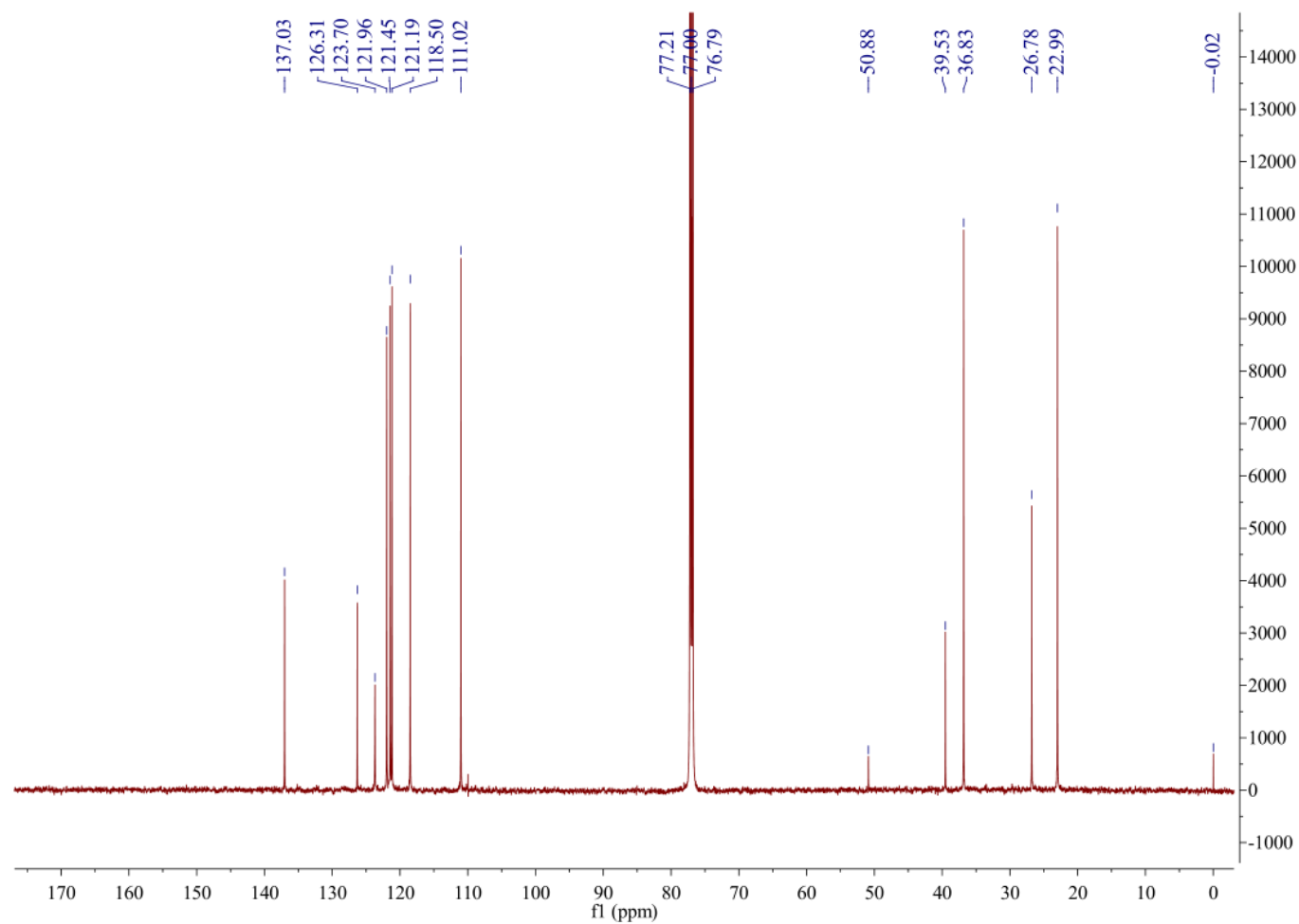


Figure S22. ^{13}C NMR spectrum of 3,3'-cyclohexylidenebis(1H-indole) (3) in CDCl_3 (150 MHz).

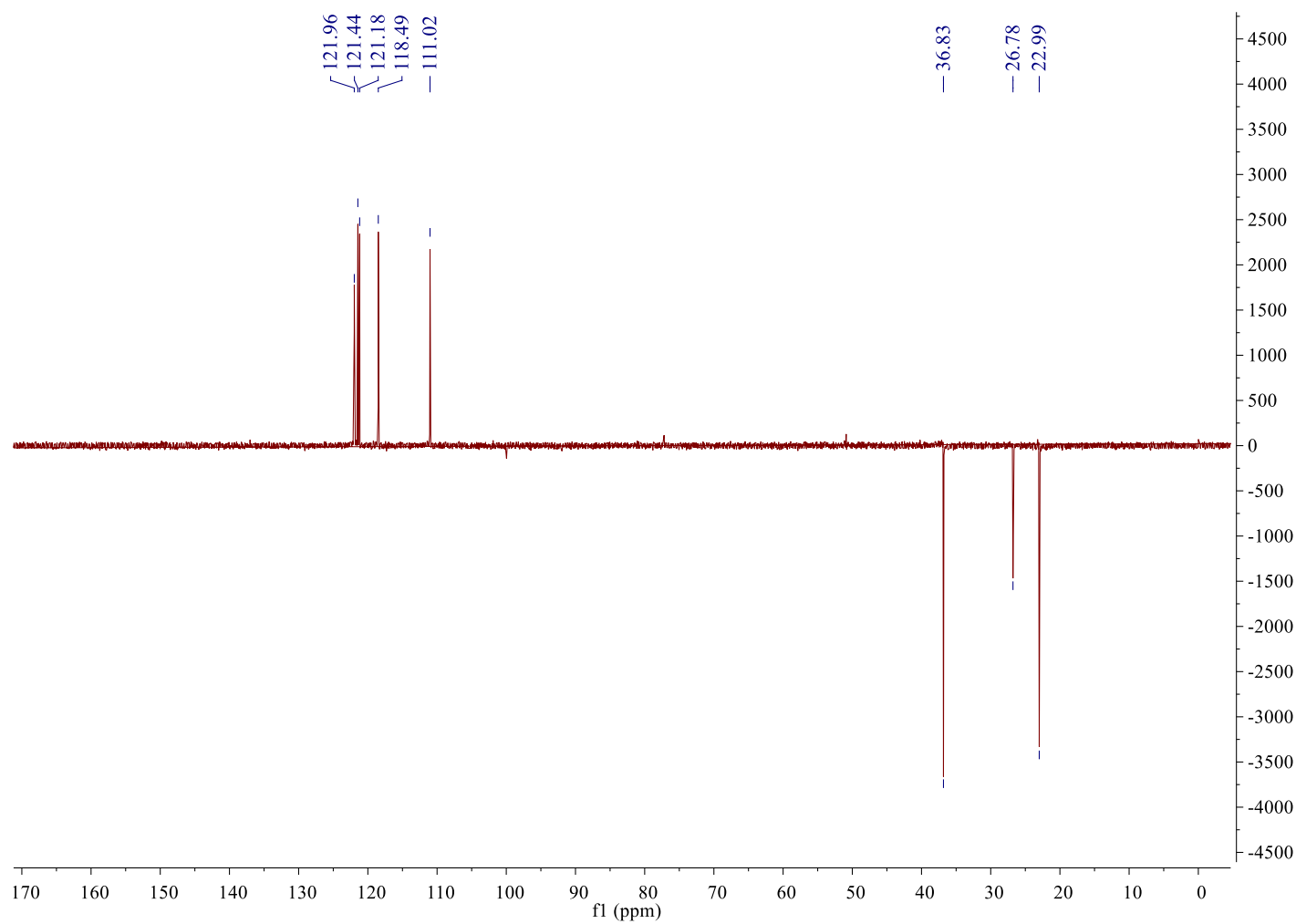


Figure S23. DEPT 135 spectrum of 3,3'-cyclohexylidenebis(1H-indole) (**3**) in CDCl₃ (150 MHz).

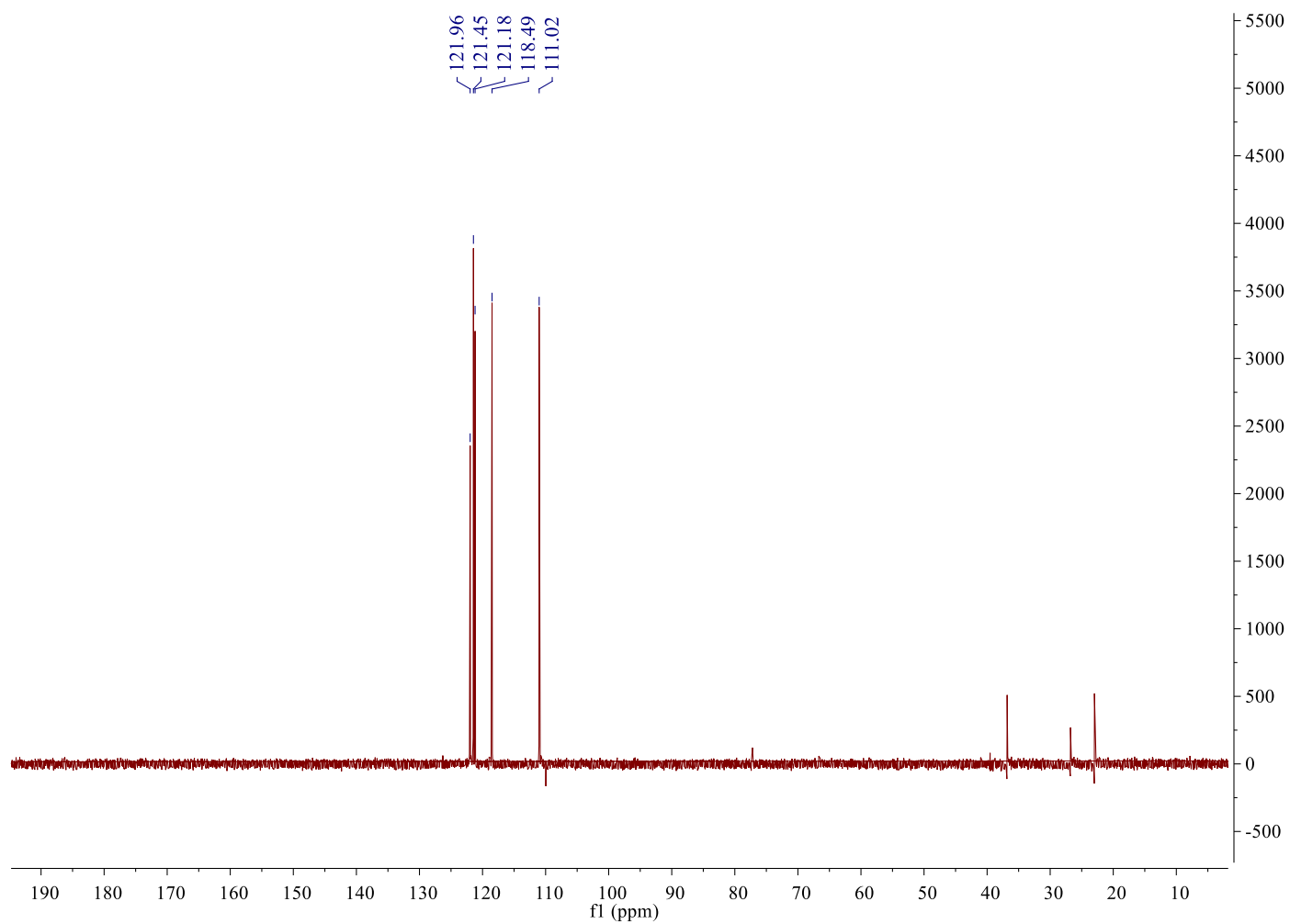


Figure S24. DEPT 90 spectrum of 3,3'-cyclohexylidenebis(1H-indole) (3) in CDCl₃ (150 MHz).

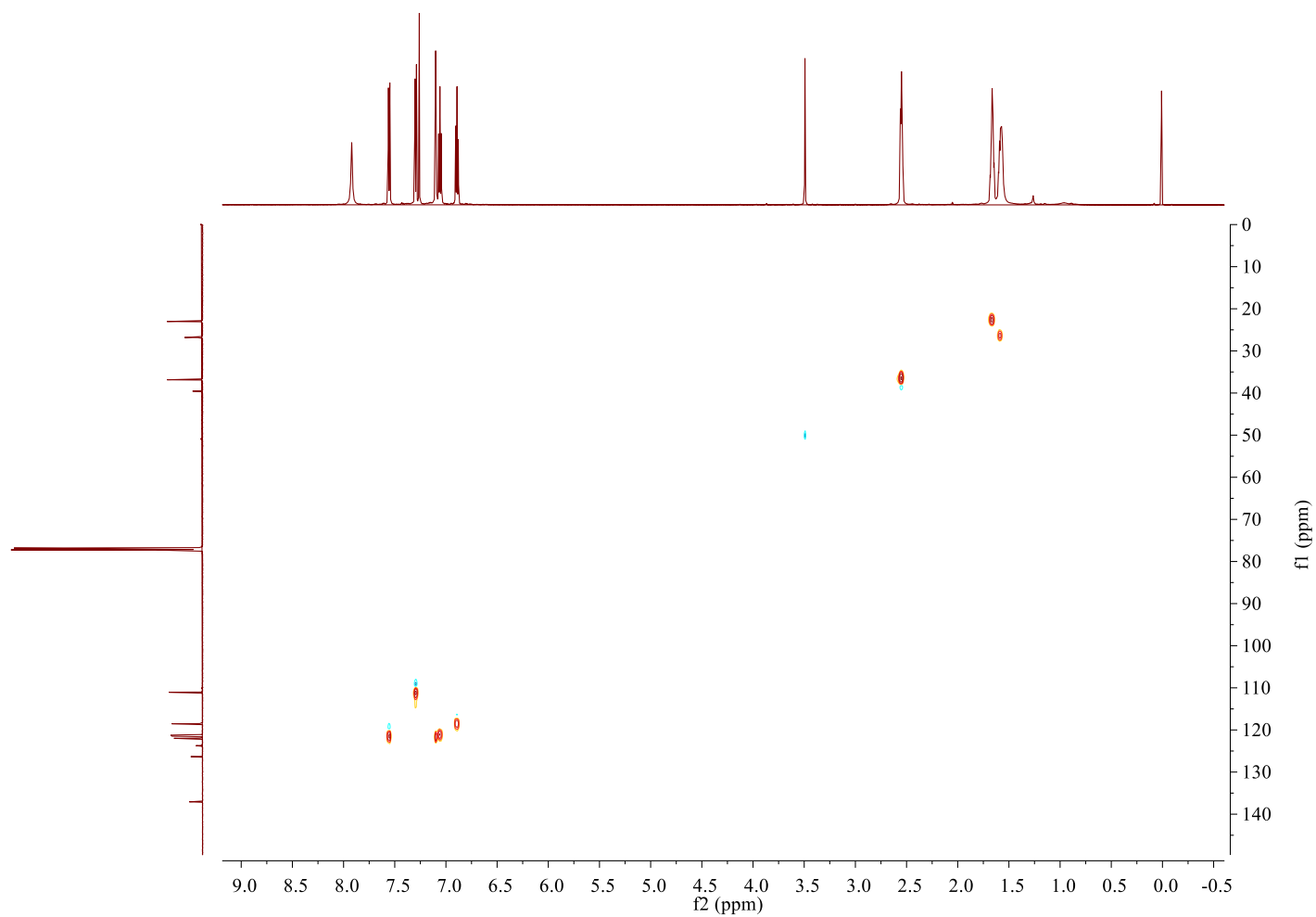


Figure S25. HMQC spectrum of 3,3'-cyclohexylidenebis(1H-indole) (**3**) in CDCl₃.

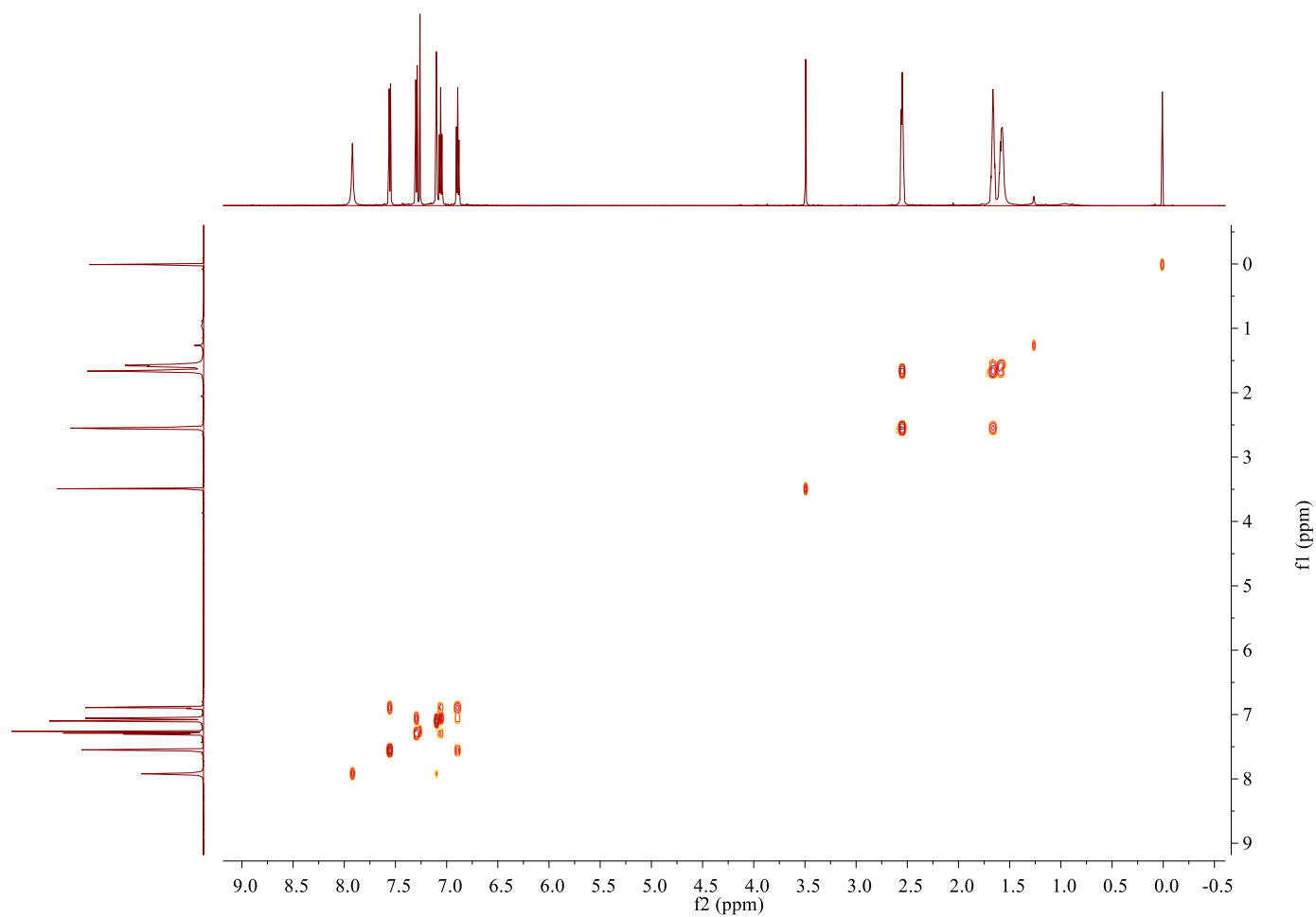


Figure S26. ^1H – ^1H COSY spectrum of 3,3'-cyclohexylidenebis(1*H*-indole) (**3**) in CDCl_3 .

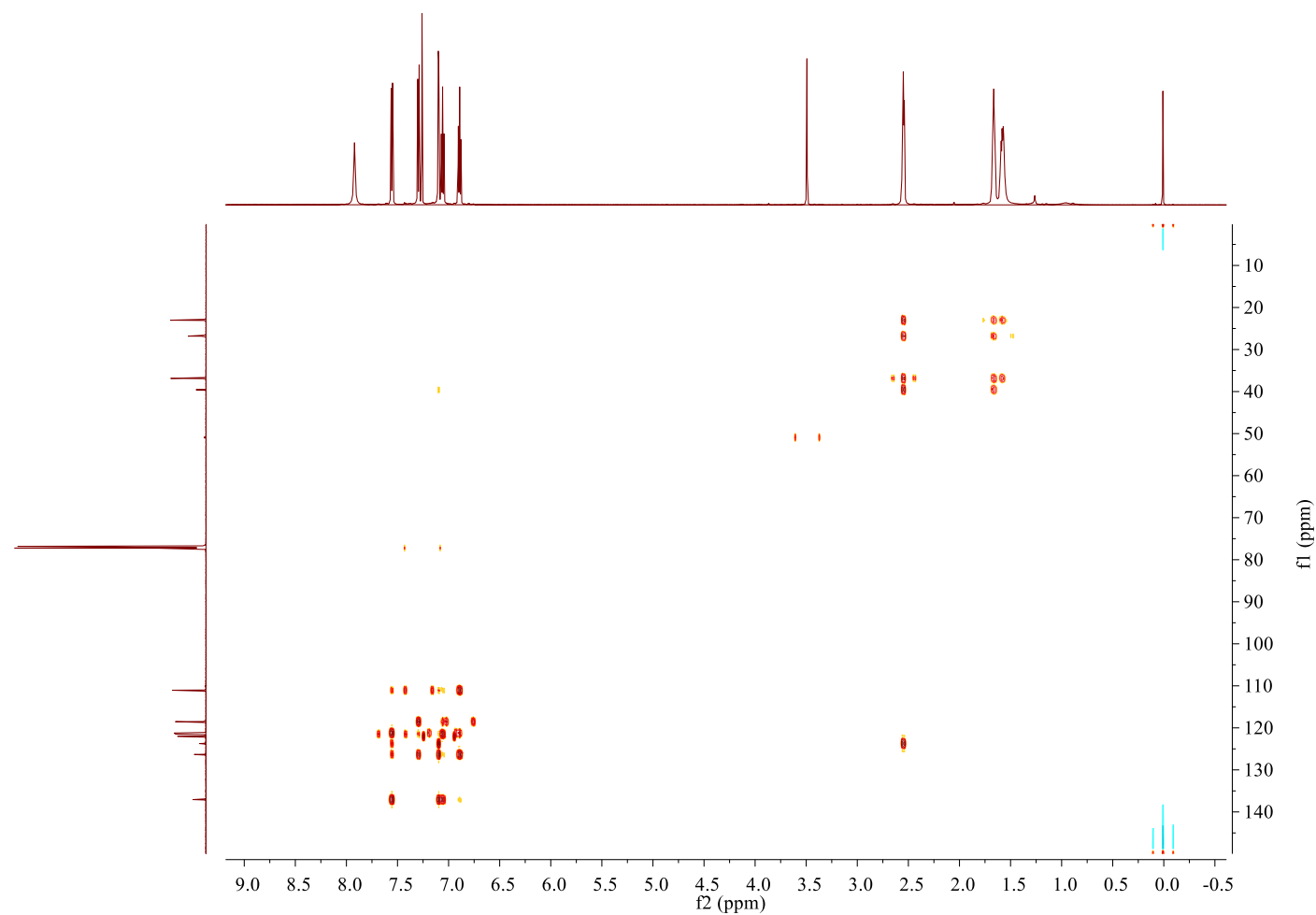


Figure S27. HMBC spectrum of 3,3'-cyclohexylidenebis(1*H*-indole) (**3**) in CDCl₃.

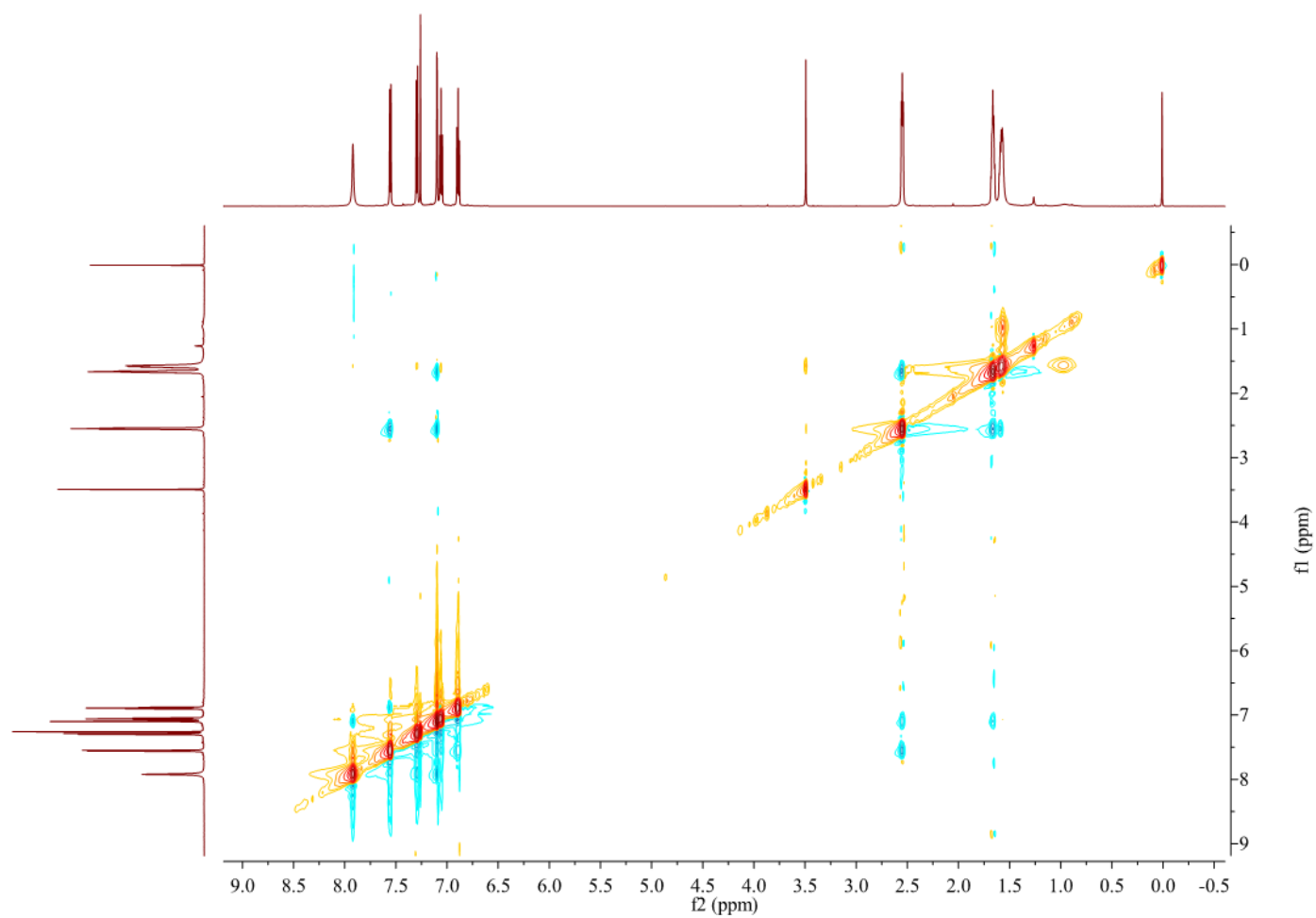


Figure S28. NOESY spectrum of 3,3'-cyclohexylidenebis(1*H*-indole) (**3**) in CDCl_3 .

