Supporting Information

Acetophenone Monomers from *Acronychia Trifoliolata*

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Figure S1. NCI-60 Human tumor cell line assay data for the crude organic extract of *A. trifoliolata*.

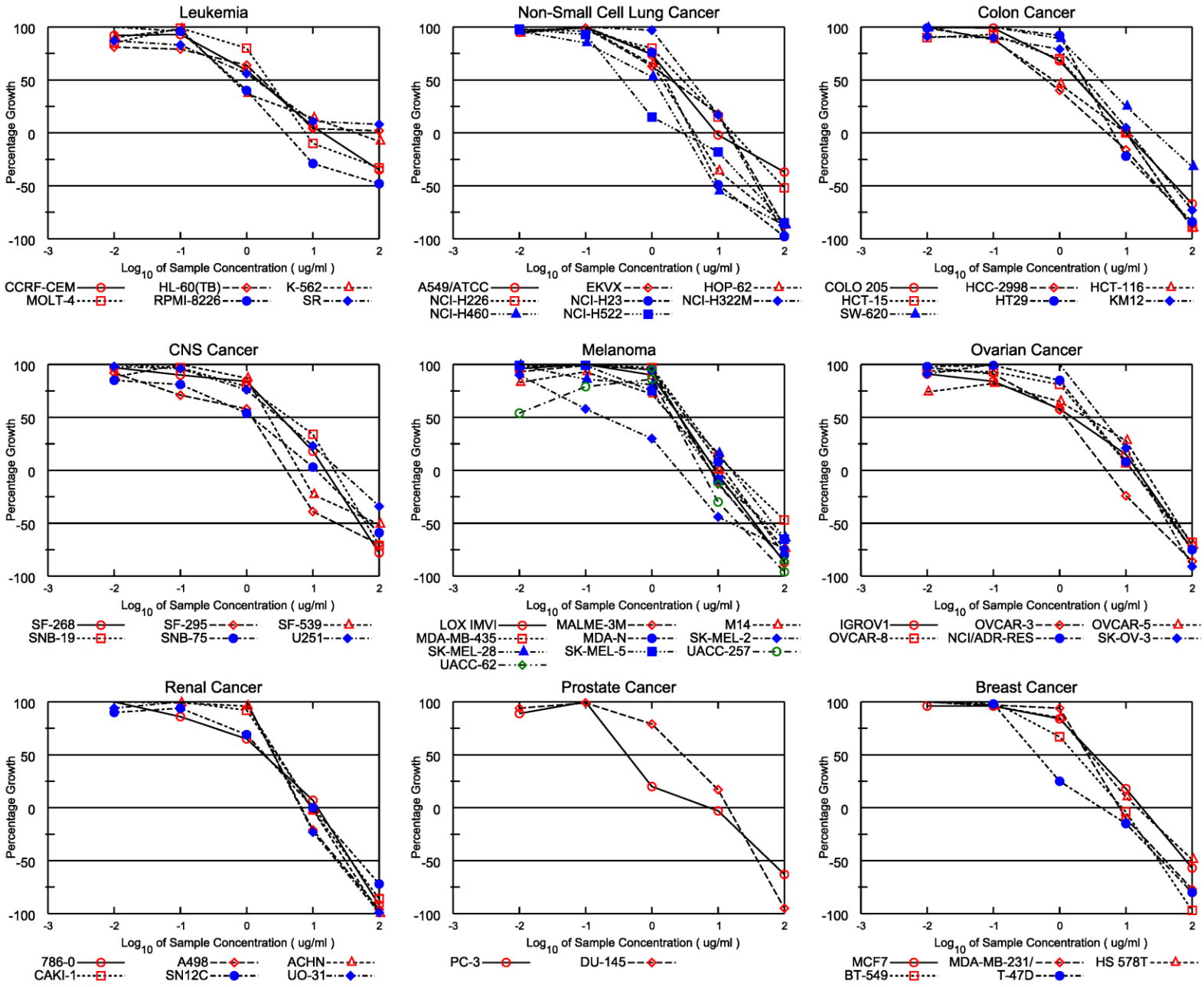


Figure S2. ^{1}H NMR spectrum of 1 (600 MHz, in $CDCl_3$).

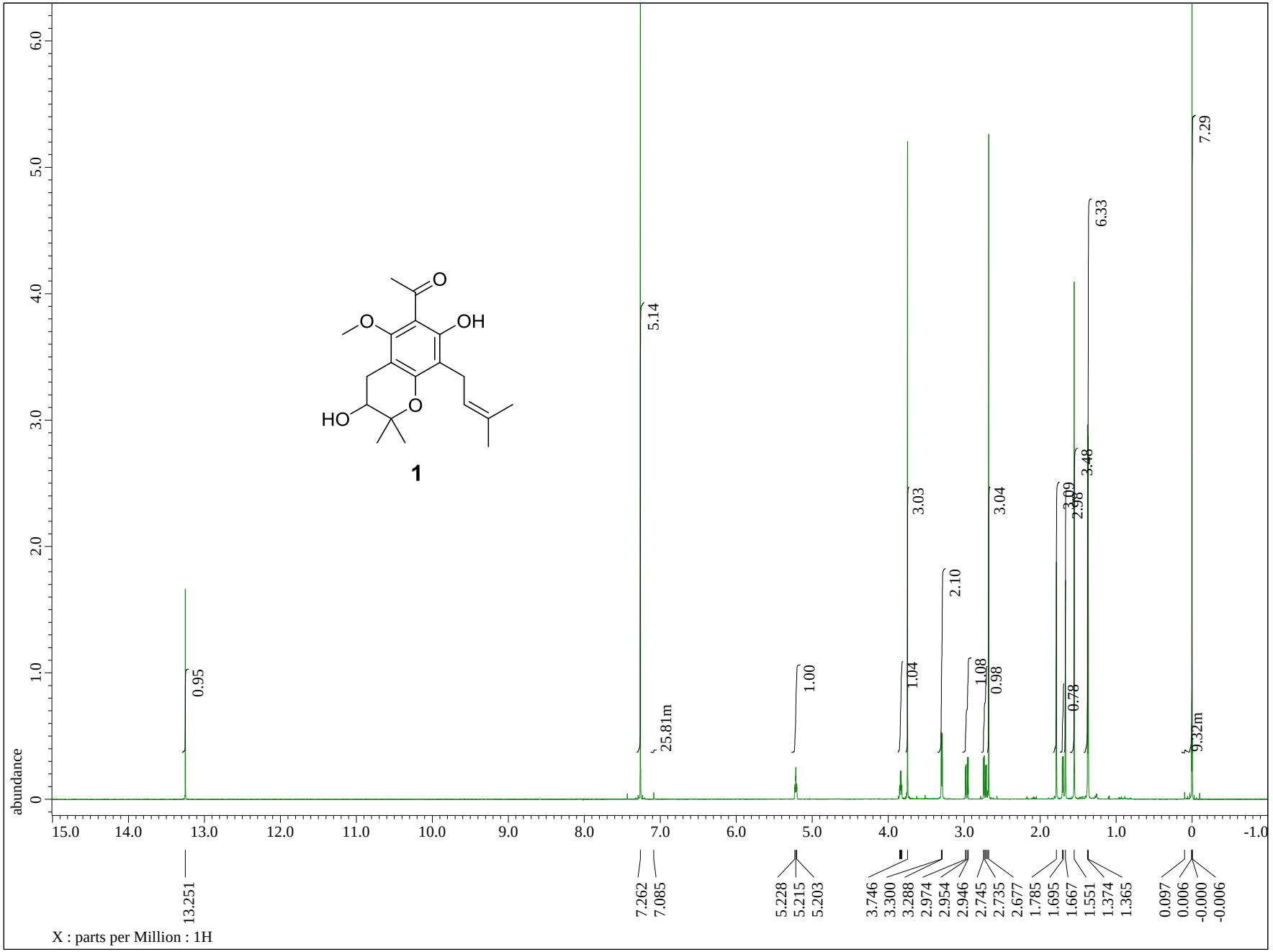


Figure S3. ^{13}C NMR spectrum of 1 (150 MHz, in $CDCl_3$).

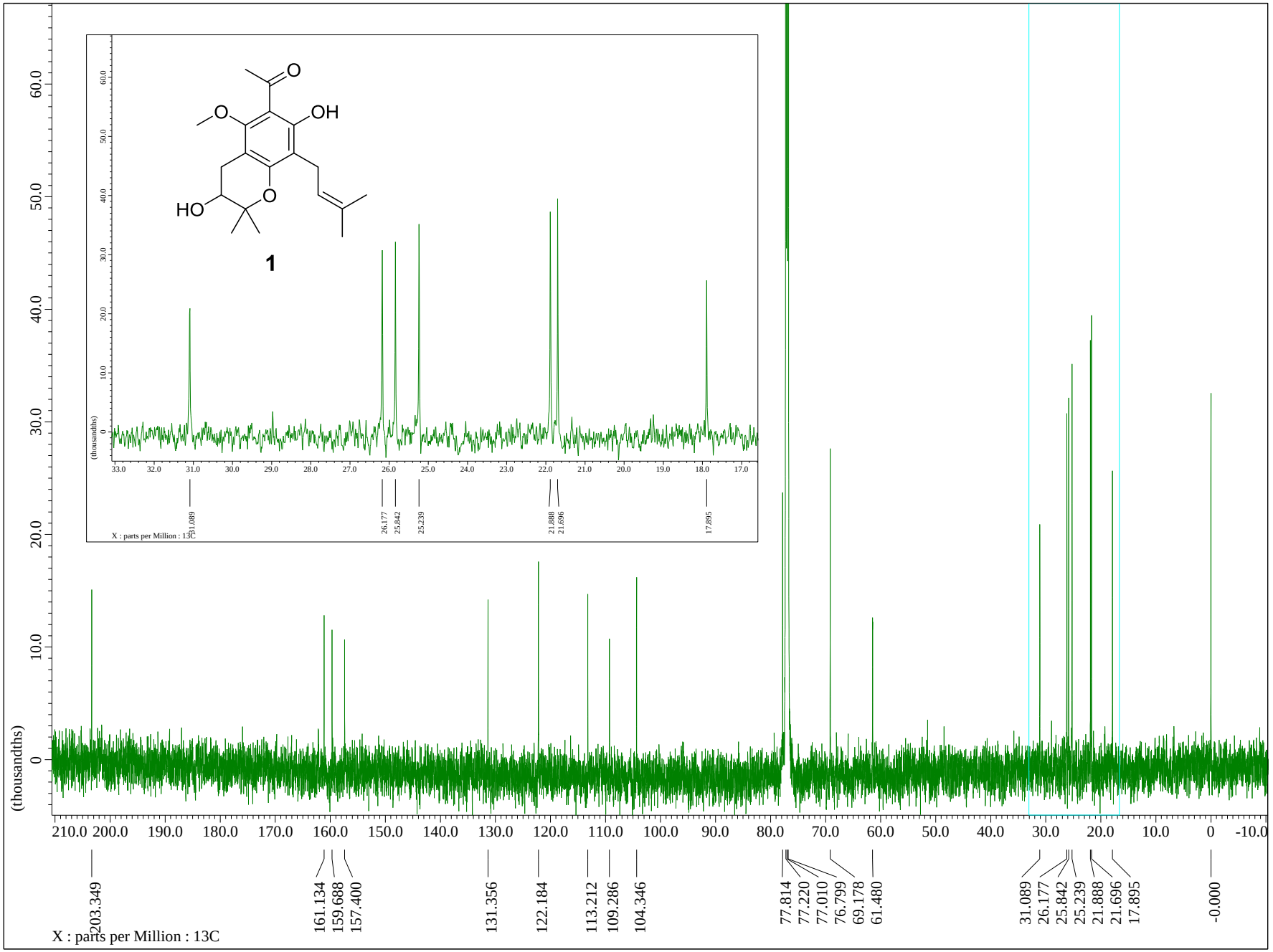


Figure S4. H-H COSY experiment of 1 (in $CDCl_3$, 400 MHz).

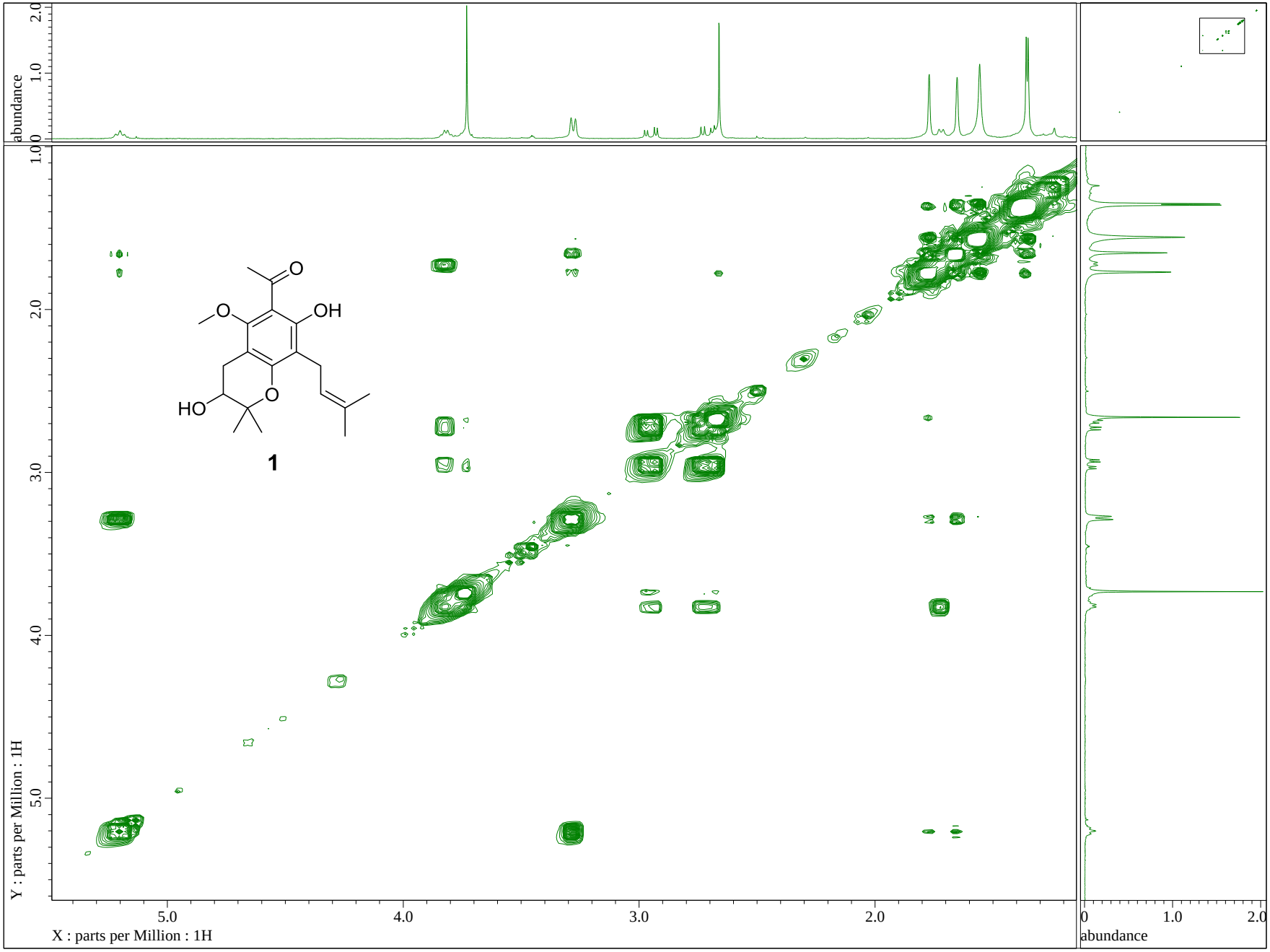


Figure S5. NOESY experiment of 1 (in $CDCl_3$).

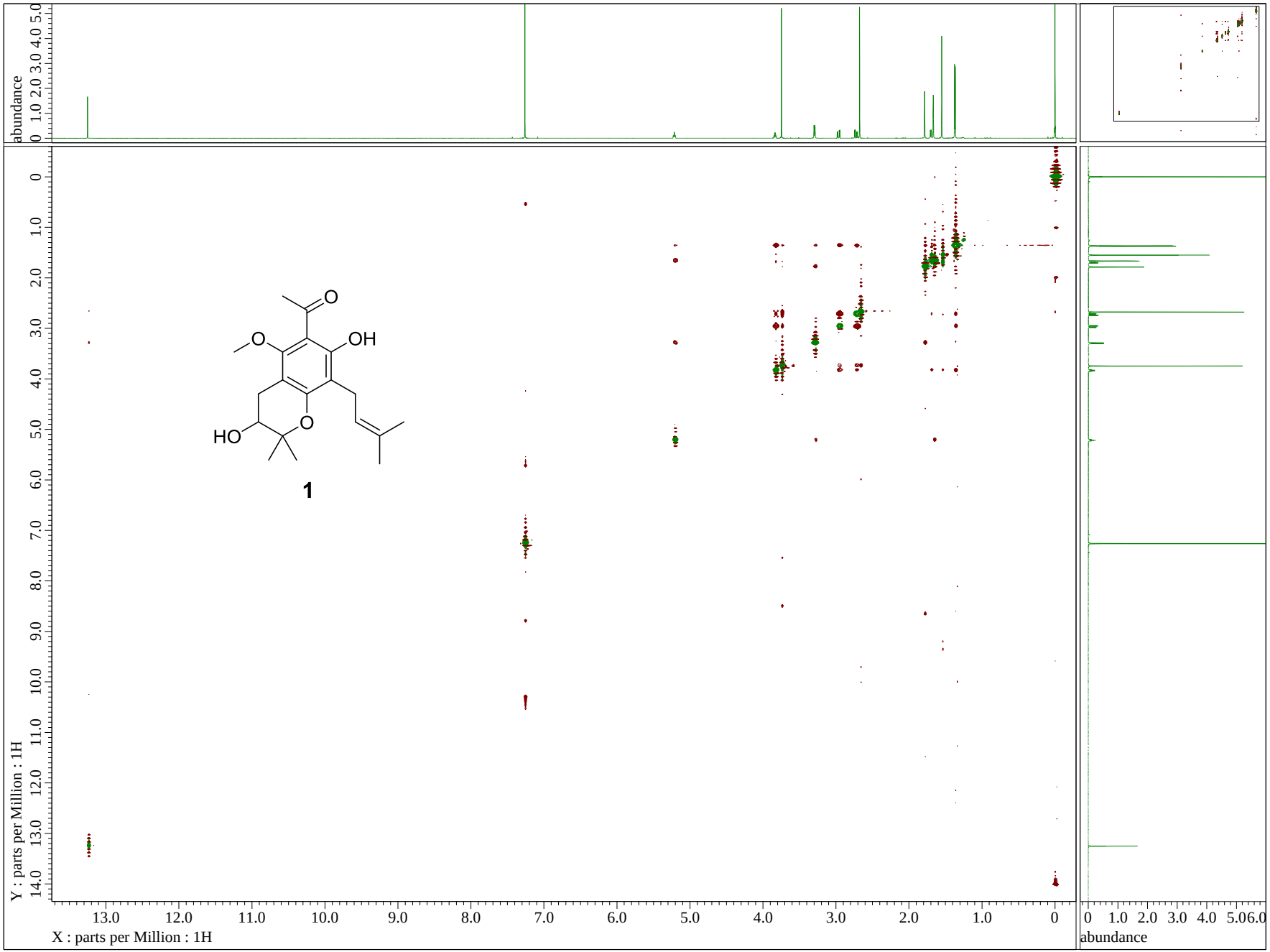


Figure S6. NOESY experiment of 1 (in $CDCl_3$).

