

Appendix

Table of Contents

Table S1. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound 1 in acetone- d_6 compared to the reported NMR data ¹ (δ in ppm, J in Hz).....	3
Table S2. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound 2 in acetone- d_6 and CDCl_3 compared to the reported NMR data ² in CDCl_3 (δ in ppm, J in Hz)	4
Table S3. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound 3 in acetone- d_6 and CDCl_3 compared to the reported NMR data ² in CDCl_3 (δ in ppm, J in Hz)	5
Table S4. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound 4 in acetone- d_6 and CDCl_3 compared to the reported NMR data ³ in CDCl_3 (δ in ppm, J in Hz)	6
Table S5. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound 6 in acetone- d_6 and CDCl_3 compared to the reported NMR data ² in CDCl_3 (δ in ppm, J in Hz)	7
Table S6. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound 6 in CD_3OD compared to the reported NMR data ⁴ in acetone- d_6 (δ in ppm, J in Hz)	8
Table S7. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound 7 in acetone- d_6 compared to the reported NMR data ⁵ (δ in ppm, J in Hz).....	9
References	9
Figure S1. ^1H NMR spectrum of nordihydroguaiaretic acid (1) in $(\text{CD}_3)_2\text{CO}$	10
Figure S2. ^{13}C NMR spectrum of nordihydroguaiaretic acid (1) in $(\text{CD}_3)_2\text{CO}$	11
Figure S3. HMQC NMR spectrum of nordihydroguaiaretic acid (1) in $(\text{CD}_3)_2\text{CO}$	12
Figure S4. ^1H NMR spectrum of 3'- <i>O</i> -methylnordihydroguaiaretic acid (2) in $(\text{CD}_3)_2\text{CO}$	13
Figure S5. ^1H NMR spectrum of 3'- <i>O</i> -methylnordihydroguaiaretic acid (2) in CDCl_3	14
Figure S6. ^{13}C NMR spectrum of 3'- <i>O</i> -methylnordihydroguaiaretic acid (2) in $(\text{CD}_3)_2\text{CO}$	15
Figure S7. ^{13}C DEPT-135 NMR spectrum of 3'- <i>O</i> -methylnordihydroguaiaretic acid (2) in $(\text{CD}_3)_2\text{CO}$	16
Figure S8. HMQC NMR spectrum of 3'- <i>O</i> -methylnordihydroguaiaretic acid (2) in $(\text{CD}_3)_2\text{CO}$	17
Figure S9. ^1H NMR spectrum of 3'-demethoxy-6- <i>O</i> -demethylisoguaiacin (3) in $(\text{CD}_3)_2\text{CO}$	18
Figure S10. ^1H NMR spectrum of 3'-demethoxy-6- <i>O</i> -demethylisoguaiacin (3) in CDCl_3	19
Figure S11. ^{13}C NMR spectrum of 3'-demethoxy-6- <i>O</i> -demethylisoguaiacin (3) in $(\text{CD}_3)_2\text{CO}$	20
Figure S12. HMQC spectrum of 3'-demethoxy-6- <i>O</i> -demethylisoguaiacin (3) in $(\text{CD}_3)_2\text{CO}$	21
Figure S13. HMBC spectrum of 3'-demethoxy-6- <i>O</i> -demethylisoguaiacin (3) in $(\text{CD}_3)_2\text{CO}$	22
Figure S14. ^1H NMR spectrum of nor-isoguaiacin (4) in $(\text{CD}_3)_2\text{CO}$	23
Figure S15. ^1H NMR spectrum of nor-isoguaiacin (4) in CDCl_3	24
Figure S16. ^{13}C NMR spectrum of nor-isoguaiacin (4) in $(\text{CD}_3)_2\text{CO}$	25
Figure S17. ^{13}C DEPT 135 NMR spectrum of nor-isoguaiacin (4) in $(\text{CD}_3)_2\text{CO}$	26

Figure S18. HMQC NMR spectrum of nor-isoguaicin (4) in (CD ₃) ₂ CO.....	27
Figure S19. ¹ H NMR spectrum of 3'-demethoxyisoguaiaicin (5) in (CD ₃) ₂ CO	28
Figure S20. ¹³ C NMR spectrum of 3'-demethoxyisoguaiaicin (5) in (CD ₃) ₂ CO	29
Figure S21. ¹³ C DEPT-135 NMR spectrum of 3'-demethoxyisoguaiaicin (5) in (CD ₃) ₂ CO.....	30
Figure S22. HMQC NMR spectrum of 3'-demethoxyisoguaiaicin (5) in (CD ₃) ₂ CO	31
Figure S23. ¹ H NMR spectrum of 6, 3'-di- <i>O</i> -demethoxy-isoguaiaicin (6) in CD ₃ OD.....	32
Figure S24. ¹³ C NMR spectrum of 6, 3'-di- <i>O</i> -demethoxy-isoguaiaicin (6) in CD ₃ OD.....	33
Figure S25. ¹³ C DEPT-135 NMR spectrum of 6, 3'-di- <i>O</i> -demethoxy-isoguaiaicin (6) in CD ₃ OD	34
Figure S26. ¹ H NMR spectrum of 3'-hydroxy-4-epi-larreatricin (7) in (CD ₃) ₂ CO	35
Figure S27. ¹³ C NMR spectrum of 3'-hydroxy-4-epi-larreatricin (7) in (CD ₃) ₂ CO	36
Figure S28. ¹³ C DEPT-135 NMR spectrum of 3'-hydroxy-4-epi-larreatricin (7) in (CD ₃) ₂ CO.....	37
Figure S29. ¹³ C DEPT-90 NMR spectrum of 3'-hydroxy-4-epi-larreatricin (7) in (CD ₃) ₂ CO.....	38
Figure S30. HMQC NMR spectrum of 3'-hydroxy-4-epi-larreatricin (7) in (CD ₃) ₂ CO	39
Figure S31. ¹ H NMR spectrum of (7 <i>R</i> , 7' <i>R</i>)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8 <i>R</i> , 8' <i>S</i>)-8, 8'- dimethyltetrahydrofuran (8) in (CD ₃) ₂ CO	40
Figure S32. ¹³ C NMR spectrum of of (7 <i>R</i> , 7' <i>R</i>)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8 <i>R</i> , 8' <i>S</i>)-8, 8'- dimethyltetrahydrofuran (8) in (CD ₃) ₂ CO	41
Figure S33. ¹³ C DEPT-135 NMR spectrum of of (7 <i>R</i> , 7' <i>R</i>)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8 <i>R</i> , 8' <i>S</i>)-8, 8'-dimethyltetrahydrofuran (8) in (CD ₃) ₂ CO	42
Figure S34. ¹³ C DEPT-90 NMR spectrum of of (7 <i>R</i> , 7' <i>R</i>)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8 <i>R</i> , 8' <i>S</i>)- 8, 8'-dimethyltetrahydrofuran (8) in (CD ₃) ₂ CO.....	43
Figure S35. HMQC NMR spectrum of (7 <i>R</i> , 7' <i>R</i>)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8 <i>R</i> , 8' <i>S</i>)-8, 8'- dimethyltetrahydrofuran (8) in (CD ₃) ₂ CO	44
Figure S36. HMBC NMR spectrum of of (7 <i>R</i> , 7' <i>R</i>)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8 <i>R</i> , 8' <i>S</i>)-8, 8'- dimethyltetrahydrofuran (8) in (CD ₃) ₂ CO	45
Figure S37. NOESY NMR spectrum of of (7 <i>R</i> , 7' <i>R</i>)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8 <i>R</i> , 8' <i>S</i>)-8, 8'- dimethyltetrahydrofuran (8) in (CD ₃) ₂ CO	46
Figure S38. NOESY NMR spectrum of of (7 <i>R</i> , 7' <i>R</i>)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8 <i>R</i> , 8' <i>S</i>)-8, 8'- dimethyltetrahydrofuran (8) in (CD ₃) ₂ CO	47
Figure S39. ¹ H NMR spectrum of 3-methoxy-6, 7, 4'-trihydroxyflavone (9) in CDCl ₃ and CD ₃ OD.....	48
Figure S40. ¹³ C NMR spectrum of 3-methoxy-6, 7, 4'-trihydroxyflavone (9) in CDCl ₃ and CD ₃ OD.....	49
Figure S41. ¹³ C DEPT-135 NMR spectrum of 3-methoxy-6, 7, 4'-trihydroxyflavone (9) in CDCl ₃ and CD ₃ OD.....	50
Figure S42. ¹³ C DEPT-90 NMR spectrum of 3-methoxy-6, 7, 4'-trihydroxyflavone (9) in CDCl ₃ and CD ₃ OD.....	51
Figure S43. HMQC NMR spectrum of 3-methoxy-6, 7, 4'-trihydroxyflavone (9) in CDCl ₃ and CD ₃ OD.....	52
Figure S44. HMBC NMR spectrum of 3-methoxy-6, 7, 4'-trihydroxyflavone (9) in CDCl ₃ and CD ₃ OD.....	53

Table S1. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound **1** in acetone- d_6 compared to the reported NMR data¹ (δ in ppm, J in Hz)

Position	1		Reported	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1a/4a	2.21 dd (13.3, 9.2)	39.2 CH ₂	2.20 dd (9.0, 4.2)	39.2 CH ₂
1b/4b	2.70 dd (13.3, 5.0)	-	2.68 dd (8.4, 4.8)	-
2/3	1.74 m	40.2 CH	1.72 m	40.1 CH
5/6	0.83 d (6.64)	16.6 CH ₃	0.82 d (6.64)	16.5 CH ₃
1'/1''	-	134.4 C	-	134.4 C
2'/2''	6.69 d (1.8)	115.8 CH	6.68 d (1.8)	115.8 CH
3'/3''	-	143.7 C	-	143.7 C
4'/4''	-	145.6 C	-	145.6 C
5'/5''	6.73 d (7.9)	116.9 CH	6.73 d (7.8)	116.9 CH
6'/6''	6.52 dd (7.9, 1.8)	121.3 CH	6.52 dd (6.0, 1.8)	121.3 CH

Table S2. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound **2** in acetone- d_6 and CDCl_3 compared to the reported NMR data² in CDCl_3 (δ in ppm, J in Hz)

Position	2 ^a		2 ^b	Reported ^b
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1	2.25 dd ^c	39.1 CH ₂	2.25 dd (13.1, 9.3)	2.25 dd (13.4, 9.3)
	2.75 dd (13.4, 4.8)		2.71 dd (13.3, 4.8)	2.71 dd (13.4, 4.7)
2,3	1.75 m	39.9, 40.0 CH	1.73 m	1.72 m
4	2.24 dd ^c	39.3 CH ₂	2.25 dd (13.3, 9.4)	2.25 dd (13.5, 9.3)
	2.69 dd (13.4, 5.40)		2.68 dd (13.3, 5.0)	2.68 dd (13.5, 5.2)
5,6	0.82 d, 0.84 d (6.8)	16.4, 16.6 CH ₃	0.82 d, 0.83 d (6.6)	0.82 d, 0.83 d (6.7)
1'	-	134.1 C	-	-
2'	6.71 d (1.9)	116.9 CH	6.61 brd (1.9)	6.61 d (1.9)
3'	-	148.1 C	-	-
4'	-	145.4 C	-	-
5'	6.75 d (8.2)	115.4 CH	6.82 d (8.0)	6.82 d (8.0)
6'	6.63 dd (8.0, 1.9)	122.3 CH	6.64 dd (8.0, 1.9)	6.64 dd (8.0, 1.9)
1''	-	134.3 C	-	-
2''	6.75 d (2.1)	113.2 CH	6.67 brd (2.0)	6.67 d (2.0)
3''	-	143.8 C	-	-
4''	-	145.7 C	-	-
5''	6.73 d (8.0)	115.8 CH	6.77 d (8.0)	6.77 d (8.0)
6''	6.54 dd (7.9, 1.6)	121.2 CH	6.58 brdd (8.0, 2.0)	6.58 dd (8.0, 2.0)
OMe	3.81 s	56.1 OCH ₃	3.86 s	3.86 s
OH	7.58 brs		5.03 brs, 5.45 s	5.00, 5.15, 5.45 s

^a In acetone- d_6

^b In CDCl_3

^c Overlapped signals

Table S3. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound **3** in acetone- d_6 and CDCl_3 compared to the reported NMR data² in CDCl_3 (δ in ppm, J in Hz)

Position	3 ^a		3 ^b	Reported ^b
	δ_{H}	δ_{C}	δ_{H}	δ_{H}
1	3.59 d (6.3)	50.8 CH	3.57 d (6.2)	3.59 d (6.2)
2	1.89 m	41.8 CH	1.89 m	1.90 m
3	2.03 m	30.1 CH	1.99 m	2.01 m
4a	2.81 dd (16.2, 5.2)	35.7 CH ₂	2.83 dd (16.4, 5.5)	2.84 dd (16.3, 5.3)
4b	2.39 dd (16.2, 7.2)		2.41 dd (16.4, 7.2)	2.42 dd (16.3, 7.2)
5	6.56 s	115.9 CH	6.60 s	6.62 s
6	-	144.0 C	-	-
7	-	144.4 C	-	-
8	6.23 s	117.7 CH	6.29 s	6.31 s
9	-	128.1 C	-	-
10	-	130.7 C	-	-
11	0.88 d (6.9)	16.1 CH ₃	0.87 d (6.9)	0.87 d (6.9)
12	0.89 d (6.9)	16.3 CH ₃	0.88 d (6.9)	0.88 d (6.9)
1'	-	139.3 C	-	-
2'	6.85 d (8.4)	130.8 CH	6.86 d (8.5)	6.89 d (8.5)
3'	6.71 d (8.4)	115.7 CH	6.69 d (8.5)	6.72 d (8.5)
4'	-	156.3 C	-	-
5'	6.71 d (8.4)	115.7 CH	6.69 d (8.5)	6.72 d (8.5)
6'	6.85 d (8.4)	130.8 CH	6.86 d (8.5)	6.89 d (8.5)
OH	8.06, 7.46, 7.43		5.25 s, 5.35 s	very broad

^a In acetone- d_6

^b In CDCl_3

Table S4. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound **4** in acetone- d_6 and CDCl_3 compared to the reported NMR data³ in CDCl_3 (δ in ppm, J in Hz)