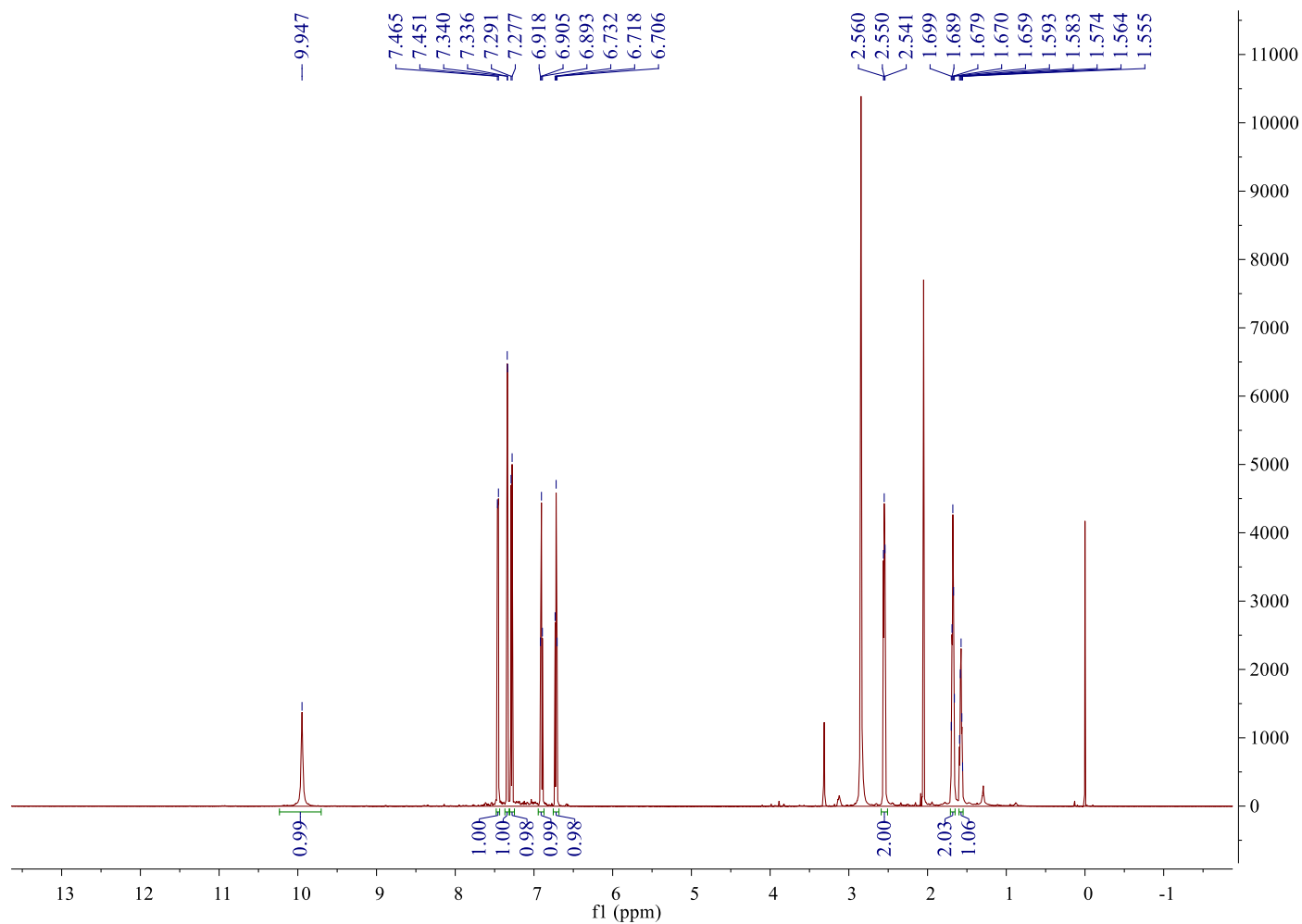


Figure S29. ^1H NMR spectrum of 3,3'-cyclohexylidenebis(1H-indole) (3) in acetone- d_6 (600 MHz).

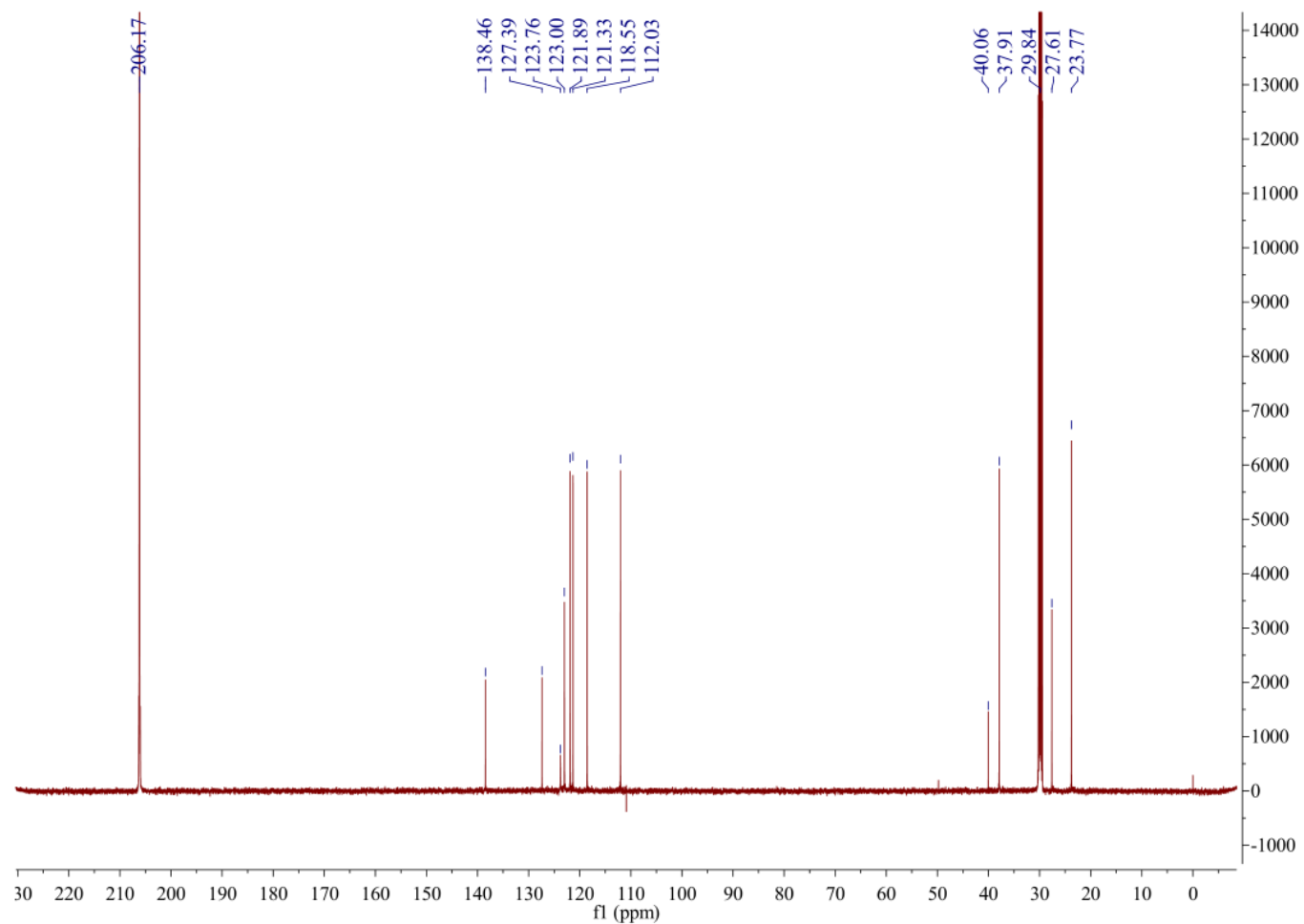


Figure S30. ^{13}C NMR spectrum of 3,3'-cyclohexylidenebis(1H-indole) (**3**) in acetone- d_6 (150 MHz).

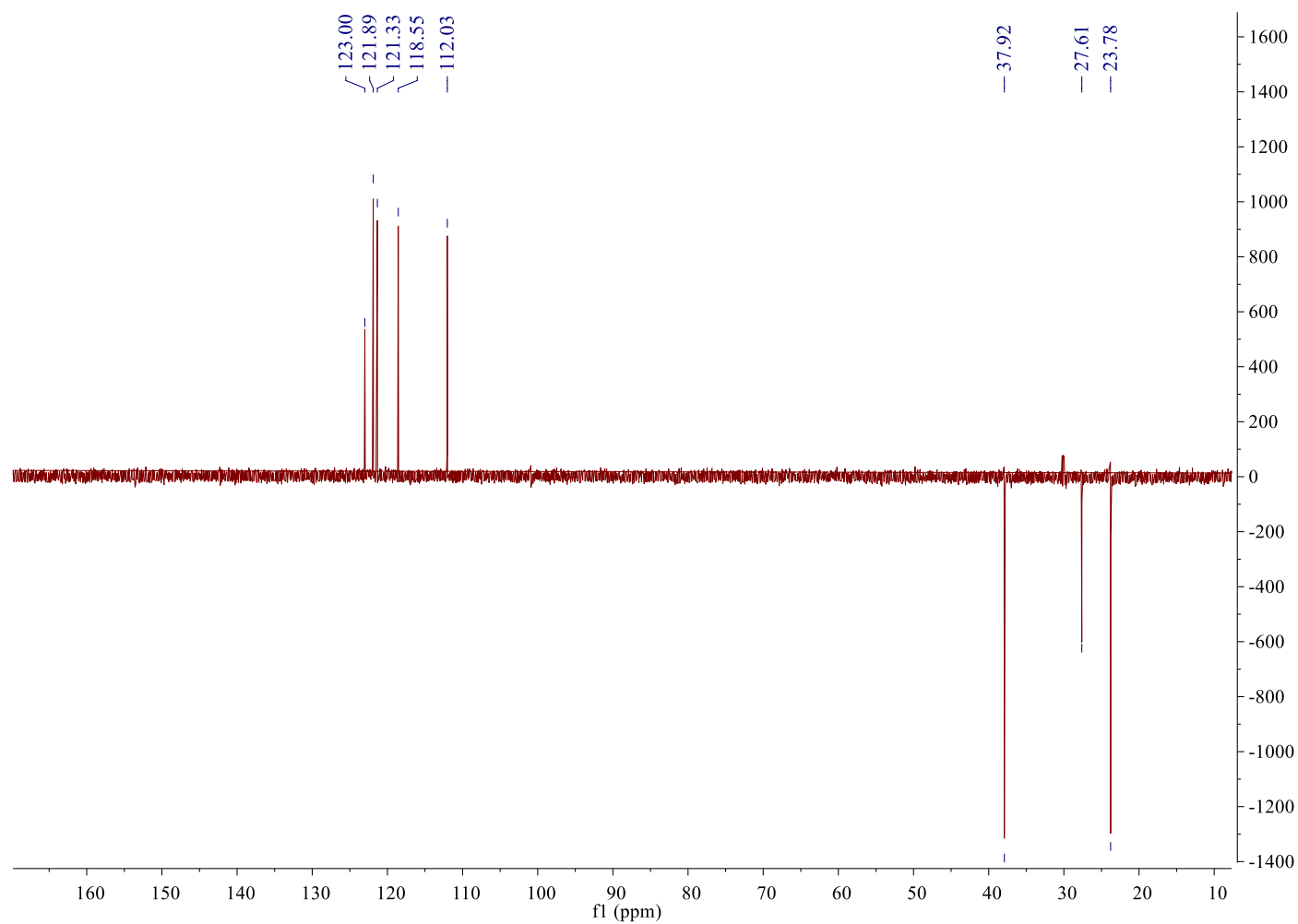


Figure S31. DEPT 135 spectrum of 3,3'-cyclohexylidenebis(1*H*-indole) (**3**) in acetone-*d*₆ (150 MHz).

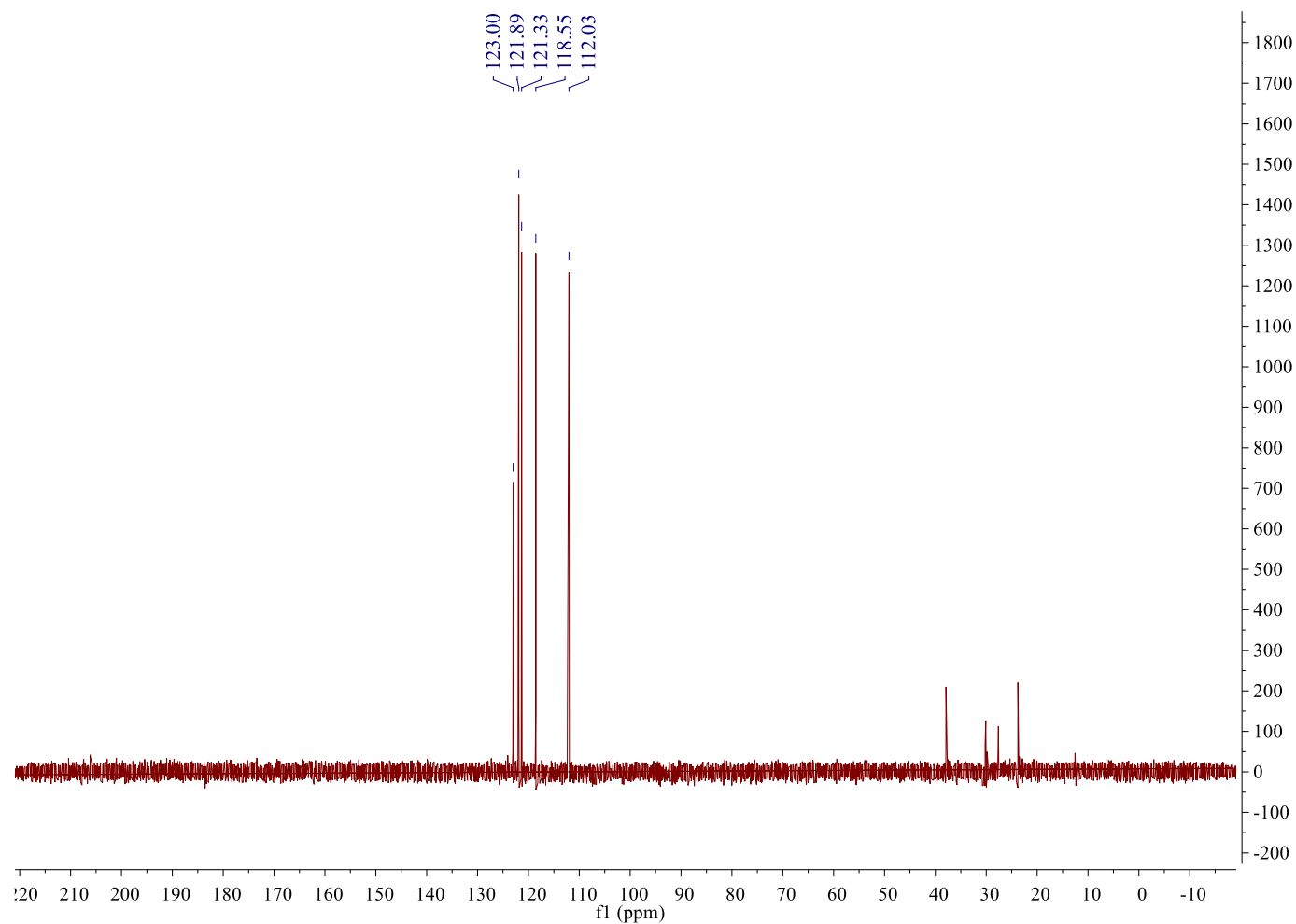


Figure S32. DEPT 90 spectrum of 3,3'-cyclohexylidenebis(1*H*-indole) (**3**) in acetone-*d*₆ (150 MHz).

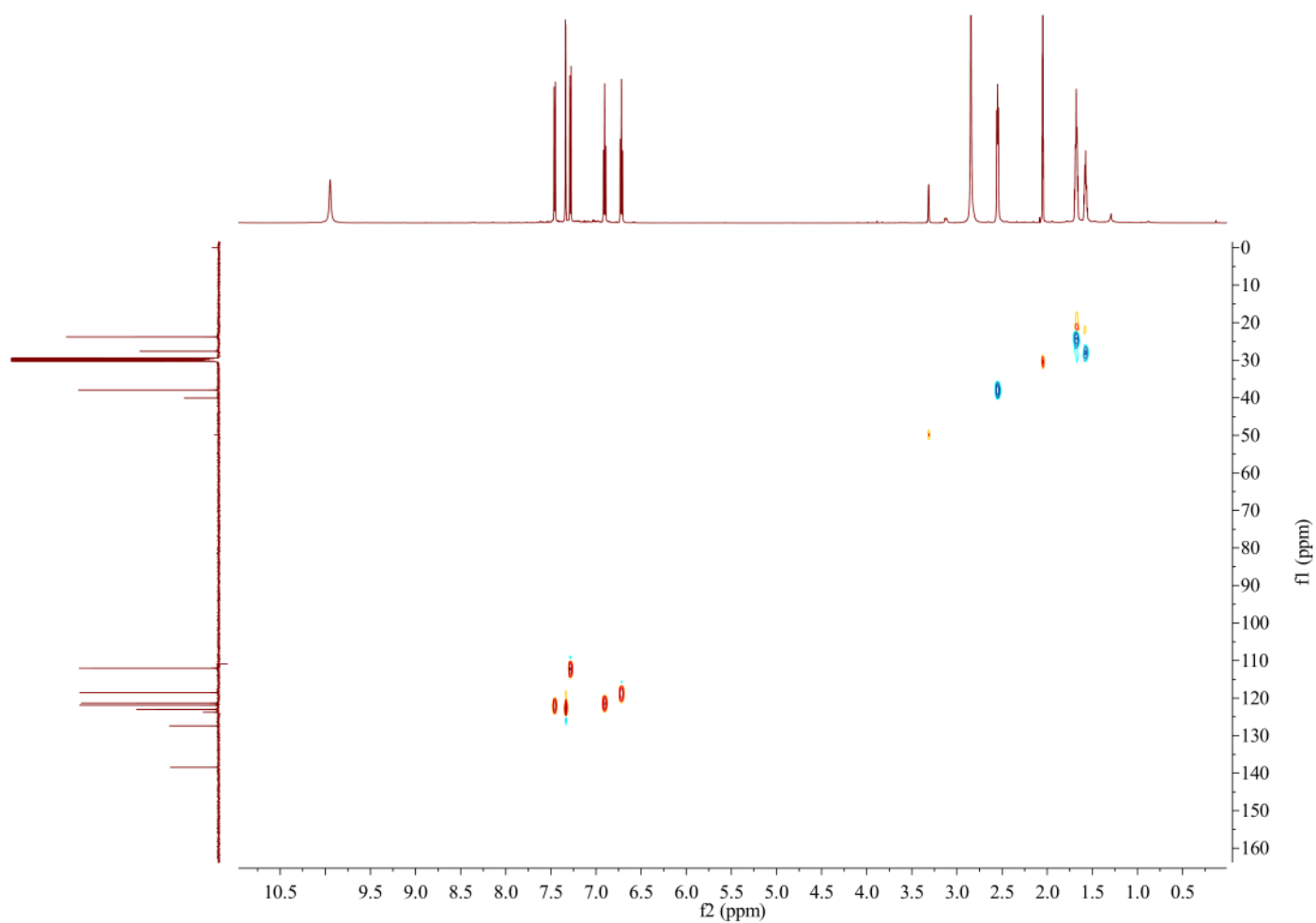
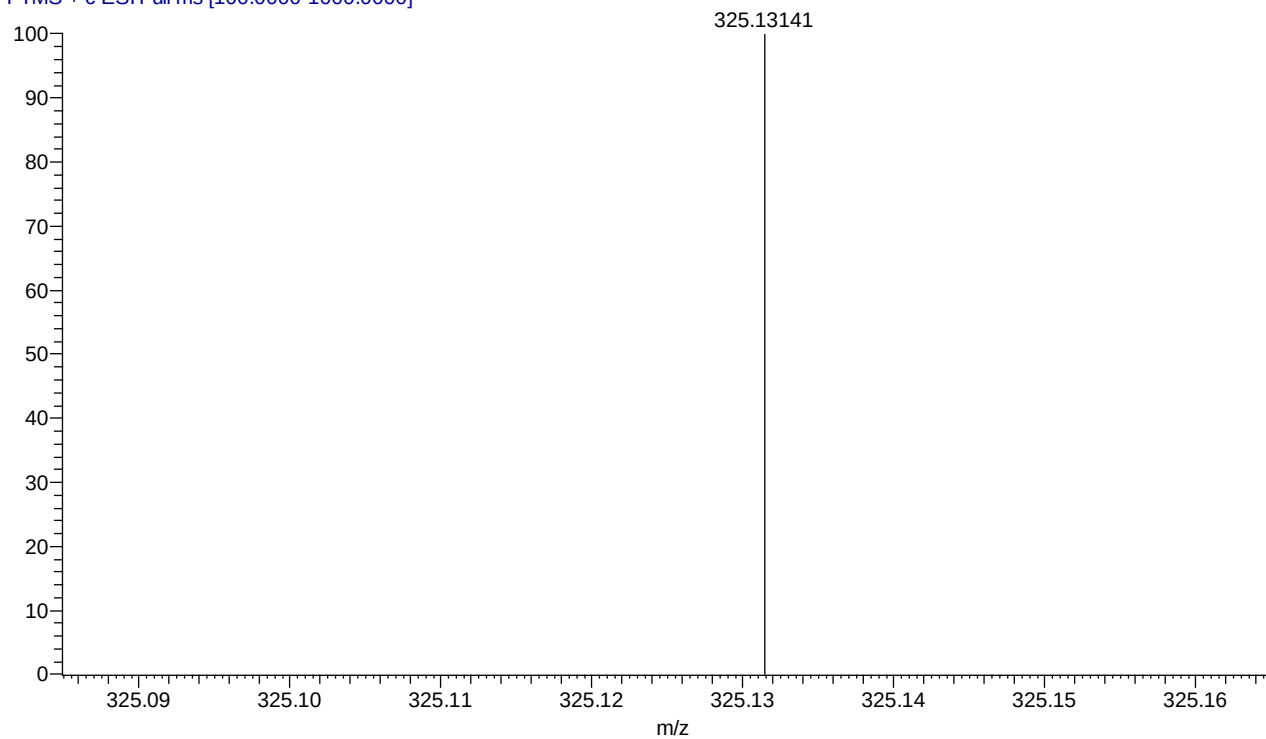


Figure S33. HMQC spectrum of 3,3'-cyclohexylidenebis(1*H*-indole) (**3**) in acetone- d_6 .

17010A0134-1_171011180146 #6-9 RT: 0.04-0.07 AV: 4 NL: 4.14E6
T: FTMS + c ESI Full ms [100.0000-1000.0000]



SPECTRUM - simulation:

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
325.1314	325.13113	0.85	12.5	C20 H18 O N2 Na

Figure S34. HR-(+)ESI-MS spectrum of 3,3-bis(3-indolyl) butan-2-one (**4**).

