Supplementary Information

Capsisteroids A–F, Withanolides from the Leaves of *Solanum capsicoides*

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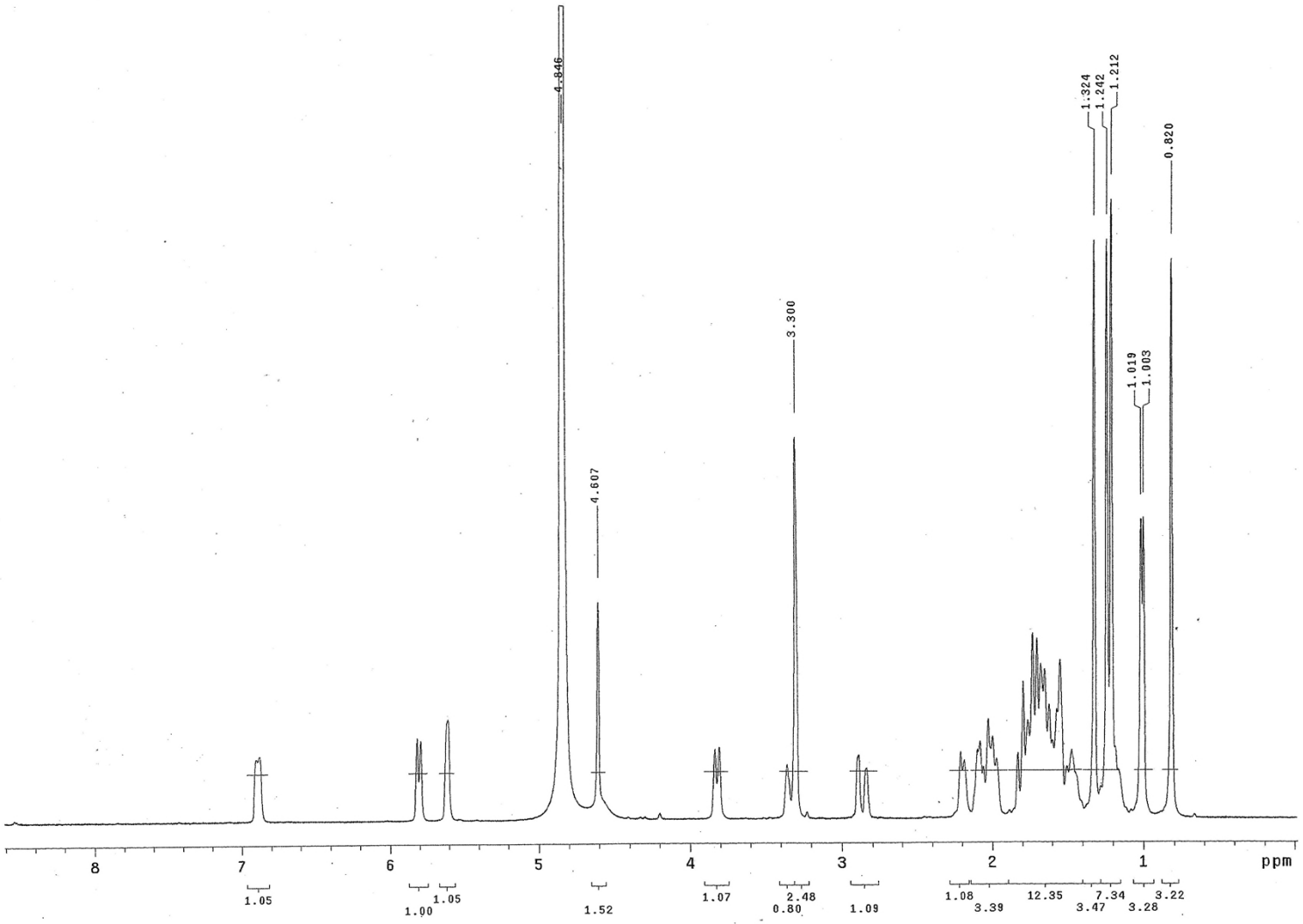
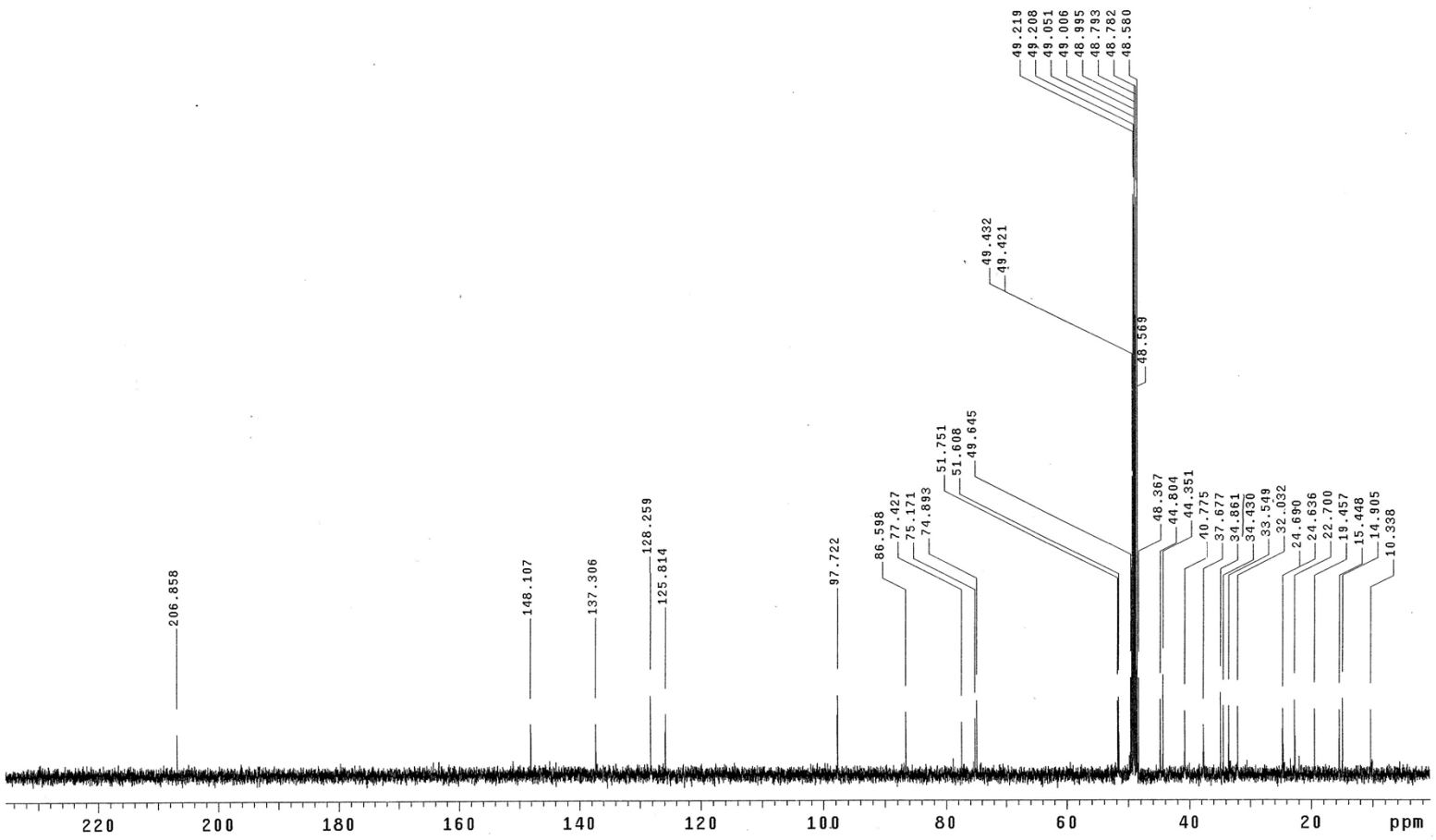
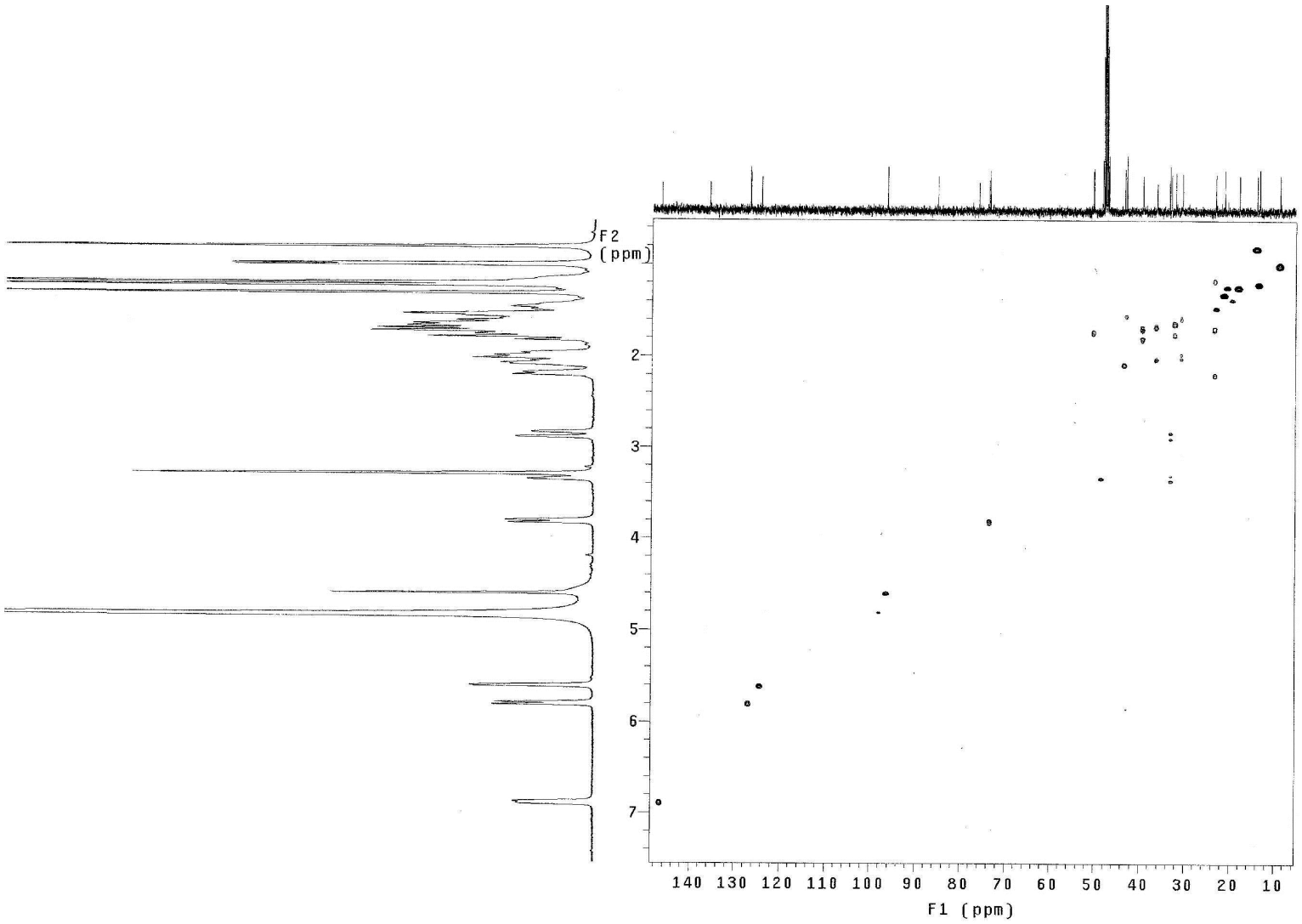


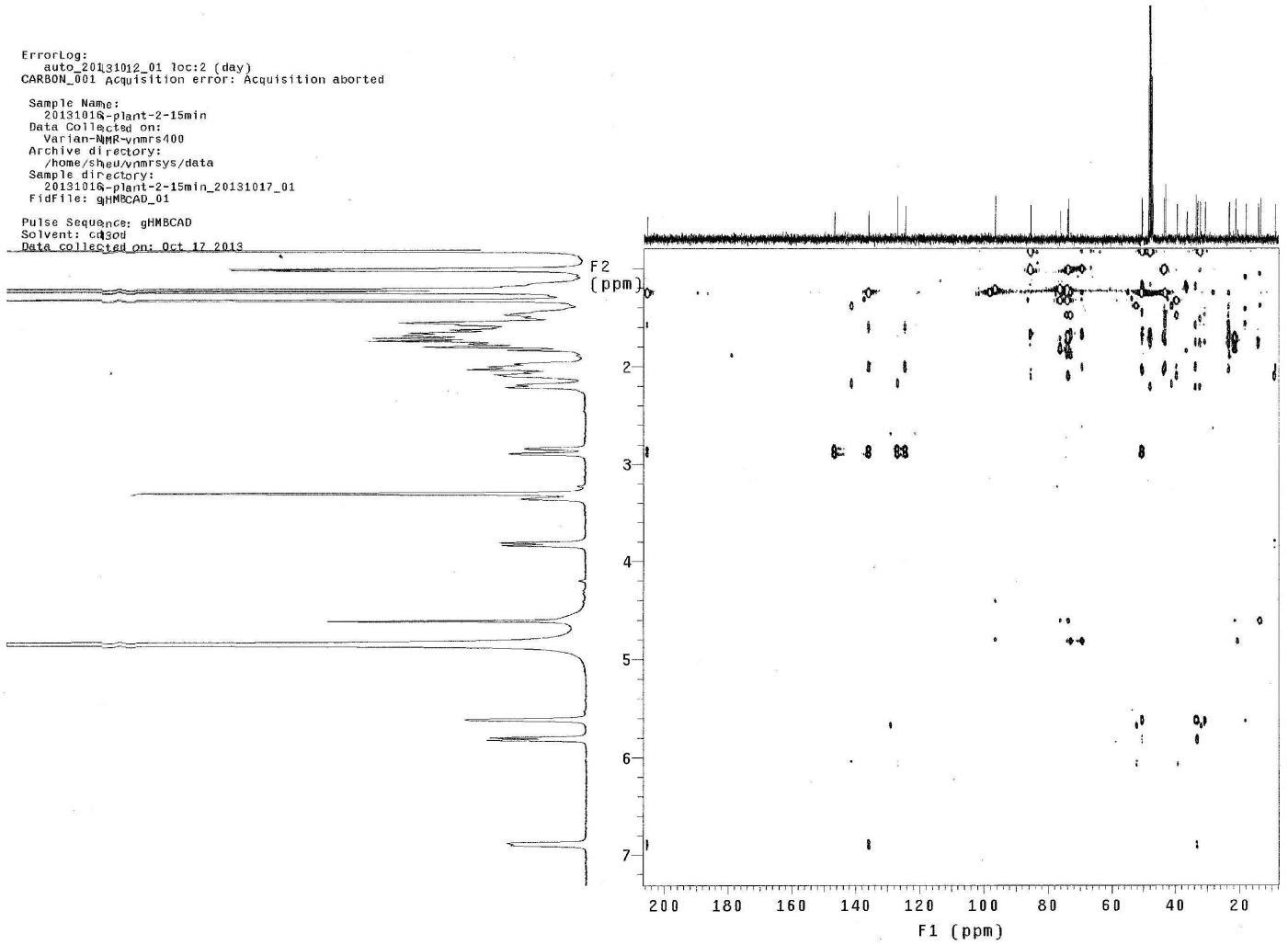
S1. ^{1}H NMR spectrum of **1** in methanol-d_4 at 400 MHz.



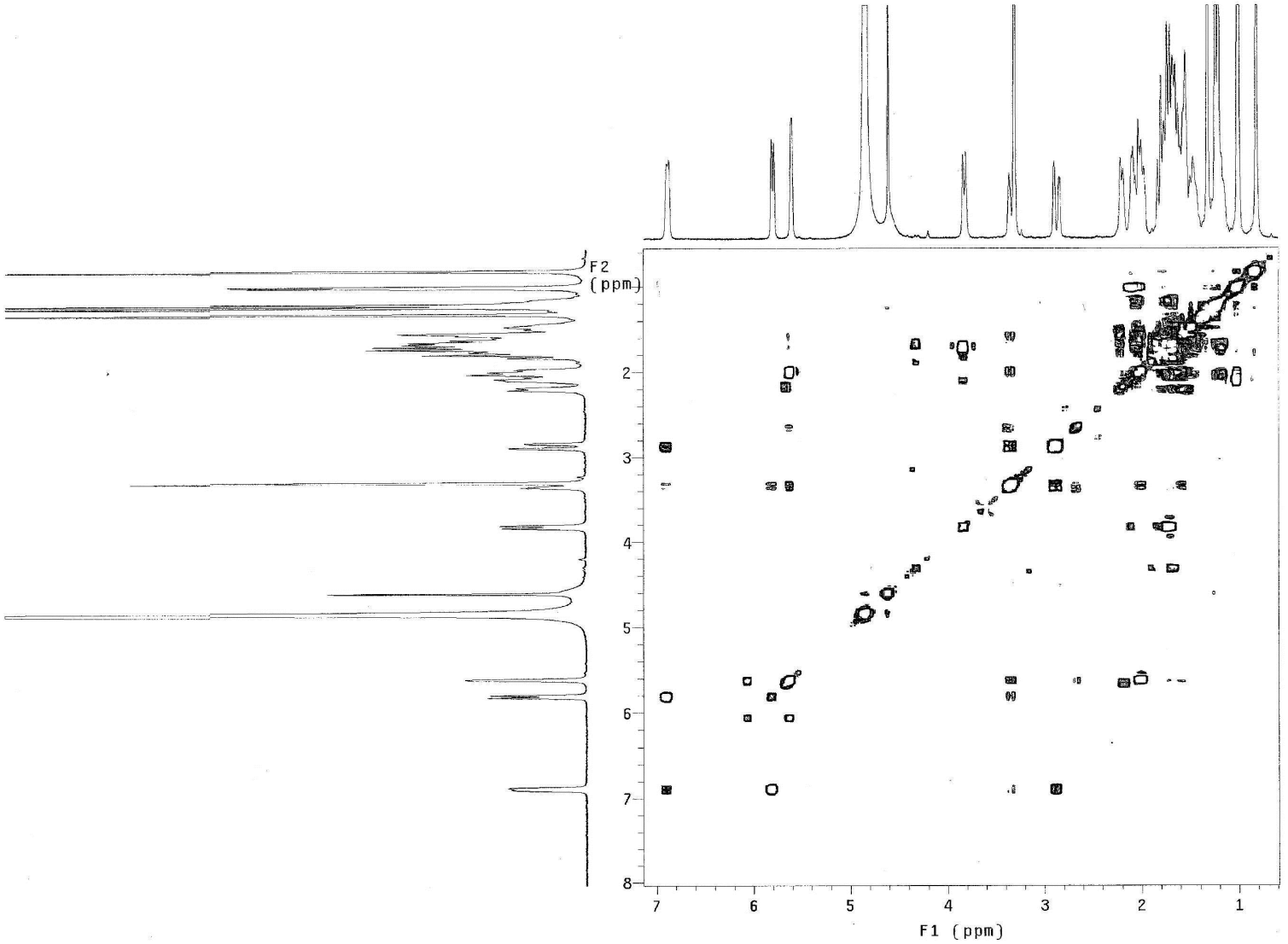
S2. ^{13}C NMR spectrum of **1** in methanol-d_4 at 100 MHz.



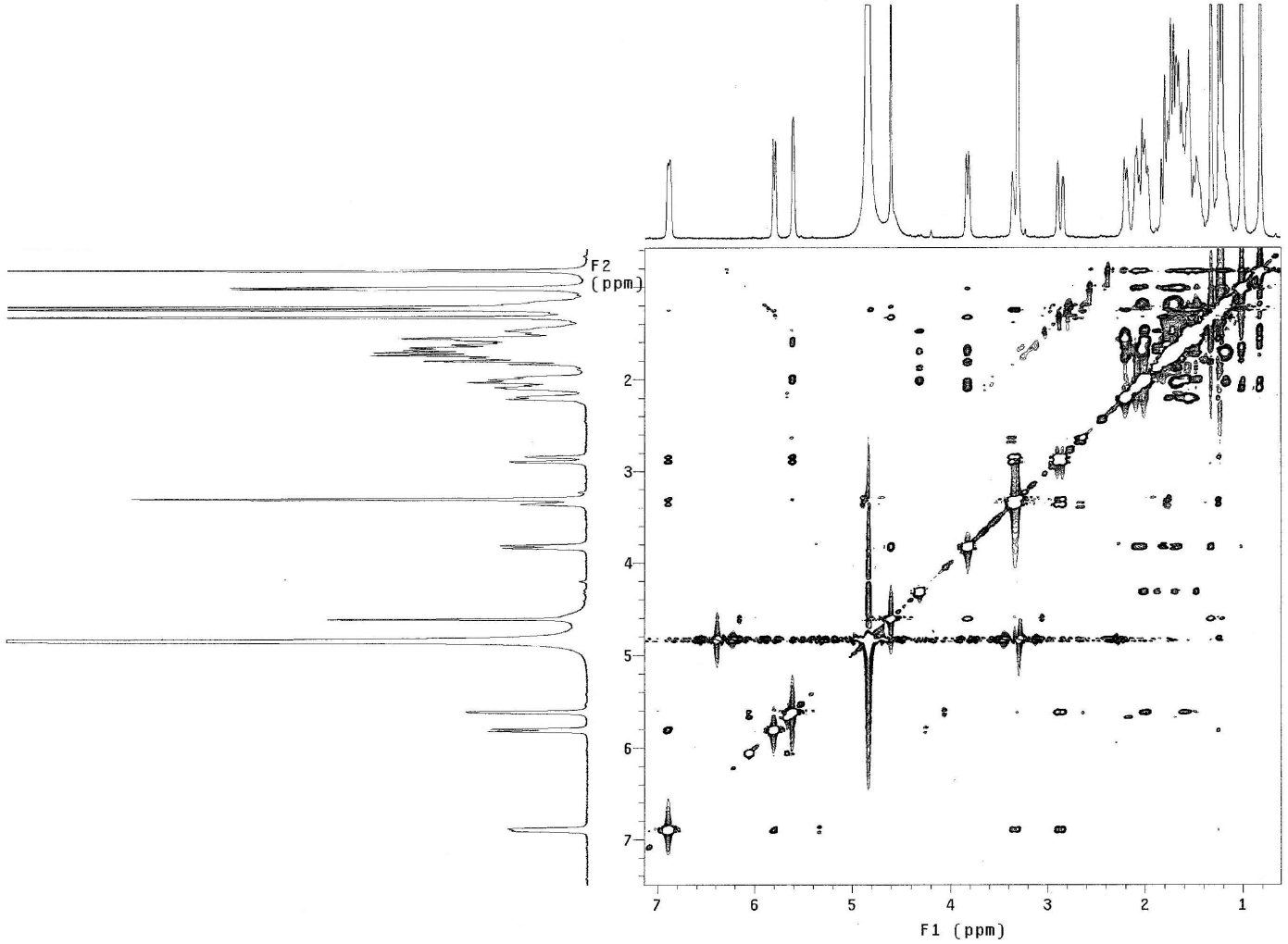
S3. HSQC spectrum of **1** in methanol-d_4 at 100 MHz.