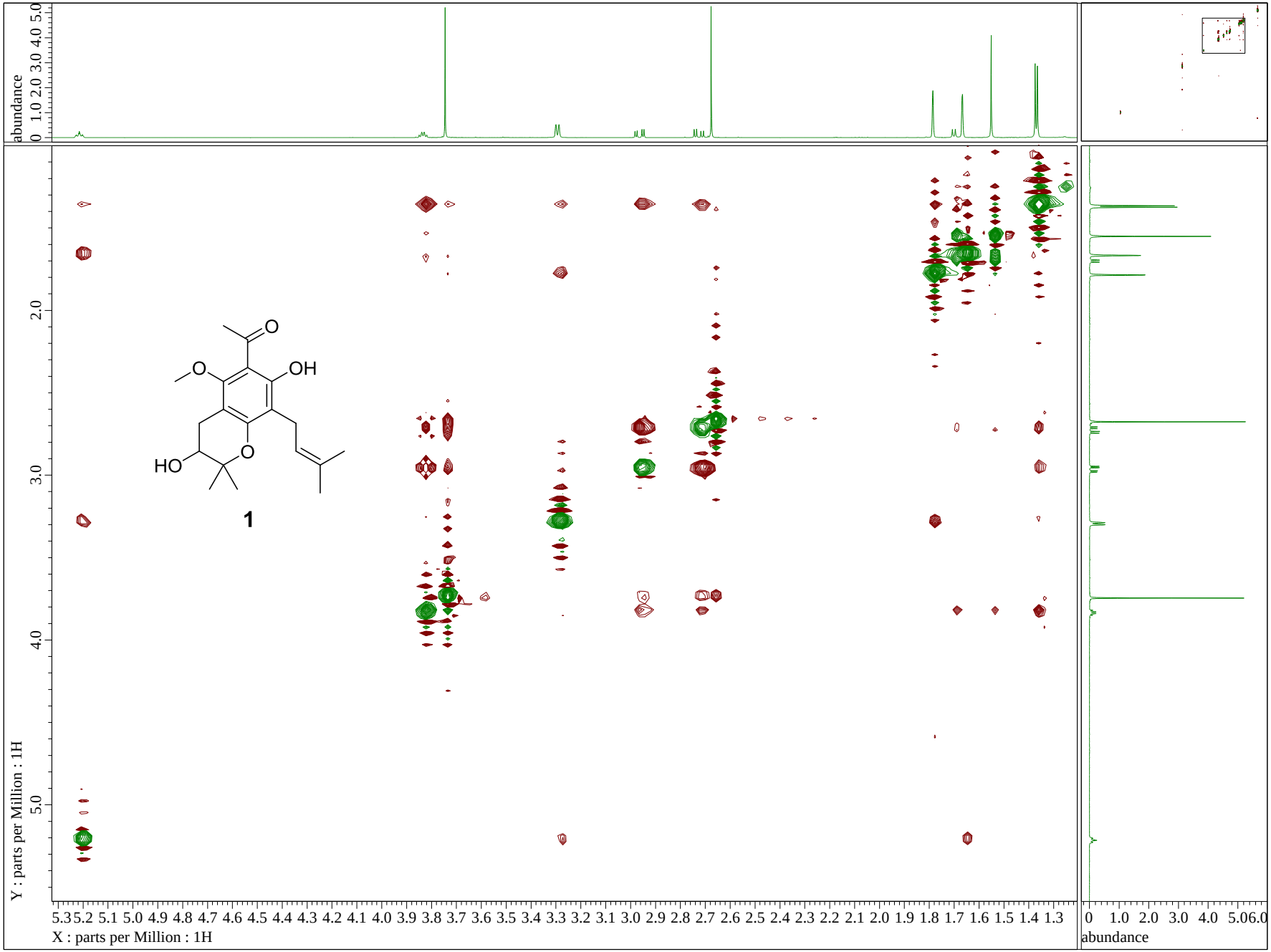


Figure S7. HMQC experiment of 1 (in $CDCl_3$).

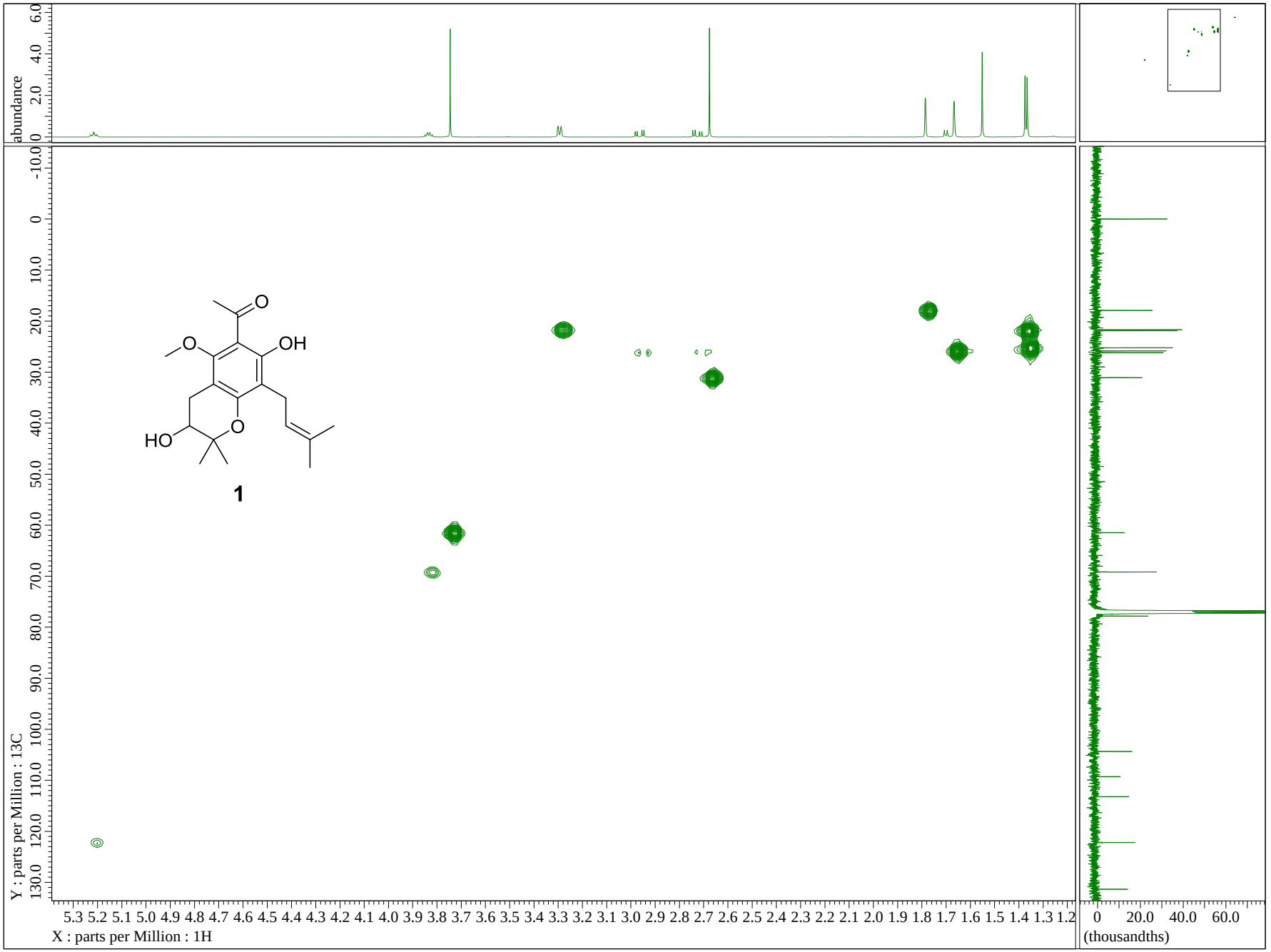


Figure S8. HMBC experiment of 1 (in $CDCl_3$).

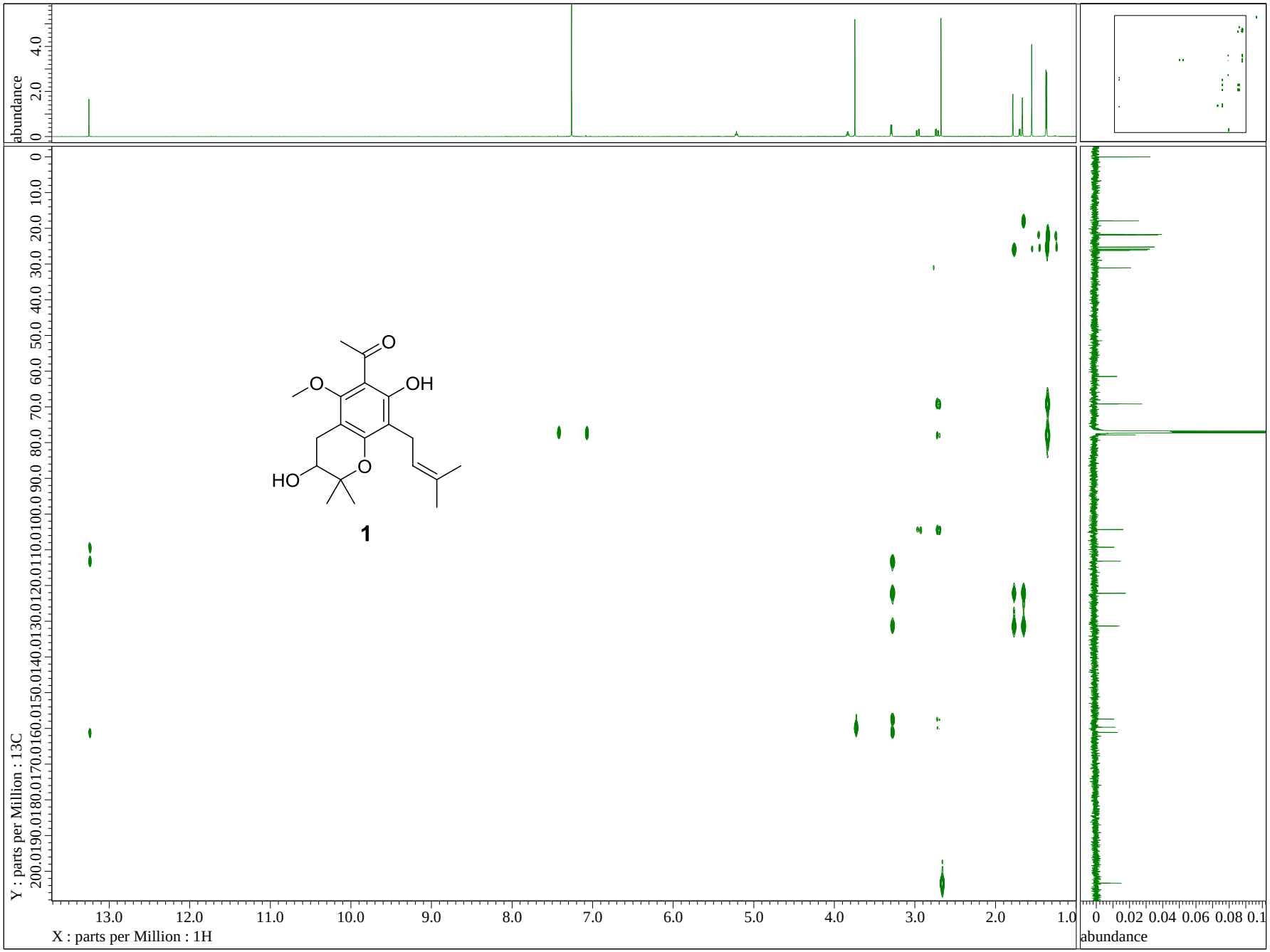


Figure S9. HMBC experiment of 1 (in $CDCl_3$).

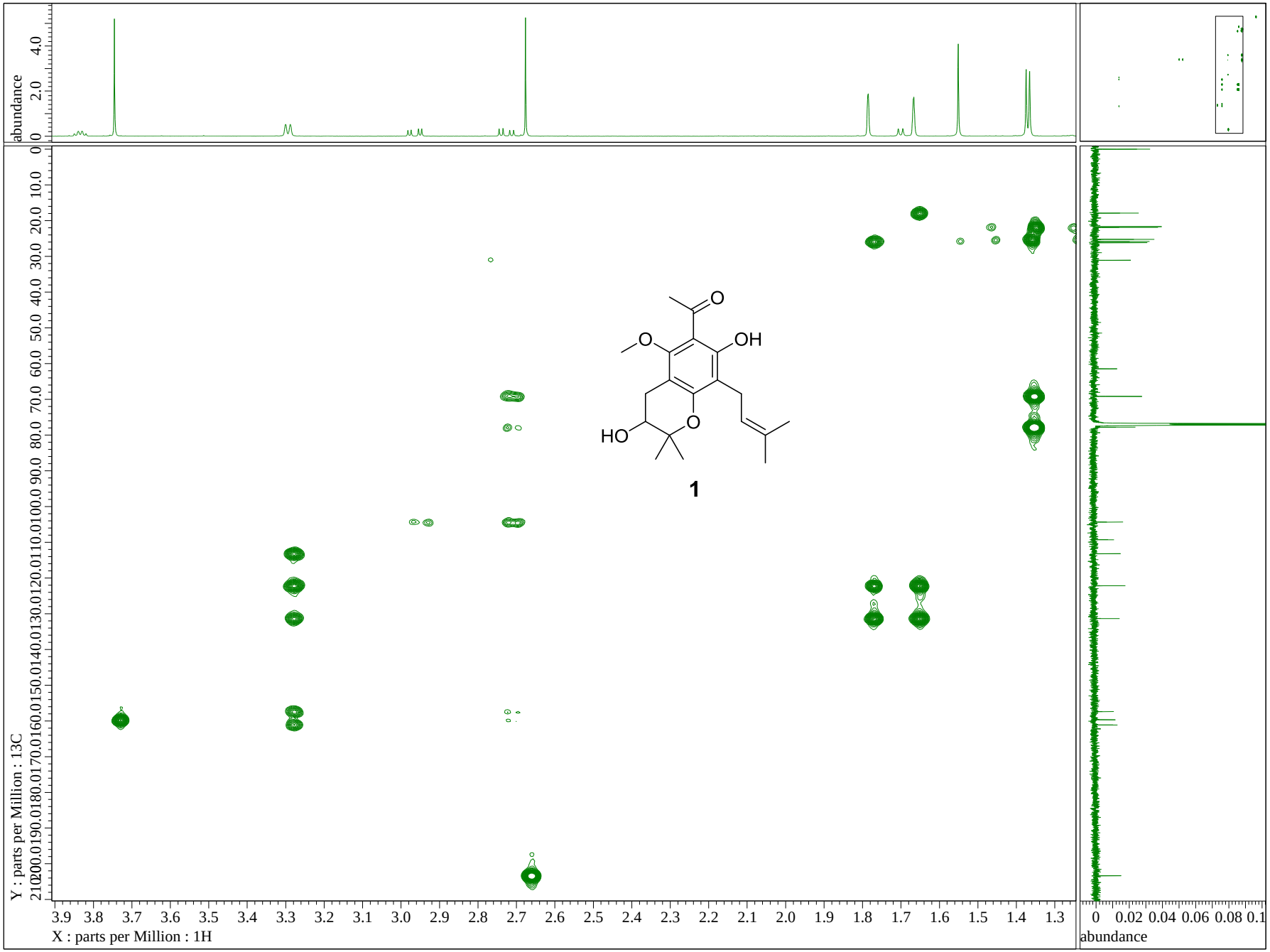


Figure S10. ^{1}H NMR spectrum of 2 (600 MHz, in $CDCl_3$).

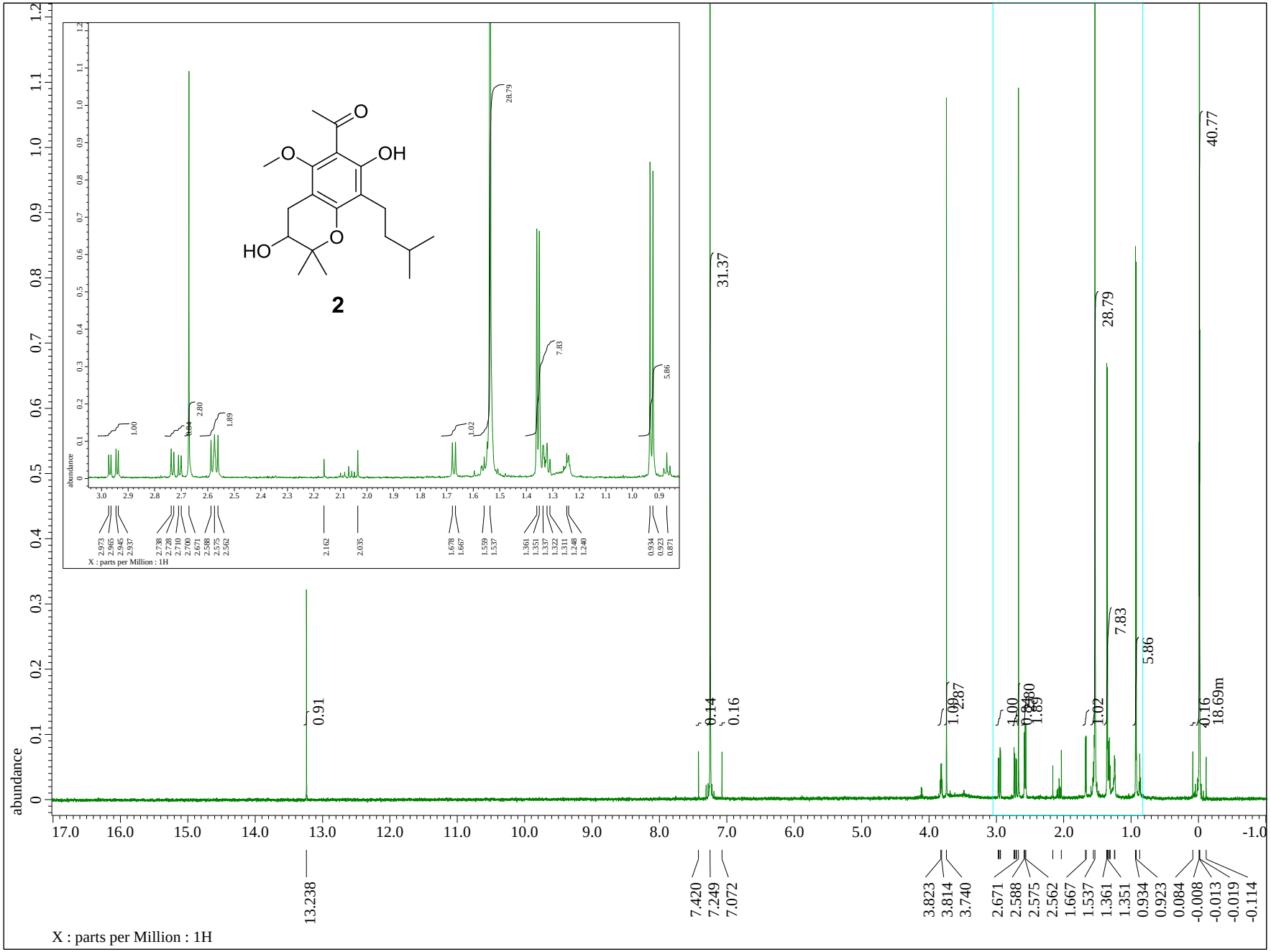


Figure S11. H-H COSY experiment of 2 (in $CDCl_3$).

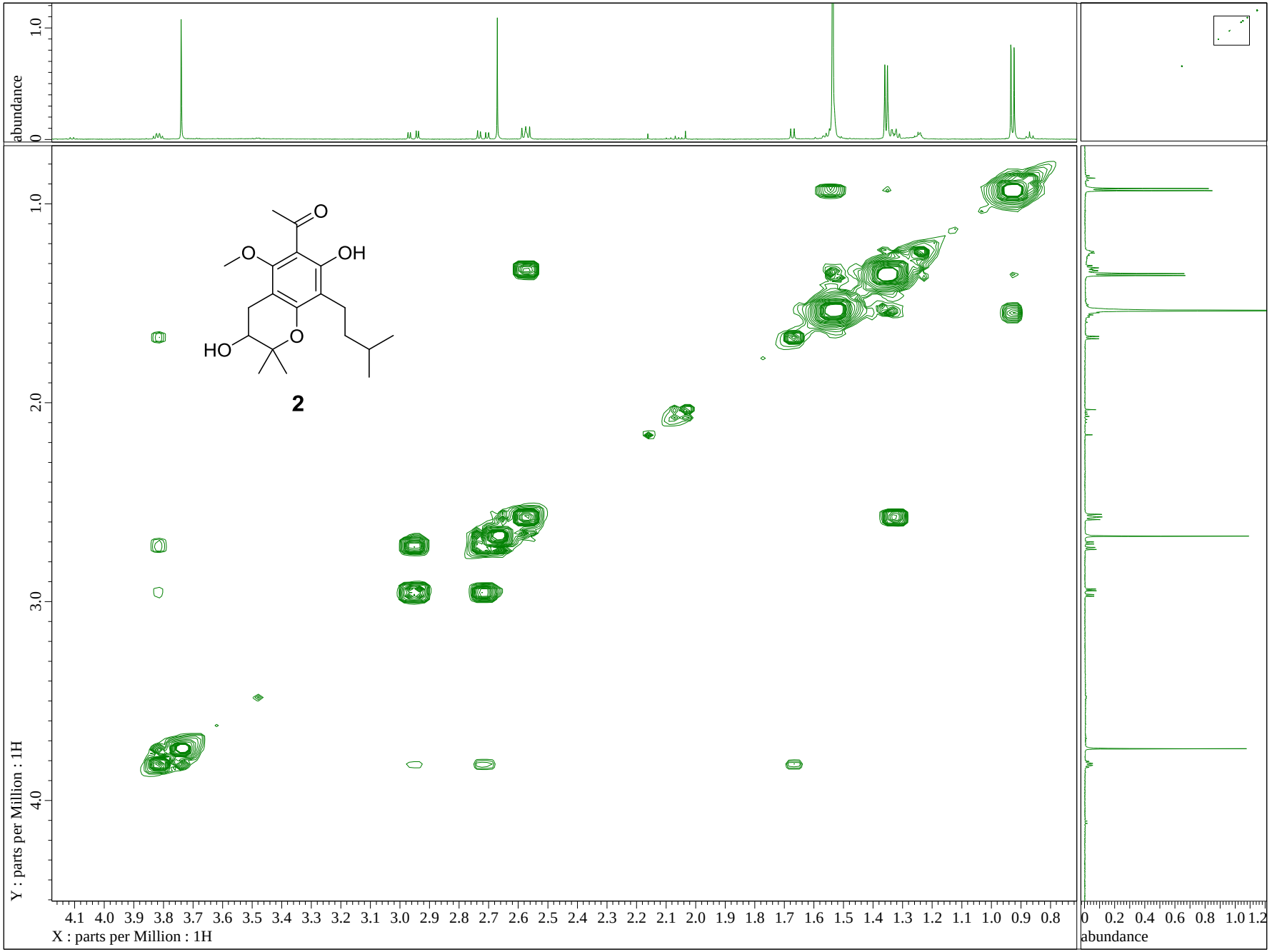


Figure S12. NOESY experiment of 2 (in $CDCl_3$).