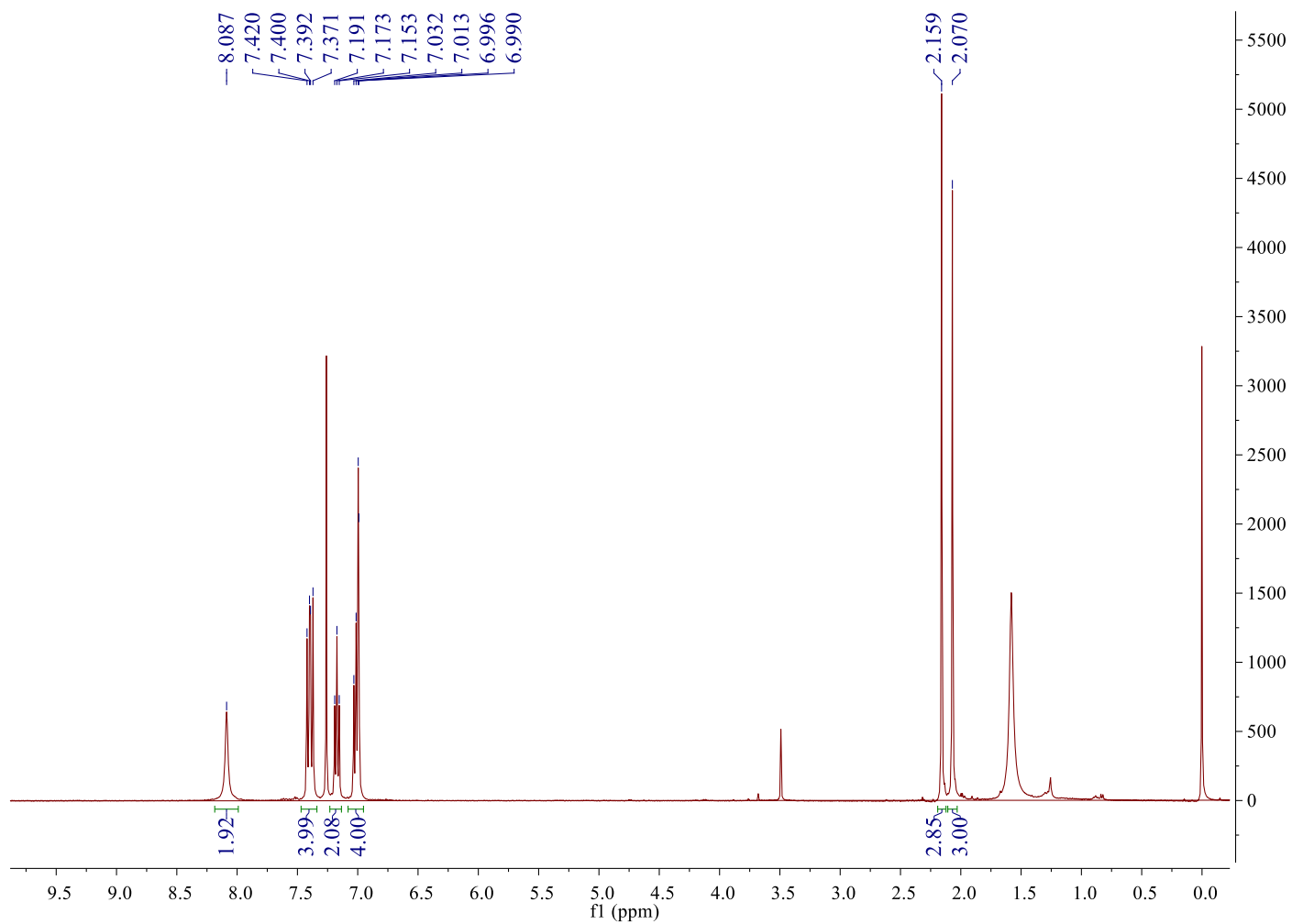


Figure S35. ^1H NMR spectrum of 3,3-bis(3-indolyl) butan-2-one (**4**) in CDCl_3 (400 MHz).

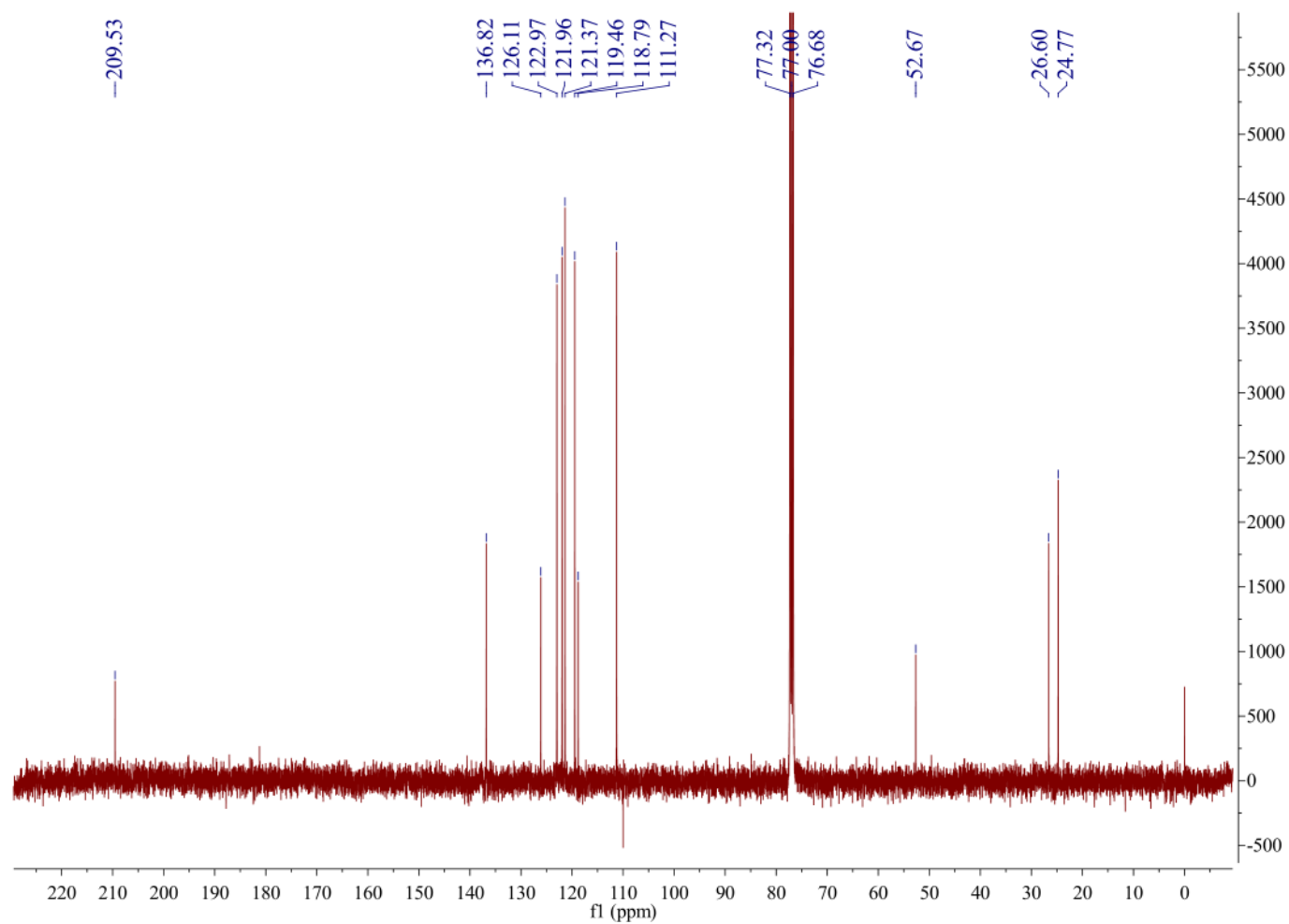
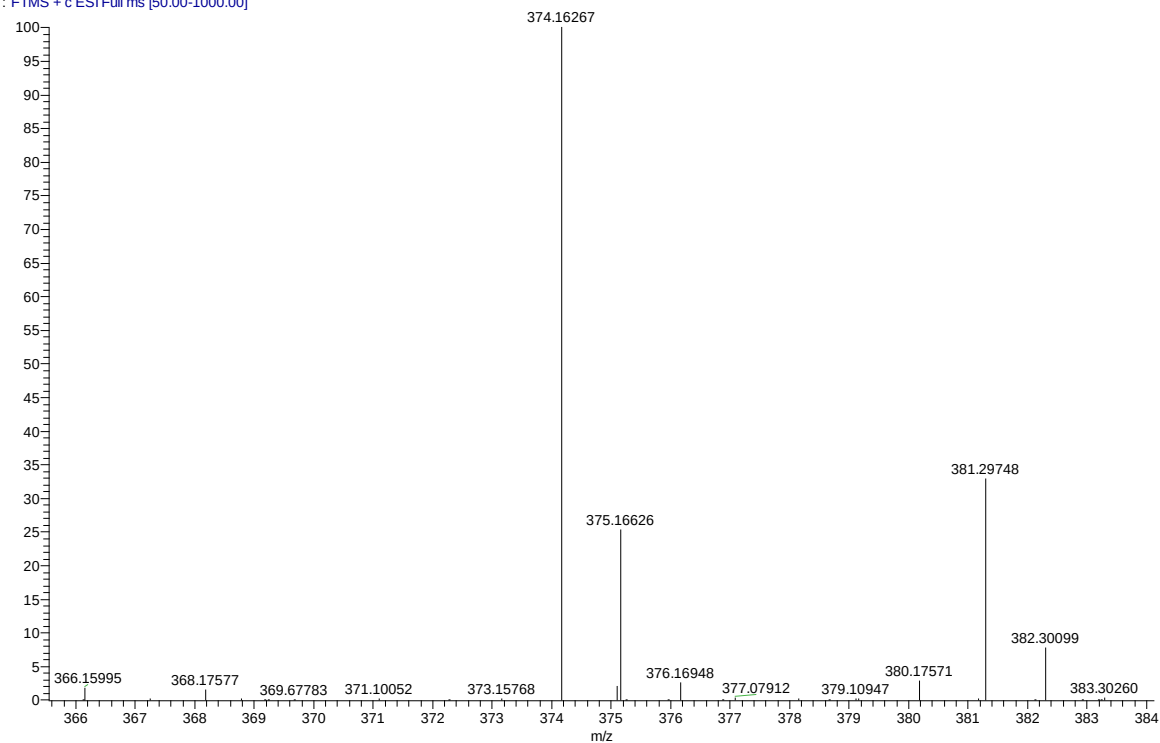


Figure S36. ^{13}C NMR spectrum of 3,3-bis(3-indolyl)butan-2-one (**4**) in CDCl_3 (100 MHz).

1708A0315 170816150827 #19-28 RT: 0.09-0.13 AV: 10 NL: 1.33E5
T: FTMS + c ESI Full ms [50.00-1000.00]



SPECTRUM - simulation:

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
374.16267	374.16277	-0.26	15.5	C24 H21 N3 Na

Figure S37. HR-(+)ESI-MS spectrum of 2-[2,2-di(1*H*-indol-3-yl) ethyl] aniline (**5**).

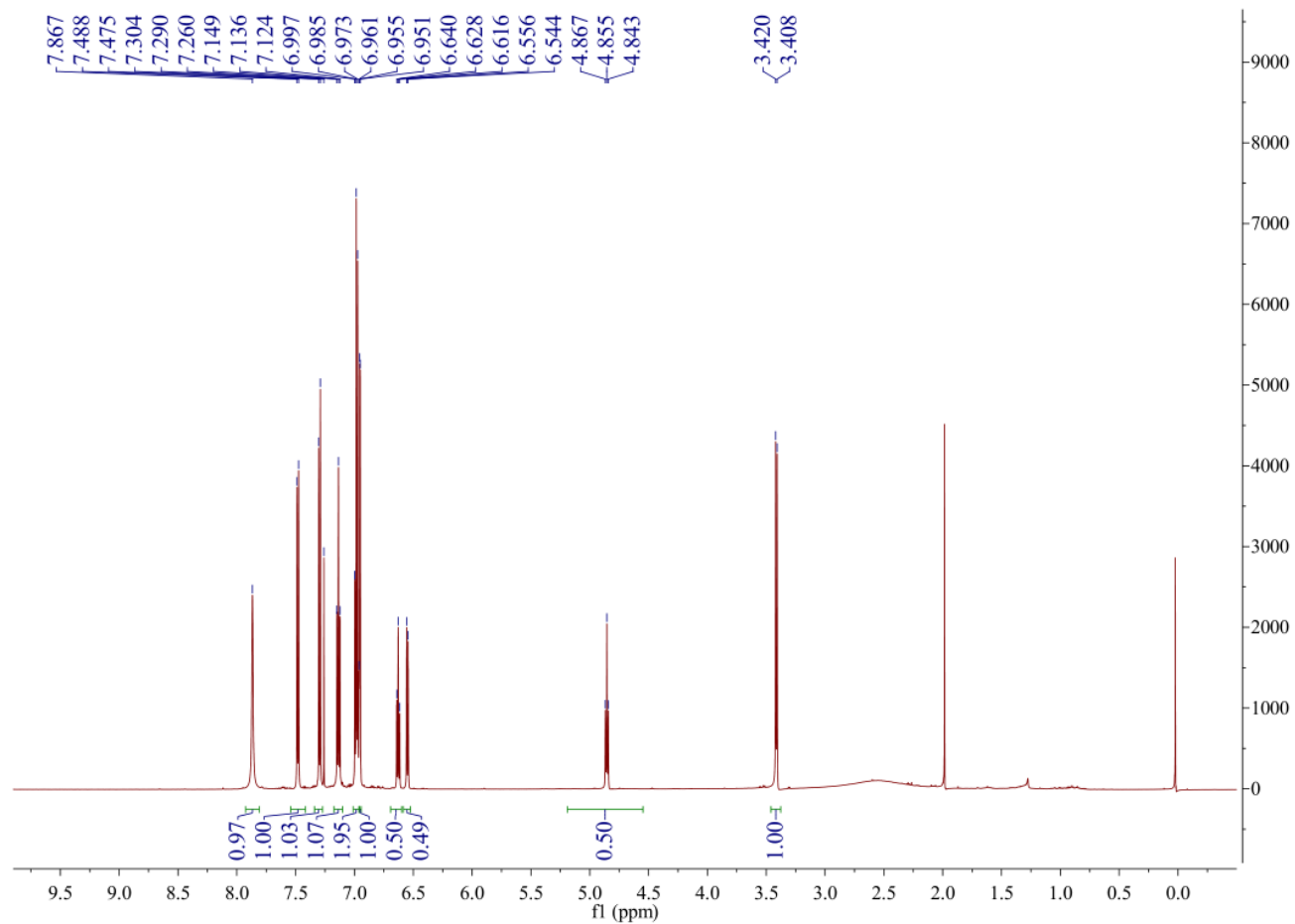


Figure S38. ^1H NMR spectrum of 2-[2,2-di(1*H*-indol-3-yl) ethyl] aniline (5) in CDCl_3 (600 MHz).

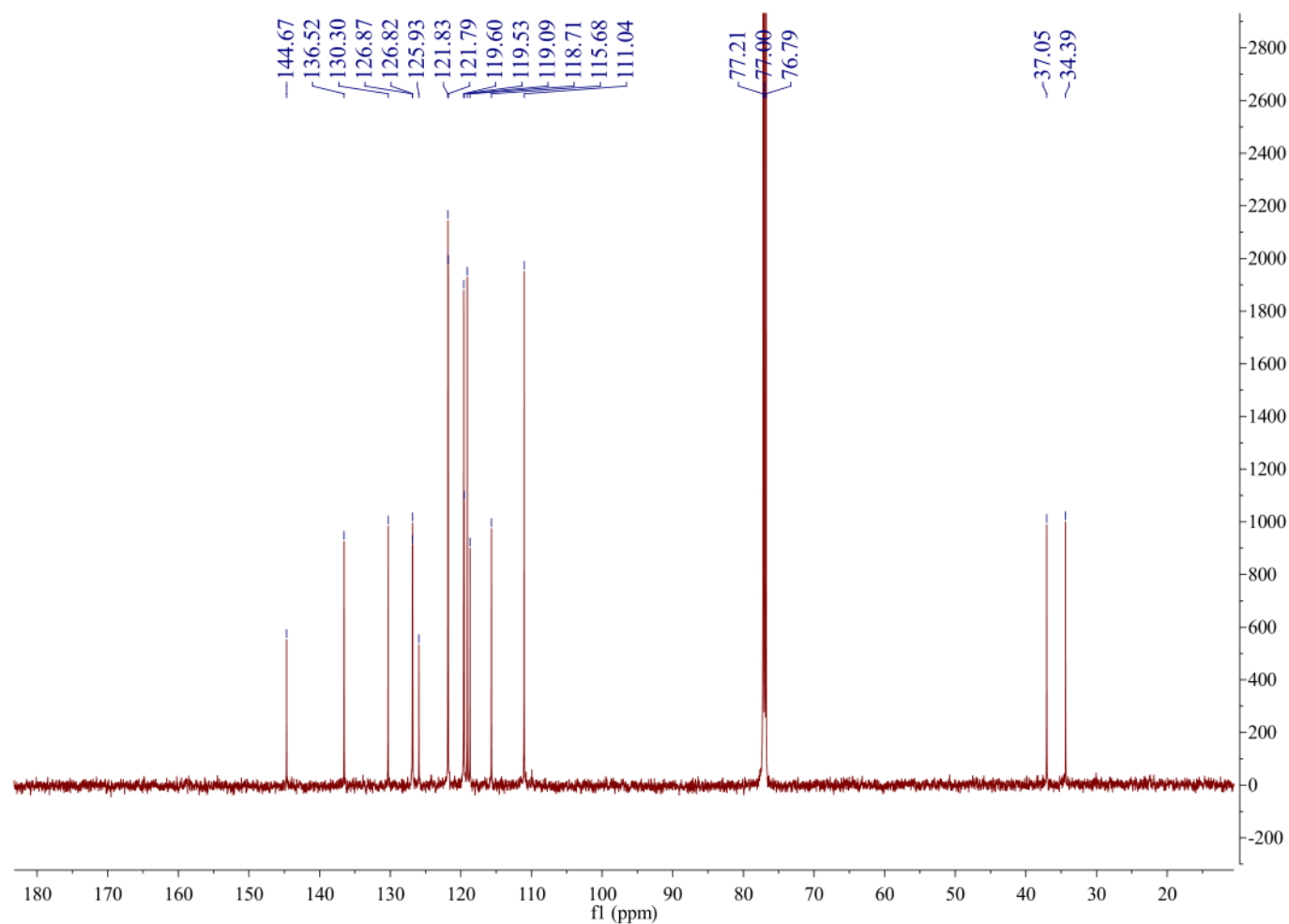


Figure S39. ^{13}C NMR spectrum of 2-[2,2-di(1*H*-indol-3-yl) ethyl] aniline (5) in CDCl_3 (150 MHz).

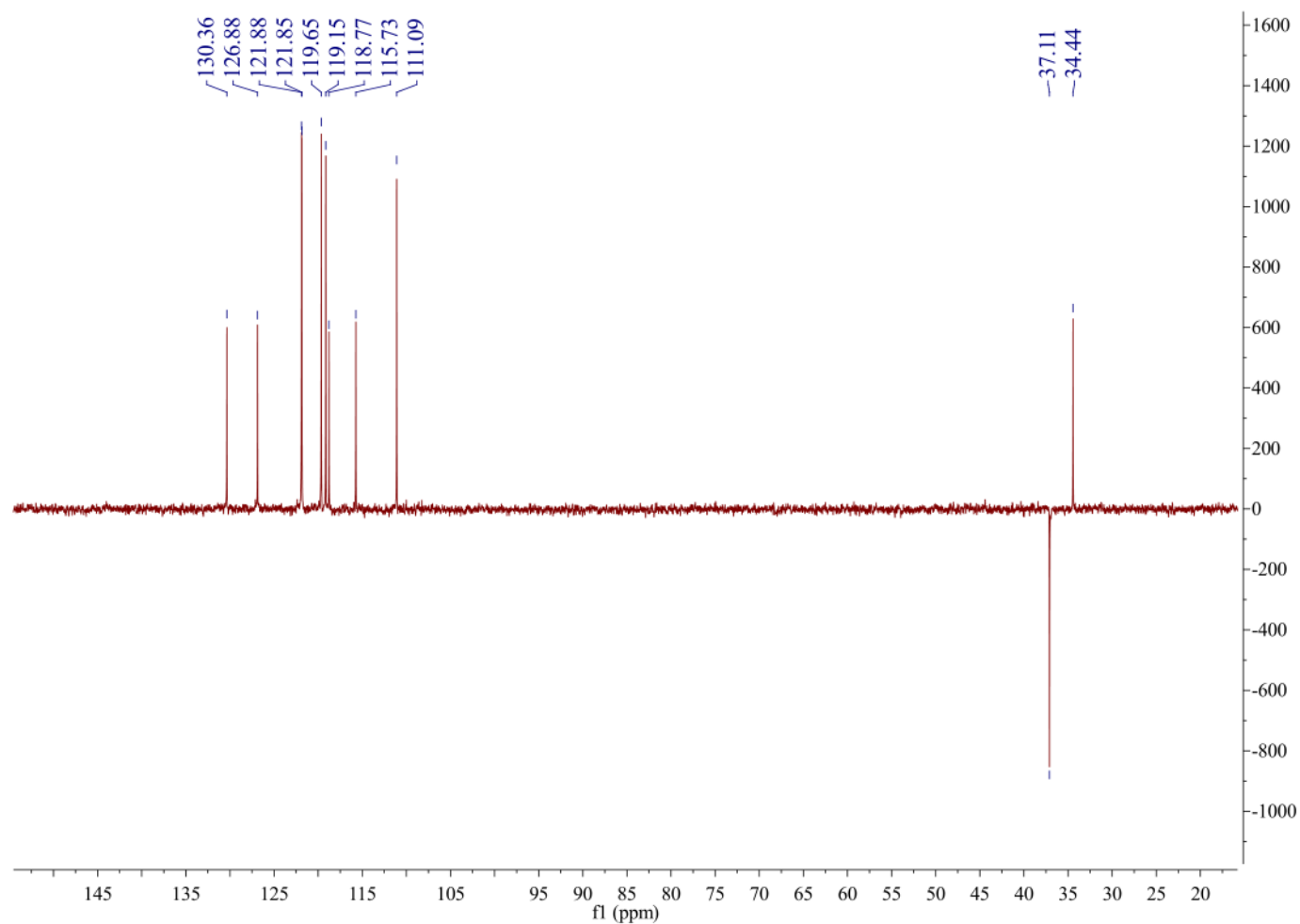


Figure S40. DEPT 135 spectrum of 2-[2,2-di(1*H*-indol-3-yl) ethyl] aniline (**5**) in CDCl₃ (150 MHz).

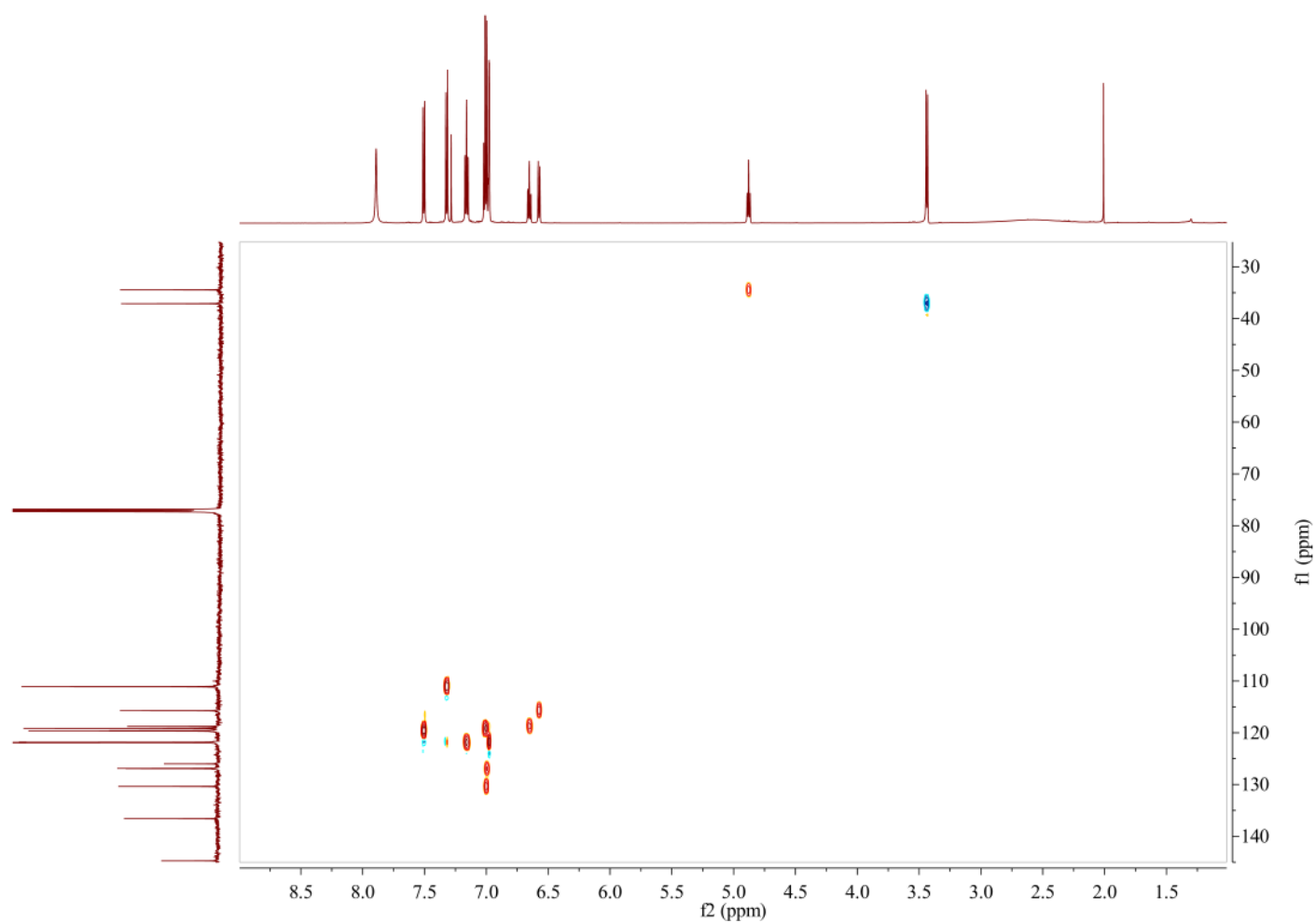


Figure S41. HMQC spectrum of 2-[2,2-di(1*H*-indol-3-yl) ethyl] aniline (**5**) in CDCl_3 .