Position	4 ^a		4 ^b		Reported ^b	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1	3.55 d (6.8)	51.0 CH	3.56 d (6.8)	50.5 CH	3.56 d (6.5)	50.3 CH
2	2.01 m	30.4 CH	2.0 m	29.4 CH	2.0 dd (6.6, 3.0)	29.1 CH
3	1.94 dt (6.9, 3.0)	41.5 CH	1.91 dt (6.8, 3.0)	40.7 CH	1.91 dt (6.9, 6.5)	40.5 CH
4a	2.39 dd (16.3, 6.9)	35.7 CH ₂	2.41 dd (16.4, 7.0)	35.1 CH ₂	2.41 dd (16.5, 6.9)	34.8 CH ₂
4b	2.84 dd (16.3, 5.3)		2.83 dd (16.4, 5.3)		2.83 dd (16.5, 6.9)	
5	6.56 s	115.8 CH	6.32 s	115.0 CH	6.29 s	114.7 CH
6	-	143.8 C	-	141.4 C	-	142.1 C
7	-	144.3 C	-	142.1 C	-	142.5 C
8	6.25 s	117.5 CH	6.61 s	116.8 CH	6.58 s	116.6 CH
9	-	128.0 C	-	129.3 C	-	129.7 C
10	-	130.4 C	-	131.0 C	-	128.3 C
11	0.874 d (6.9)	16.2 CH	0.87 d (6.8)	15.9 CH ₃	0.87 d (6.9)	15.6 CH ₃
12	0.867 d (6.9)	15.9 CH	0.88 d (6.8)	16.0 CH ₃	0.88 d (6.9)	15.7 CH ₃
1'	-	139.7 C	-	139.2 C	-	139.3 C
2'	6.70 d (2.0)	113.3 CH	6.52 d (1.8)	111.3 CH	6.54 s	111.8 CH
3'	-	148.0 C	-	146.4 C	-	146.4 C
4'	-	145.5 C	-	143.8 C	-	143.4 C
5'	6.71 s (8.1)	115.1 CH	6.79 d (8.0)	113.6 CH	6.74 d (7.8)	113.8 CH
6'	6.46 dd (8.1, 2.0)	122.5 CH	6.50 dd (8.0, 1.8)	121.9 CH	6.4 dd (8.1, 1.9)	121.8 CH
OMe	3.76	56.2 OCH ₃	3.80 s	55.8 OCH ₃	3.79 s	55.7 OCH ₃

^a In acetone- d_6

^b In CDCl_3

Table S5. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound **6** in acetone- d_6 and CDCl_3 compared to the reported NMR data² in CDCl_3 (δ in ppm, J in Hz)

Position	5^a		5^b	Reported ^b
	δ_{H}	δ_{C}	δ_{H}	δ_{H}
1	3.59 d (6.4)	50.8 CH	3.61 d (6.1)	3.61 d (6.2)
2	1.90 m	41.7 CH	1.90 m	1.90 m
3	2.02 m	30.0 CH	2.0 m	2.02 m
4a	2.88 dd (16.3, 5.4)	35.8 CH ₂	2.87 dd (6.2, 5.0)	2.87 dd (16.2, 7.2)
4b	2.45 dd (16.3, 7.3)		2.45 dd (16.2, 7.2)	2.45 dd (16.2, 7.2)
5	6.66 s	112.3 CH	6.57 s	6.57 s
6	-	145.4 C	-	-
7	-	156.3 C	-	-
8	6.26 s	117.4 CH	6.39 s	6.39 s
9	-	127.6 C	-	-
10	-	131.5 C	-	-
11	0.87 d (6.9)	16.0 CH ₃	0.88 d (6.9)	0.88 d (6.9)
12	0.88 d (6.9)	16.2 CH ₃	0.89 d (6.9)	0.89 d (8.9)
1'	-	139.0 C	-	-
2'	6.86 d (8.5)	130.7 CH	6.87 d (8.5)	6.87 d (8.5)
3'	6.72 d (8.5)	115.6 CH	6.70 d (8.5)	6.70 d (8.5)
4'	-	146.8 C	-	-
5'	6.72 d (8.5)	115.6 CH	6.70 d (8.5)	6.70 d (8.5)
6'	6.86 d (8.5)	130.7 CH	6.87 d (8.5)	6.87 d (8.5)
OMe	3.80 s	56.1 OCH ₃	3.86 s	3.86
OH	8.0, s, 7.1, s		4.85 s, 5.32 s	4.78 s, 5.35 s

^a In acetone- d_6

^b In CDCl_3

Table S6. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound **6** in CD_3OD compared to the reported NMR data⁴ in acetone- d_6 (δ in ppm, J in Hz)

Position	6 ^a		Reported ^b	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1	3.48 d (6.4)	51.5 CH	3.51 d (6.3)	50.8 CH
2	1.88 dt (6.8, 2.8)	42.2 CH	1.88 m	41.5 CH
3	2.01 m	30.6 CH	2.02 m	29.8 CH
4a	2.38 dd (16.4, 7.2)	36.0 CH_2	2.37 dd (16.5, 7.7)	35.4 CH_2
4b	2.80 dd (16.4, 5.6)		2.80 dd (16.5, 5.4)	
5	6.50 s	116.0 or 115.8 CH	6.56 s	115.5 or 115.7 CH
6, 7	-	144.2, 144.1 C	-	143.7 C
8	6.25 s	118.1 CH	6.26 s	117.6 CH
9	-	128.5 C	-	128.0 C
10	-	140.6 C	-	140.0 C
11,12	0.88 dd (7.2, 3.2)	16.2, 16.1 CH_3	0.87 d (6.8)	16.0, 16.2 CH_3
1'	-	130.9 C	-	130.3 C
2'	6.43 d (2.0)	117.3 CH	6.44 brs	116.8 CH
3'	-	145.8 C	-	145.2 C
4'	-	144.5 C	-	144.0 C
5'	6.66 d (8.0)	116.0 or 115.8 CH	6.71 d (8.7)	115.5 or 115.7 CH
6'	6.39 dd (8.0, 2.0)	121.6 CH	6.43 dd (8.7, 2.1)	121.2 CH

^a In CD_3OD

^b In acetone- d_6

Table S7. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) data for compound **7** in acetone- d_6 compared to the reported NMR data⁵ (δ in ppm, J in Hz)

Position	7		Reported	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1	-	135.9	-	135.8
2	6.91 d (1.9)	114.2	6.92 d (92.1)	114.2
3	-	145.8	-	145.8
4	-	145.2	-	145.1
5	6.79 d (7.5)	115.7	6.79 d (7.7)	115.7
6	6.72 dd (7.9, 1.9)	118.7	6.74 dd (7.7, 2.1)	118.7
7	4.56 d (8.9)	88.8	4.56 d (8.4)	88.8
8	1.72 m	52.0	1.72 m	52.0
9	1.01 d (6.0)	14.0	1.10 d (5.4)	14.0
1'	-	134.8	-	134.8
2', 6'	7.23 d (7.5)	128.4	7.24	128.4
3', 5'	6.81 d (8.6)	115.8	6.82 d (8.6)	115.8
4'	-	157.6	-	157.6
7'	4.54 d (8.9)	88.8	4.54 d (8.4)	88.8
8'	1.72 m	51.9	1.72 m	51.9
9'	0.99 d (6.0)	14.1	0.99 d (5.4)	14.1

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Figure S1. ^1H NMR spectrum of nordihydroguaiaretic acid (**1**) in $(\text{CD}_3)_2\text{CO}$

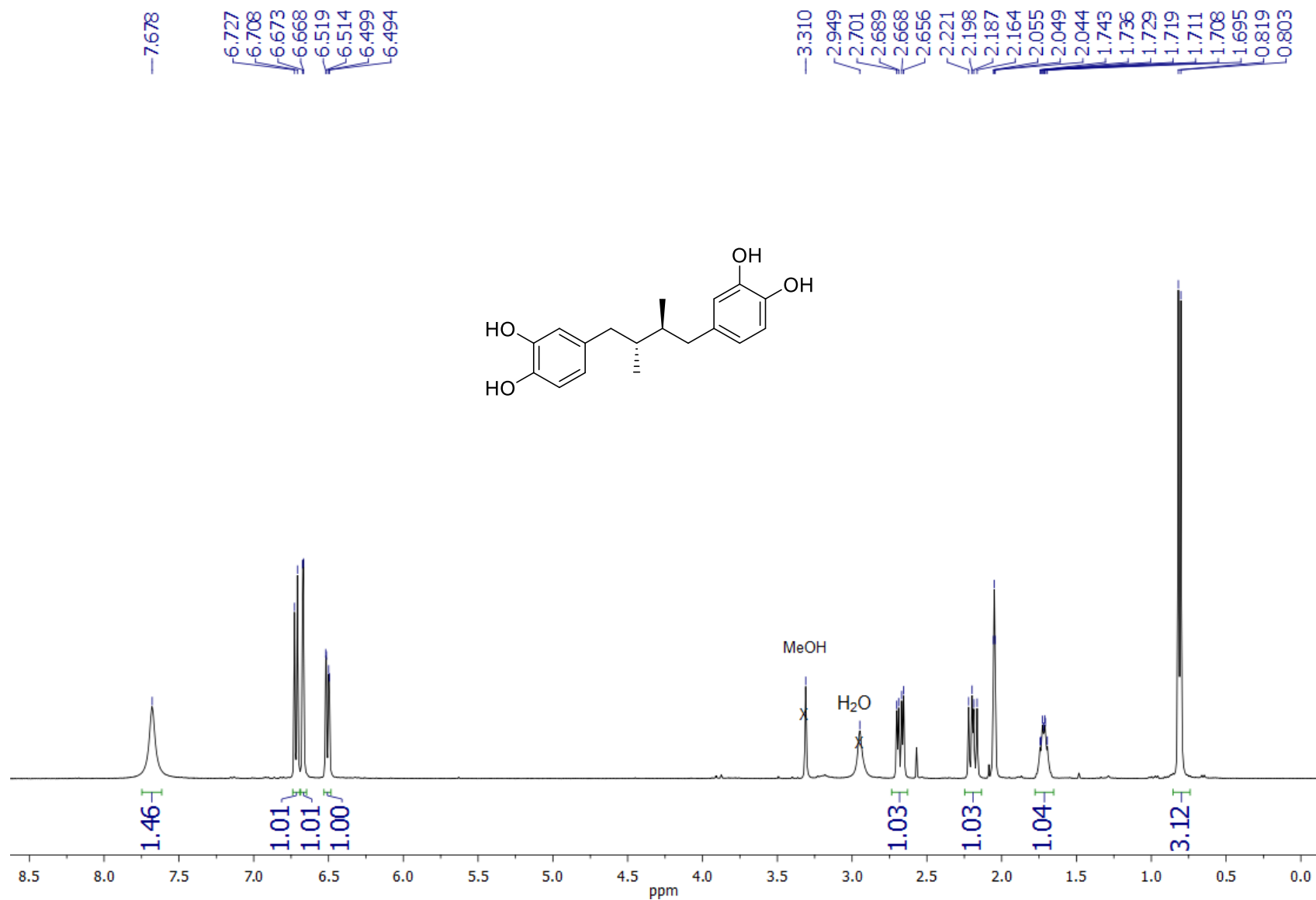


Figure S2. ^{13}C NMR spectrum of nordihydroguaiaretic acid (**1**) in $(\text{CD}_3)_2\text{CO}$

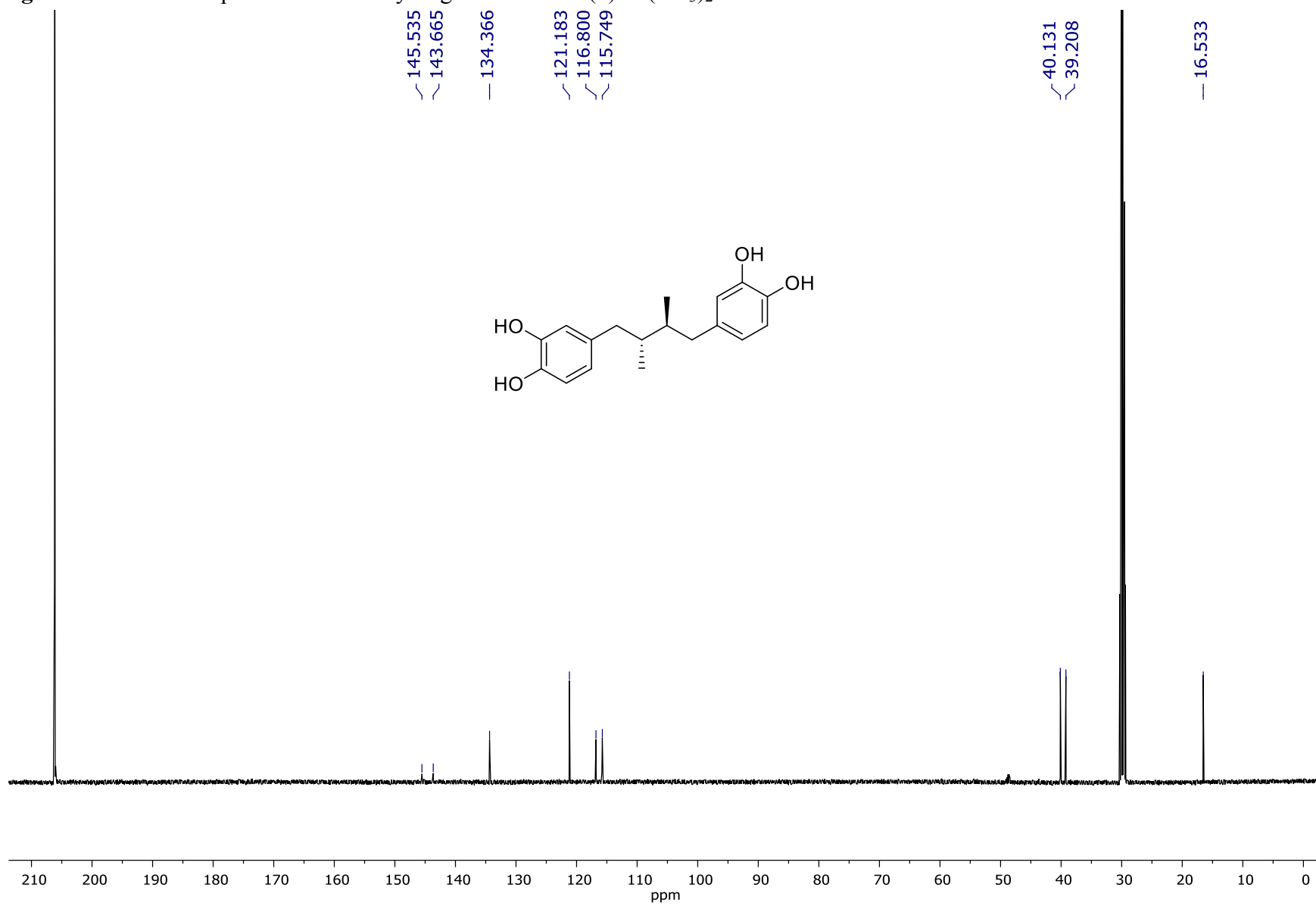


Figure S3. HMQC NMR spectrum of nordihydroguaiaretic acid (**1**) in $(\text{CD}_3)_2\text{CO}$



Figure S4. ^1H NMR spectrum of 3'-*O*-methylnordihydroguaiaretic acid (**2**) in $(\text{CD}_3)_2\text{CO}$