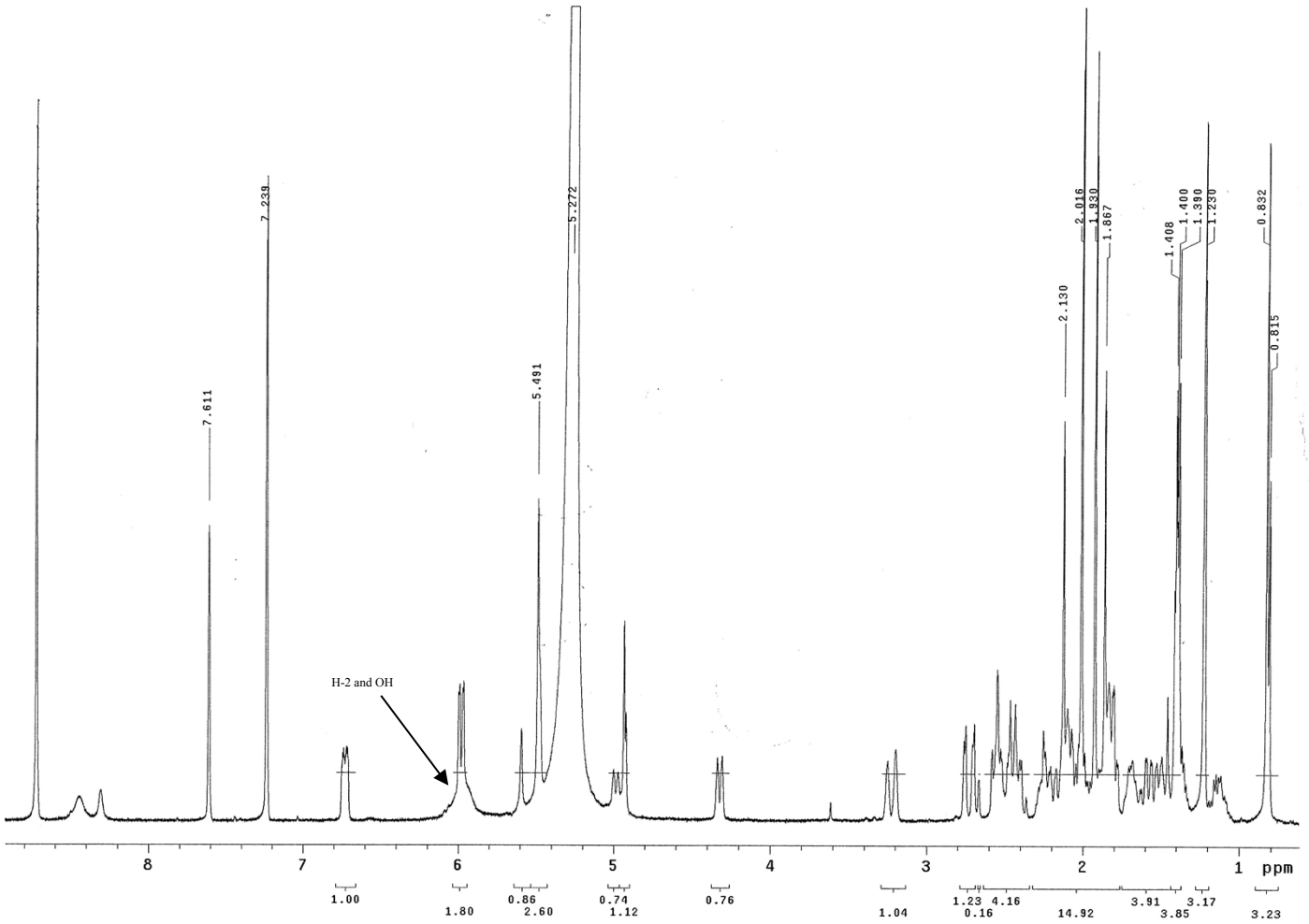
S4. HMBC spectrum of **1** in methanol-d_4 at 100 MHz.



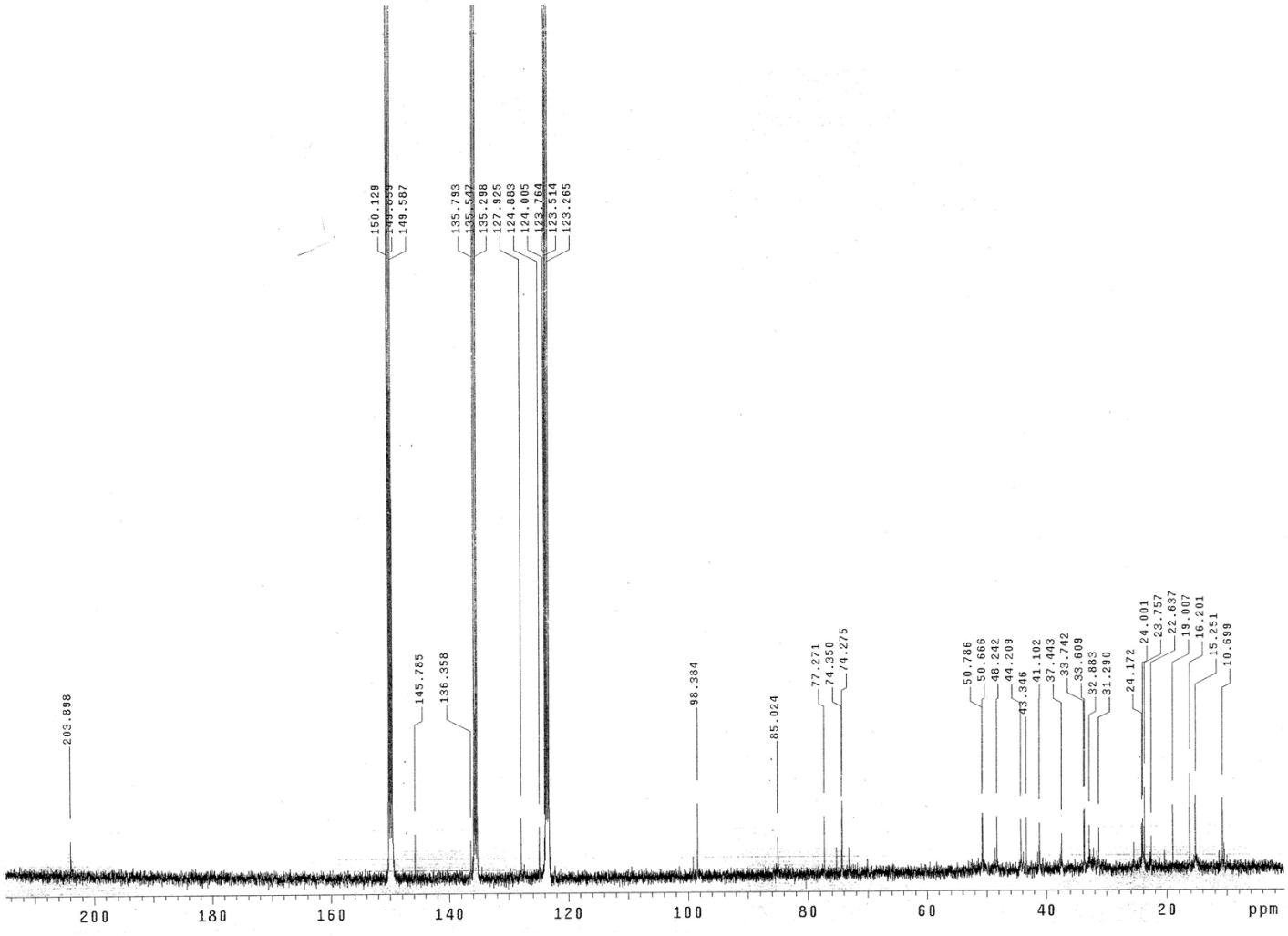
S5. COSY spectrum of **1** in methanol-d_4 at 100 MHz.



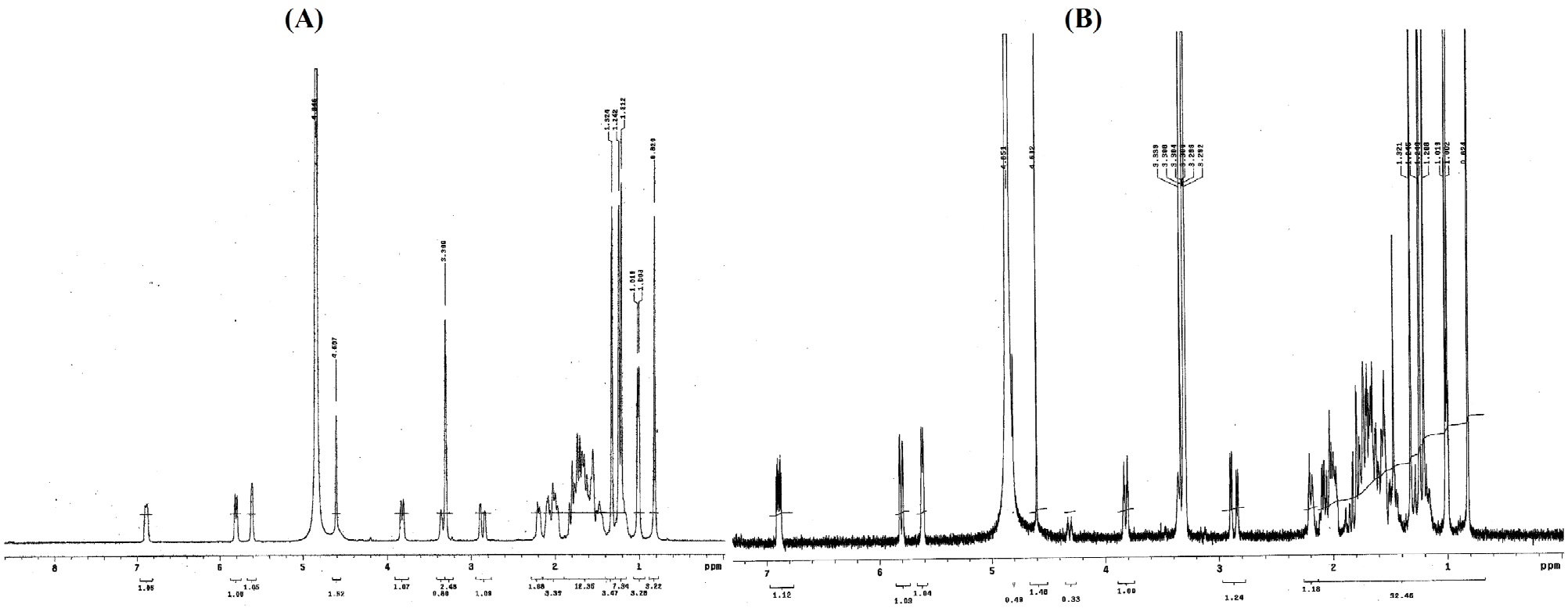
S6. NOESY spectrum of **1** in methanol-d_4 at 100 MHz.



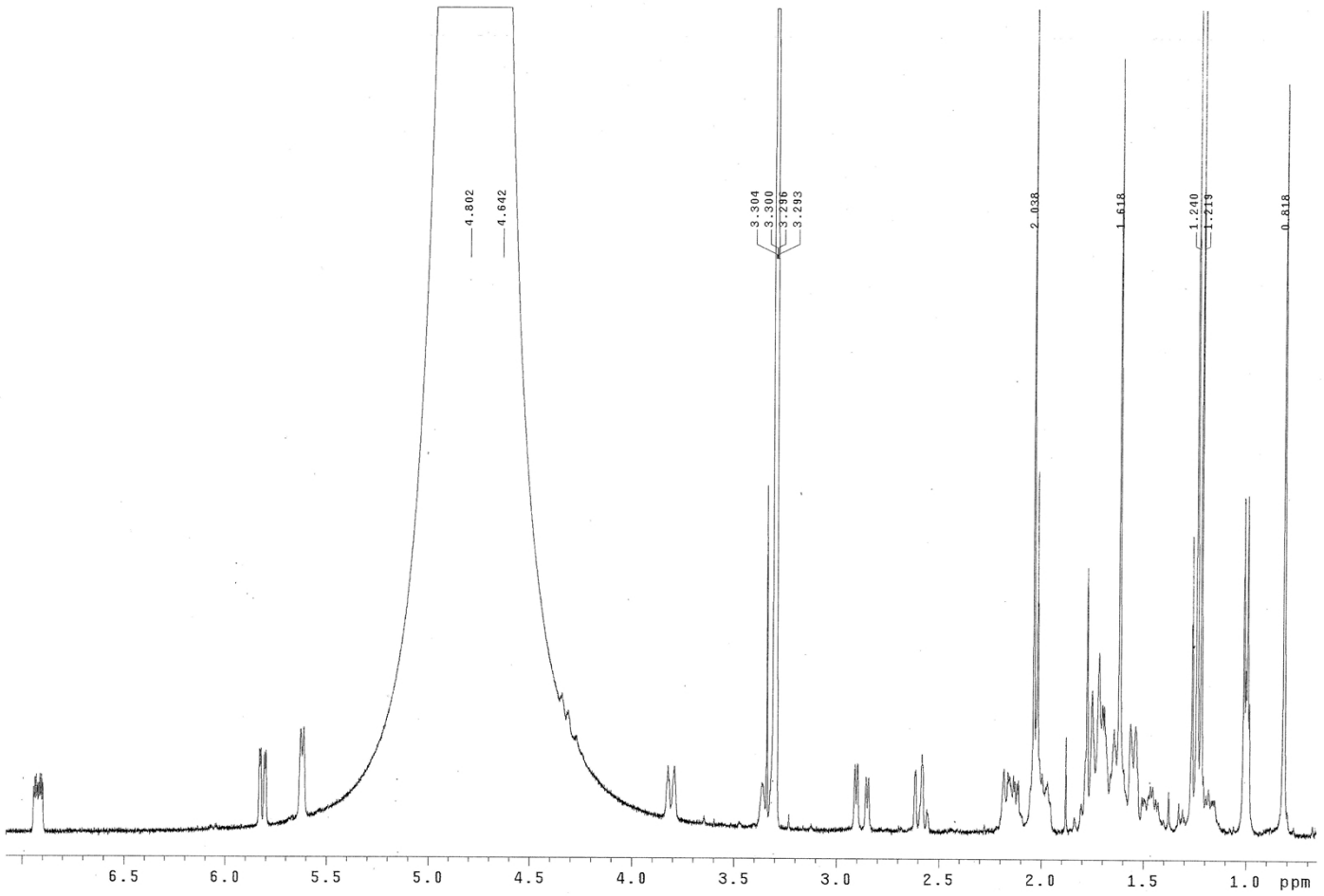
S7. ^{1}H NMR spectrum of **1** in pyridine-d_5 at 400 MHz.



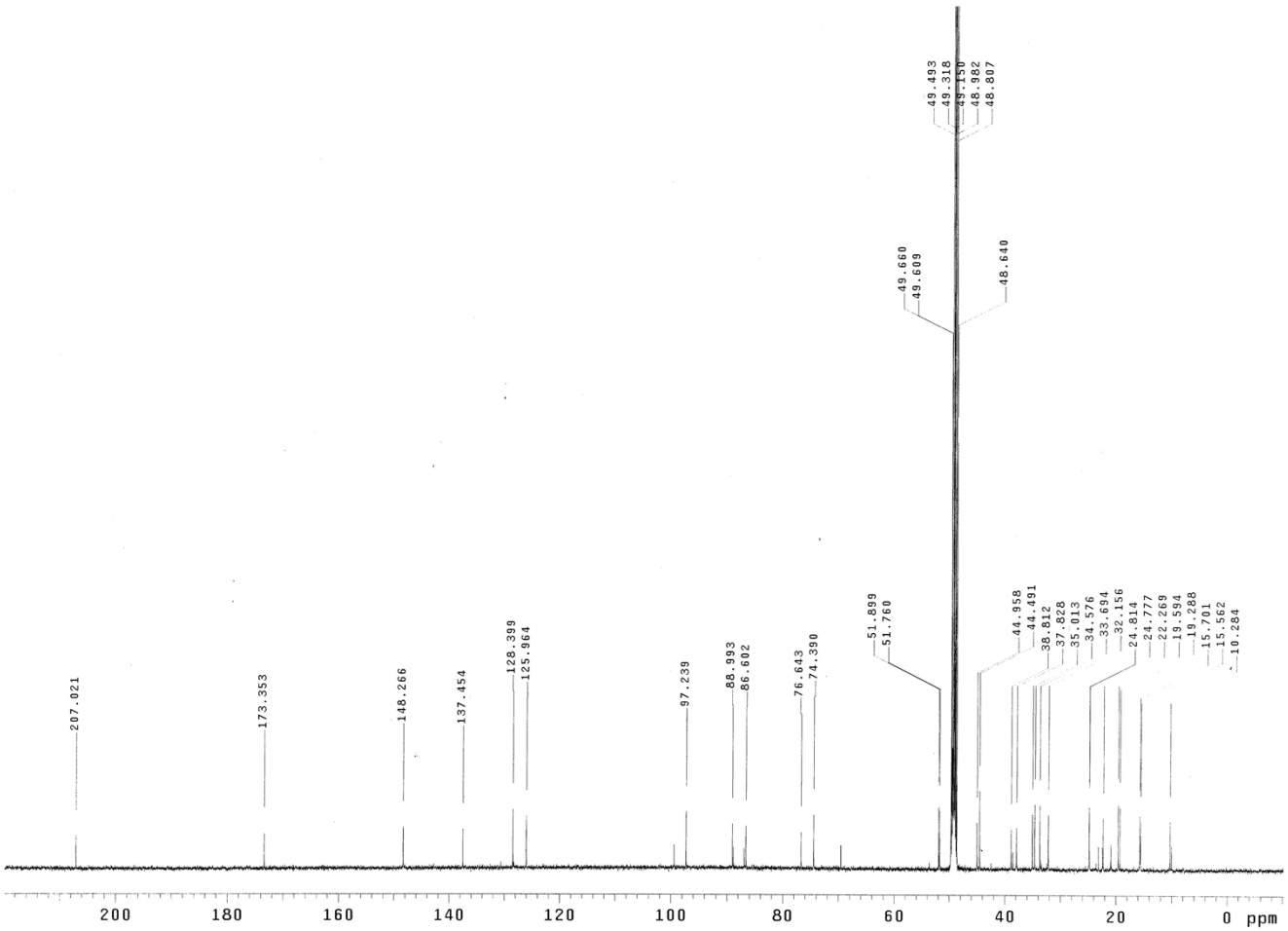
S8. ^{13}C NMR spectrum of **1** in pyridine-d_5 at 100 MHz.



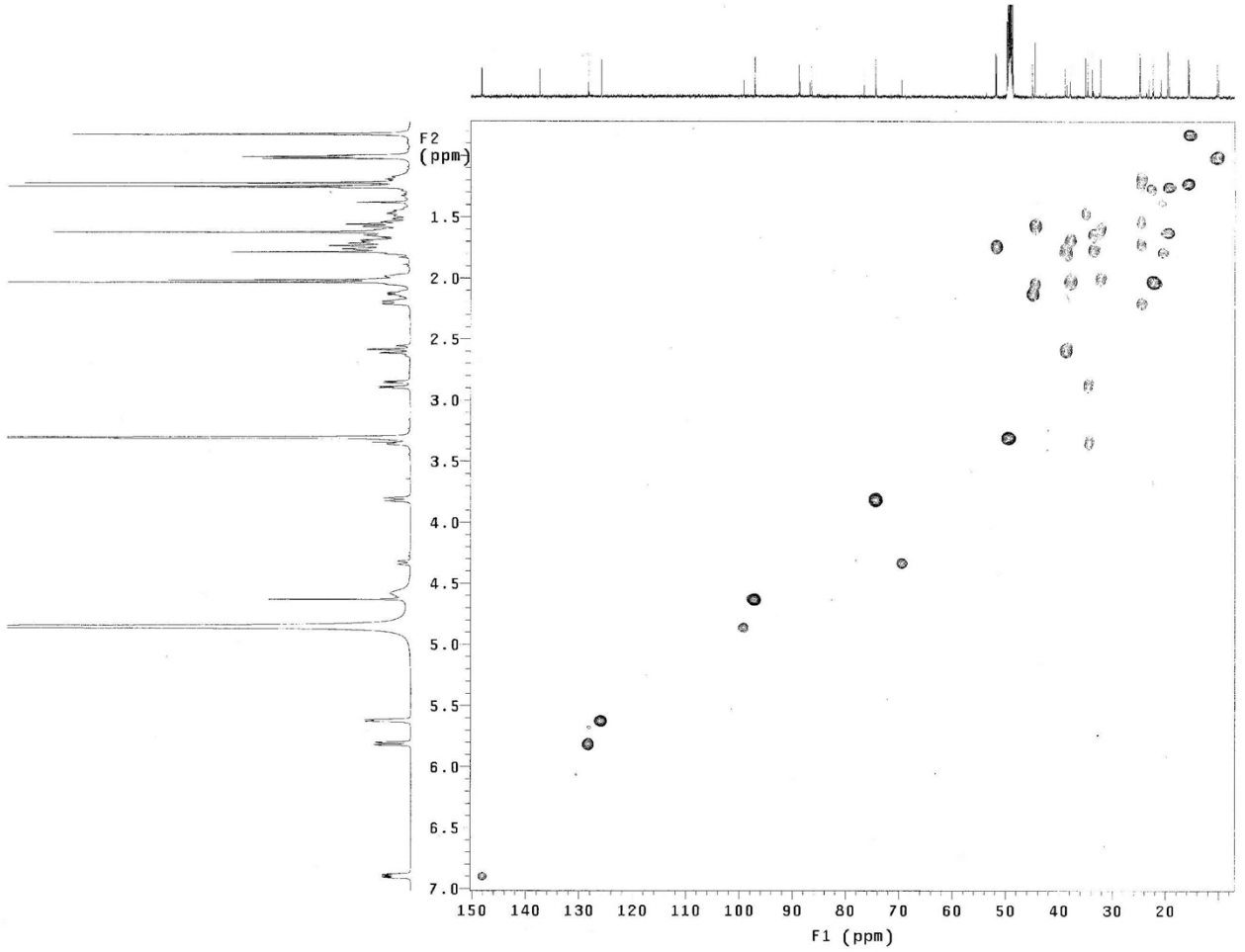
S9. (A) 26*S* conformer of pure compound **1 (B)** 3:1 epimeric (26*S*/*R*) mixture of compound **1**



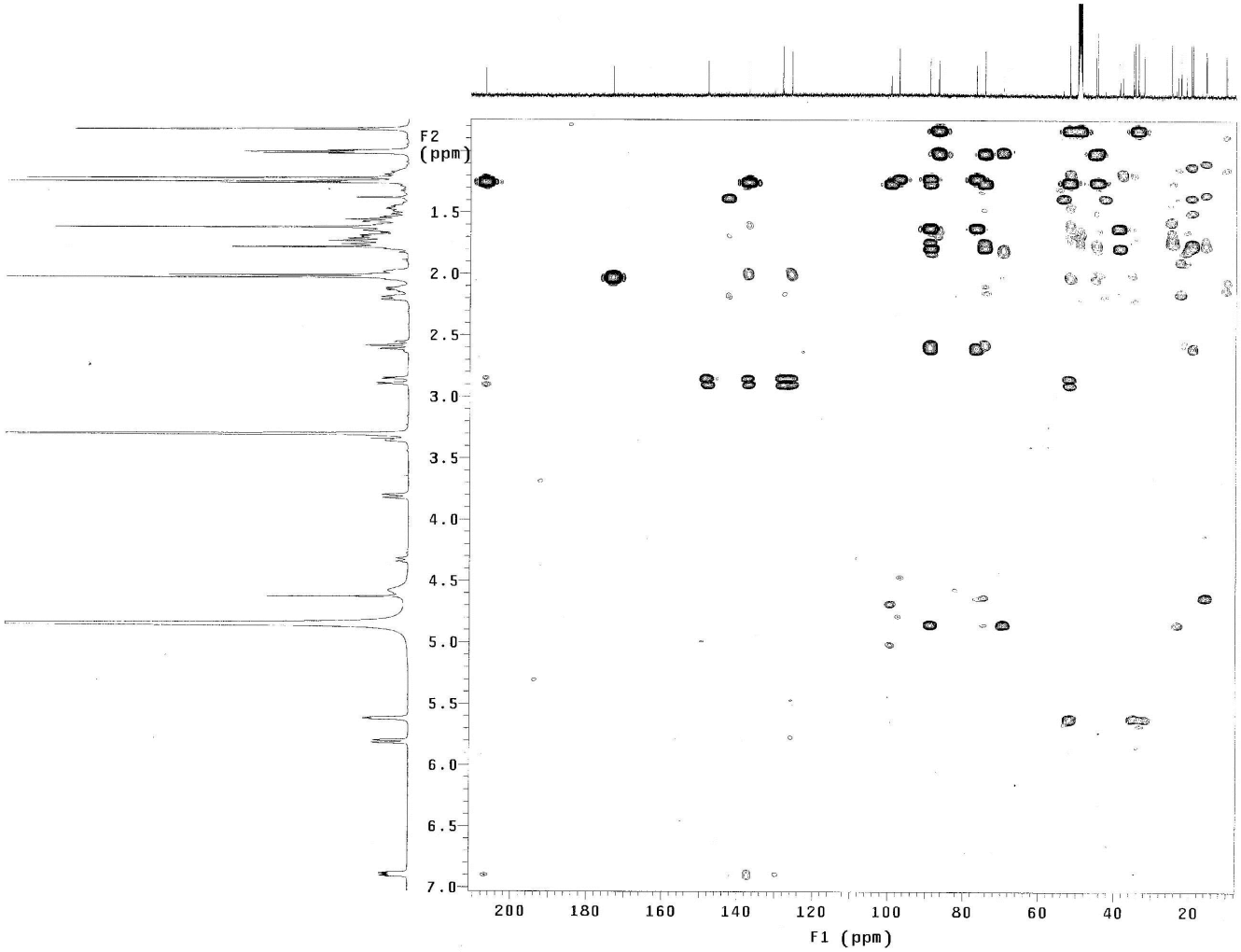
S10. ^{1}H NMR spectrum of **2** in methanol-d_4 at 400 MHz.