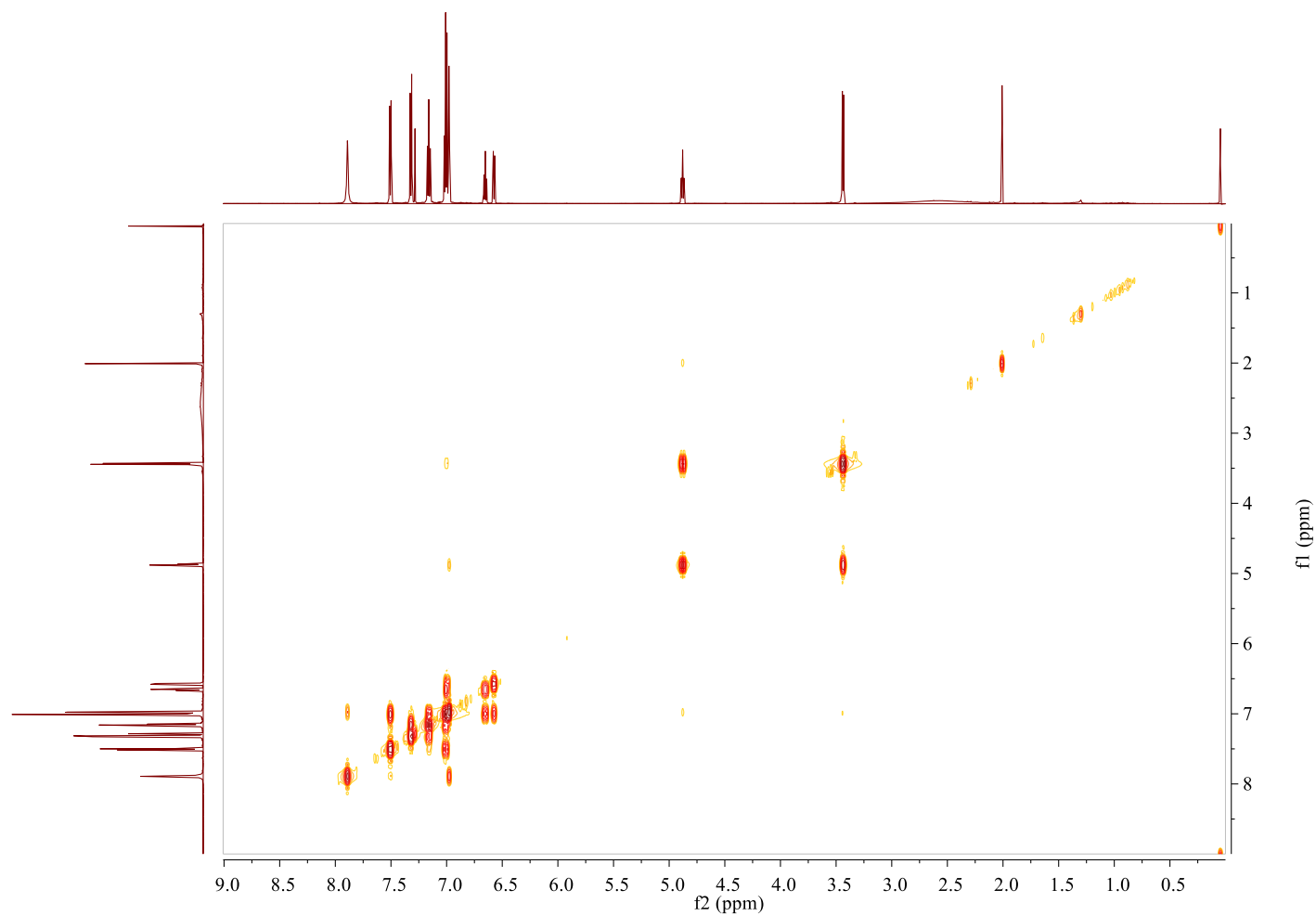


Figure S42. ^1H - ^1H COSY spectrum of 2-[2,2-di(1*H*-indol-3-yl) ethyl] aniline (**5**) in CDCl_3 .

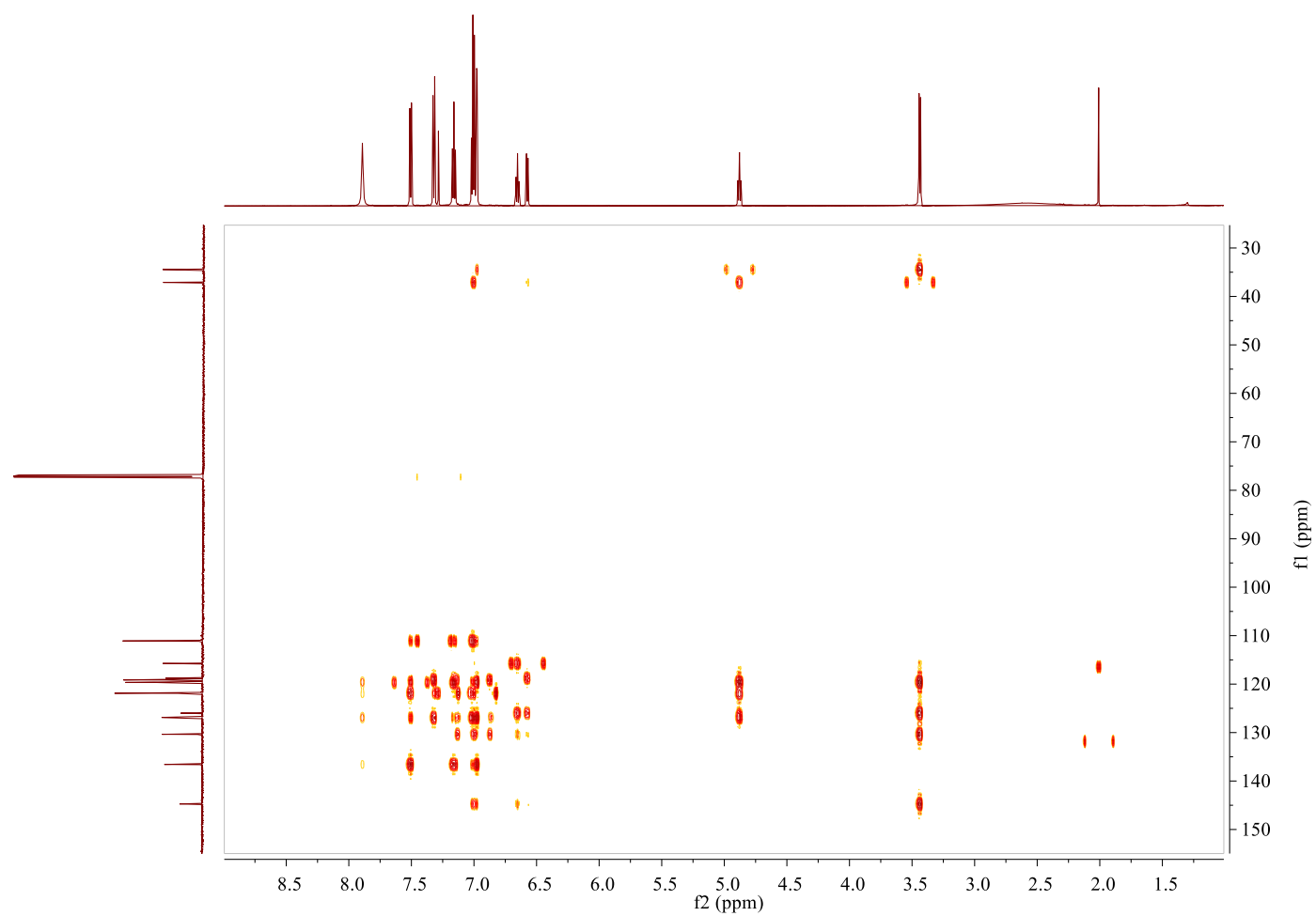


Figure S43. HMBC spectrum of 2-[2,2-di(1*H*-indol-3-yl) ethyl] aniline (**5**) in CDCl₃.

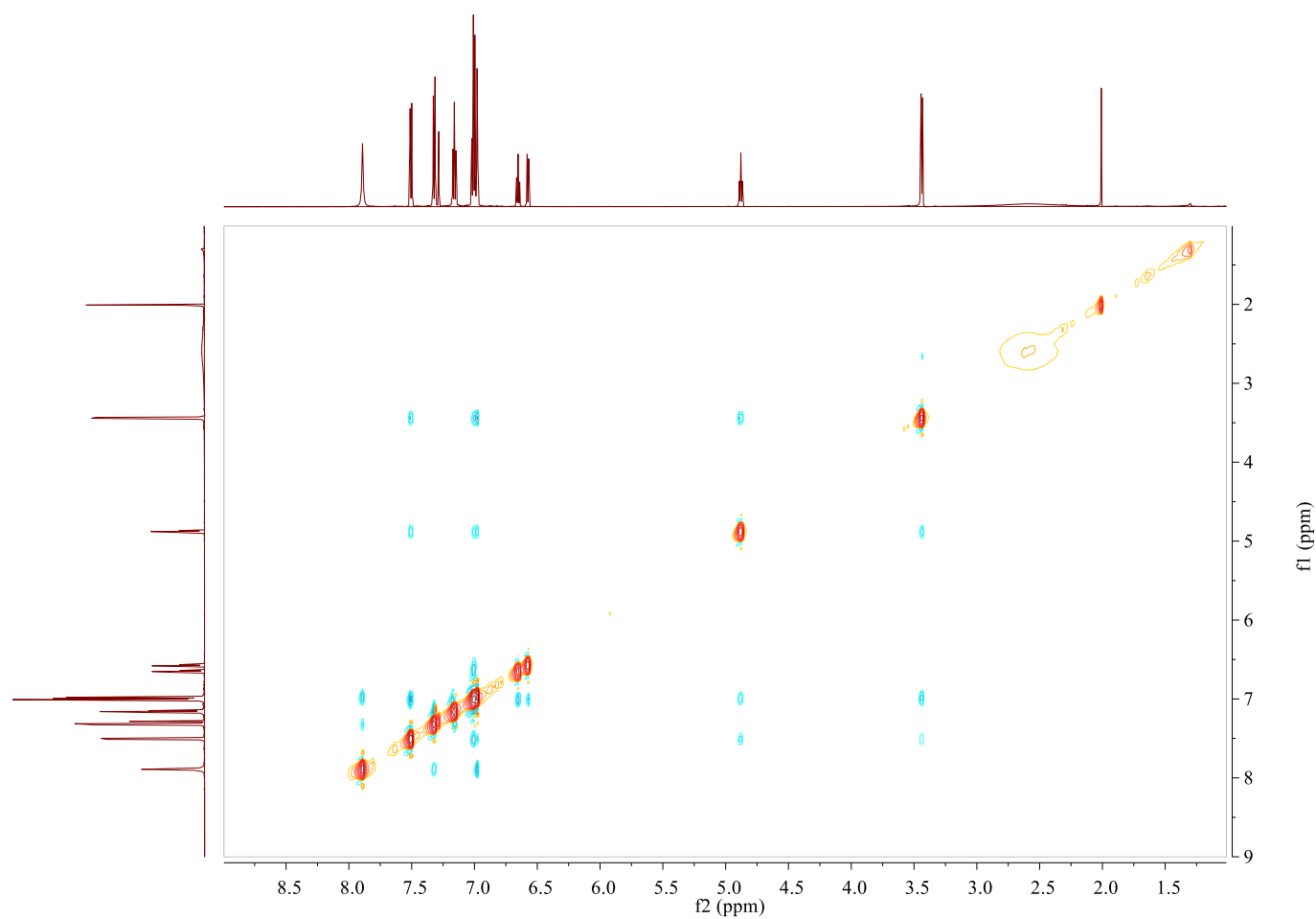


Figure S44. NOESY spectrum of 2-[2,2-di(1*H*-indol-3-yl) ethyl] aniline (**5**) in CDCl₃.

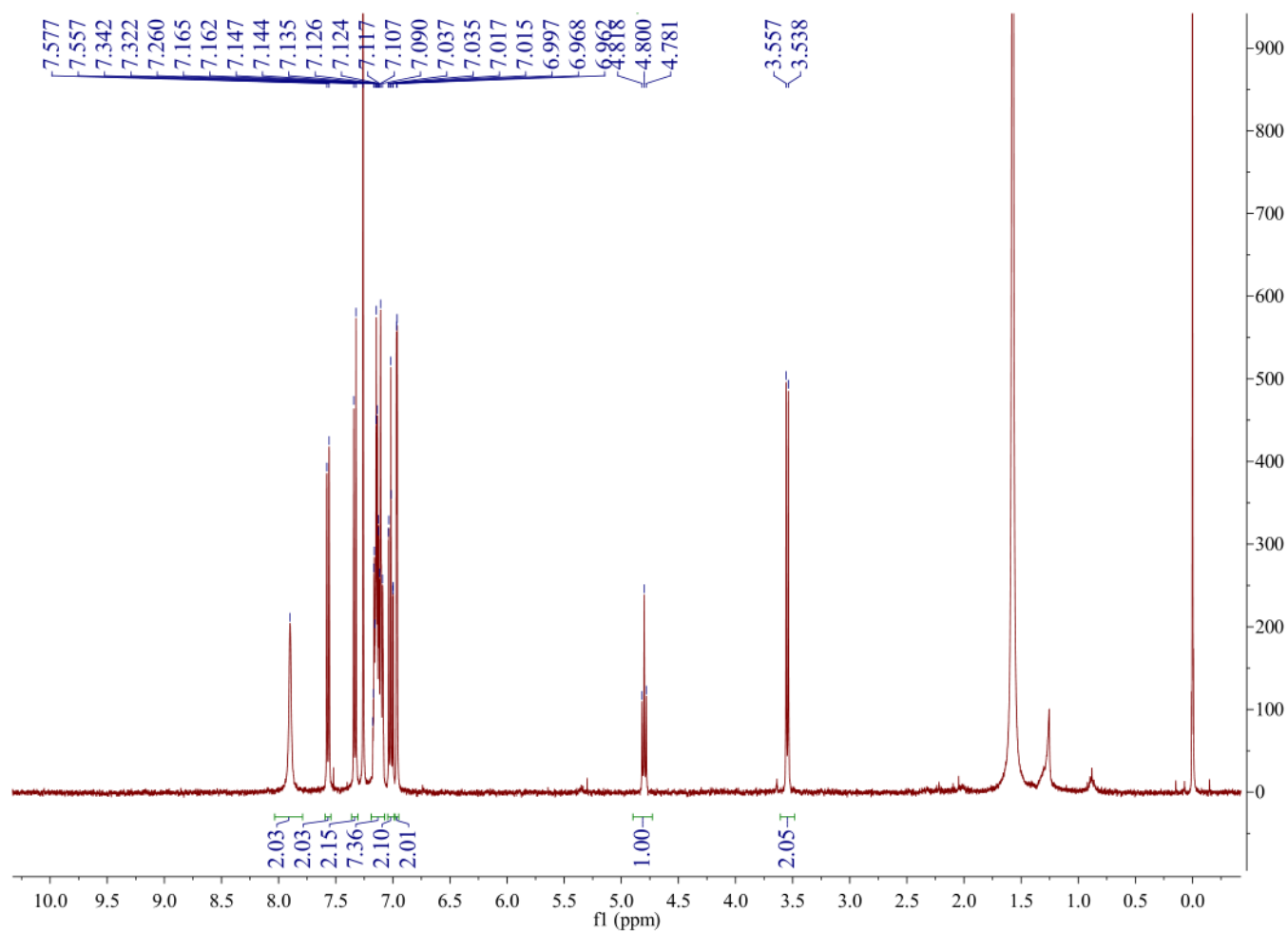


Figure S45. ¹H NMR spectrum of 3,3'-Diindolyl(phenyl)methane (**6**) in CDCl₃ (400 MHz).

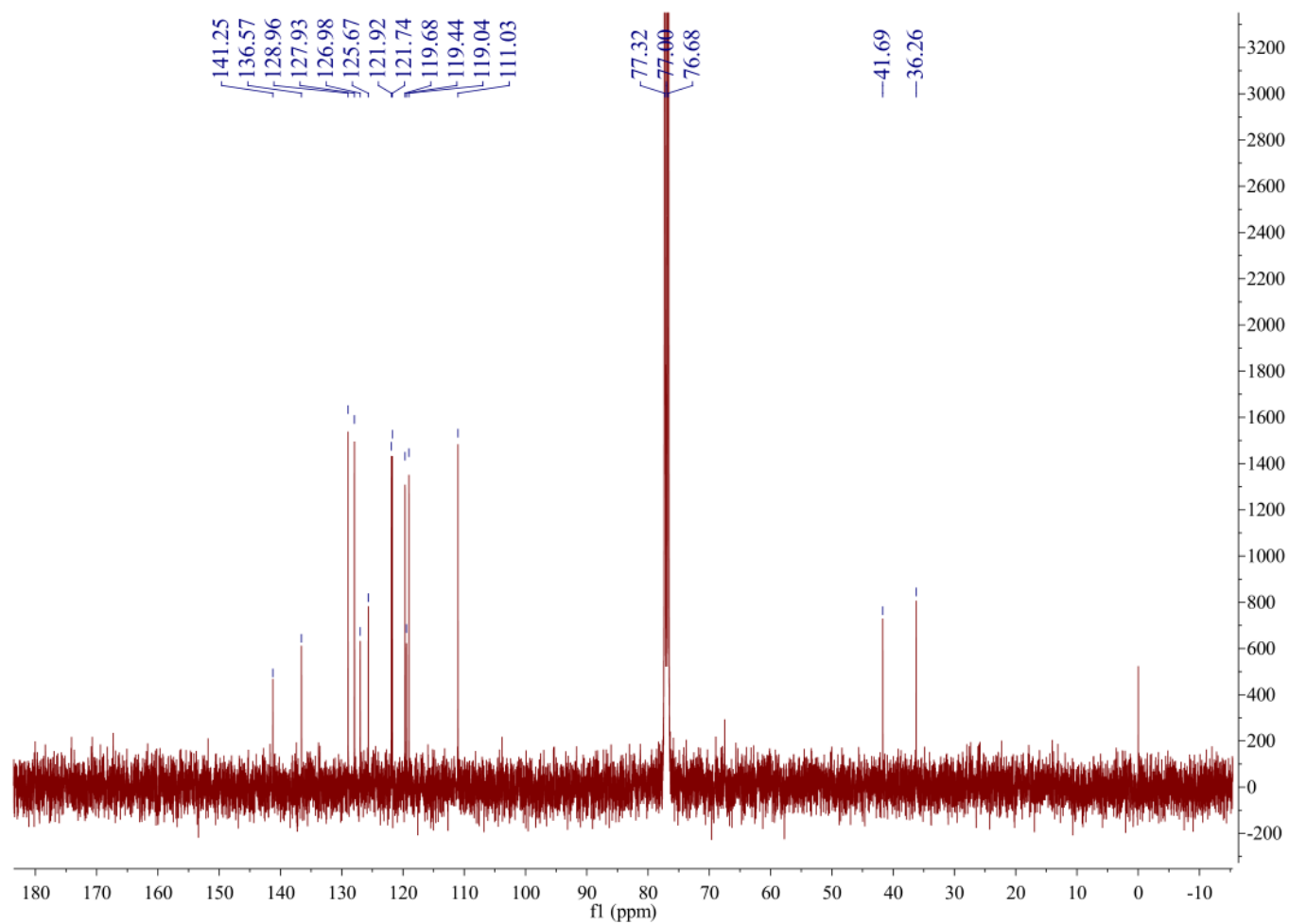


Figure S46. ^{13}C NMR spectrum of 3,3'-Diindolyl(phenyl)methane (**6**) in CDCl_3 (100 MHz).

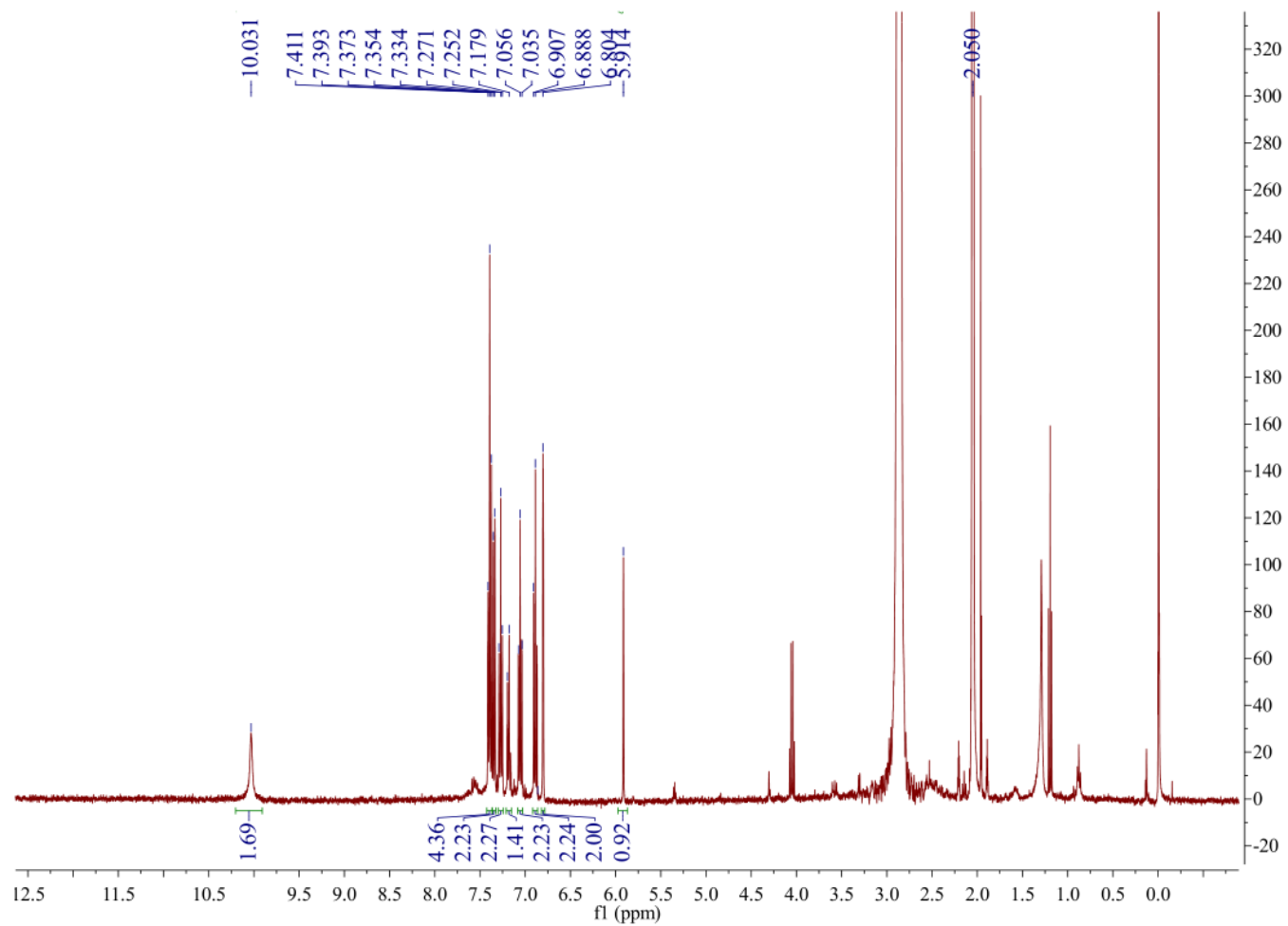


Figure S47. ^1H NMR spectrum of 1,1-(3,3'-Diindolyl)-2-phenylethane (7) in acetone- d_6 (400 MHz).

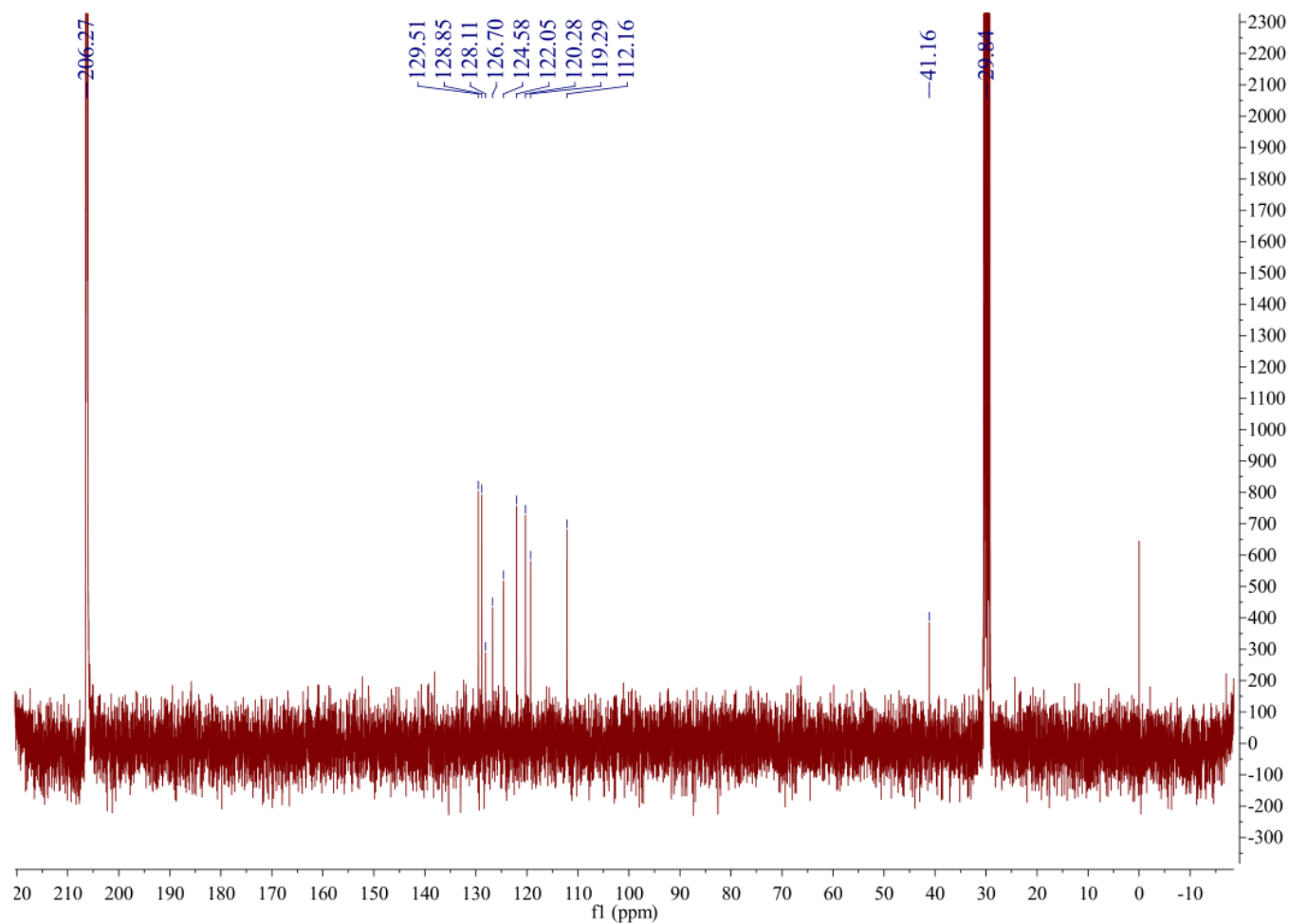


Figure S48. ^{13}C NMR spectrum of 1,1-(3,3'-Diindolyl)-2-phenylethane (7) in acetone- d_6 (100 MHz).