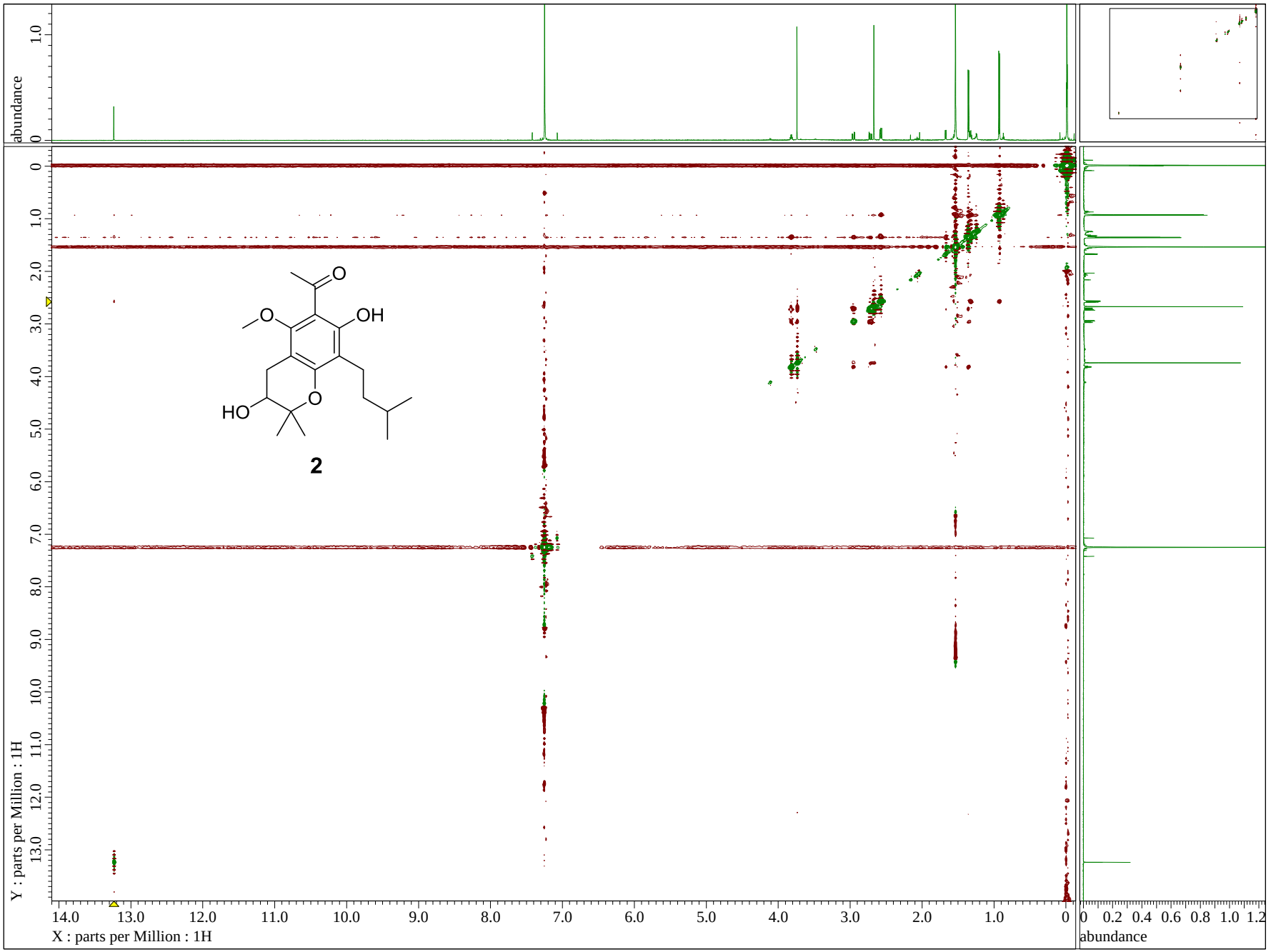


Figure S13. NOESY experiment of 2 (in $CDCl_3$).

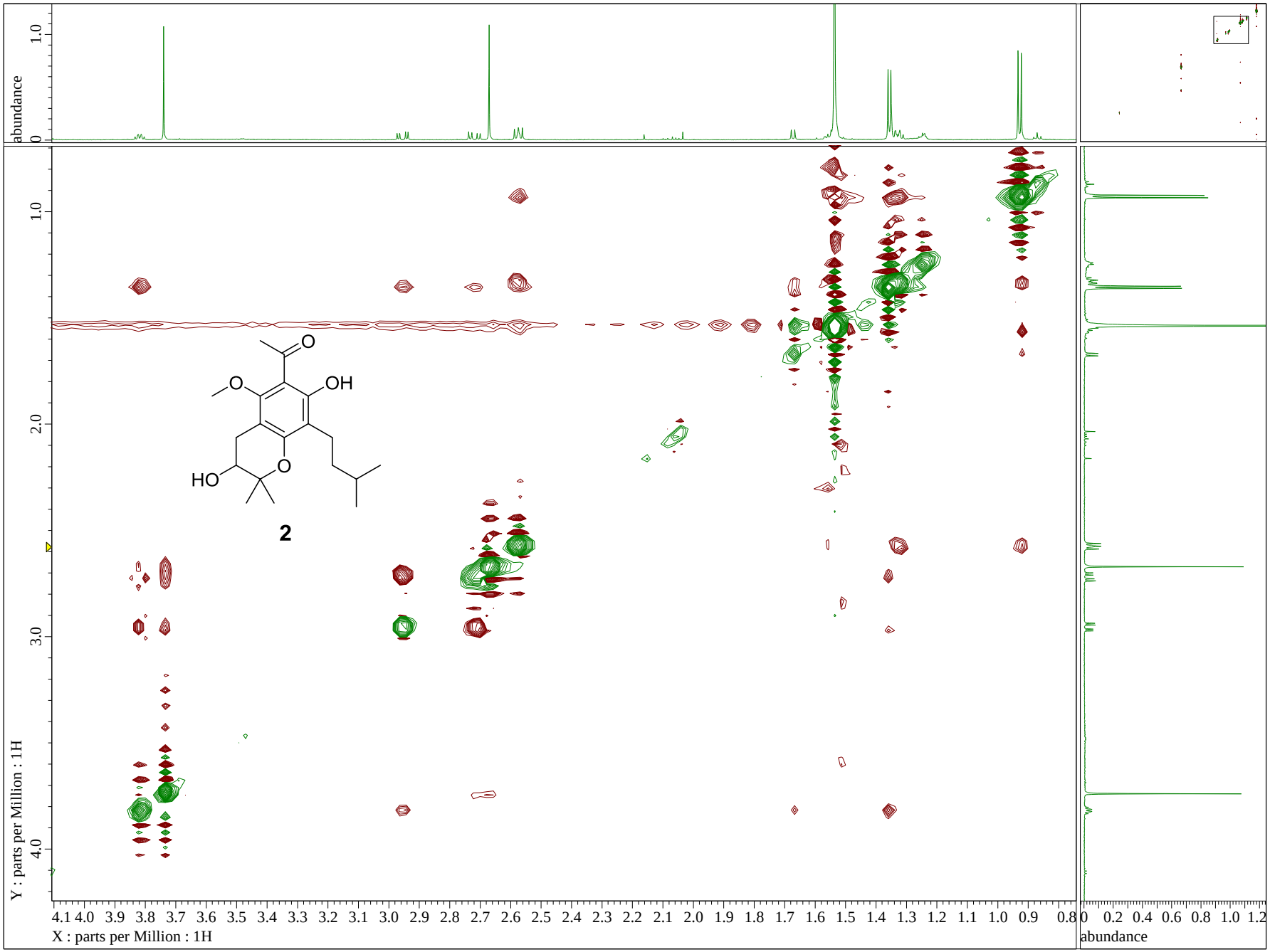


Figure S14. ^{1}H NMR spectrum of 3 (600 MHz, in $CDCl_3$).

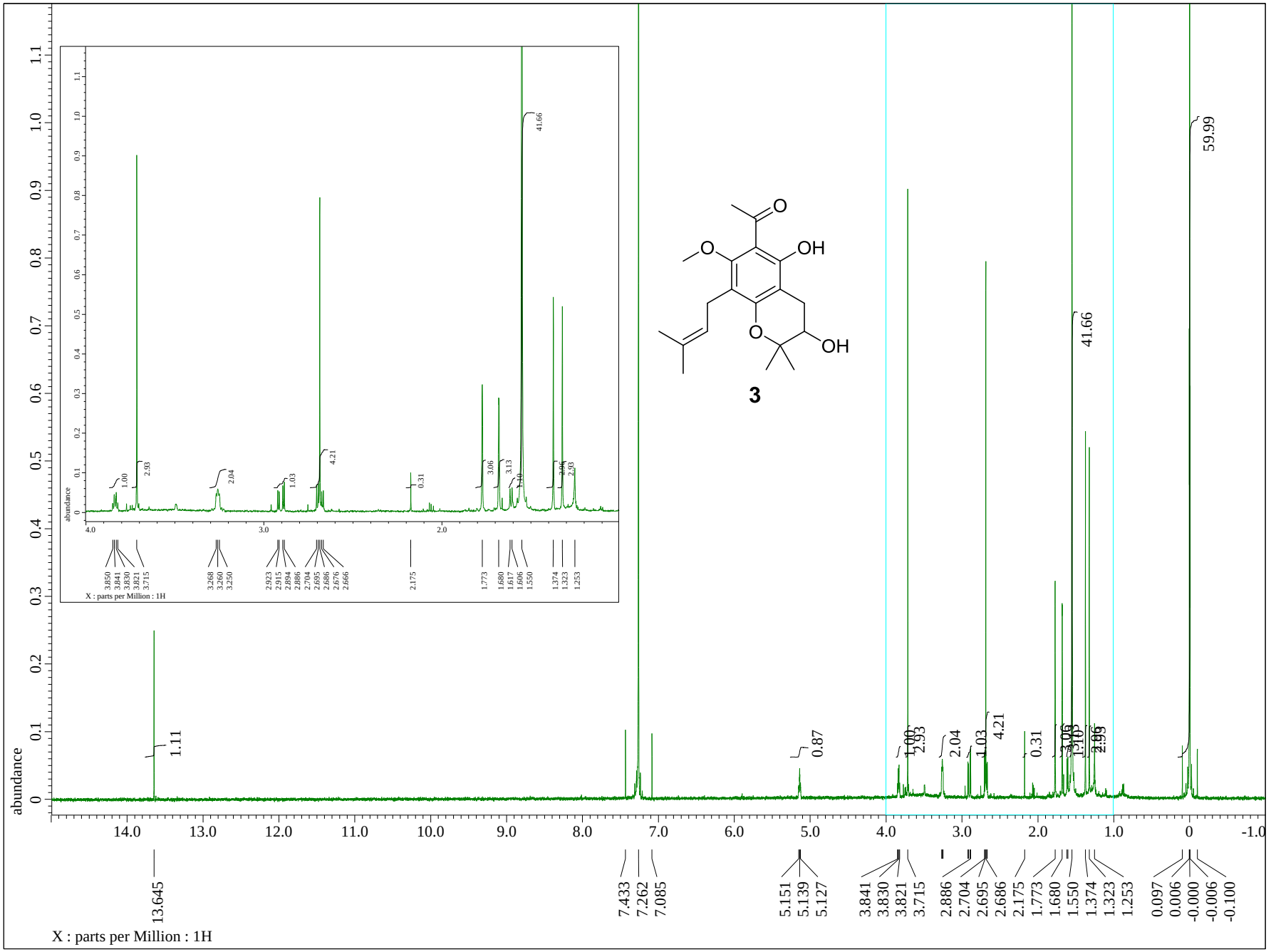


Figure S15. H-H COSY experiment of 3 (in $CDCl_3$).

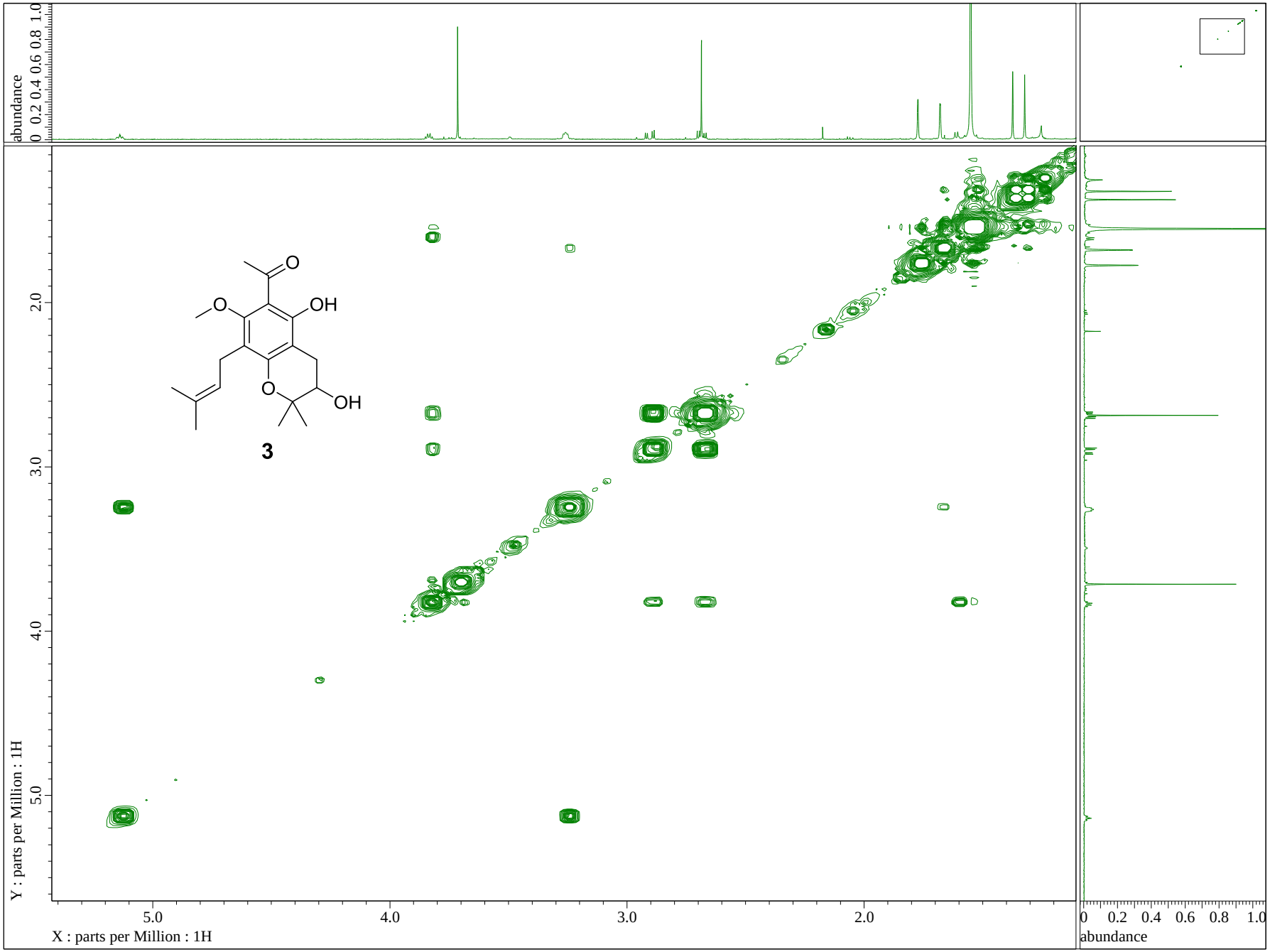


Figure S16. NOESY experiment of 3 (in $CDCl_3$).

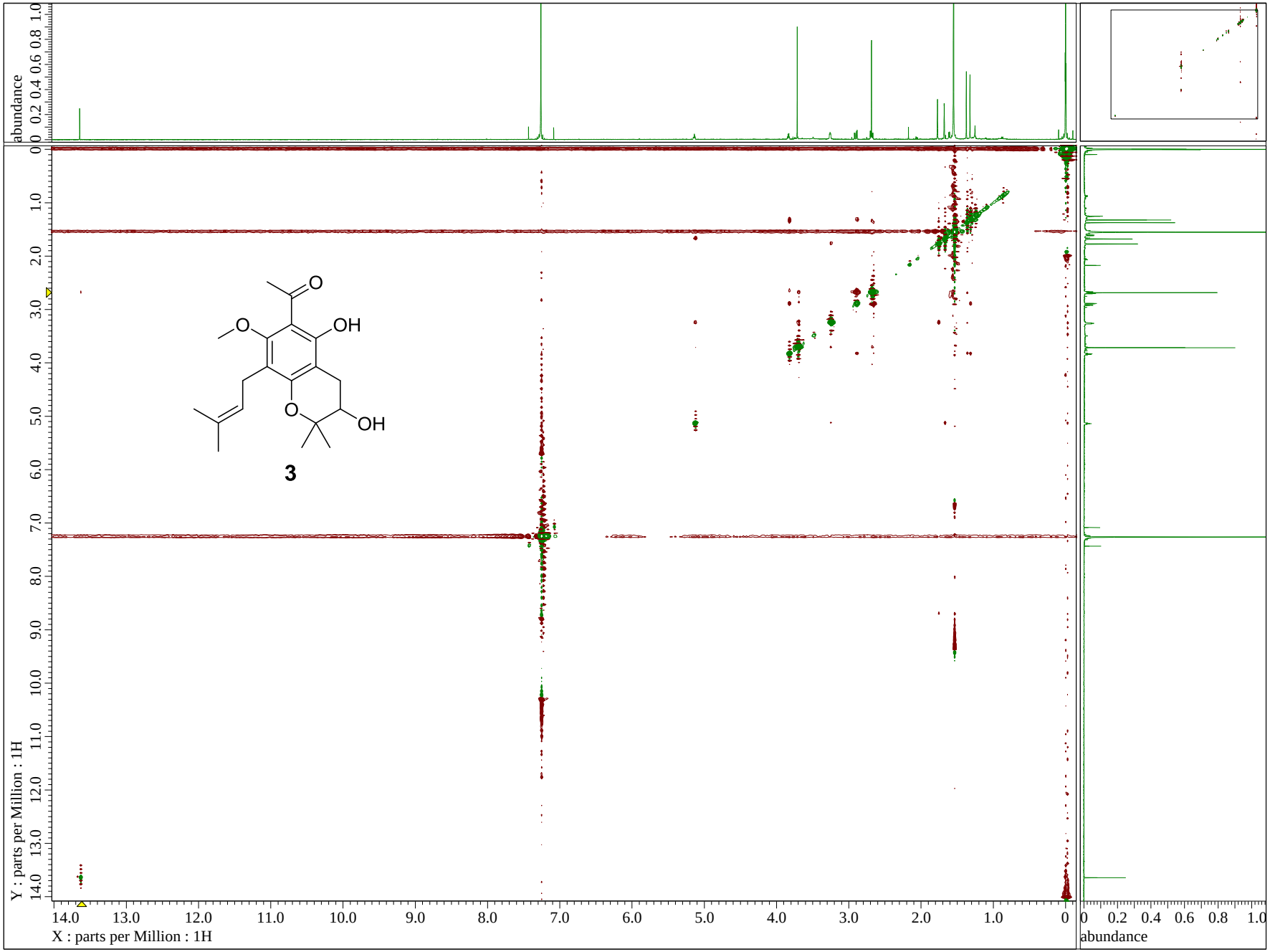


Figure S17. NOESY experiment of 3 (in $CDCl_3$).