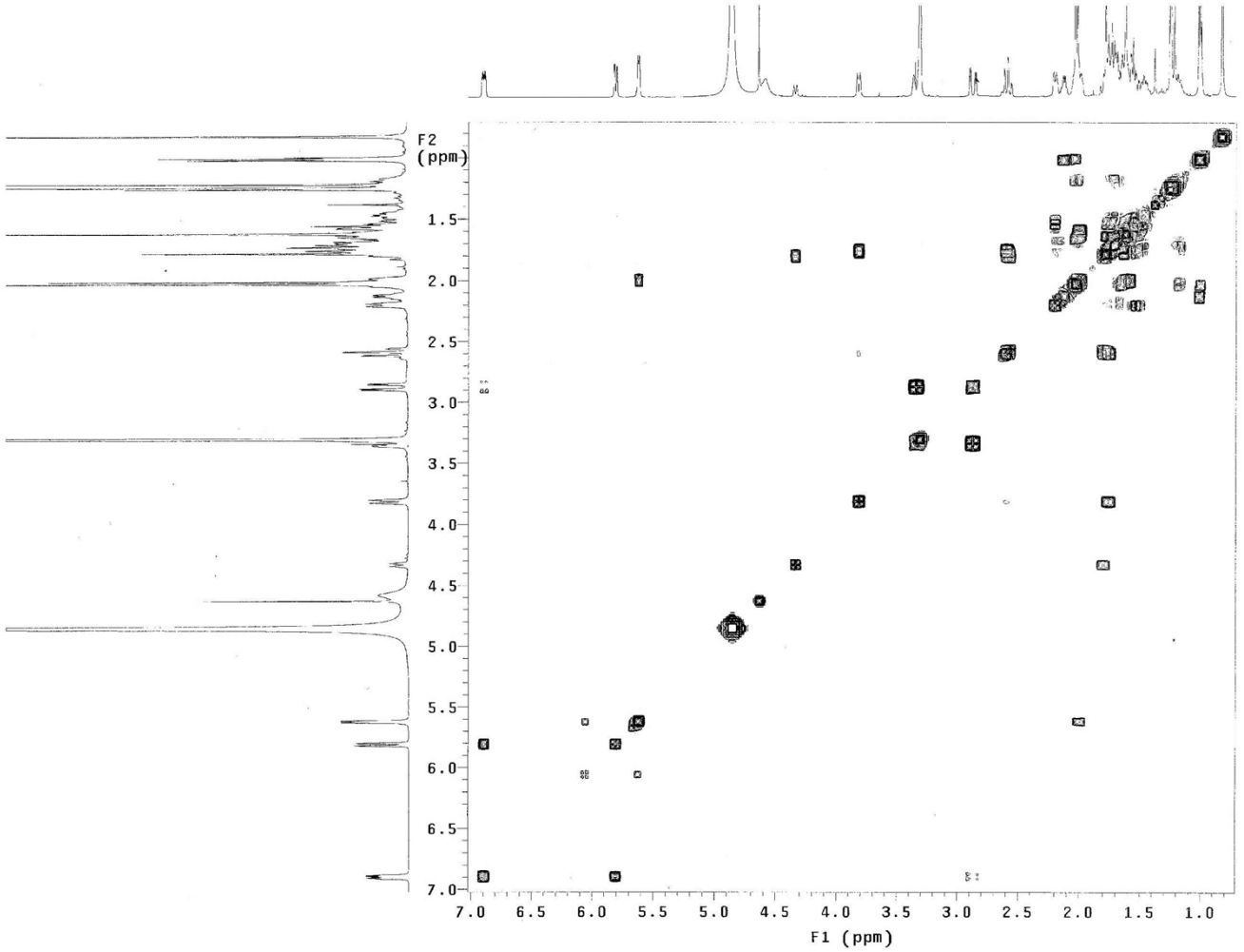
S11. ^{13}C NMR spectrum of **2** in methanol-d_4 at 100 MHz.



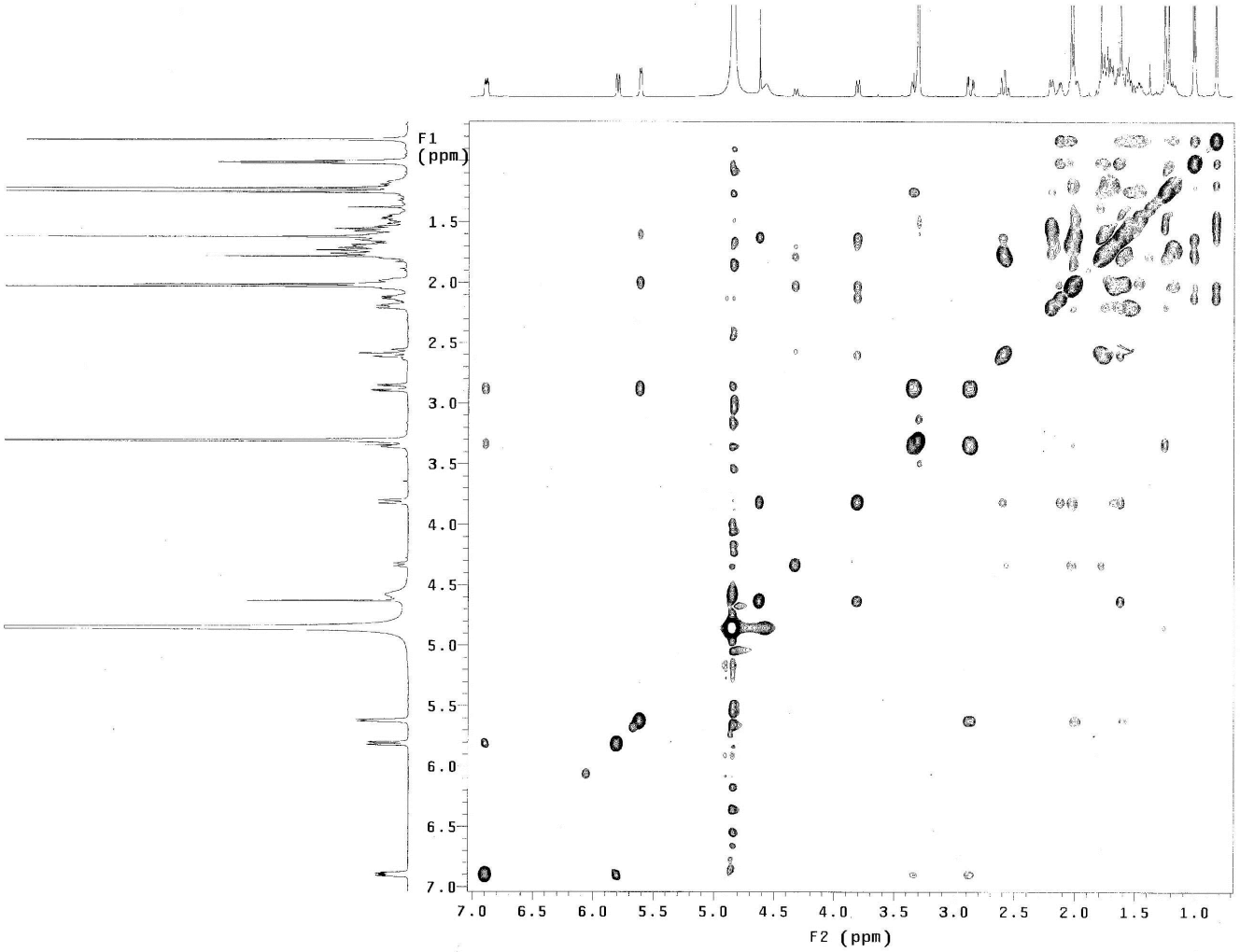
S12. HSQC spectrum of **2** in methanol-d_4 at 100 MHz.



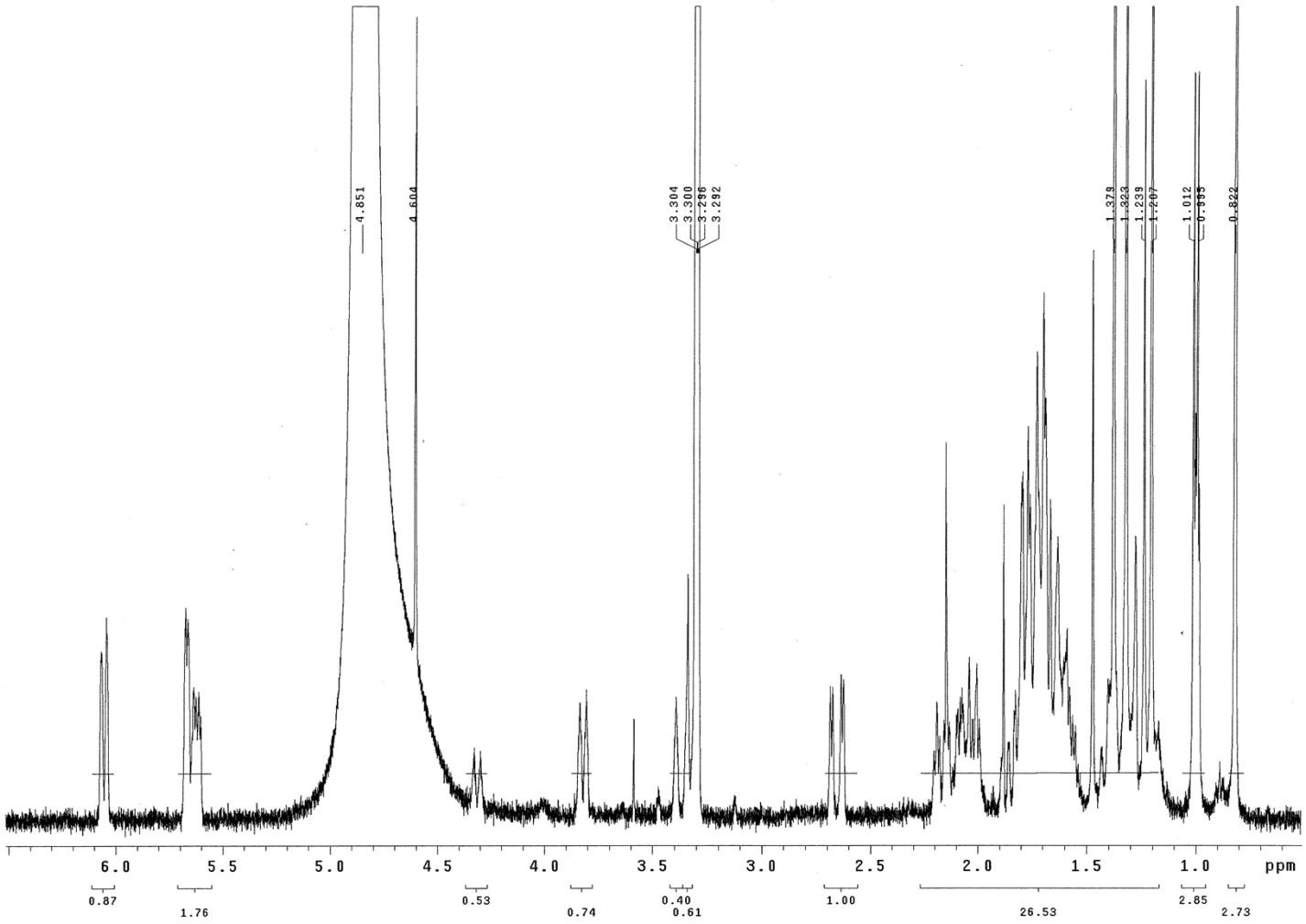
S13. HMBC spectrum of **2** in methanol-d_4 at 100 MHz.



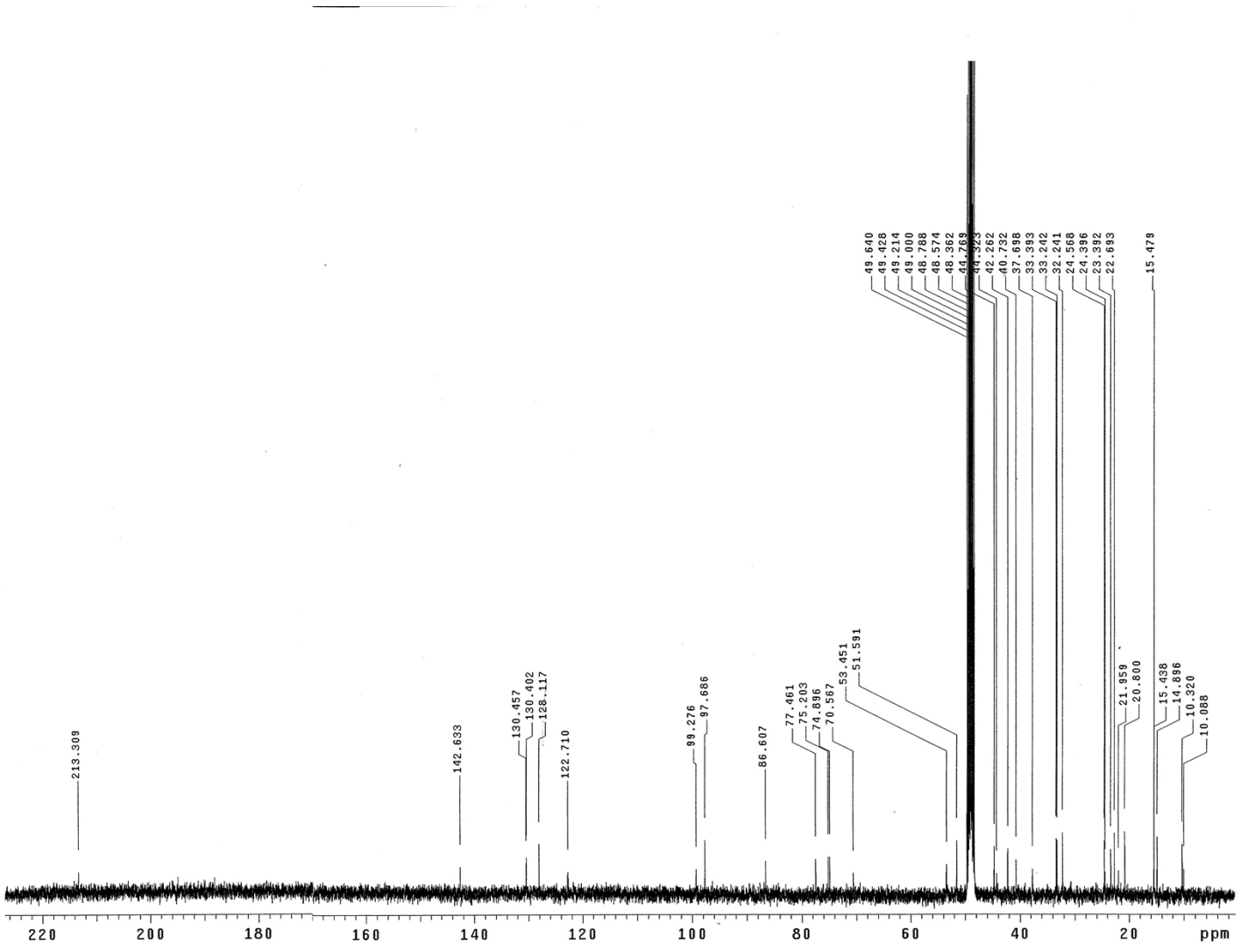
S14. COSY spectrum of **2** in methanol-d_4 at 100 MHz



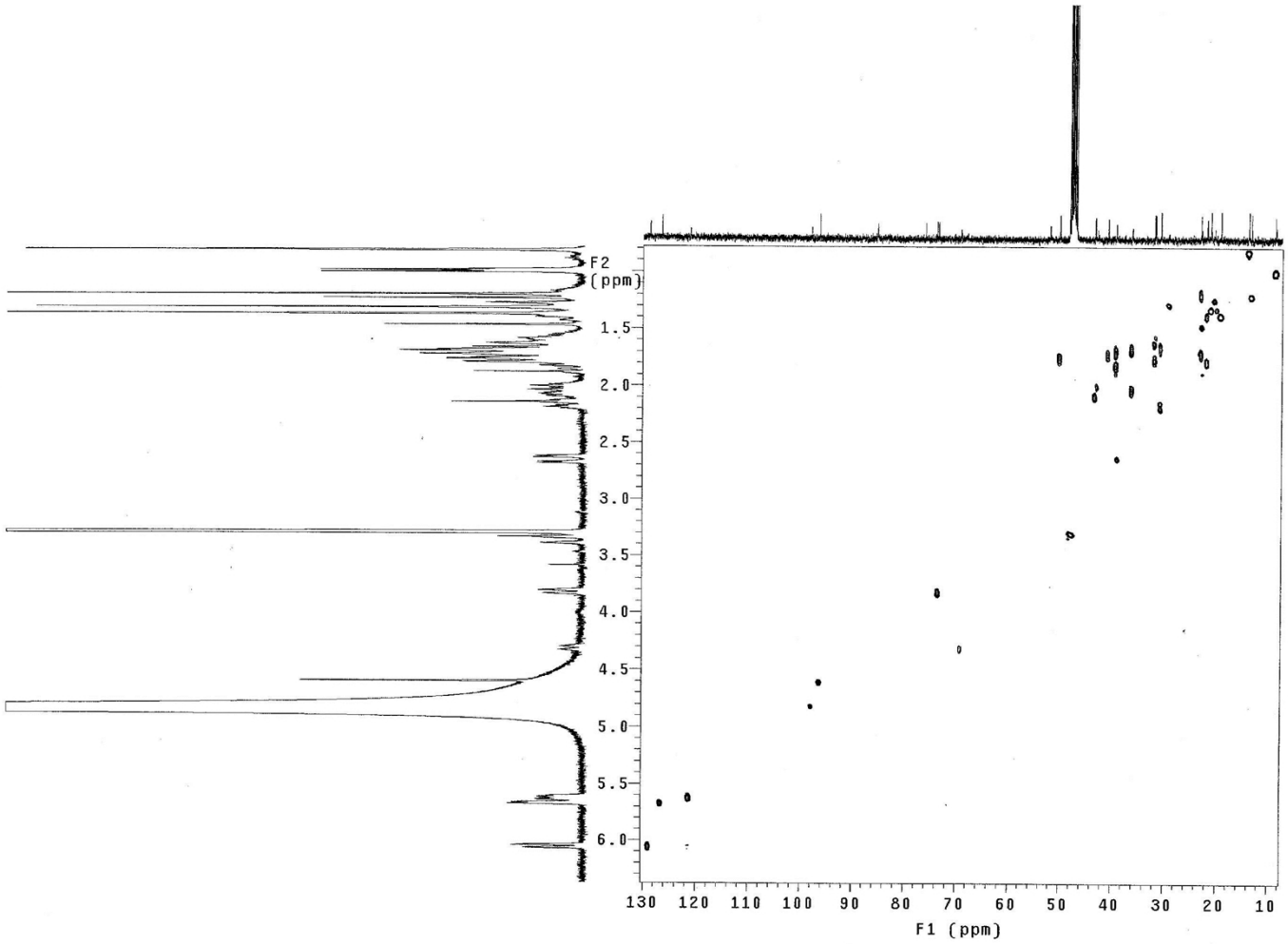
S15. NOESY spectrum of **2** in methanol-d_4 at 100 MHz



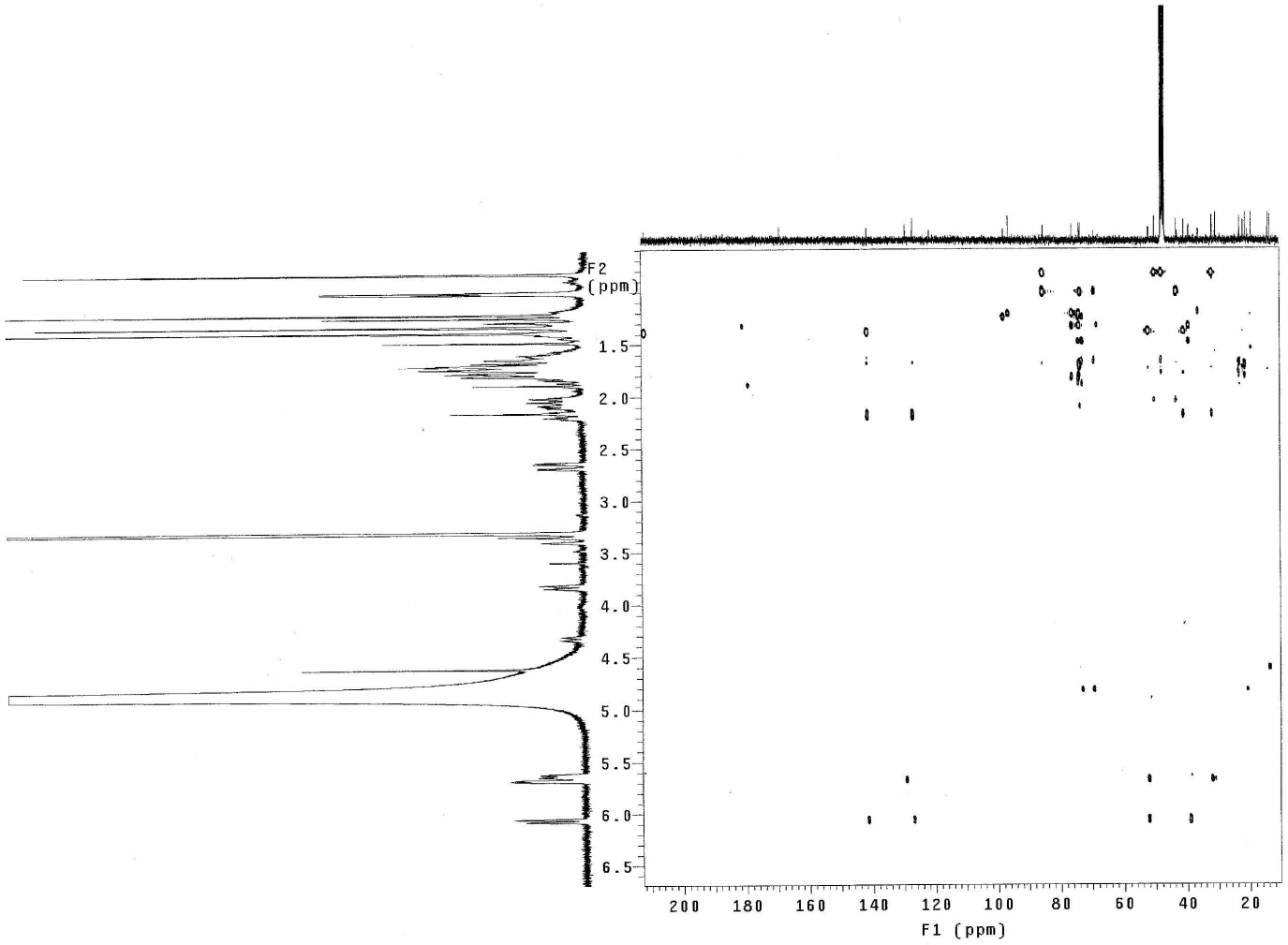
S16. ^{1}H NMR spectrum of **3** in methanol-d_4 at 400 MHz.