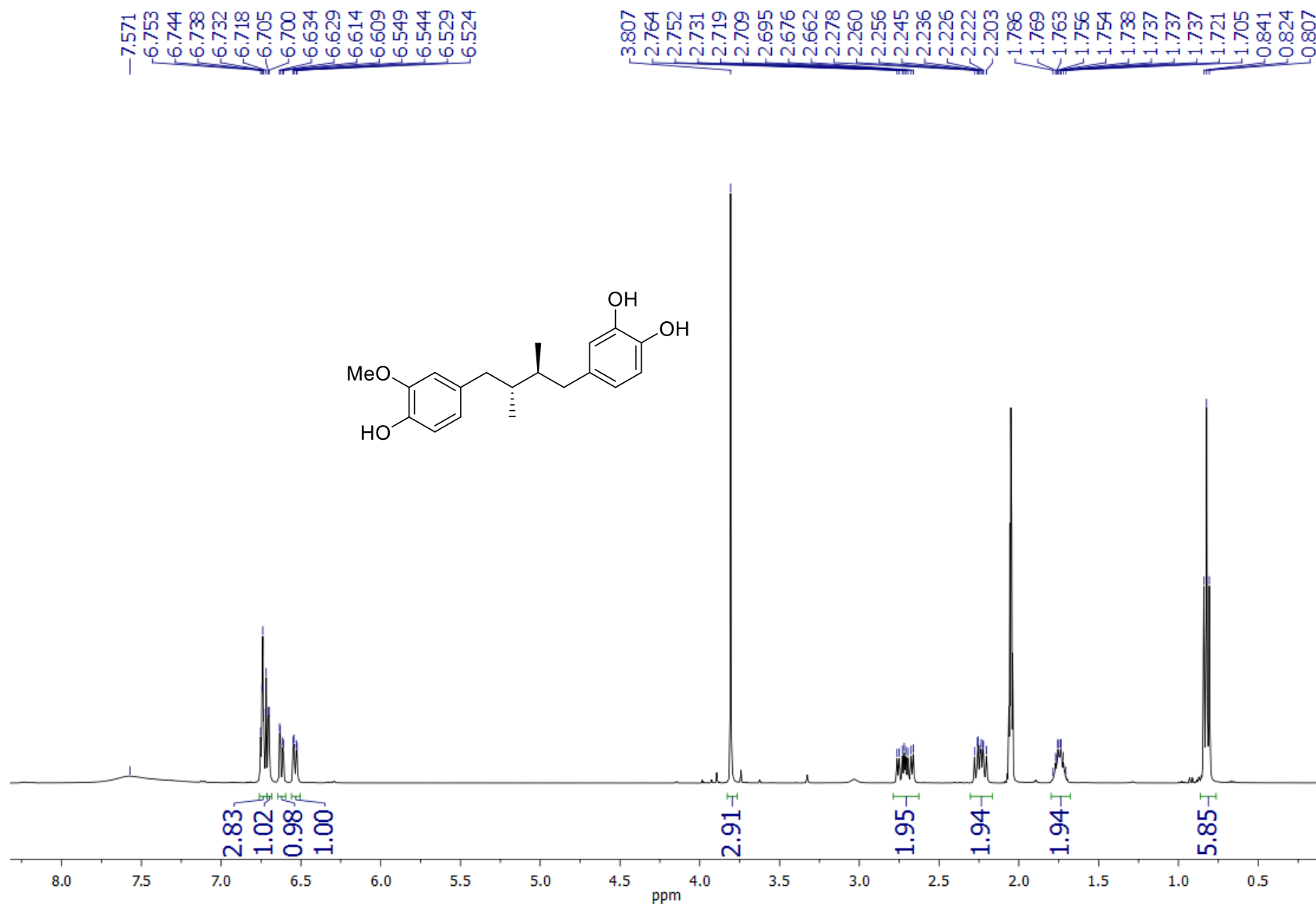


Figure S5. ^1H NMR spectrum of 3'-*O*-methylnordihydroguaiaretic acid (**2**) in CDCl_3

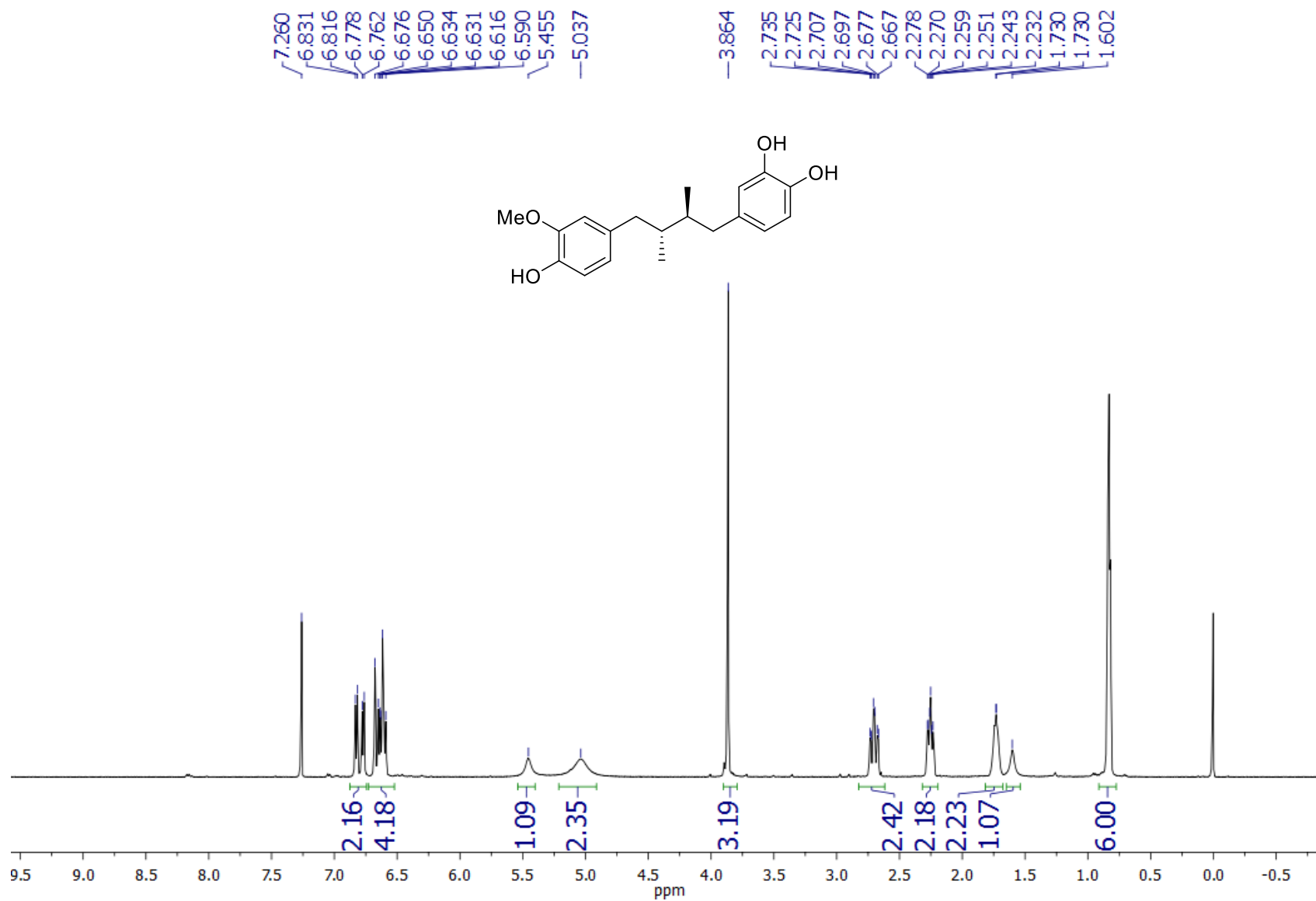


Figure S6. ^{13}C NMR spectrum of 3'-*O*-methylnordihydroguaiaretic acid (**2**) in $(\text{CD}_3)_2\text{CO}$

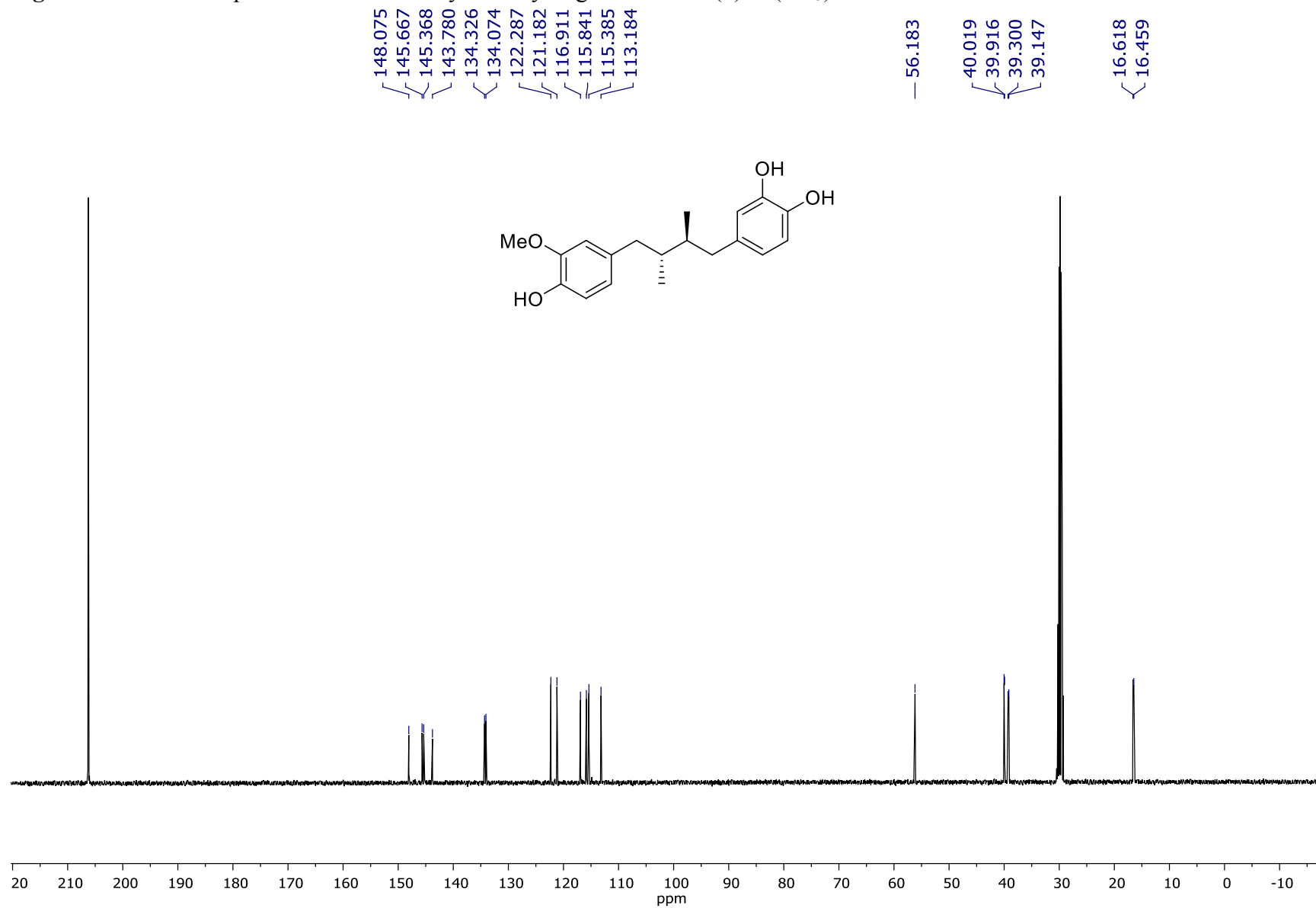


Figure S7. ^{13}C DEPT-135 NMR spectrum of 3'-*O*-methylnordihydroguaiaretic acid (**2**) in $(\text{CD}_3)_2\text{CO}$

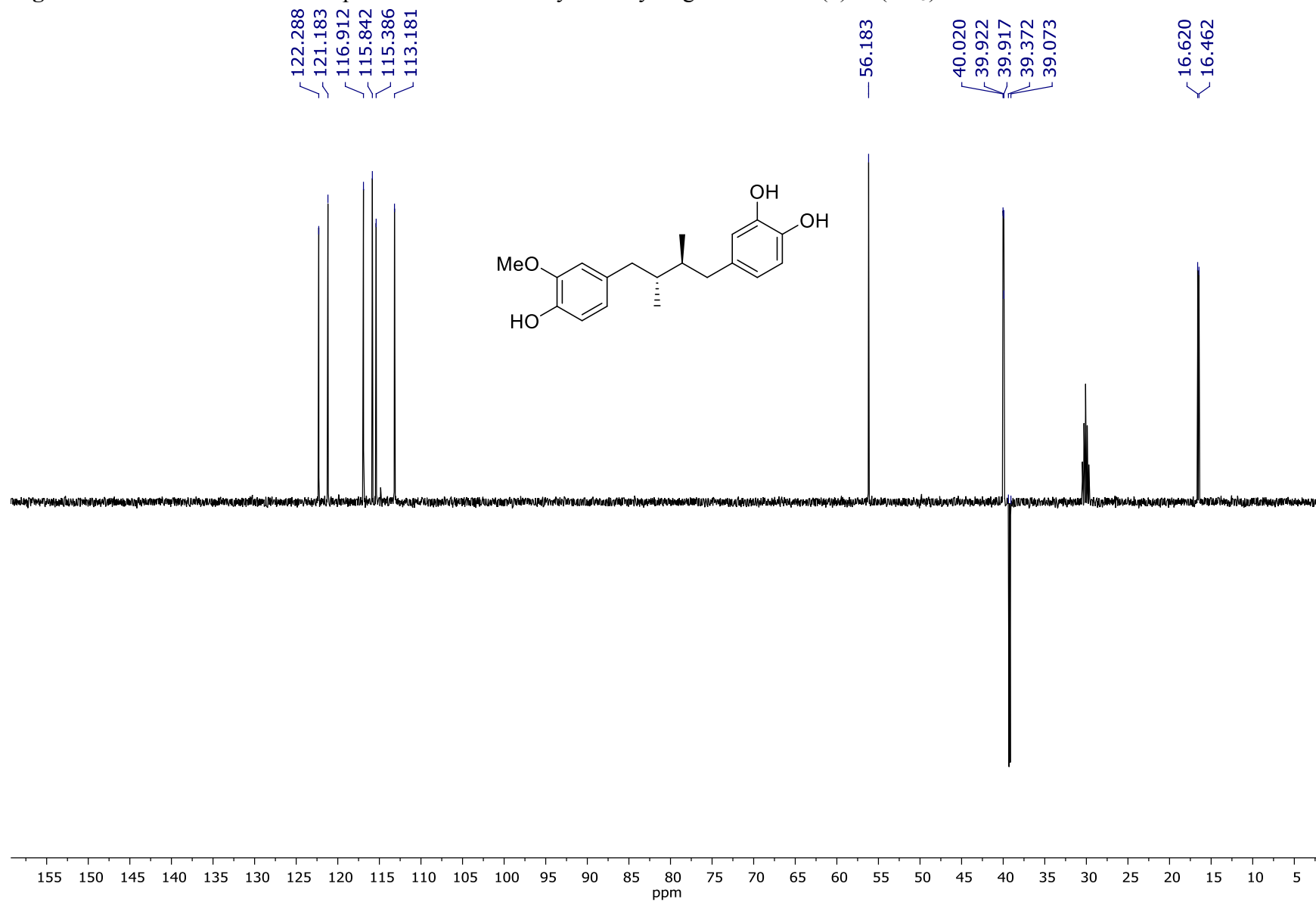


Figure S8. HMQC NMR spectrum of 3'-*O*-methylnordihydroguairetic acid (**2**) in (CD₃)₂CO