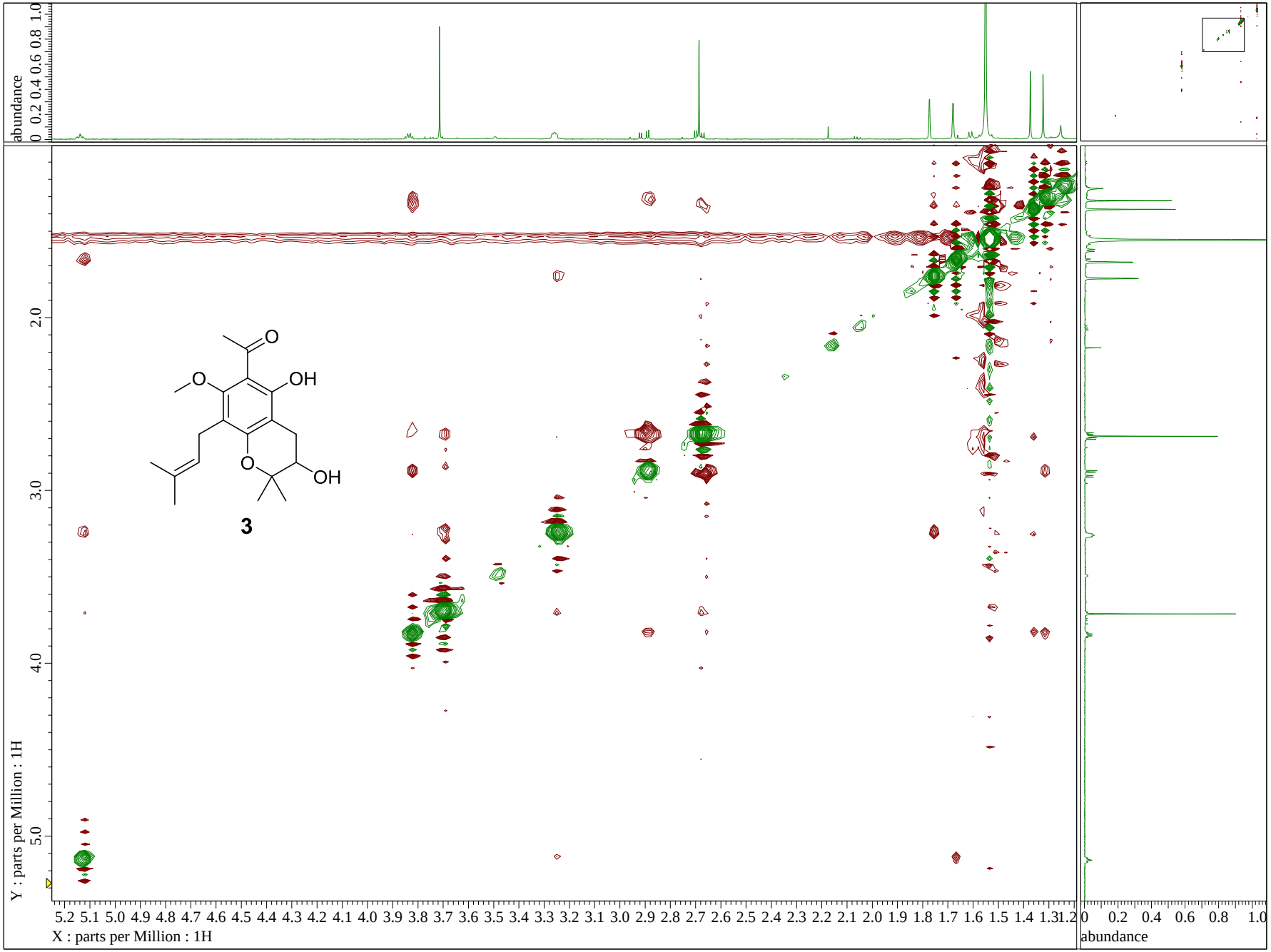


Figure S18. ^{1}H NMR spectrum of 4 (600 MHz, in $CDCl_3$).

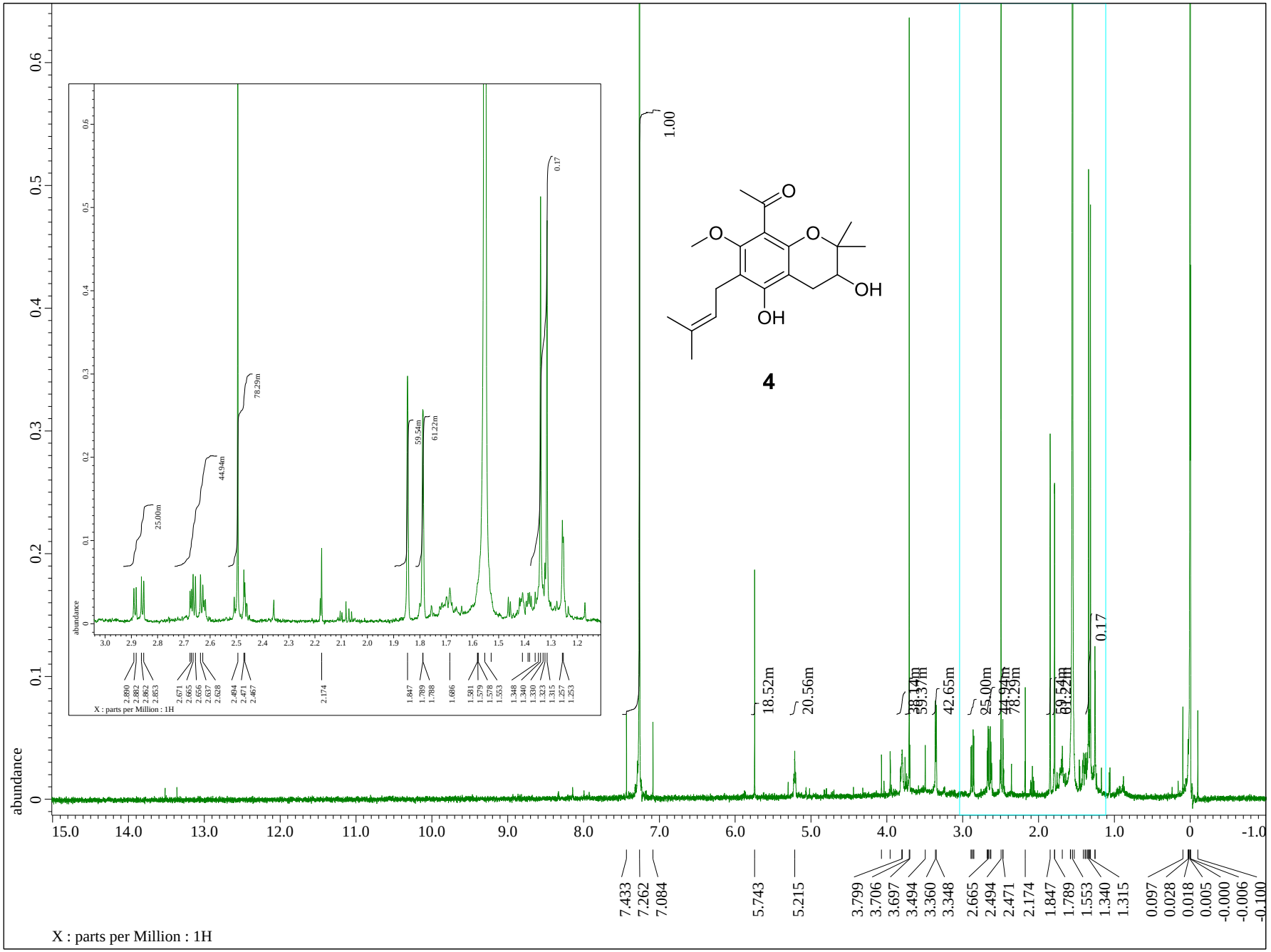


Figure S19. H-H COSY experiment of 4 (in $CDCl_3$).

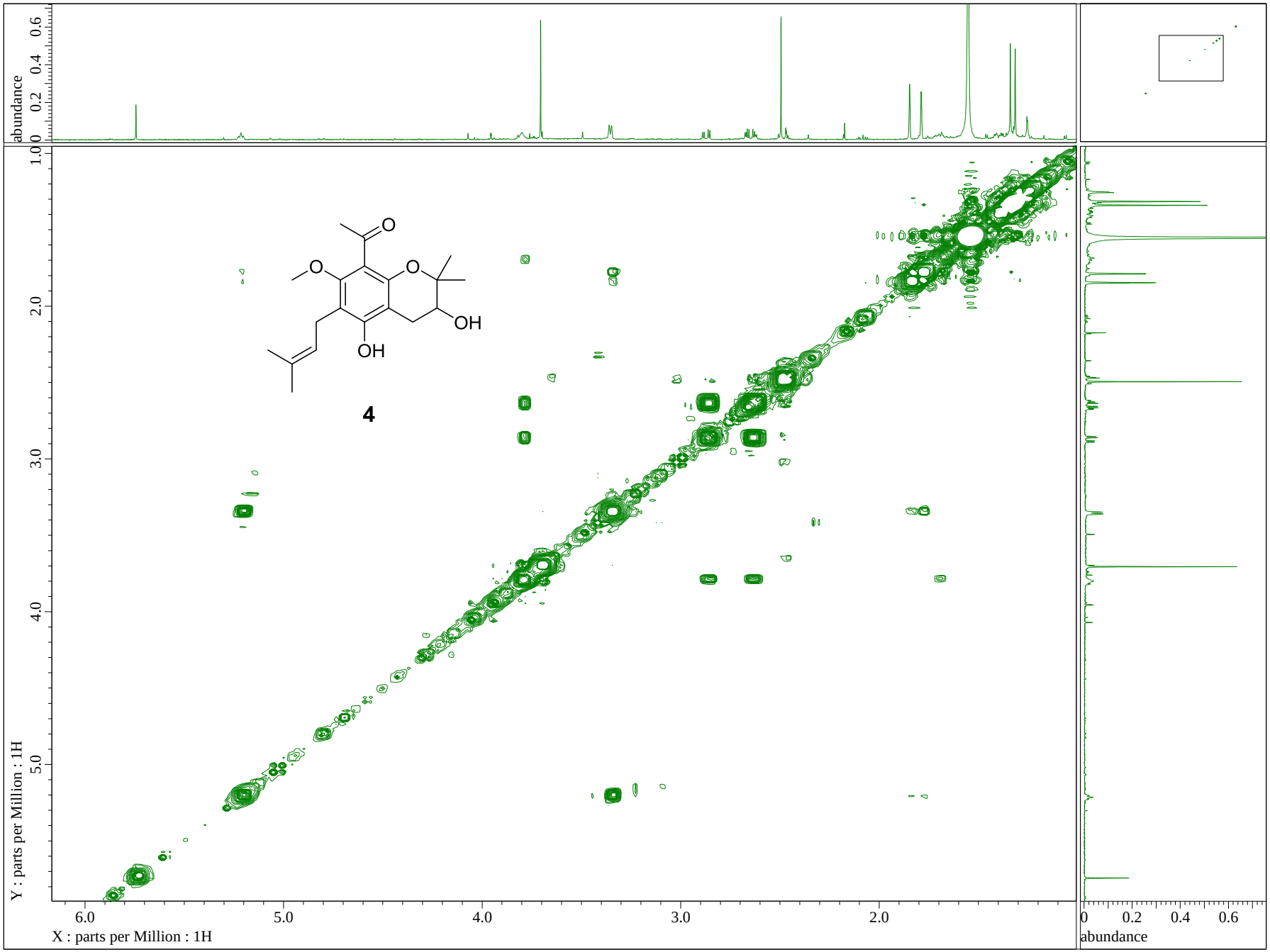


Figure S20. NOESY experiment of 4 (in $CDCl_3$).

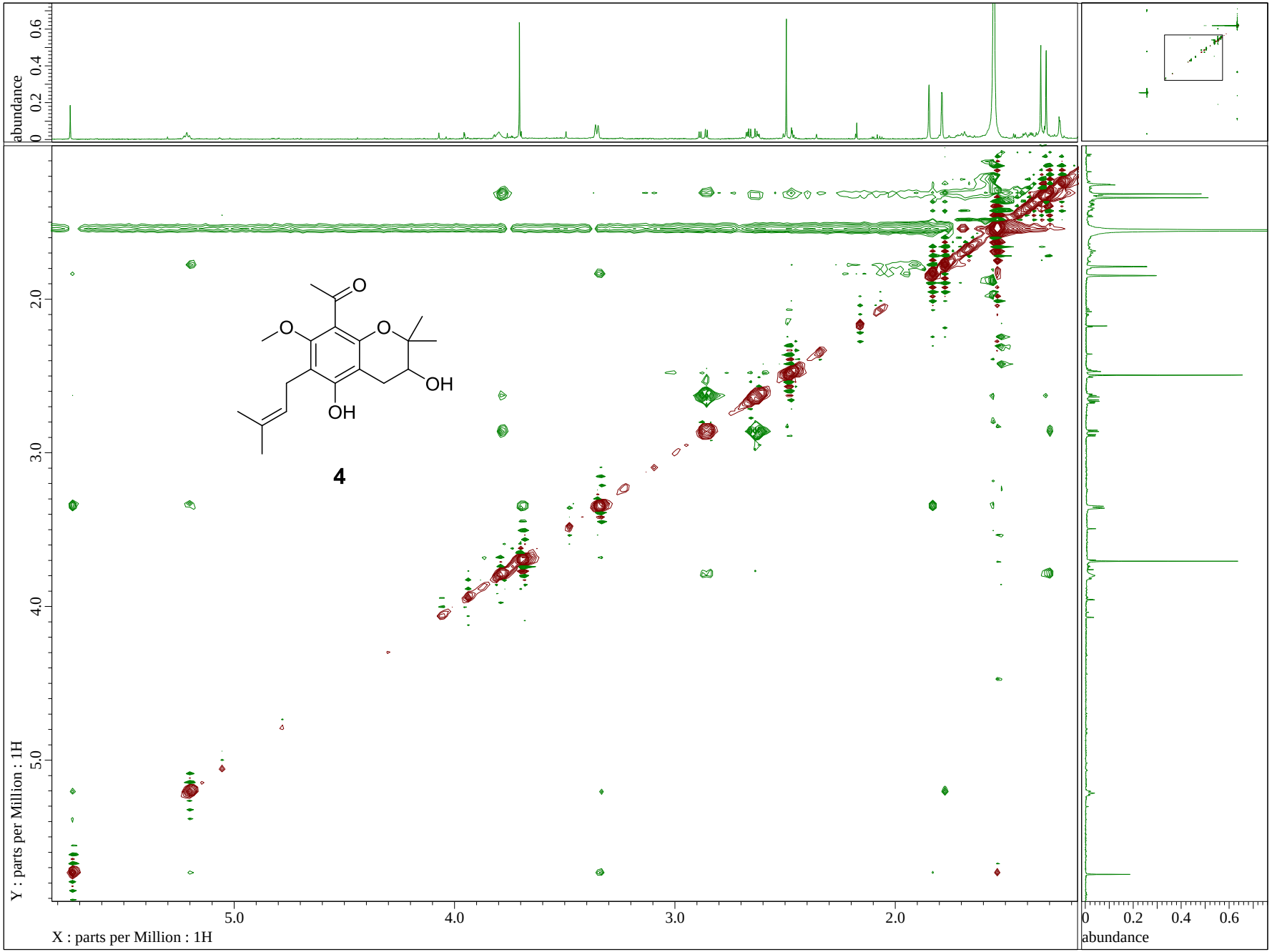


Figure S21. ^{1}H NMR spectrum of 5 (600 MHz, in $CDCl_3$).

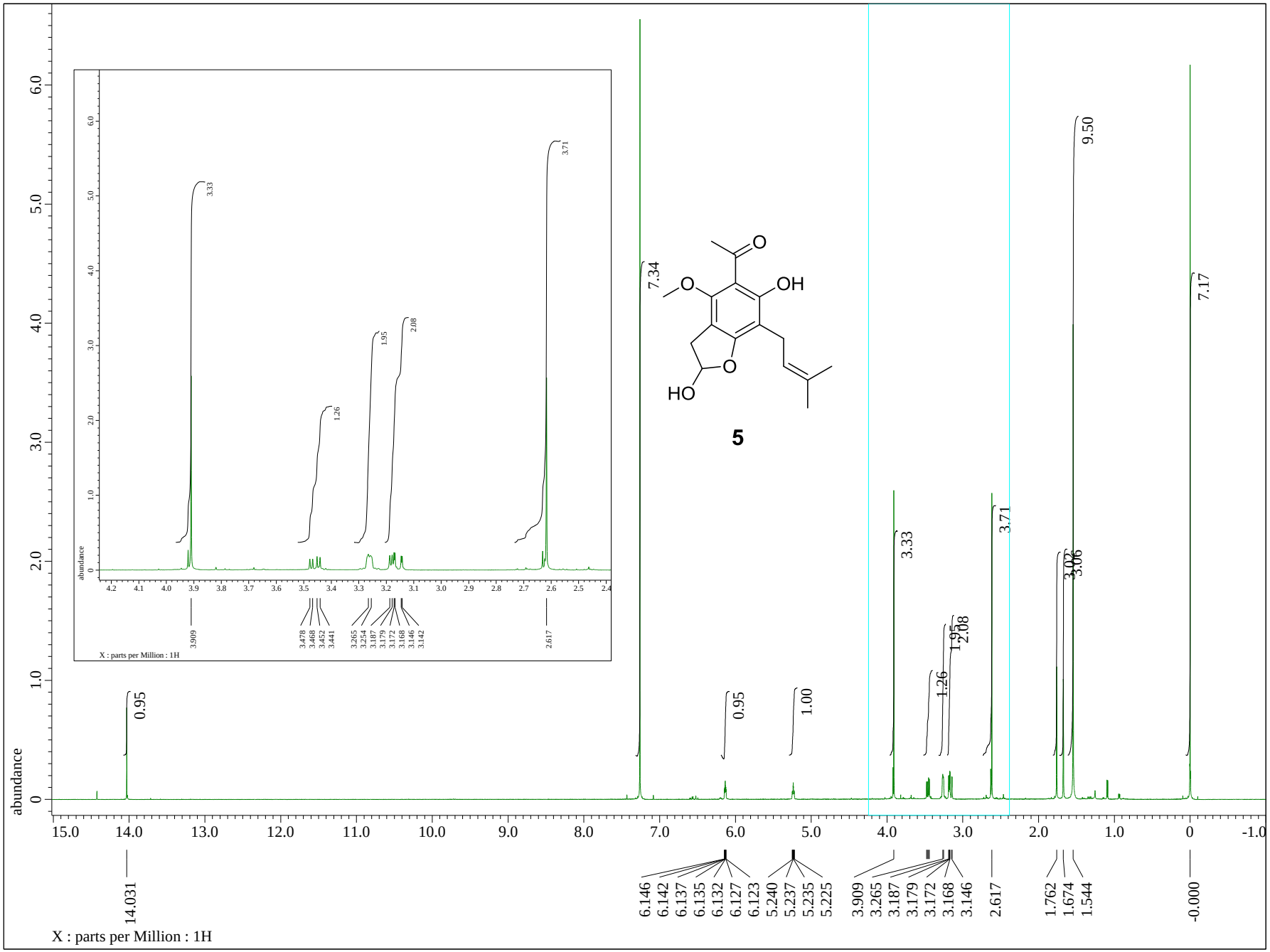


Figure S22. ^{13}C NMR spectrum of **5** (150 MHz, in $CDCl_3$).

