

Supplementary Data

Isochromans and Related Constituents from an Endophytic Fungus *Annulohypoxylon truncatum* of *Zizania caduciflora* and Their Anti-inflammatory Effects

Wei Li,[†] Changyeol Lee,[‡] Sung Hee Bang,[‡] Jin Yeul Ma,[†] Soonok Kim,[§] Young-Sang Koh^{||}, and Sang Hee Shim^{‡,*}

[†] KM Application Center, Korea Institute of Oriental Medicine, Daegu 41062, Republic of Korea

[‡] College of Pharmacy, Duksung Women's University, Seoul 01369, Republic of Korea

[§] National Institute of Biological Resources, Incheon 22689, Republic of Korea

^{||} School of Medicine and Brain Korea 21 PLUS Program, and Institute of Medical Science, Jeju National University, Jeju 690-756, Republic of Korea

*Correspondence to:

Sang Hee Shim Ph.D.

College of Pharmacy, Duksung Women's University, Seoul 01369, Republic of Korea.

Tel.: +82 2 901 8774. Fax: +82 2 901 8386 E-mail address: sangheeshim@duksung.ac.kr(S. H. Shim).

Contents

Figure S1. HR-ESI-MS spectrum of compound 1 -----	5
Figure S2. ^1H NMR spectrum of compound 1 in pyridine- d_5 (600 MHz) -----	6
Figure S3. ^{13}C NMR spectrum of compound 1 in pyridine- d_5 (150 MHz) -----	7
Figure S4. HMQC spectrum of compound 1 -----	8
Figure S5. HMBC spectrum of compound 1 -----	9
Figure S6. COSY spectrum of compound 1 -----	10
Figure S7. NOESY spectrum of compound 1 -----	11
Figure S8. HR-ESI-MS spectrum of compound 2 -----	12
Figure S9. ^1H NMR spectrum of compound 2 in methanol- d_4 (600 MHz) -----	13
Figure S10. ^{13}C NMR spectrum of compound 2 in methanol- d_4 (150MHz) -----	14
Figure S11. HMQC spectrum of compound 2 -----	15
Figure S12. HMBC spectrum of compound 2 -----	16
Figure S13. COSY spectrum of compound 2 -----	17
Figure S14. NOESY spectrum of compound 2 -----	18
Figure S15. HR-ESI-MS spectrum of compound 3 -----	19
Figure S16. ^1H NMR spectrum of compound 3 in methanol- d_4 (600 MHz) -----	20
Figure S17. ^{13}C NMR spectrum of compound 3 in methanol- d_4 (150MHz) -----	21
Figure S18. HMQC spectrum of compound 3 -----	22
Figure S19. HMBC spectrum of compound 3 -----	23

Figure S20. COSY spectrum of compound 3	24
Figure S21. NOESY spectrum of compound 3	25
Figure S22. HR-ESI-MS spectrum of compound 4	26
Figure S23. ^1H NMR spectrum of compound 4 in chloroform- <i>d</i> (600 MHz)	27
Figure S24. ^{13}C NMR spectrum of compound 4 in chloroform- <i>d</i> (150MHz)	28
Figure S25. HMQC spectrum of compound 4	29
Figure S26. HMBC spectrum of compound 4	30
Figure S27. COSY spectrum of compound 4	31
Figure S28. NOESY spectrum of compound 4	32
Figure S29. HR-ESI-MS spectrum of compound 6	33
Figure S30. ^1H NMR spectrum of compound 6 in pyridine- <i>d</i> ₅ (600 MHz)	34
Figure S31. ^{13}C NMR spectrum of compound 6 in pyridine- <i>d</i> ₅ (150 MHz)	35
Figure S32. HMQC spectrum of compound 6	36
Figure S33. HMBC spectrum of compound 6	37
Figure S34. COSY spectrum of compound 6	38
Figure S35. NOESY spectrum of compound 6	39
Figure S36. HR-ESI-MS spectrum of compound 7	40
Figure S37. ^1H NMR spectrum of compound 7 in pyridine- <i>d</i> ₅ (600 MHz)	41
Figure S38. ^{13}C NMR spectrum of compound 7 in pyridine- <i>d</i> ₅ (150 MHz)	42
Figure S39. HMQC spectrum of compound 7	43
Figure S40. HMBC spectrum of compound 7	44

Figure S41. COSY spectrum of compound 7 -----	45
Figure S42. NOESY spectrum of compound 7 -----	46
Figure S43. HR-ESI-MS spectrum of compound 8 -----	47
Figure S44. ^1H NMR spectrum of compound 8 in methanol- d_4 (600 MHz) -----	48
Figure S45. ^{13}C NMR spectrum of compound 8 in methanol- d_4 (150MHz) -----	49
Figure S46. HMQC spectrum of compound 8 -----	50
Figure S47. HMBC spectrum of compound 8 -----	51
Figure S48. COSY spectrum of compound 8 -----	52
Figure S49. NOESY spectrum of compound 8 -----	53

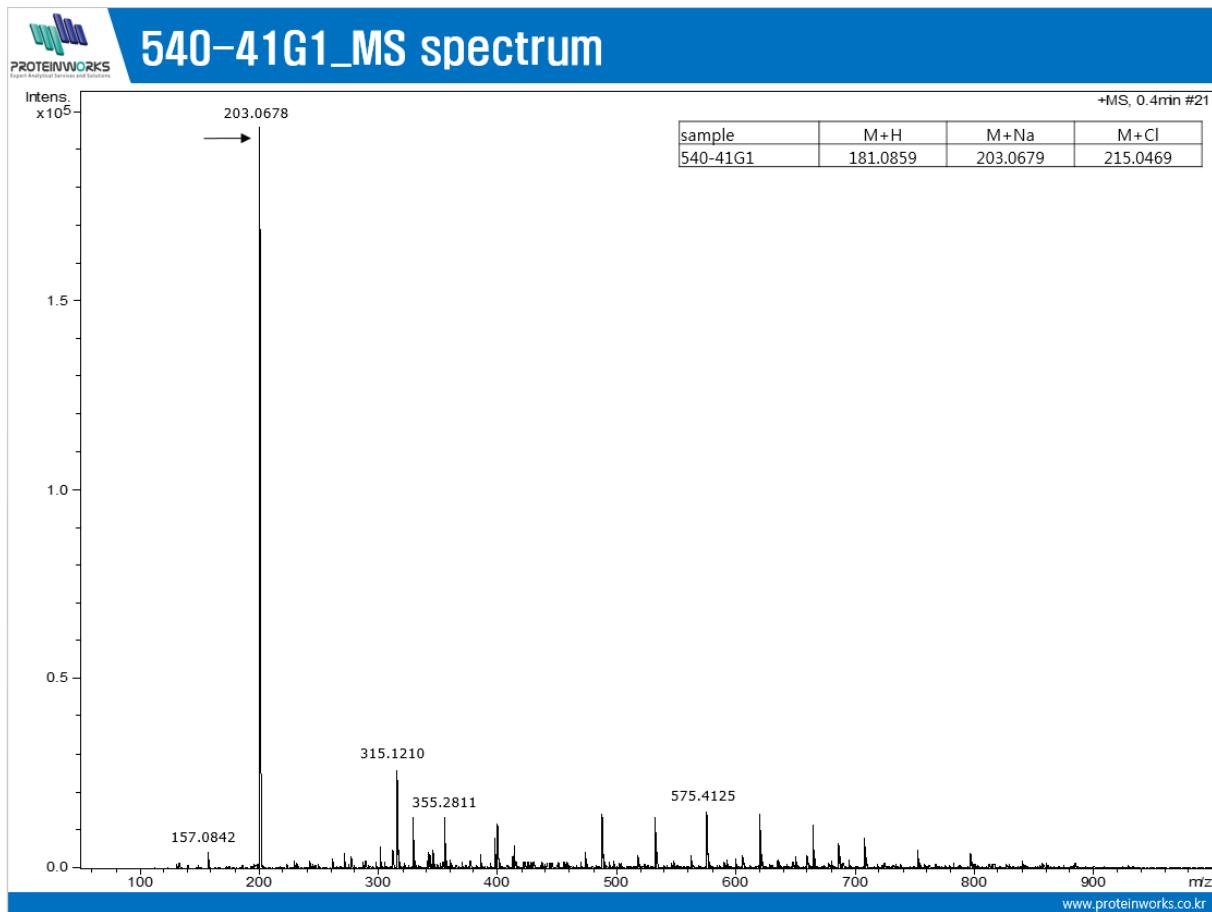


Figure S1. HR-ESI-MS spectrum of compound 1

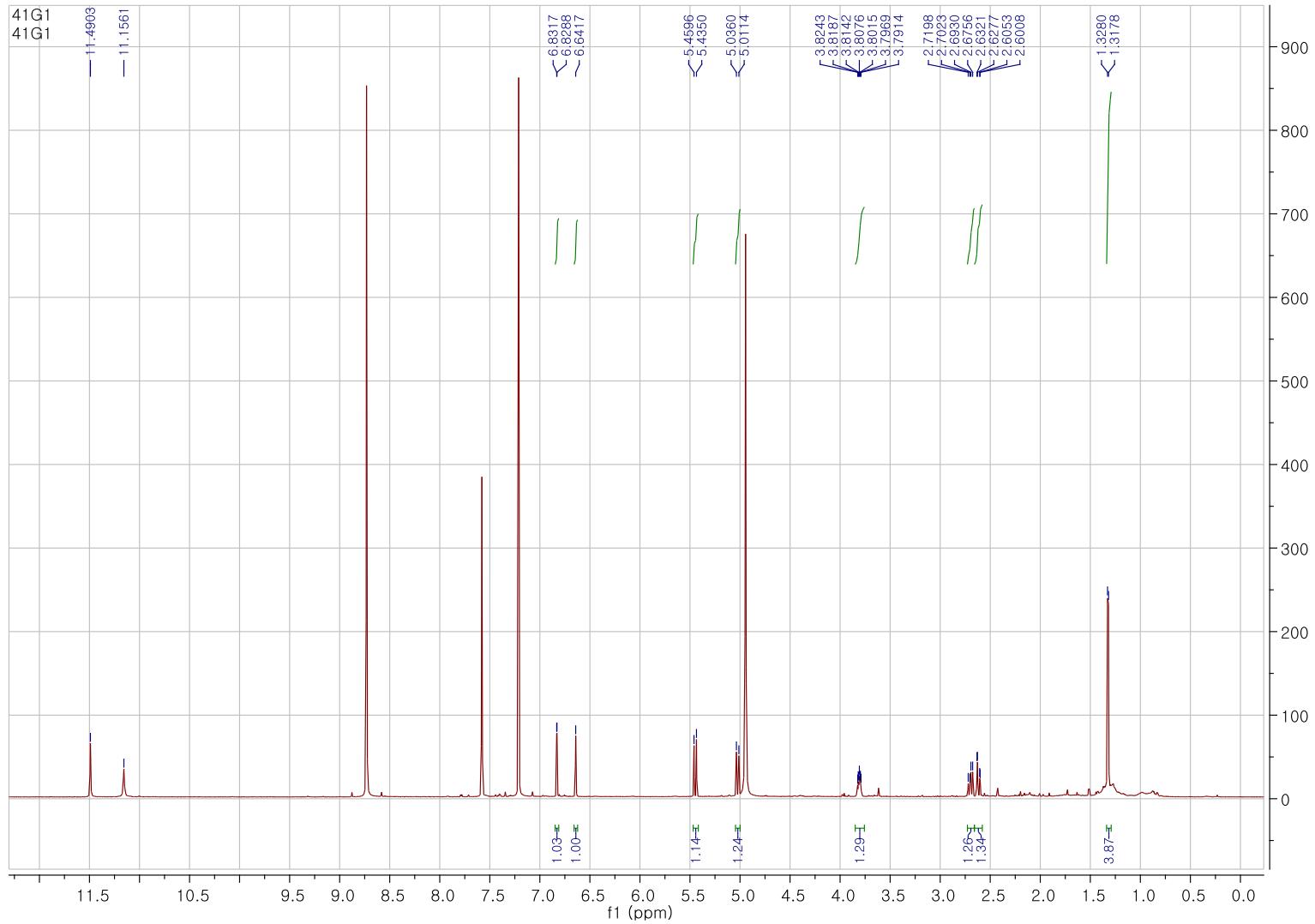


Figure S2. ^1H NMR spectrum of compound **1** in pyridine- d_5 (600 MHz)

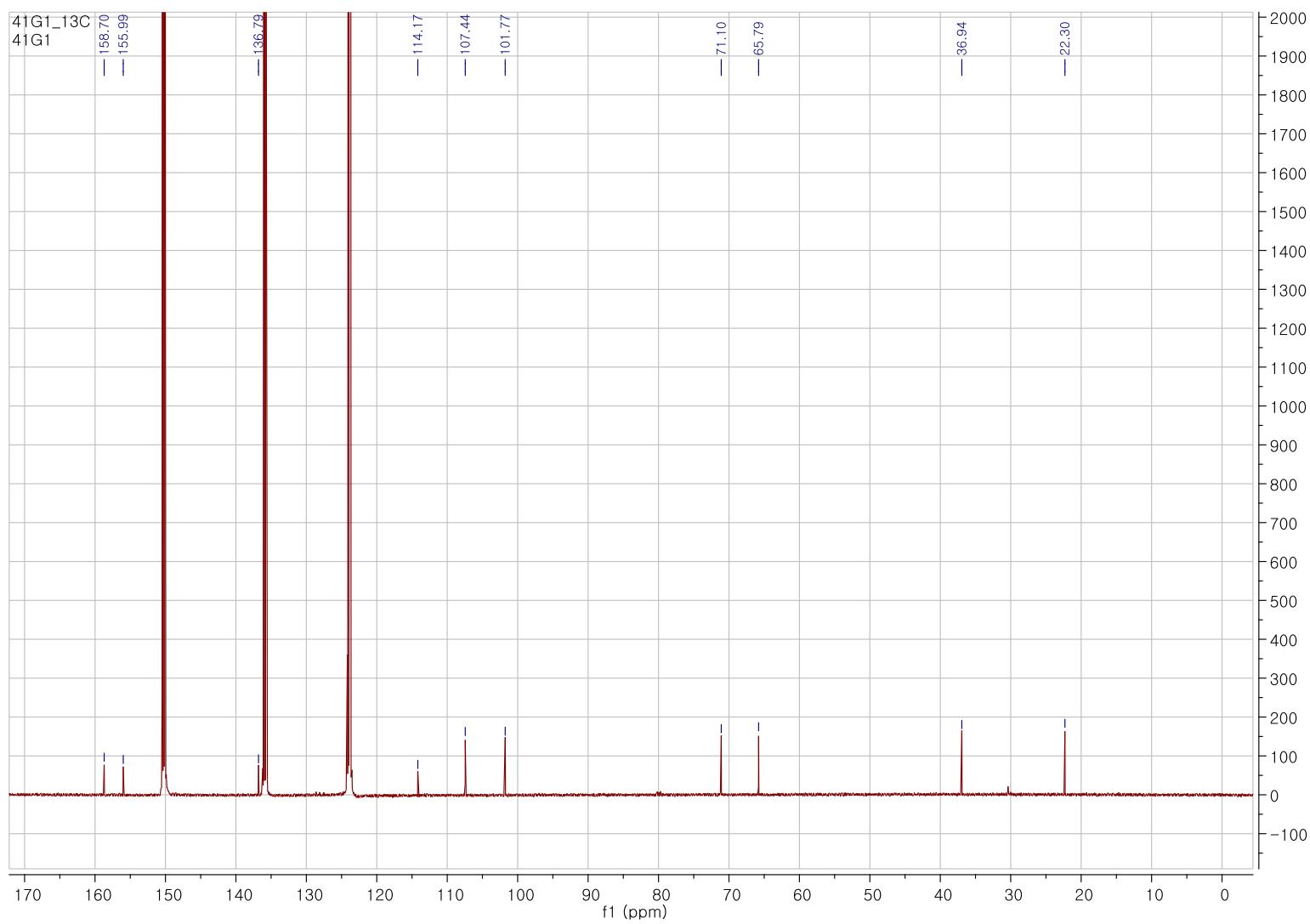


Figure S3. ^{13}C NMR spectrum of compound **1** in pyridine- d_5 (150 MHz)