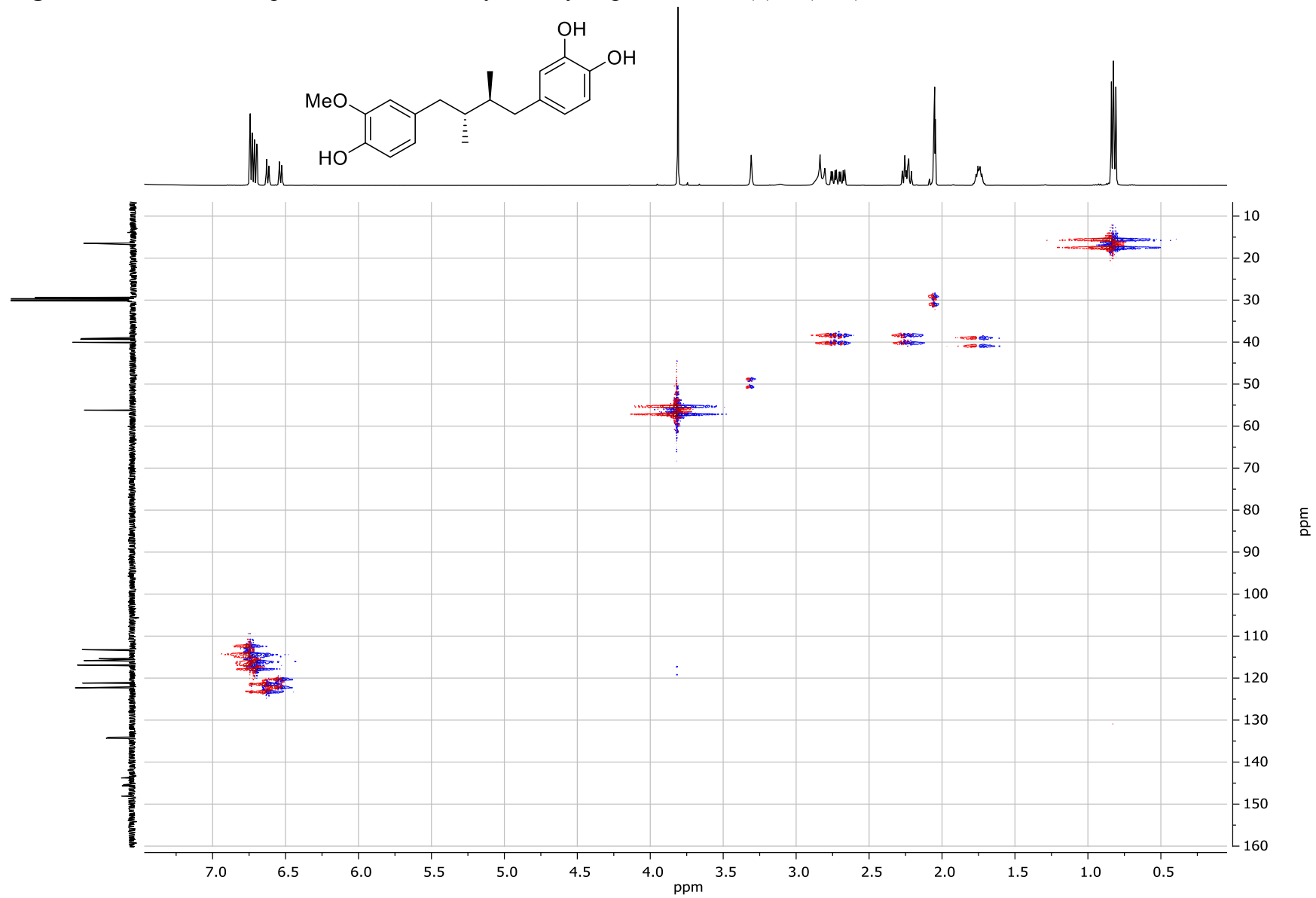


Figure S9. ¹H NMR spectrum of 3'-demethoxy-6-O-demethylisoguaiacin (**3**) in (CD₃)₂CO

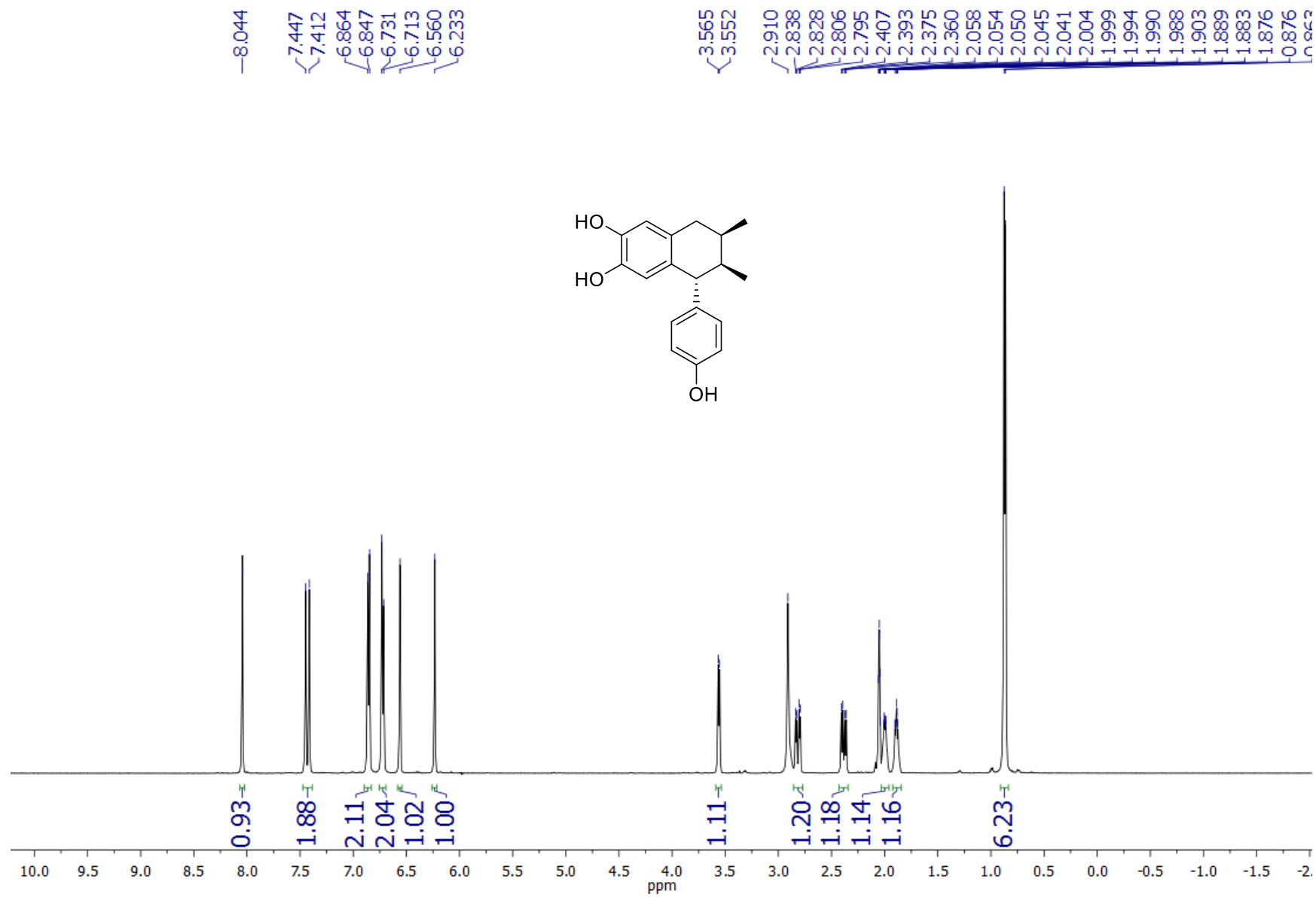


Figure S10. ^1H NMR spectrum of 3'-demethoxy-6-*O*-demethylisoguaiacin (**3**) in CDCl_3

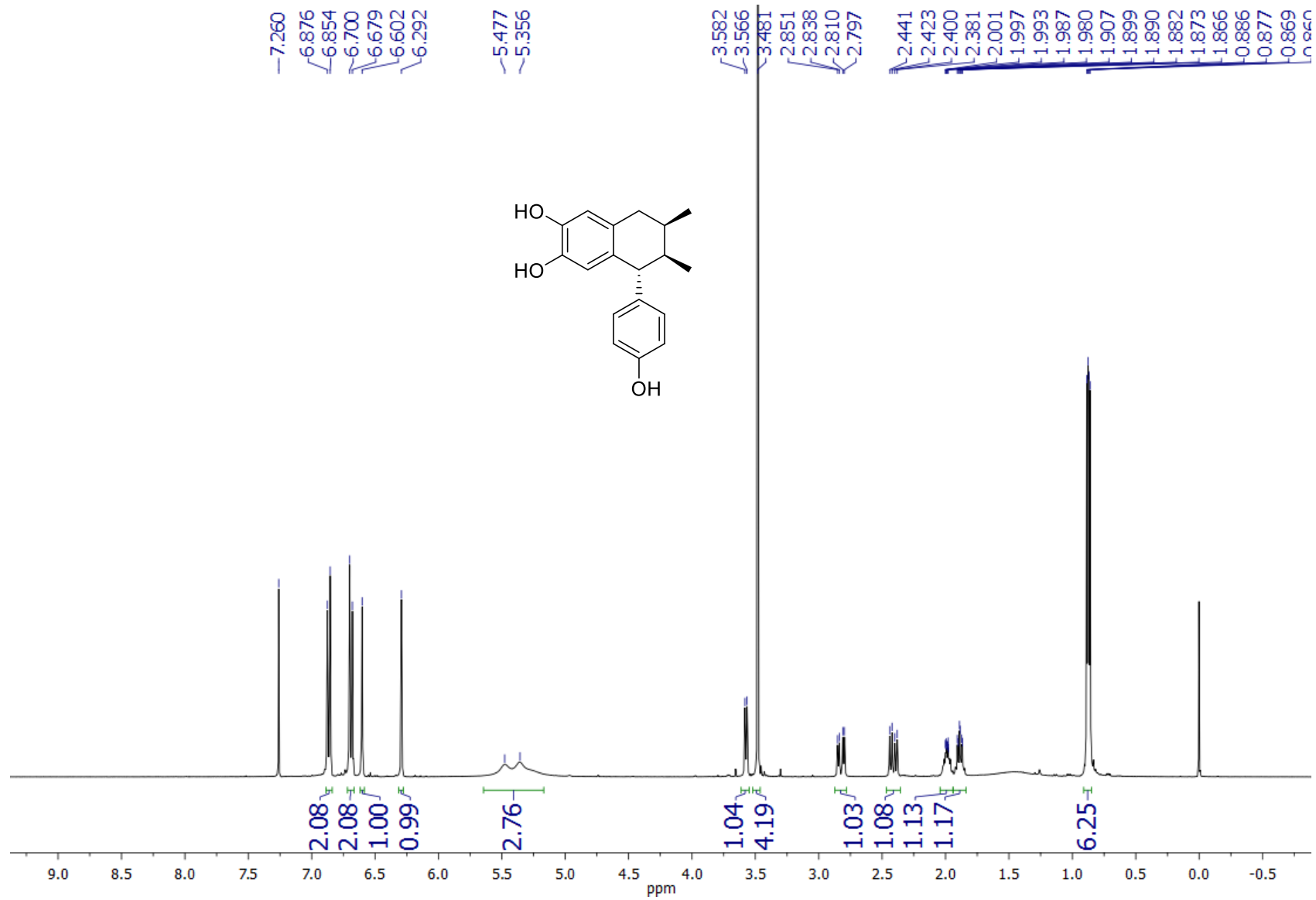


Figure S11. ^{13}C NMR spectrum of 3'-demethoxy-6-*O*-demethylisoguaiacin (**3**) in $(\text{CD}_3)_2\text{CO}$

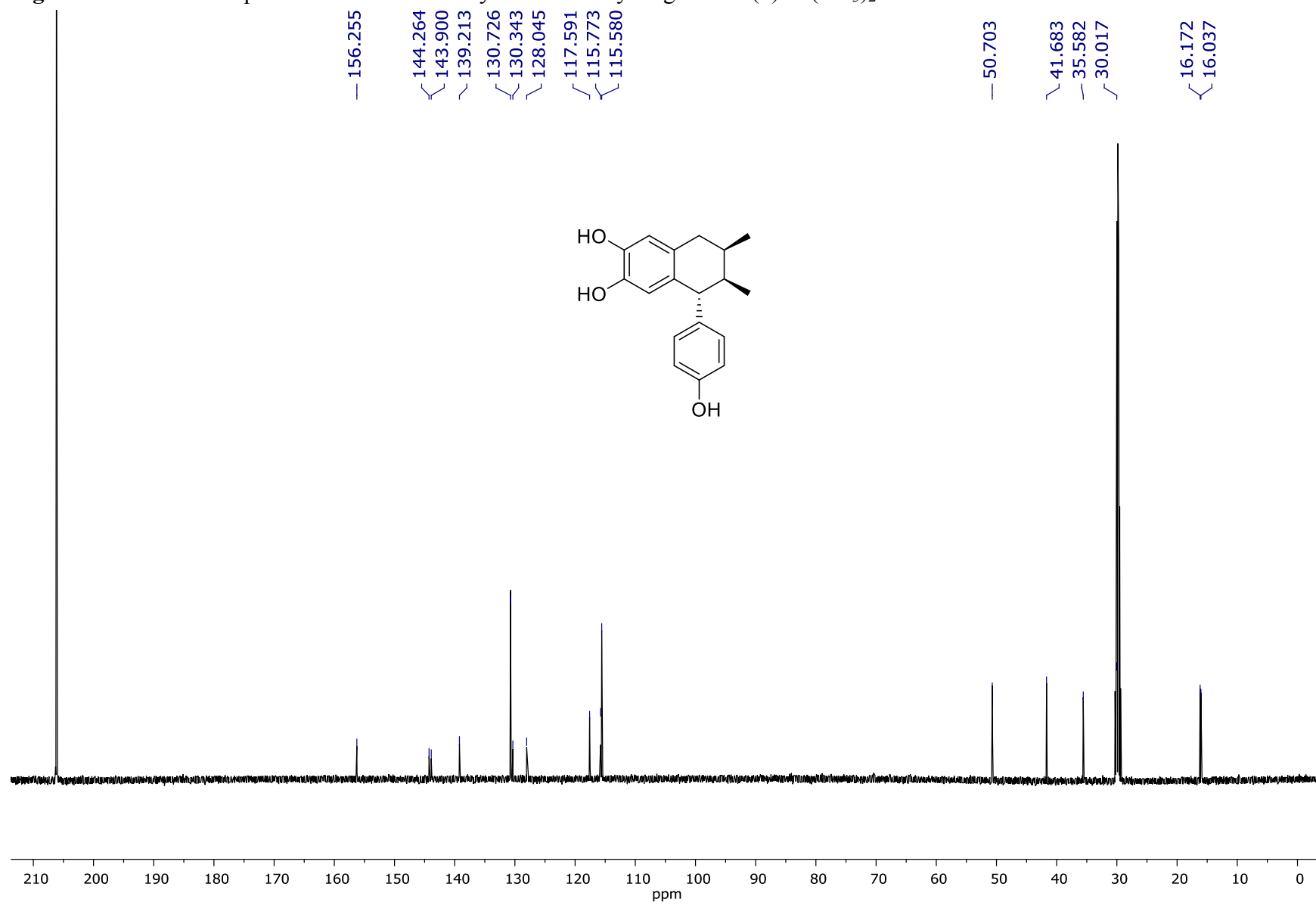


Figure S12. HMQC spectrum of 3'-demethoxy-6-*O*-demethylisoguaiacin (**3**) in (CD₃)₂CO