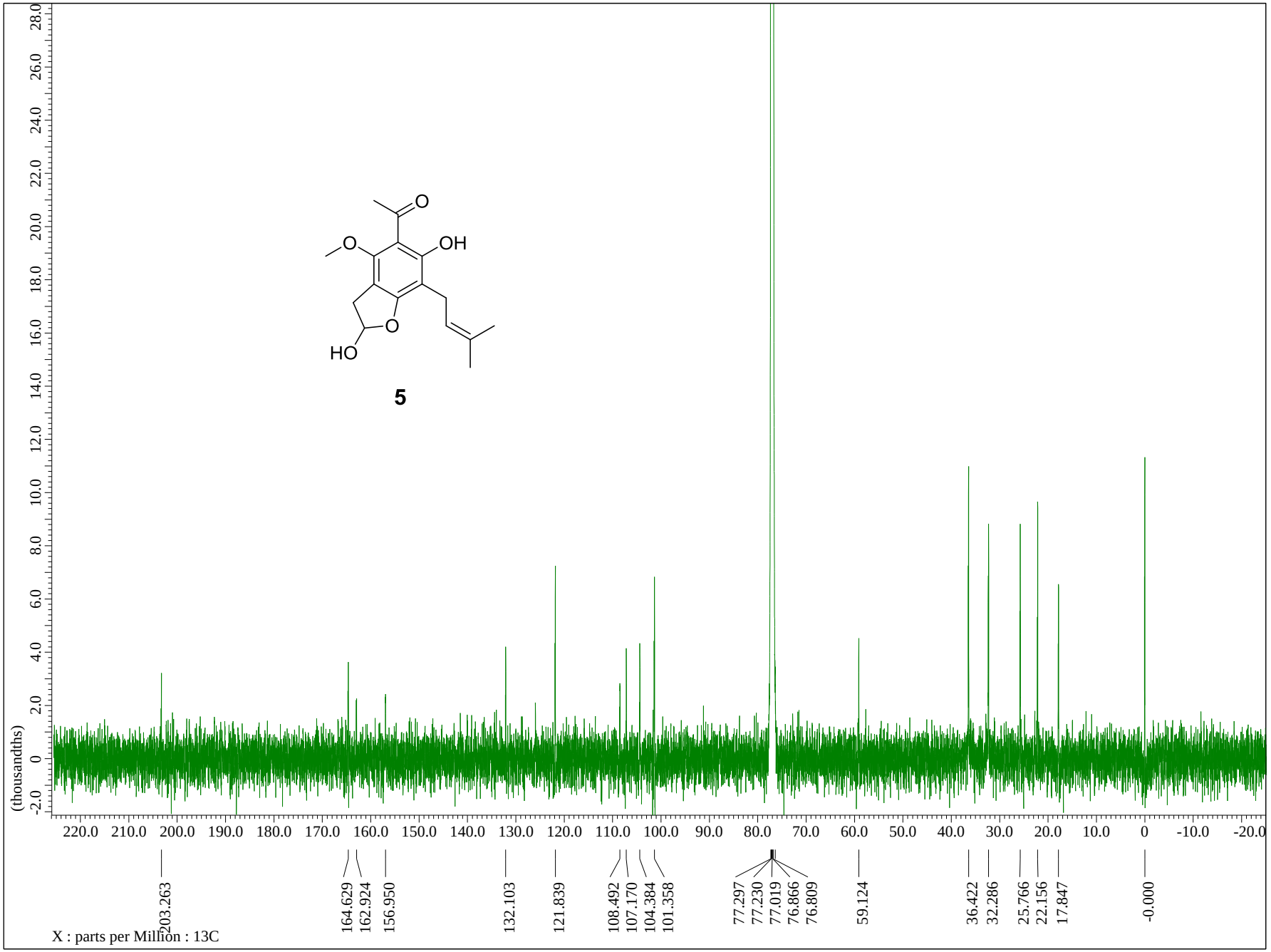


Figure S23. H-H COSY experiment of 5 (in $CDCl_3$).

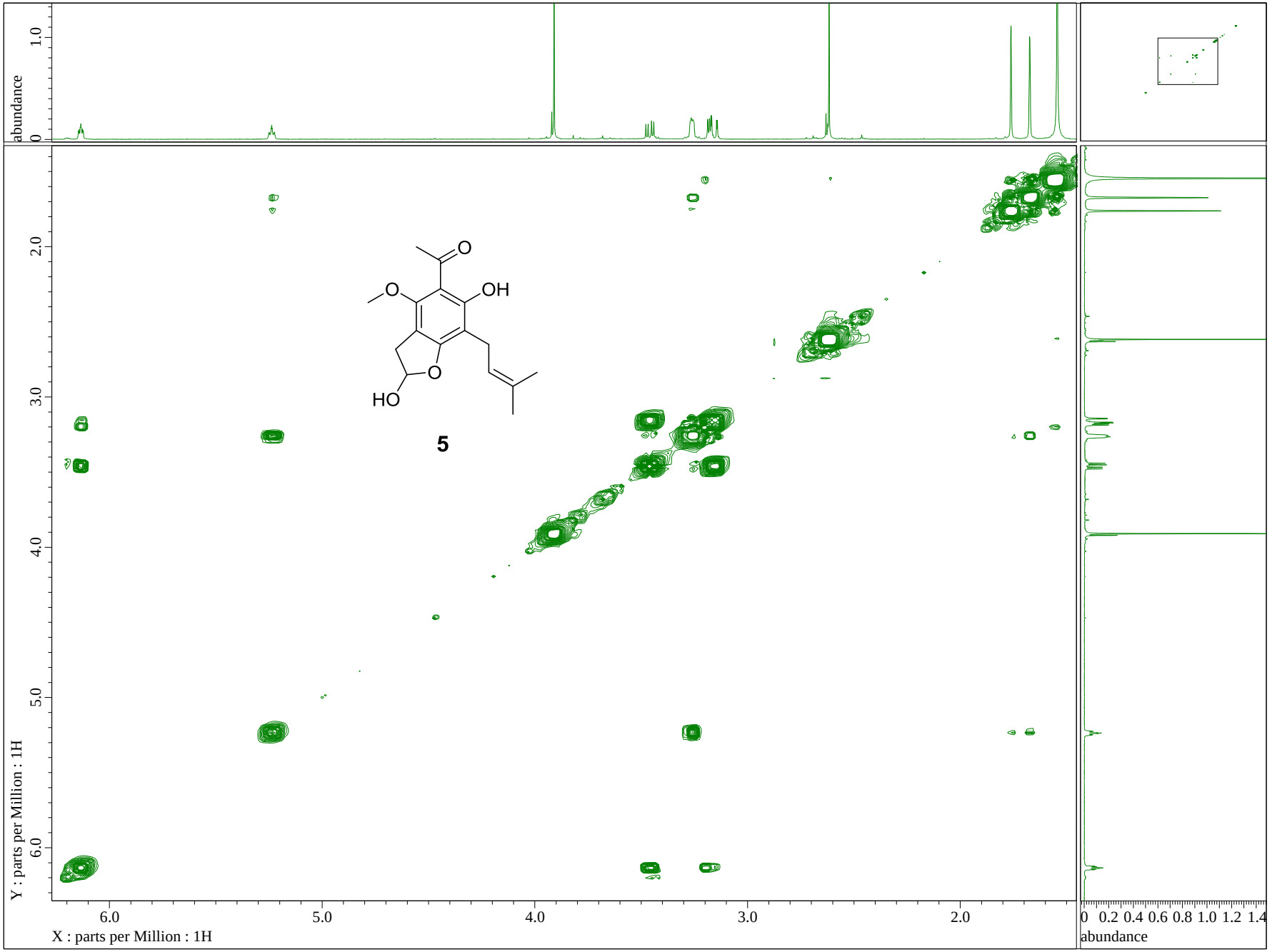


Figure S24. NOESY experiment of 5 (in $CDCl_3$).

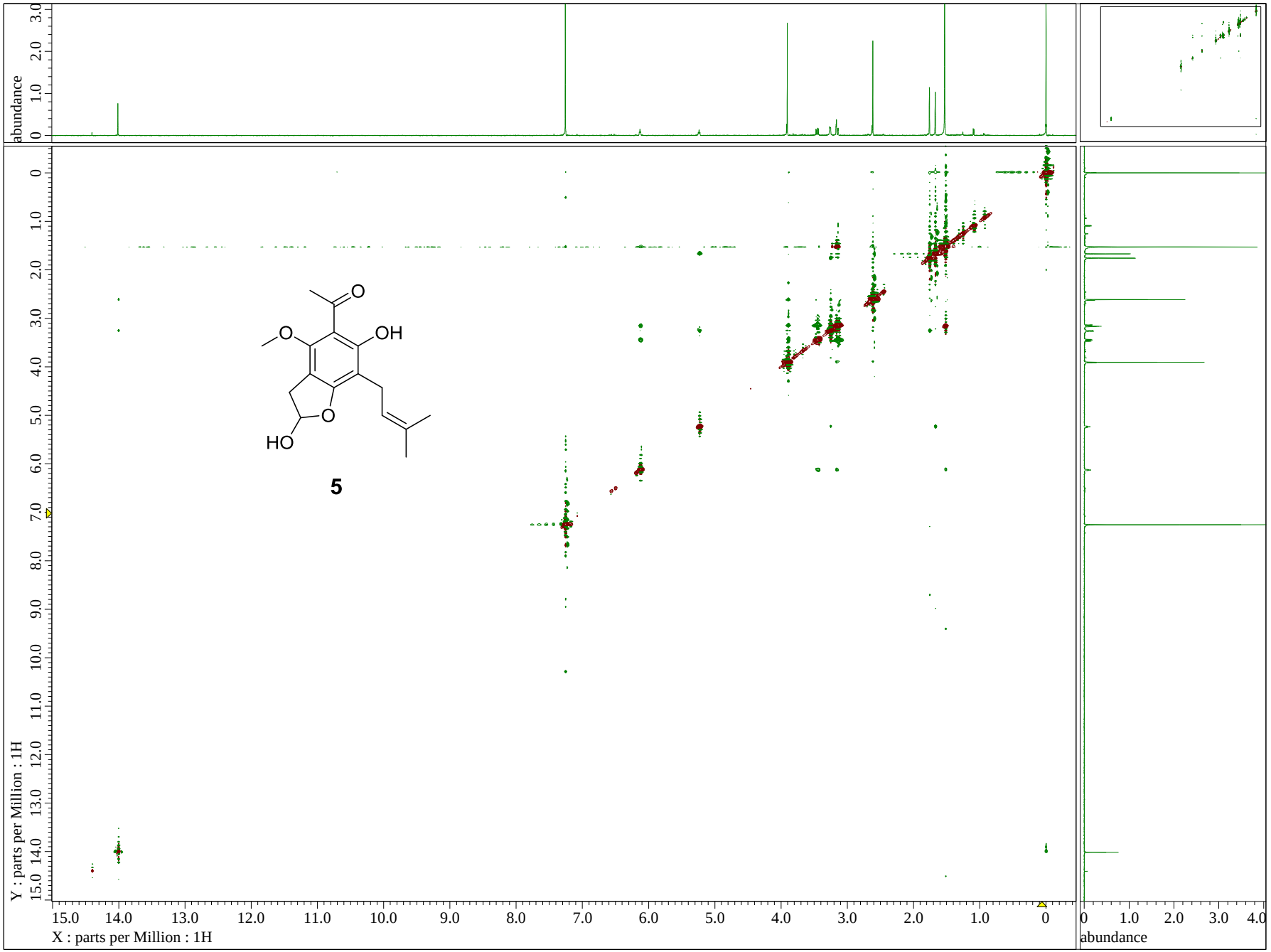


Figure S25. NOESY experiment of 5 (in $CDCl_3$).

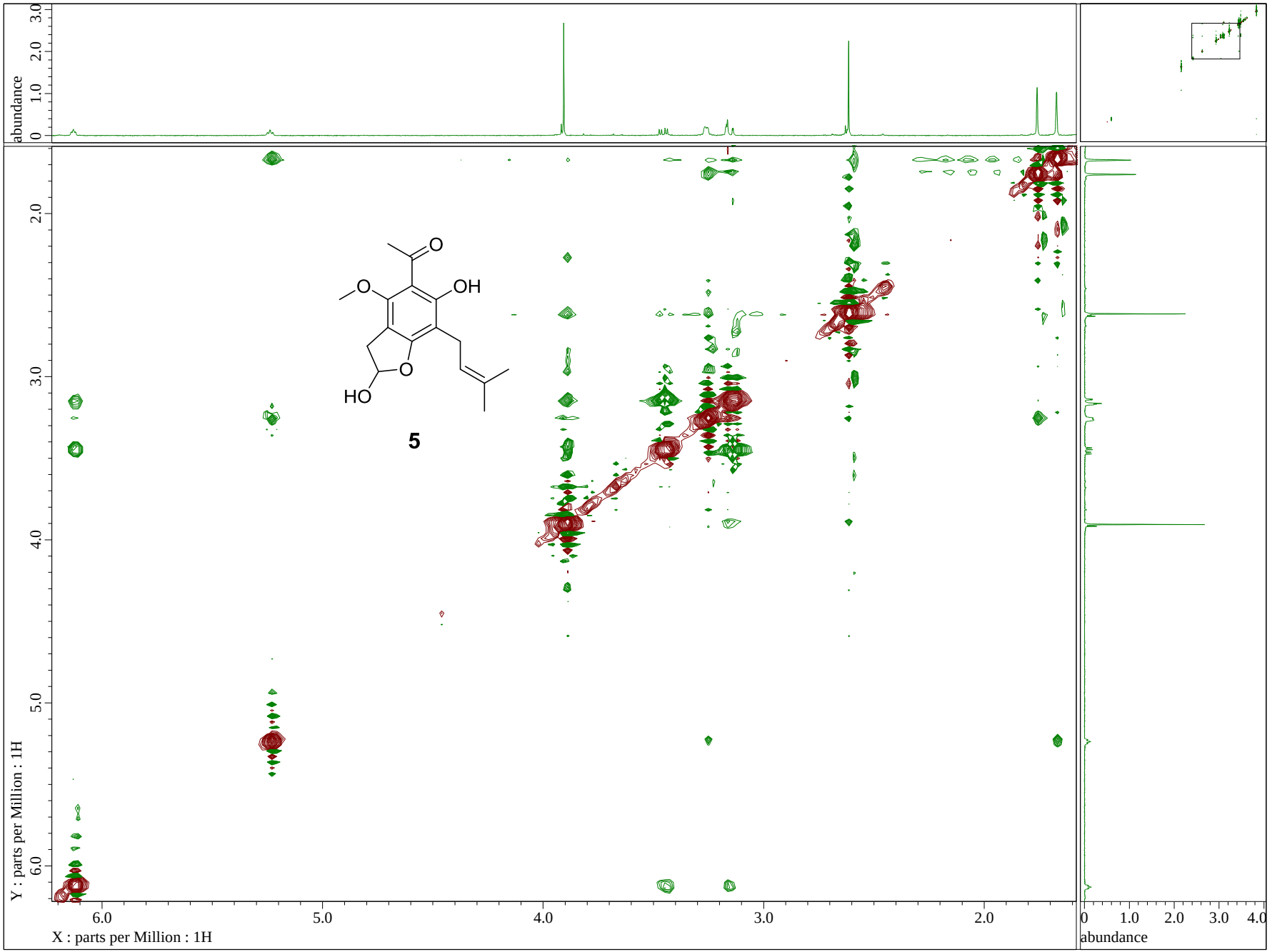


Figure S26. HMQC experiment of 5 (in $CDCl_3$).

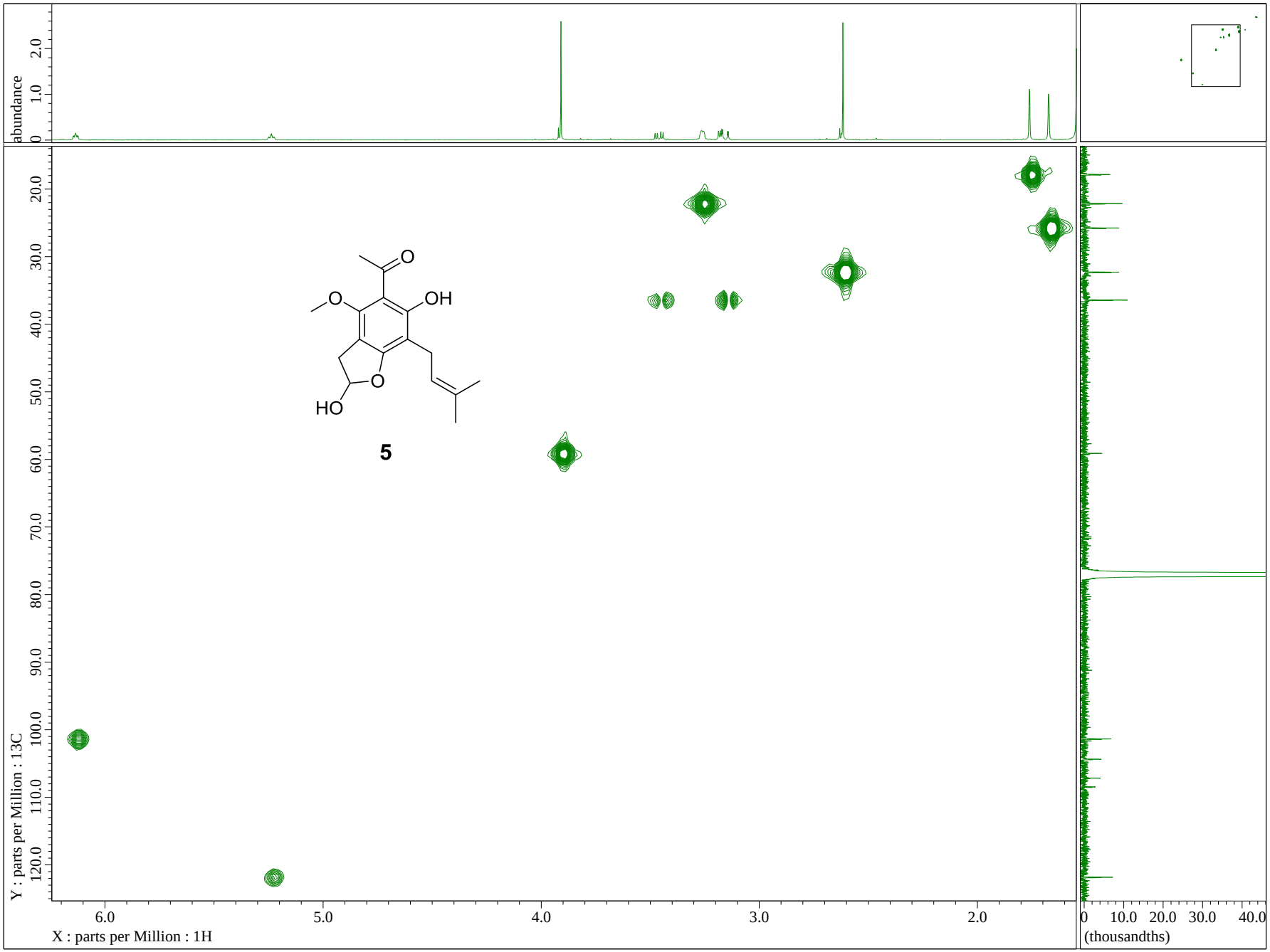


Figure S27. HMBC experiment of 5 (in $CDCl_3$).

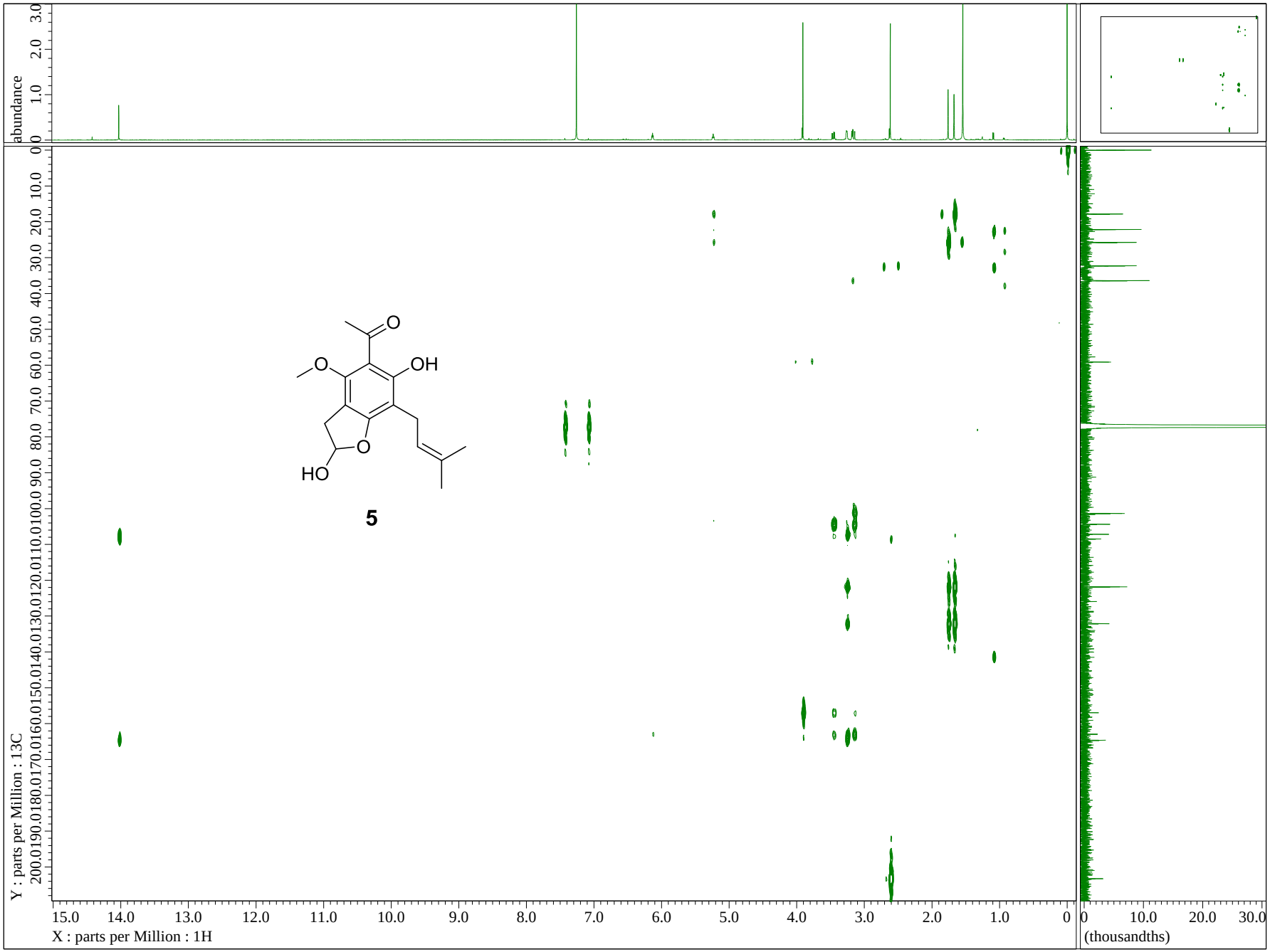


Figure S28. HMBC experiment of 5 (in $CDCl_3$).