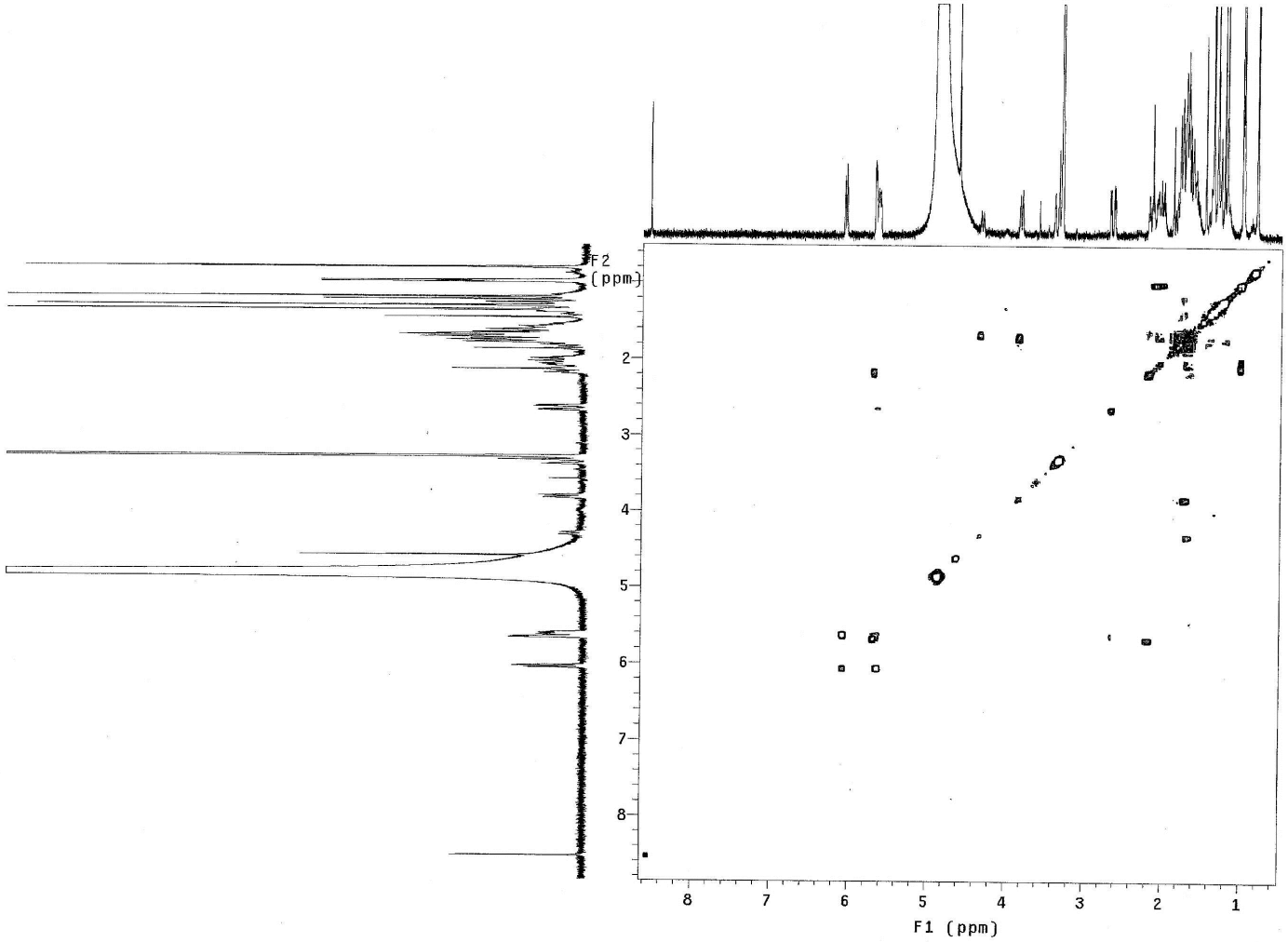
S17. ^{13}C NMR spectrum of **3** in methanol-d_4 at 100 MHz.



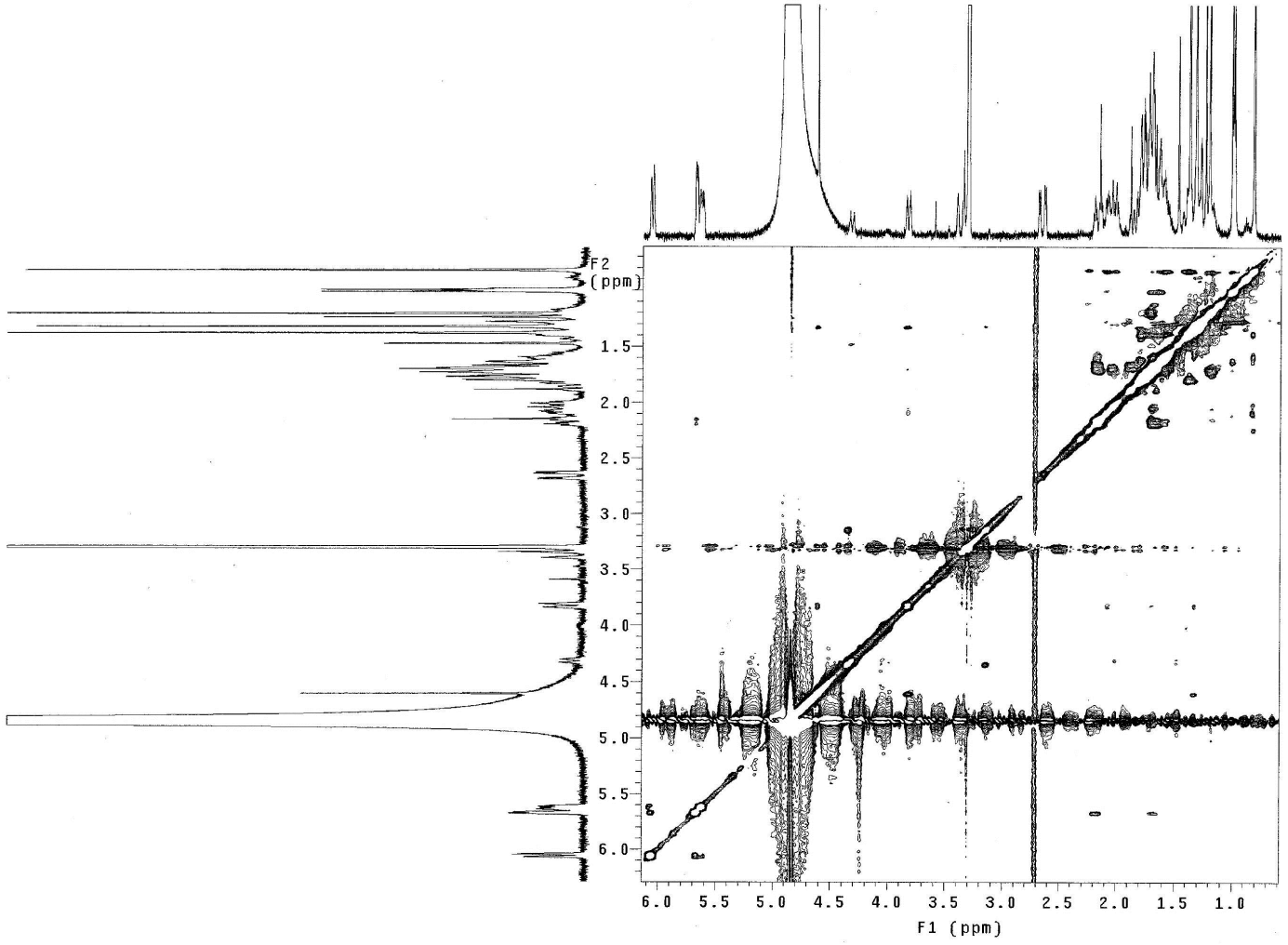
S18. HSQC spectrum of **3** in methanol-d_4 at 100 MHz.



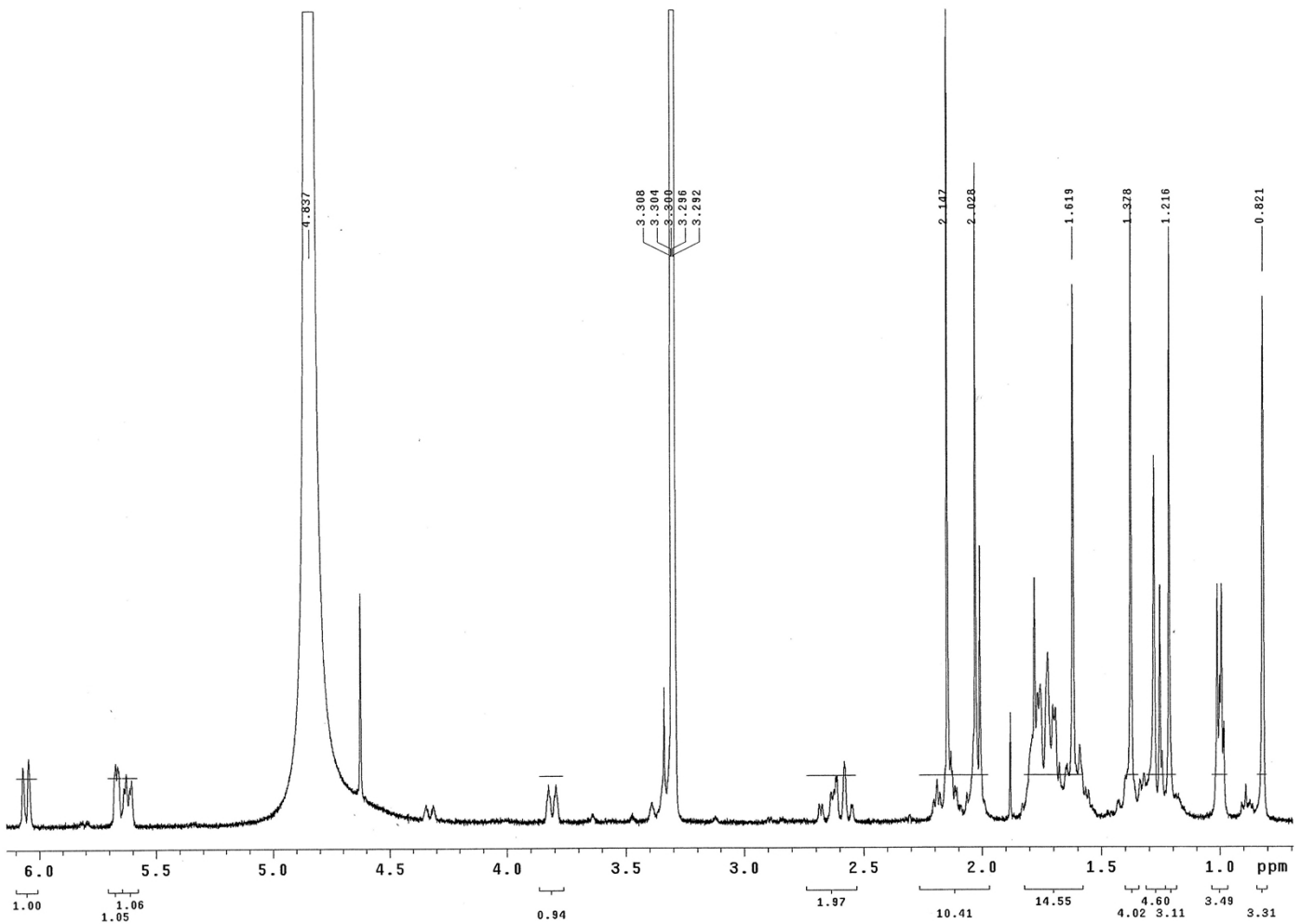
S19. HMBC spectrum of **3** in methanol-d_4 at 100 MHz.



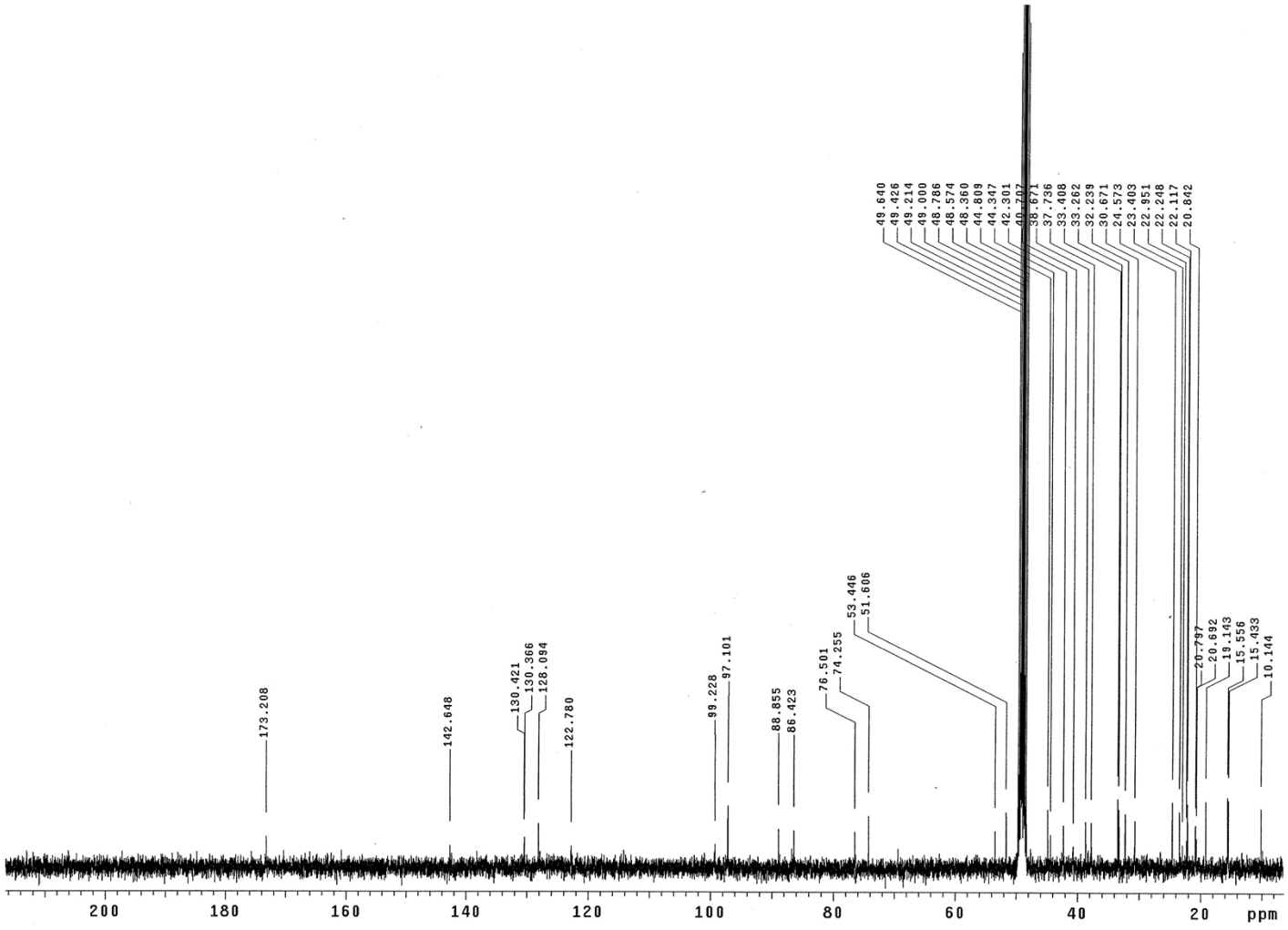
S20. COSY spectrum of **3** in methanol-d_4 at 100 MHz.



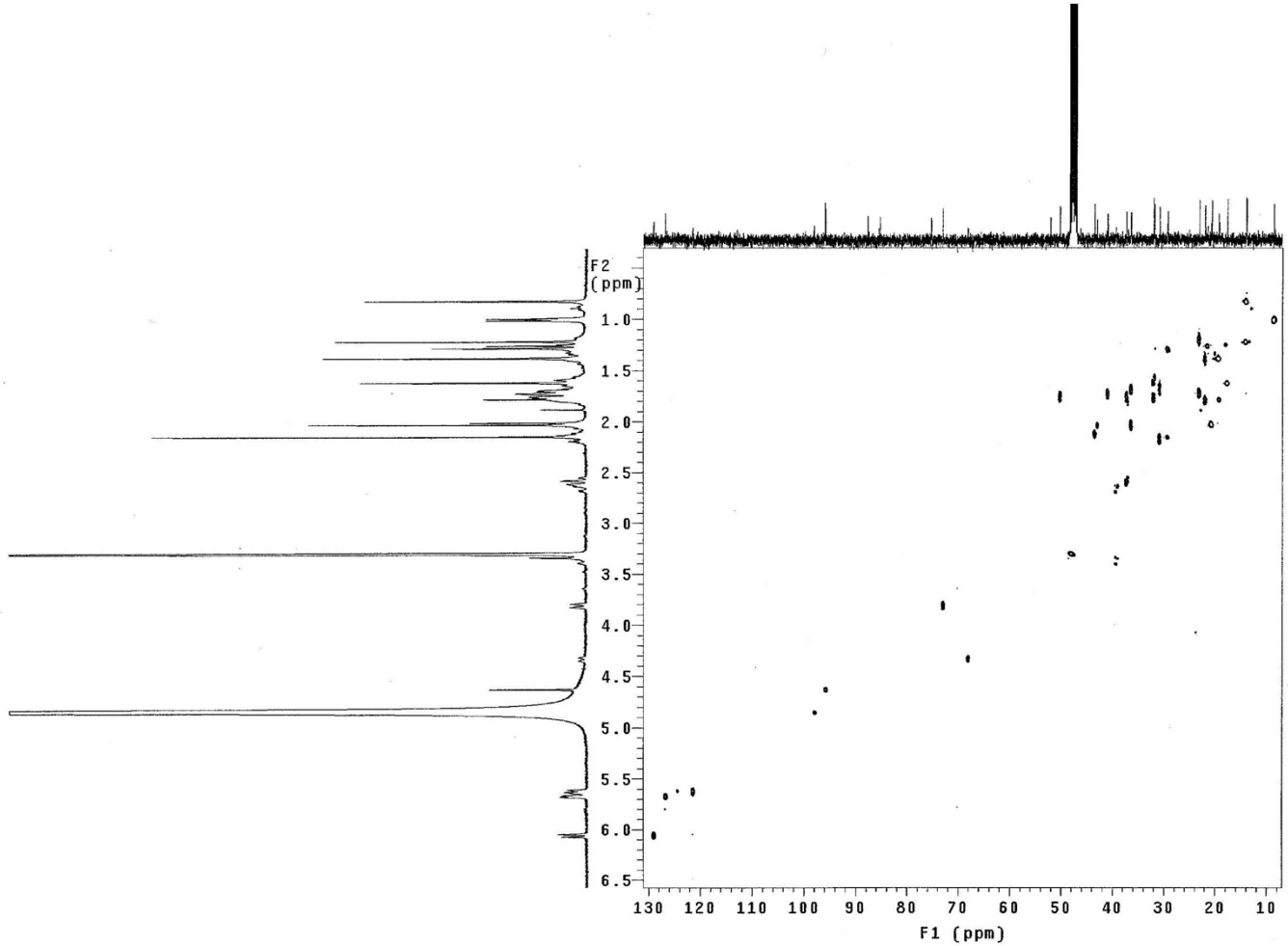
S21. NOESY spectrum of **3** in methanol-d_4 at 100 MHz.



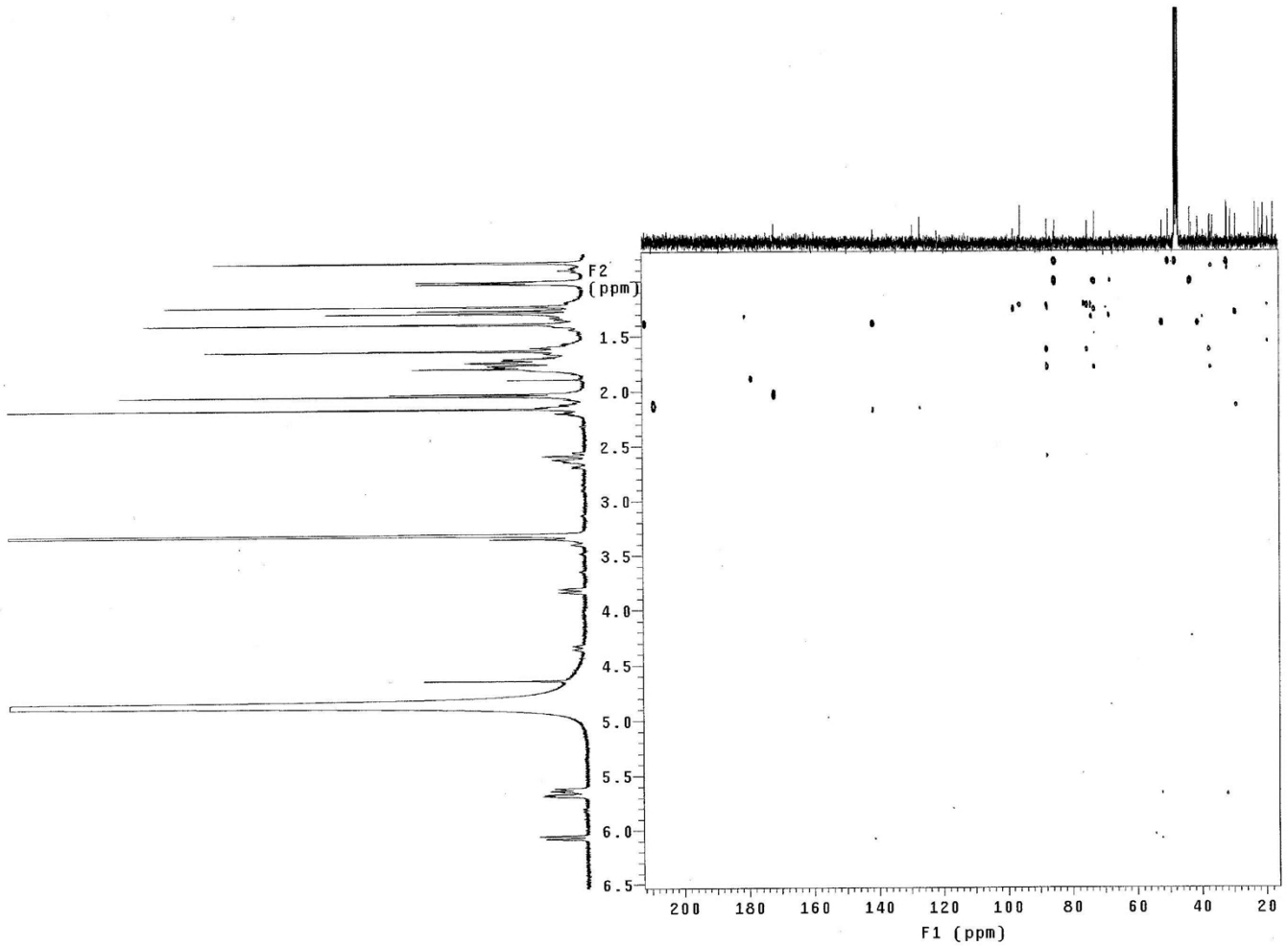
S22. ^{1}H NMR spectrum of **4** in methanol-d_4 at 400 MHz.