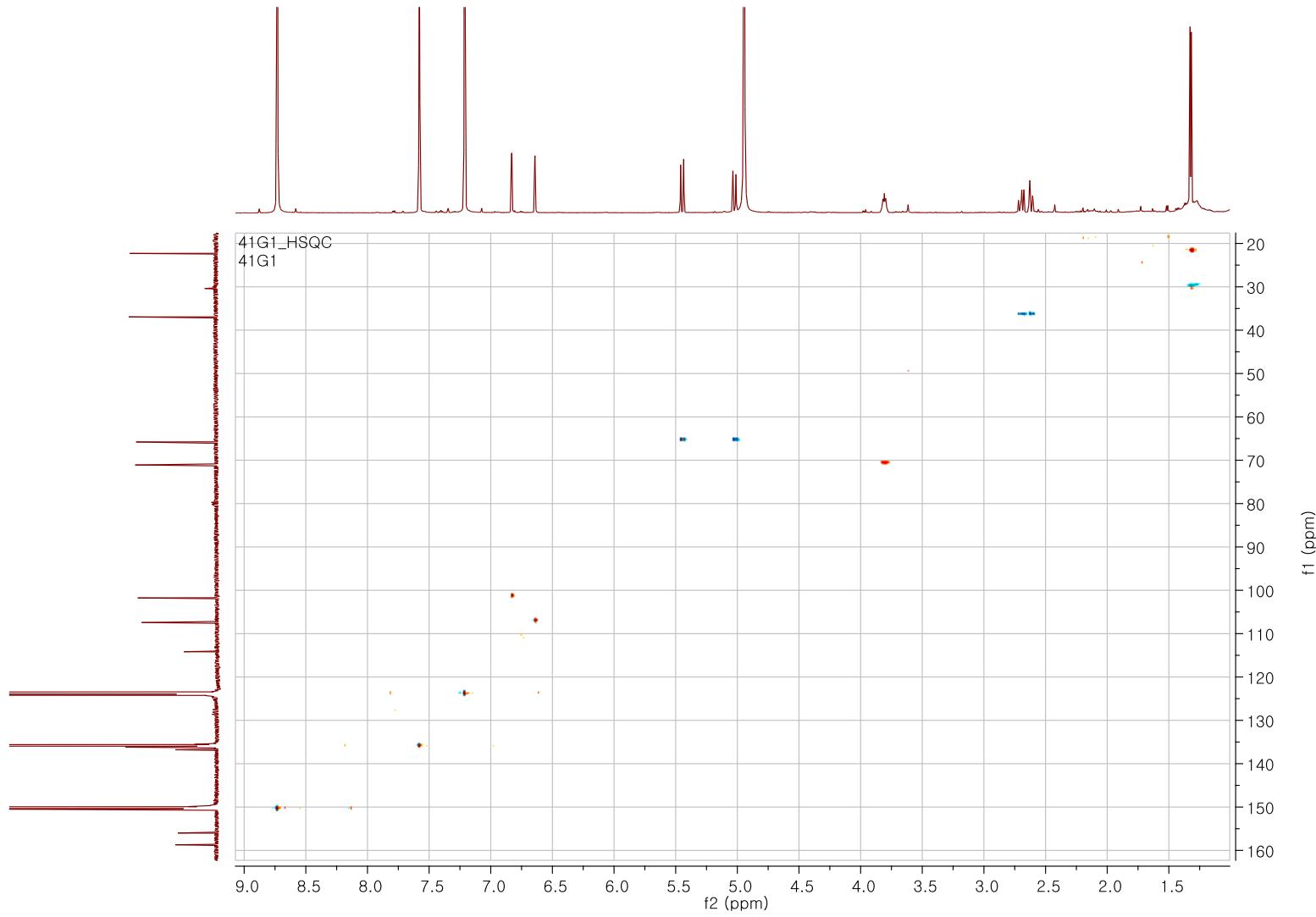


Figure S4. HMQC spectrum of compound **1**

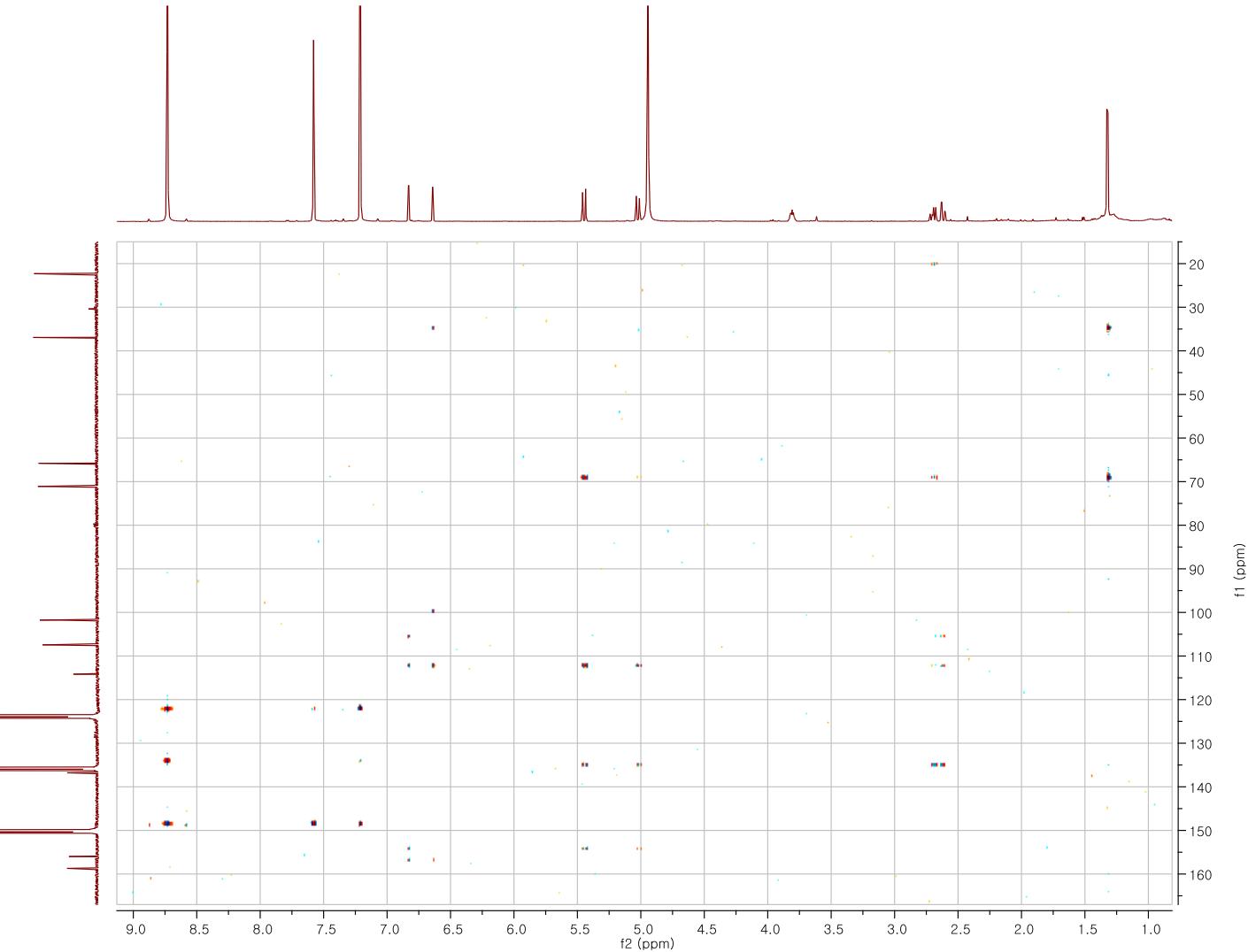


Figure S5. HMBC spectrum of compound **1**

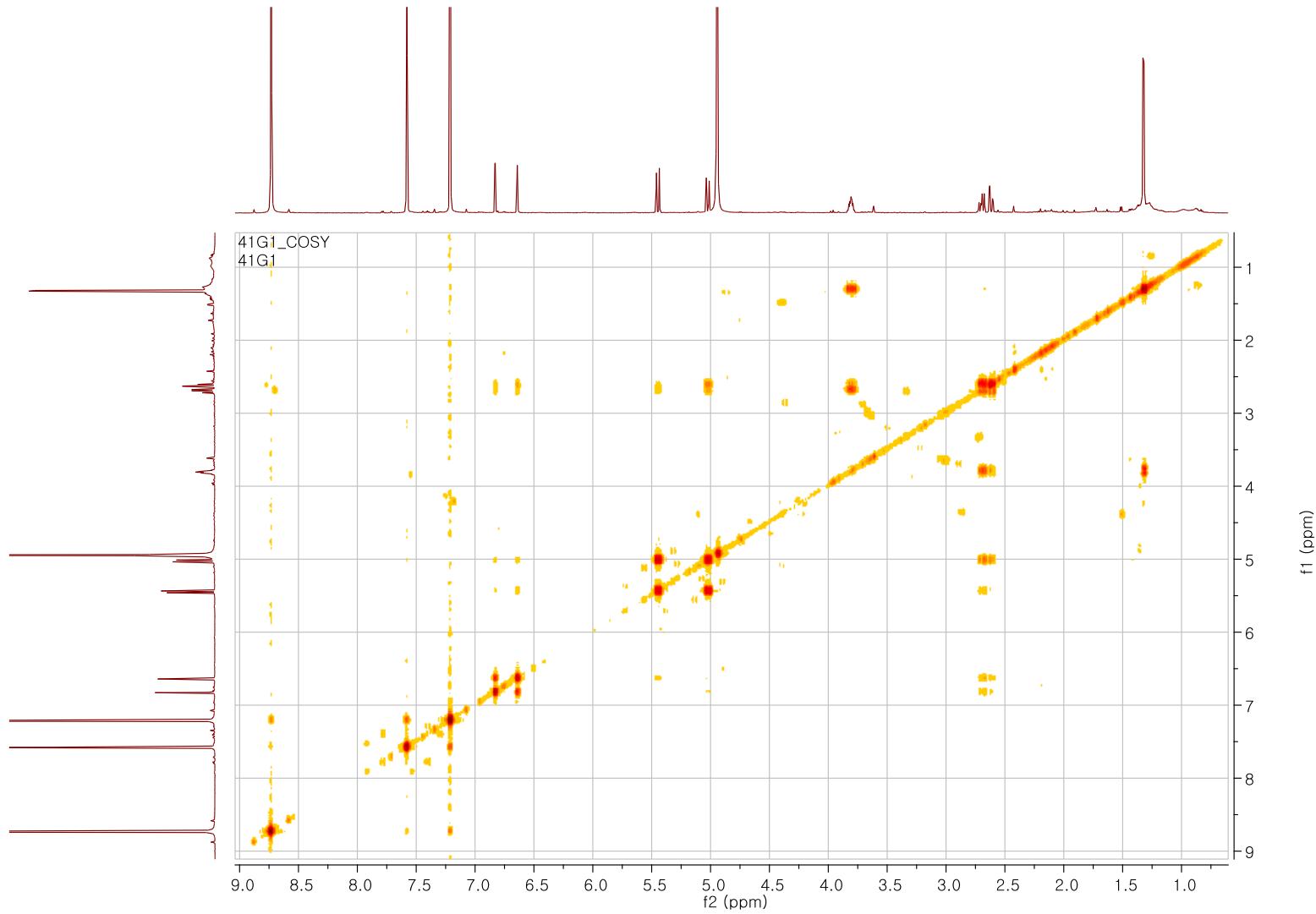


Figure S6. COSY spectrum of compound **1**

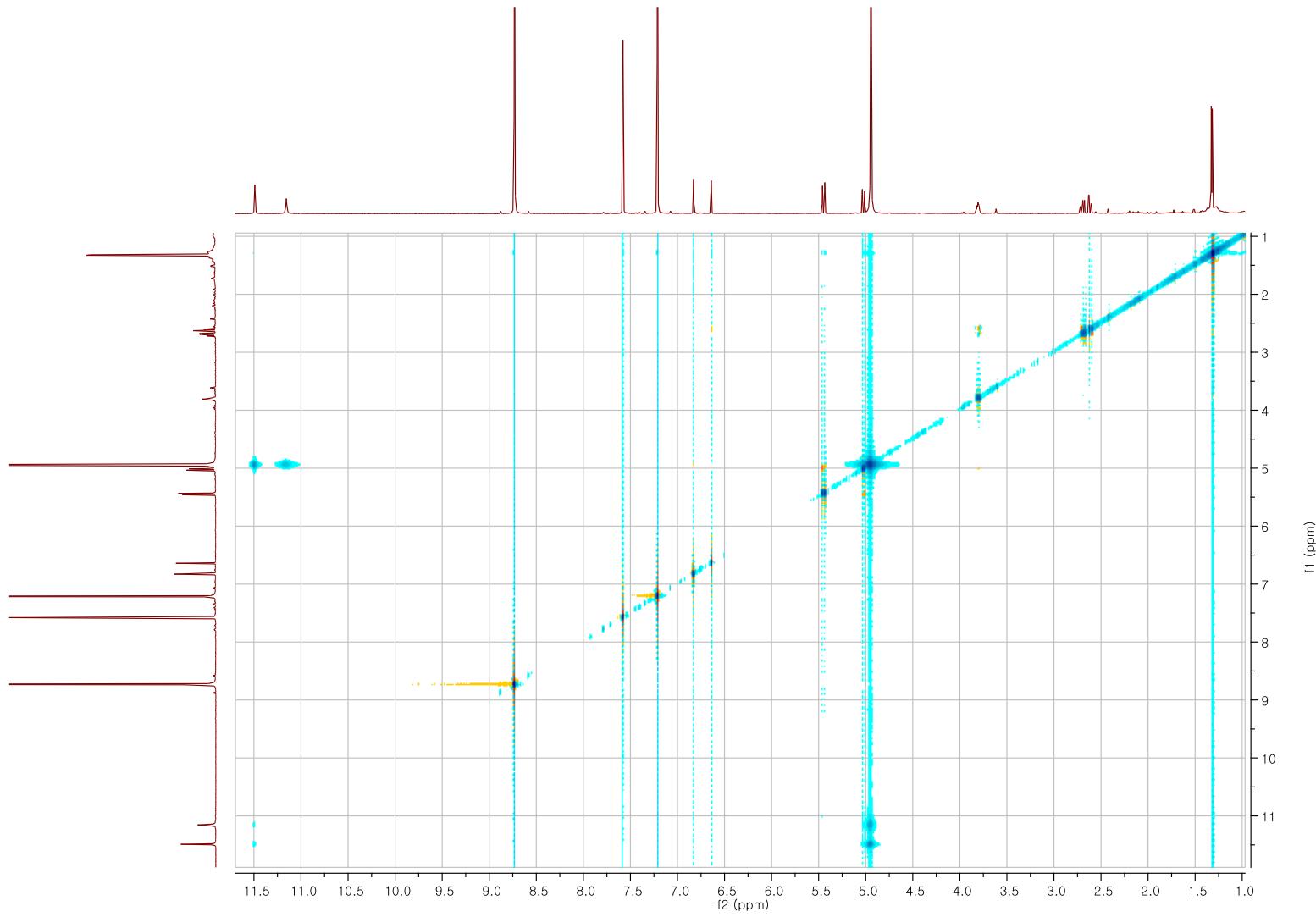


Figure S7. NOESY spectrum of compound **1**

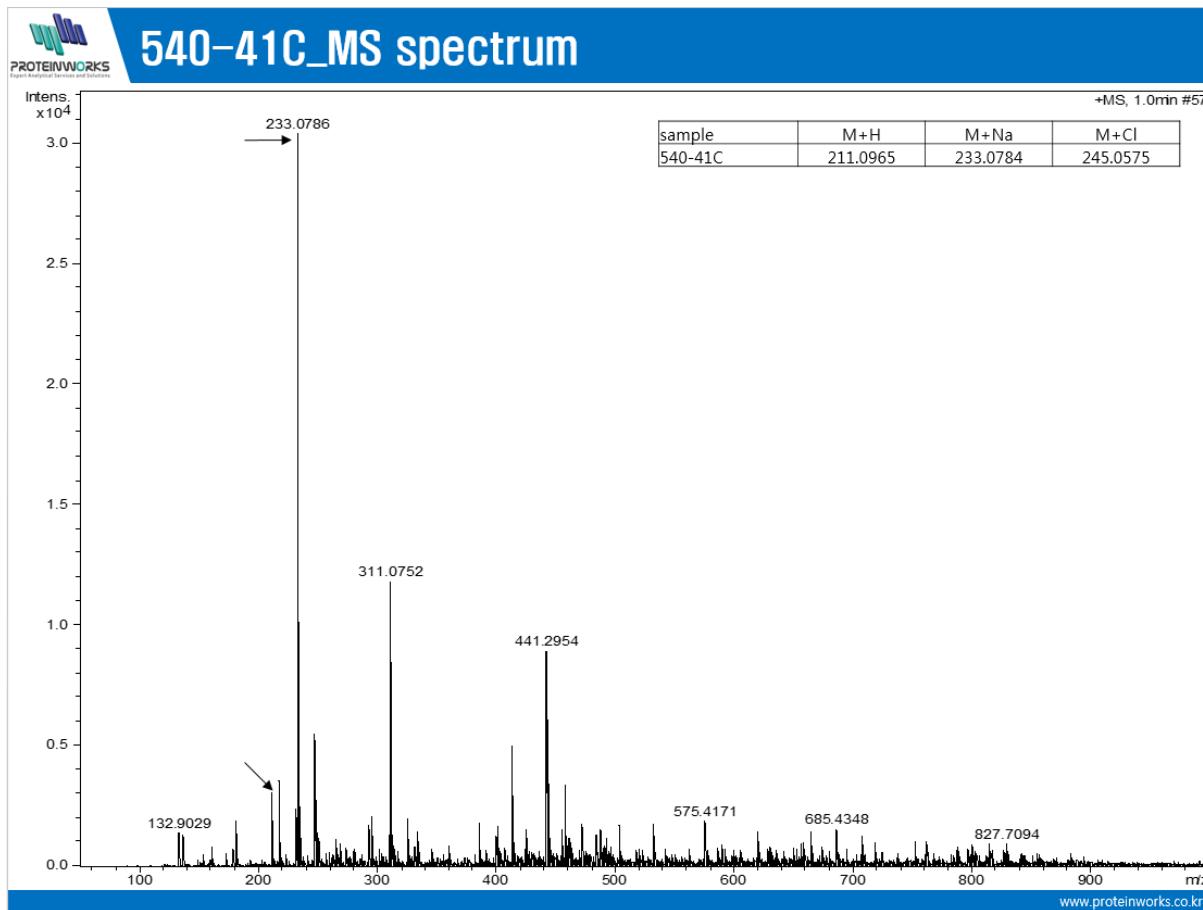


Figure S8. HR-ESI-MS spectrum of compound 2

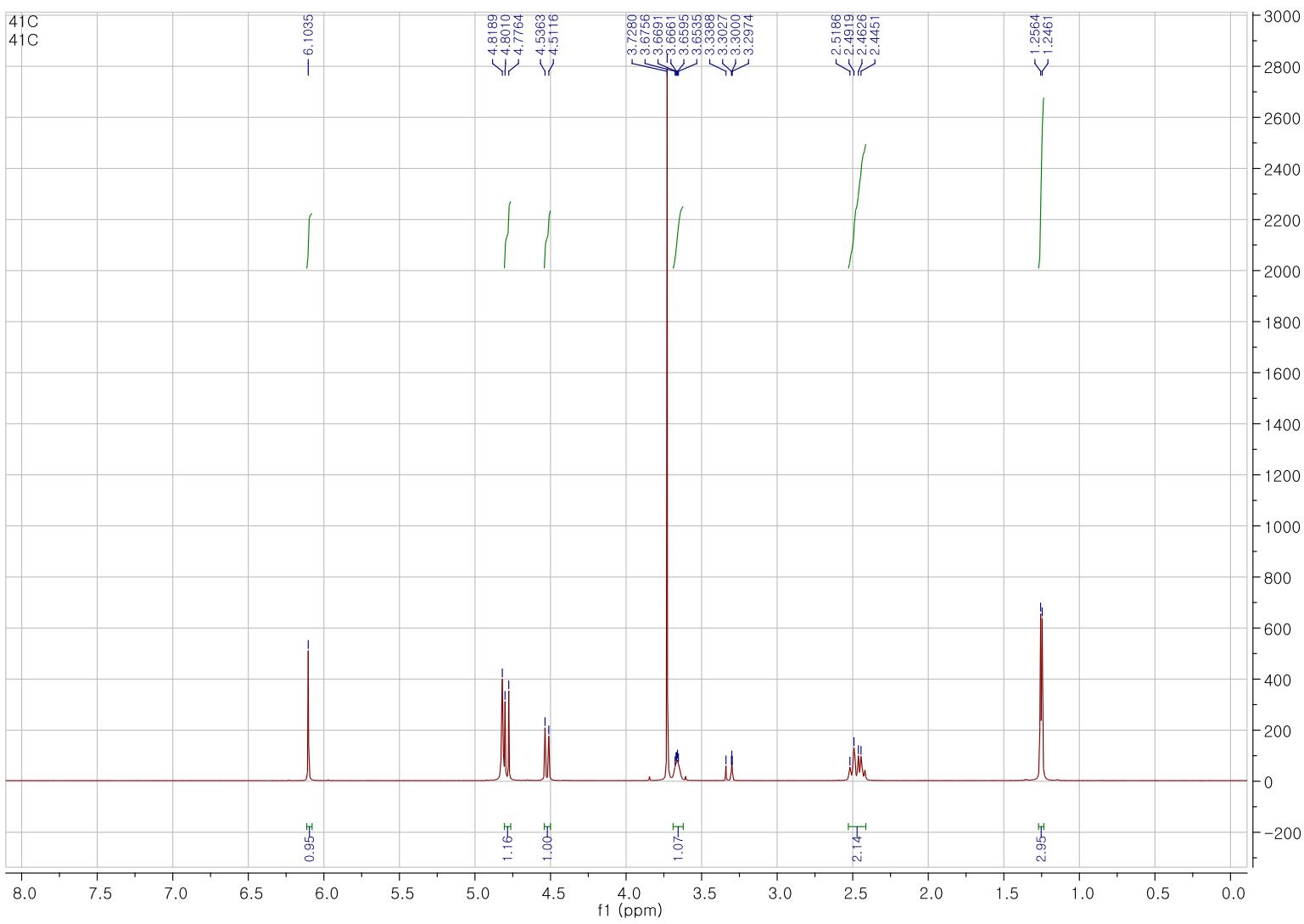


Figure S9. ^1H NMR spectrum of compound 2 in methanol- d_4 (600 MHz)

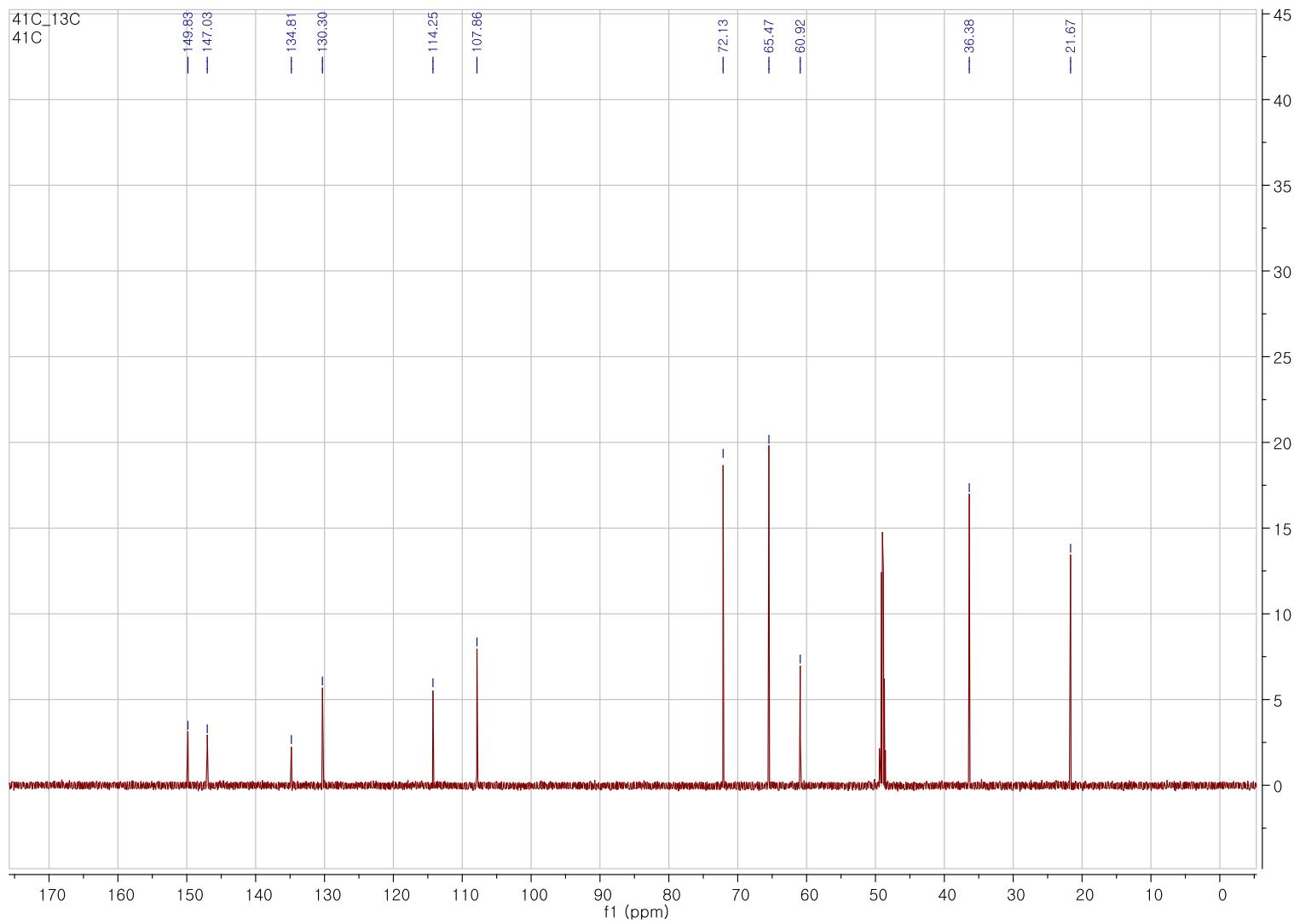


Figure S10. ^{13}C NMR spectrum of compound **2** in methanol- d_4 (150MHz)