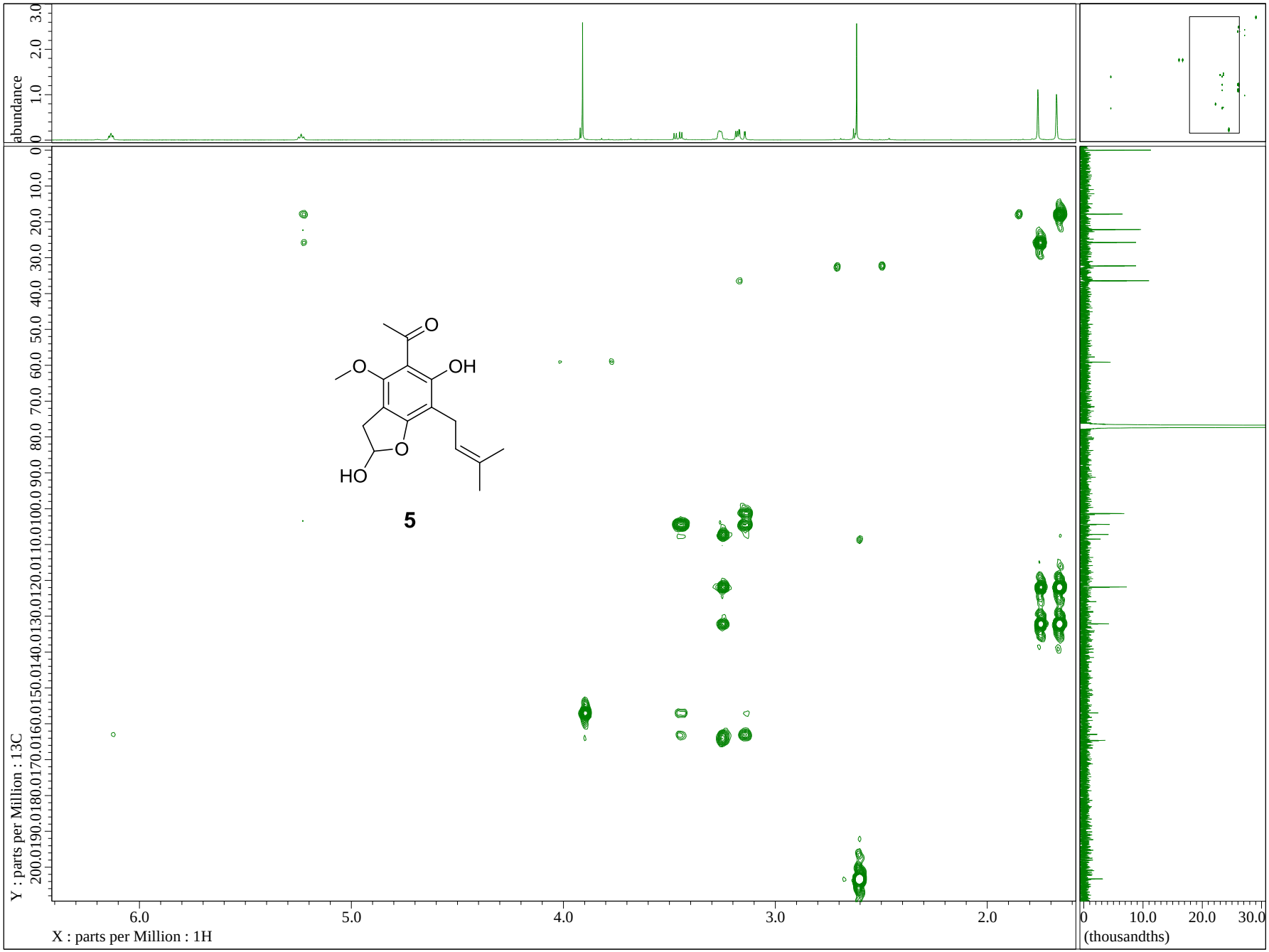


Figure S29. ^{1}H NMR spectrum of 6 (600 MHz, in $CDCl_3$).

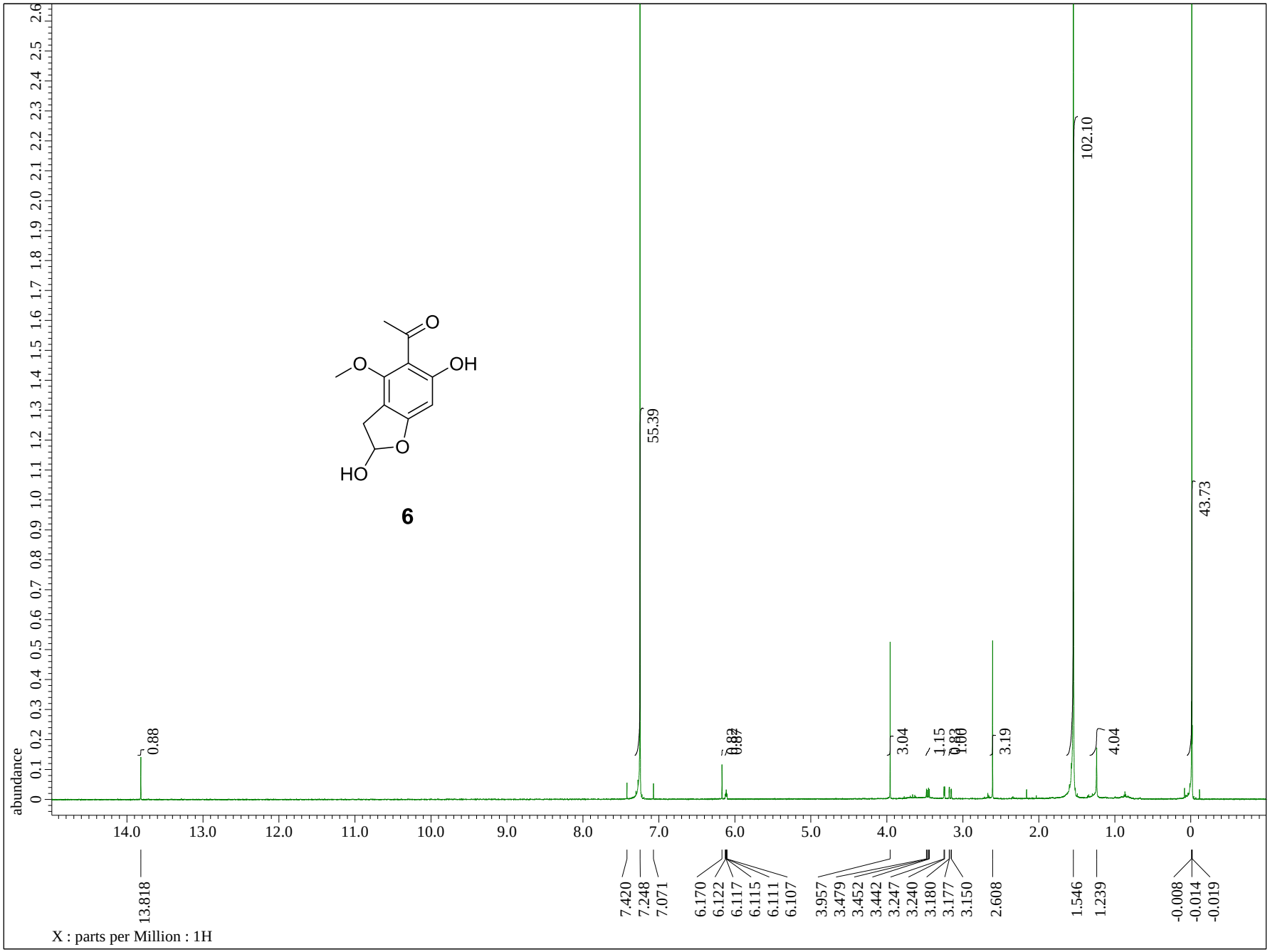


Figure S30. H-H COSY experiment of 6 (in $CDCl_3$).

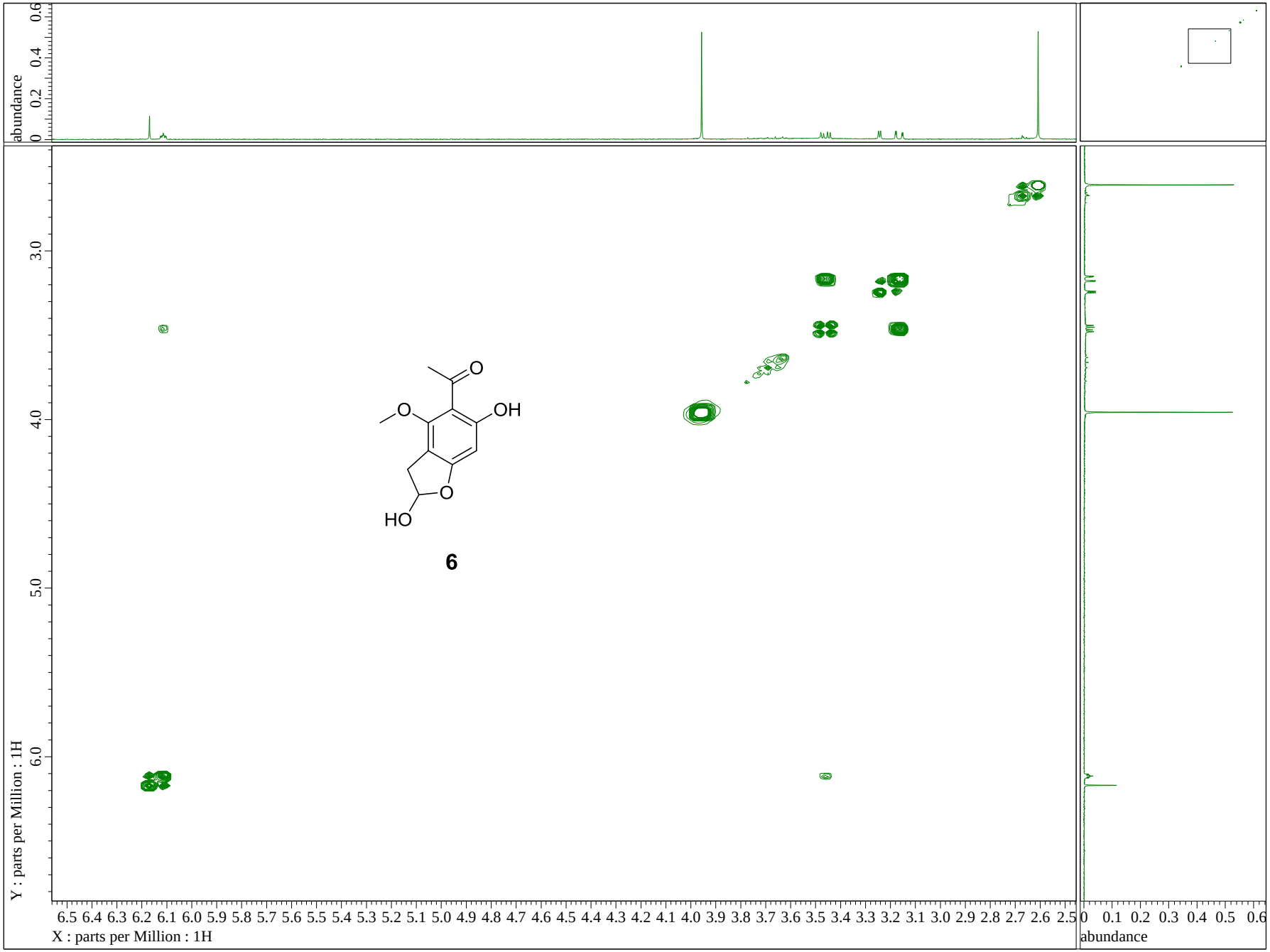


Figure S31. NOESY experiment of 6 (in $CDCl_3$).

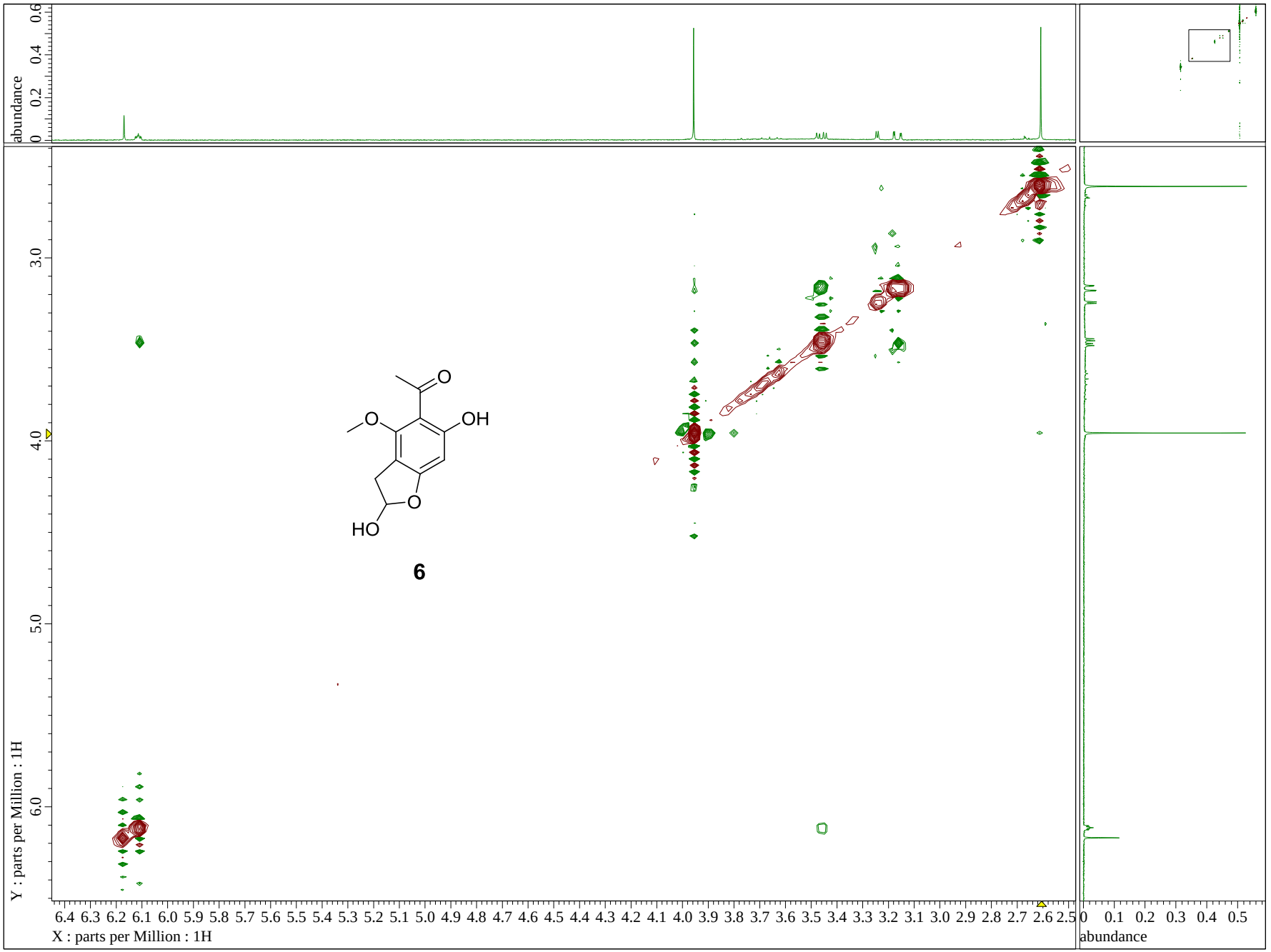


Figure S32. ^{1}H NMR spectrum of 7 (600 MHz, in $CDCl_3$).

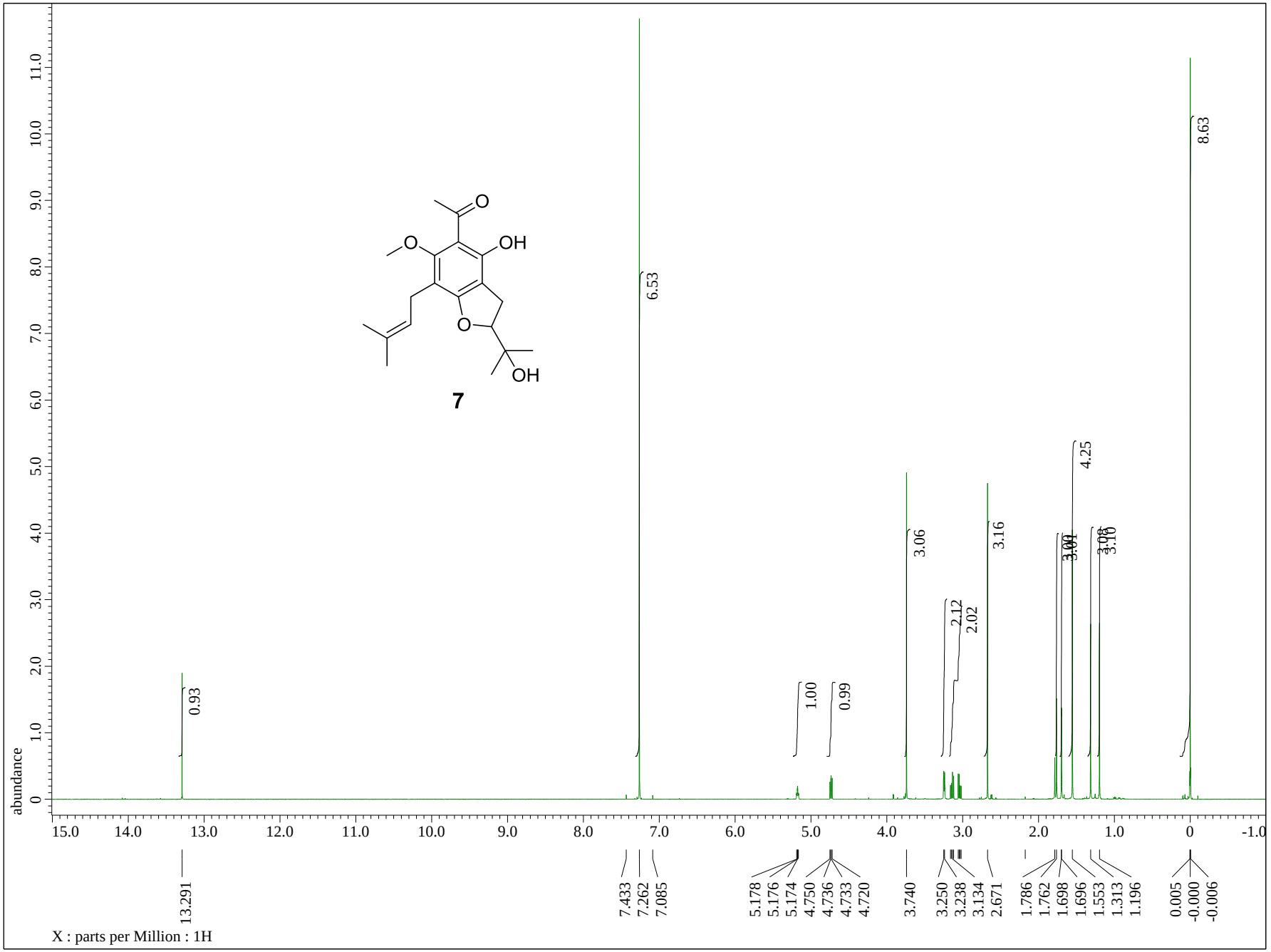


Figure S33. ^{13}C NMR spectrum of 7 (150 MHz, in $CDCl_3$).