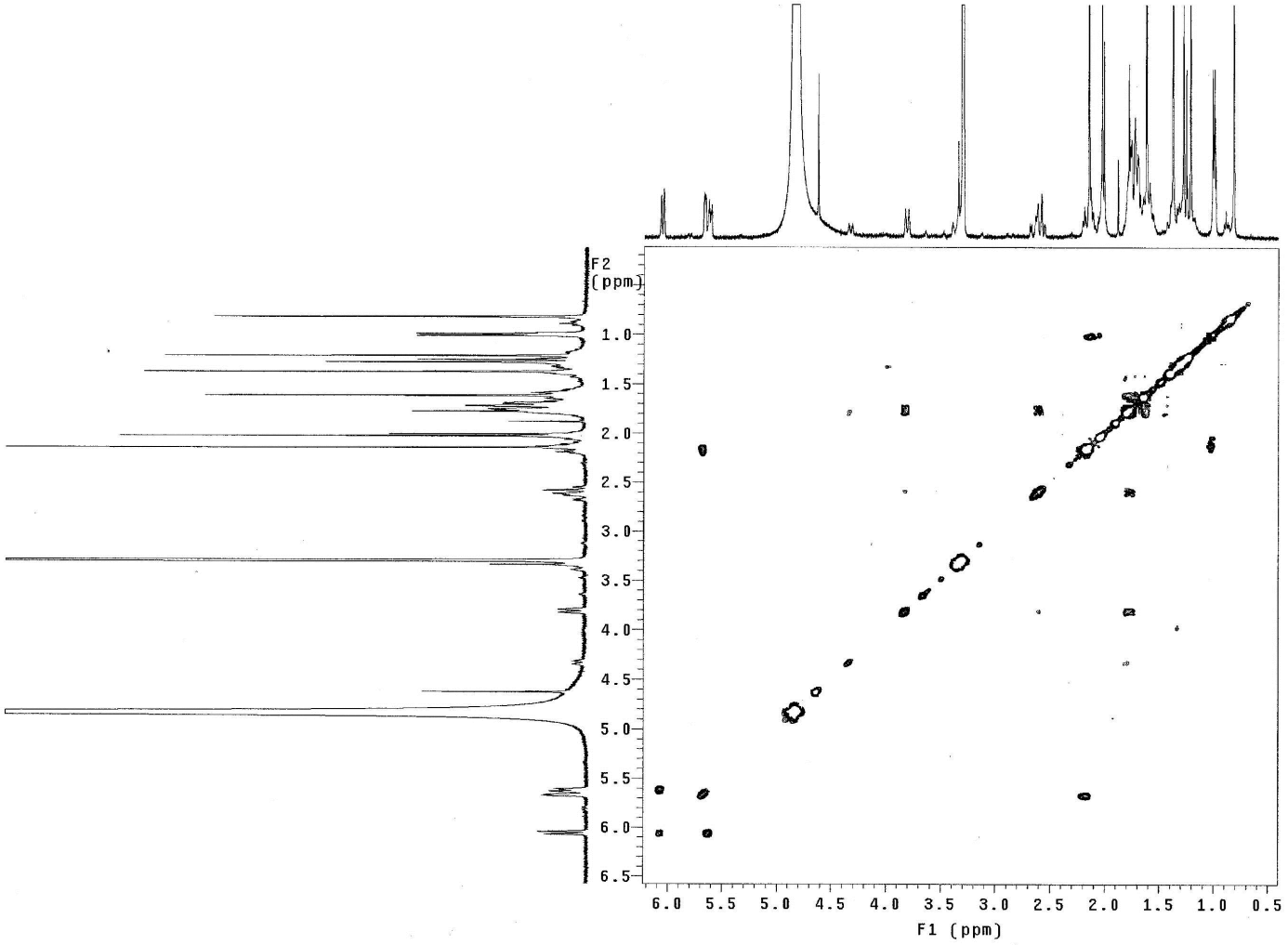
S23. ^{13}C NMR spectrum of **4** in methanol-d_4 at 100 MHz.



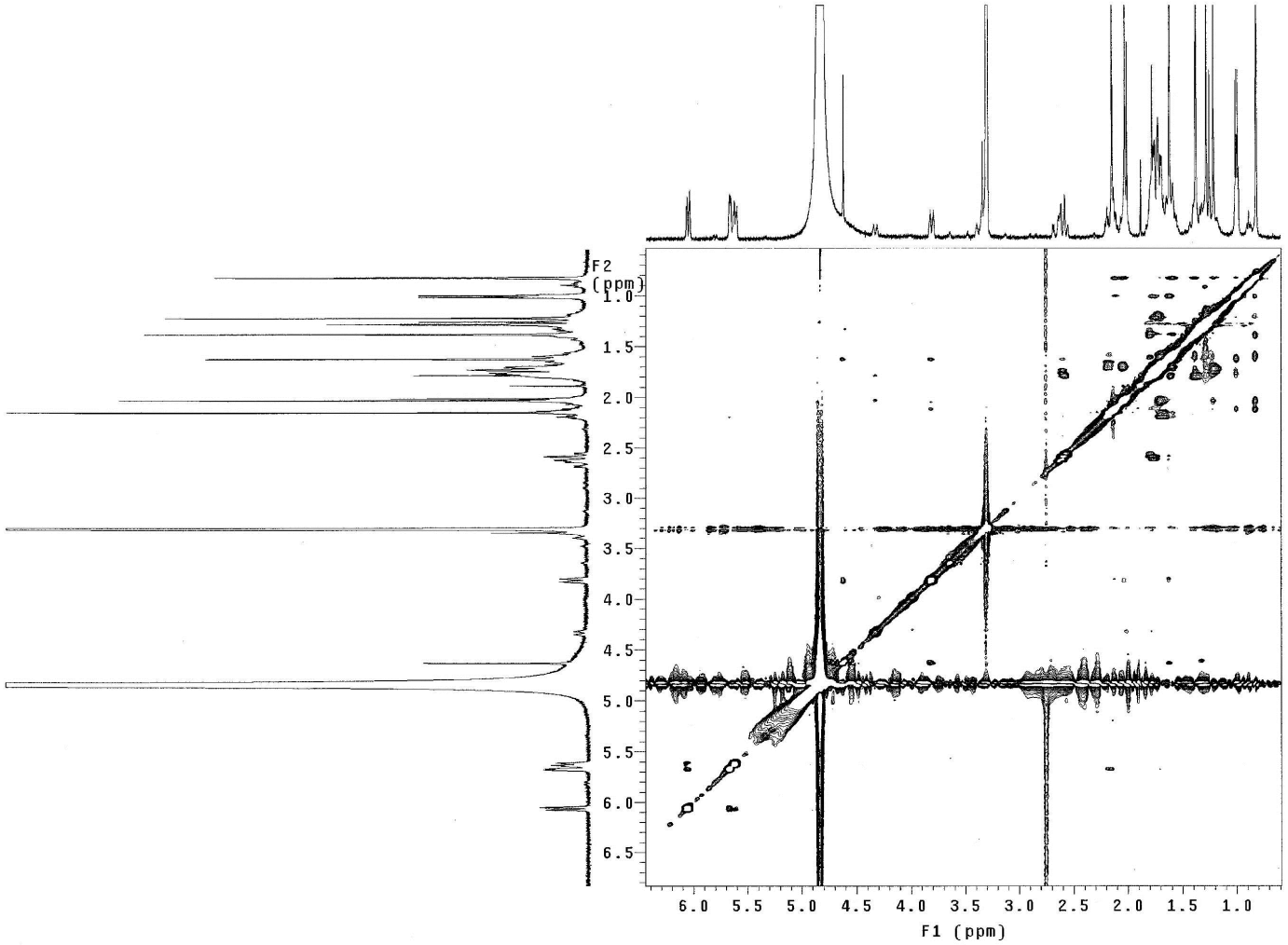
S24. HSQC spectrum of **4** in methanol-d_4 at 100 MHz.



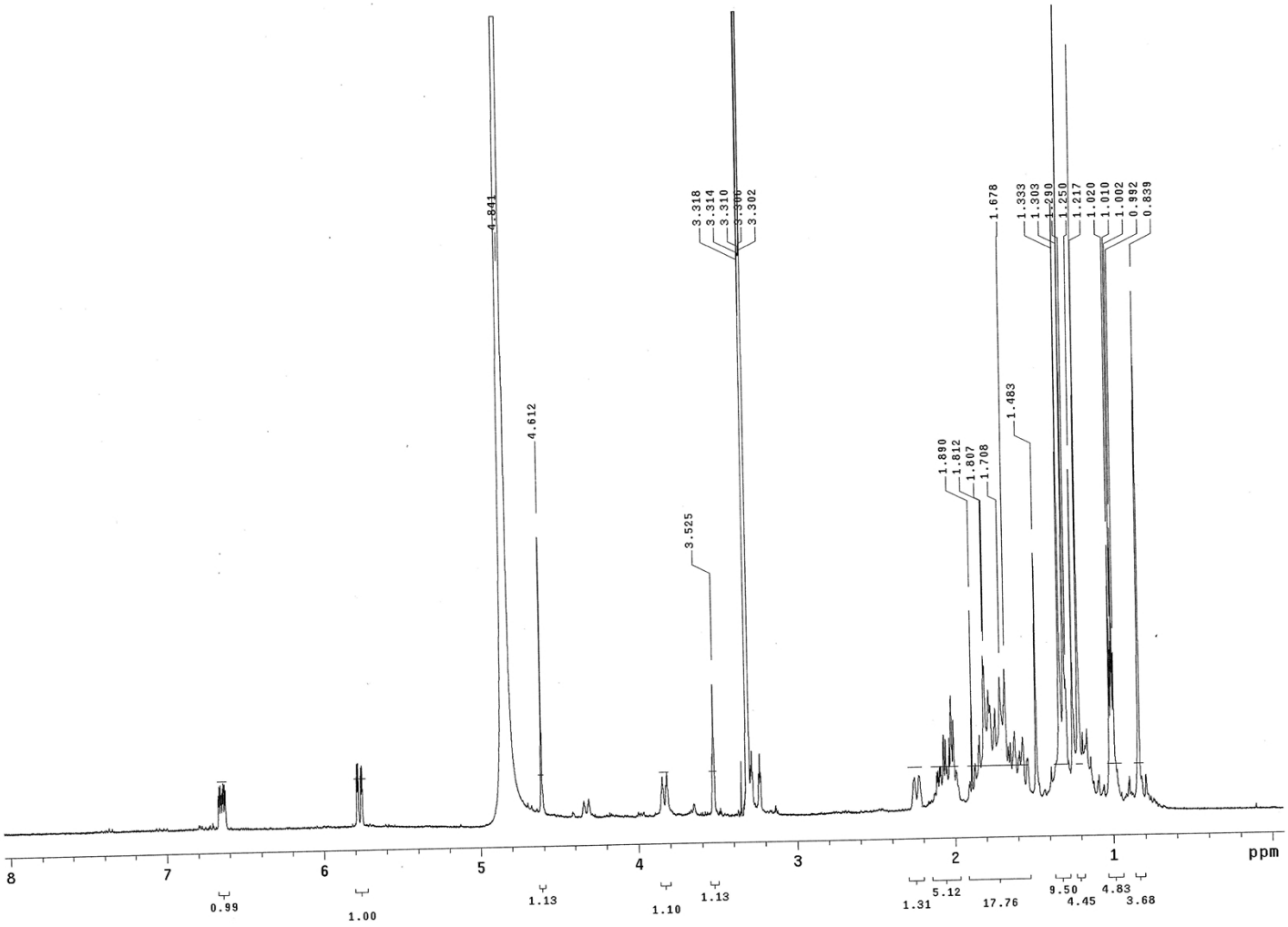
S25. HMBC spectrum of **4** in methanol-d_4 at 100 MHz.



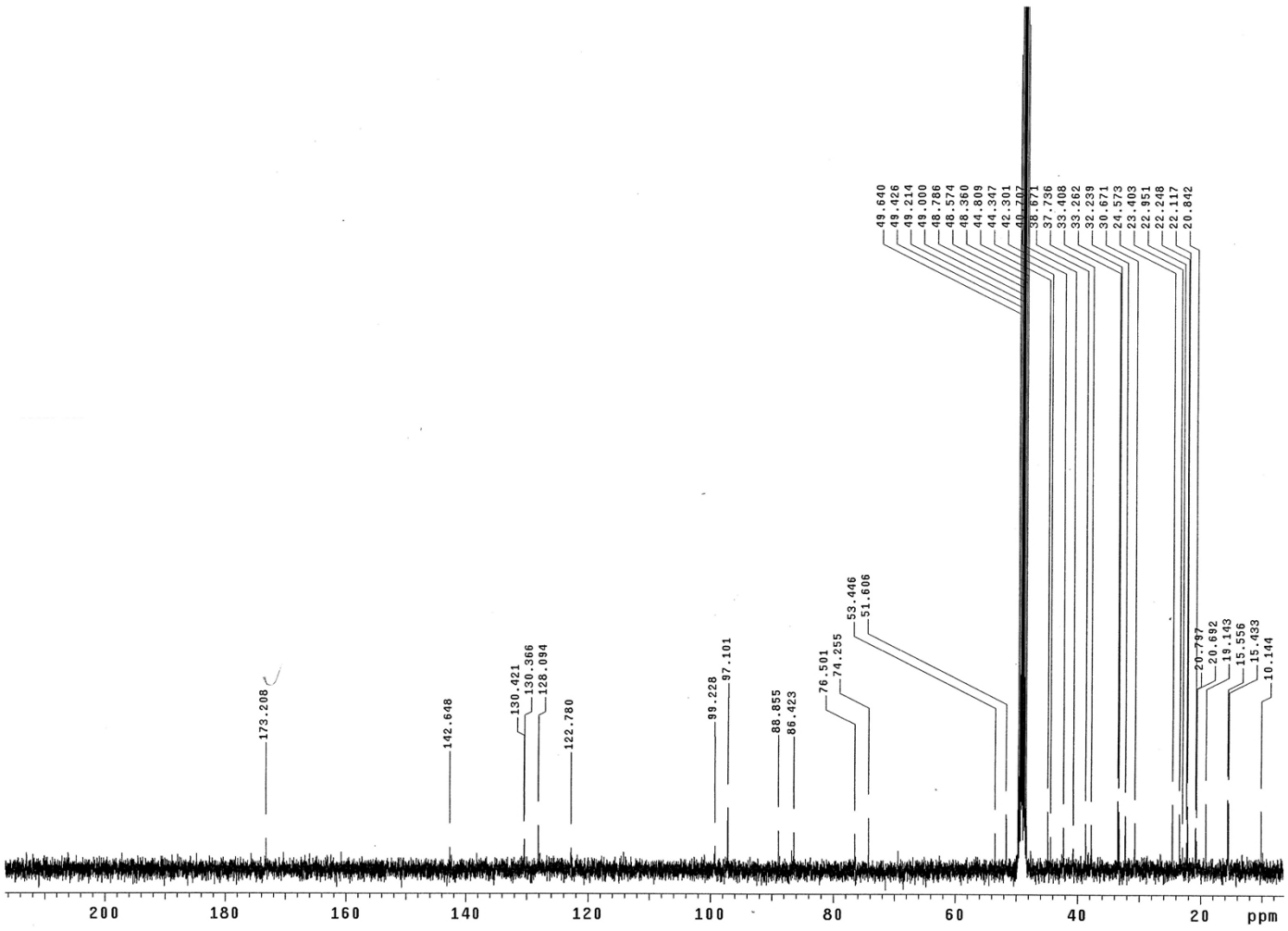
S26. COSY spectrum of **4** in methanol-d_4 at 100 MHz.



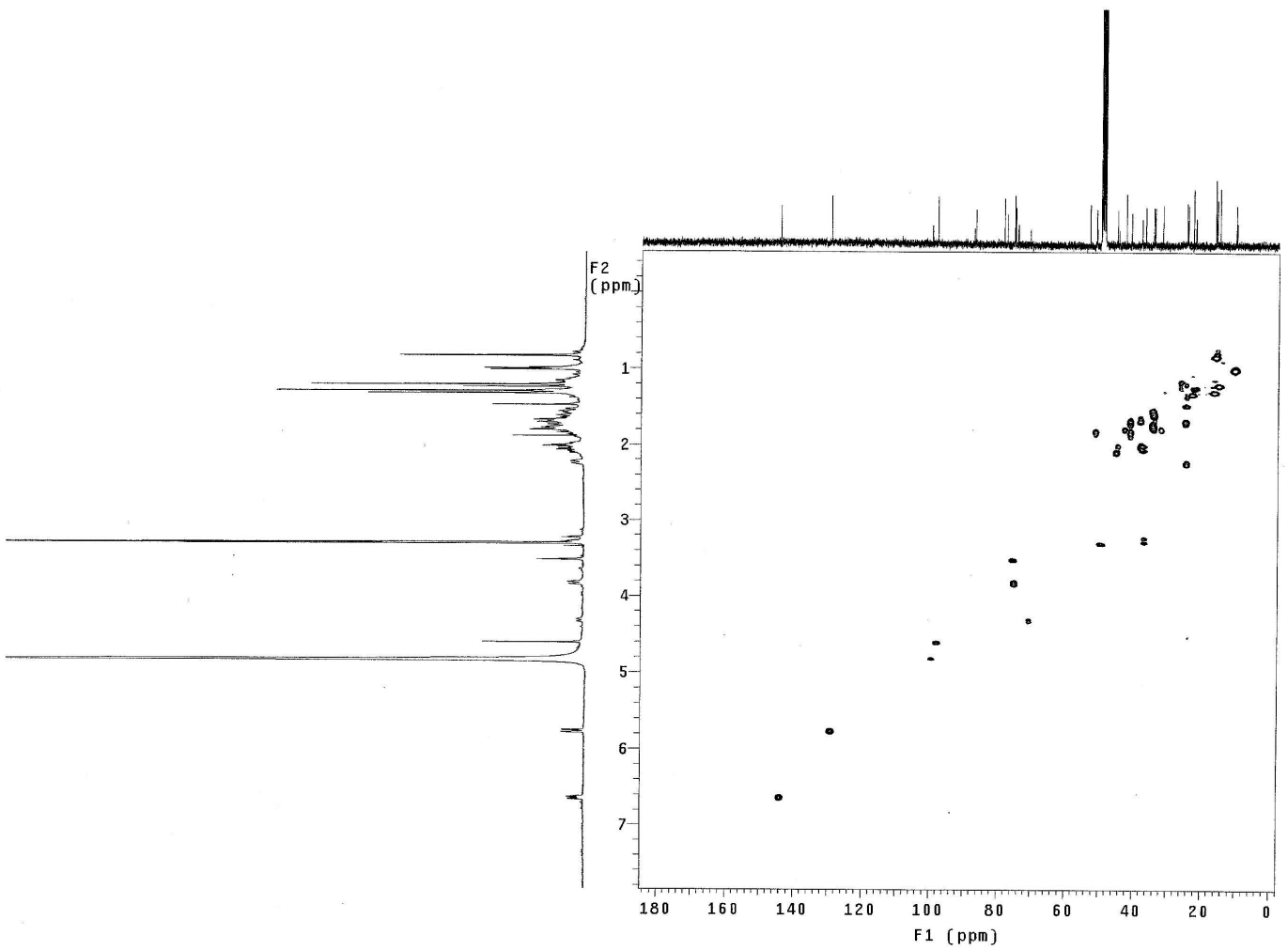
S27. NOESY spectrum of **4** in methanol-d_4 at 100 MHz.



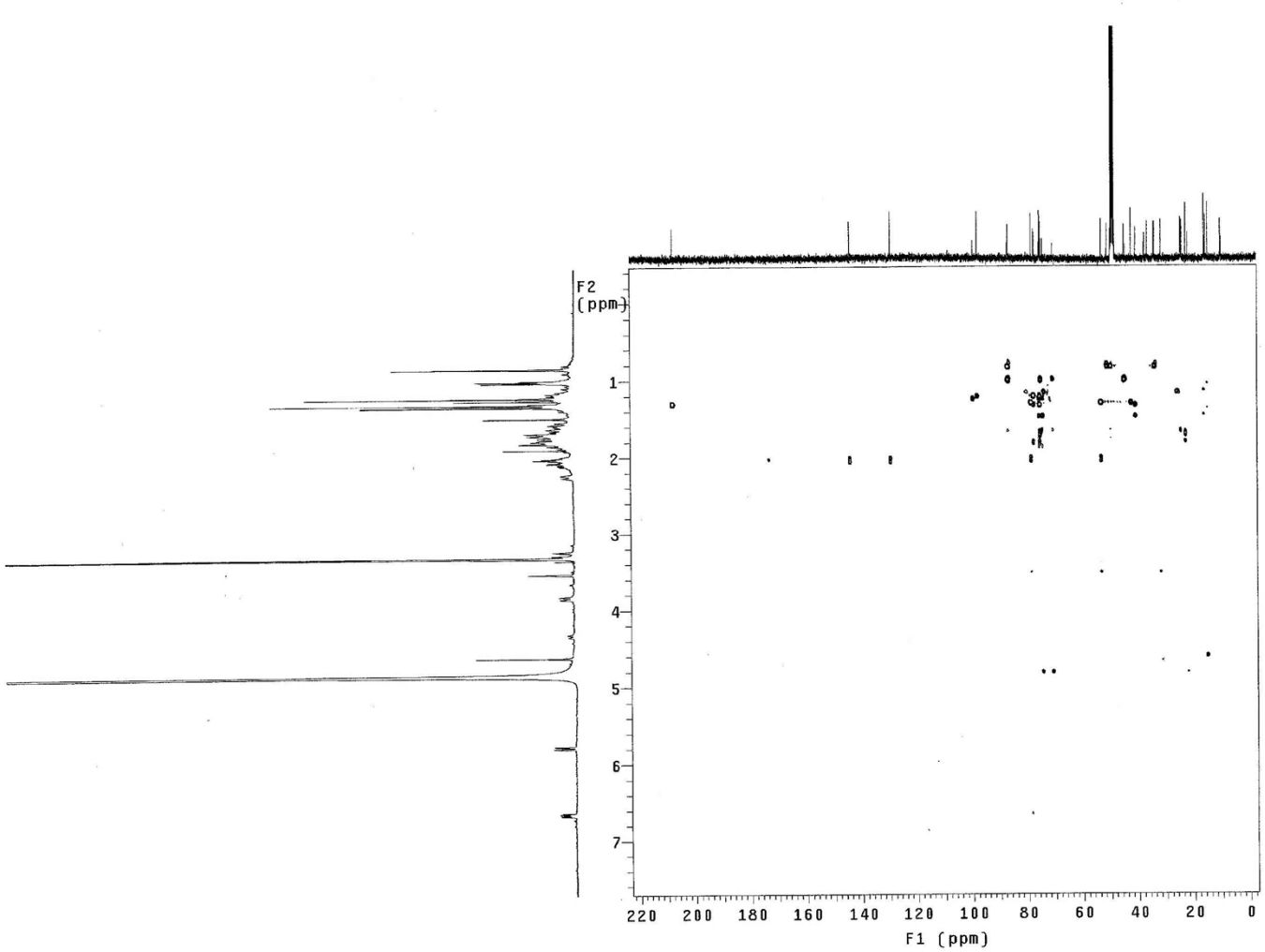
S28. ^{1}H NMR spectrum of **5** in methanol-d_4 at 400 MHz.