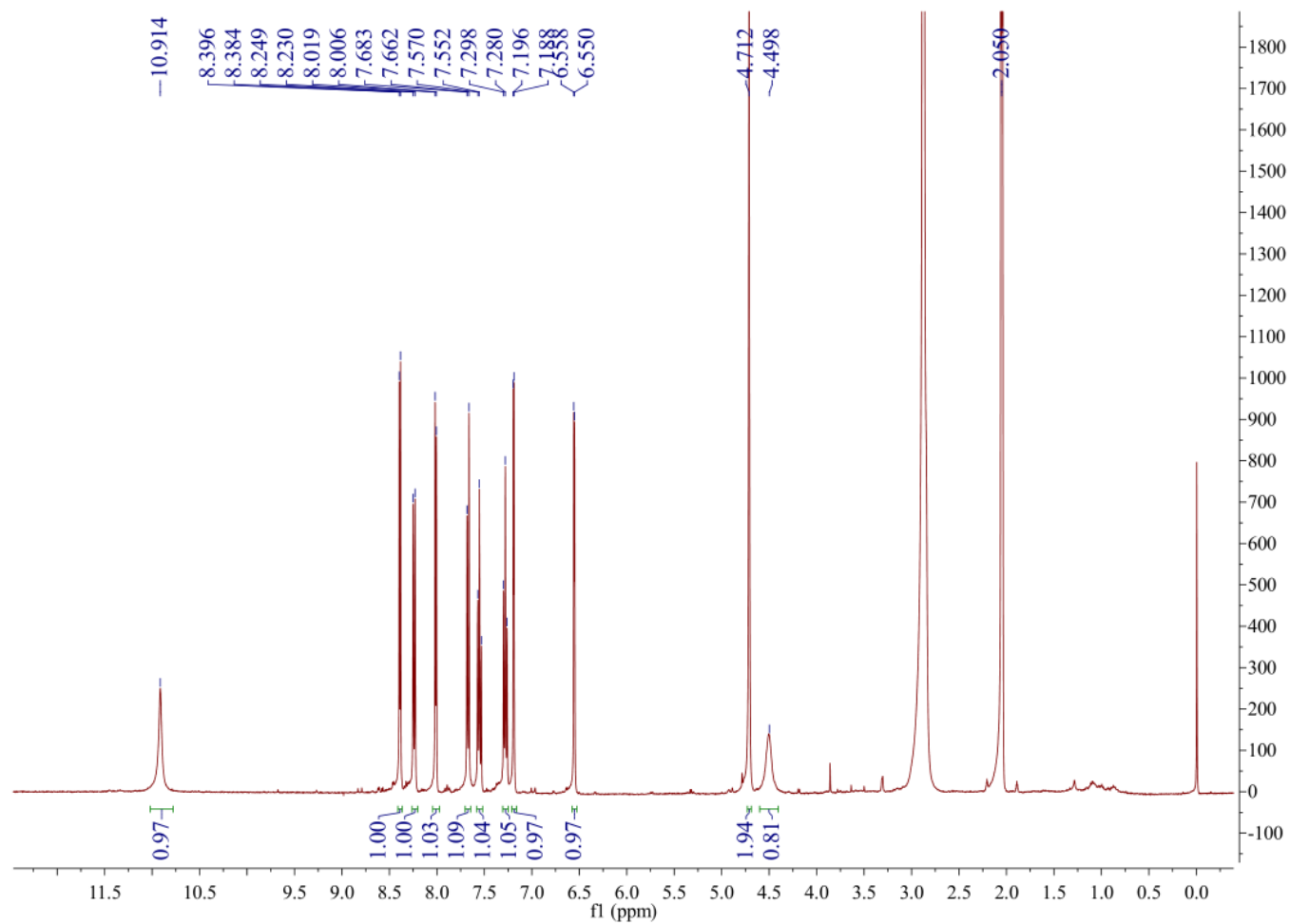


Figure S49. ^1H NMR spectrum of perlolyrin (**8**) in acetone- d_6 (400 MHz).

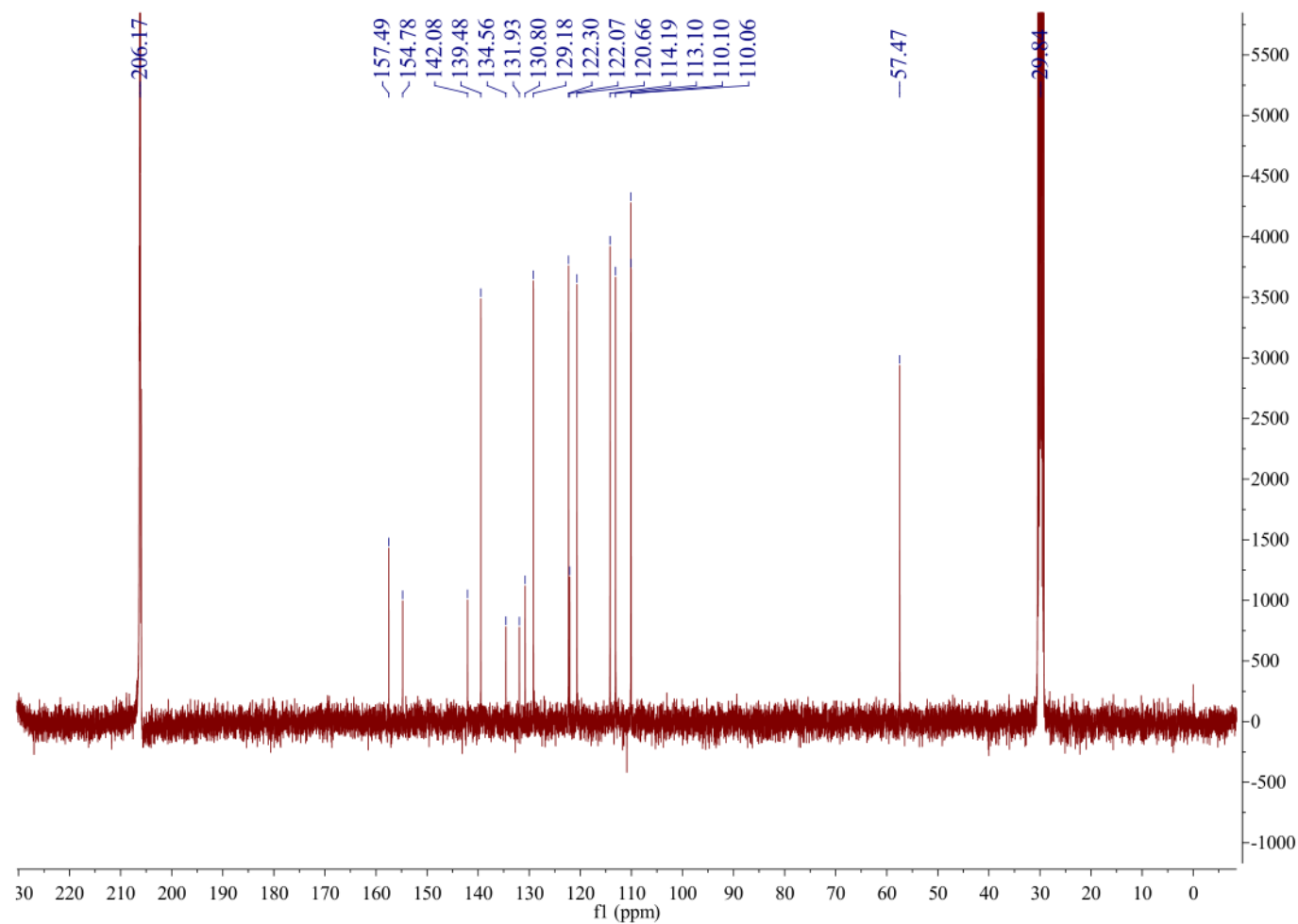


Figure S50. ¹³C NMR spectrum of perlolyrin (**8**) in acetone-*d*₆ (100 MHz).

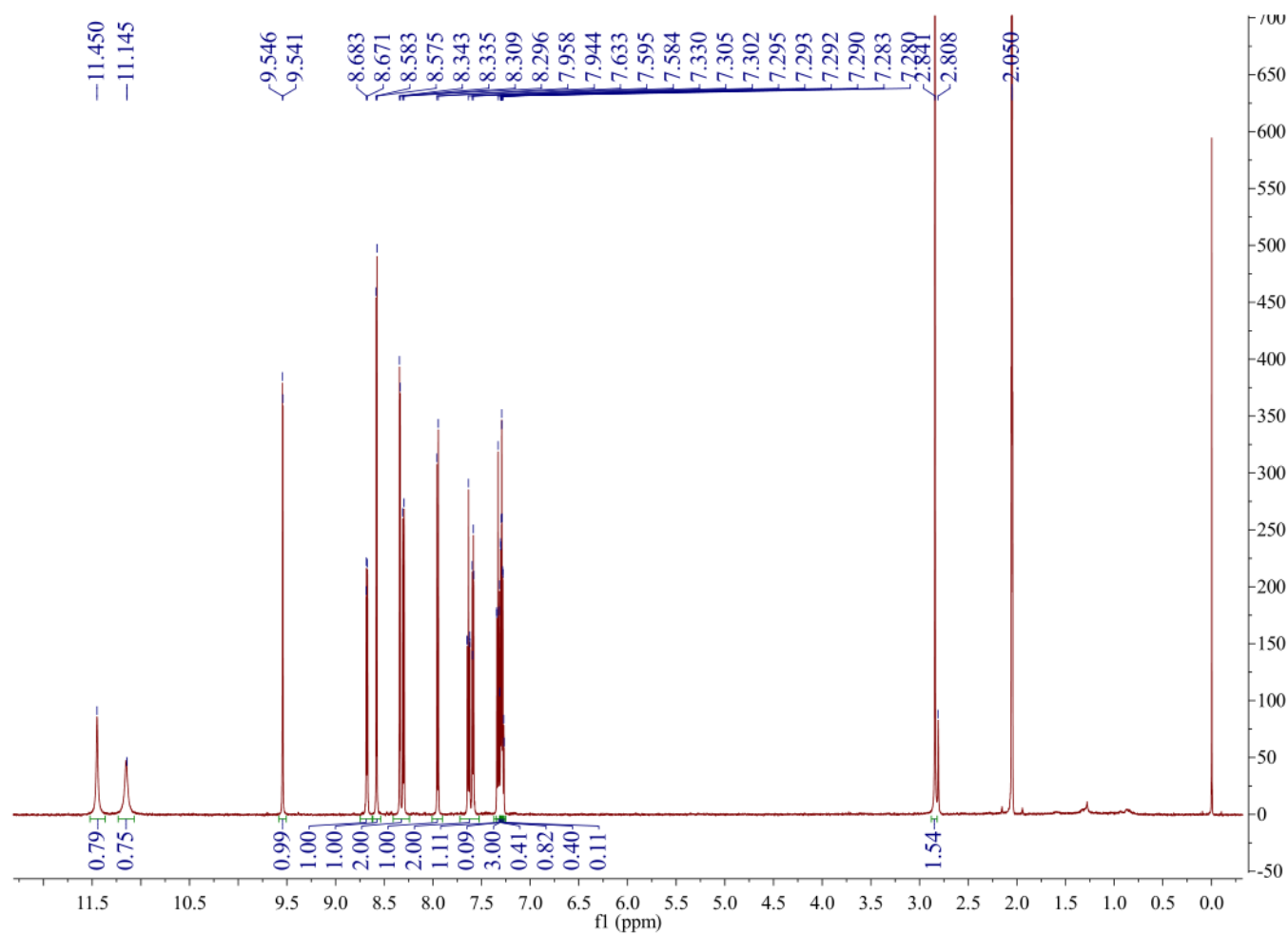


Figure S51. ^1H NMR spectrum of pityriacitrin (**9**) in acetone- d_6 (600 MHz).

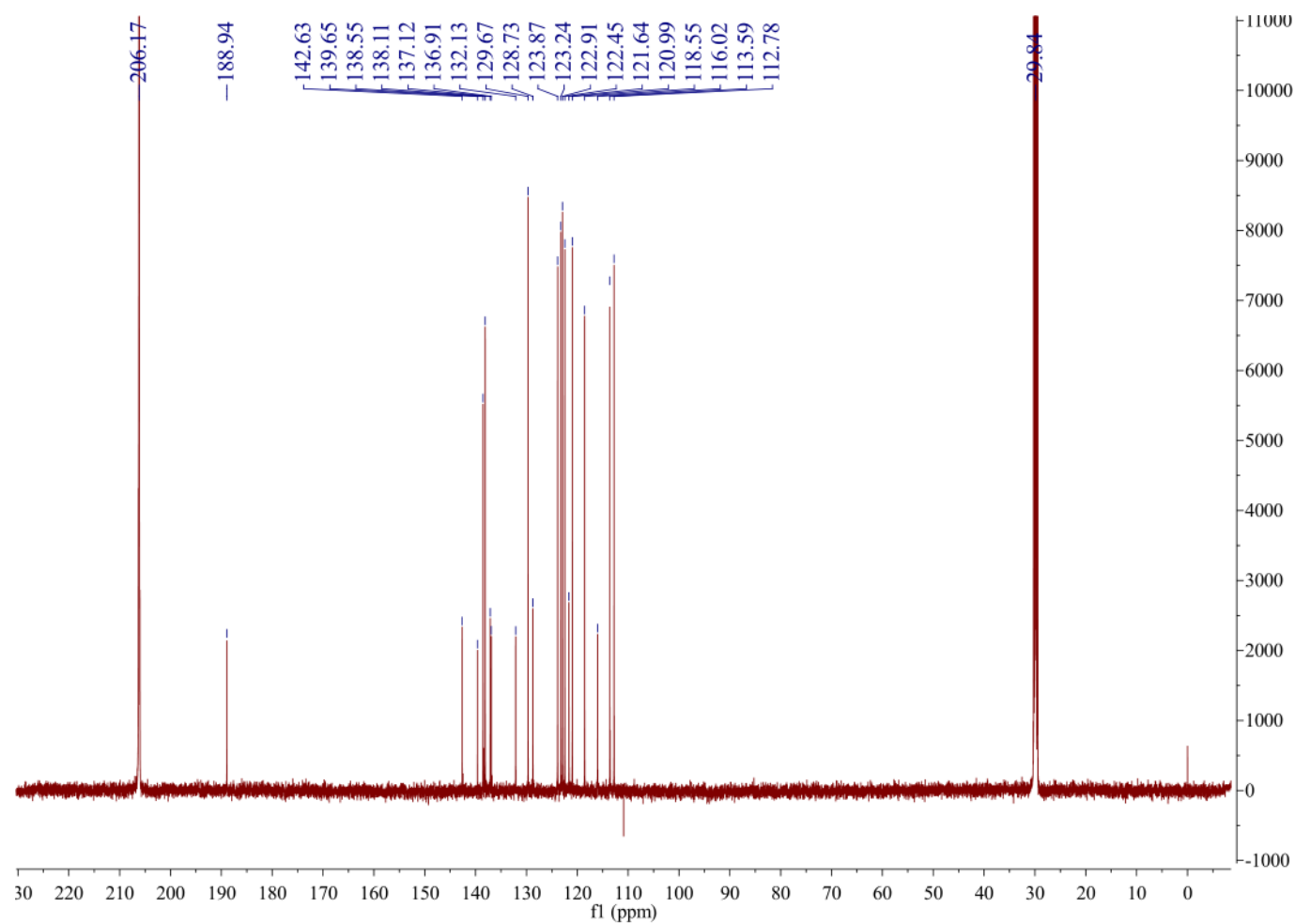


Figure S52. ¹³C NMR spectrum of pityriacitrin (**9**) in acetone-*d*₆ (150 MHz).

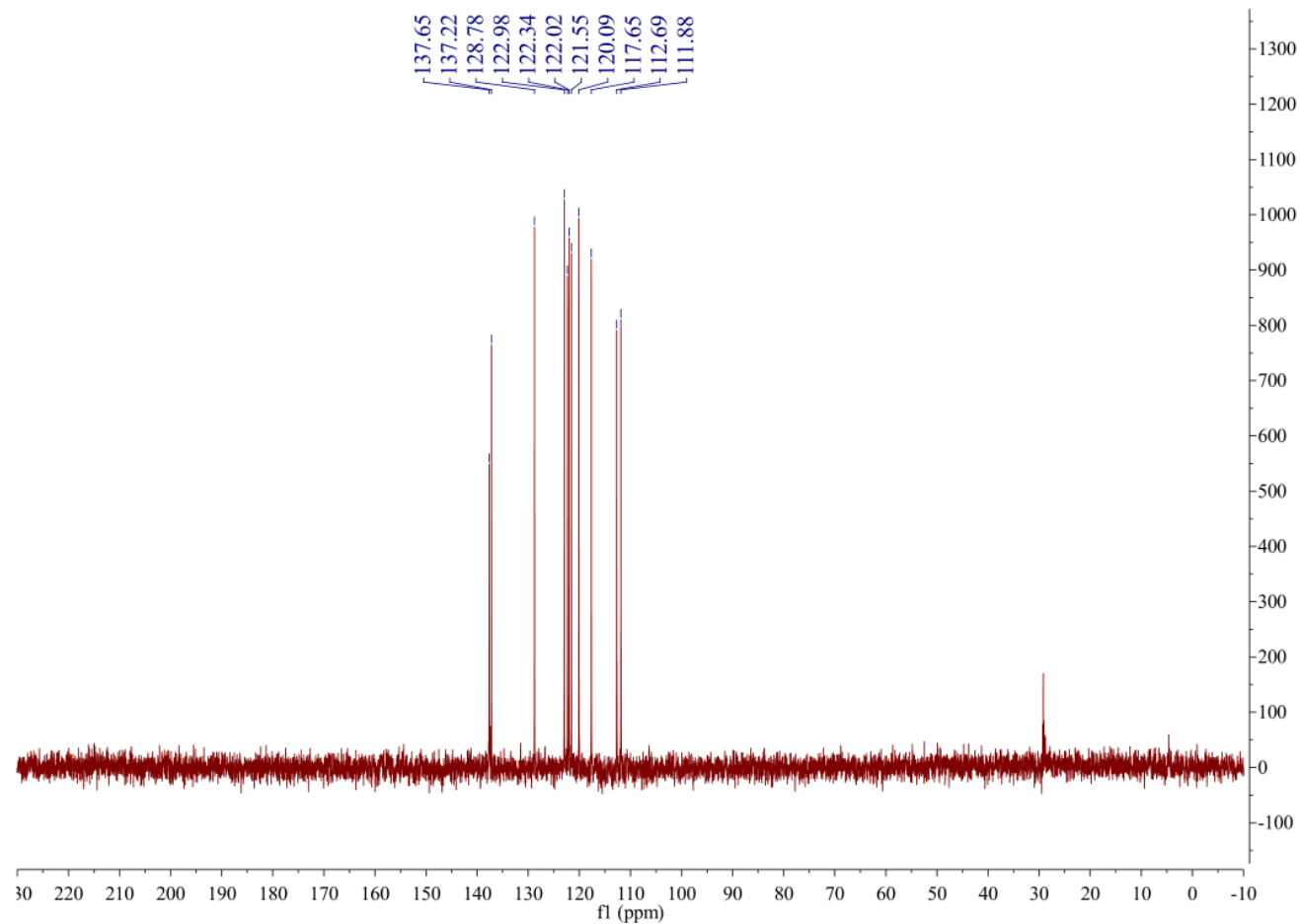


Figure S53. DEPT 135 spectrum of pityriacitrin (**9**) in acetone- d_6 (150 MHz).

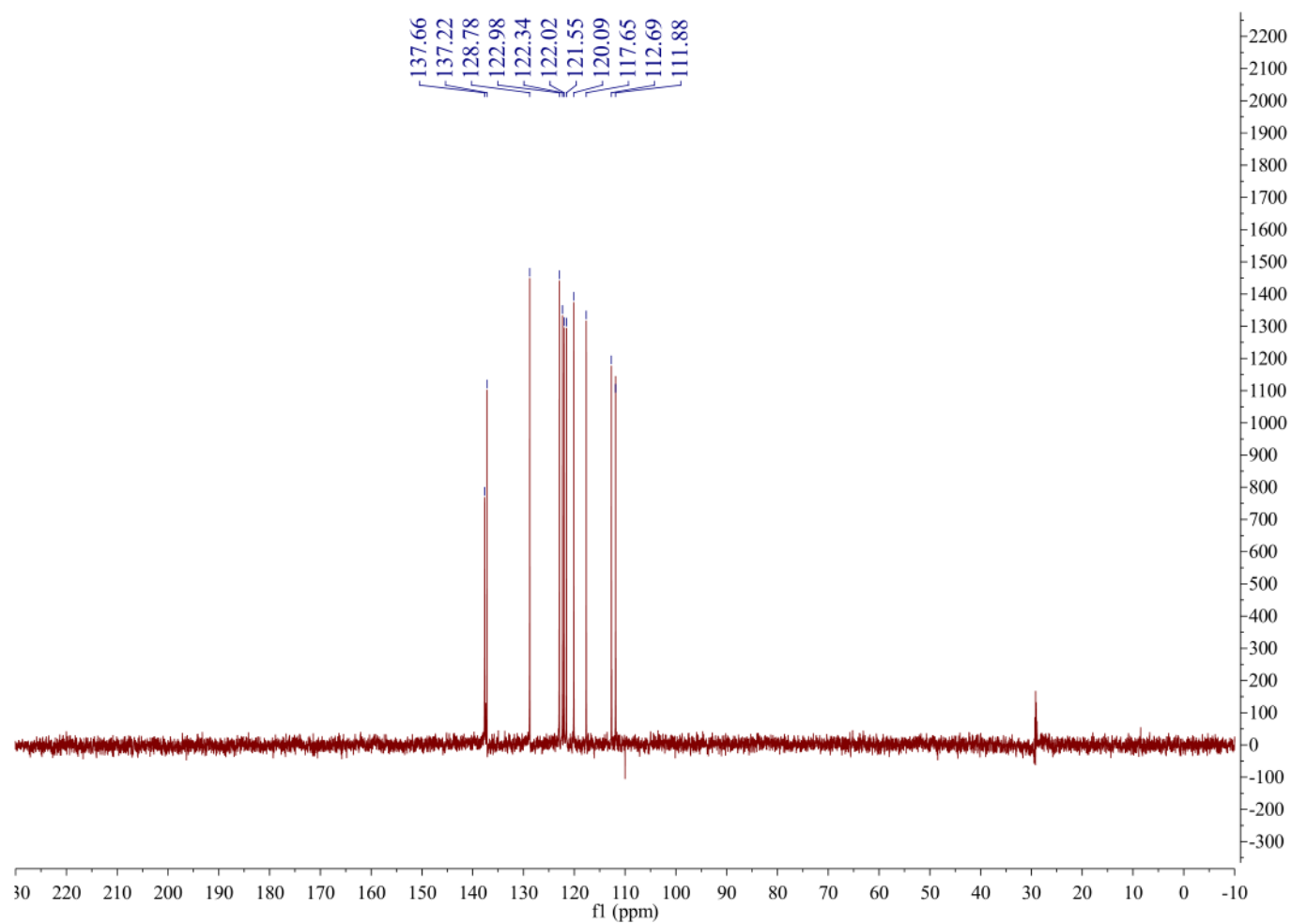


Figure S54. DEPT 90 spectrum of pityriacitrin (**9**) in acetone- d_6 (150 MHz).