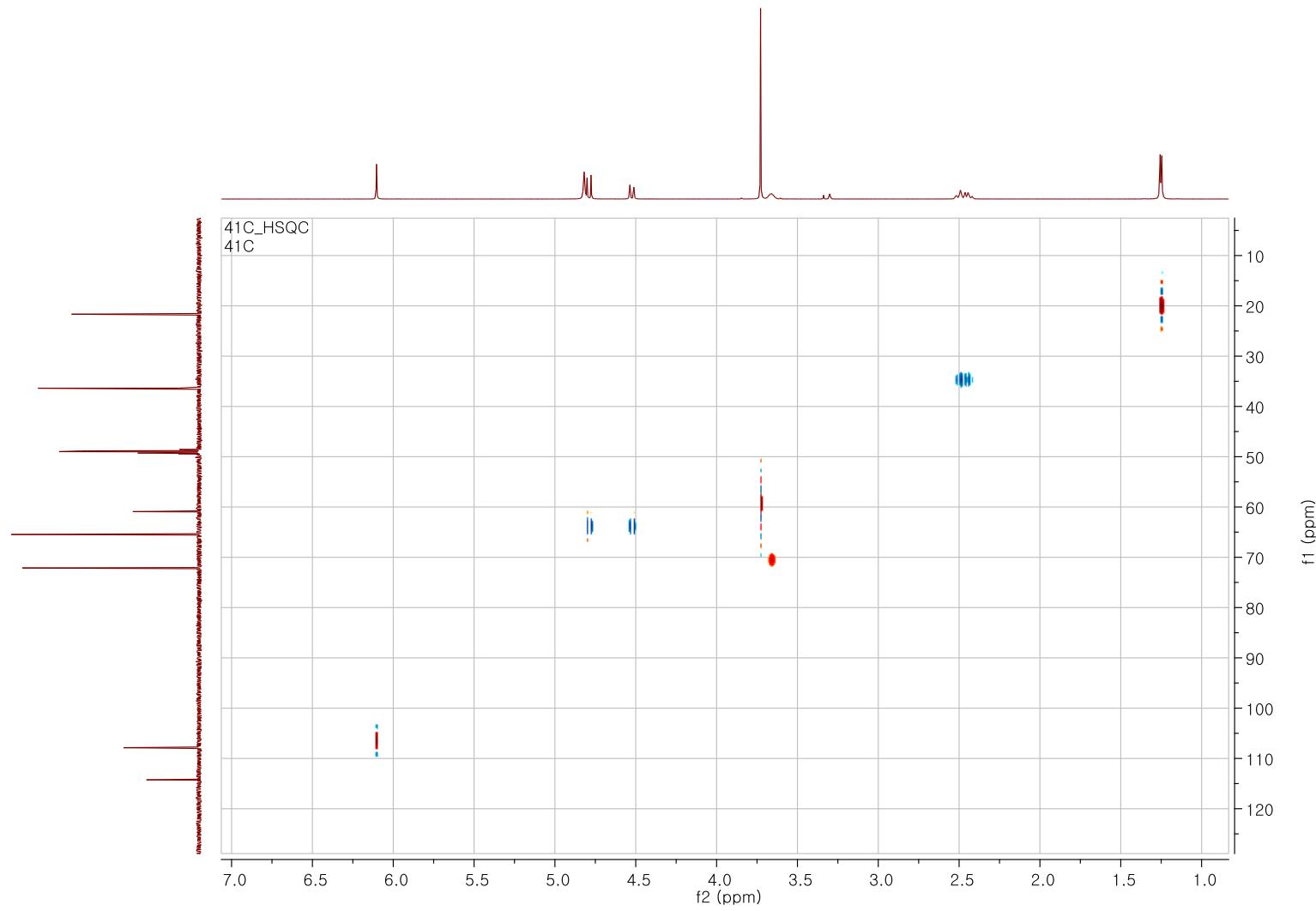


Figure S11. HMQC spectrum of compound 2

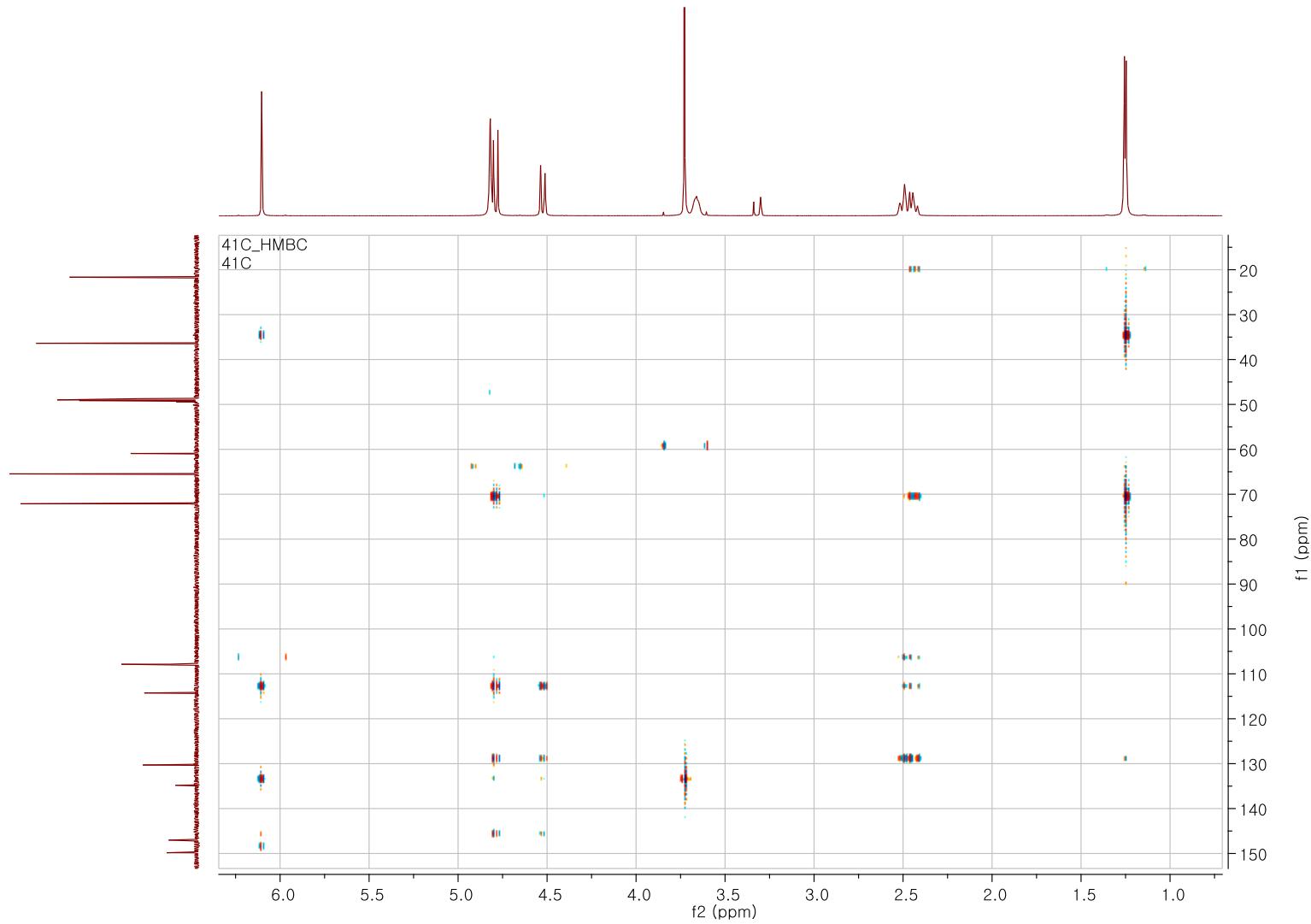


Figure S12. HMBC spectrum of compound 2

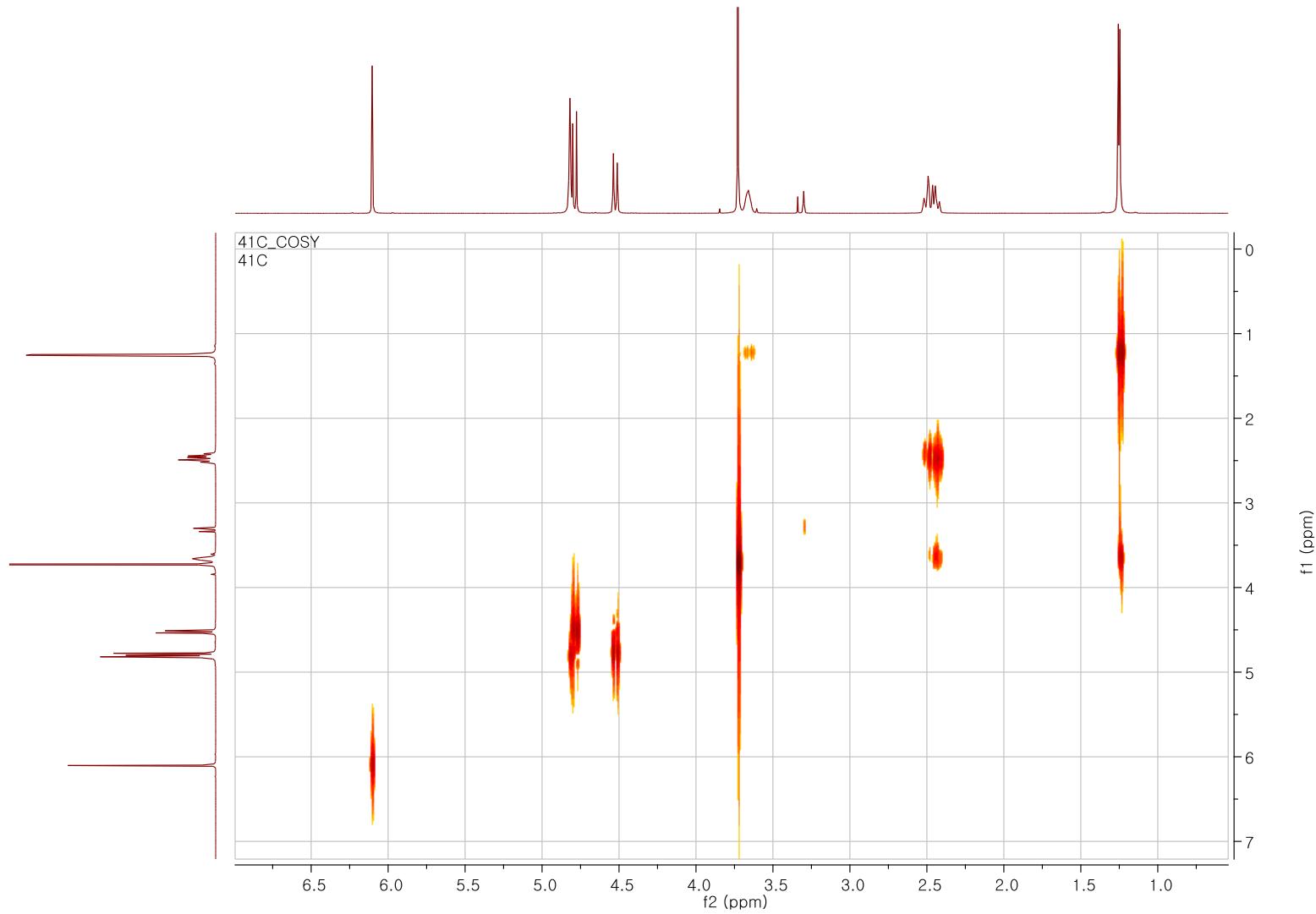


Figure S13. COSY spectrum of compound 2

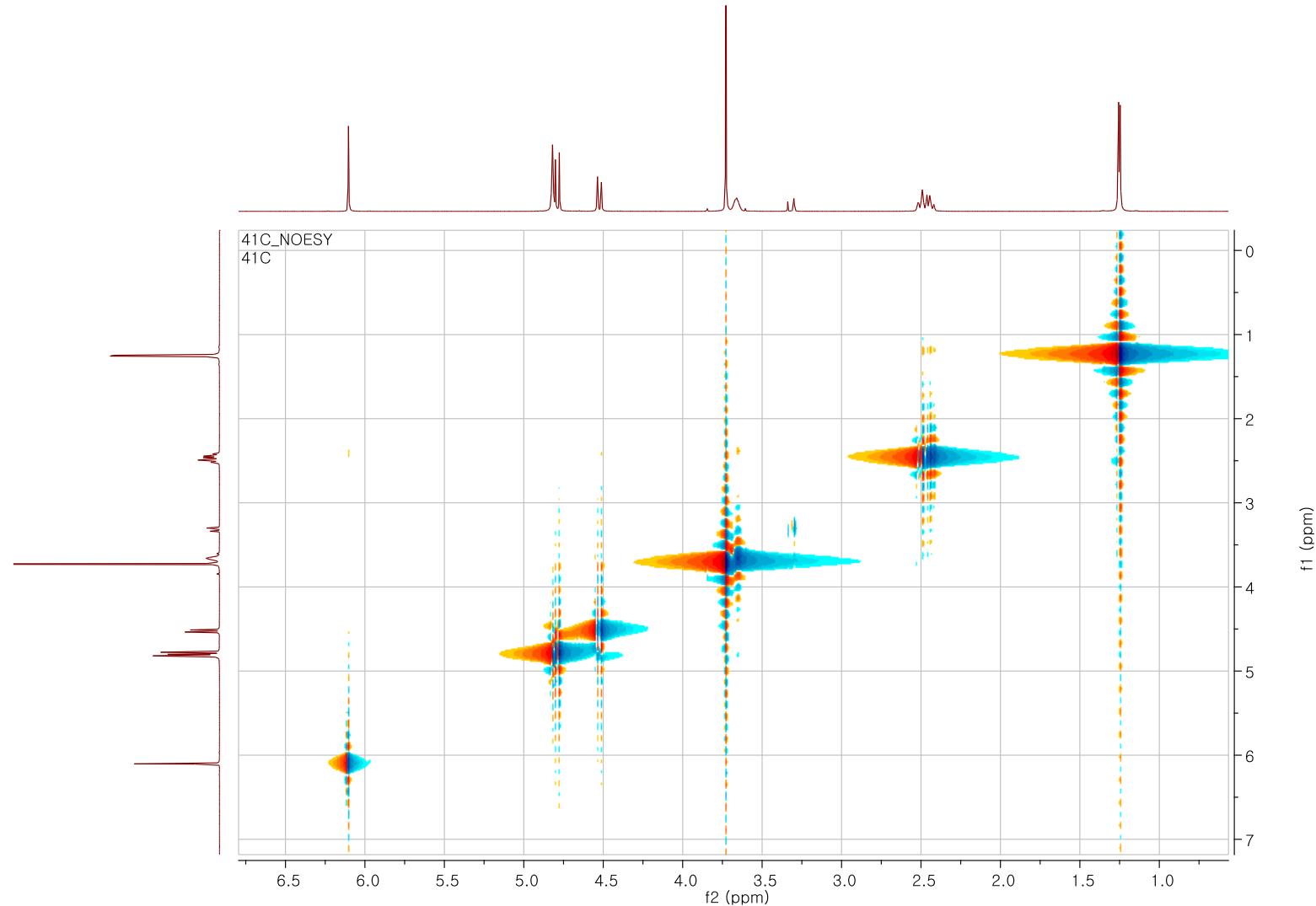


Figure S14. NOESY spectrum of compound 2



540-45E1_MS spectrum

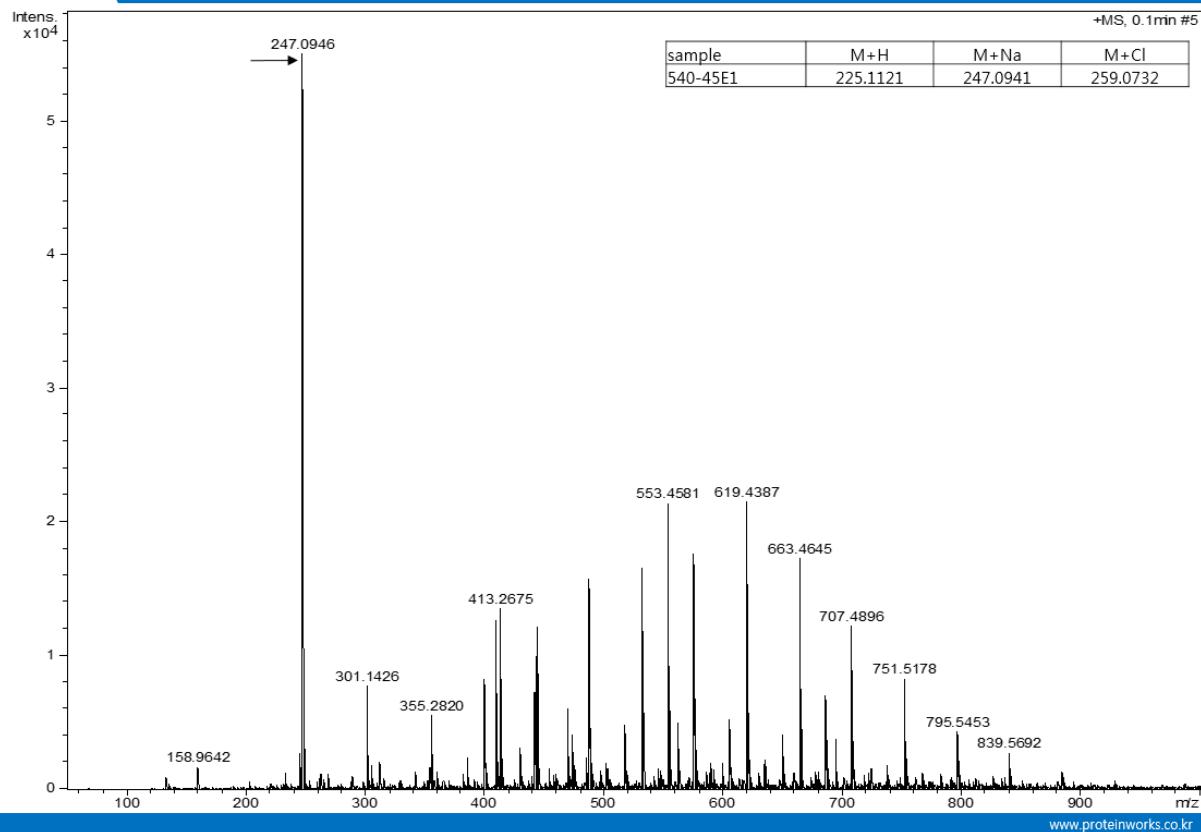


Figure S15. HR-ESI-MS spectrum of compound 3

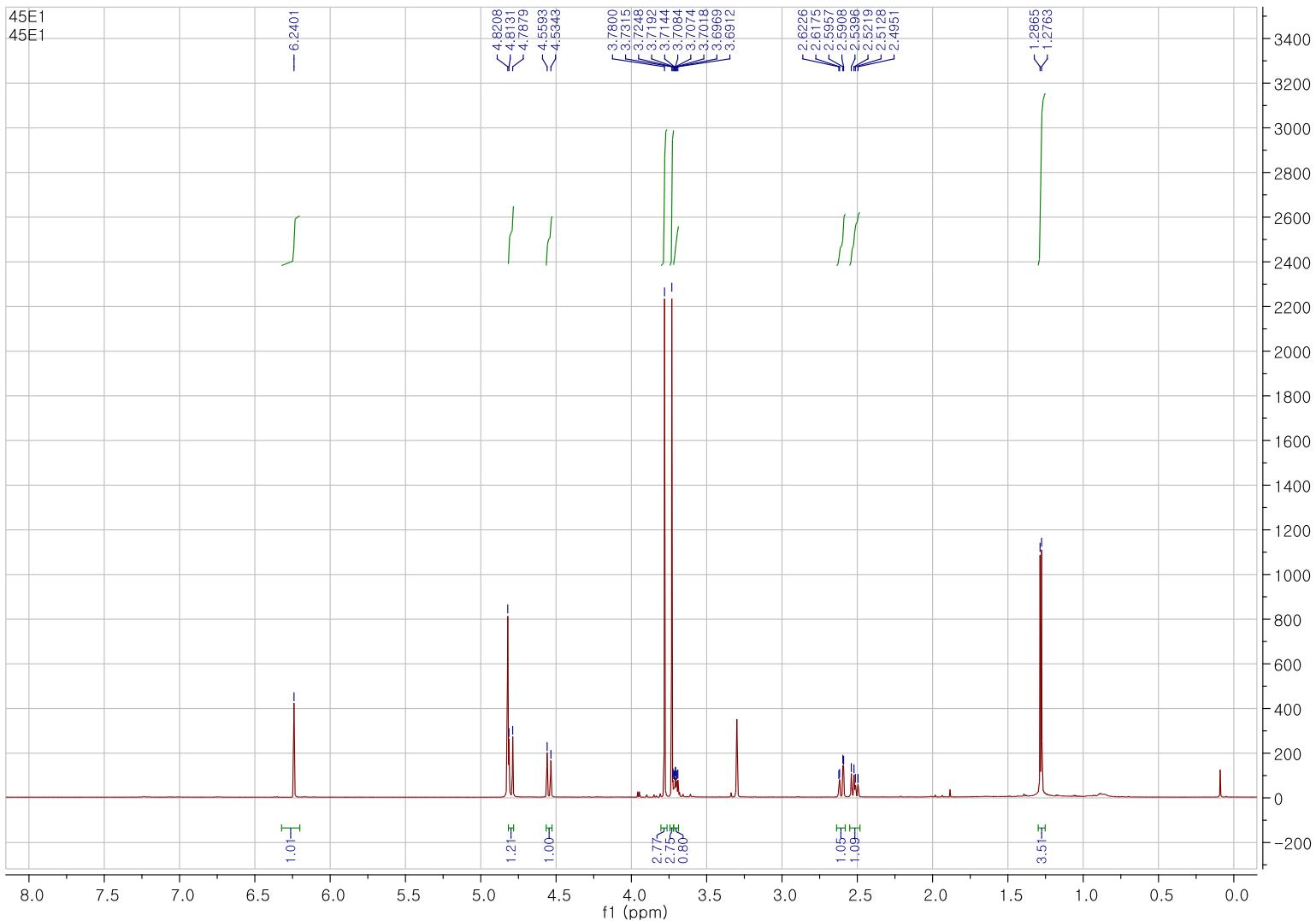


Figure S16. ^1H NMR spectrum of compound **3** in methanol- d_4 (600 MHz)

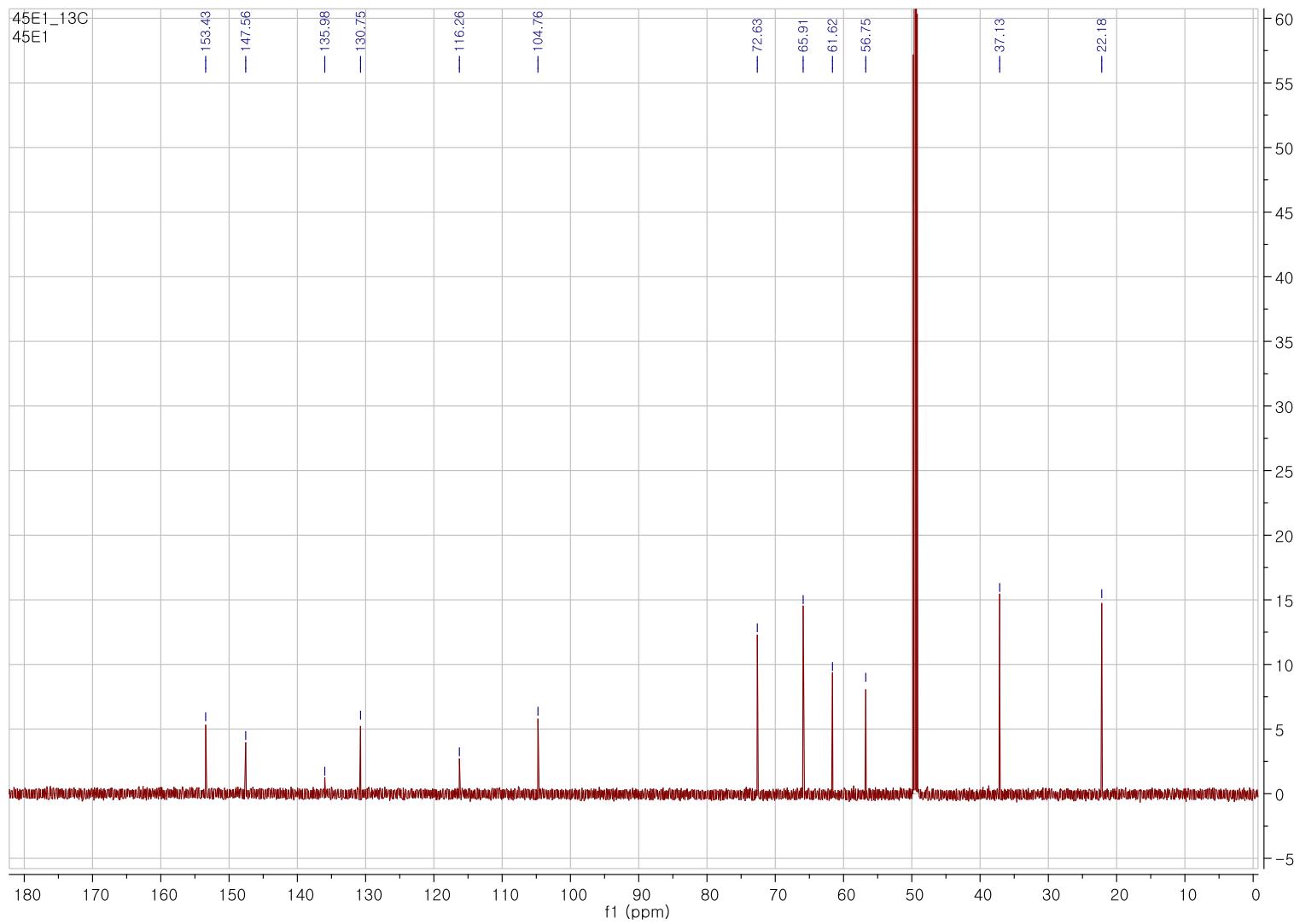


Figure S17. ¹³C NMR spectrum of compound **3** in methanol-*d*₄ (150MHz)