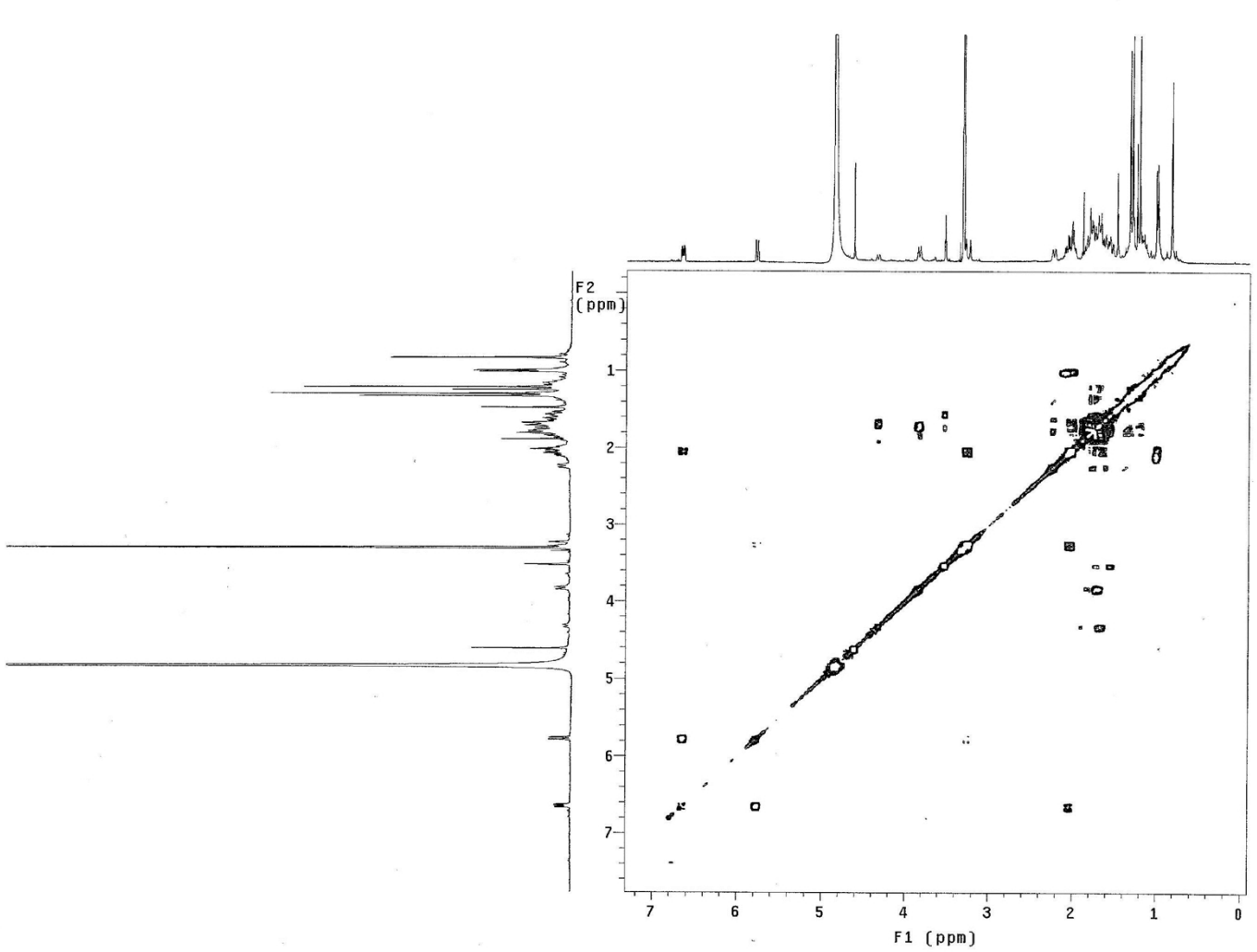
S29. ^{13}C NMR spectrum of **5** in methanol-d_4 at 100 MHz.



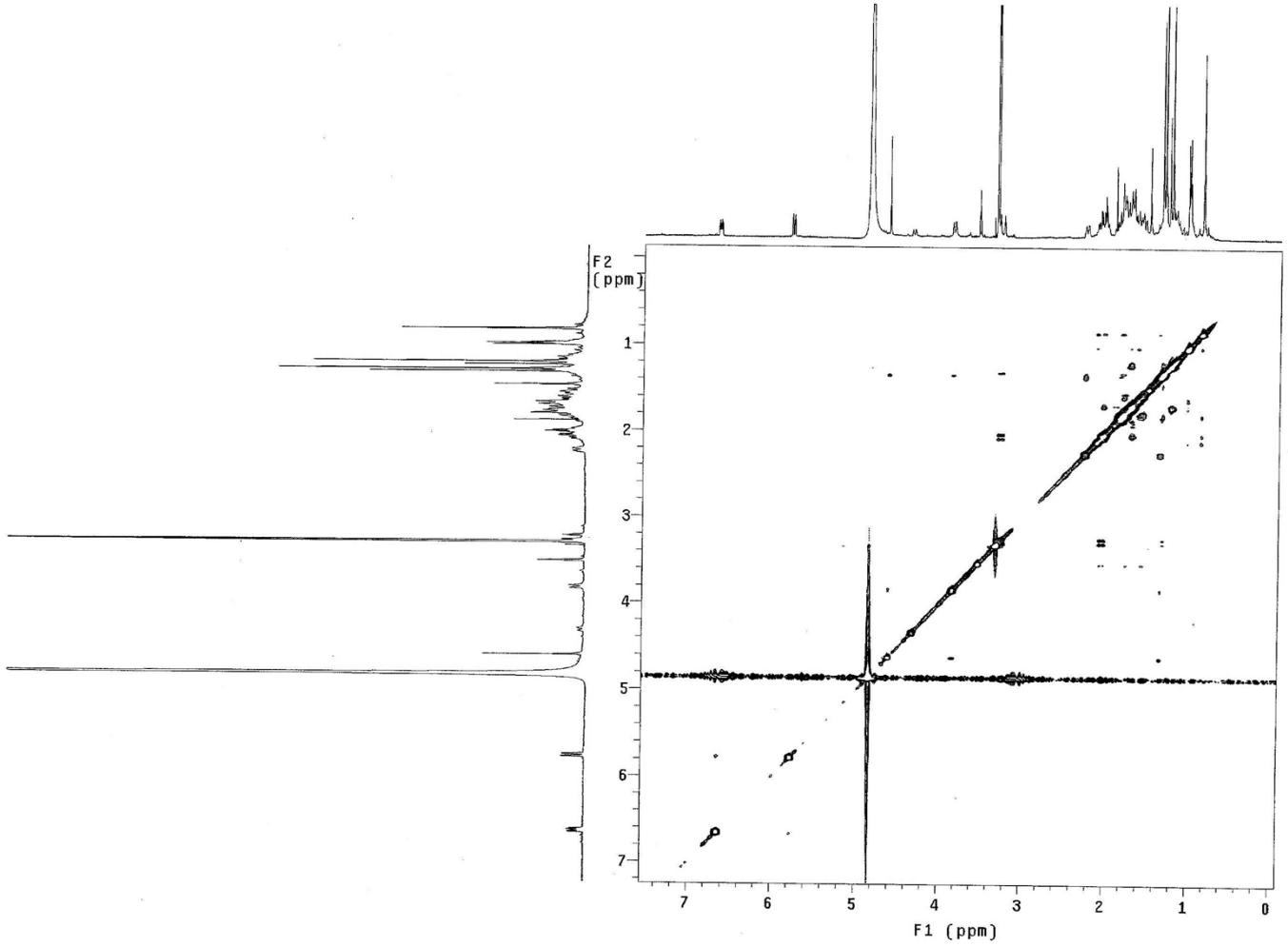
S30. HSQC spectrum of **5** in methanol-d_4 at 100 MHz.



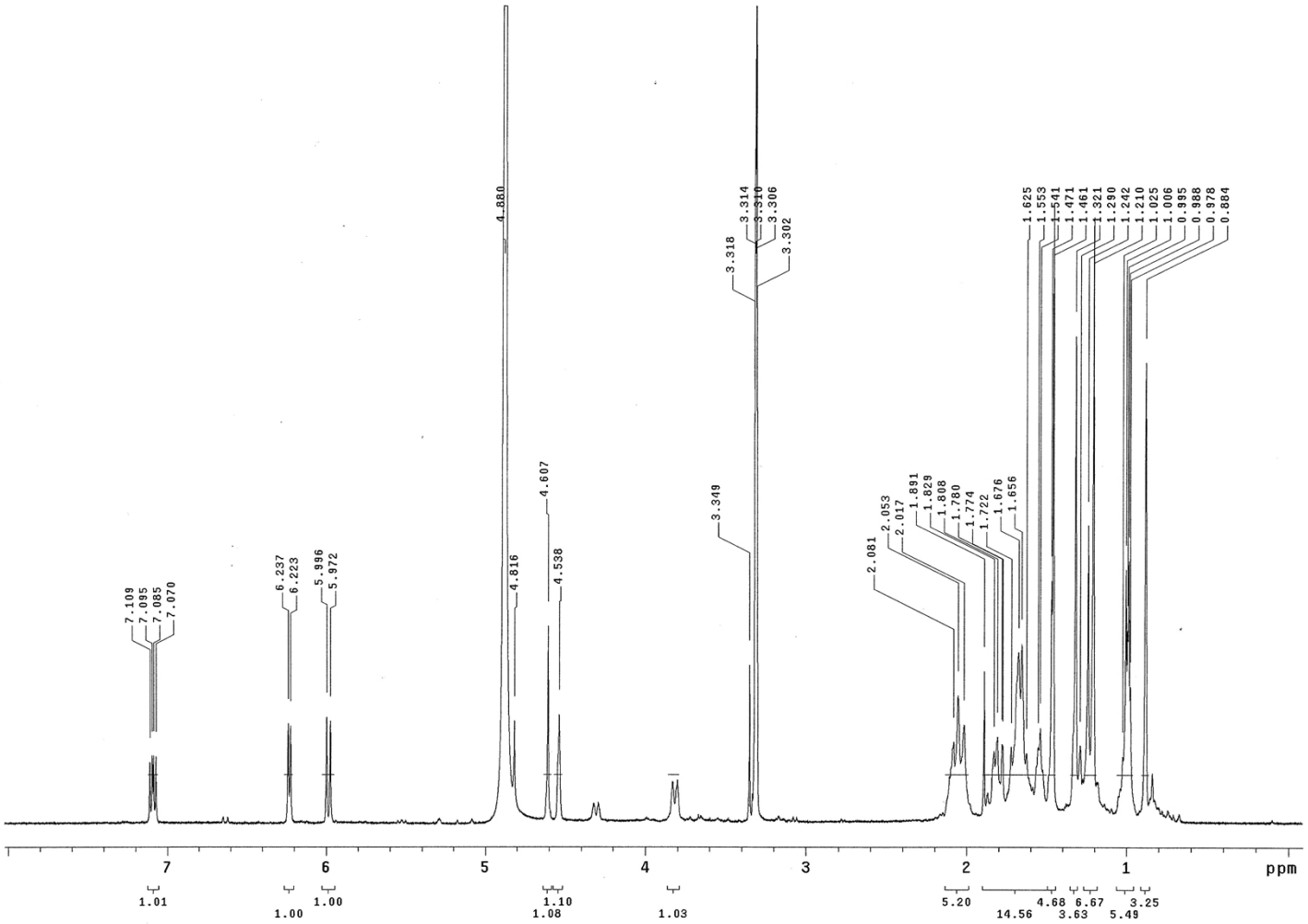
S31. HMBC spectrum of **5** in methanol-d_4 at 100 MHz.



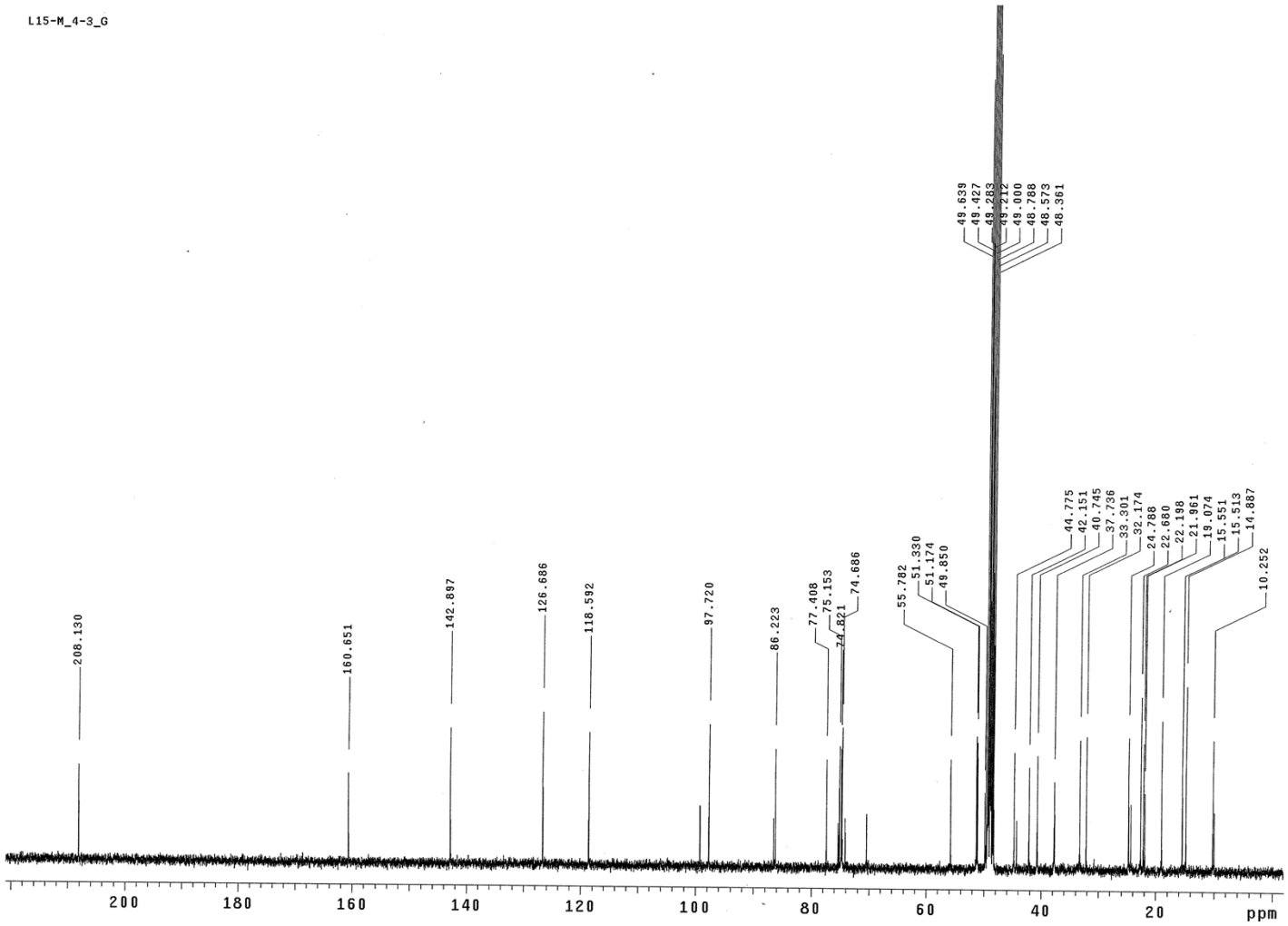
S32. COSY spectrum of **5** in methanol-d_4 at 100 MHz.



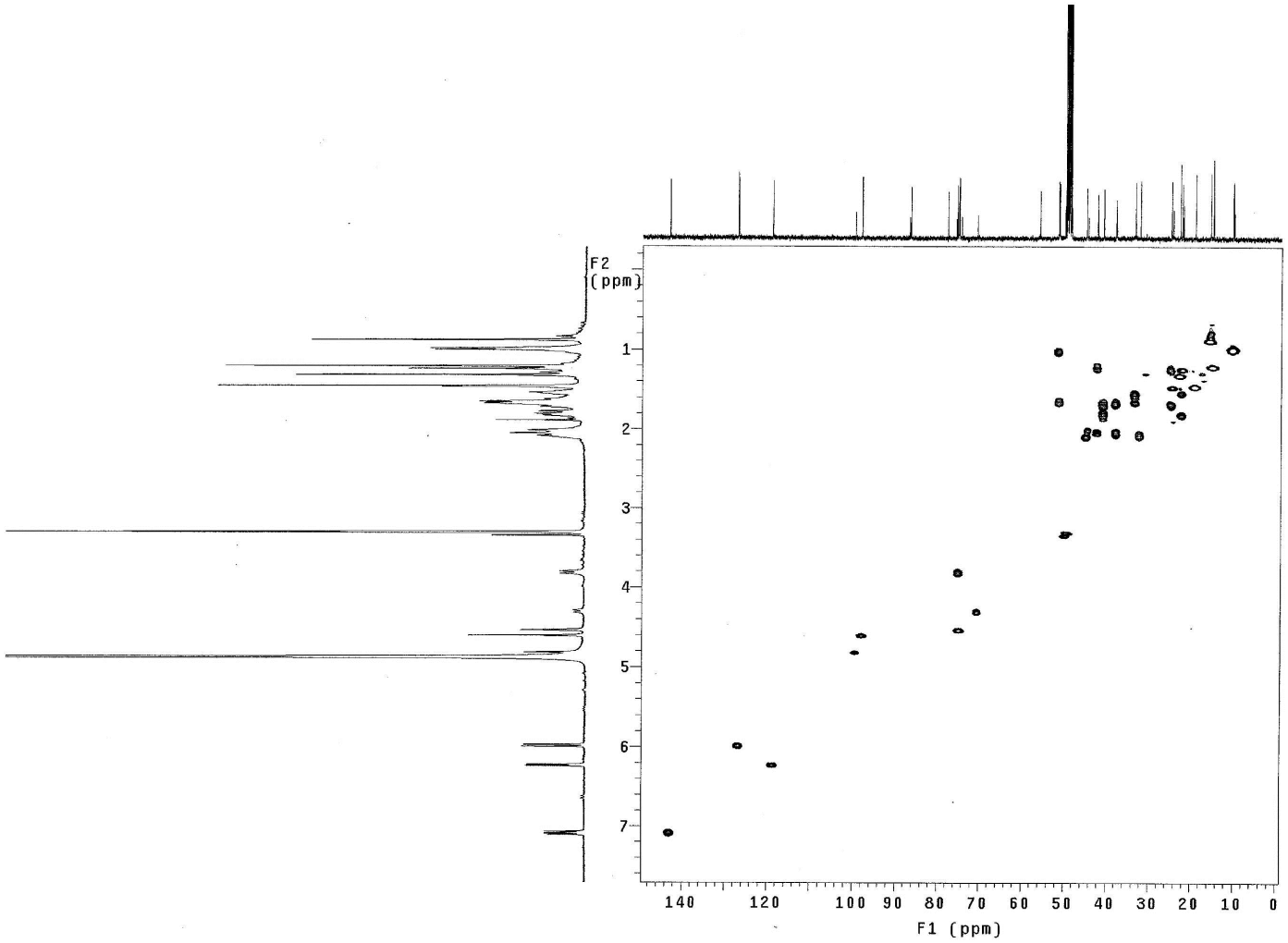
S33. NOESY spectrum of **5** in methanol-d_4 at 100 MHz.



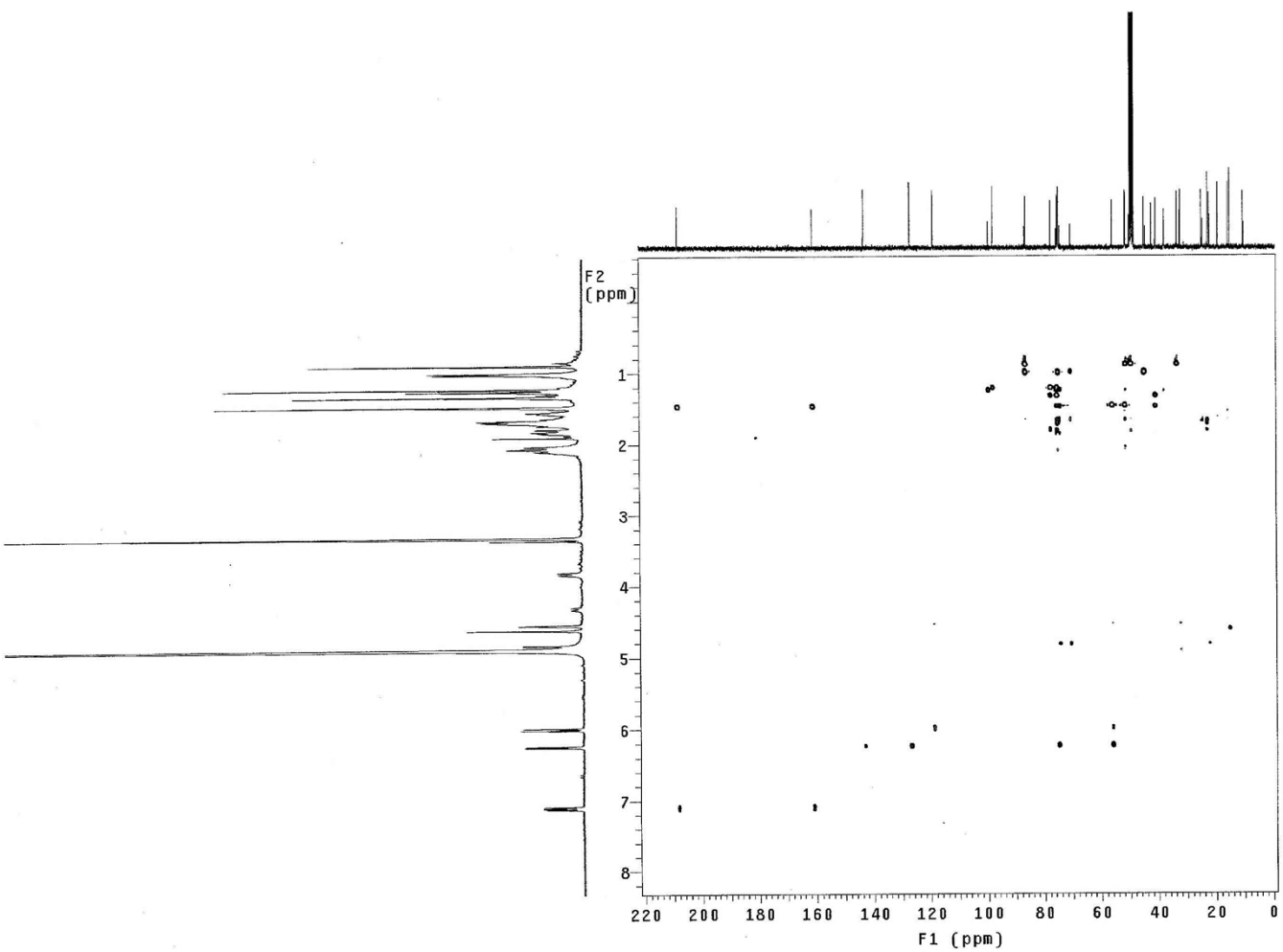
S34. ^{1}H NMR spectrum of **6** in methanol-d_4 at 400 MHz.