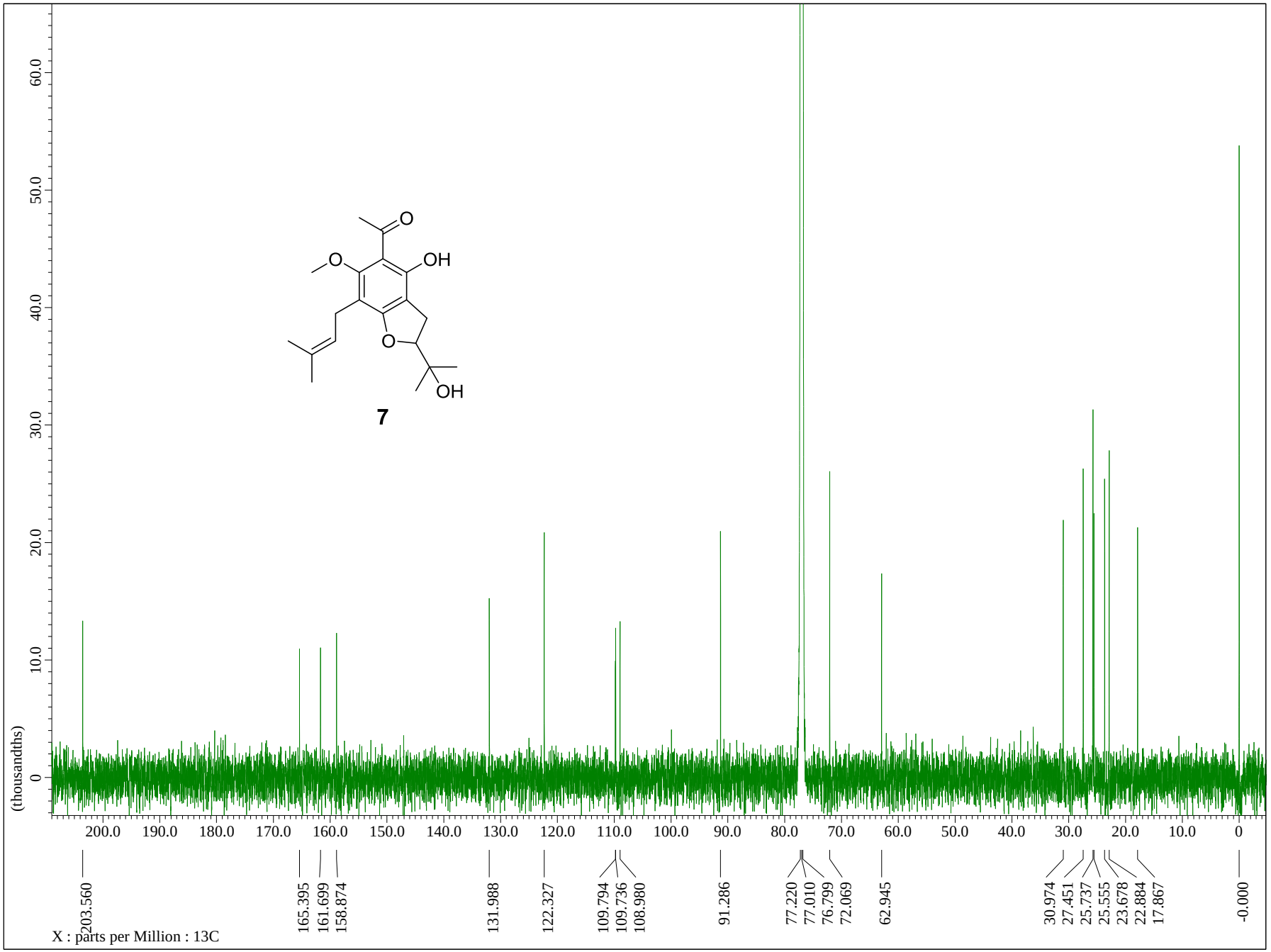


Figure S34. H-H COSY experiment of 7 (in $CDCl_3$).

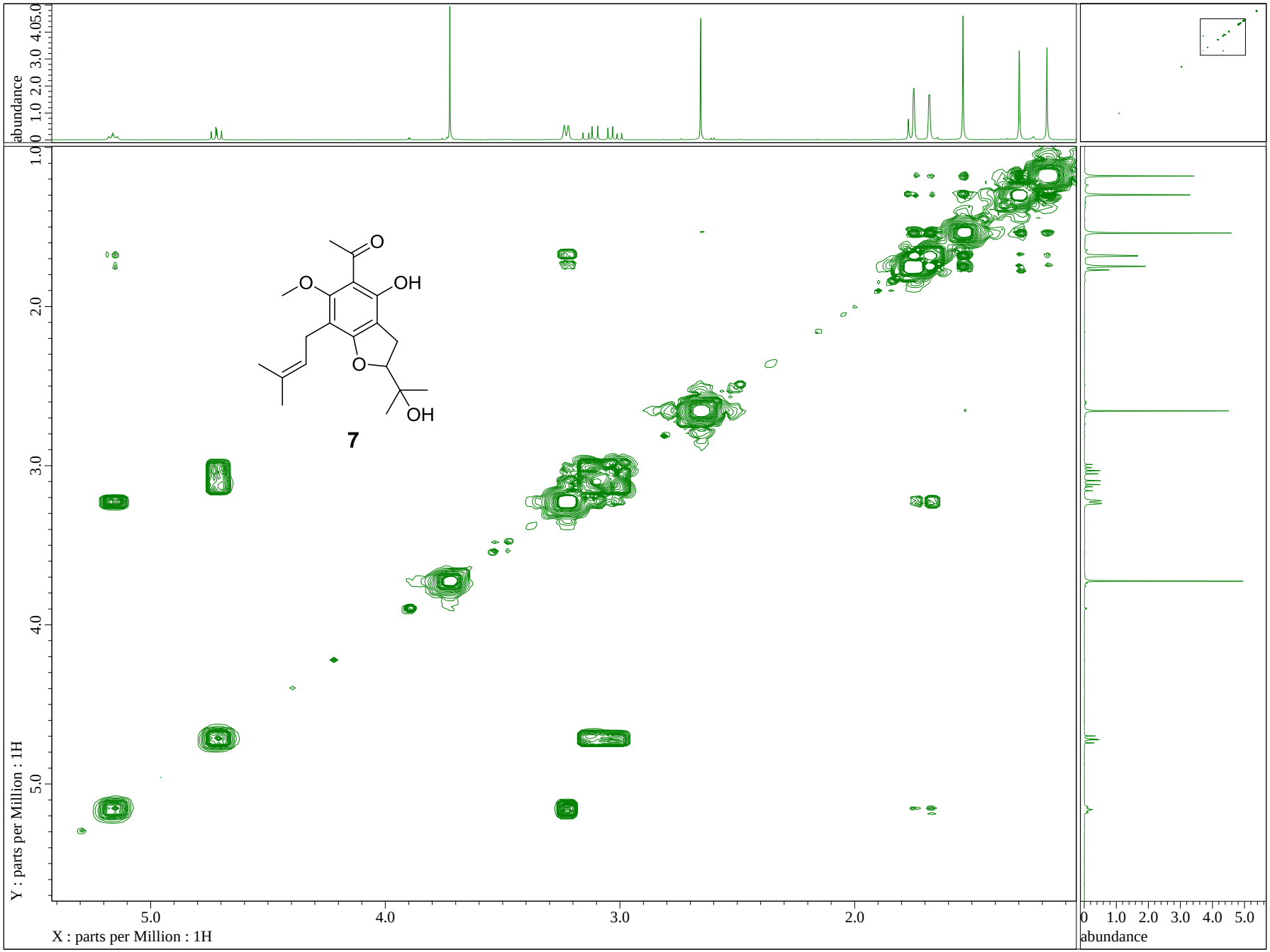


Figure S35. NOESY experiment of 7 (in $CDCl_3$).

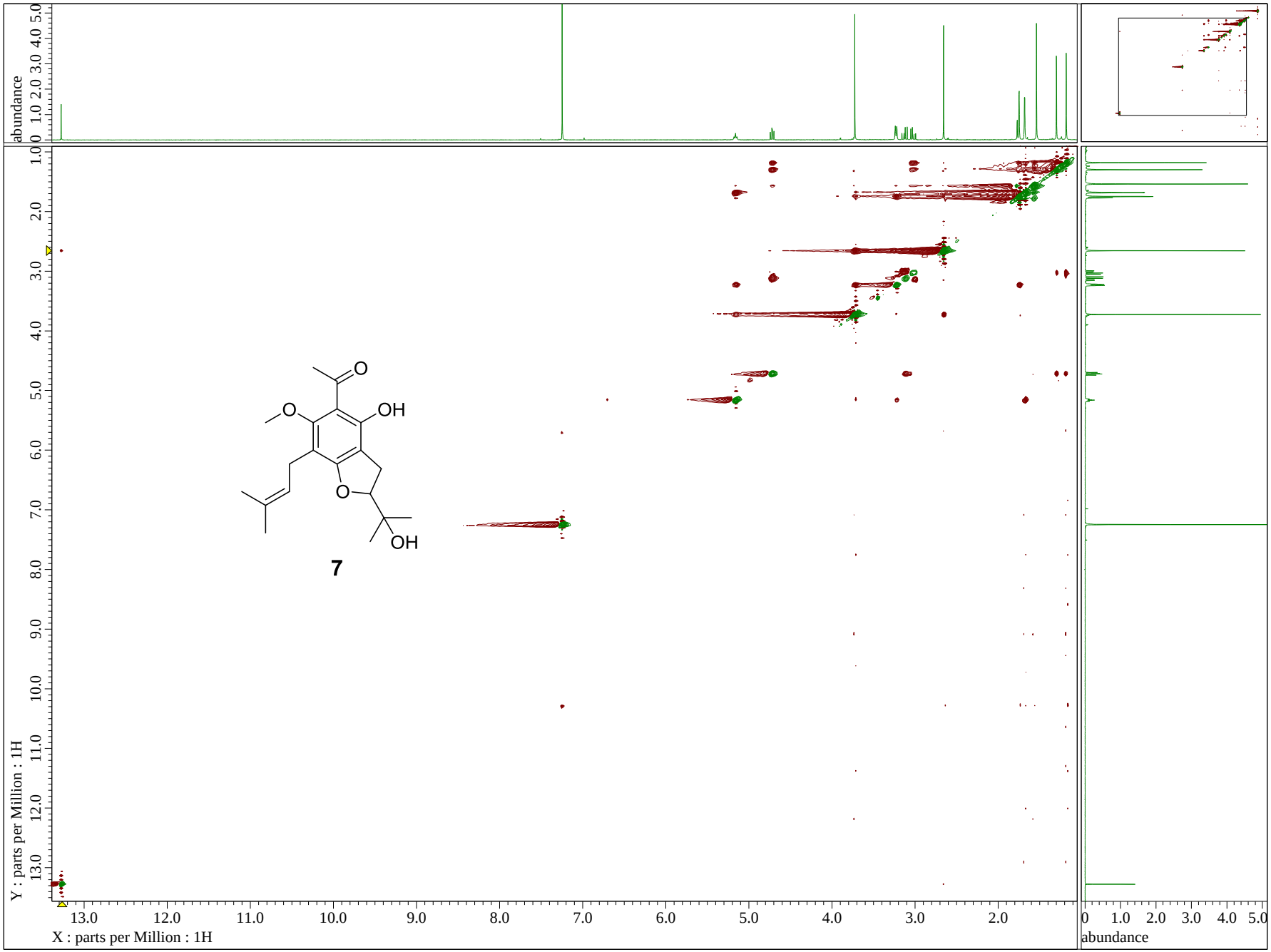


Figure S36. HMQC experiment of 7 (in $CDCl_3$).

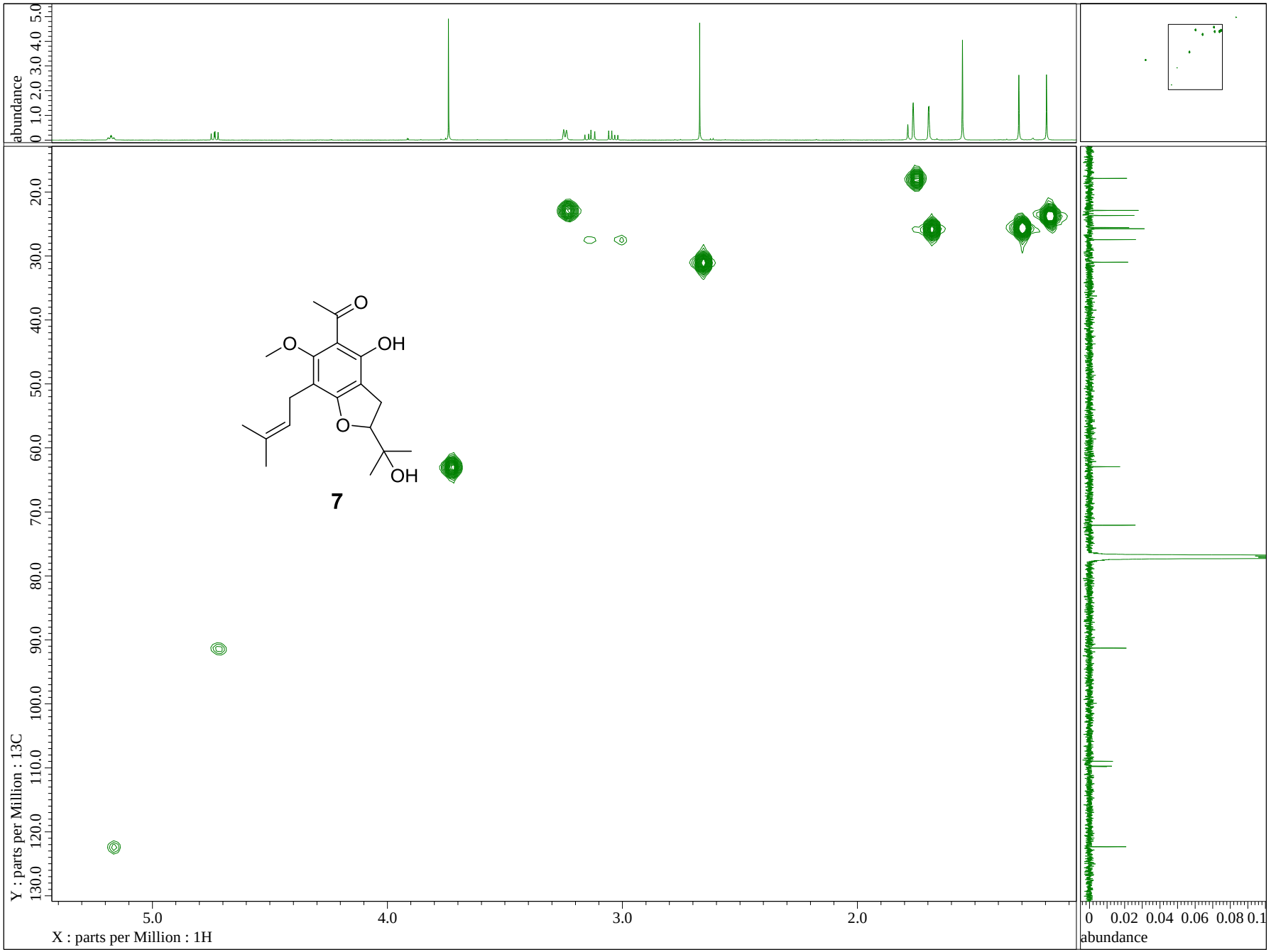


Figure S37. HMBC experiment of 7 (in $CDCl_3$).

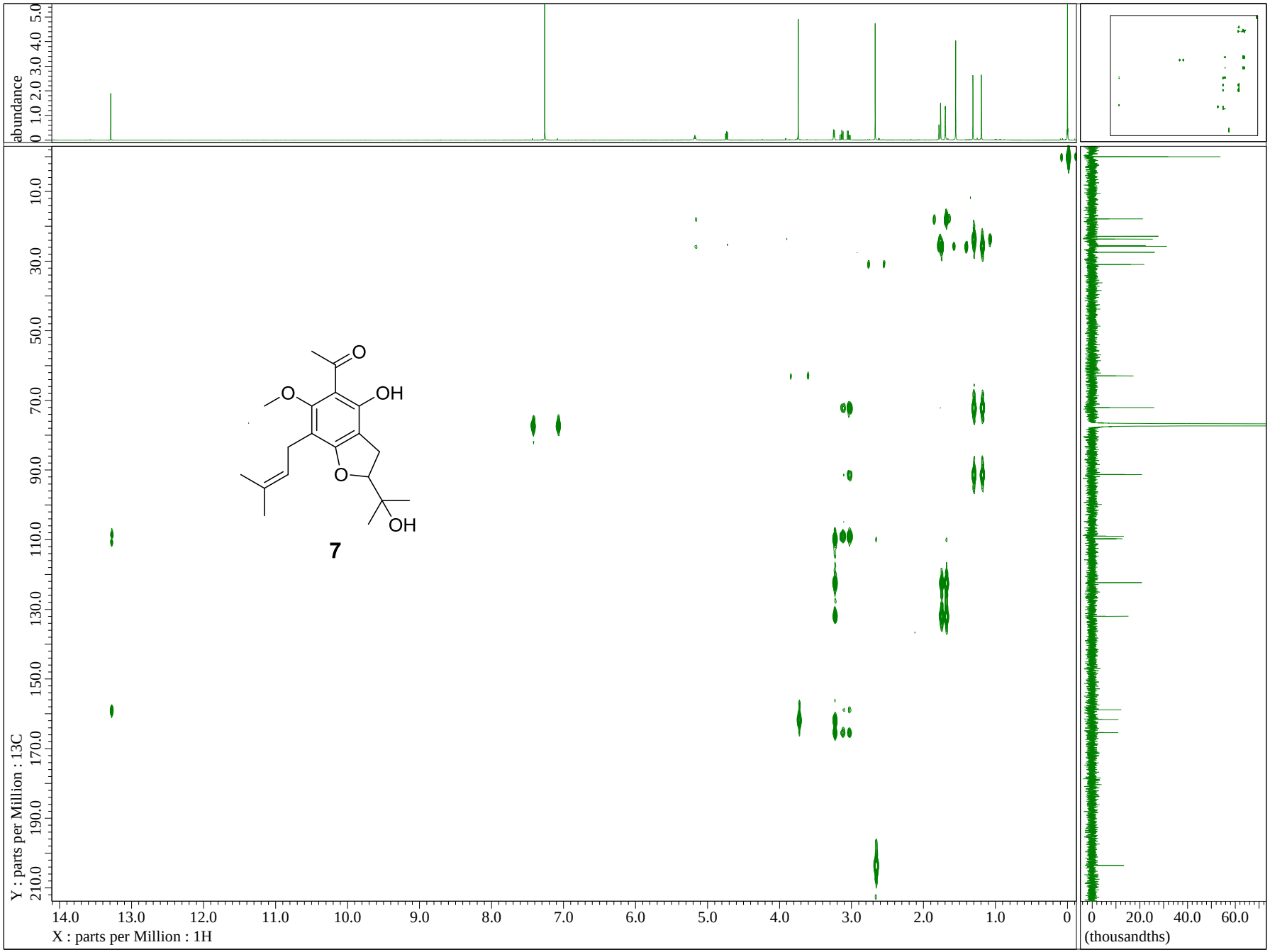


Figure S38. HMBC experiment of 7 (in $CDCl_3$).

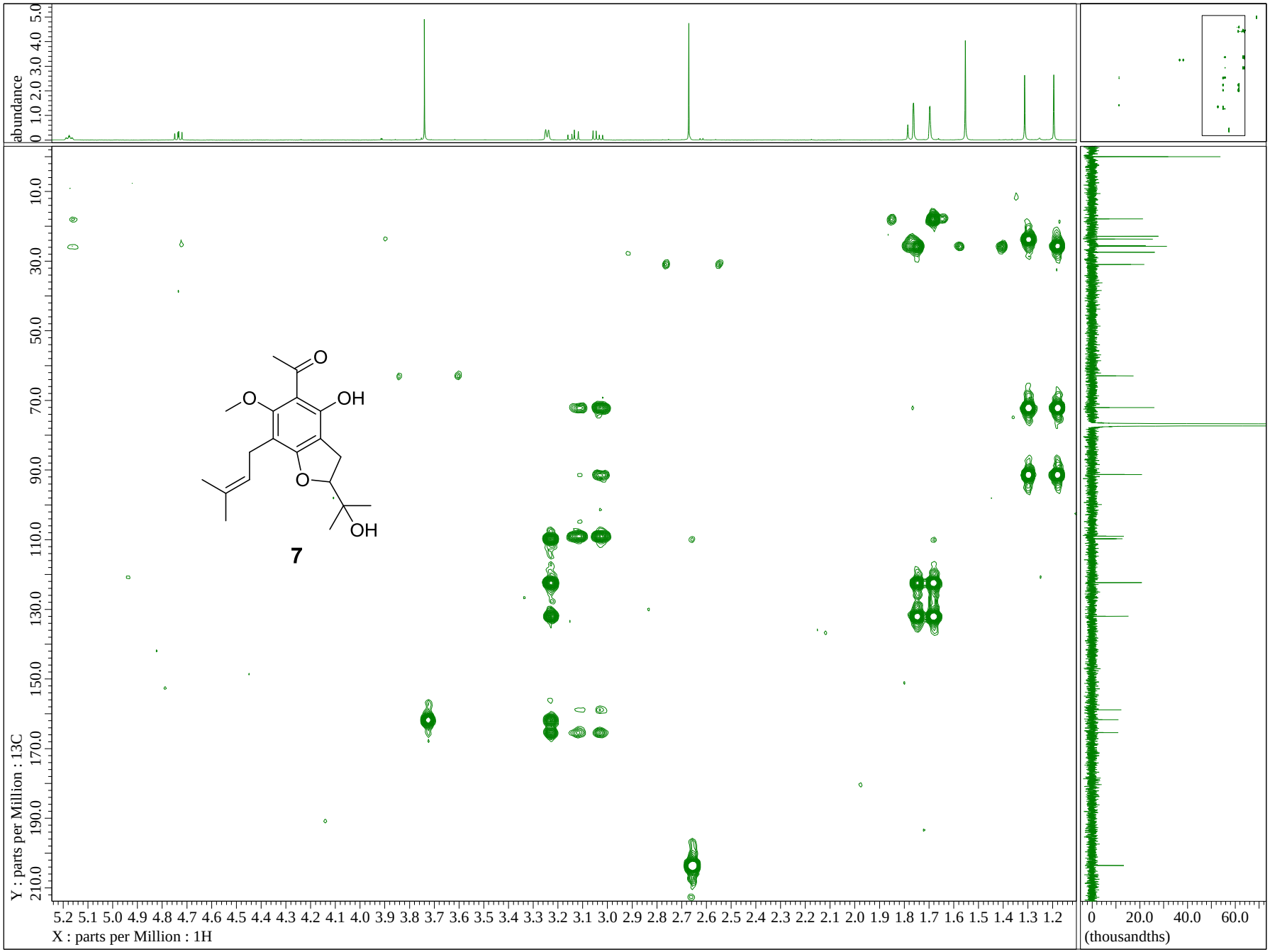


Figure S39. ^{1}H NMR spectrum of 8 (600 MHz, in acetone-d_6).