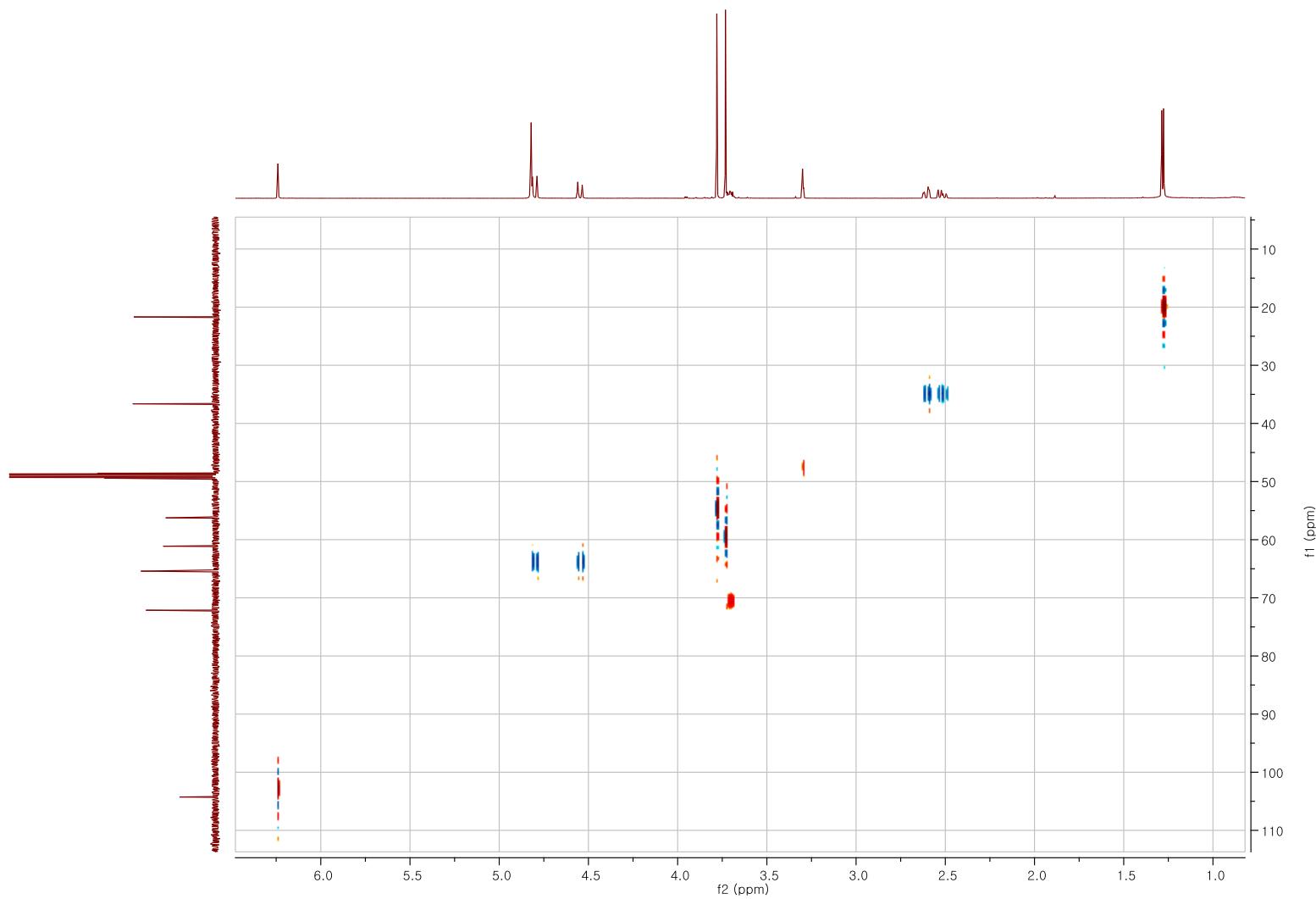


Figure S18. HMQC spectrum of compound 3

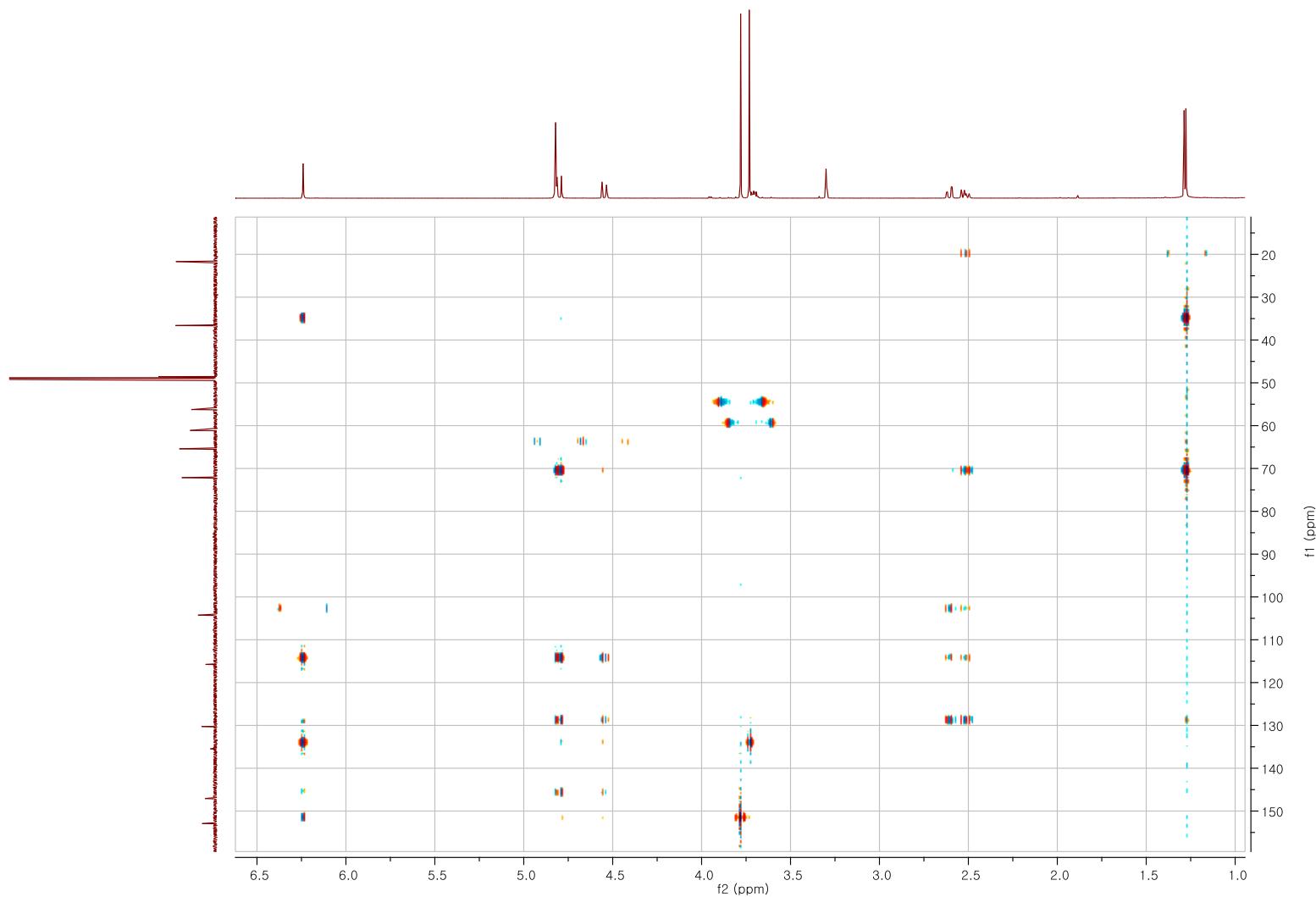


Figure S19. HMBC spectrum of compound 3

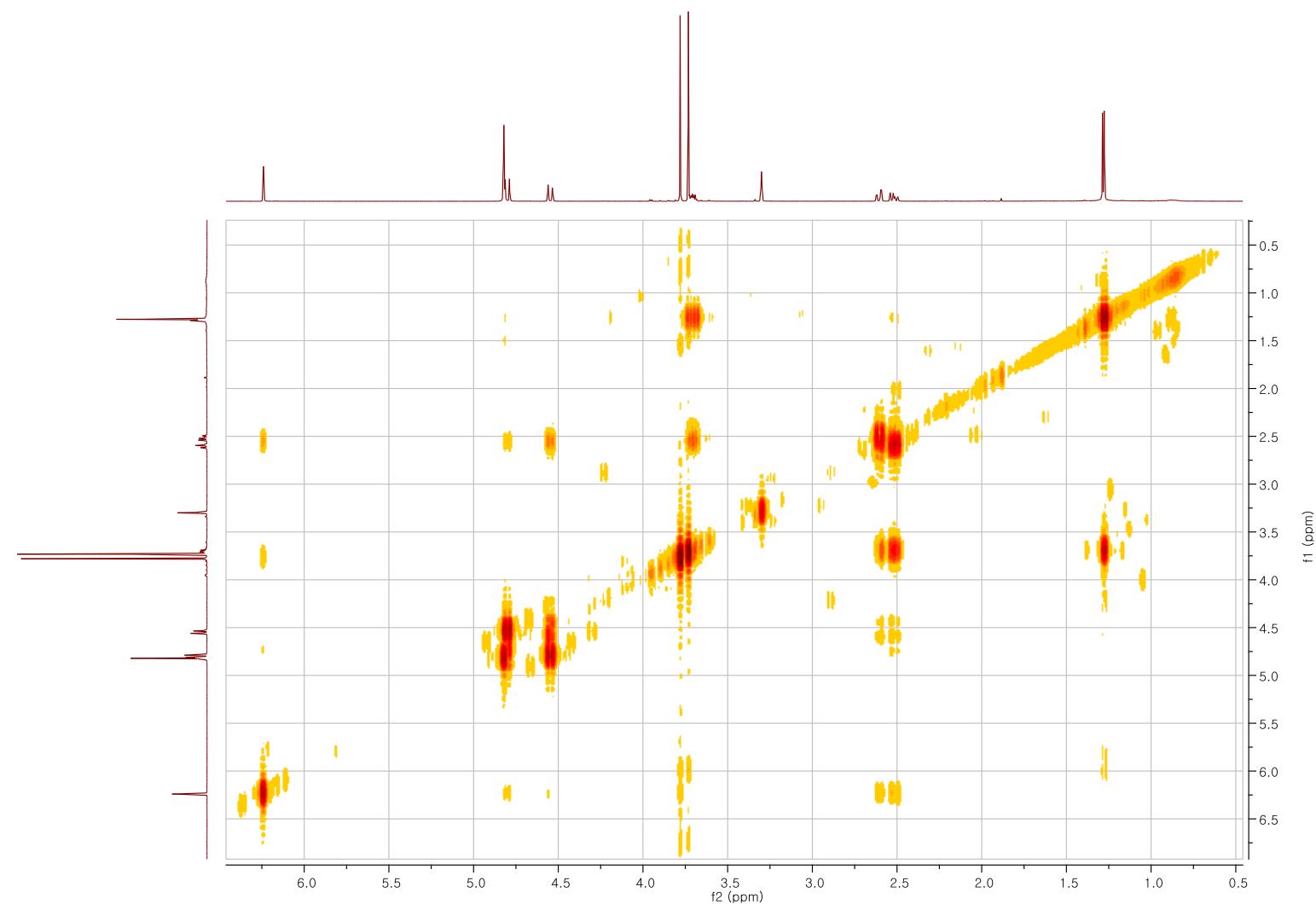


Figure S20. COSY spectrum of compound **3**

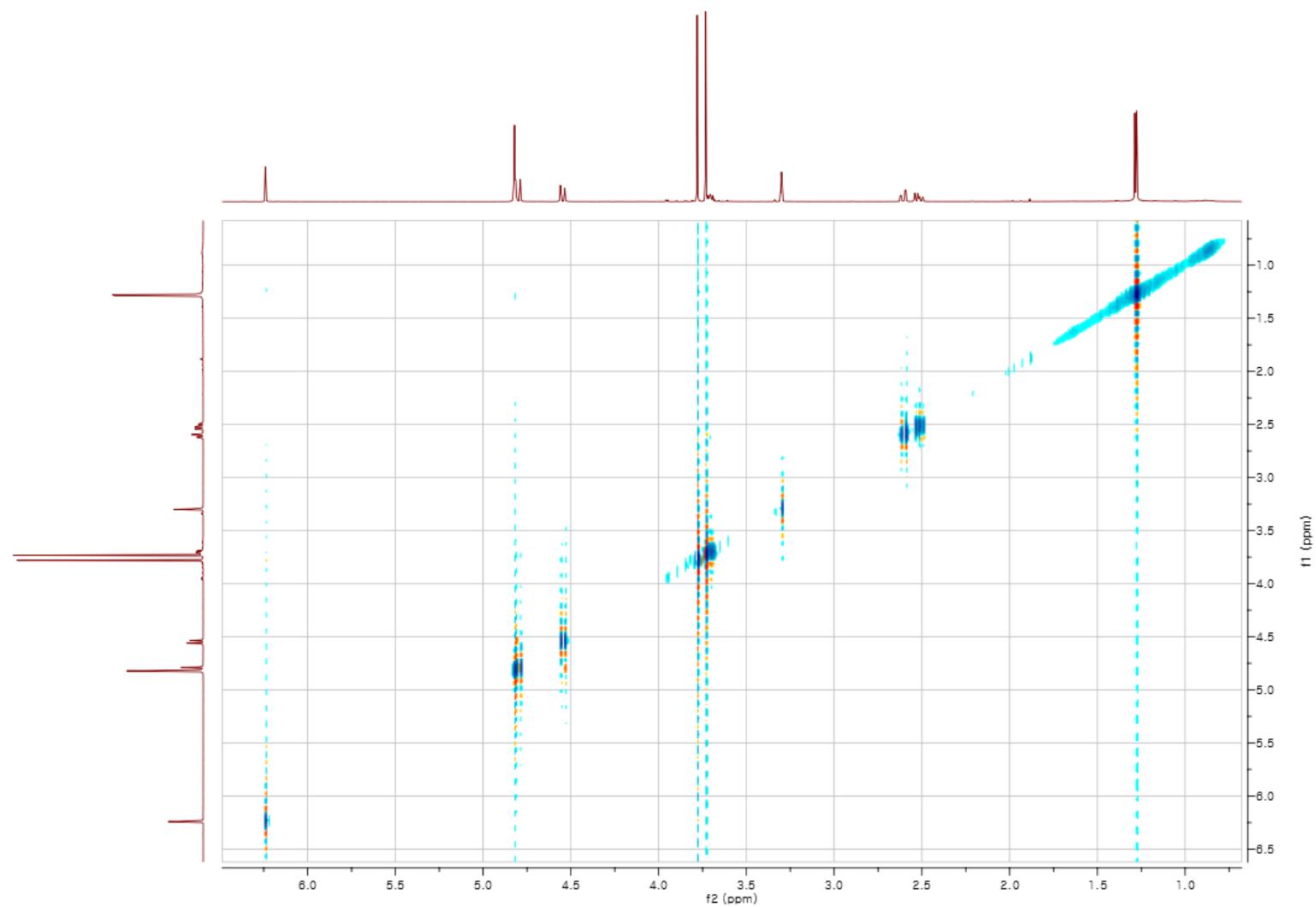


Figure S21. NOESY spectrum of compound **3**

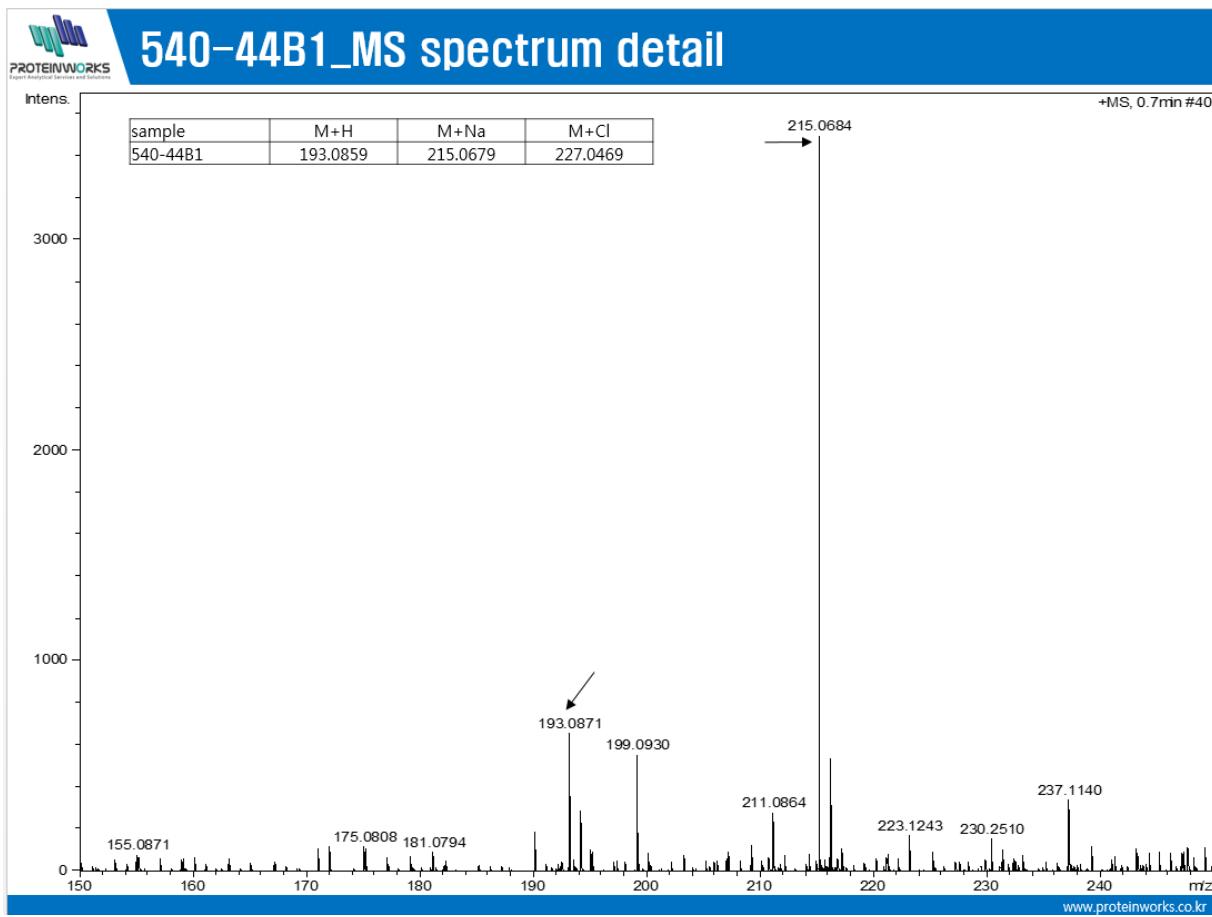


Figure S22. HR-ESI-MS spectrum of compound 4

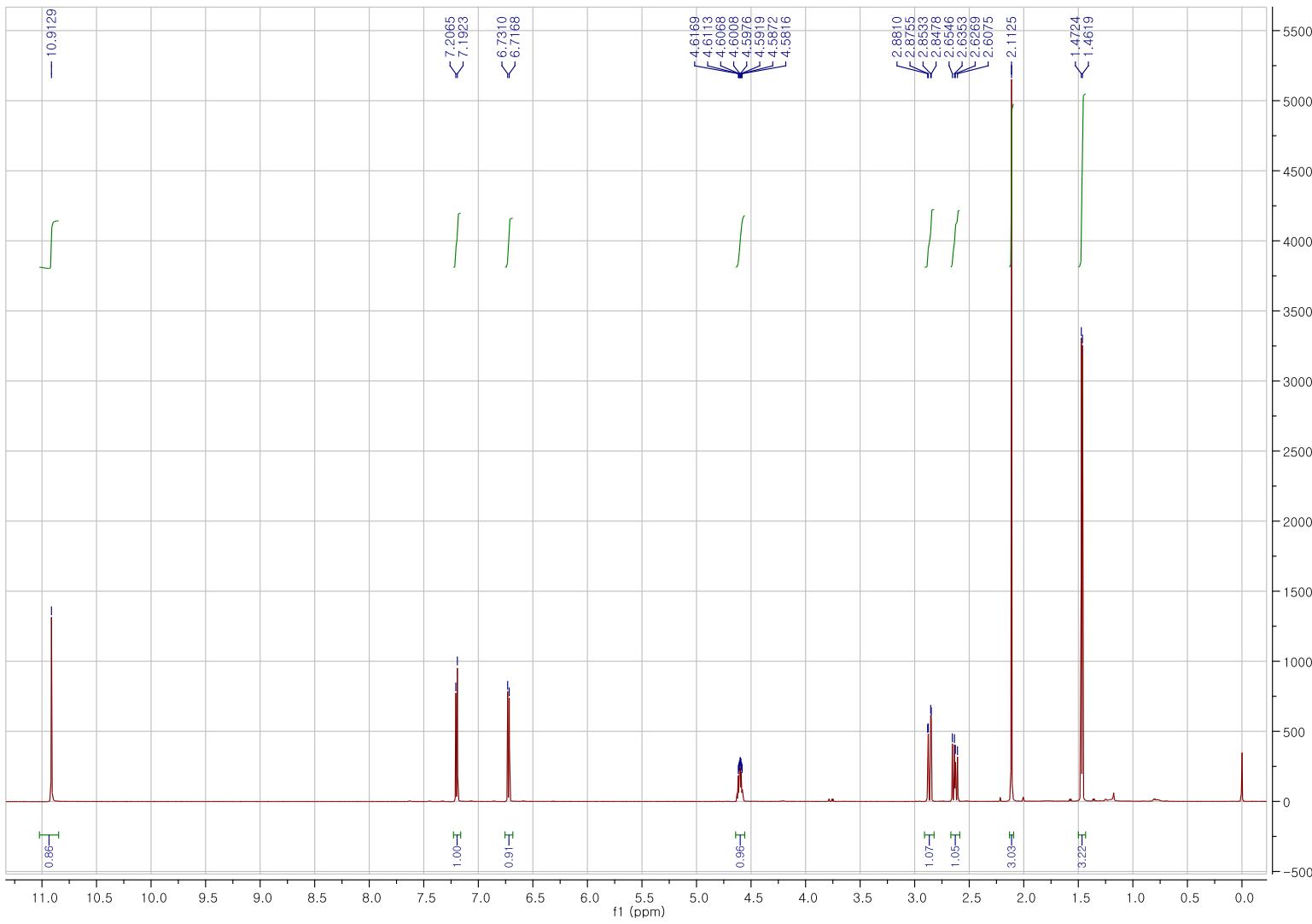


Figure S23. ^1H NMR spectrum of compound **4** in chloroform-*d* (600 MHz)

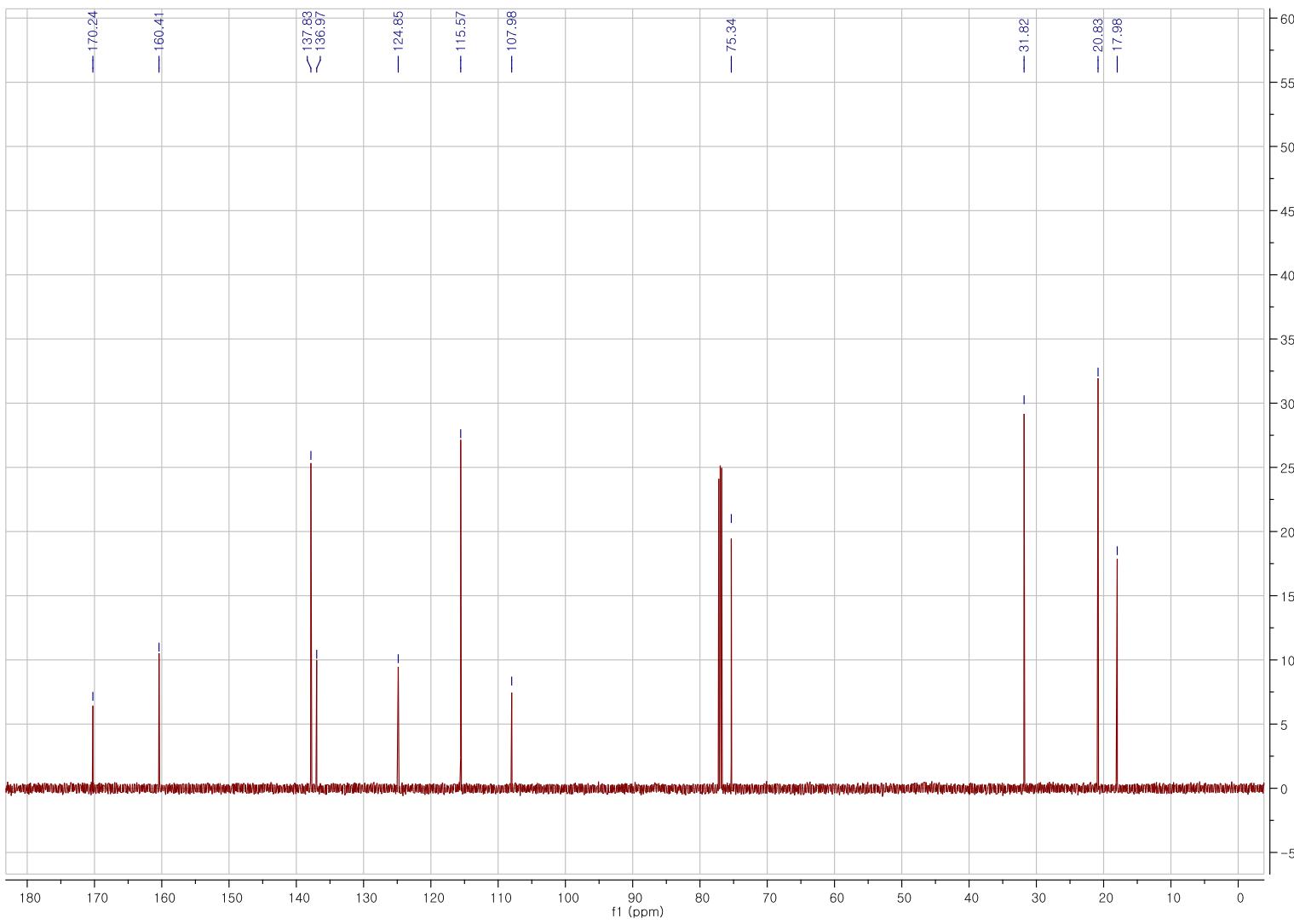


Figure S24. ^{13}C NMR spectrum of compound **4** in chloroform-*d* (150MHz)