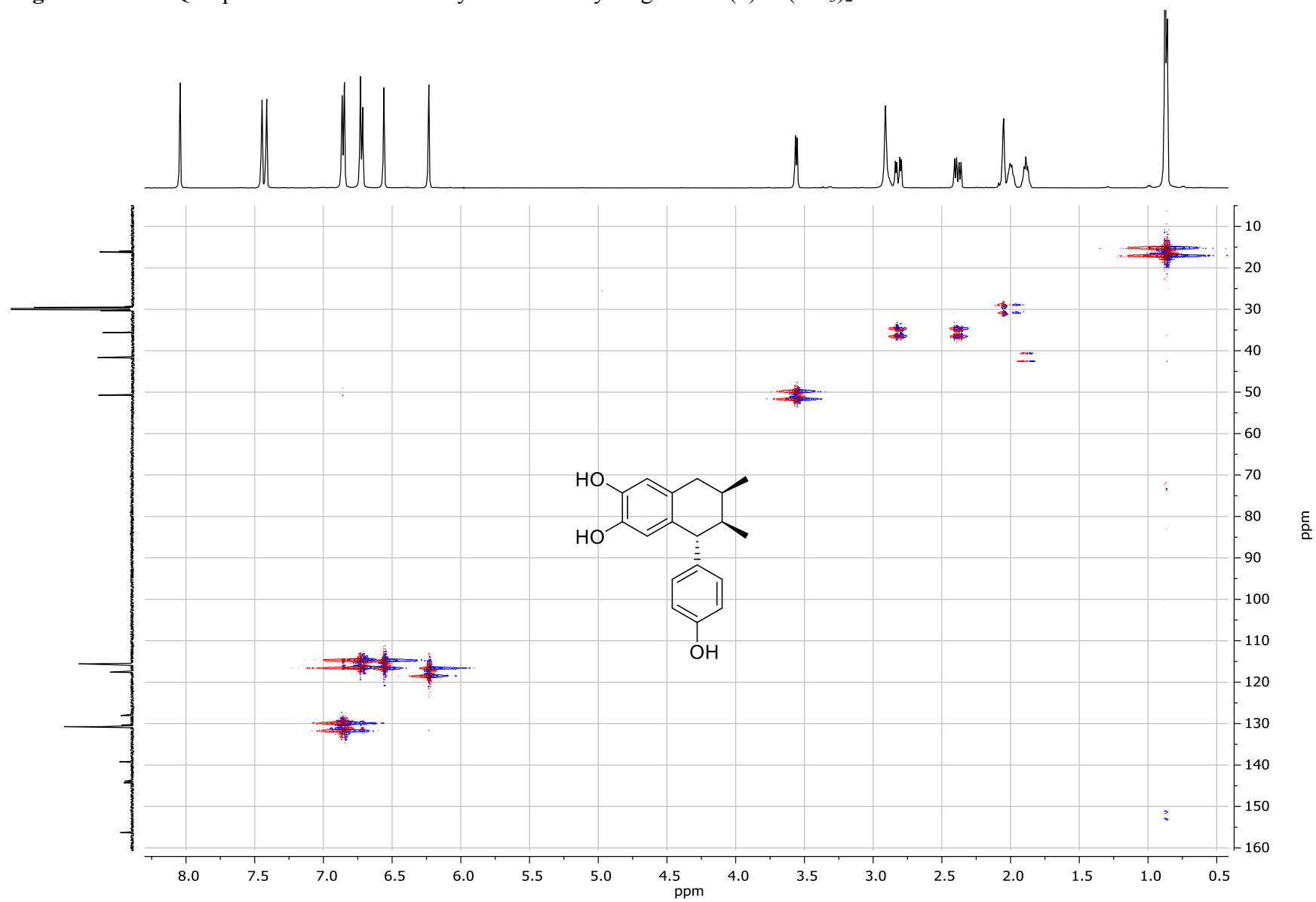


Figure S13. HMBC spectrum of 3'-demethoxy-6-*O*-demethylisoguaiacin (**3**) in (CD₃)₂CO

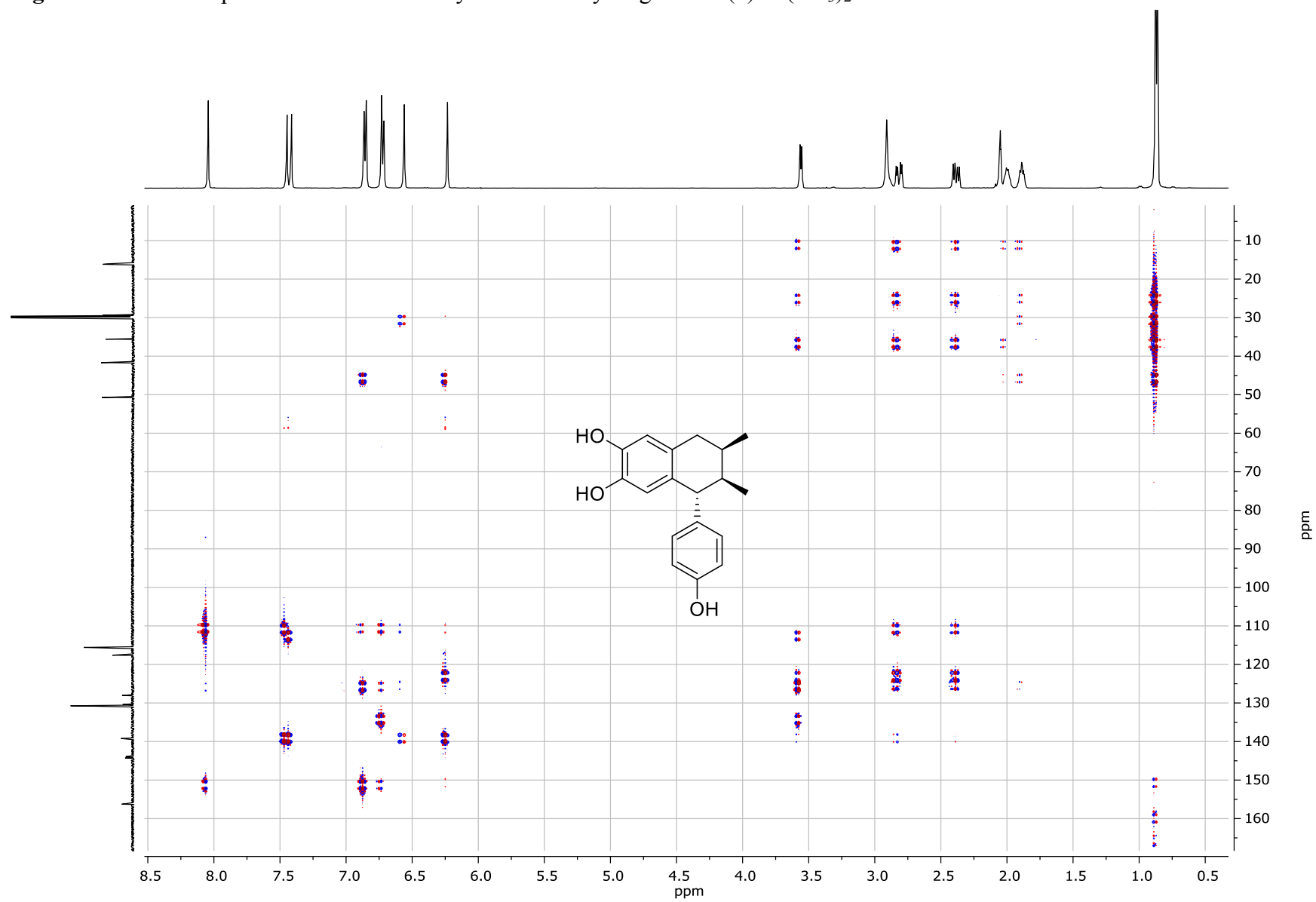


Figure S14. ¹H NMR spectrum of nor-isogaucin (4) in (CD₃)₂CO

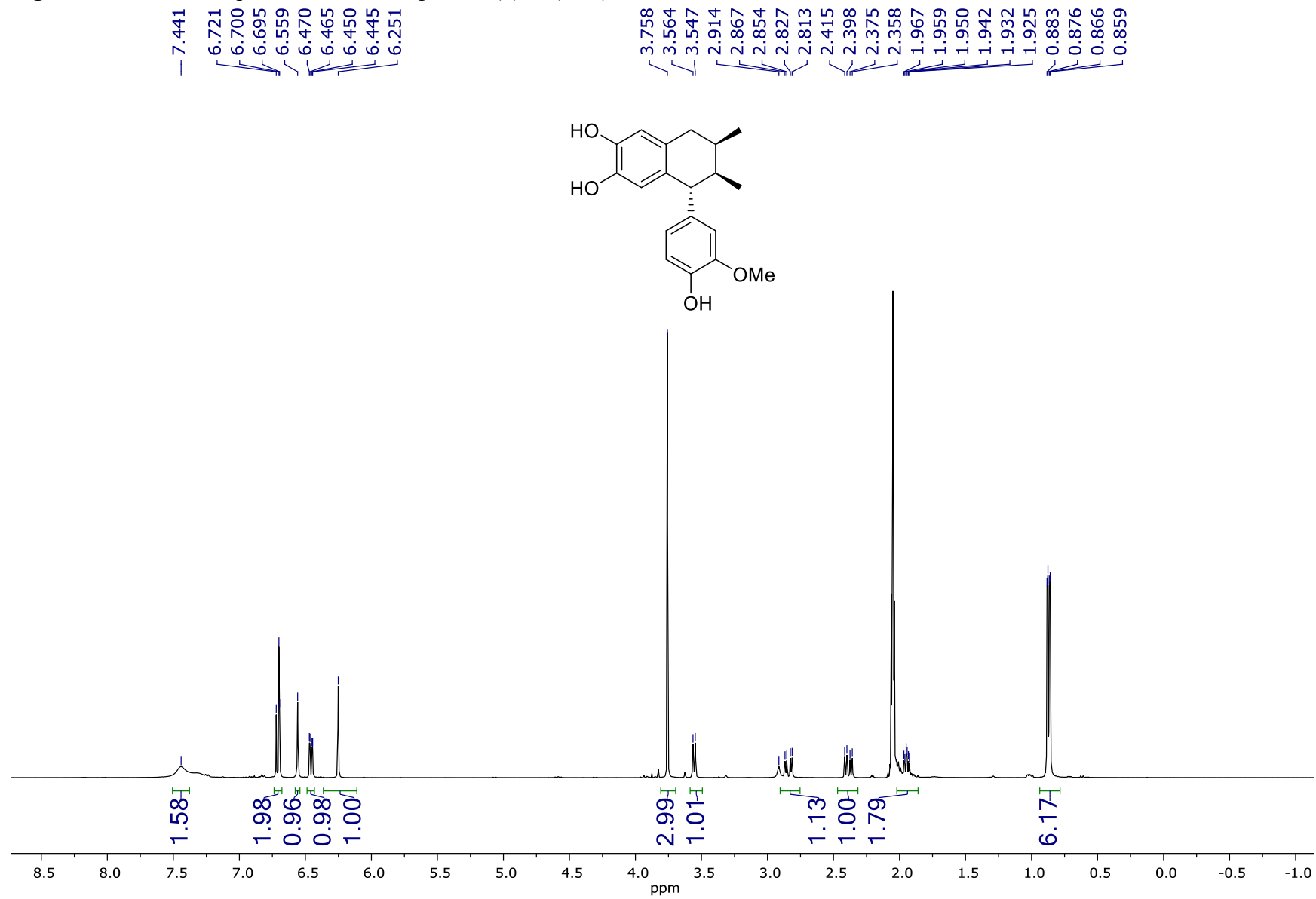


Figure S15. ¹H NMR spectrum of nor-isogaicic acid (4) in CDCl₃

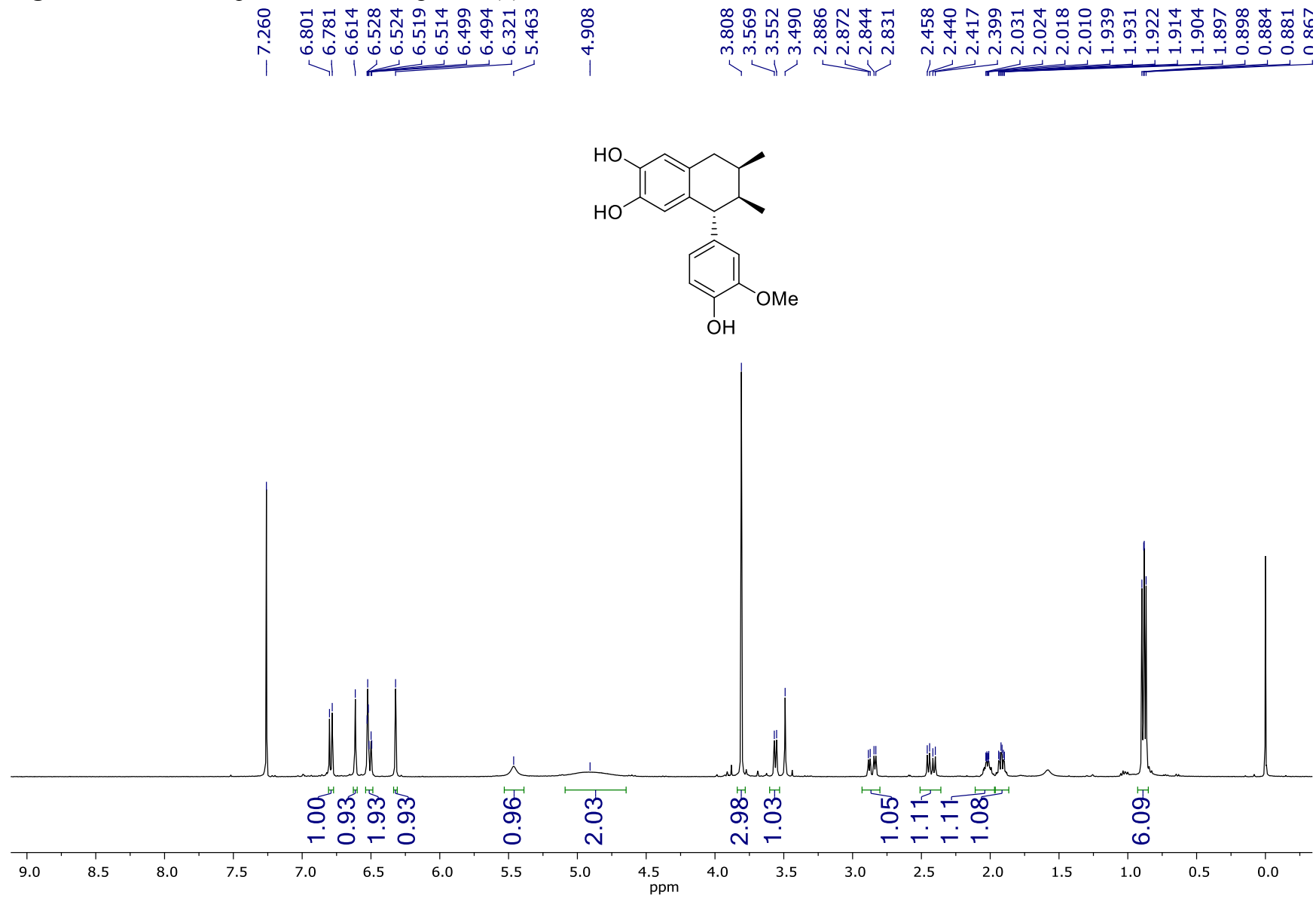


Figure S16. ^{13}C NMR spectrum of nor-isogaucin (**4**) in $(\text{CD}_3)_2\text{CO}$