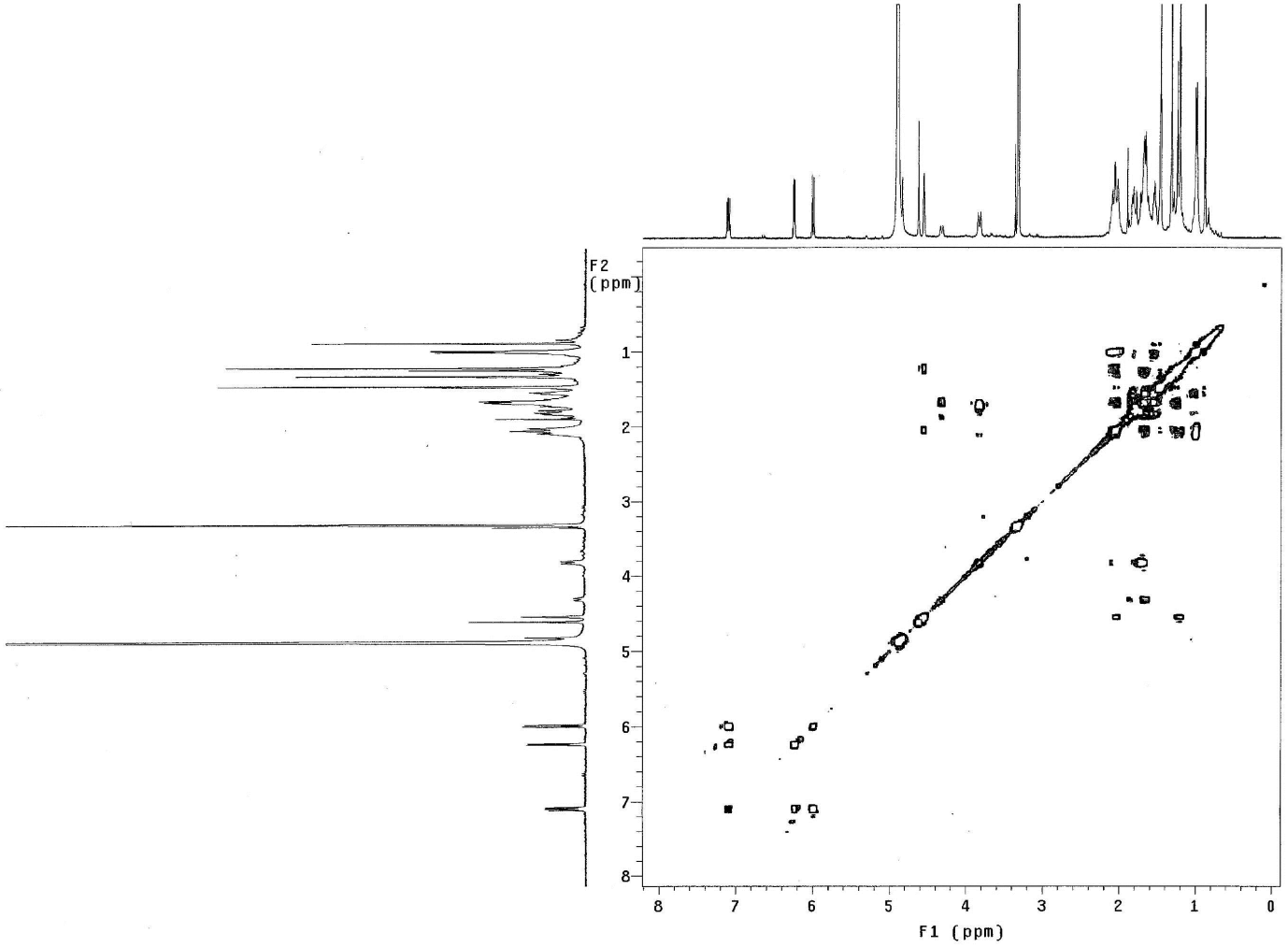
S35. ^{13}C NMR spectrum of **6** in methanol-d_4 at 100 MHz.



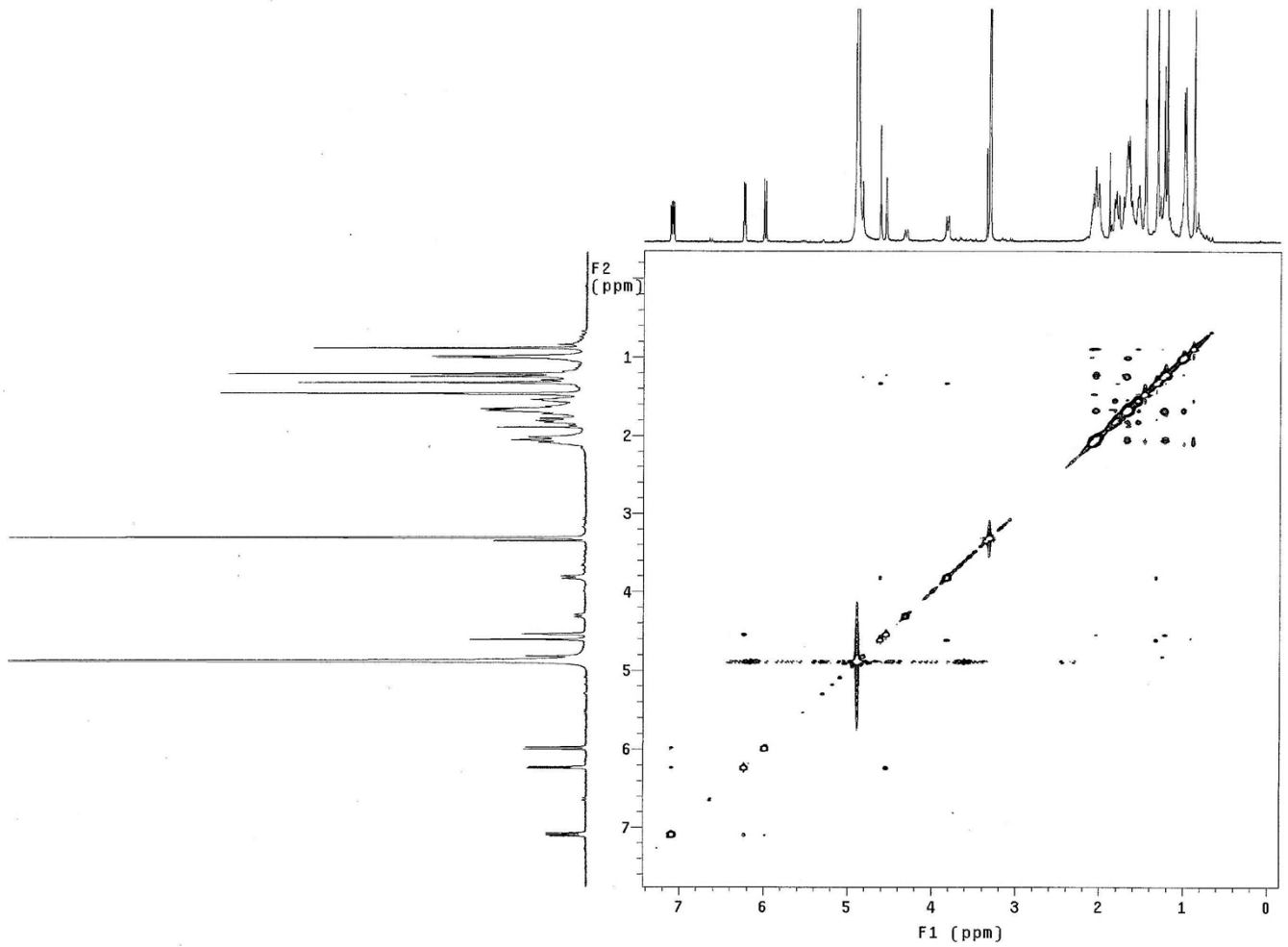
S36. HSQC spectrum of **6** in methanol-d_4 at 100 MHz.



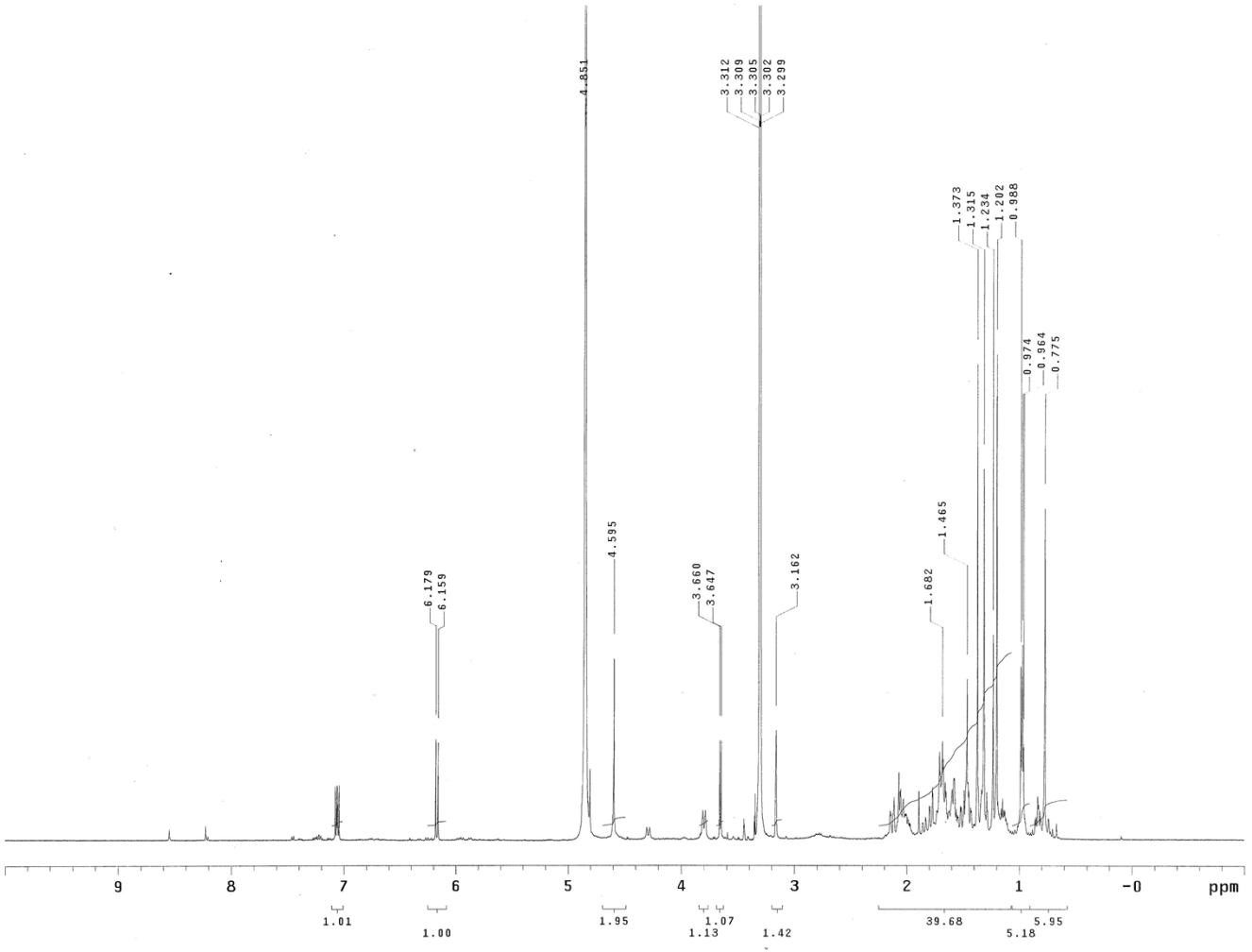
S37. HMBC spectrum of **6** in methanol-d_4 at 100 MHz.



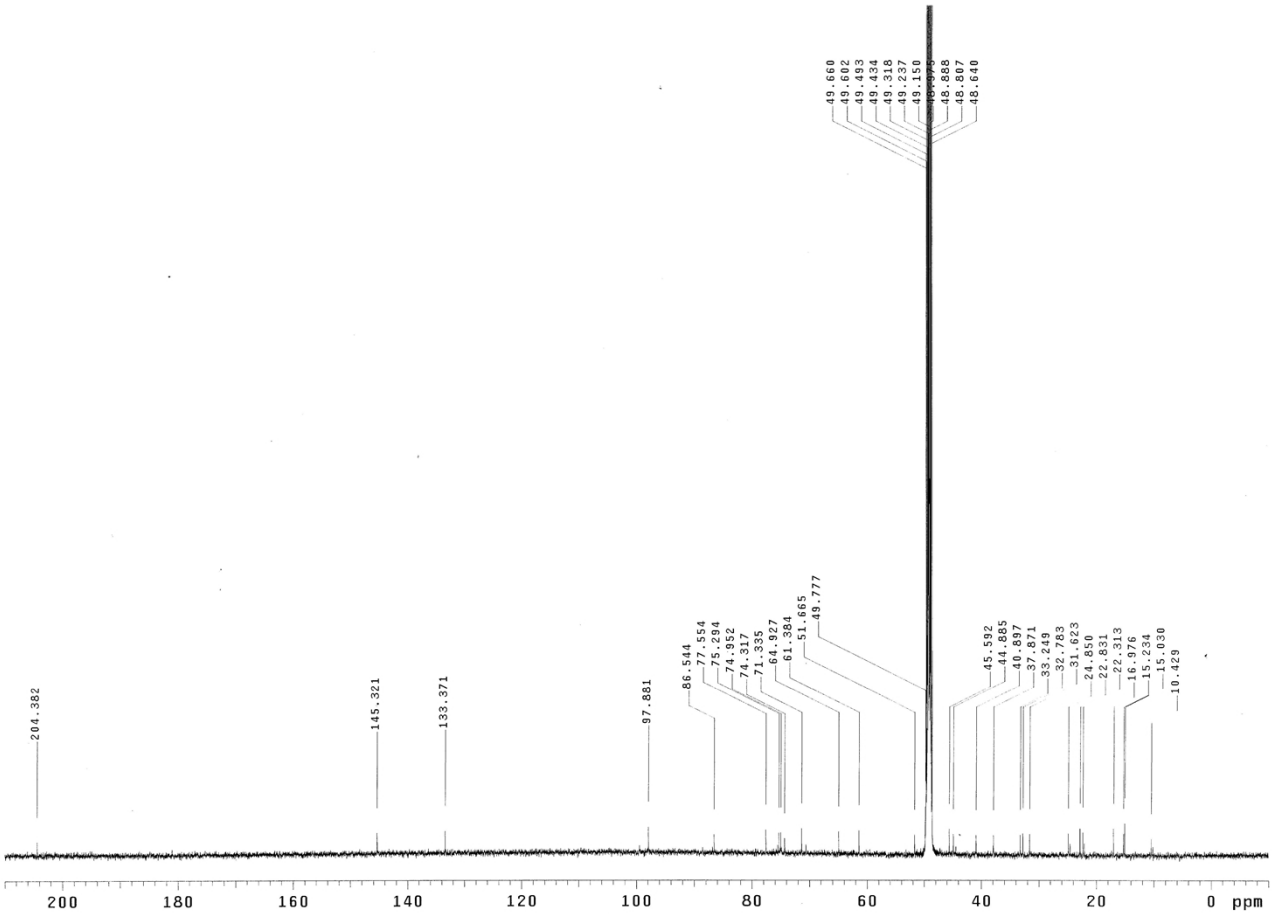
S38. COSY spectrum of **6** in methanol-d_4 at 100 MHz.



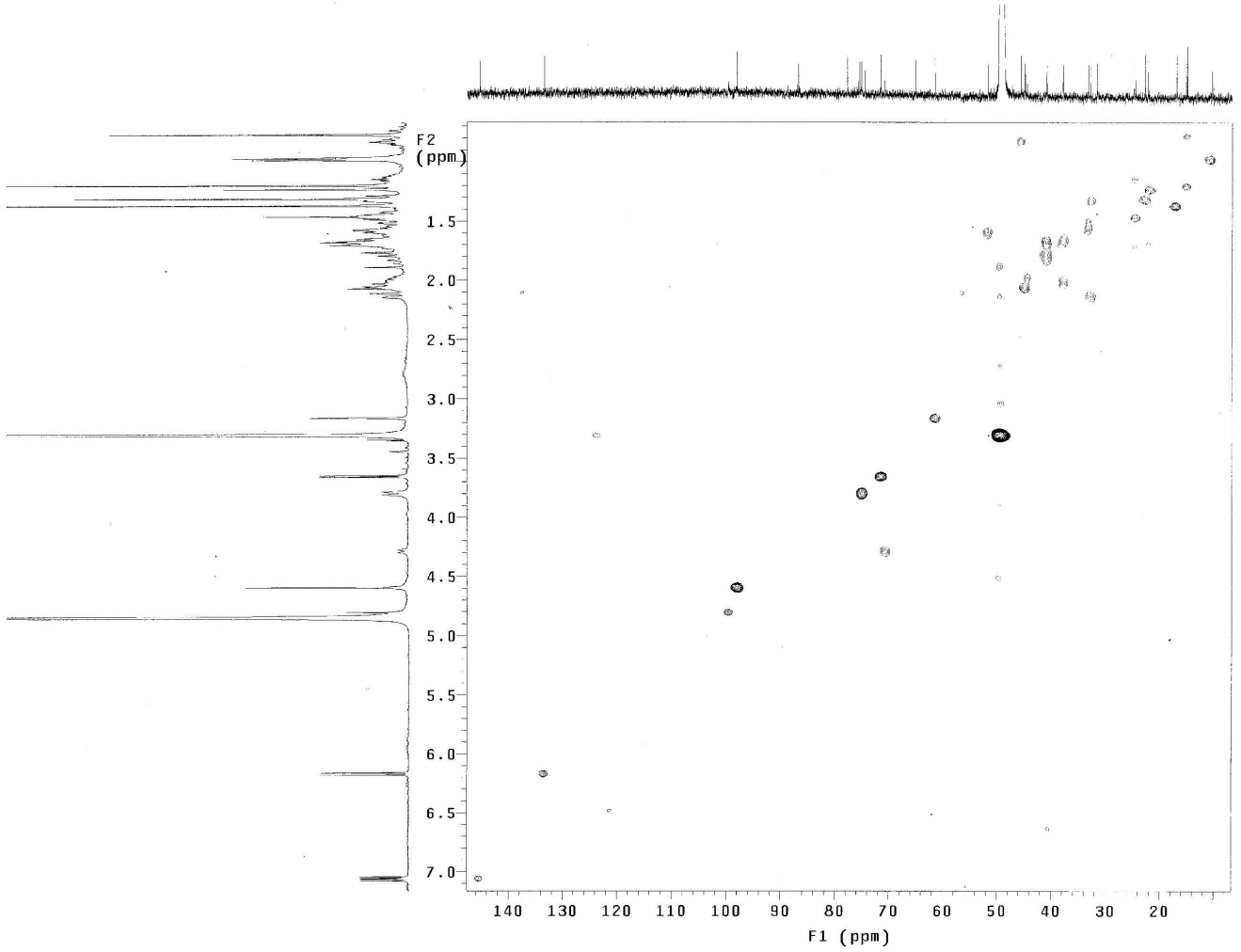
S39. NOESY spectrum of **6** in methanol-d_4 at 100 MHz.



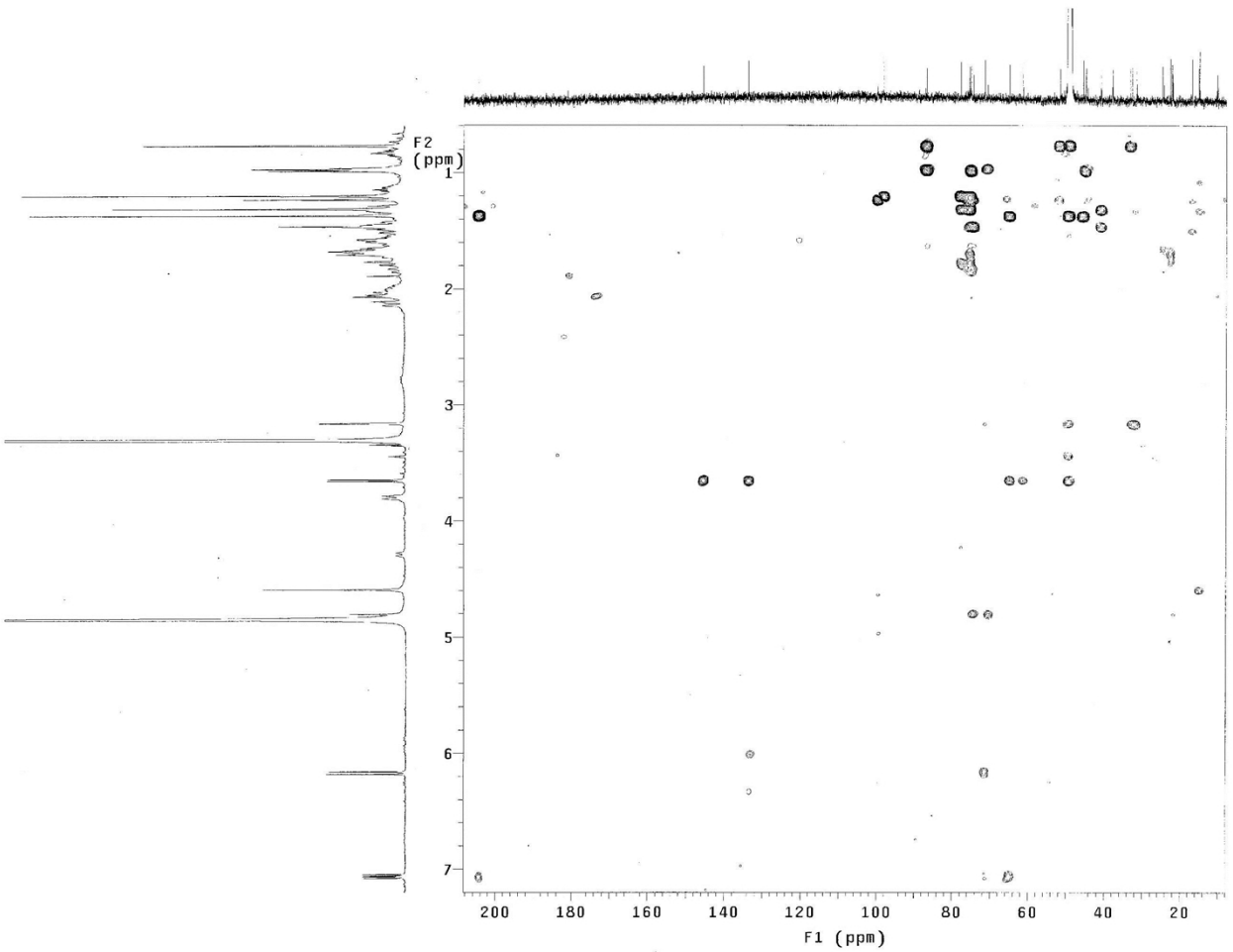
S40. [1]H NMR spectrum of **7** in methanol-d_4 at 400 MHz.



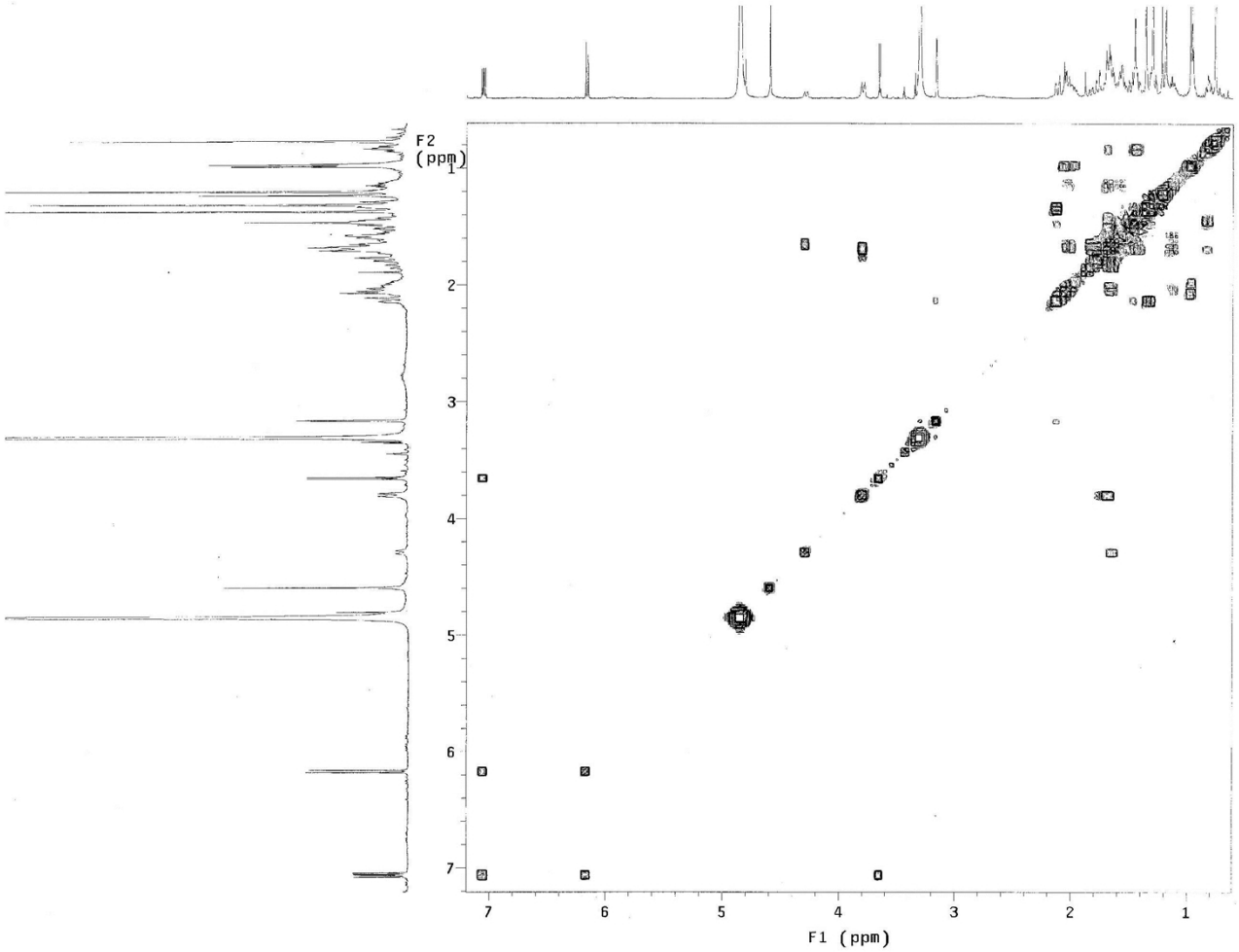
S41. ^{13}C NMR spectrum of **7** in methanol-d_4 at 100 MHz.