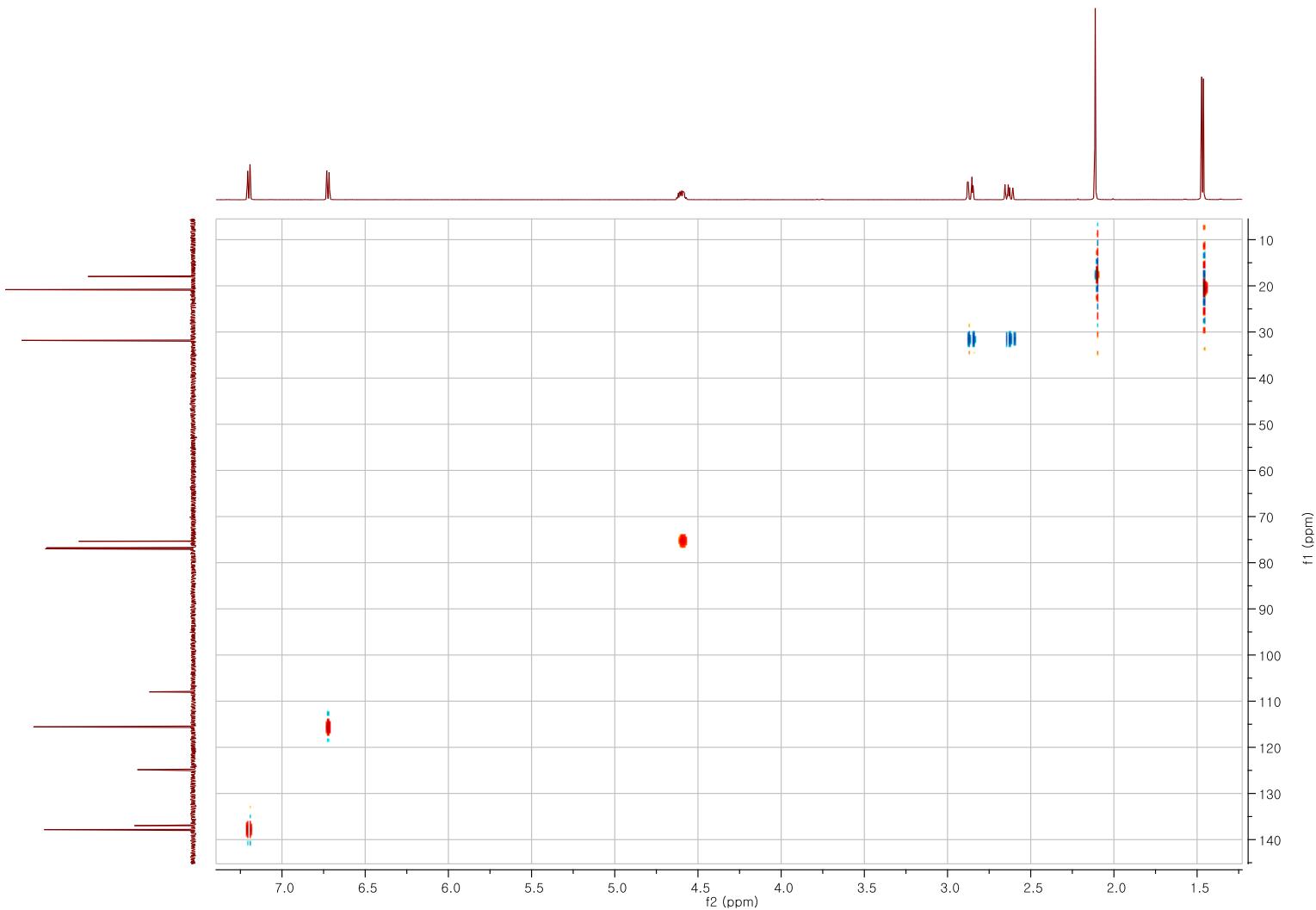


Figure S25. HMQC spectrum of compound 4

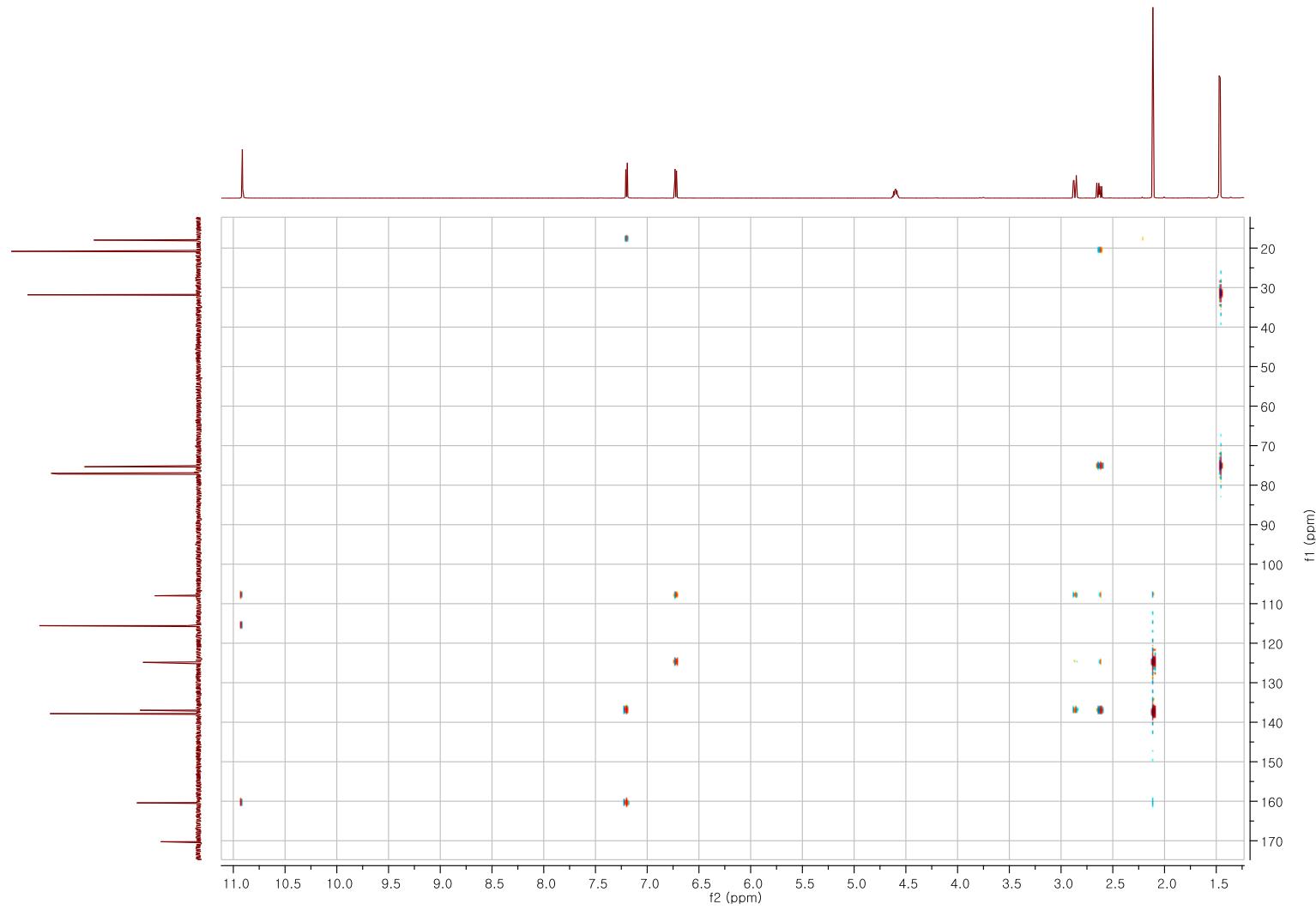


Figure S26. HMBC spectrum of compound 4

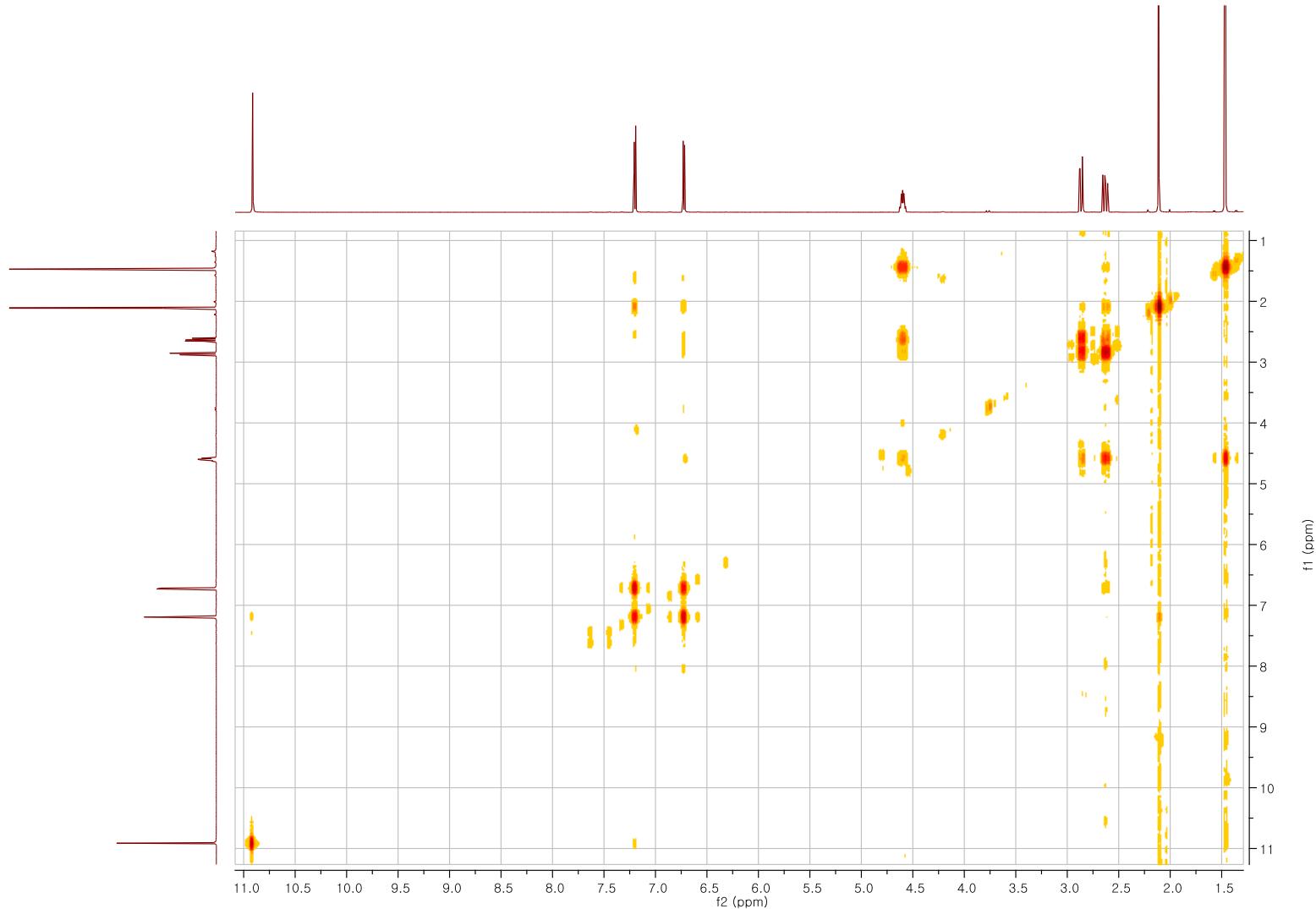


Figure S27. COSY spectrum of compound 4

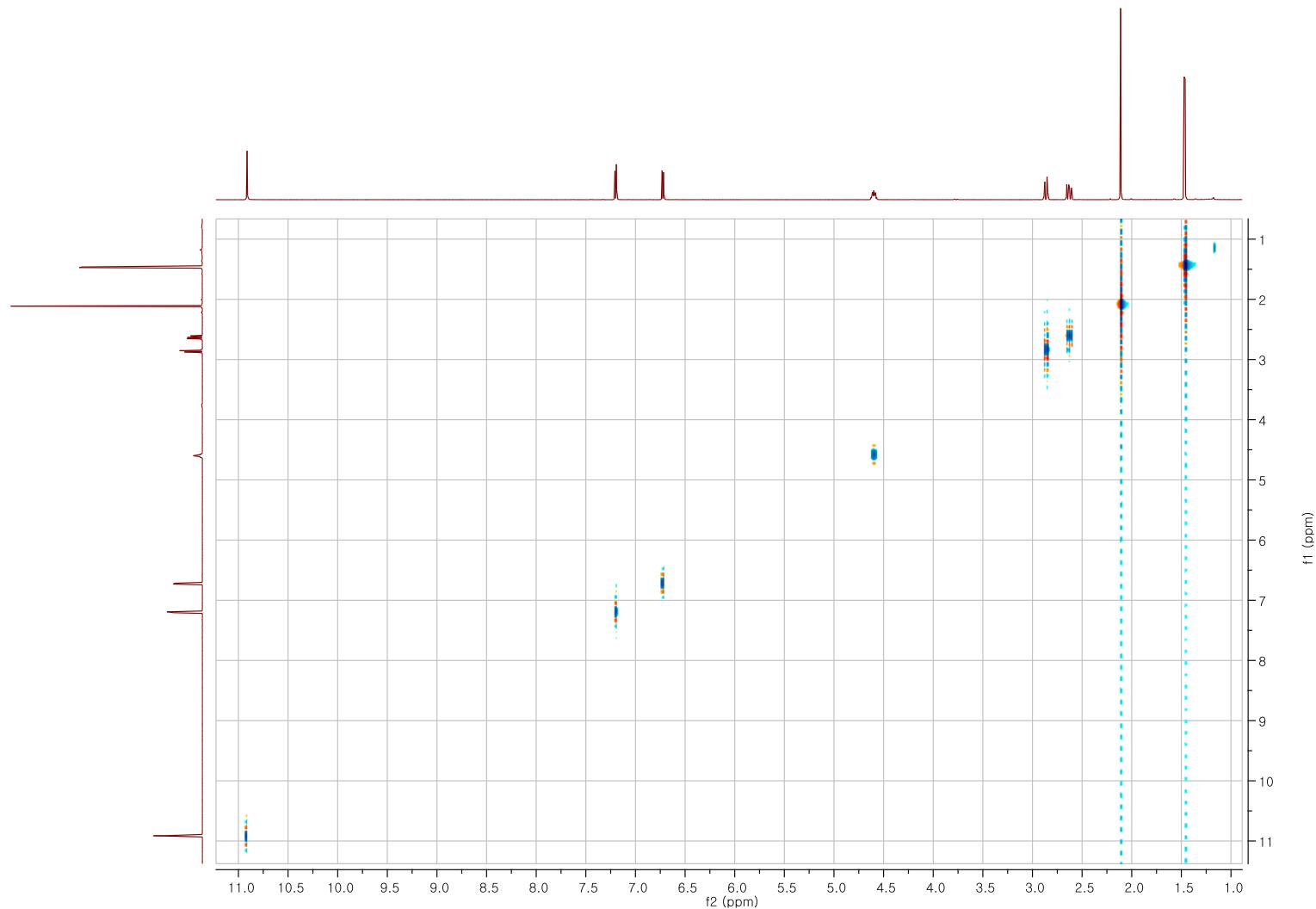


Figure S28. NOESY spectrum of compound 4

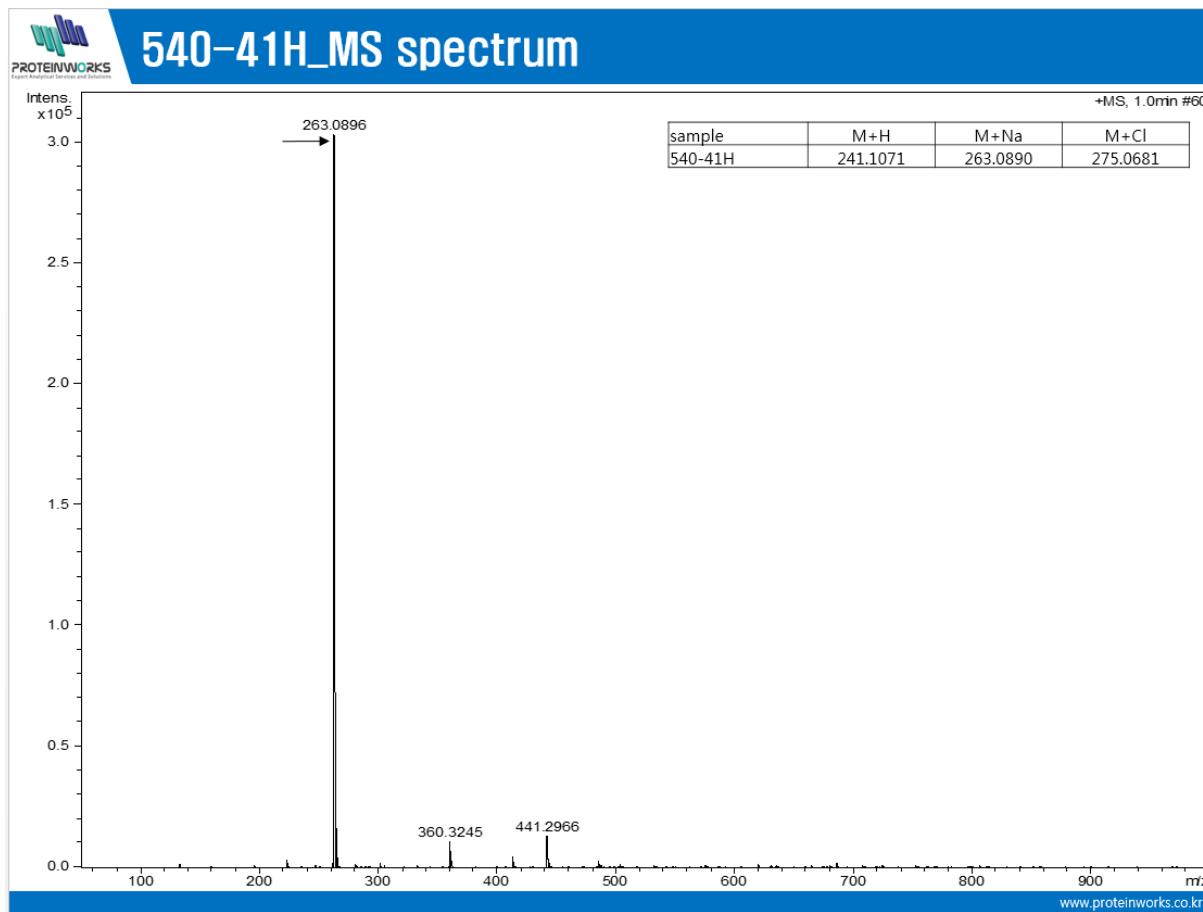


Figure S29. HR-ESI-MS spectrum of compound **6**

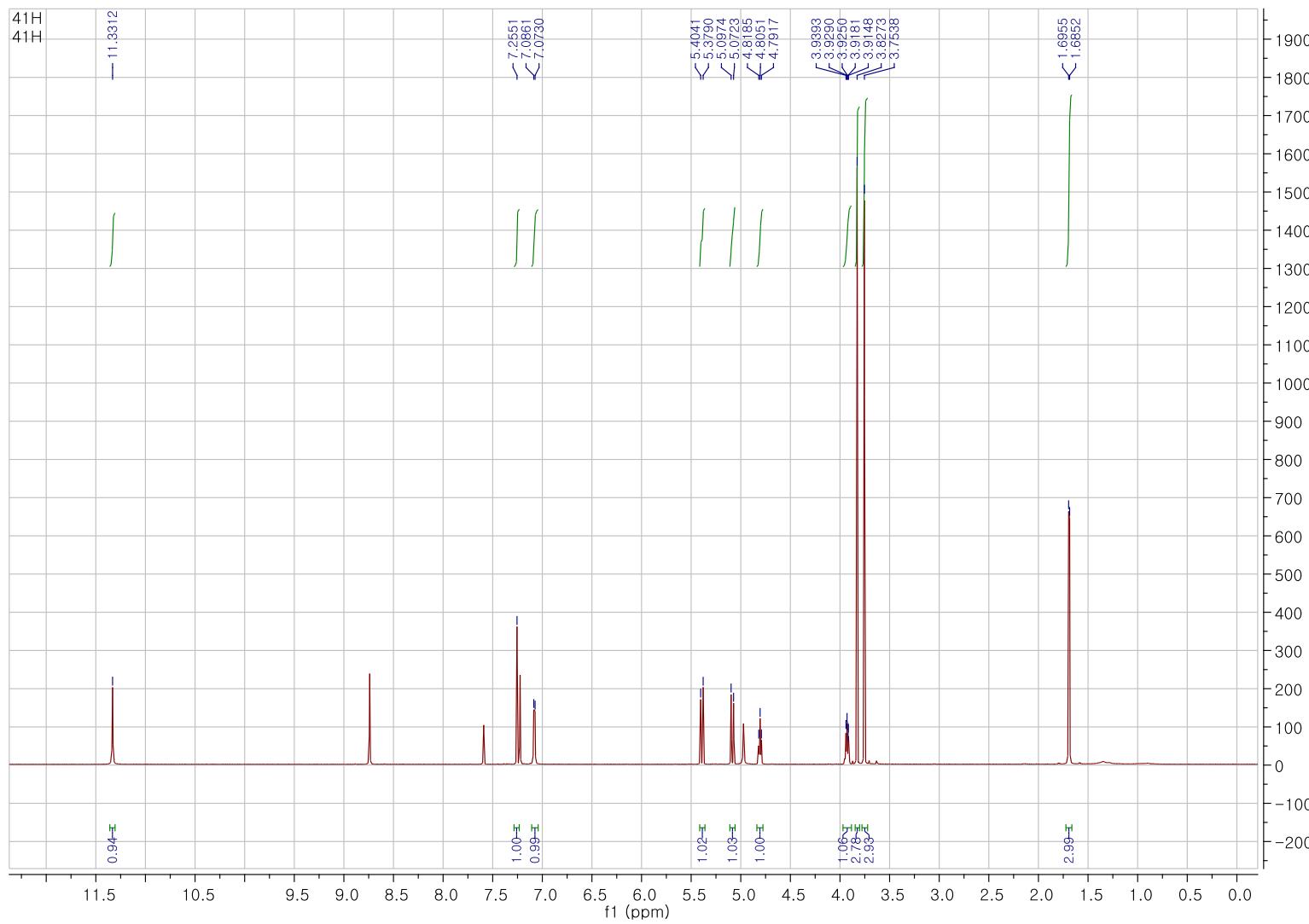


Figure S30. ¹H NMR spectrum of compound **6** in pyridine-*d*₅ (600 MHz)