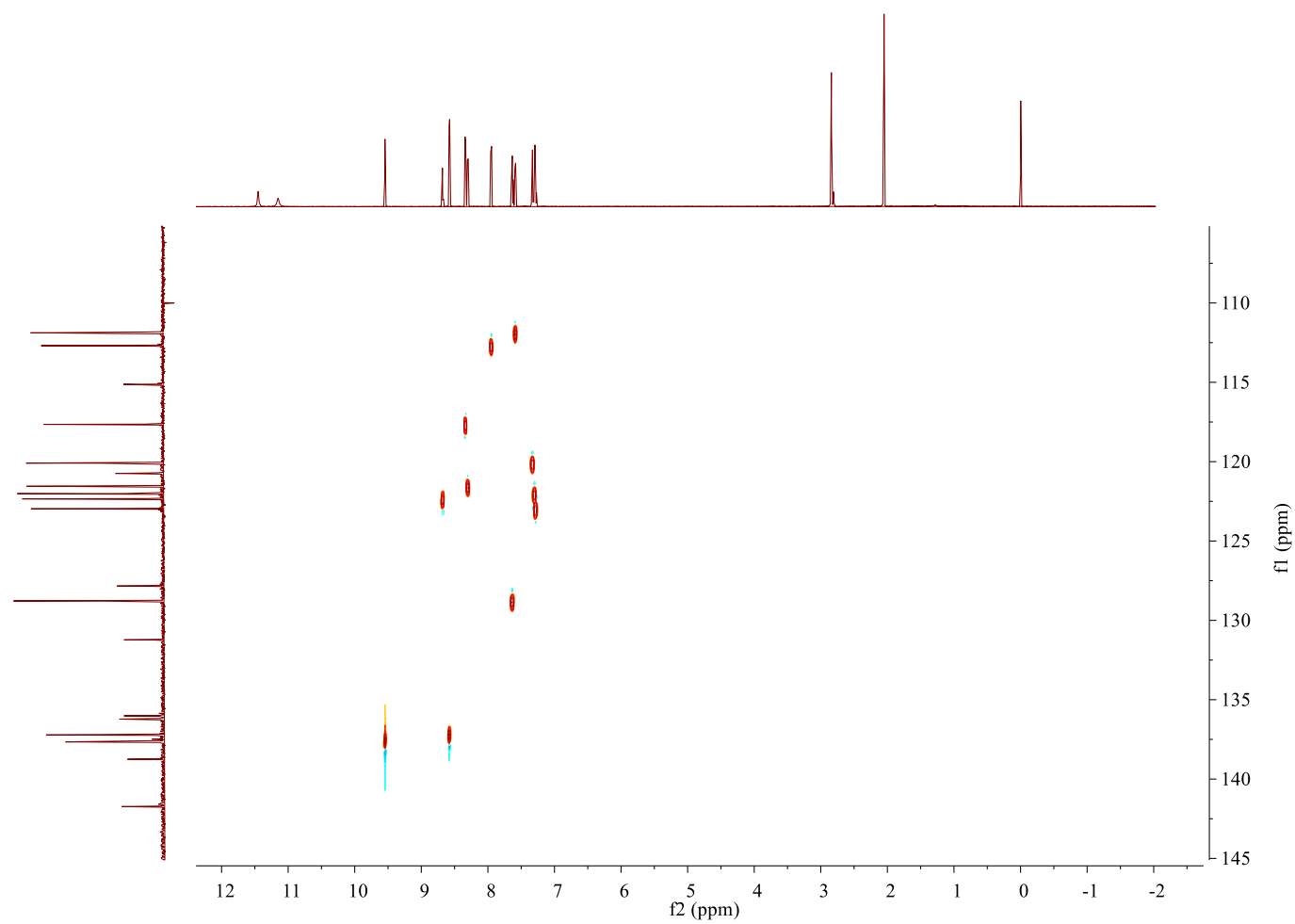


Figure S55. HMQC spectrum of pityriacitrin (**9**) in acetone- d_6 .

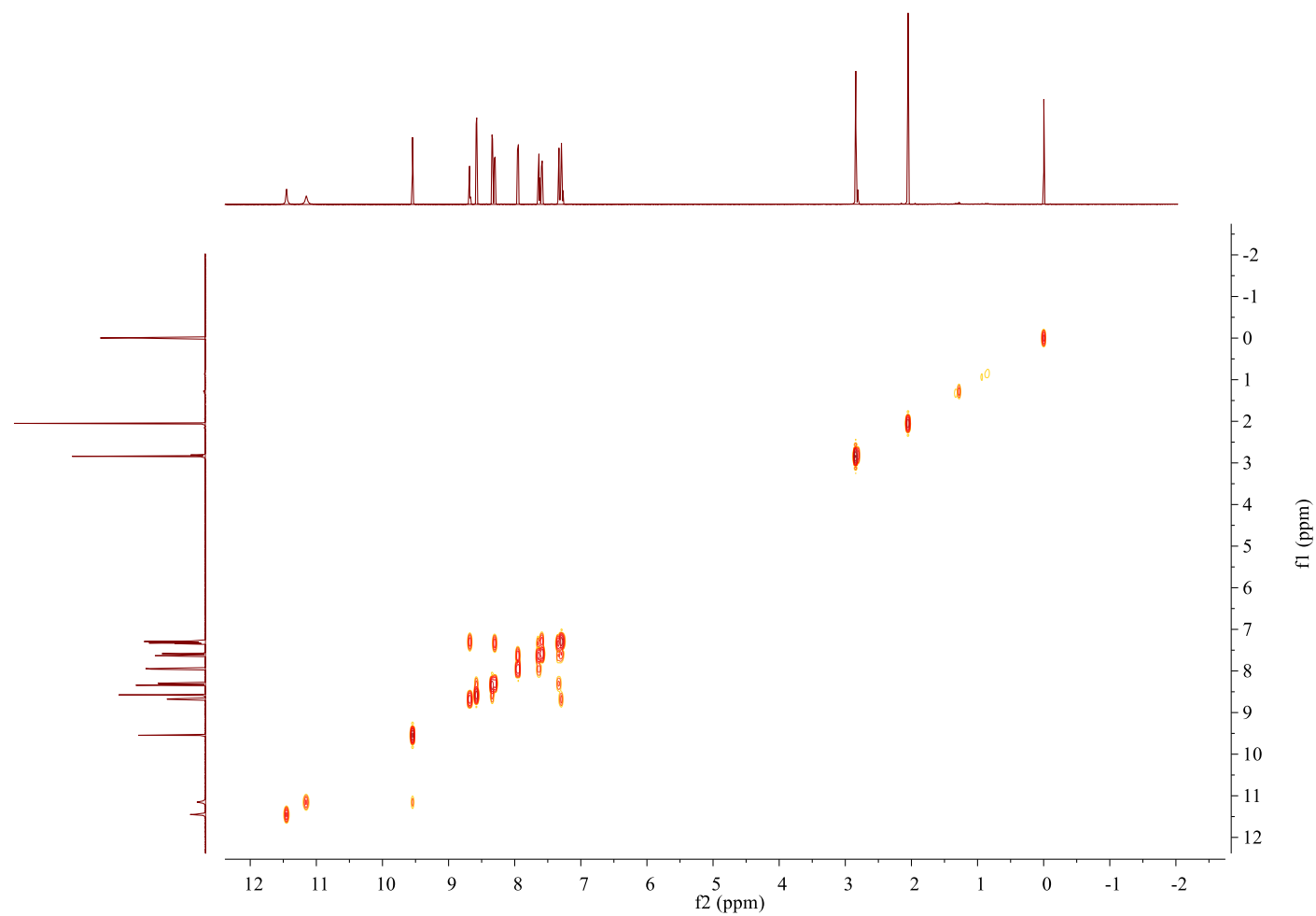


Figure S56. ^1H - ^1H COSY spectrum of pityriacitrin (**9**) in acetone- d_6 .

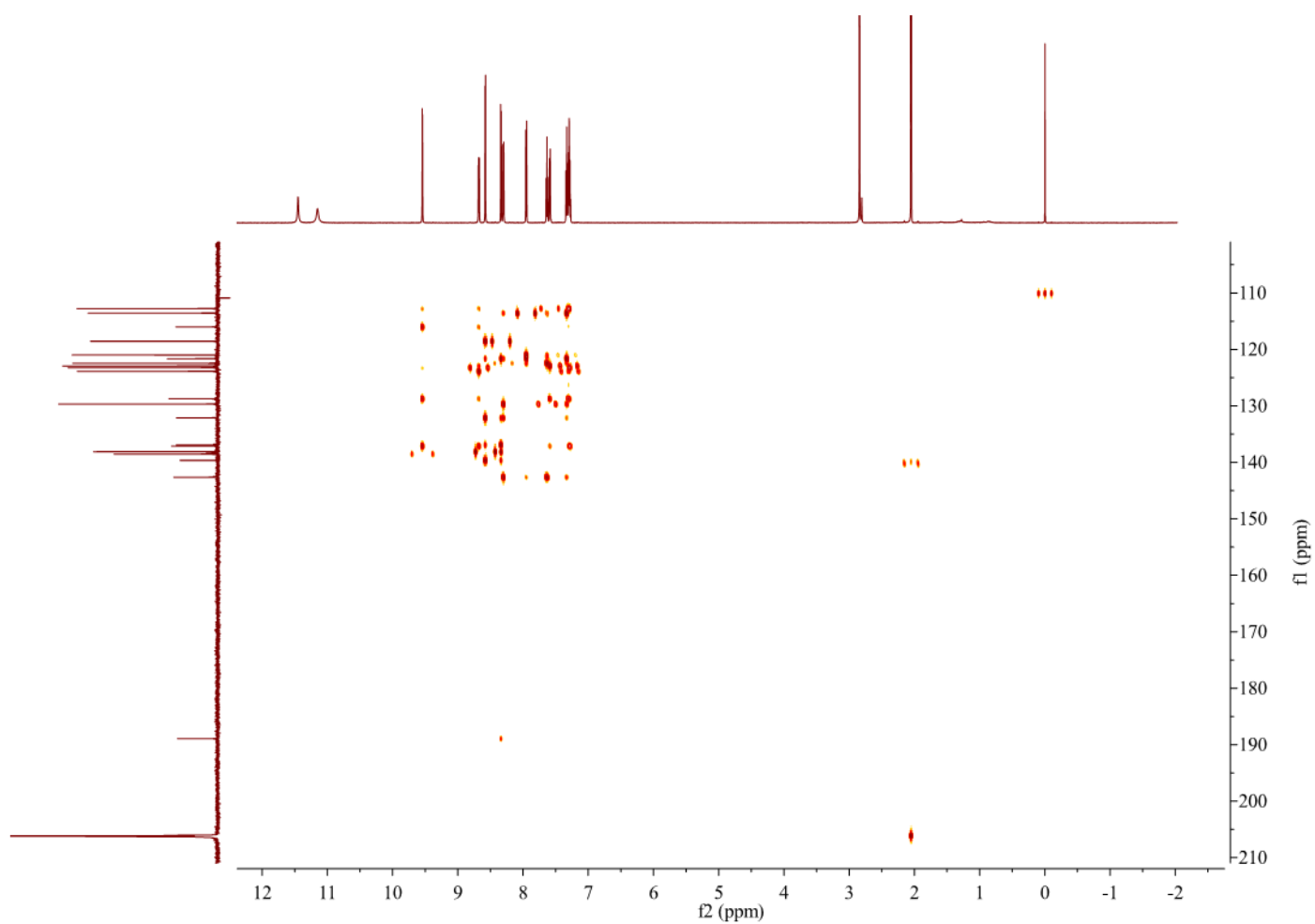


Figure S57. HMBC spectrum of pityriacitrin (**9**) in acetone- d_6 .

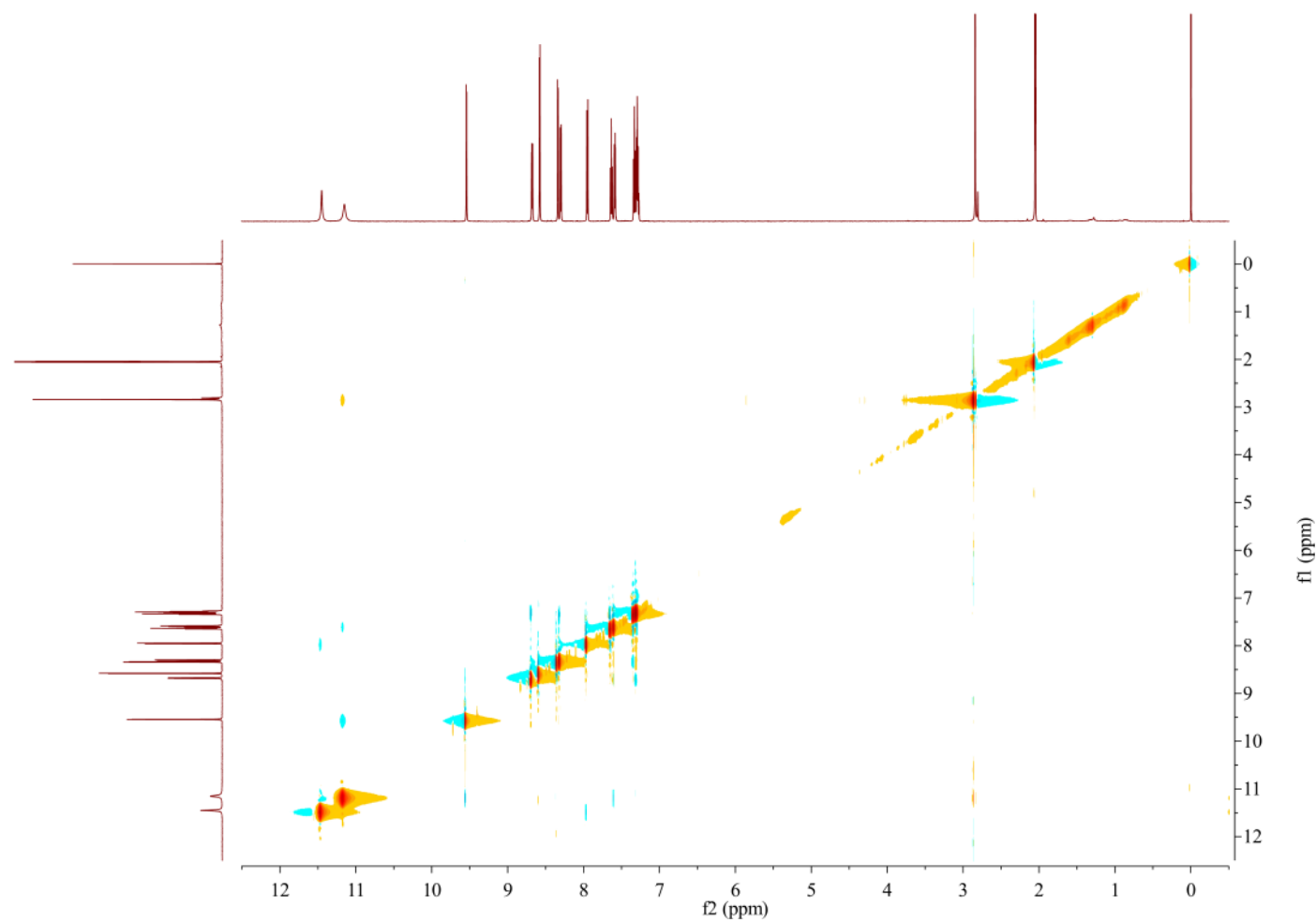


Figure S58. NOESY spectrum of pityriacitrin (**9**) in acetone- d_6 .

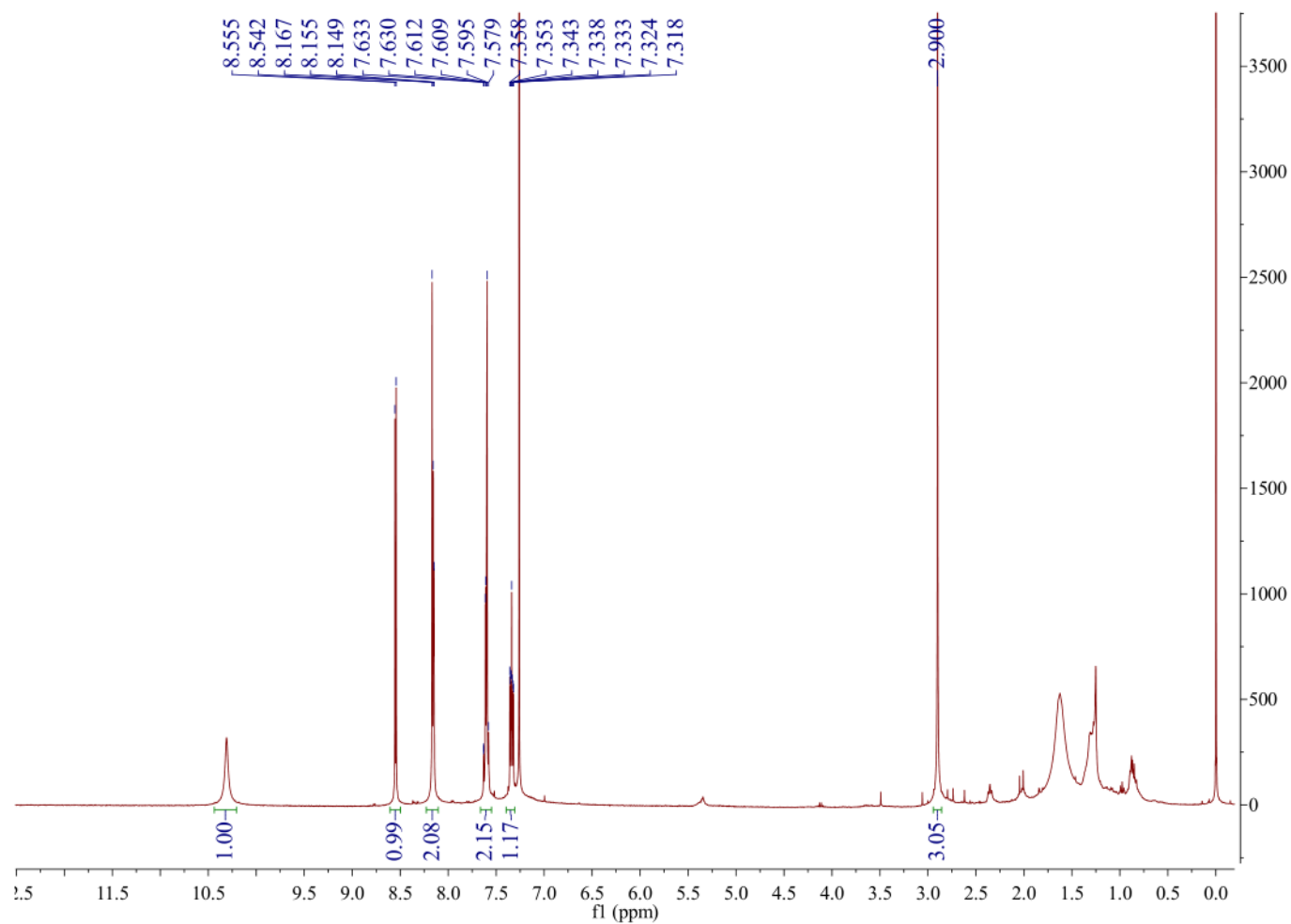


Figure S59. ¹H NMR spectrum of 1-acetyl-β-carboline (**10**) in CDCl₃ (400 MHz).

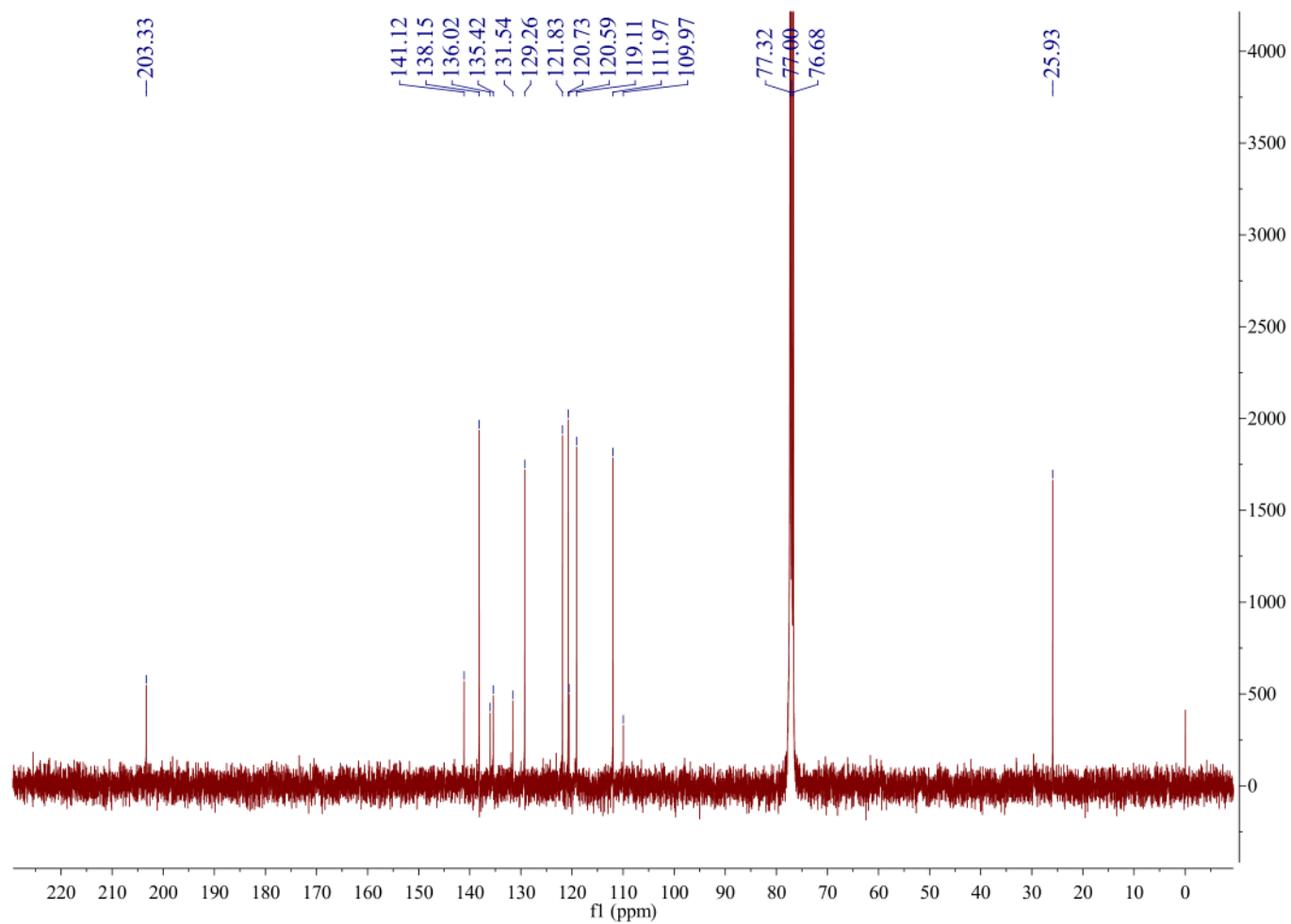


Figure S60. ^{13}C NMR spectrum of 1-acetyl- β -carboline (**10**) in CDCl_3 (100 MHz).

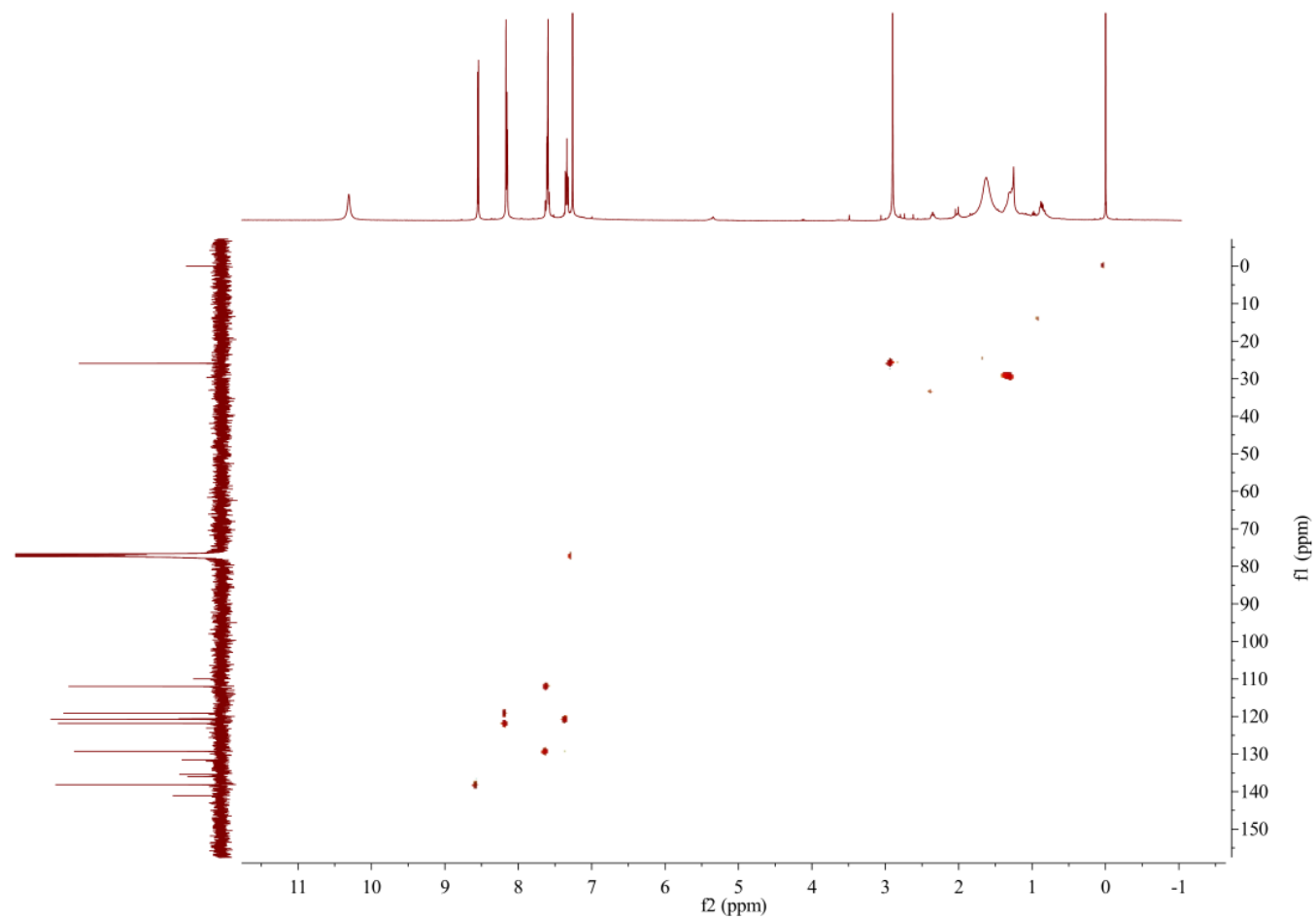


Figure S61. HMQC spectrum of 1-acetyl- β -carboline (**10**) in CDCl₃.