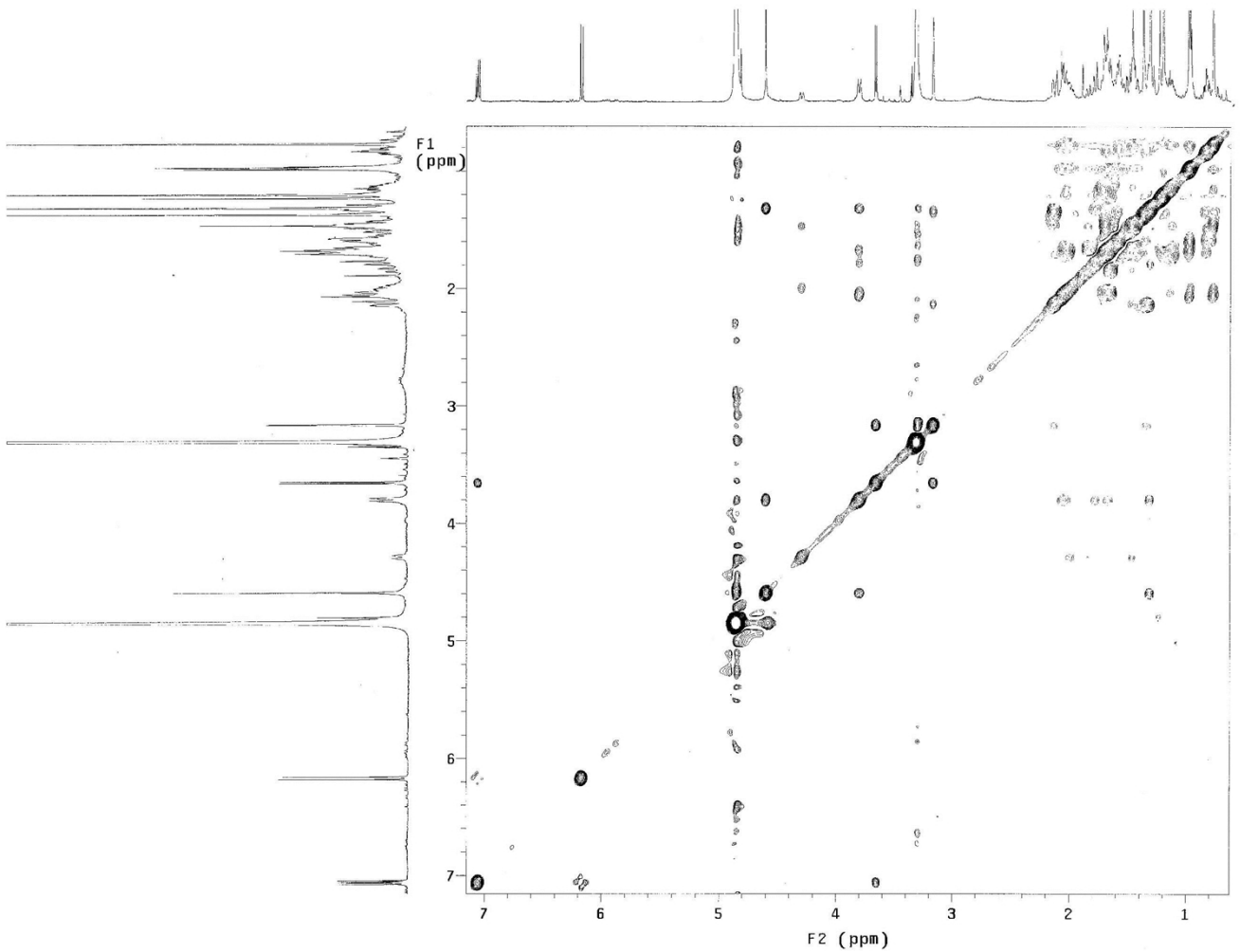
S42. HSQC spectrum of **7** in methanol-d_4 at 100 MHz.



S43. HMBC spectrum of **7** in methanol-d_4 at 100 MHz.



S44. COSY spectrum of **7** in methanol-d_4 at 100 MHz.



S45. NOESY spectrum of **7** in methanol-d_4 at 100 MHz.

S46. Crystal data and structure refinement for cu_130829LT_0m.

Identification code	CU_130829LT_0M	
Empirical formula	C28 H47 O8.50	
Formula weight	519.65	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 7.5227(4) Å	α= 90°.
	b = 9.6240(6) Å	β= 90°.
	c = 37.396(2) Å	γ = 90°.
Volume	2707.4(3) $Å^3$	
Z	4	
Density (calculated)	1.275 Mg/m^3	
Absorption coefficient	0.758 mm^{-1}	
F(000)	1132	
Crystal size	0.50 x 0.30 x 0.03 mm^3	
Theta range for data collection	2.363 to 66.257°.	
Index ranges	-8<=h<=6, -11<=k<=10, -39<=l<=44	
Reflections collected	13445	
Independent reflections	4384 [R(int) = 0.0520]	
Completeness to theta = 67.679°	92.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9492 and 0.7735	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4384 / 3 / 344	
Goodness-of-fit on F^2	1.113	
Final R indices [I>2sigma(I)]	R1 = 0.0936, wR2 = 0.2351	
R indices (all data)	R1 = 0.0943, wR2 = 0.2355	
Absolute structure parameter	0.3(7)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.416 and -0.443 $e.Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for cu_130829LT_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7774(12)	3387(8)	10925(2)	25(2)
C(2)	8176(13)	3085(9)	11295(2)	32(2)
C(3)	9668(12)	3482(10)	11449(2)	31(2)
C(4)	11068(12)	4305(11)	11260(2)	37(2)
C(5)	10788(11)	4363(8)	10862(2)	24(2)
C(6)	12216(11)	4313(8)	10643(2)	27(2)
C(7)	12124(10)	4421(8)	10249(2)	22(2)
C(8)	10311(10)	5026(8)	10123(2)	18(2)
C(9)	8778(9)	4319(7)	10317(2)	17(2)
C(10)	8890(10)	4484(7)	10729(2)	17(2)
C(11)	6985(10)	4808(9)	10155(2)	26(2)
C(12)	6849(10)	4746(9)	9747(2)	25(2)
C(13)	8369(9)	5497(7)	9568(2)	17(2)
C(14)	10108(10)	4863(8)	9722(2)	19(2)
C(15)	11596(11)	5430(8)	9481(2)	25(2)
C(16)	10698(10)	5612(9)	9112(2)	24(2)
C(17)	8701(11)	5238(7)	9156(2)	21(2)
C(18)	8294(11)	7065(8)	9638(2)	26(2)
C(19)	8117(11)	5905(9)	10856(2)	26(2)
C(20)	7536(10)	6093(8)	8901(2)	21(2)
C(21)	5543(11)	5711(9)	8940(2)	26(2)
C(22)	8122(11)	5981(8)	8512(2)	24(2)
C(23)	7605(13)	4639(9)	8314(2)	33(2)
C(24)	8147(12)	4687(9)	7924(2)	31(2)
C(25)	7229(13)	6004(9)	7750(2)	32(2)
C(26)	7752(12)	7287(9)	7971(2)	29(2)
C(27)	5224(13)	5826(11)	7724(3)	41(2)
C(28)	10157(15)	4689(12)	7874(3)	48(3)
O(1)	6523(9)	2826(6)	10775(2)	33(2)
O(2)	8418(7)	3794(5)	9072(2)	21(1)
O(3)	7412(12)	3437(7)	7771(2)	49(2)
O(4)	7918(10)	6186(7)	7398(2)	42(2)
O(5)	6832(10)	8426(7)	7841(2)	43(2)
O(6)	7248(9)	7135(6)	8333(2)	31(1)

O(7)	8743(9)	881(7)	7972(2)	46(2)
O(8)	6999(11)	3732(9)	7010(2)	58(2)
O(9)	10240(19)	9160(13)	8484(3)	39(3)

Bond lengths [Å] and angles [°] for cu_130829LT_0m.

C(1)-O(1)	1.221(11)
C(1)-C(2)	1.446(12)
C(1)-C(10)	1.535(11)
C(2)-C(3)	1.319(13)
C(2)-H(2)	0.9500
C(3)-C(4)	1.495(13)
C(3)-H(3)	0.9500
C(4)-C(5)	1.505(12)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.353(12)
C(5)-C(10)	1.517(11)
C(6)-C(7)	1.476(11)
C(6)-H(6)	0.9500
C(7)-C(8)	1.556(10)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(14)	1.513(11)
C(8)-C(9)	1.524(10)
C(8)-H(8)	1.0000
C(9)-C(10)	1.549(10)
C(9)-C(11)	1.553(10)
C(9)-H(9)	1.0000
C(10)-C(19)	1.562(10)
C(11)-C(12)	1.528(11)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.509(11)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(18)	1.533(10)
C(13)-C(14)	1.555(10)
C(13)-C(17)	1.581(11)
C(14)-C(15)	1.538(11)
C(14)-H(14)	1.0000
C(15)-C(16)	1.546(11)
C(15)-H(15A)	0.9900

C(15)-H(15B)	0.9900
C(16)-C(17)	1.554(11)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-O(2)	1.441(9)
C(17)-C(20)	1.536(10)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(22)	1.521(11)
C(20)-C(21)	1.550(11)
C(20)-H(20)	1.0000
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-O(6)	1.454(9)
C(22)-C(23)	1.540(11)
C(22)-H(22)	1.0000
C(23)-C(24)	1.514(12)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-O(3)	1.443(11)
C(24)-C(28)	1.524(15)
C(24)-C(25)	1.584(11)
C(25)-O(4)	1.426(11)
C(25)-C(27)	1.521(14)
C(25)-C(26)	1.537(12)
C(26)-O(5)	1.385(11)
C(26)-O(6)	1.412(10)
C(26)-H(26)	1.0000
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800

O(2)-H(2A)	0.8400
O(3)-H(3A)	0.8400
O(4)-H(4)	0.8400
O(5)-H(5)	0.8400
O(7)-H(7C)	0.9632
O(7)-H(7D)	0.9614
O(8)-H(8A)	0.9681
O(8)-H(8B)	0.9716
O(9)-H(9A)	1.0281
O(9)-H(9B)	0.9916

O(1)-C(1)-C(2)	120.8(8)
O(1)-C(1)-C(10)	120.4(7)
C(2)-C(1)-C(10)	118.7(7)
C(3)-C(2)-C(1)	122.6(8)
C(3)-C(2)-H(2)	118.7
C(1)-C(2)-H(2)	118.7
C(2)-C(3)-C(4)	123.1(8)
C(2)-C(3)-H(3)	118.4
C(4)-C(3)-H(3)	118.4
C(3)-C(4)-C(5)	112.8(8)
C(3)-C(4)-H(4A)	109.0
C(5)-C(4)-H(4A)	109.0
C(3)-C(4)-H(4B)	109.0
C(5)-C(4)-H(4B)	109.0
H(4A)-C(4)-H(4B)	107.8
C(6)-C(5)-C(4)	119.3(7)
C(6)-C(5)-C(10)	123.4(7)
C(4)-C(5)-C(10)	117.4(7)
C(5)-C(6)-C(7)	124.4(7)
C(5)-C(6)-H(6)	117.8
C(7)-C(6)-H(6)	117.8
C(6)-C(7)-C(8)	111.7(6)
C(6)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7A)	109.3
C(6)-C(7)-H(7B)	109.3
C(8)-C(7)-H(7B)	109.3
H(7A)-C(7)-H(7B)	107.9
C(14)-C(8)-C(9)	110.5(6)

C(14)-C(8)-C(7)	110.5(6)
C(9)-C(8)-C(7)	110.5(6)
C(14)-C(8)-H(8)	108.4
C(9)-C(8)-H(8)	108.4
C(7)-C(8)-H(8)	108.4
C(8)-C(9)-C(10)	112.8(6)
C(8)-C(9)-C(11)	109.6(6)
C(10)-C(9)-C(11)	113.9(6)
C(8)-C(9)-H(9)	106.7
C(10)-C(9)-H(9)	106.7
C(11)-C(9)-H(9)	106.7
C(5)-C(10)-C(1)	107.8(6)
C(5)-C(10)-C(9)	111.7(6)
C(1)-C(10)-C(9)	112.0(6)
C(5)-C(10)-C(19)	108.5(6)
C(1)-C(10)-C(19)	104.6(6)
C(9)-C(10)-C(19)	111.9(6)
C(12)-C(11)-C(9)	115.9(6)
C(12)-C(11)-H(11A)	108.3
C(9)-C(11)-H(11A)	108.3
C(12)-C(11)-H(11B)	108.3
C(9)-C(11)-H(11B)	108.3
H(11A)-C(11)-H(11B)	107.4
C(13)-C(12)-C(11)	111.9(7)
C(13)-C(12)-H(12A)	109.2
C(11)-C(12)-H(12A)	109.2
C(13)-C(12)-H(12B)	109.2
C(11)-C(12)-H(12B)	109.2
H(12A)-C(12)-H(12B)	107.9
C(12)-C(13)-C(18)	111.6(6)
C(12)-C(13)-C(14)	106.6(6)
C(18)-C(13)-C(14)	110.7(6)
C(12)-C(13)-C(17)	118.5(6)
C(18)-C(13)-C(17)	109.1(6)
C(14)-C(13)-C(17)	99.6(6)
C(8)-C(14)-C(15)	118.1(6)
C(8)-C(14)-C(13)	114.3(6)
C(15)-C(14)-C(13)	104.8(6)
C(8)-C(14)-H(14)	106.3

C(15)-C(14)-H(14)	106.3
C(13)-C(14)-H(14)	106.3
C(14)-C(15)-C(16)	104.2(6)
C(14)-C(15)-H(15A)	110.9
C(16)-C(15)-H(15A)	110.9
C(14)-C(15)-H(15B)	110.9
C(16)-C(15)-H(15B)	110.9
H(15A)-C(15)-H(15B)	108.9
C(15)-C(16)-C(17)	107.6(6)
C(15)-C(16)-H(16A)	110.2
C(17)-C(16)-H(16A)	110.2
C(15)-C(16)-H(16B)	110.2
C(17)-C(16)-H(16B)	110.2
H(16A)-C(16)-H(16B)	108.5
O(2)-C(17)-C(20)	107.2(6)
O(2)-C(17)-C(16)	110.1(6)
C(20)-C(17)-C(16)	111.2(6)
O(2)-C(17)-C(13)	109.9(6)
C(20)-C(17)-C(13)	115.6(6)
C(16)-C(17)-C(13)	102.7(6)
C(13)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(10)-C(19)-H(19A)	109.5
C(10)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(10)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(22)-C(20)-C(17)	113.0(6)
C(22)-C(20)-C(21)	110.7(7)
C(17)-C(20)-C(21)	111.5(7)
C(22)-C(20)-H(20)	107.1
C(17)-C(20)-H(20)	107.1
C(21)-C(20)-H(20)	107.1
C(20)-C(21)-H(21A)	109.5

C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(6)-C(22)-C(20)	104.8(7)
O(6)-C(22)-C(23)	107.7(6)
C(20)-C(22)-C(23)	116.5(7)
O(6)-C(22)-H(22)	109.2
C(20)-C(22)-H(22)	109.2
C(23)-C(22)-H(22)	109.2
C(24)-C(23)-C(22)	111.7(7)
C(24)-C(23)-H(23A)	109.3
C(22)-C(23)-H(23A)	109.3
C(24)-C(23)-H(23B)	109.3
C(22)-C(23)-H(23B)	109.3
H(23A)-C(23)-H(23B)	107.9
O(3)-C(24)-C(23)	104.7(7)
O(3)-C(24)-C(28)	109.4(8)
C(23)-C(24)-C(28)	112.7(8)
O(3)-C(24)-C(25)	109.7(7)
C(23)-C(24)-C(25)	107.6(7)
C(28)-C(24)-C(25)	112.4(8)
O(4)-C(25)-C(27)	108.4(7)
O(4)-C(25)-C(26)	107.8(8)
C(27)-C(25)-C(26)	112.3(8)
O(4)-C(25)-C(24)	108.6(7)
C(27)-C(25)-C(24)	111.6(8)
C(26)-C(25)-C(24)	108.0(7)
O(5)-C(26)-O(6)	106.5(7)
O(5)-C(26)-C(25)	108.5(7)
O(6)-C(26)-C(25)	111.3(7)
O(5)-C(26)-H(26)	110.1
O(6)-C(26)-H(26)	110.1
C(25)-C(26)-H(26)	110.1
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5

H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(24)-C(28)-H(28A)	109.5
C(24)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(24)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(17)-O(2)-H(2A)	109.5
C(24)-O(3)-H(3A)	109.5
C(25)-O(4)-H(4)	109.5
C(26)-O(5)-H(5)	109.5
C(26)-O(6)-C(22)	113.6(6)
H(7C)-O(7)-H(7D)	101.5
H(8A)-O(8)-H(8B)	101.7
H(9A)-O(9)-H(9B)	103.6

Symmetry transformations used to generate equivalent atoms:

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for cu_130829LT_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	24(5)	12(4)	39(4)	-1(3)	2(4)	0(3)
C(2)	29(5)	26(4)	40(5)	1(4)	8(4)	-14(4)
C(3)	20(5)	36(5)	37(5)	4(4)	-3(4)	2(4)
C(4)	25(5)	48(6)	36(5)	4(4)	-1(4)	-3(4)
C(5)	19(4)	20(4)	34(4)	4(3)	-7(3)	1(3)
C(6)	16(4)	16(4)	49(5)	2(4)	-4(3)	2(3)
C(7)	9(4)	24(4)	34(4)	-1(3)	2(3)	3(3)
C(8)	3(4)	17(4)	35(4)	5(3)	1(3)	-4(3)
C(9)	3(4)	6(3)	42(4)	3(3)	-2(3)	2(3)
C(10)	13(4)	6(3)	32(4)	2(3)	-2(3)	-4(3)
C(11)	8(4)	36(5)	34(4)	2(4)	2(3)	4(3)
C(12)	13(4)	27(4)	36(4)	7(3)	0(3)	8(3)
C(13)	7(4)	9(3)	35(4)	3(3)	-7(3)	3(3)
C(14)	7(4)	14(4)	38(4)	3(3)	-1(3)	3(3)
C(15)	14(4)	21(4)	41(4)	5(3)	0(4)	6(3)
C(16)	16(4)	22(4)	32(4)	5(3)	8(3)	-11(3)
C(17)	22(4)	8(3)	34(4)	4(3)	-4(3)	4(3)
C(18)	19(4)	22(4)	34(4)	3(3)	0(4)	3(3)
C(19)	17(4)	24(4)	36(4)	-3(3)	-3(3)	1(3)
C(20)	8(4)	19(4)	37(4)	3(3)	0(3)	-2(3)
C(21)	17(5)	23(4)	39(5)	8(4)	4(3)	7(3)
C(22)	16(4)	14(4)	42(5)	11(3)	-8(3)	-5(3)
C(23)	45(6)	19(4)	36(4)	-1(3)	-4(4)	8(4)
C(24)	30(5)	22(4)	40(5)	-1(4)	-3(4)	9(4)
C(25)	35(5)	28(5)	34(4)	-2(4)	-6(4)	12(4)
C(26)	21(5)	26(4)	38(5)	10(4)	-6(4)	0(4)
C(27)	35(6)	36(5)	52(6)	-1(5)	-7(5)	1(4)
C(28)	55(7)	47(6)	43(5)	9(5)	12(5)	25(6)
O(1)	29(4)	29(3)	41(3)	4(3)	5(3)	-11(3)
O(2)	16(3)	7(2)	41(3)	-2(2)	-3(2)	-1(2)
O(3)	78(6)	24(3)	44(4)	-7(3)	-9(4)	9(4)
O(4)	44(4)	40(4)	42(4)	4(3)	2(3)	-9(3)
O(5)	52(5)	33(4)	44(4)	6(3)	-10(3)	3(3)
O(6)	38(4)	23(3)	33(3)	5(2)	-6(3)	1(3)

O(7)	33(4)	37(4)	68(4)	-5(3)	5(3)	5(3)
O(8)	49(5)	64(5)	62(5)	3(4)	-7(4)	-13(4)
O(9)	44(8)	29(7)	44(7)	2(6)	-1(6)	-4(6)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)
for cu_130829LT_0m.

	x	y	z	U(eq)
H(2)	7332	2581	11432	38
H(3)	9863	3232	11692	37
H(4A)	12245	3888	11310	44
H(4B)	11074	5264	11357	44
H(6)	13354	4200	10749	32
H(7A)	12293	3488	10143	27
H(7B)	13099	5026	10164	27
H(8)	10285	6040	10181	22
H(9)	8880	3303	10266	20
H(11A)	6023	4229	10257	31
H(11B)	6770	5778	10231	31
H(12A)	6845	3763	9670	30
H(12B)	5711	5170	9671	30
H(14)	10045	3842	9675	23
H(15A)	12598	4766	9467	30
H(15B)	12045	6330	9572	30
H(16A)	11262	4992	8934	28
H(16B)	10825	6584	9029	28
H(18A)	7186	7443	9540	38
H(18B)	9309	7517	9522	38
H(18C)	8340	7238	9896	38
H(19A)	6831	5920	10816	39
H(19B)	8677	6661	10721	39
H(19C)	8360	6027	11112	39
H(20)	7662	7090	8972	25
H(21A)	4867	6133	8744	40
H(21B)	5096	6061	9169	40
H(21C)	5407	4699	8931	40
H(22)	9439	6110	8498	29
H(23A)	8187	3836	8431	40
H(23B)	6303	4504	8330	40
H(26)	9062	7451	7953	34
H(27A)	4717	6597	7587	61

H(27B)	4712	5818	7965	61
H(27C)	4953	4946	7604	61
H(28A)	10692	3981	8028	73
H(28B)	10633	5605	7937	73
H(28C)	10440	4484	7623	73
H(2A)	9259	3319	9155	32
H(3A)	7584	3438	7549	73
H(4)	8563	6898	7392	63
H(5)	7256	9156	7929	65
H(8A)	7764	4177	6836	50
H(8B)	6118	3293	6857	50
H(9A)	10965	9858	8633	50
H(9B)	9437	9758	8341	50
H(7C)	8269	1804	7943	50
H(7D)	9551	826	7773	50