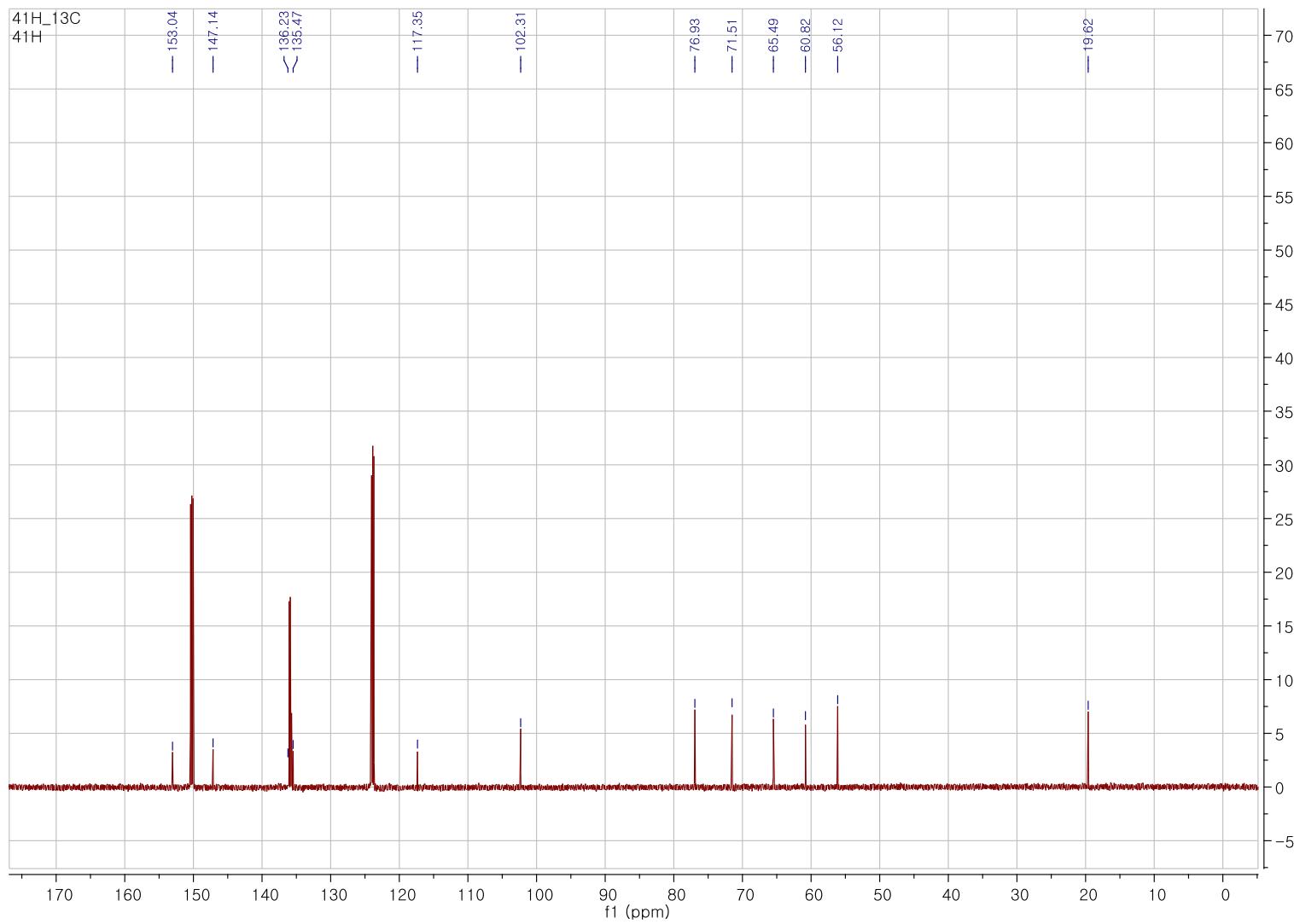


Figure S31. ^{13}C NMR spectrum of compound **6** in pyridine- d_5 (150 MHz)

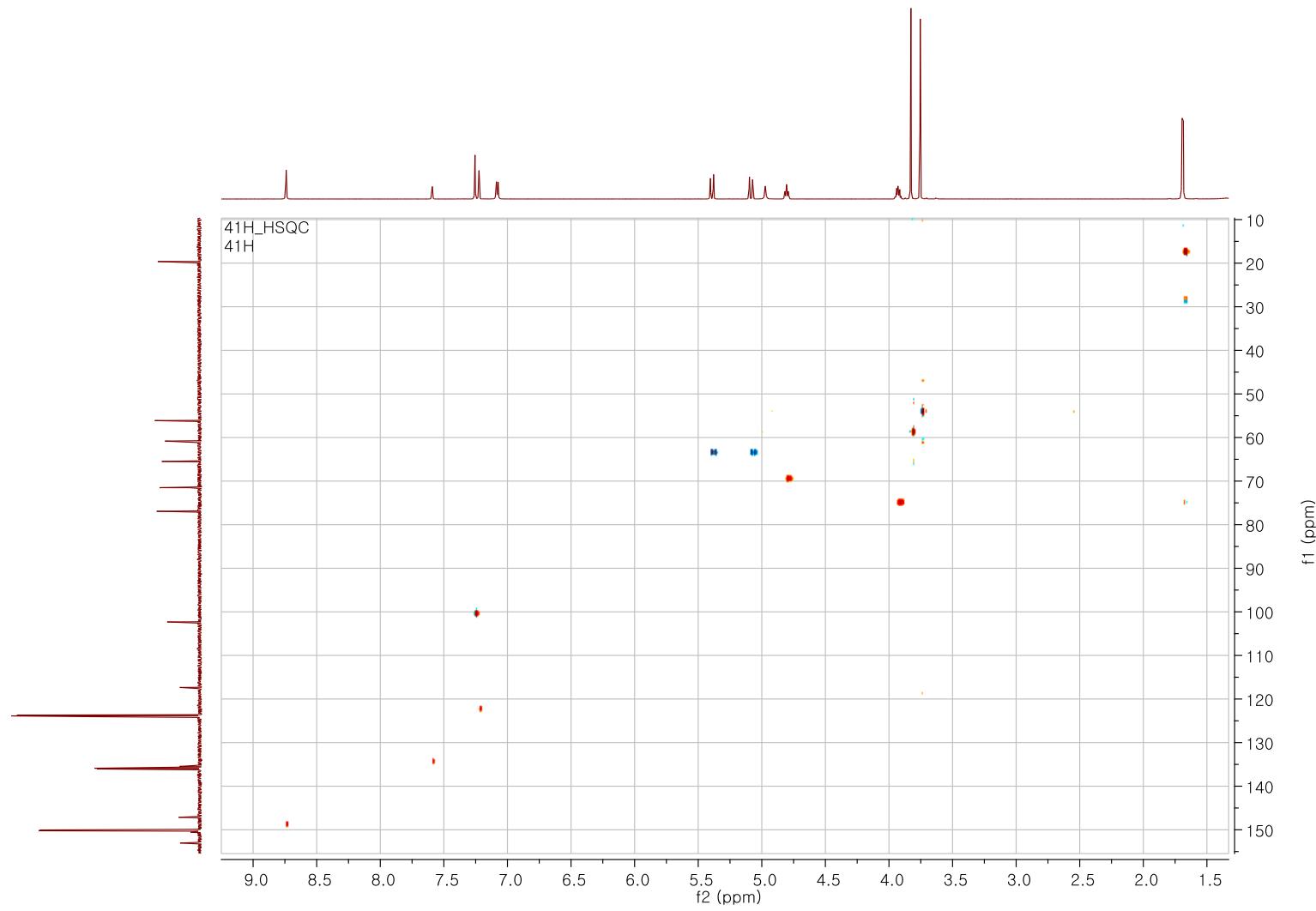


Figure S32. HMQC spectrum of compound **6**

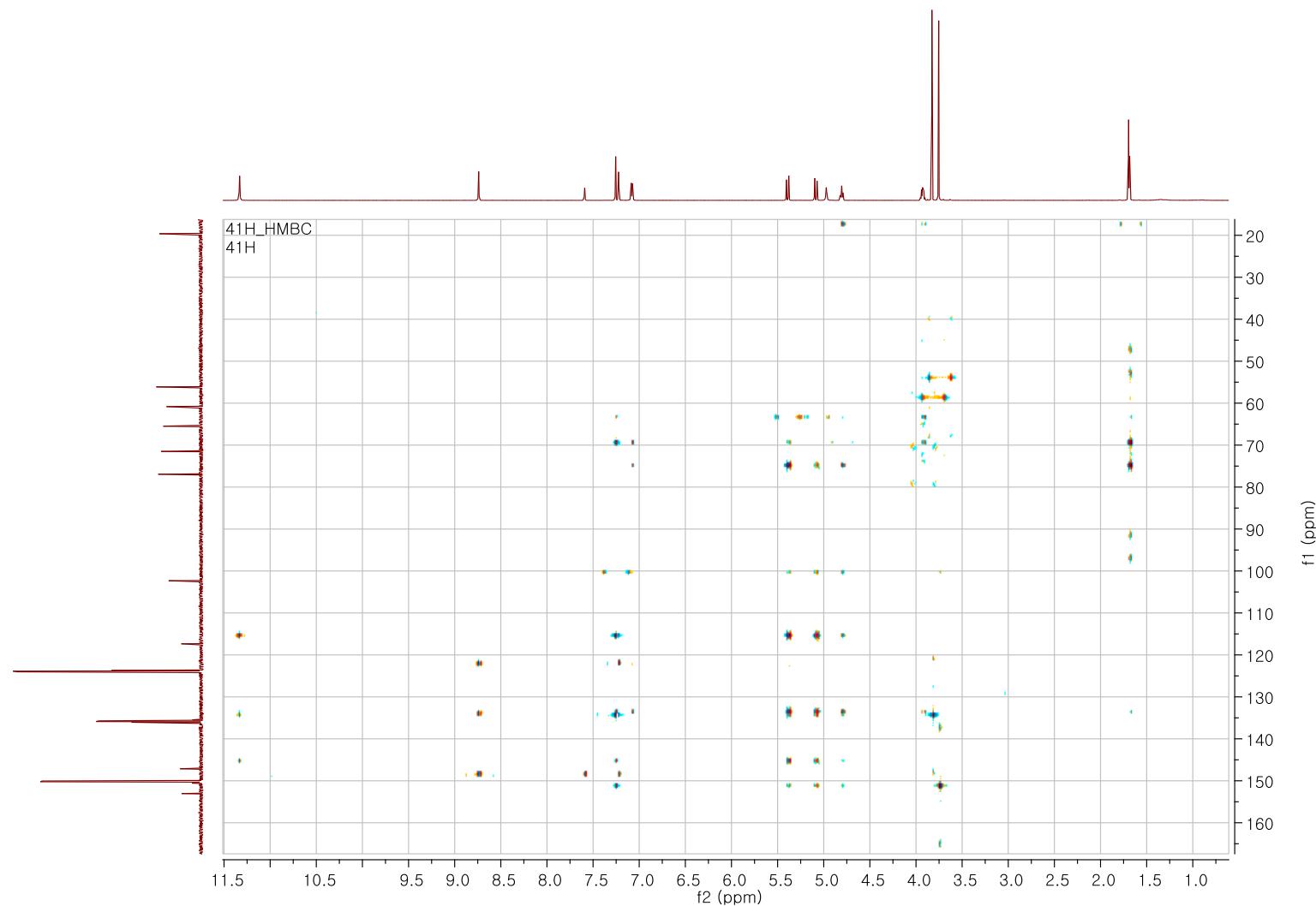


Figure S33. HMBC spectrum of compound **6**

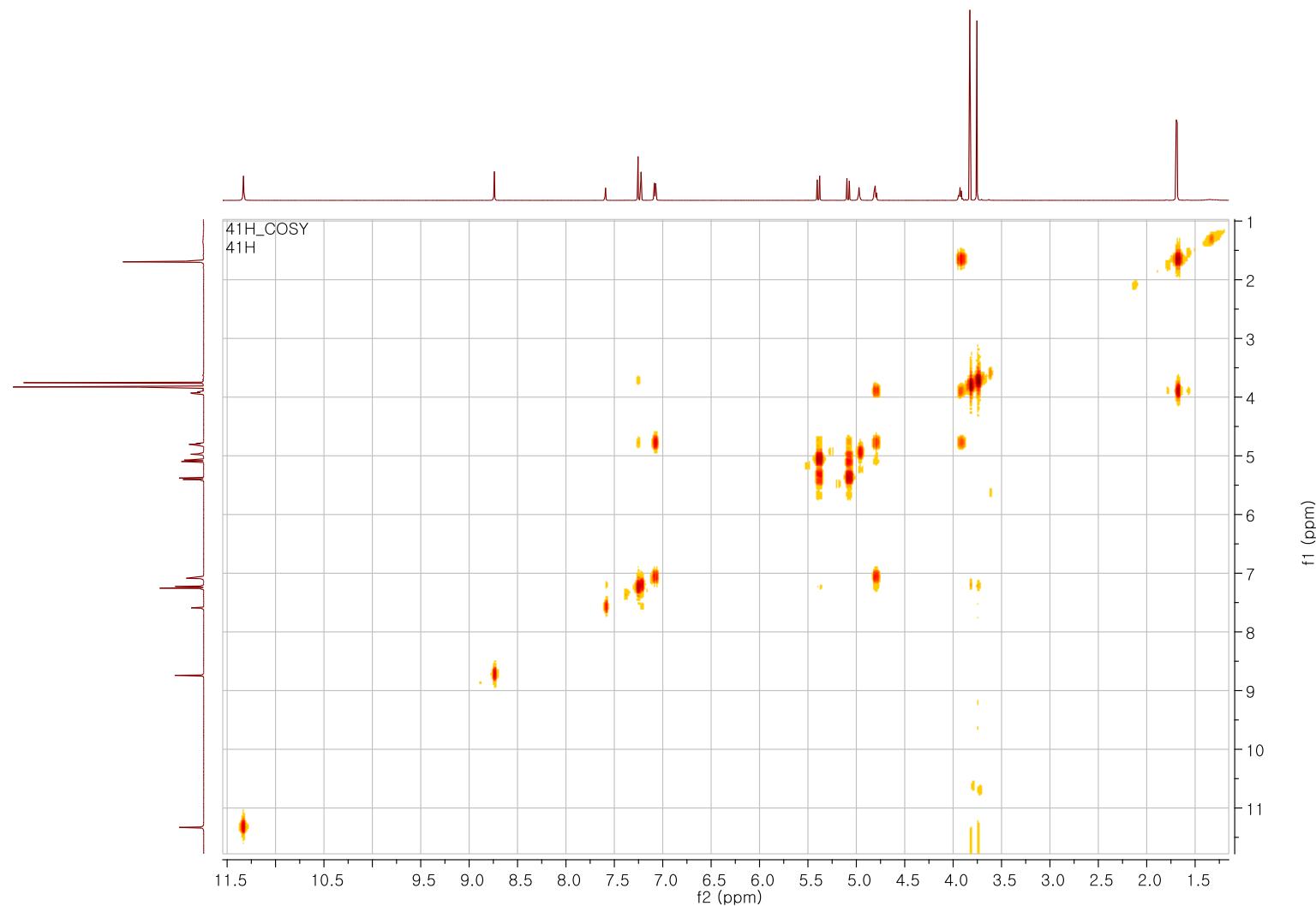


Figure S34. COSY spectrum of compound **6**

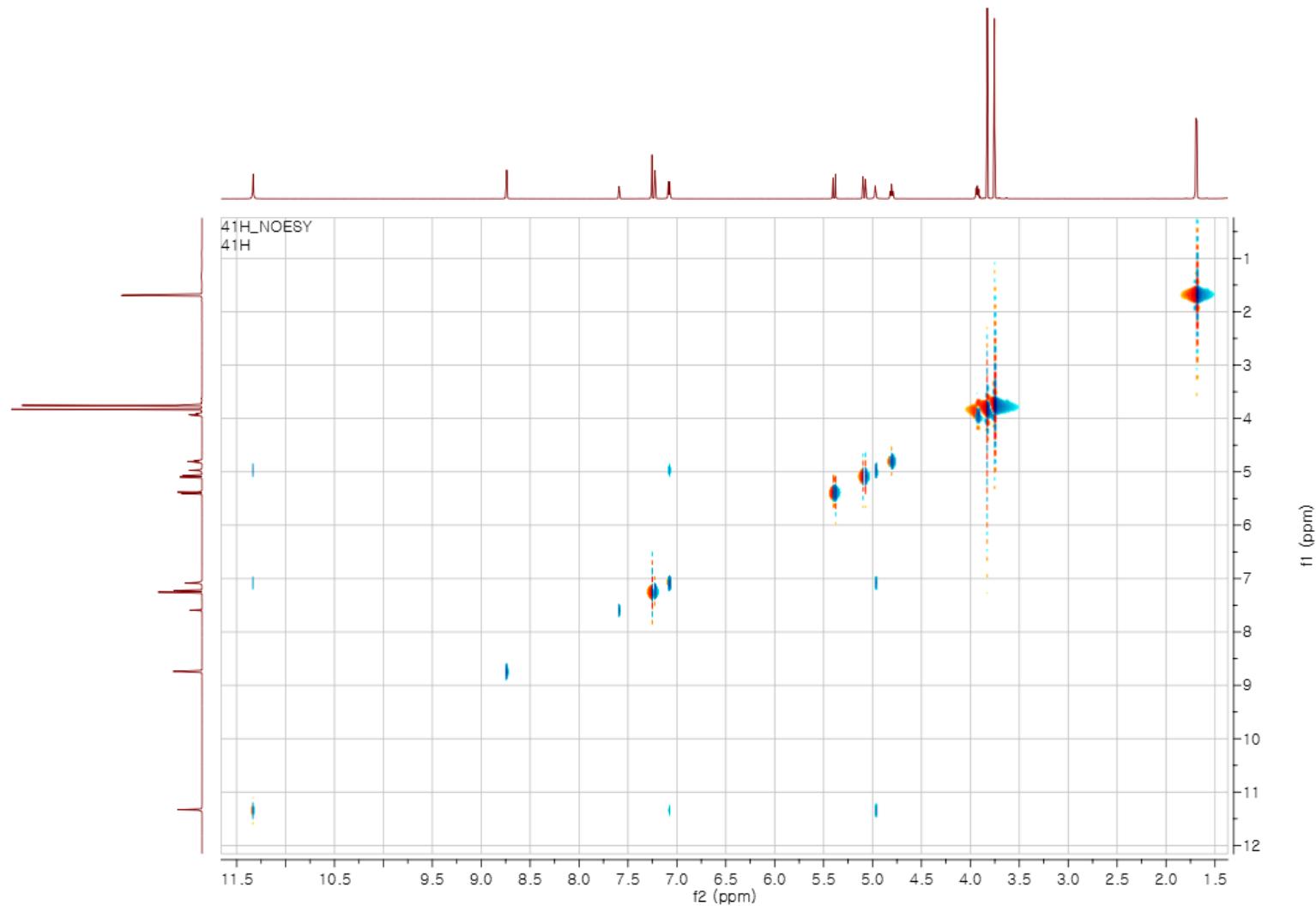


Figure S35. NOESY spectrum of compound **6**

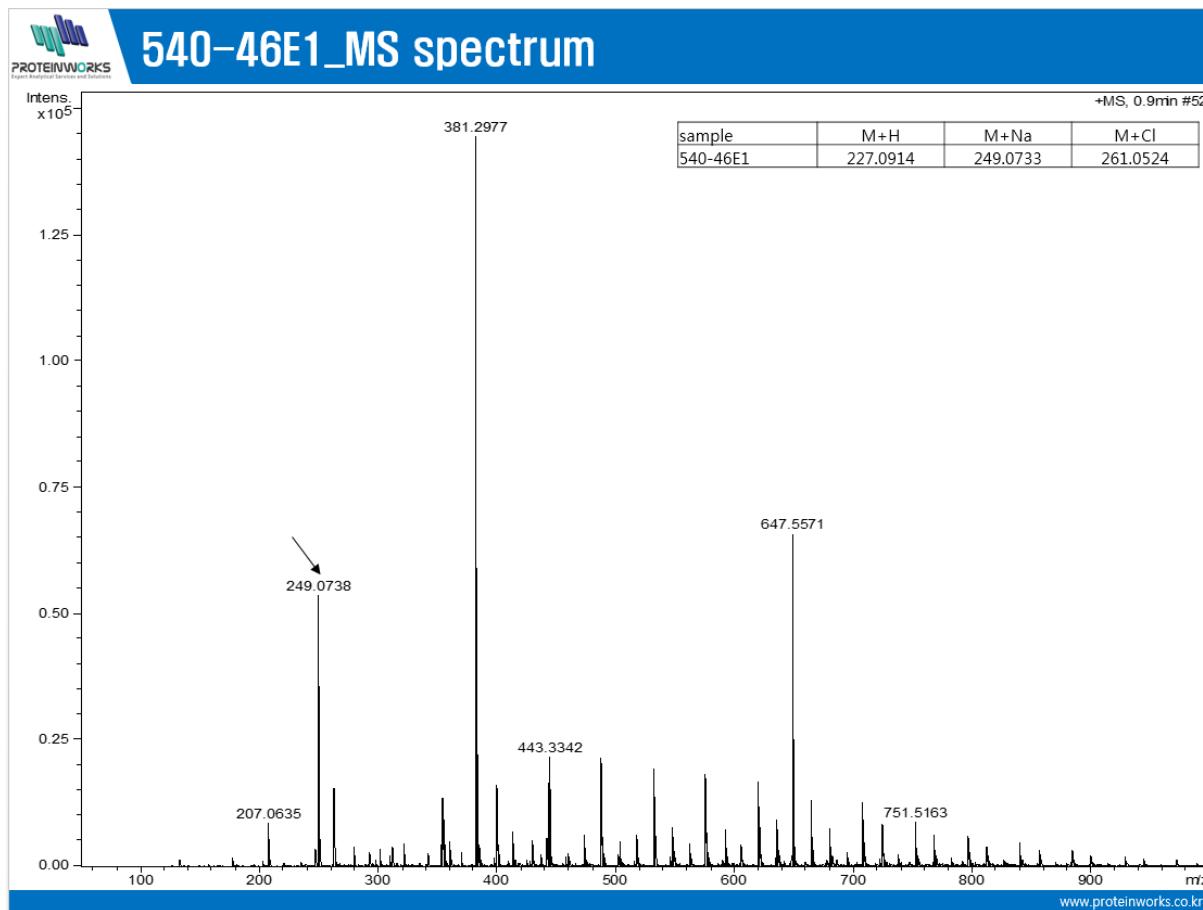


Figure S36. HR-ESI-MS spectrum of compound 7

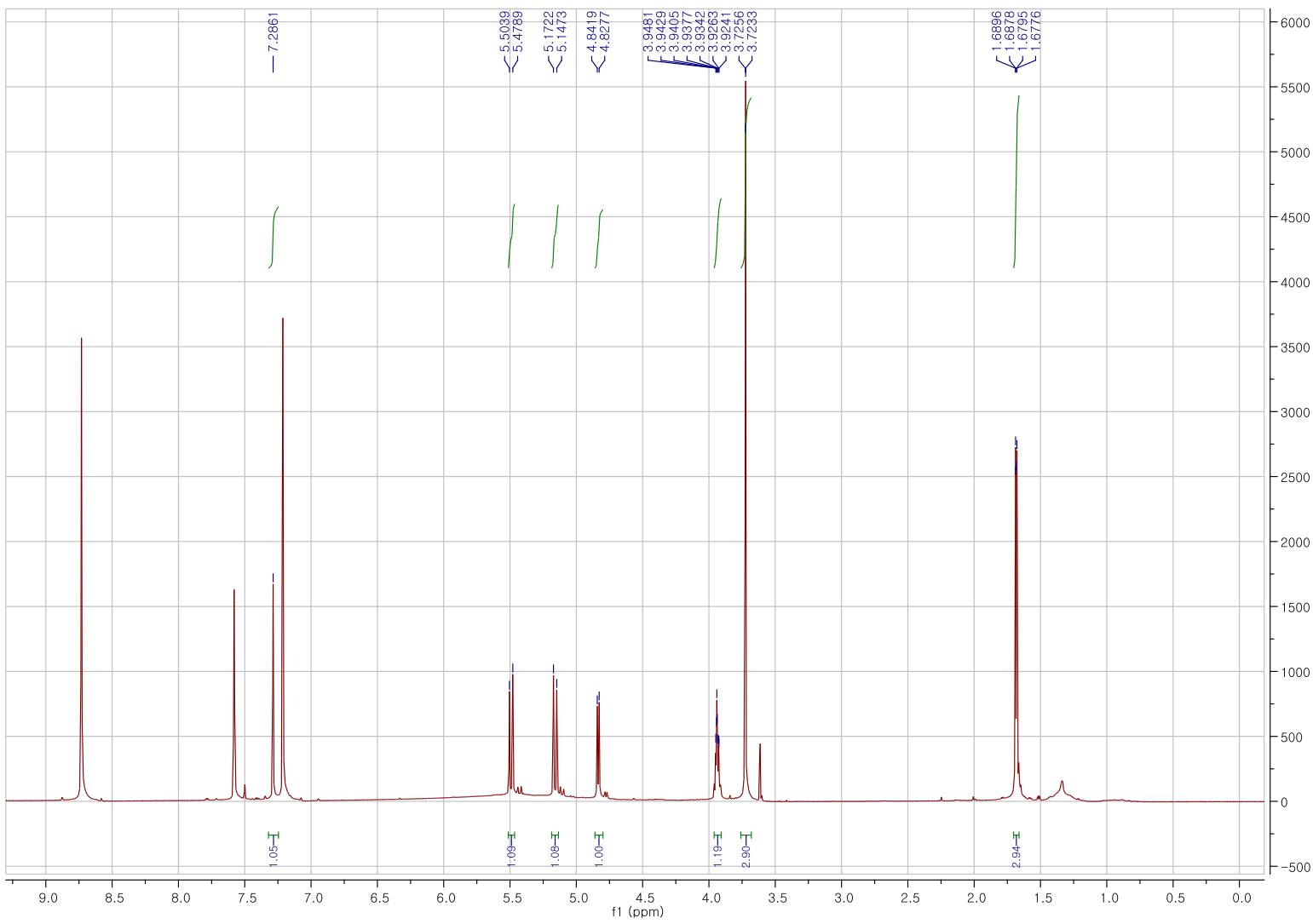


Figure S37. ^1H NMR spectrum of compound **7** in pyridine- d_5 (600 MHz)