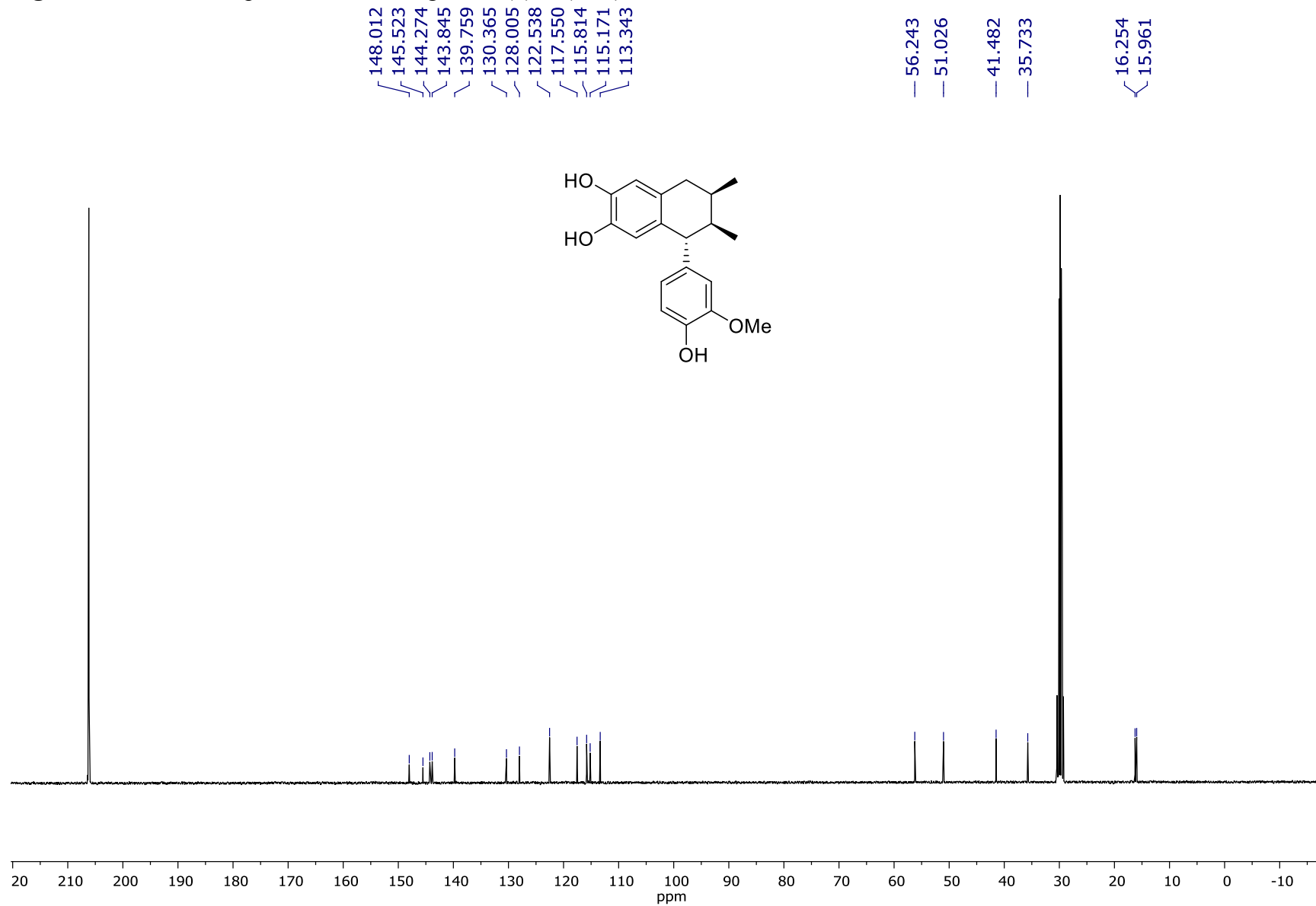


Figure S17. ^{13}C DEPT 135 NMR spectrum of nor-isogaicin (**4**) in $(\text{CD}_3)_2\text{CO}$

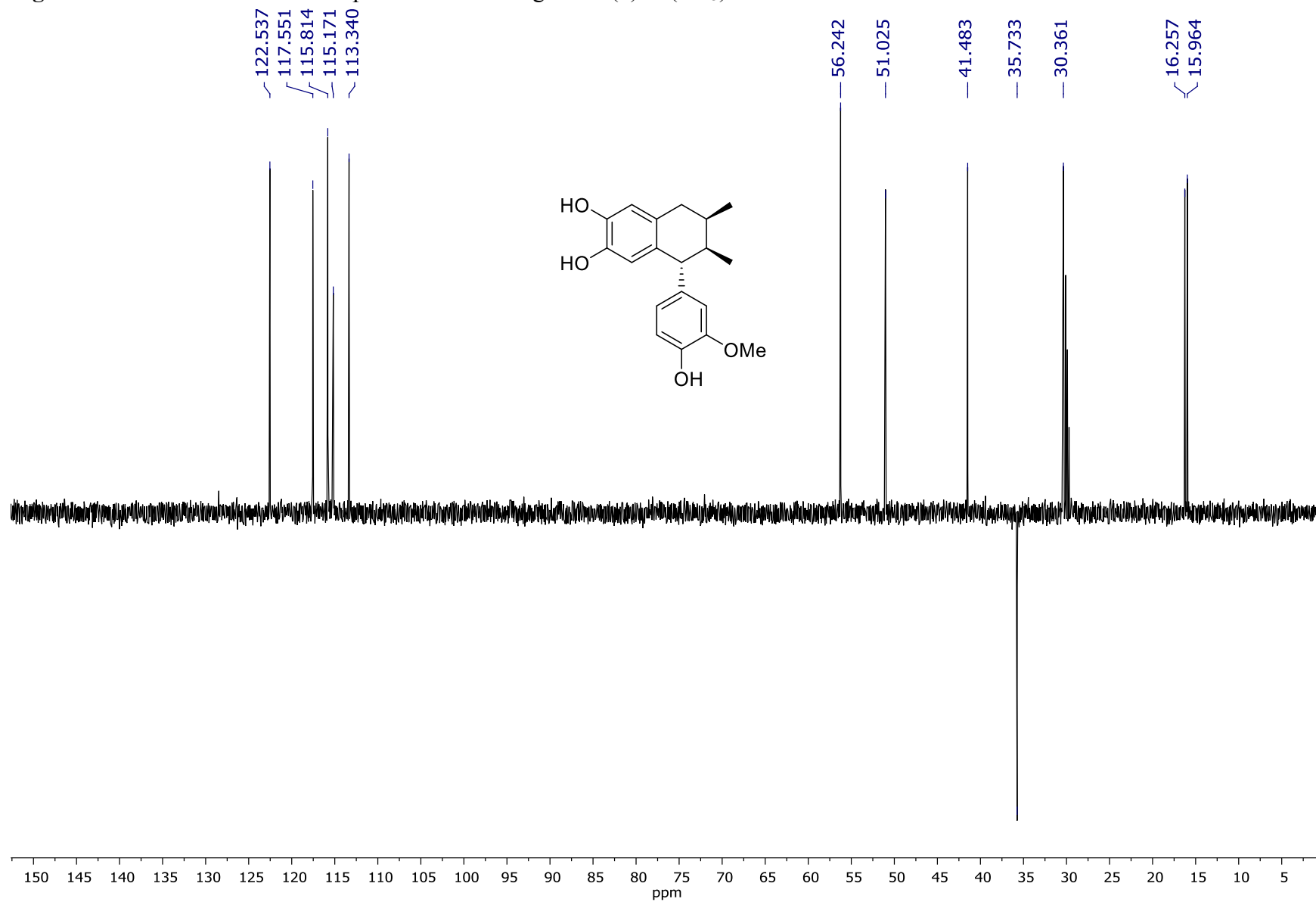


Figure S18. HMQC NMR spectrum of nor-isogaicin (4) in $(\text{CD}_3)_2\text{CO}$

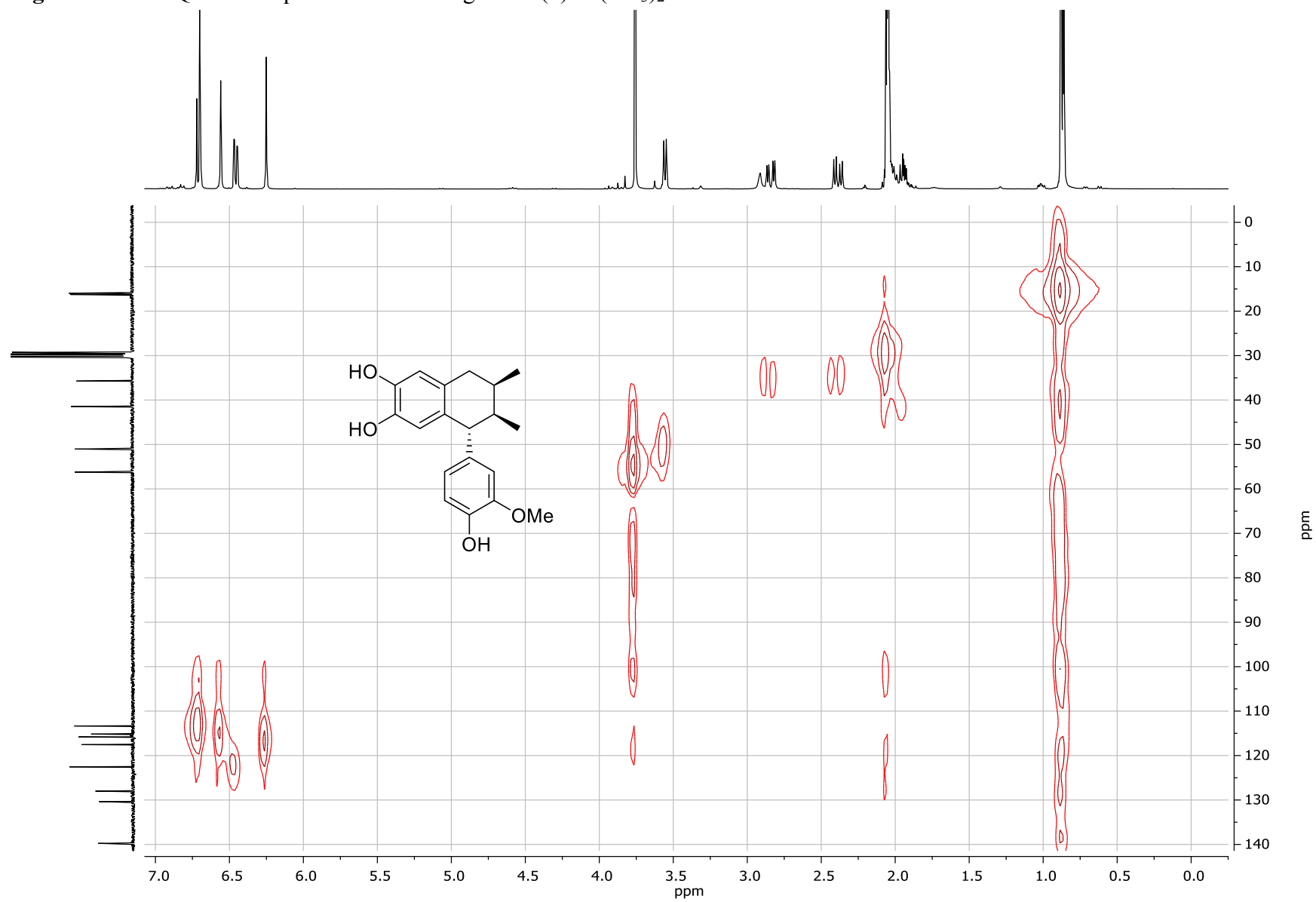


Figure S19. ^1H NMR spectrum of 3'-demethoxyisoguaiacin (**5**) in $(\text{CD}_3)_2\text{CO}$