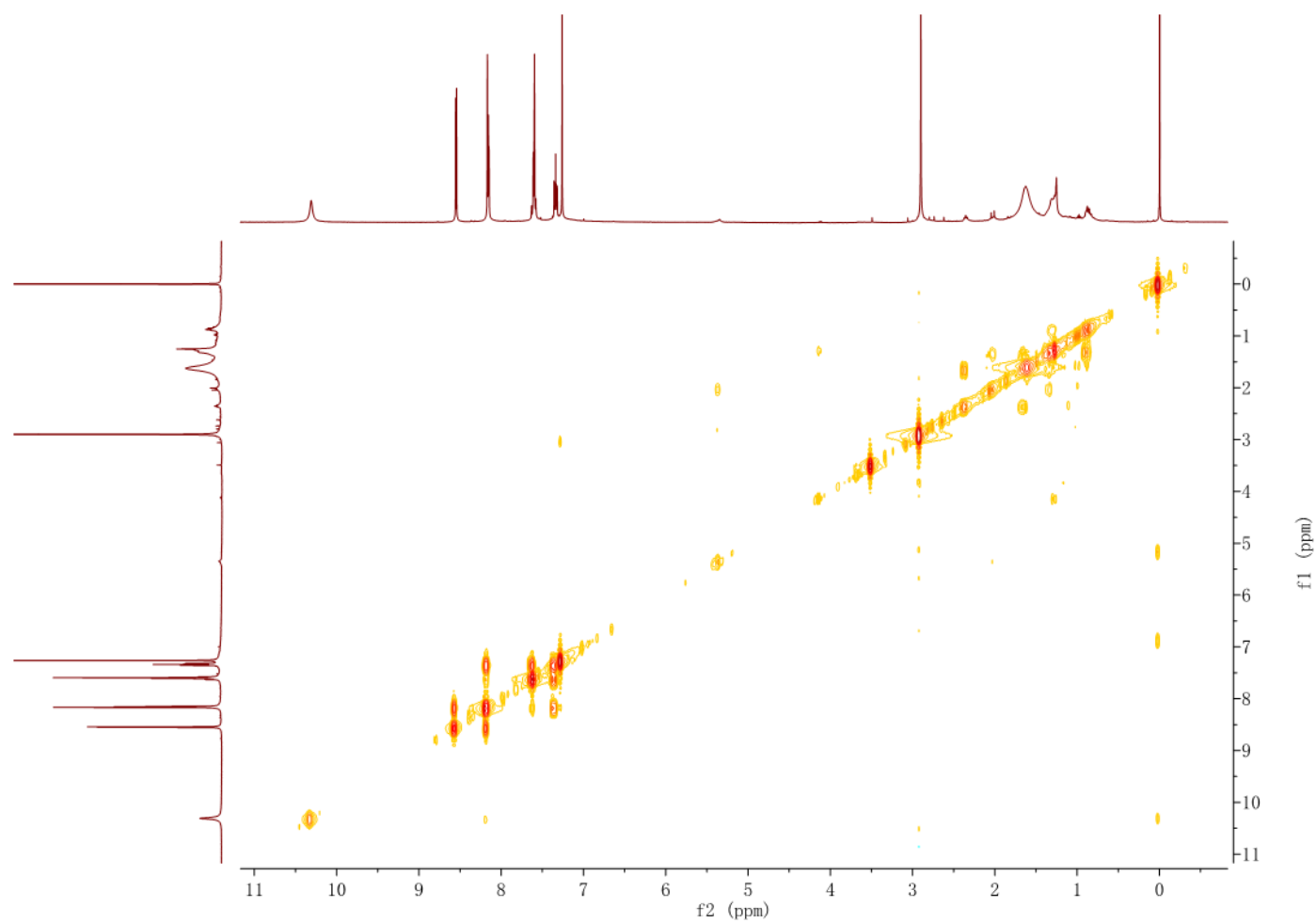


Figure S62. ^1H - ^1H COSY spectrum of 1-acetyl- β -carboline (**10**) in CDCl_3 .

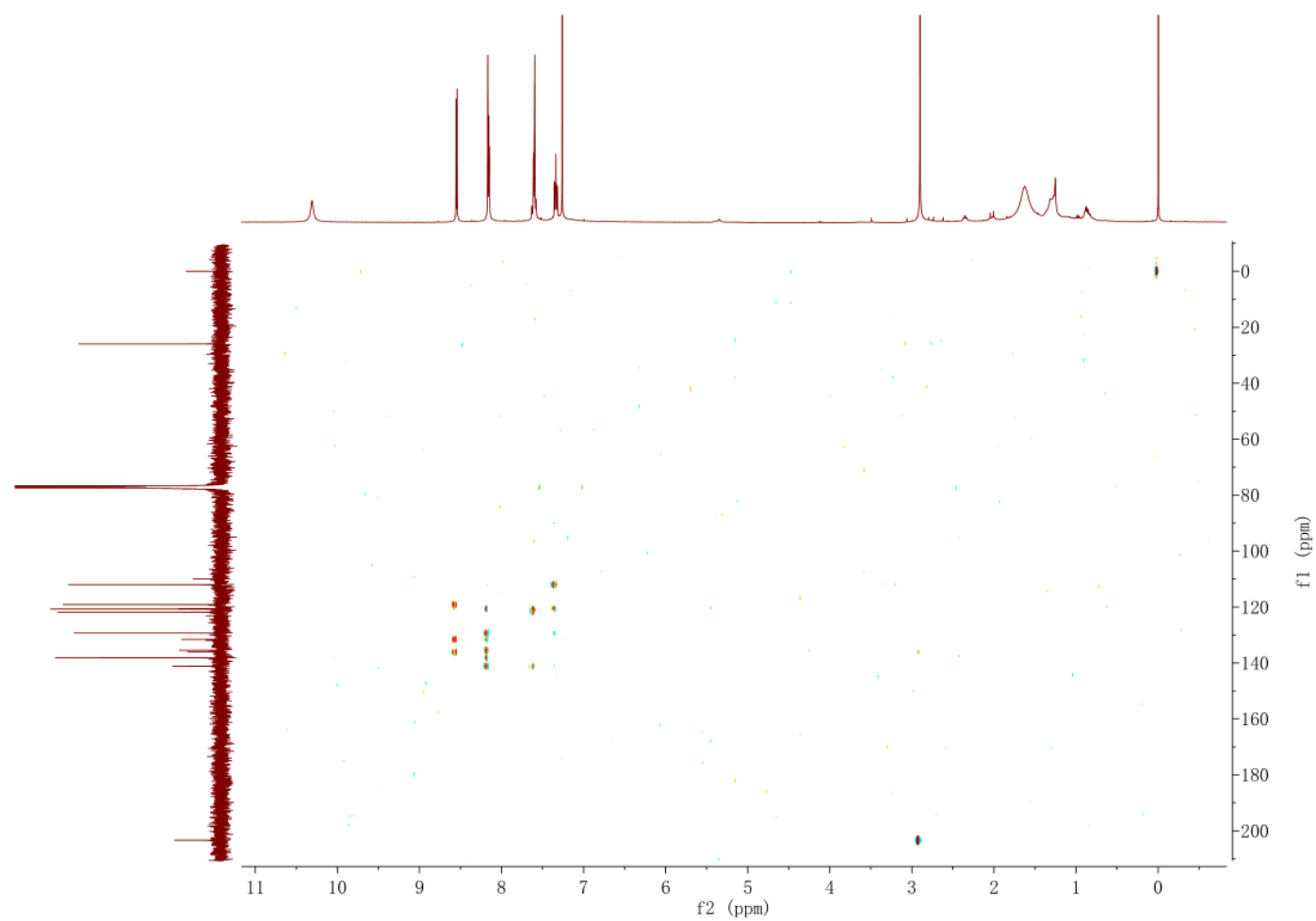


Figure S63. HMBC spectrum of 1-acetyl- β -carboline (**10**) in CDCl_3 .

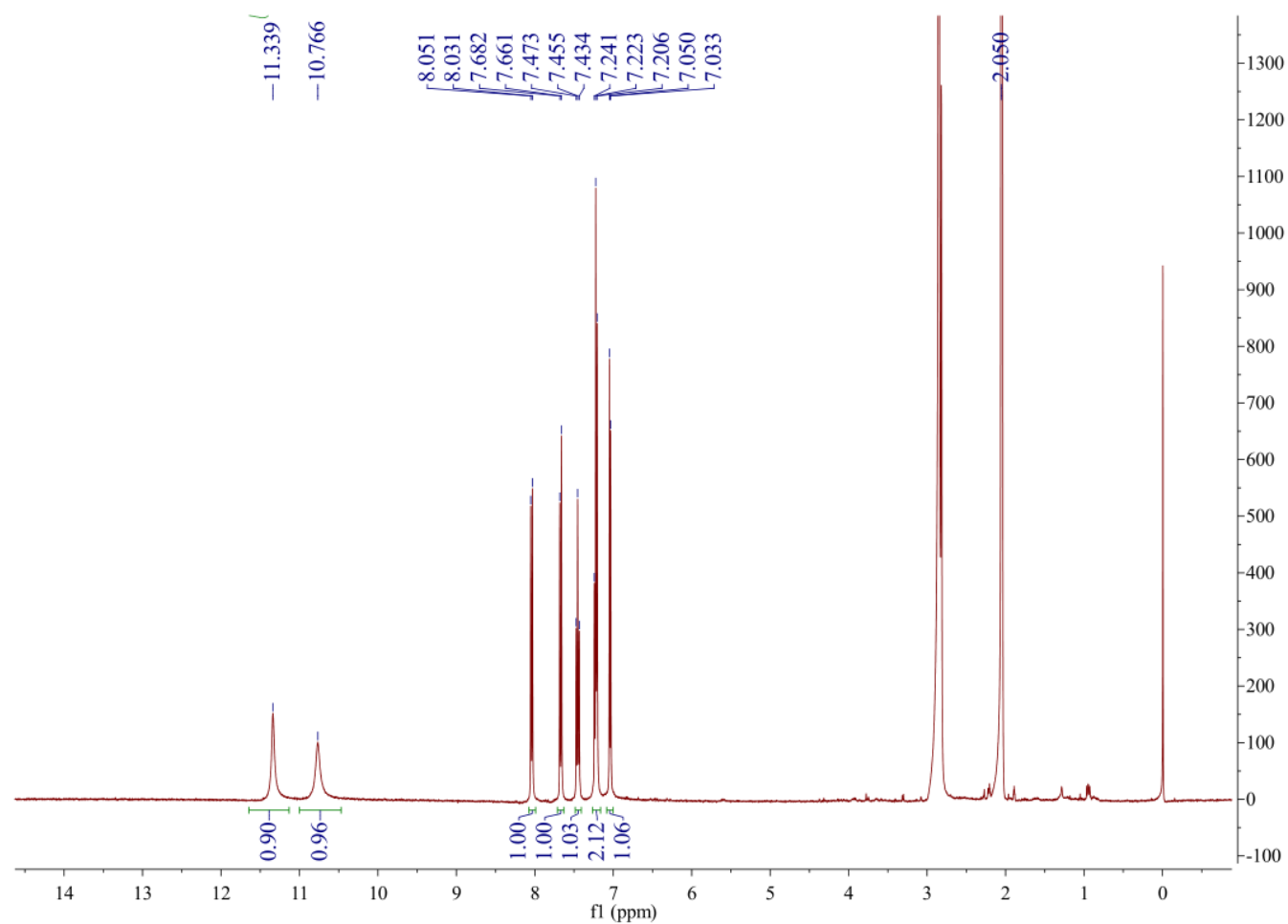


Figure S64. ^1H NMR spectrum of 3-hydroxy- β -carboline (**11**) in acetone- d_6 (400 MHz).

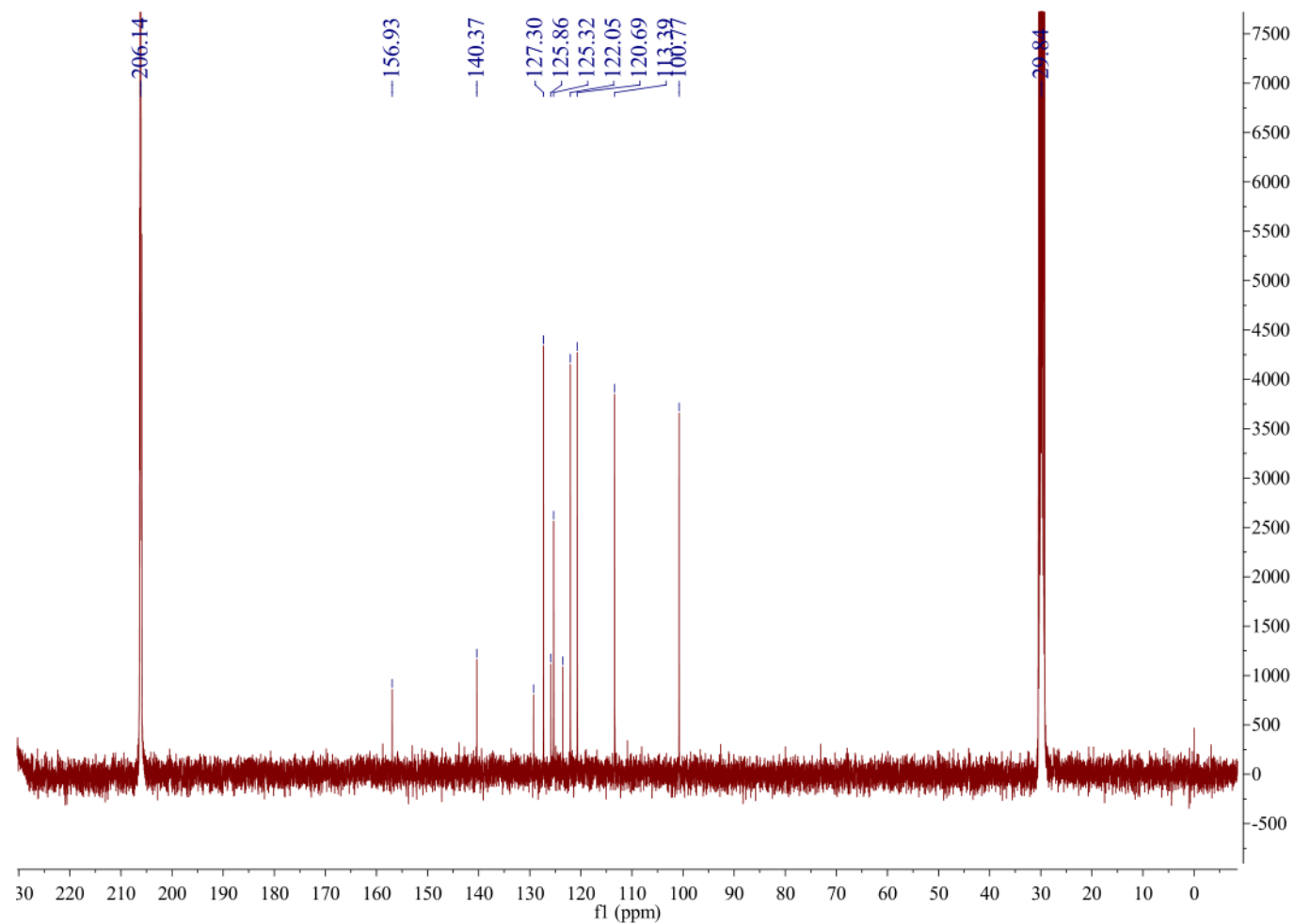


Figure S65. ^{13}C NMR spectrum of 3-hydroxy- β -carboline (**11**) in acetone- d_6 (100 MHz).

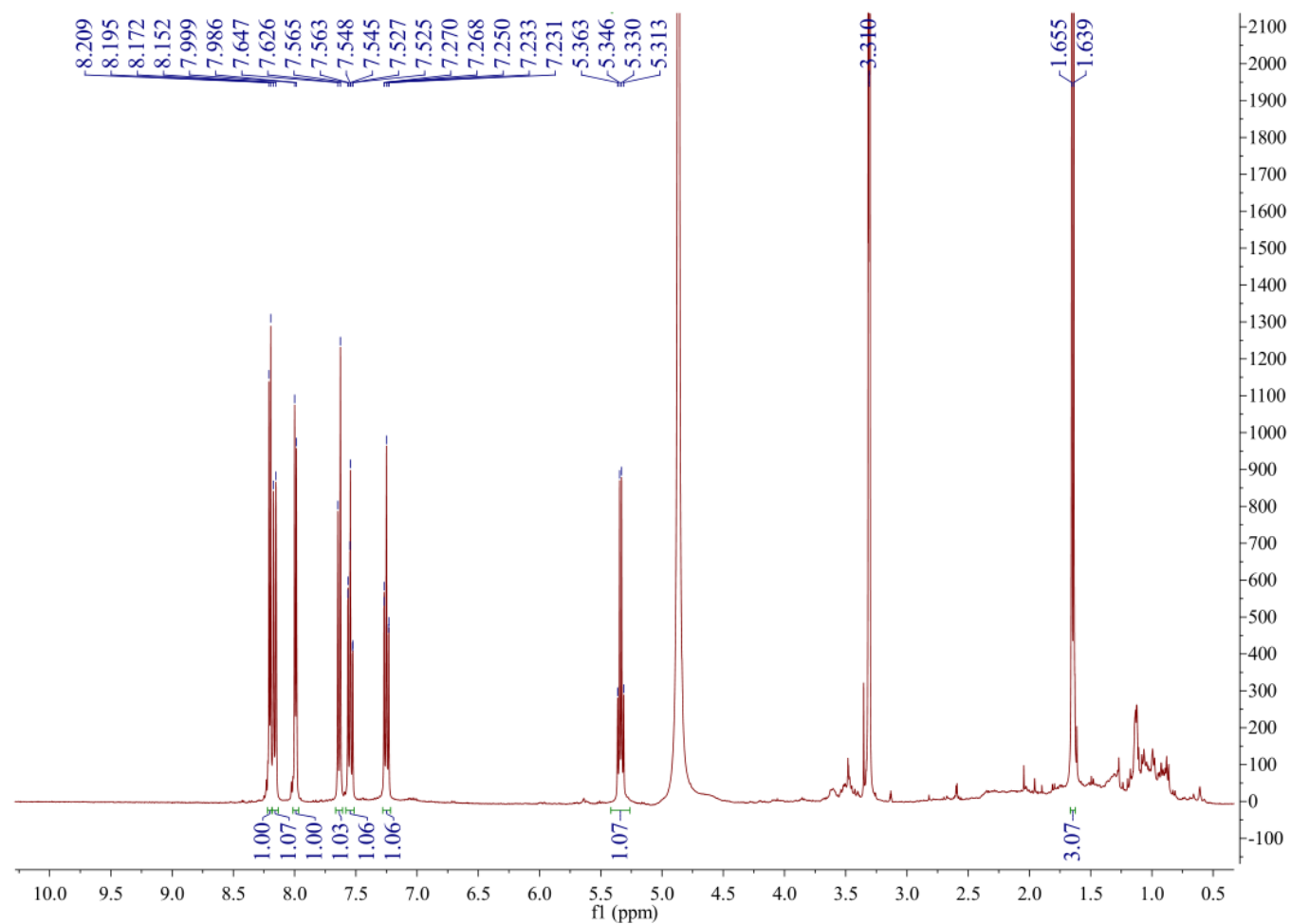


Figure S66. ^1H NMR spectrum of 1-(9*H*-pyrido [3,4-*b*] indol-1-yl) ethan-1-ol (**12**) in methanol- d_4 (400 MHz).

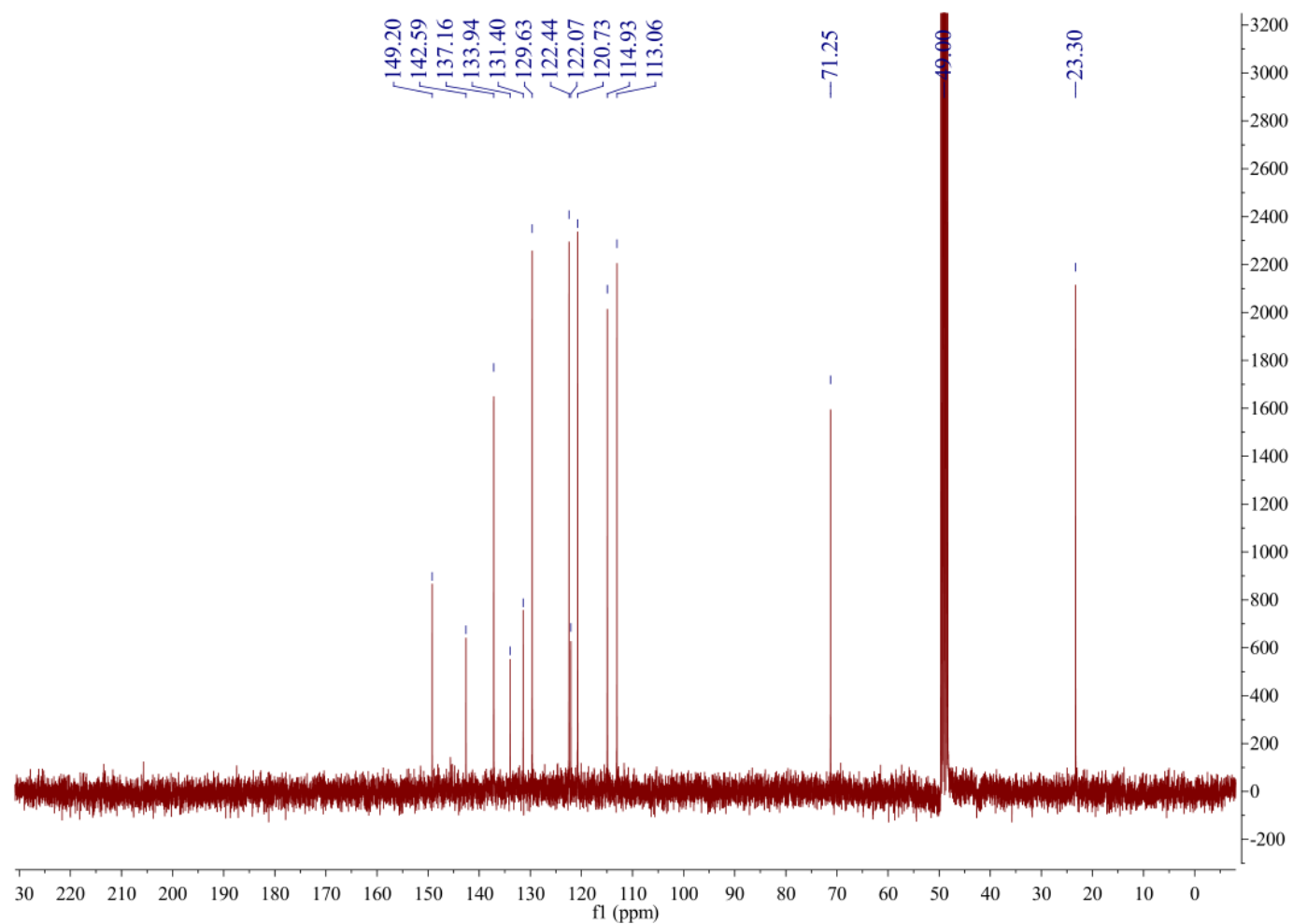


Figure S67. ^{13}C NMR spectrum of 1-(9H-pyrido [3,4-b] indol-1-yl) ethan-1-ol (**12**) in methanol- d_4 (100 MHz).