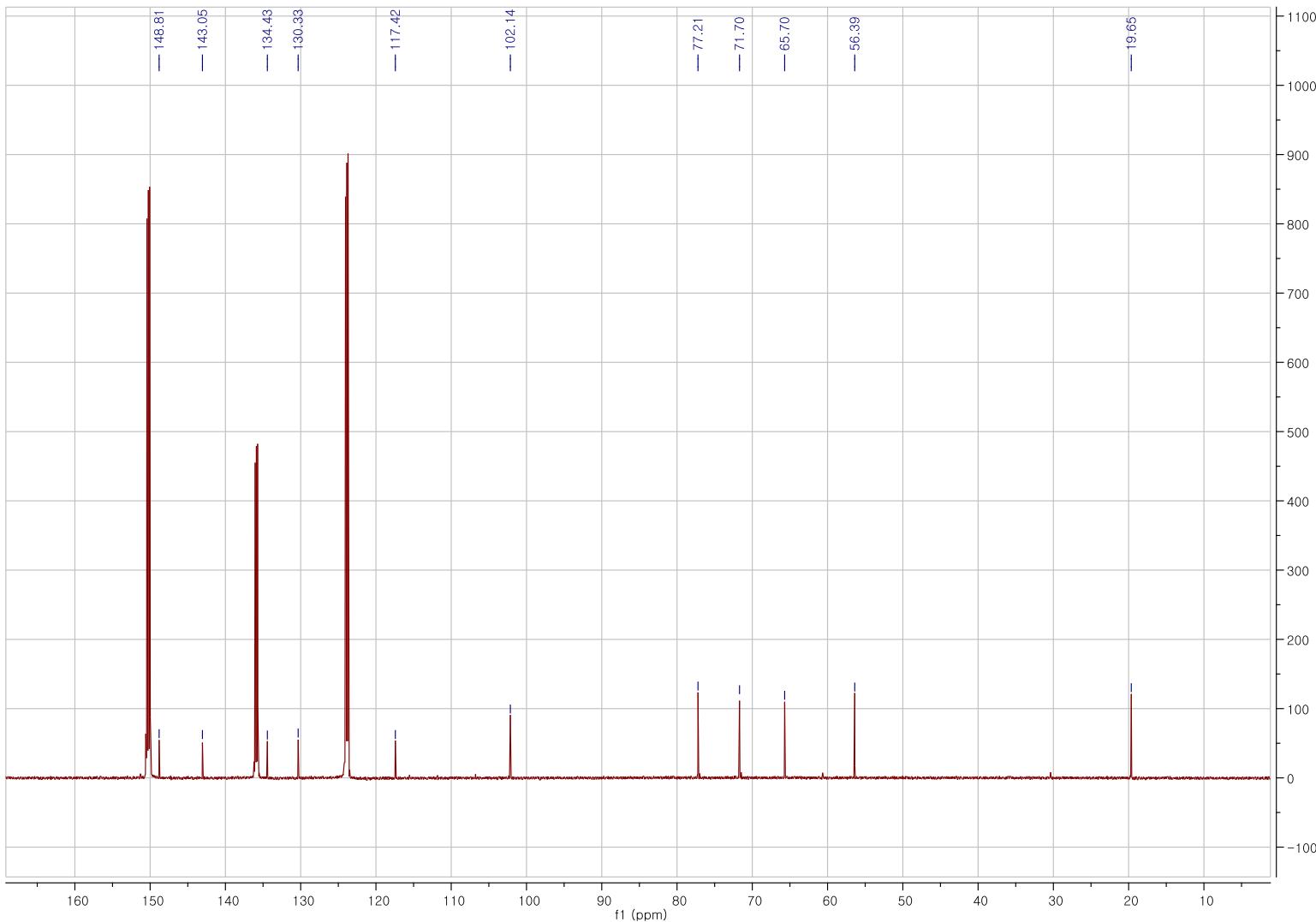


Figure S38. ^{13}C NMR spectrum of compound 7 in pyridine- d_5 (150 MHz)