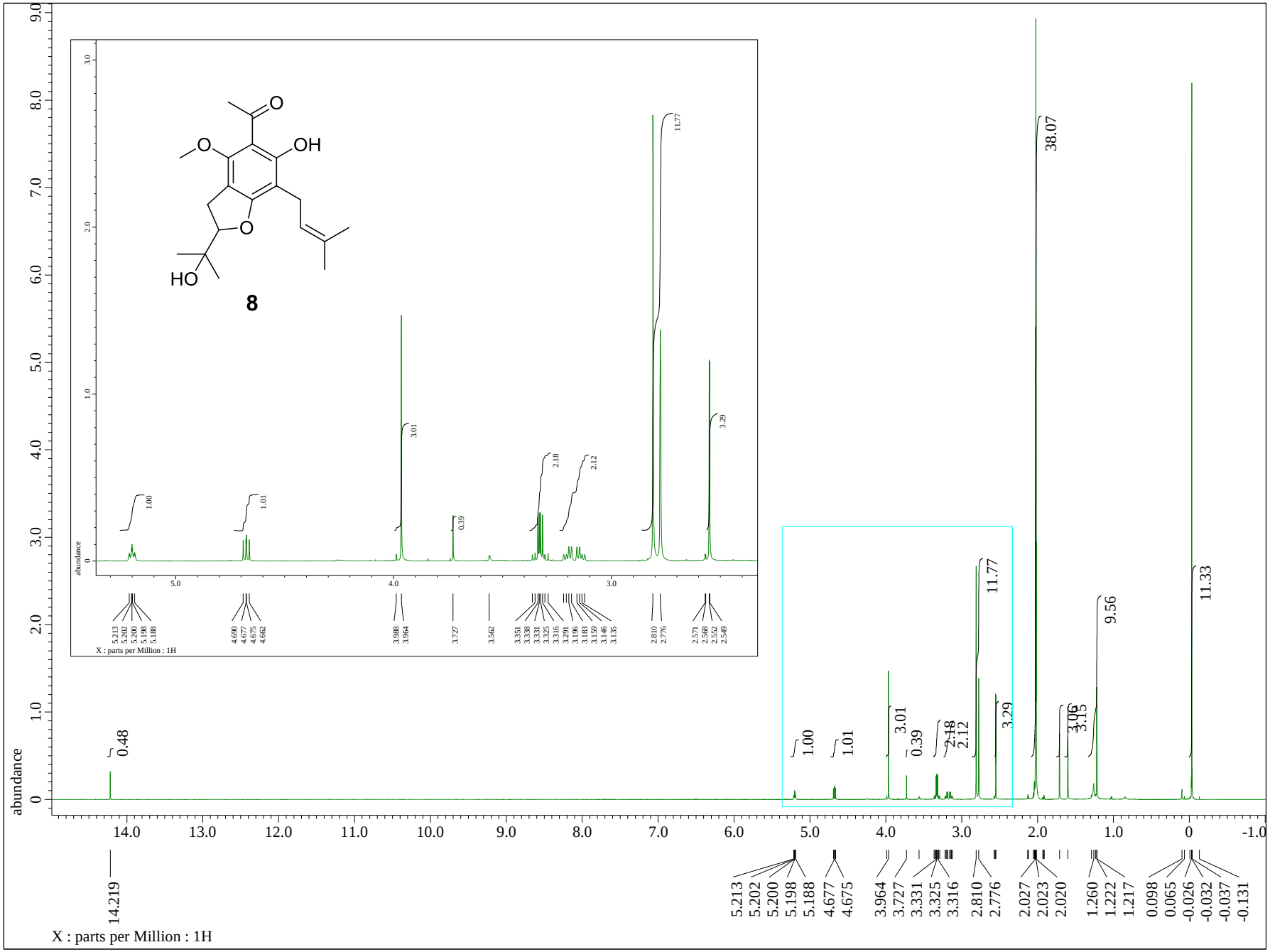


Figure S40. H-H COSY experiment of 8 (in acetone-d_6).

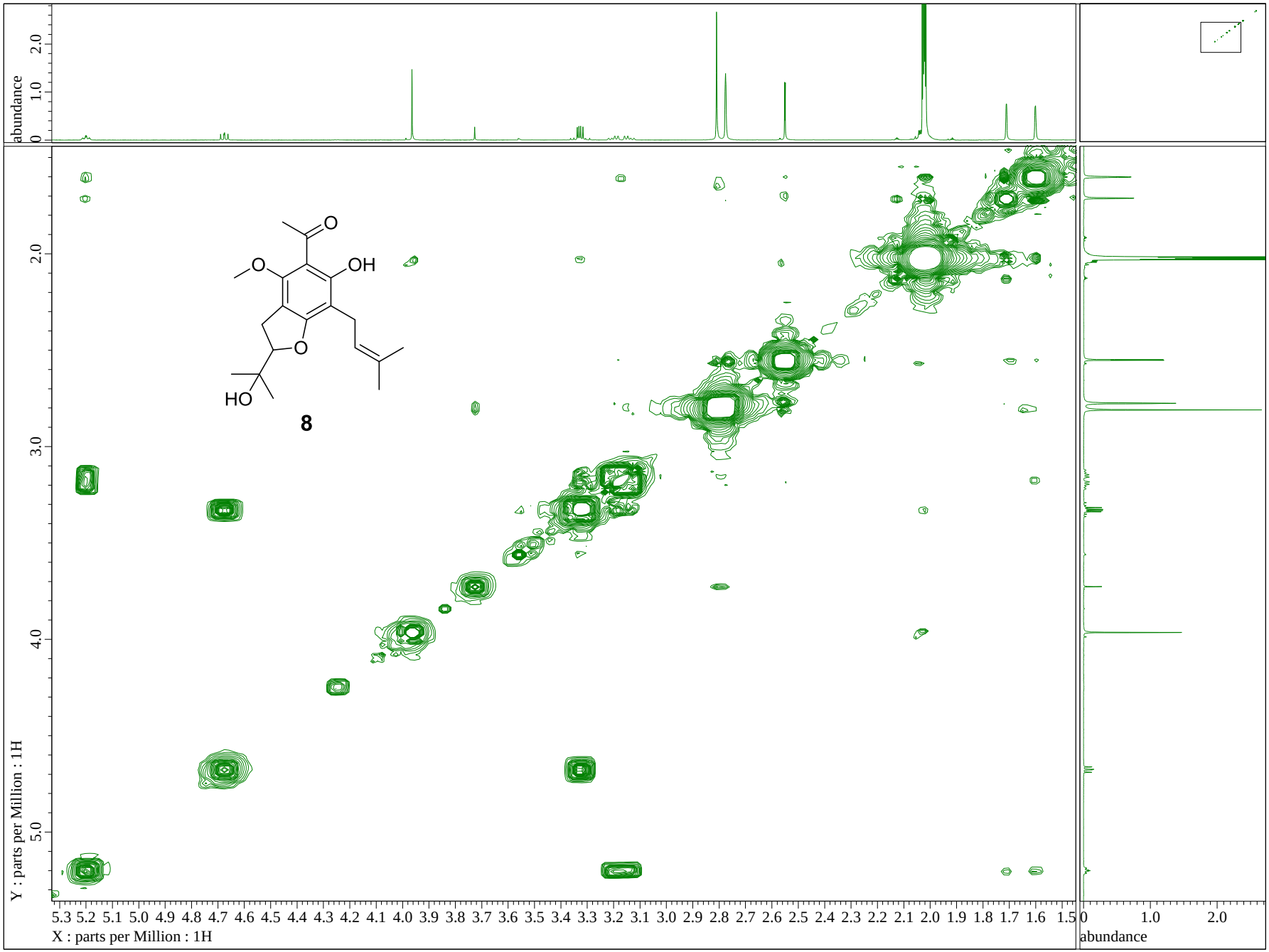


Figure S41. NOESY experiment of 8 (in acetone-d_6).

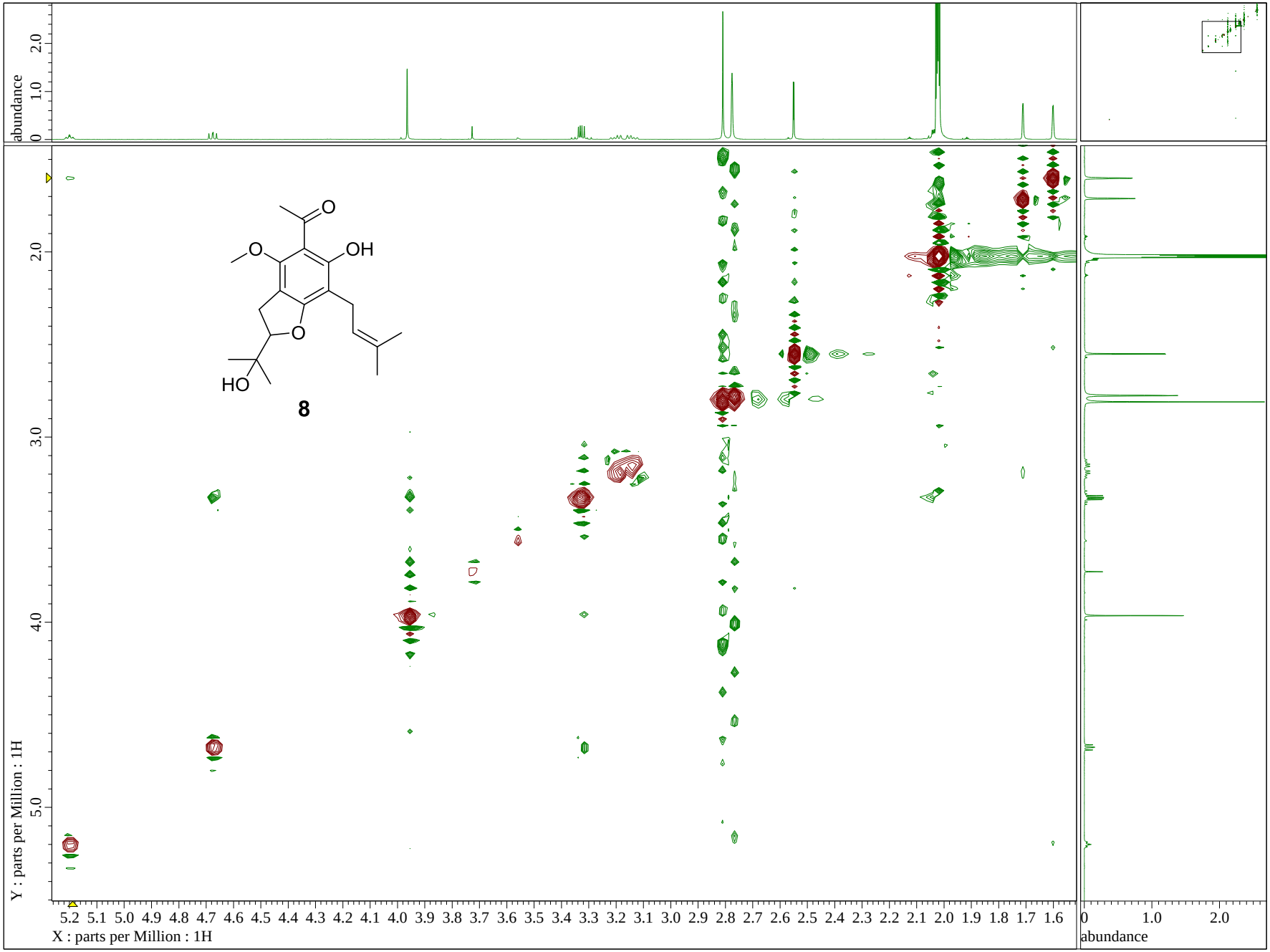
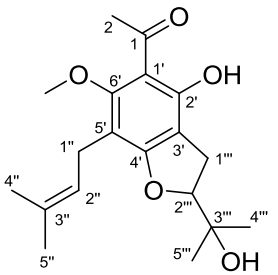


Table S42. ^{1}H and ^{13}C NMR data of 7 and 8.

	7[a]			8[b]			8[a]	
solvent	$CDCl_3$			$CDCl_3$			acetone-d_6	
position	δ_H (*J* in Hz)		δ_C	δ_H (*J* in Hz)		δ_C	δ_H (*J* in Hz)	
1			203.6			203.0		
2	2.67	s	31.0	2.61	s	32.1	2.55	s
1'			109.8			106.5		
2'			158.9			164.7		
3'			109.0			108.2		
4'			165.4			164.8		
5'			109.7			107.1		
6'			161.7			156.7		
1''	3.25	brd (6.4)	22.9	3.26	d (8.0)	22.1	3.31	dd (15.0, 9.0)
							3.34	dd (15.0, 7.2)
2''	5.18	brt (7.6)	122.3	4.64	t (8.0)	90.1	4.68	dd (9.0, 7.8)
3''			132.0			71.8		
4''	1.70	brs	25.7	1.24	s	25.7	1.217	s
5''	1.76	brs	17.9	1.36	s	25.8	1.222	s
1'''	3.04	dd (15.6, 8.0)	27.5	3.22	d (6.6)	28.9	3.14	dd (14.4, 7.8)
	3.14	dd (15.2, 10.0)					3.20	dd (14.4, 7.8)
2'''	4.74	t (10.0)	91.3	5.24	t (6.6)	121.9	5.20	t (7.5)
3'''			72.1			131.7		
4'''	1.20	s	23.7	1.67	s	25.7	1.60	brs
5'''	1.31	s	25.6	1.76	s	17.8	1.71	brs
MeO	3.74	s	62.9	3.90	s	59.1	3.96	s
OH	13.30	s		14.52	s		14.21	s

[a] Measured at 600 MHz for ^{1}H NMR and 150 MHz for ^{13}C NMR. [b] Ref. 3.



7

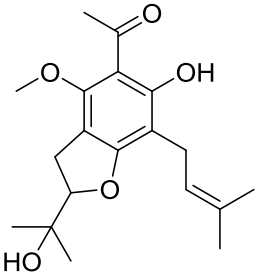


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Figure S43. HRFABMS data of 1.

Data : 分子生薬学（後藤）234　　Date : 05-Feb-2016 15:34
Instrument : MStation
Sample : 14AS_mm4
Note : NBA
Inlet : Direct　　Ion Mode : FAB+
RT : 2.35 min　　Scan# : 22
Elements : C 19/0, H 27/0, O 5/0
Mass Tolerance　　: 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
Unsaturation (U.S.) : -0.5 - 20.0

	Observed m/z	Int%					
	335.1845	100.00					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O	
1	335.1858	-4.0 / -1.3	6.5	19	27	5	

Figure S44. HRFABMS data of 2.

Data : 分子生薬学（後藤）235　　Date : 05-Feb-2016 15:40
Instrument : MStation
Sample : 14AS_mm5
Note : NBA
Inlet : Direct　　Ion Mode : FAB+
RT : 2.46 min　　Scan# : 23
Elements : C 19/0, H 29/0, O 5/0
Mass Tolerance　　: 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
Unsaturation (U.S.) : -0.5 - 20.0

	Observed m/z	Int%					
	337.2012	100.00					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O	
1	337.2015	-0.9 / -0.3	5.5	19	29	5	

Figure S45. HRFABMS data of 3.

Data : 分子生薬学（後藤）237　　Date : 05-Feb-2016 15:53
Instrument : MStation
Sample : 14AS_mm9
Note : NBA
Inlet : Direct　　Ion Mode : FAB+
RT : 2.24 min　　Scan# : 21
Elements : C 19/0, H 27/0, O 5/0
Mass Tolerance　　: 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
Unsaturation (U.S.) : -0.5 - 20.0

	Observed m/z	Int%					
	335.1850	100.00					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O	
1	335.1858	-2.5 / -0.8	6.5	19	27	5	

Figure S46. HRFABMS data of 4.

Data : 分子生薬学（後藤）236　　Date : 05-Feb-2016 15:47
Instrument : MStation
Sample : 14AS_mm6
Note : NBA
Inlet : Direct　　Ion Mode : FAB+
RT : 2.02 min　　Scan# : 19
Elements : C 19/0, H 27/0, O 5/0
Mass Tolerance　　: 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
Unsaturation (U.S.) : -0.5 - 20.0

	Observed m/z	Int%					
	335.1828	100.00					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O	
1	335.1858	-9.1 / -3.0	6.5	19	27	5	

Figure S47. HRFABMS data of 5.

Data : 分子生薬学（後藤）238　　Date : 05-Feb-2016 16:00
Instrument : MStation
Sample : 14AS_mm3
Note : NBA
Inlet : Direct　　Ion Mode : FAB+
RT : 2.83 min　　Scan# : 24
Elements : C 16/0, H 21/0, O 5/0
Mass Tolerance　　: 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
Unsaturation (U.S.) : -0.5 - 20.0

	Observed m/z	Int%					
	293.1392	100.00					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O	
1	293.1389	+1.0 / +0.3	6.5	16	21	5	

Figure S48. HRFABMS data of 6.

Data : 分子生薬学（後藤）173　　Date : 04-Jun-2015 13:27
Instrument : MStation
Sample : 15YK44C
Note : NBA
Inlet : Direct　　Ion Mode : FAB+
RT : 3.95 min　　Scan# : 26
Elements : C 11/0, H 38/0, O 5/0
Mass Tolerance　　: 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
Unsaturation (U.S.) : -0.5 - 10.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	225.0764	100.00	+0.5 / +0.1	5.5	C11 H13 O5

Figure S49. HRFABMS data of 7.

Data : 分子生薬学（後藤）233　　Date : 05-Feb-2016 15:27
Instrument : MStation
Sample : 14AS_mm2
Note : NBA
Inlet : Direct　　Ion Mode : FAB+
RT : 2.13 min　　Scan# : 20
Elements : C 19/0, H 27/0, O 5/0
Mass Tolerance　　: 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
Unsaturation (U.S.) : -0.5 - 20.0

Observed m/z	Int%
335.1845	100.00

	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	335.1858	-4.0 / -1.3	6.5	19	27	5

Figure S50. HRFABMS data of 8.

Data : 分子生薬学（後藤）240　　Date : 24-Feb-2016 13:59
Instrument : MStation
Sample : 14AS_mm1
Note : NBA
Inlet : Direct　　Ion Mode : FAB+
RT : 2.35 min　　Scan# : 22
Elements : C 19/0, H 27/0, O 5/0
Mass Tolerance　　: 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
Unsaturation (U.S.) : -0.5 - 20.0

Observed m/z	Int%
335.1814	100.00

	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	335.1858	-13.3 / -4.4	6.5	19	27	5

Table 51. Optical Rotations of 1–4, 7 and 8

*Acronyculatin I (**1**)*. $[\alpha]_D^{21}$ −2.7 (*c* 0.06, CH_3OH)

*Acronyculatin J (**2**)*. $[\alpha]_D^{21}$ +8.4 (*c* 0.02, CH_3OH).

*Acronyculatin K (**3**)*. $[\alpha]_D^{21}$ +2.0 (*c* 0.03, CH_3OH).

*Acronyculatin L (**4**)*. $[\alpha]_D^{21}$ −7.4 (*c* 0.03, CH_3OH).

*Acronyculatin O (**7**)*. $[\alpha]_D^{21}$ +0.7 (*c* 0.06, CH_3OH).

*Acronyculatin B (**8**)*. $[\alpha]_D^{21}$ +2.7 (*c* 0.04, CH_3OH).