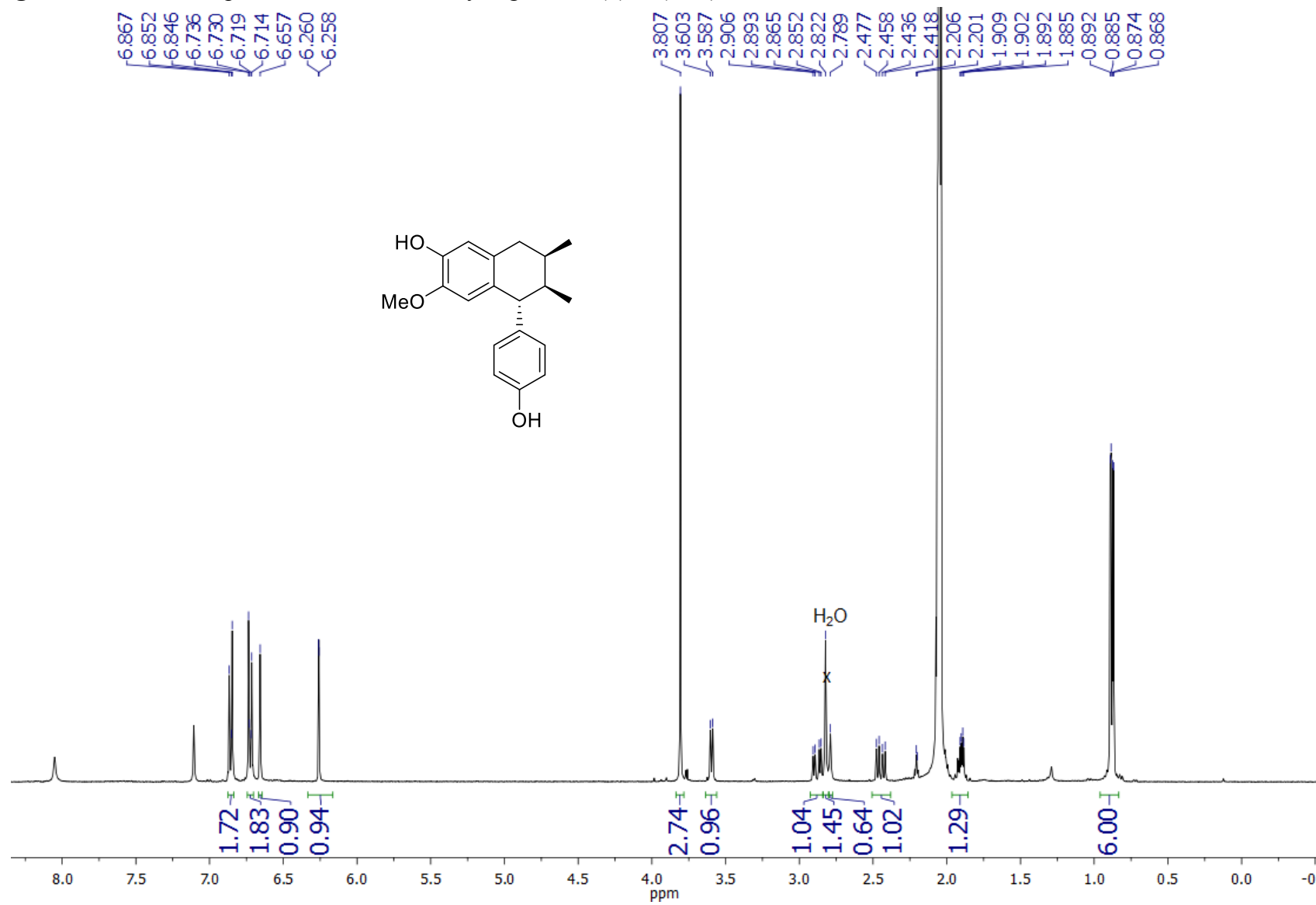


Figure S20. ^{13}C NMR spectrum of 3'-demethoxyisoguaiacin (**5**) in $(\text{CD}_3)_2\text{CO}$

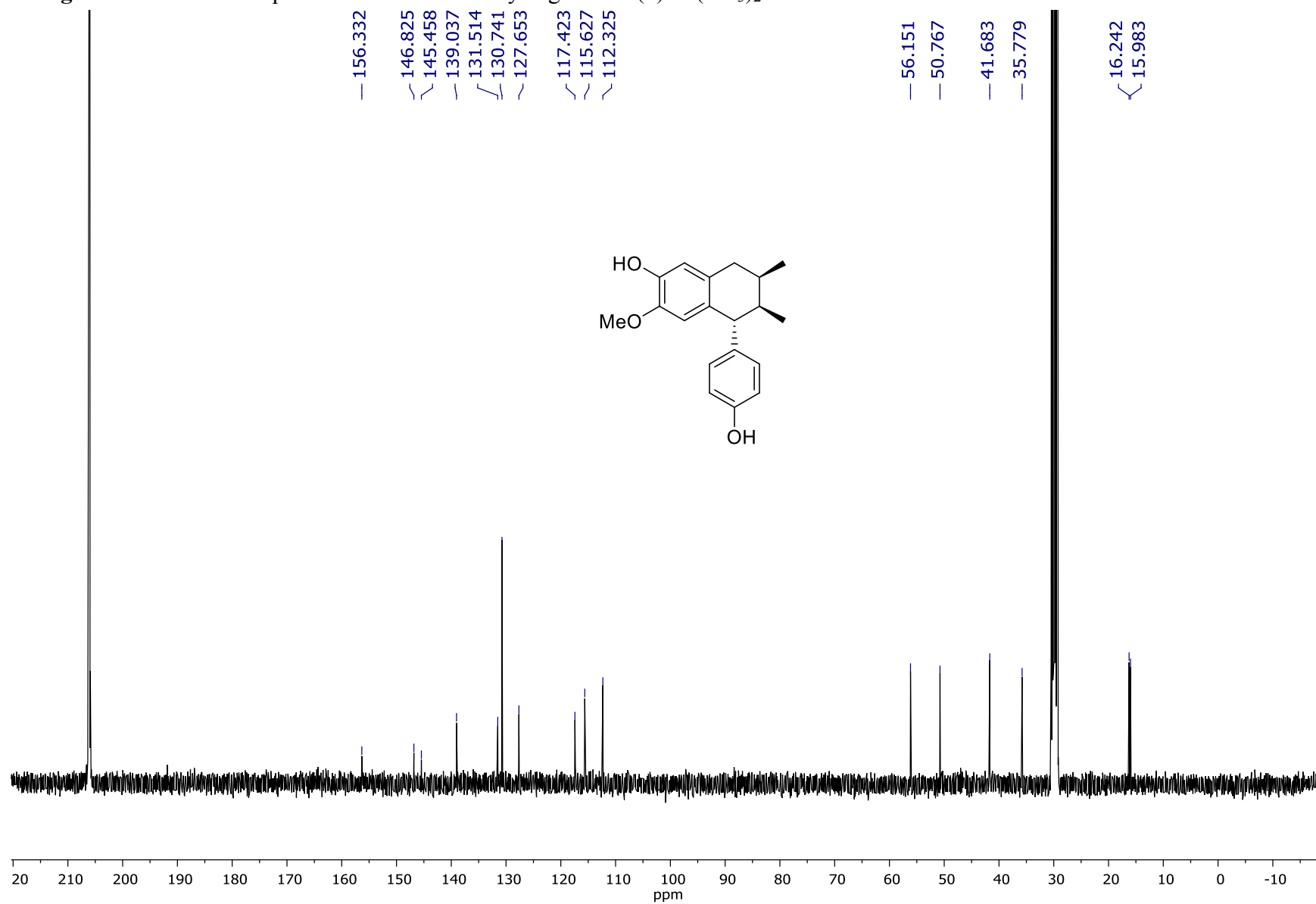


Figure S21. ^{13}C DEPT-135 NMR spectrum of 3'-demethoxyisoguaiacin (**5**) in $(\text{CD}_3)_2\text{CO}$

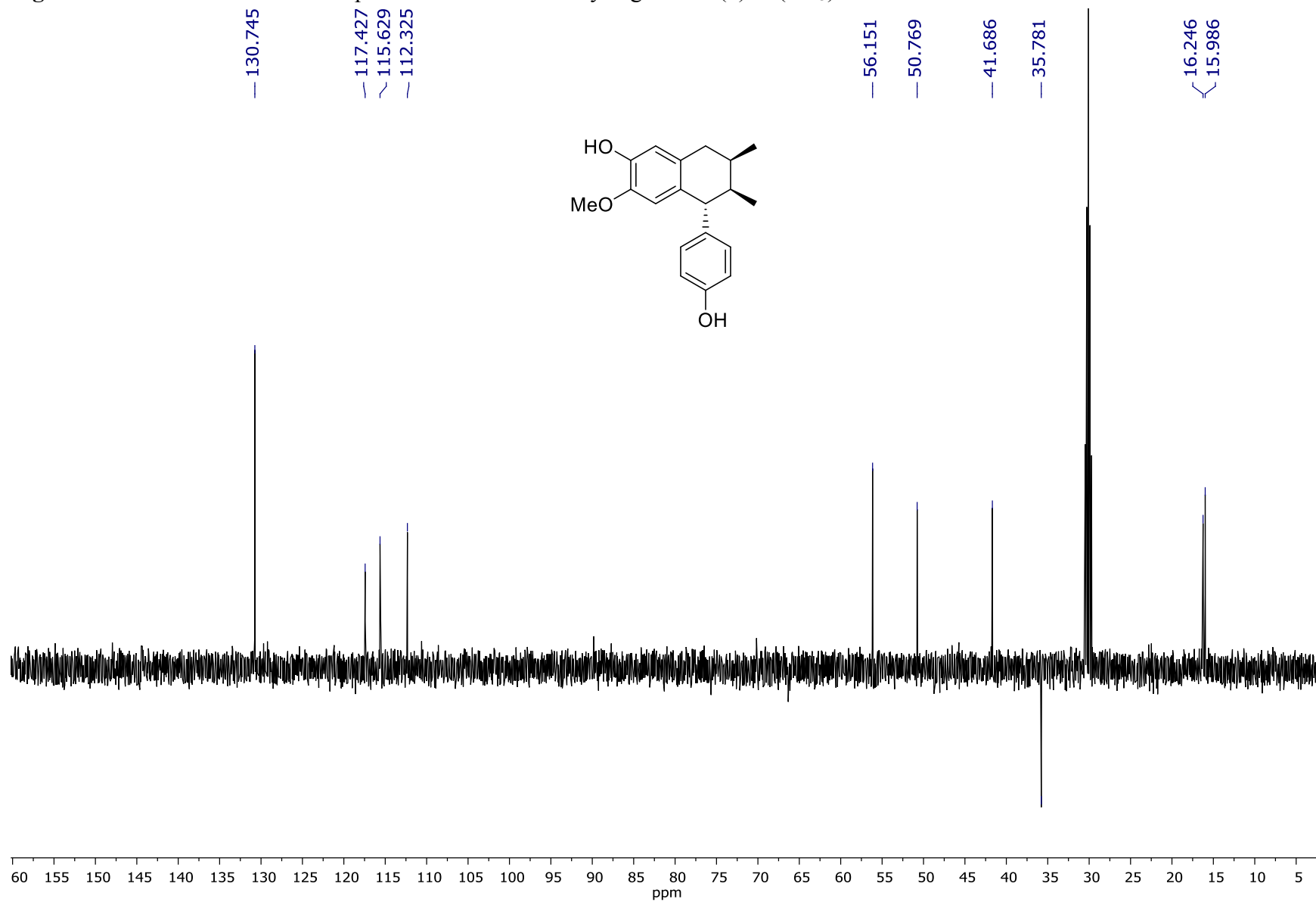


Figure S22. HMQC NMR spectrum of 3'-demethoxyisoguaiacin (**5**) in $(\text{CD}_3)_2\text{CO}$

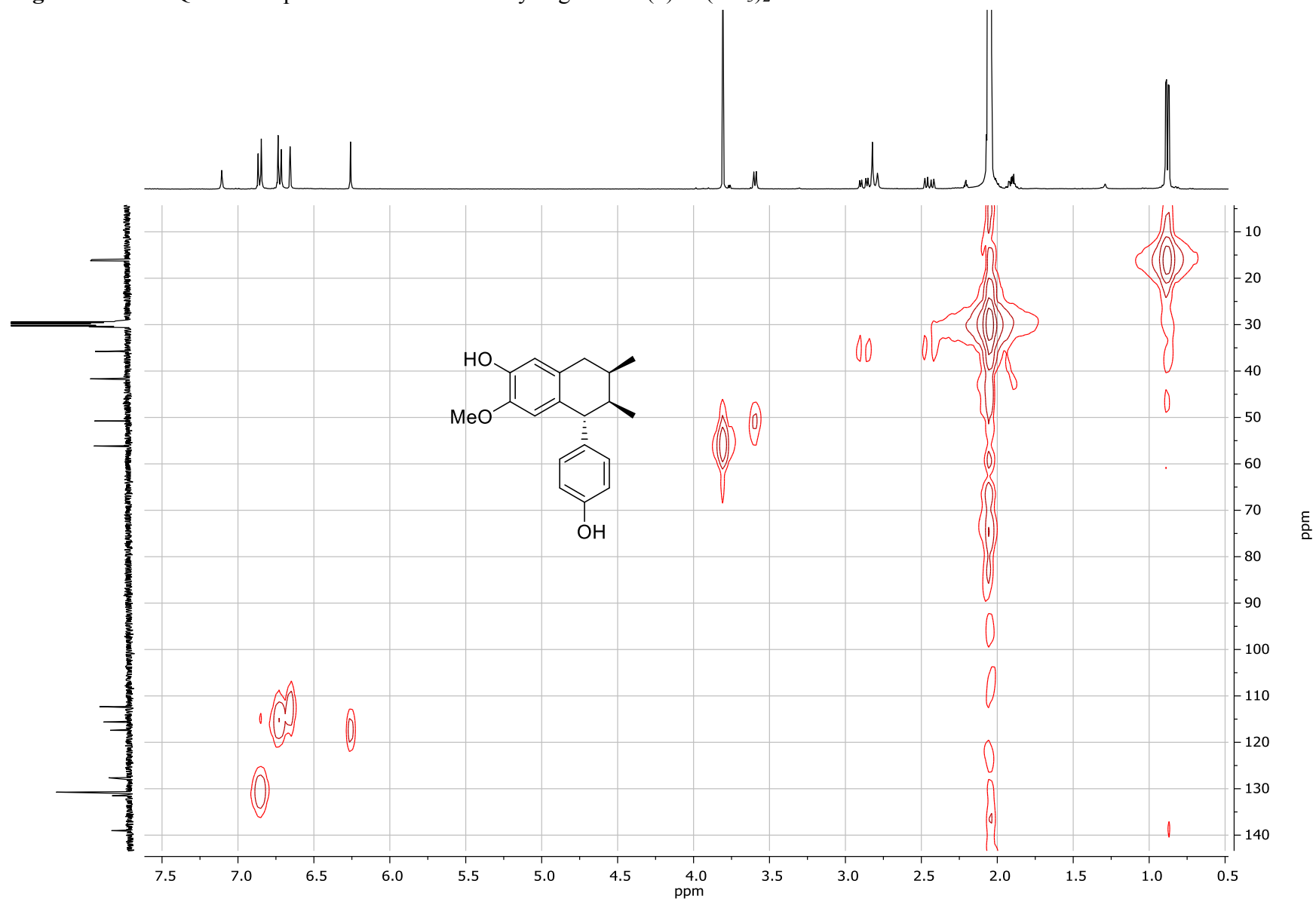


Figure S23. ^1H NMR spectrum of 6, 3'-di-*O*-demethoxy-isoguaiacin (**6**) in CD_3OD