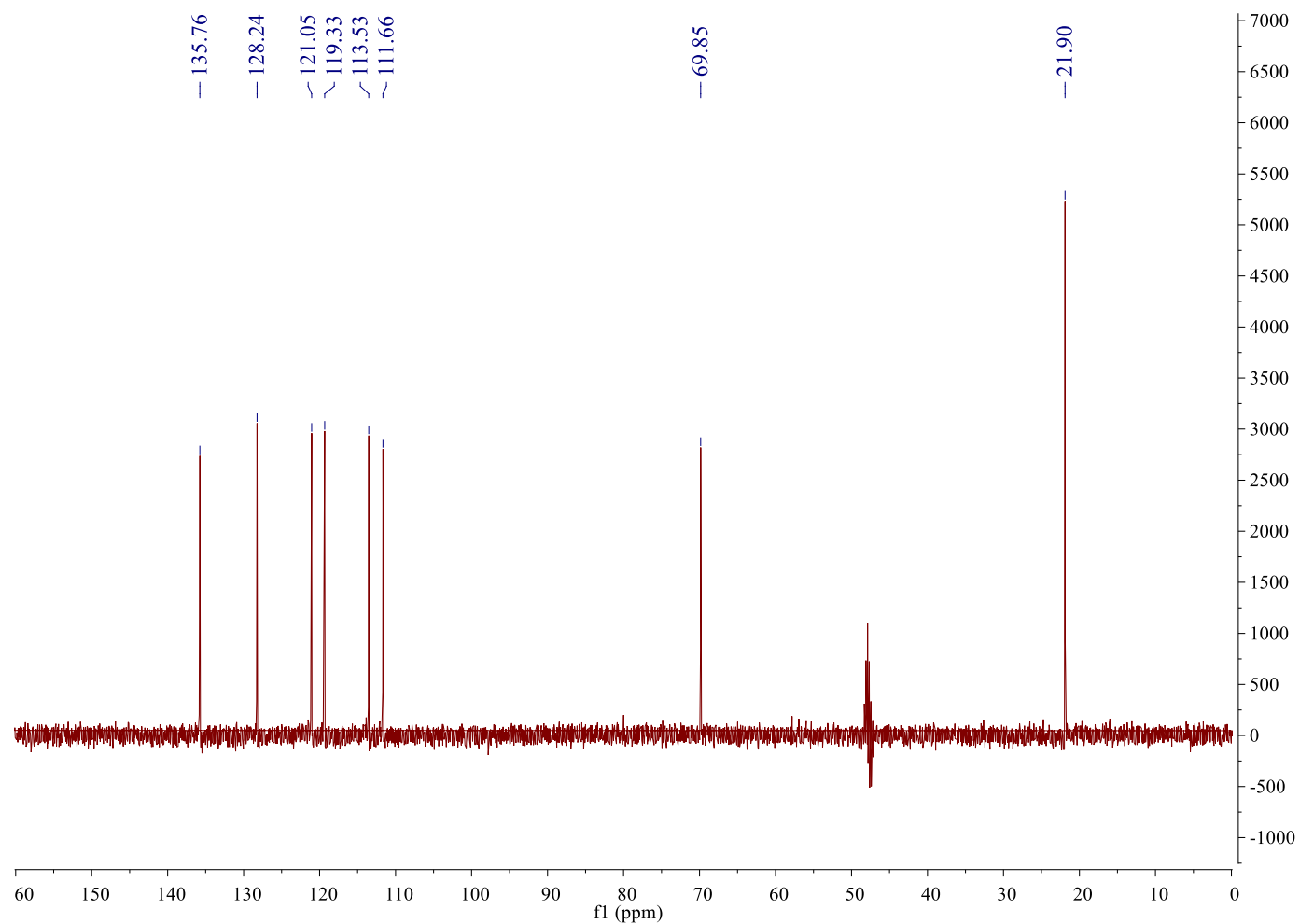


Figure S68. DEPT 135 spectrum of 1-(9H-pyrido [3,4-b] indol-1-yl) ethan-1-ol (**12**) in methanol-*d*₄ (100 MHz).

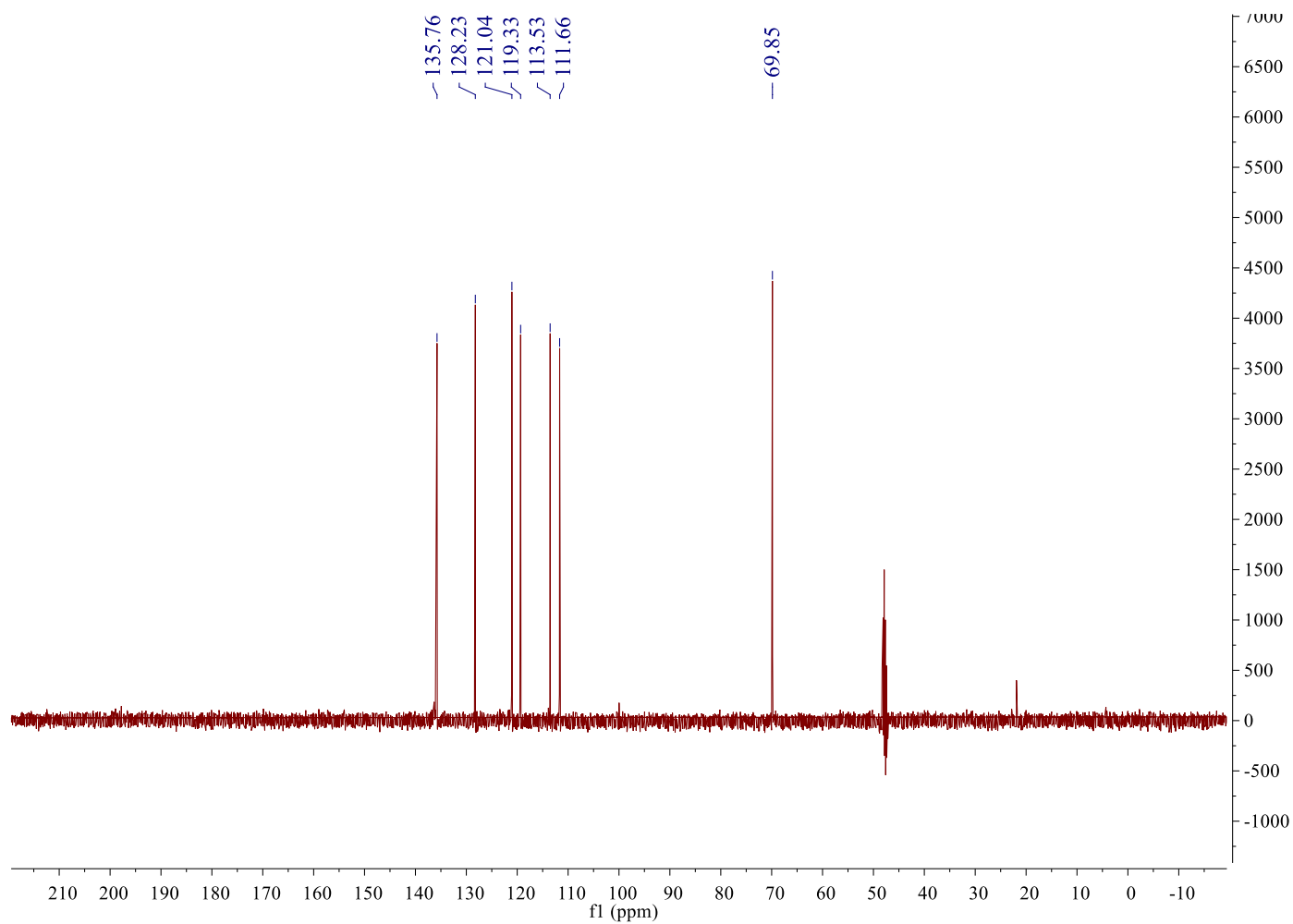


Figure S69. DEPT 90 spectrum of 1-(9H-pyrido [3,4-b] indol-1-yl) ethan-1-ol (**12**) in methanol-*d*₄ (100 MHz).

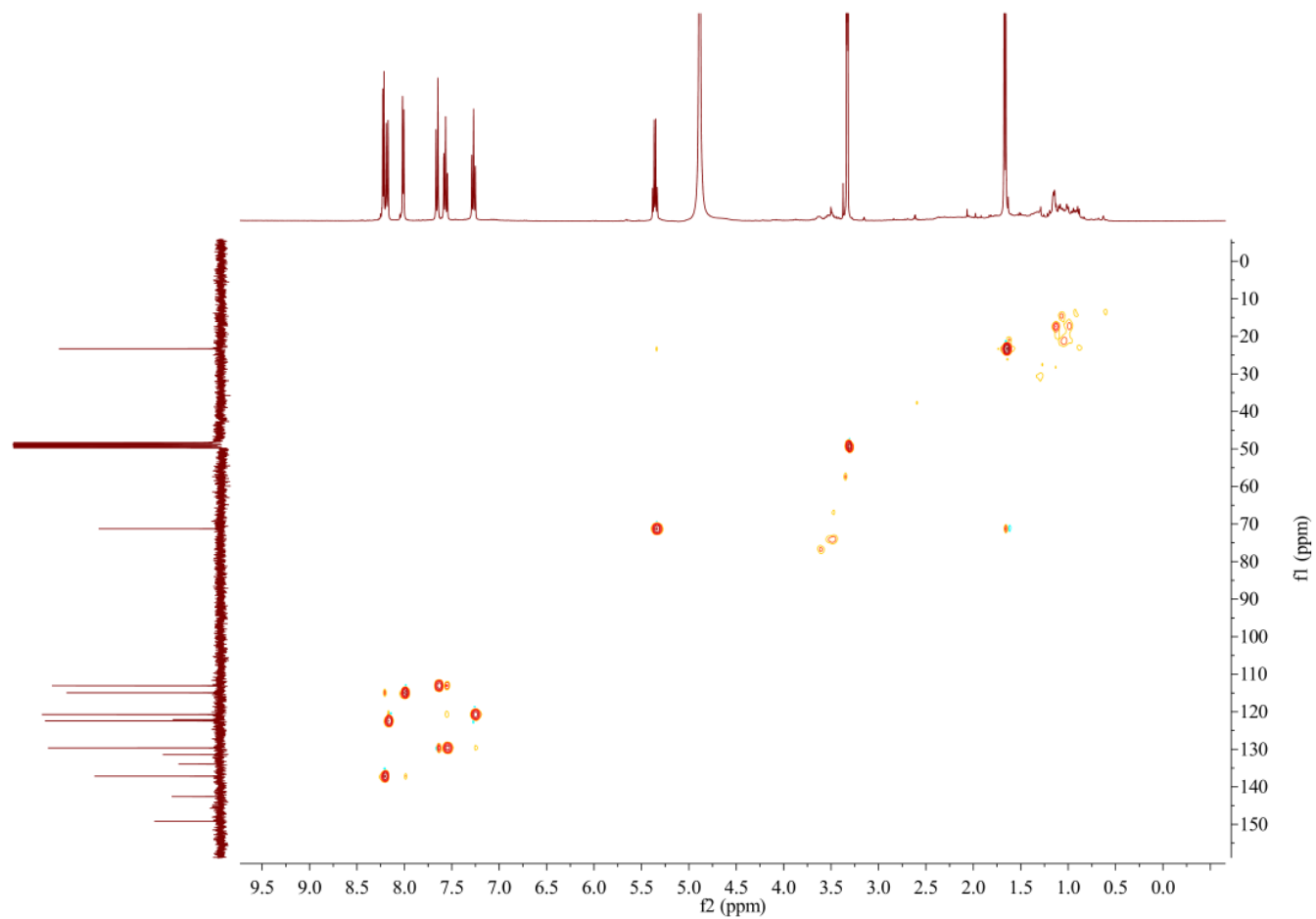


Figure S70. HMQC spectrum of 1-(9*H*-pyrido [3,4-*b*] indol-1-yl) ethan-1-ol (**12**) in methanol-*d*₄.

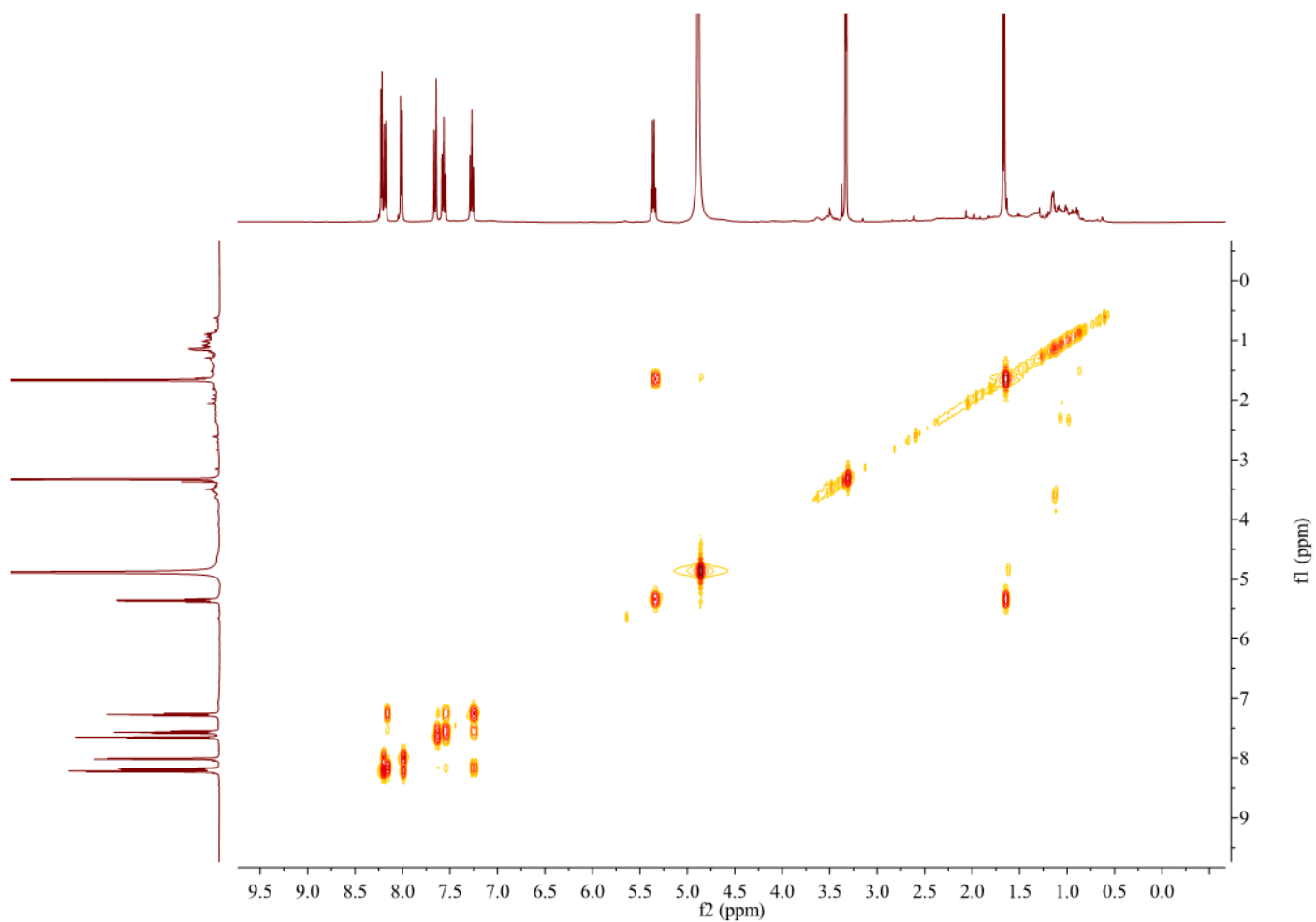


Figure S71. ^1H - ^1H COSY spectrum of 1-(9*H*-pyrido [3,4-*b*] indol-1-yl) ethan-1-ol (**12**) in methanol- d_4 .

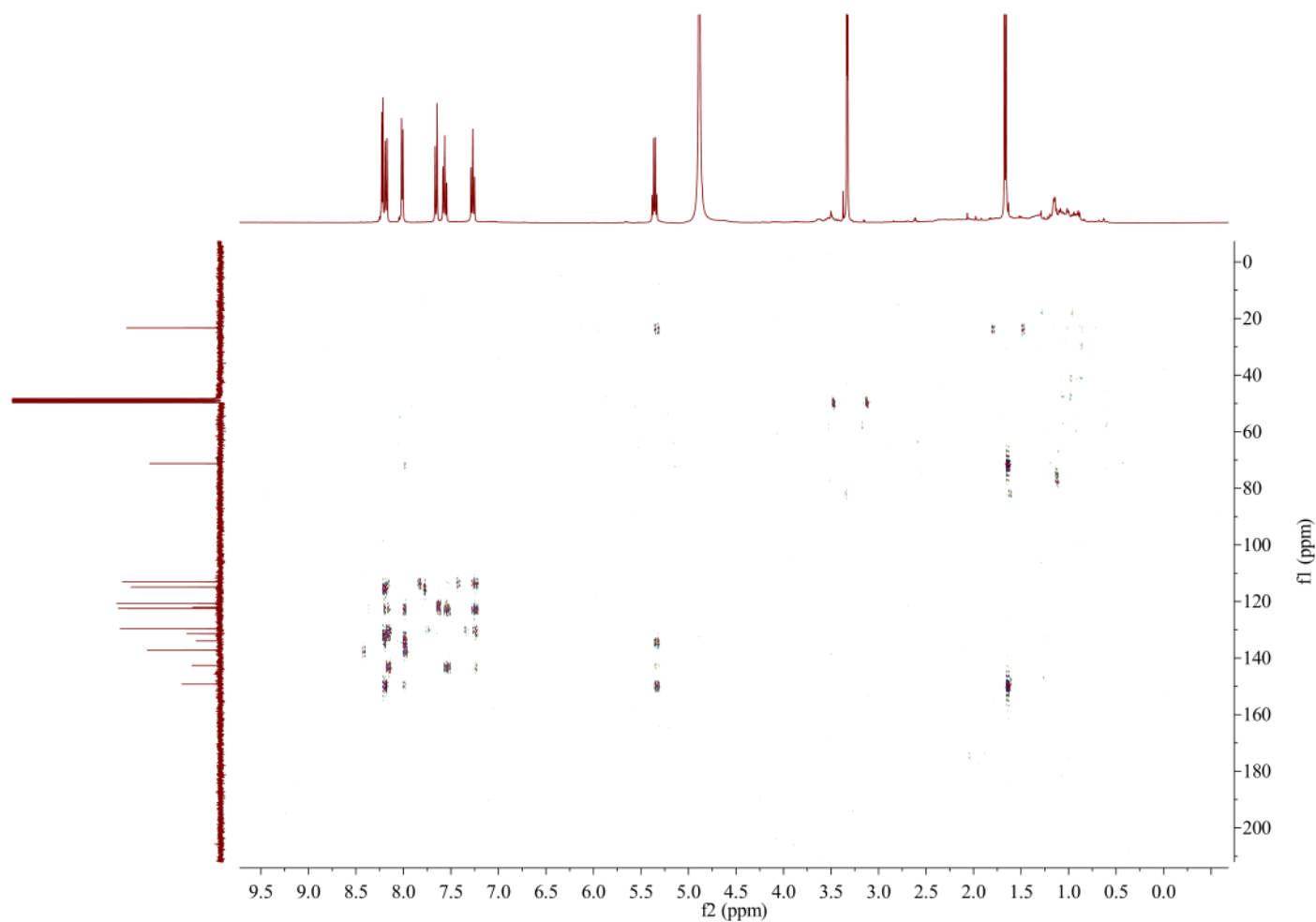


Figure S72. HMBC spectrum of 1-(9*H*-pyrido [3,4-*b*] indol-1-yl) ethan-1-ol (**12**) in methanol-*d*₄.

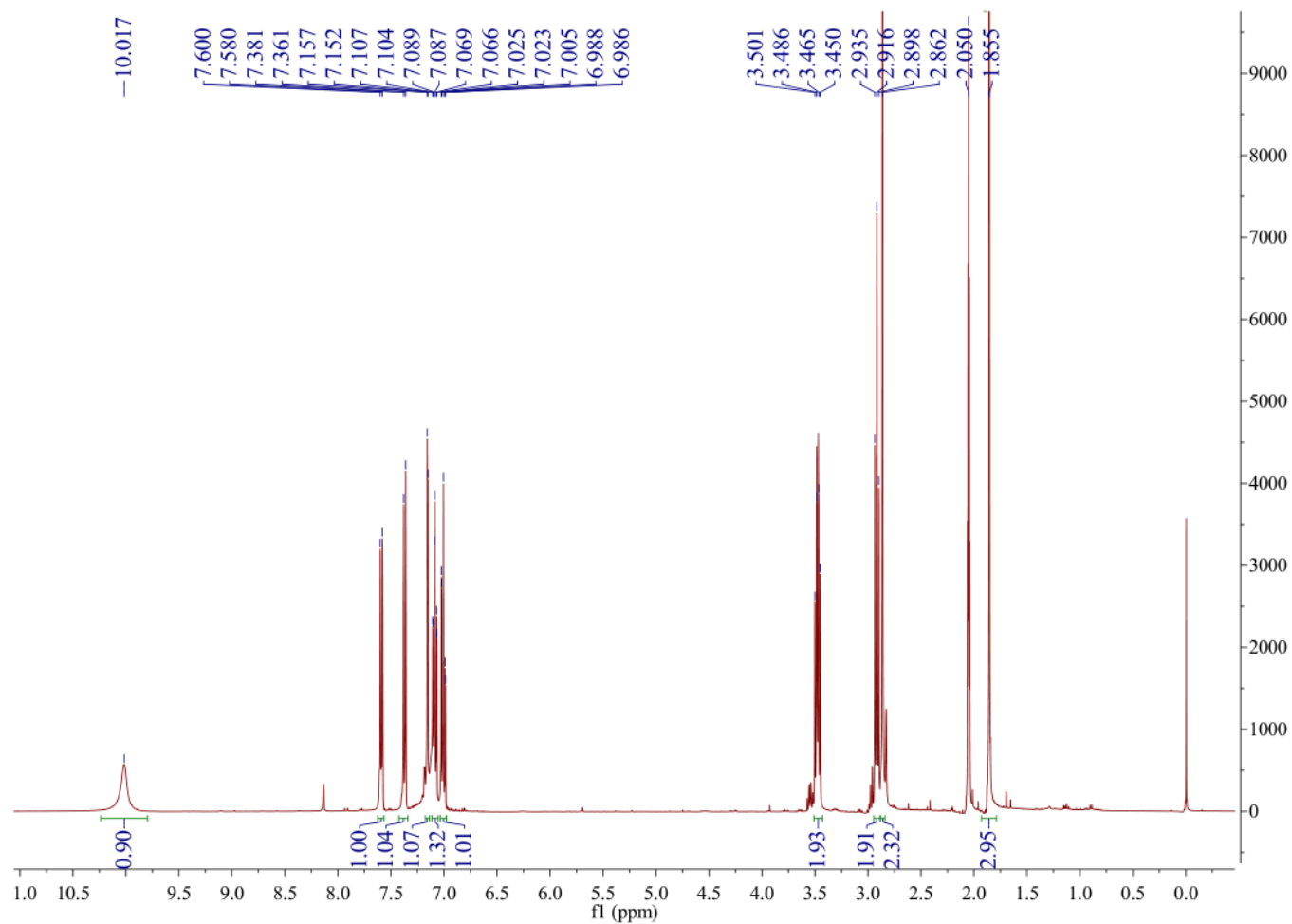


Figure S73. ¹H NMR spectrum of Nb-acetyltryptamine (**13**) in acetone-*d*₆ (400 MHz).

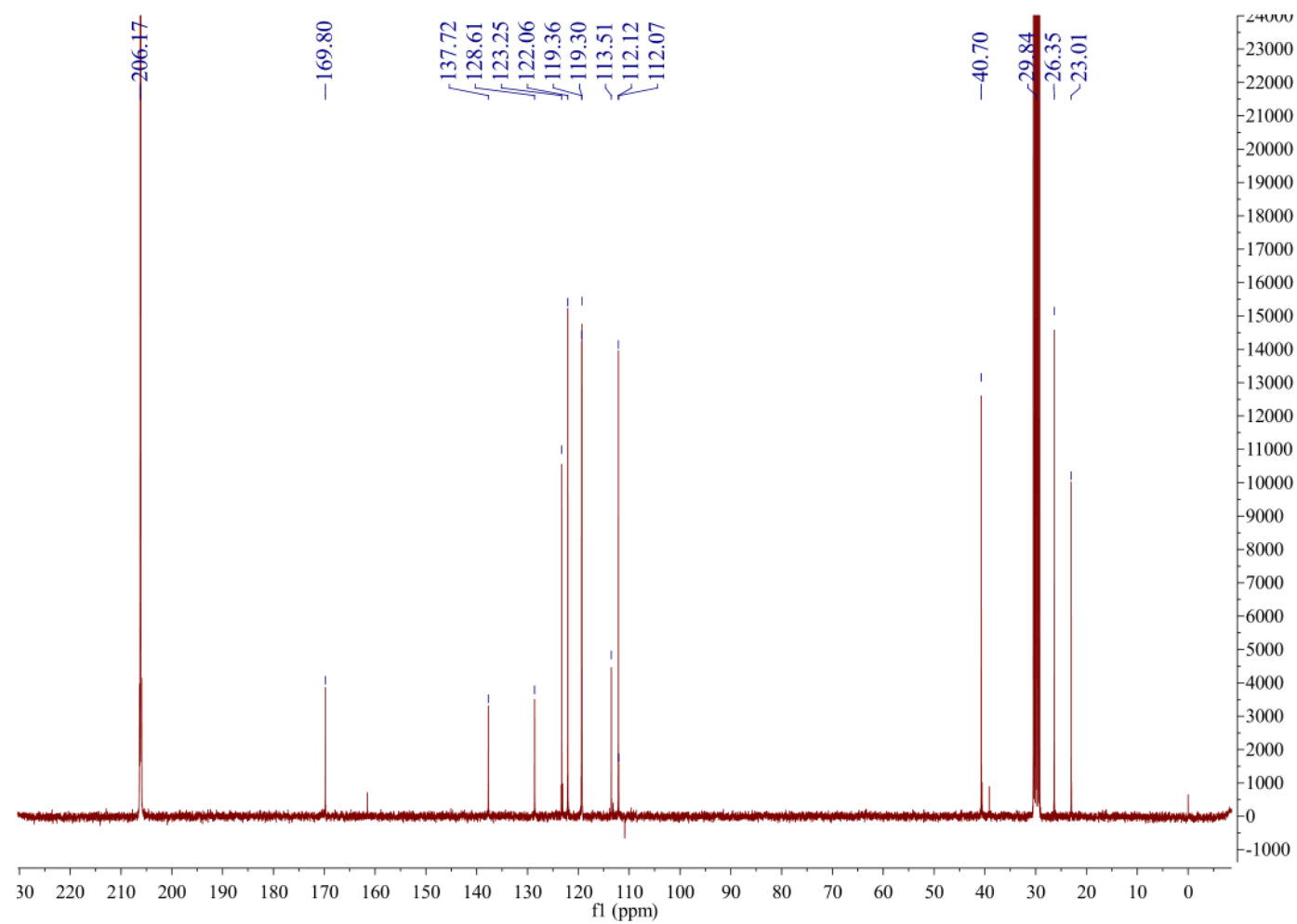


Figure S74. ^{13}C NMR spectrum of N_b -acetyltryptamine (**13**) in acetone- d_6 (100 MHz).