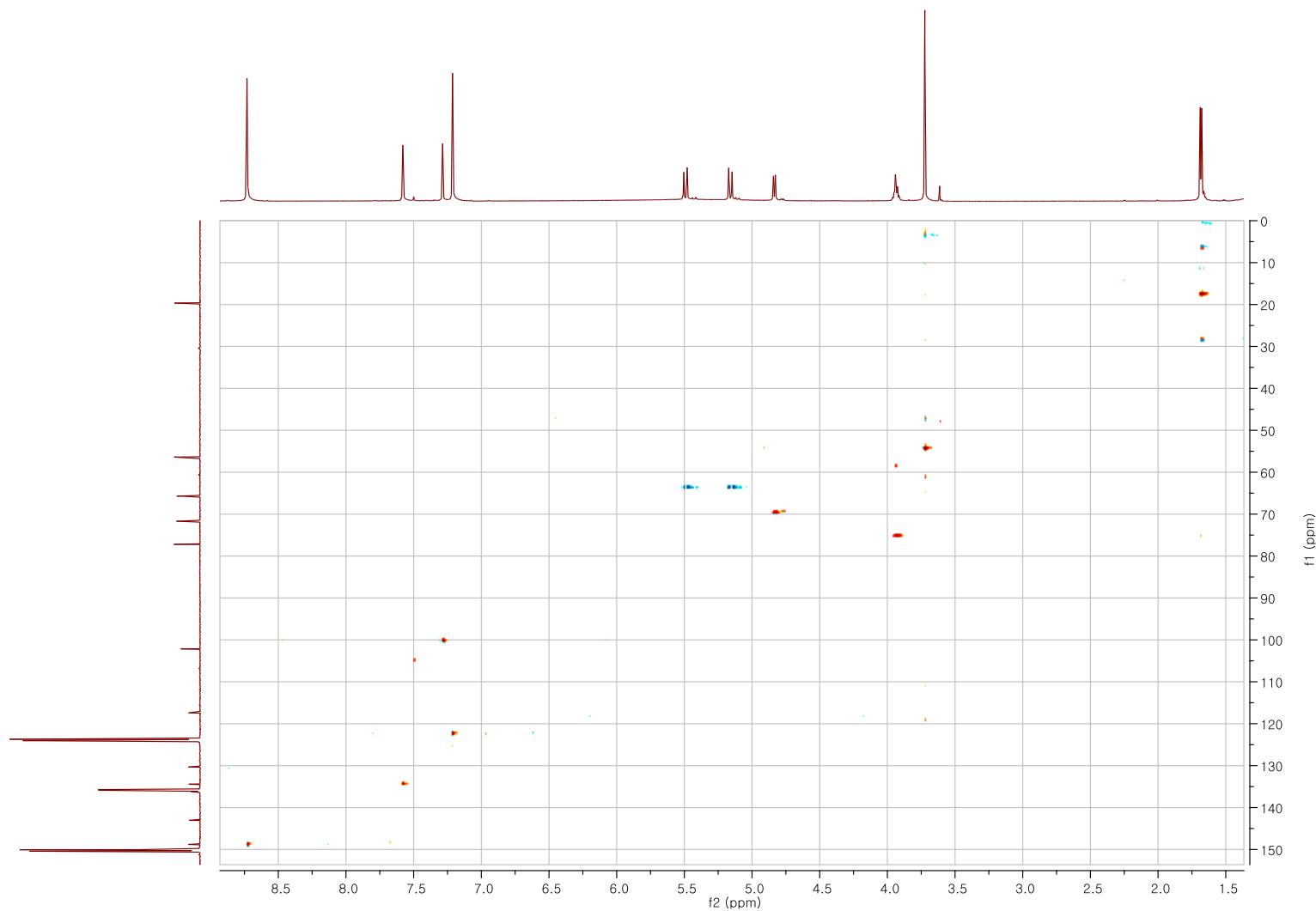


Figure S39. HMQC spectrum of compound 7

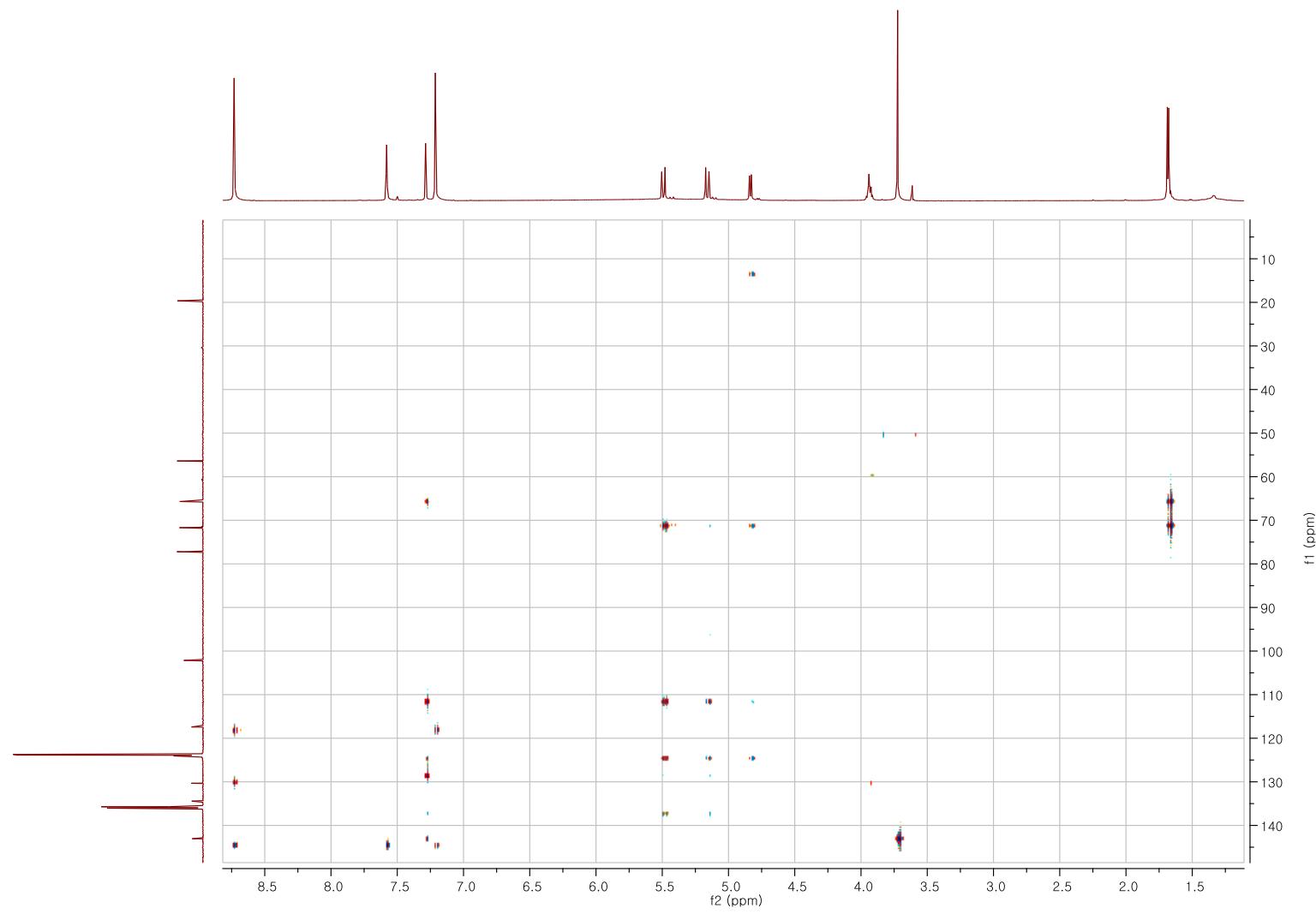


Figure S40. HMBC spectrum of compound 7

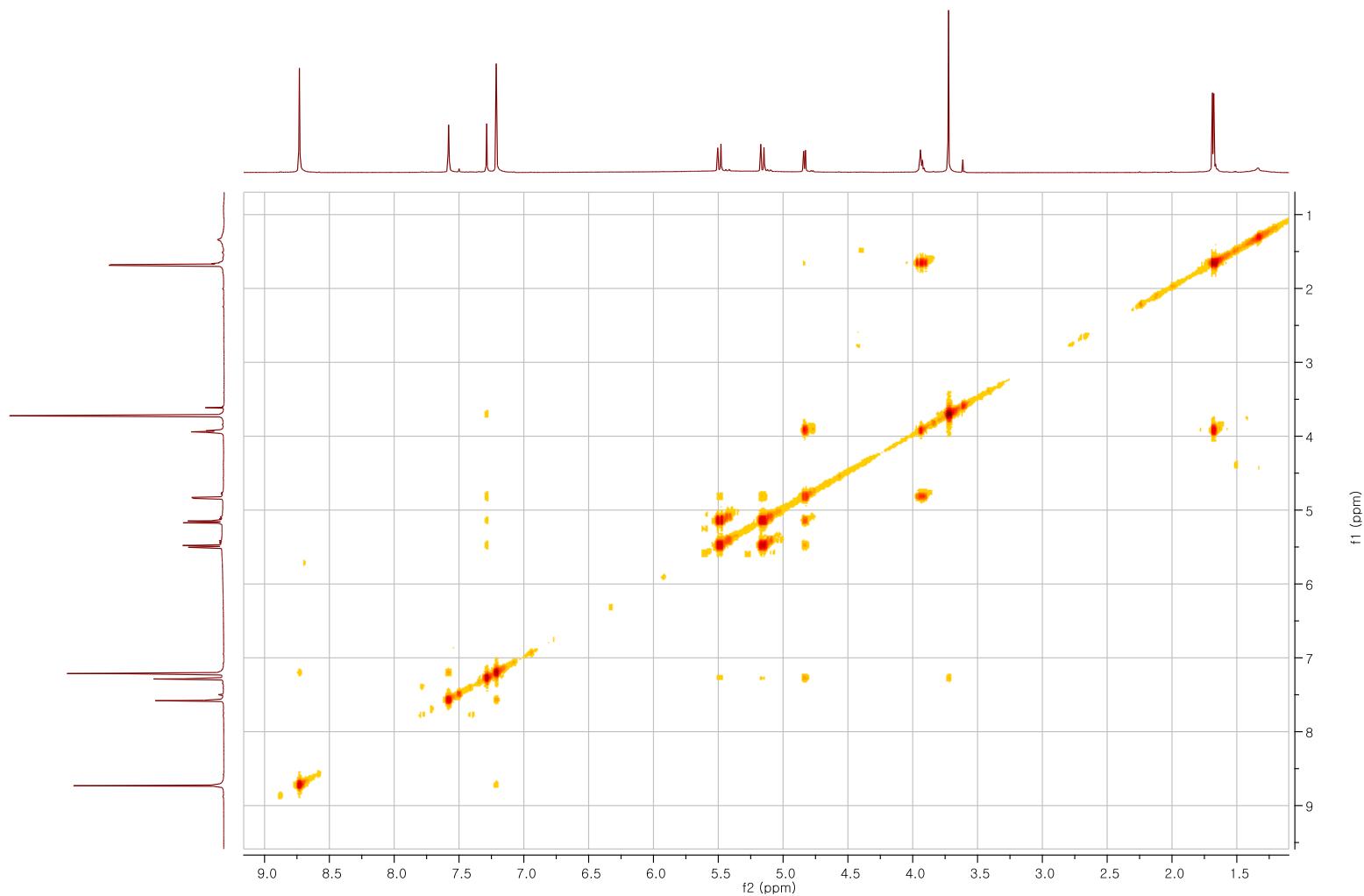


Figure S41. COSY spectrum of compound **7**

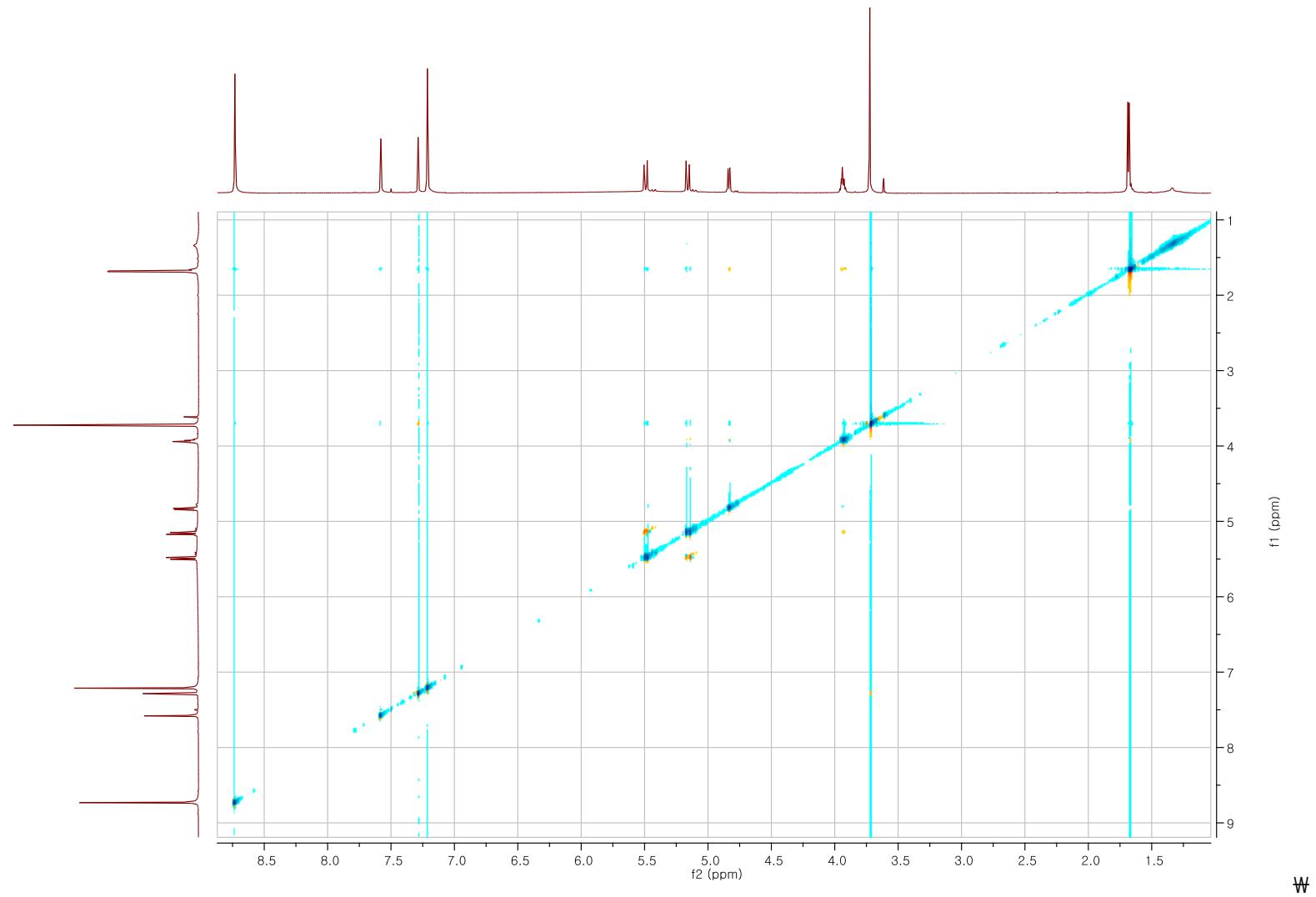


Figure S42. NOESY spectrum of compound 7

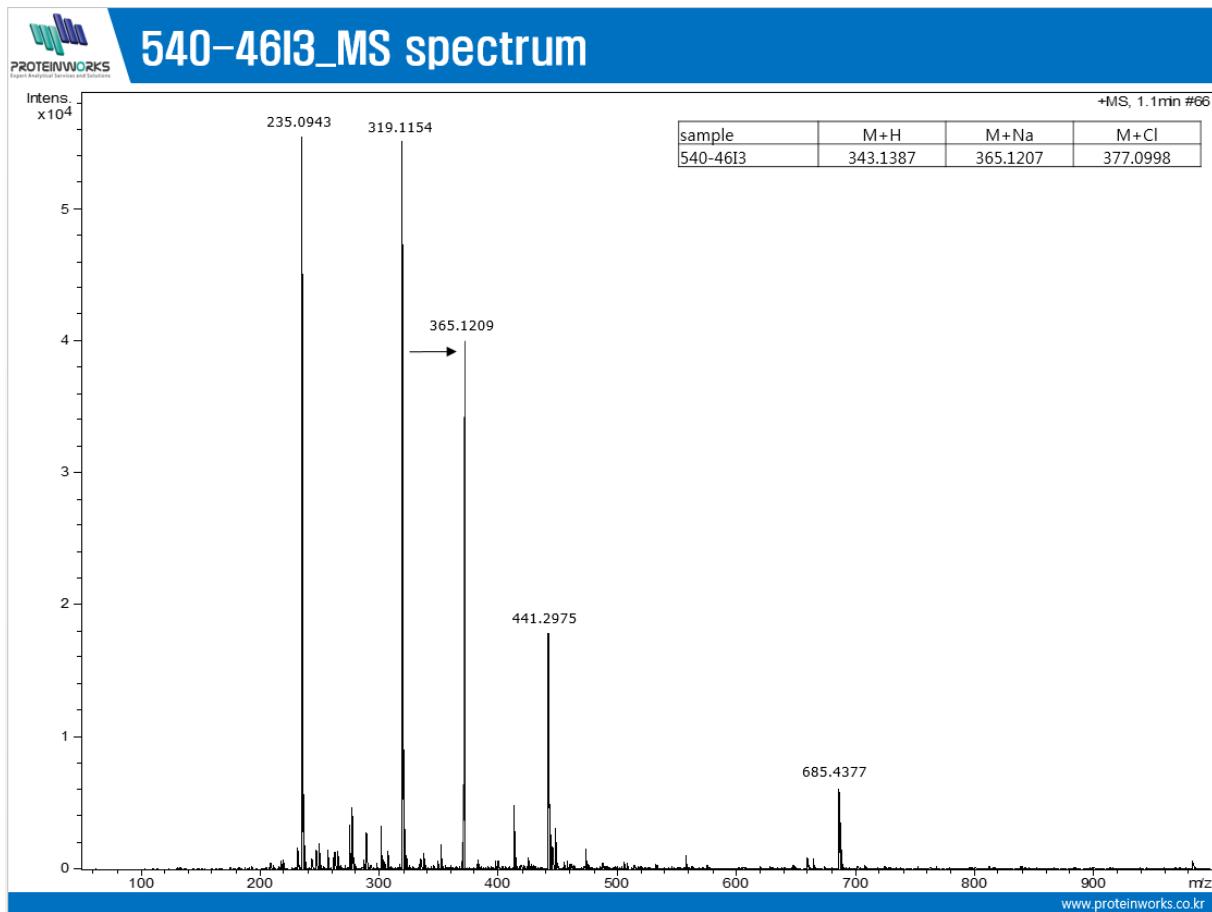


Figure S43. HR-ESI-MS spectrum of compound 8

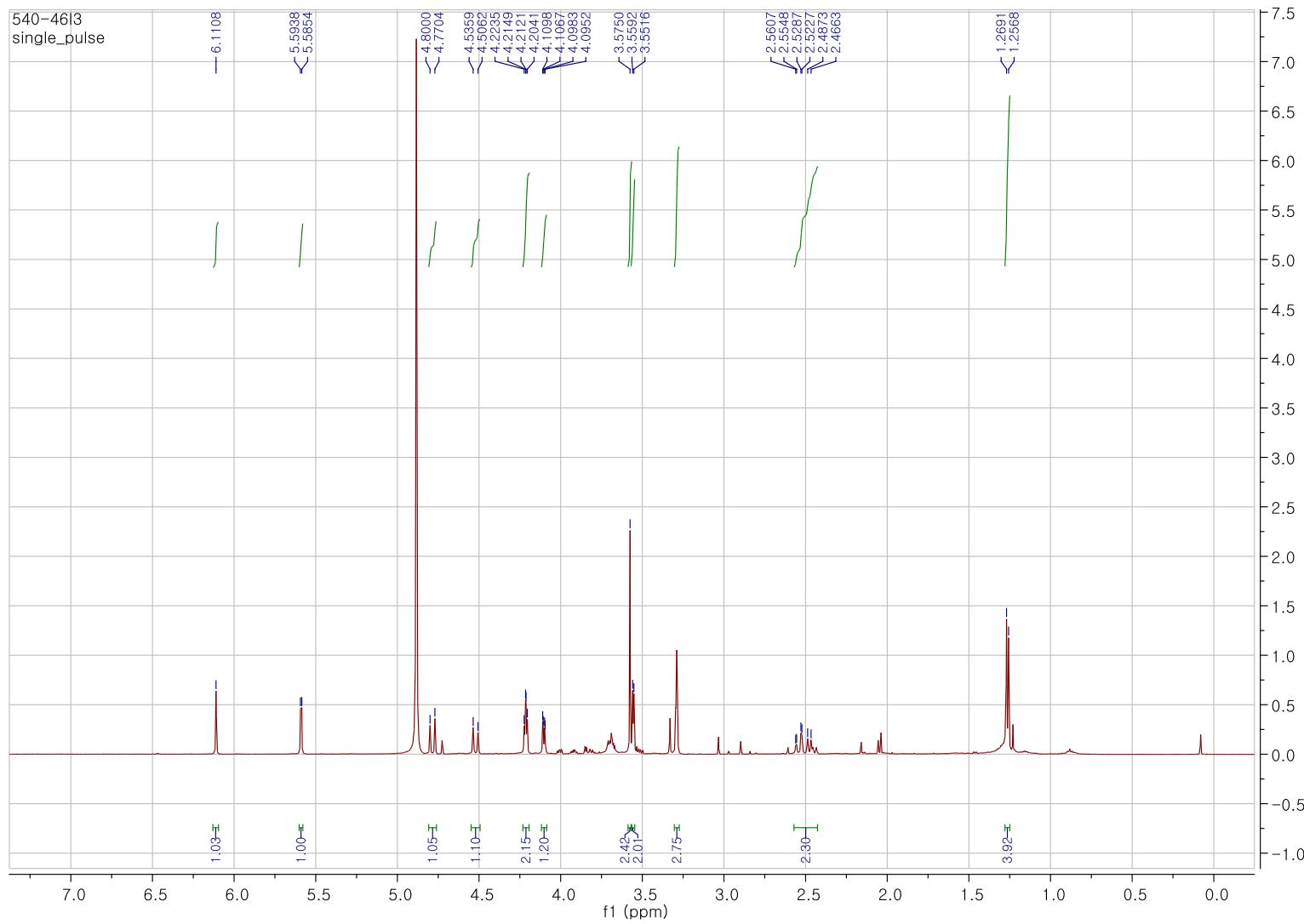


Figure S44. ^1H NMR spectrum of compound **8** in methanol- d_4 (600 MHz)

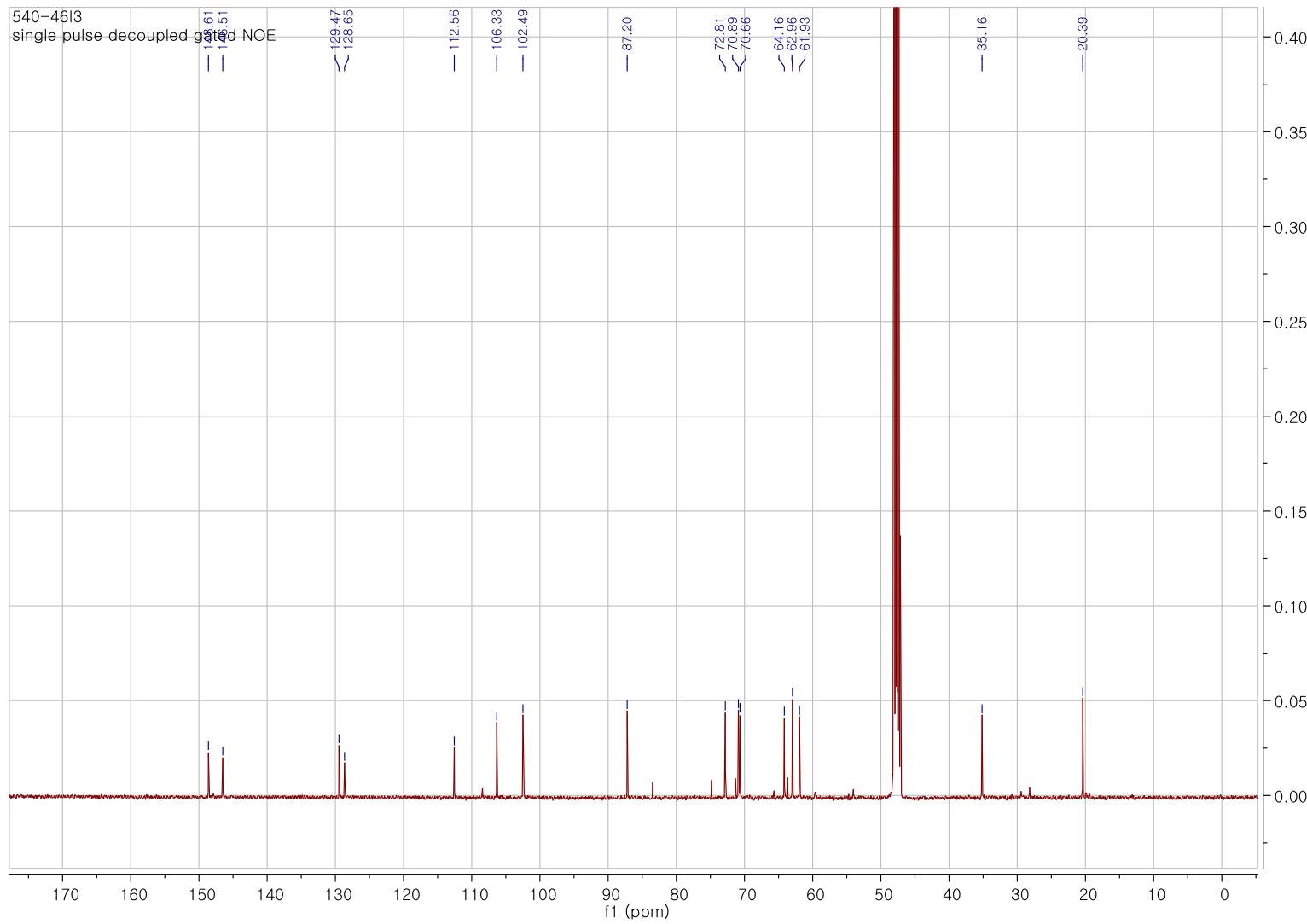


Figure S45. ^{13}C NMR spectrum of compound **8** in methanol- d_4 (150MHz)

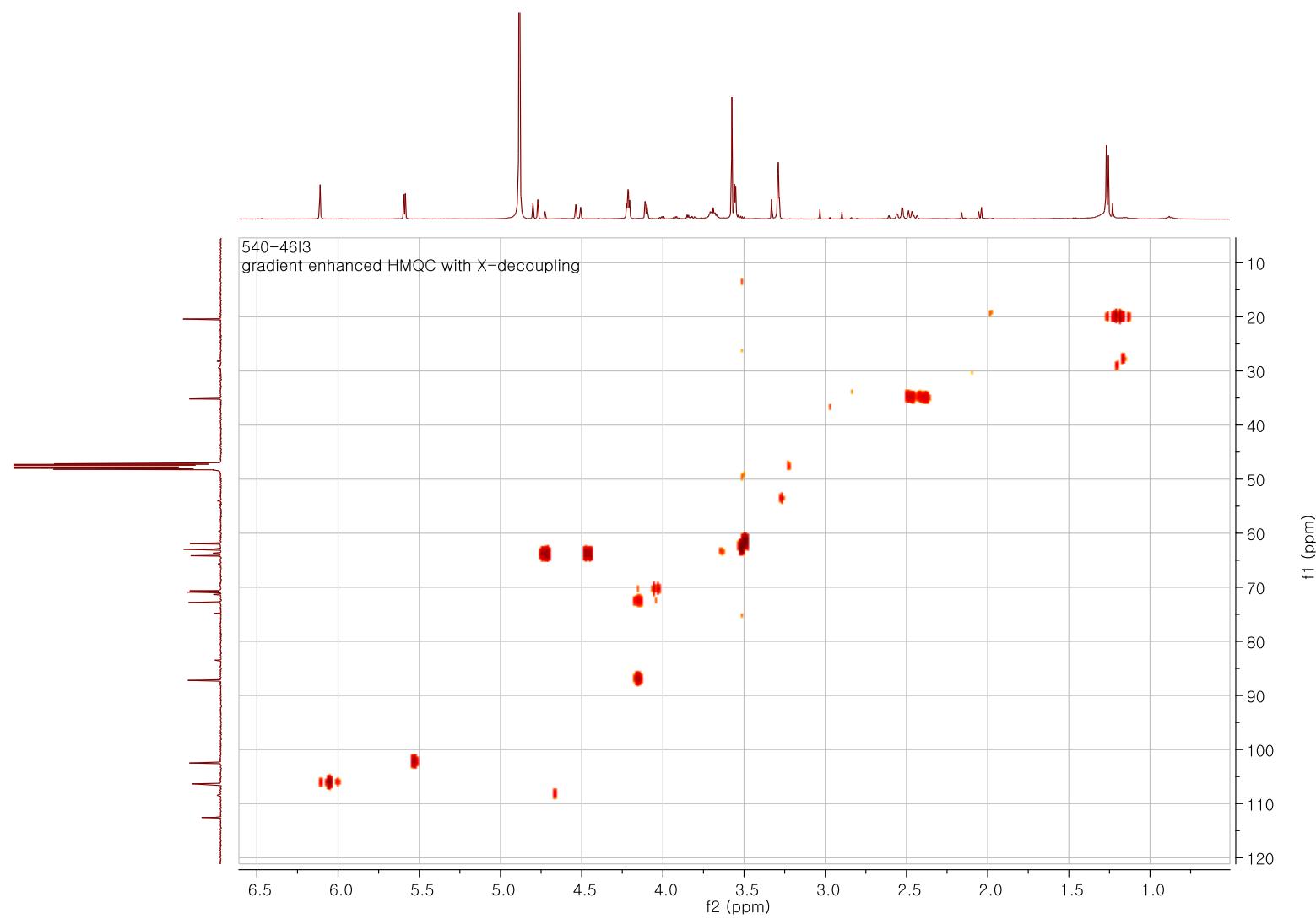


Figure S46. HMQC spectrum of compound **8**

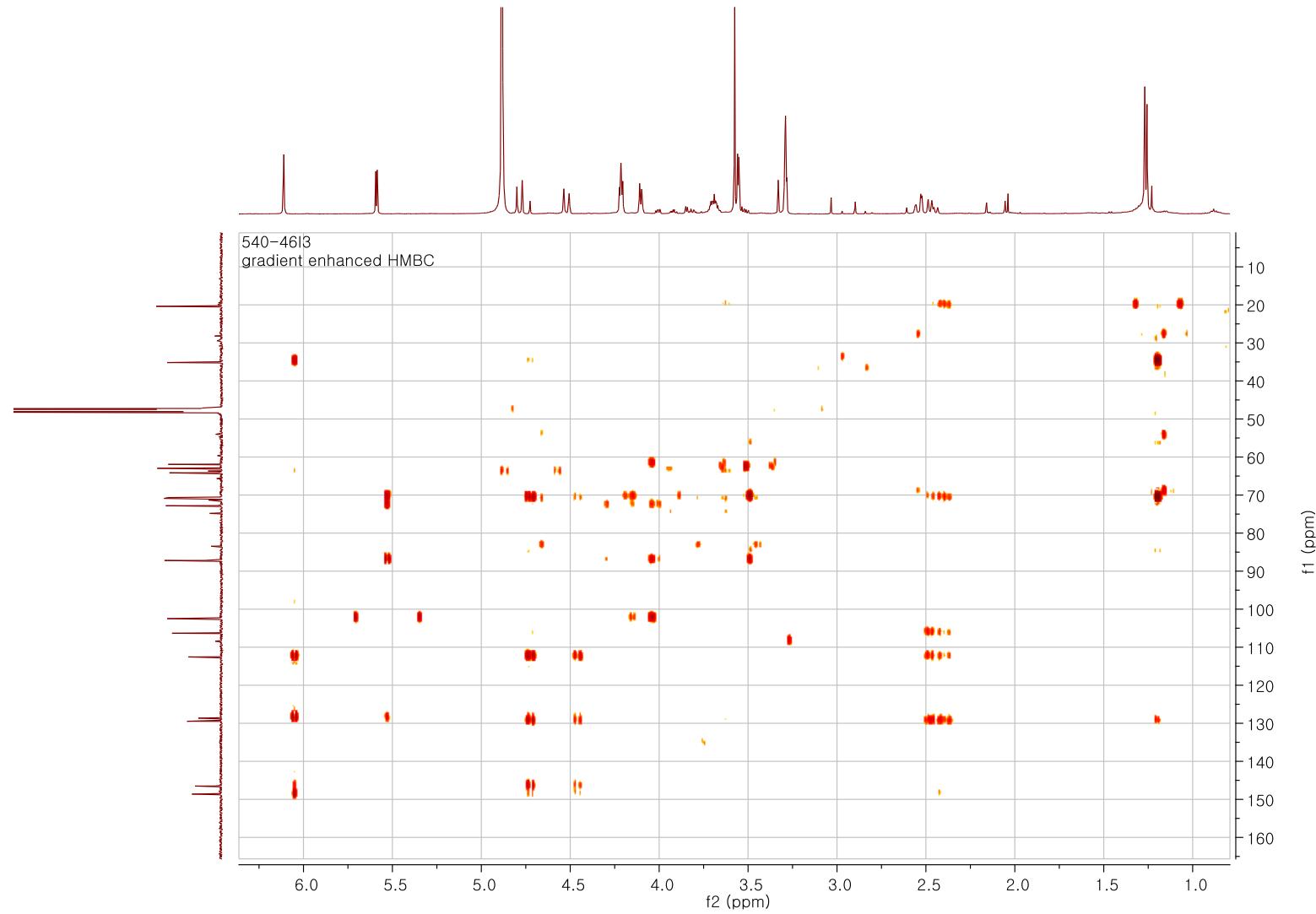


Figure S47. HMBC spectrum of compound **8**

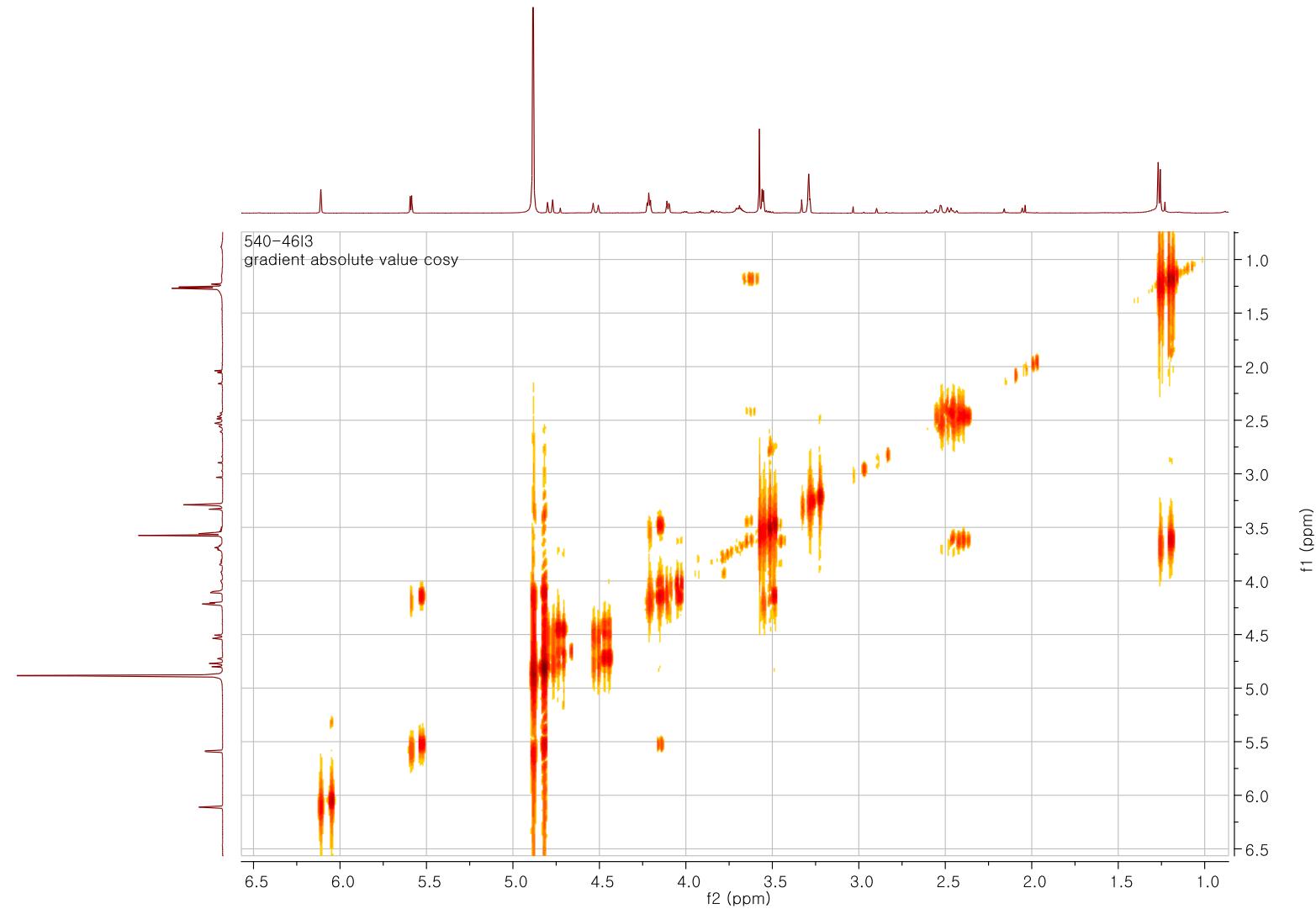


Figure S48. COSY spectrum of compound **8**

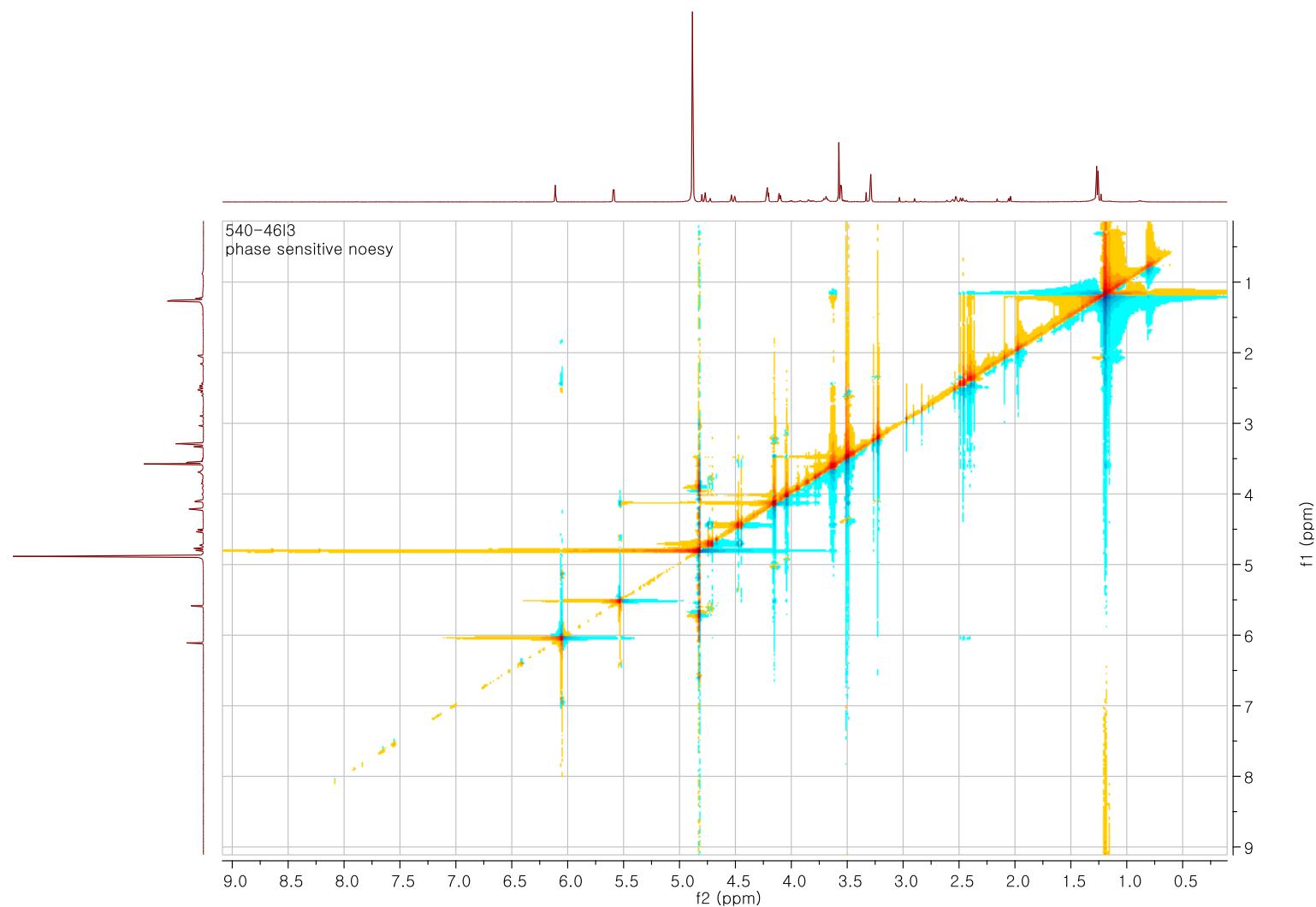


Figure S49. NOESY spectrum of compound **8**