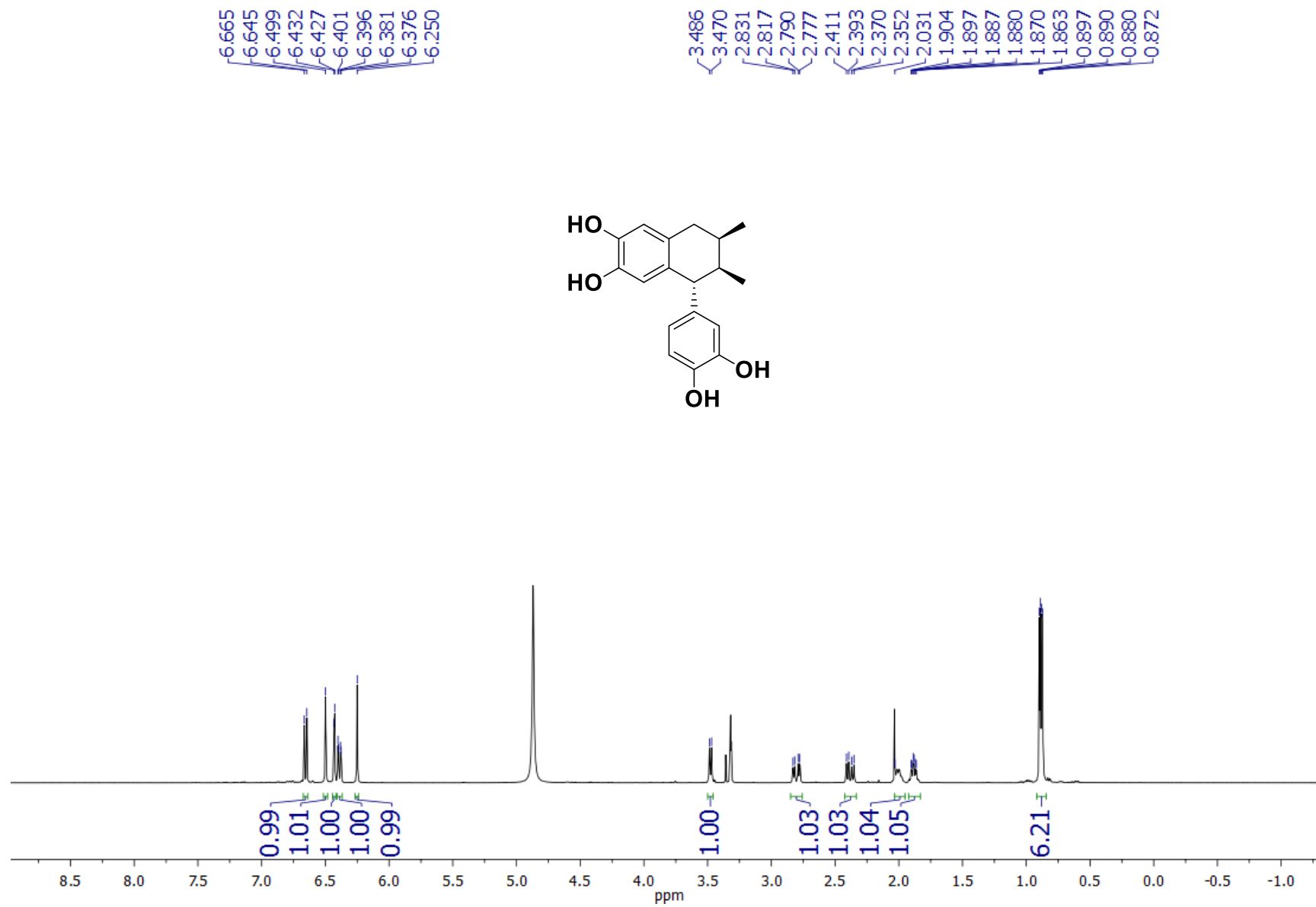


Figure S24. ^{13}C NMR spectrum of 6, 3'-di-*O*-demethoxy-isoguaiacin (**6**) in CD_3OD

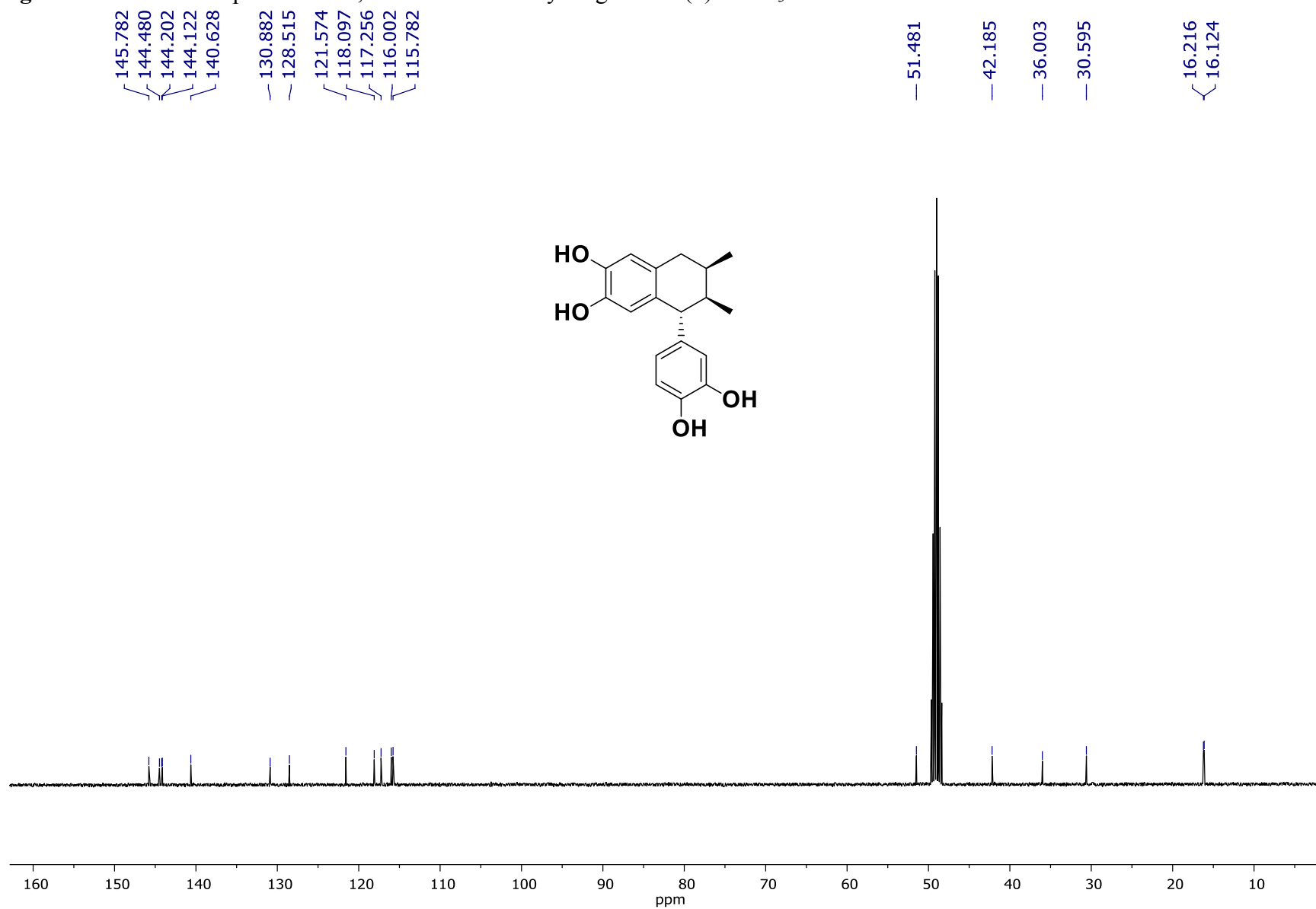


Figure S25. ^{13}C DEPT-135 NMR spectrum of 6, 3'-di-*O*-demethoxy-isoguaiacin (**6**) in CD_3OD

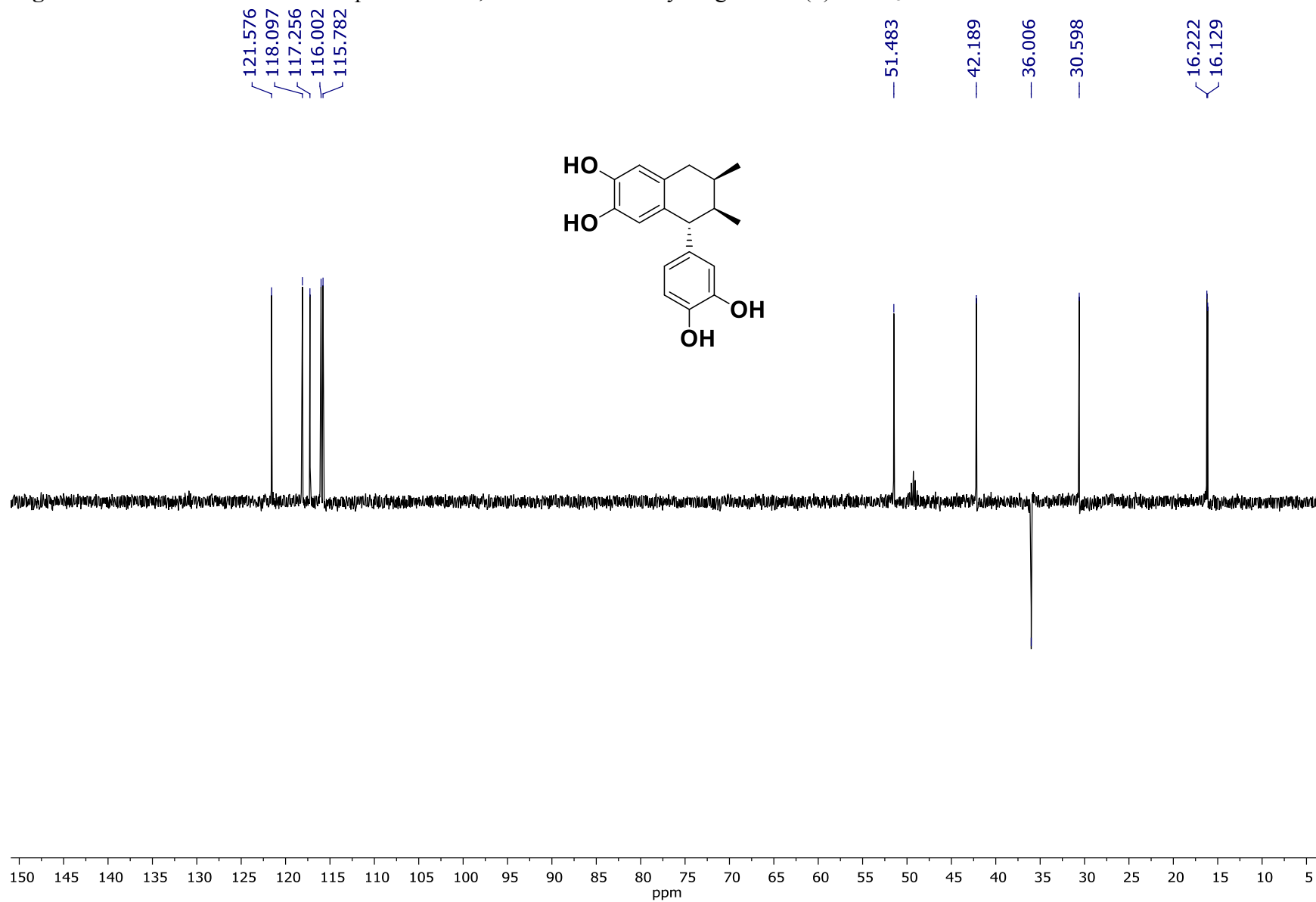


Figure S26. ¹H NMR spectrum of 3'-hydroxy-4-epi-larreatricin (**7**) in (CD₃)₂CO

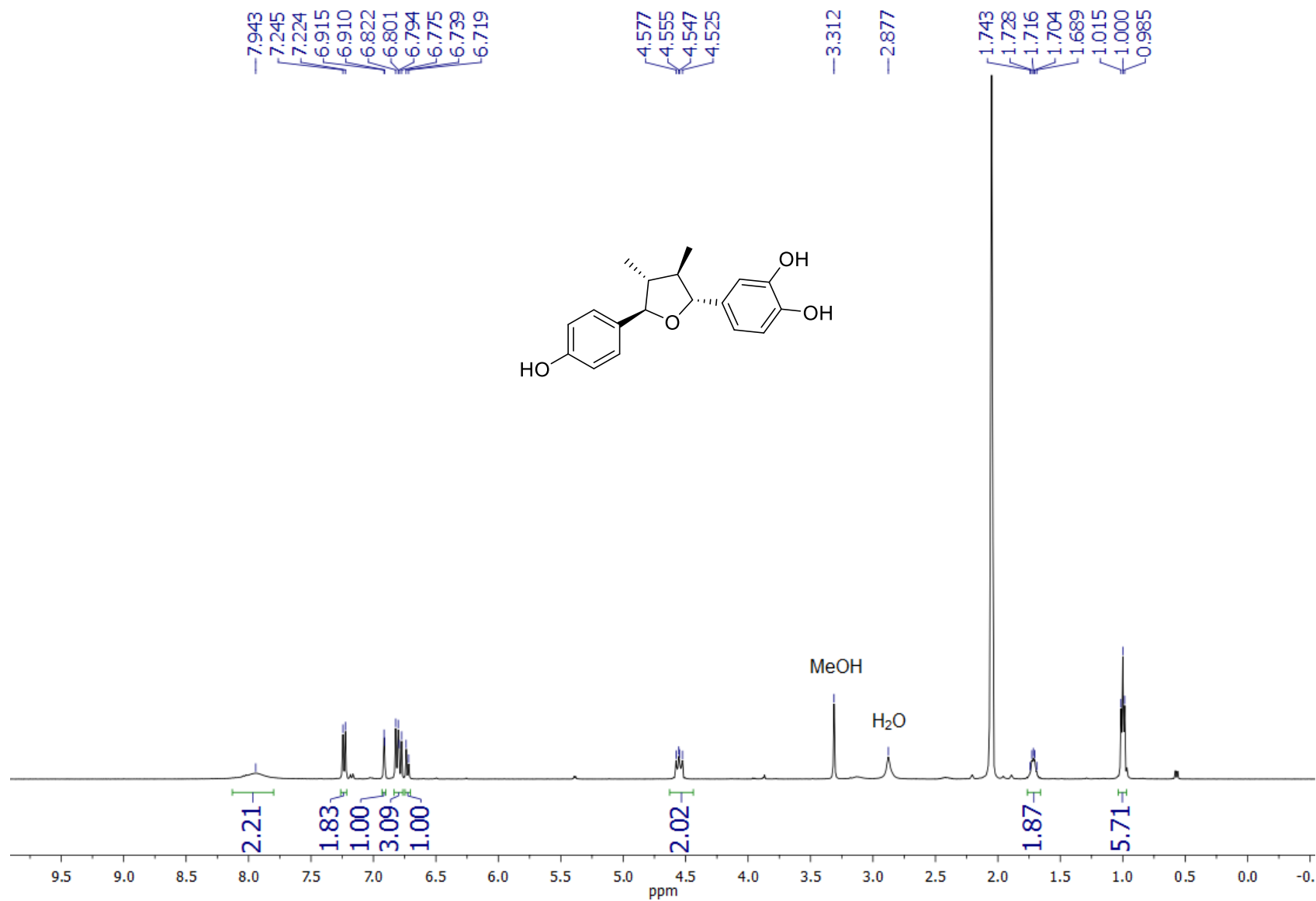


Figure S27. ^{13}C NMR spectrum of 3'-hydroxy-4-epi-larreatricin (7) in $(\text{CD}_3)_2\text{CO}$

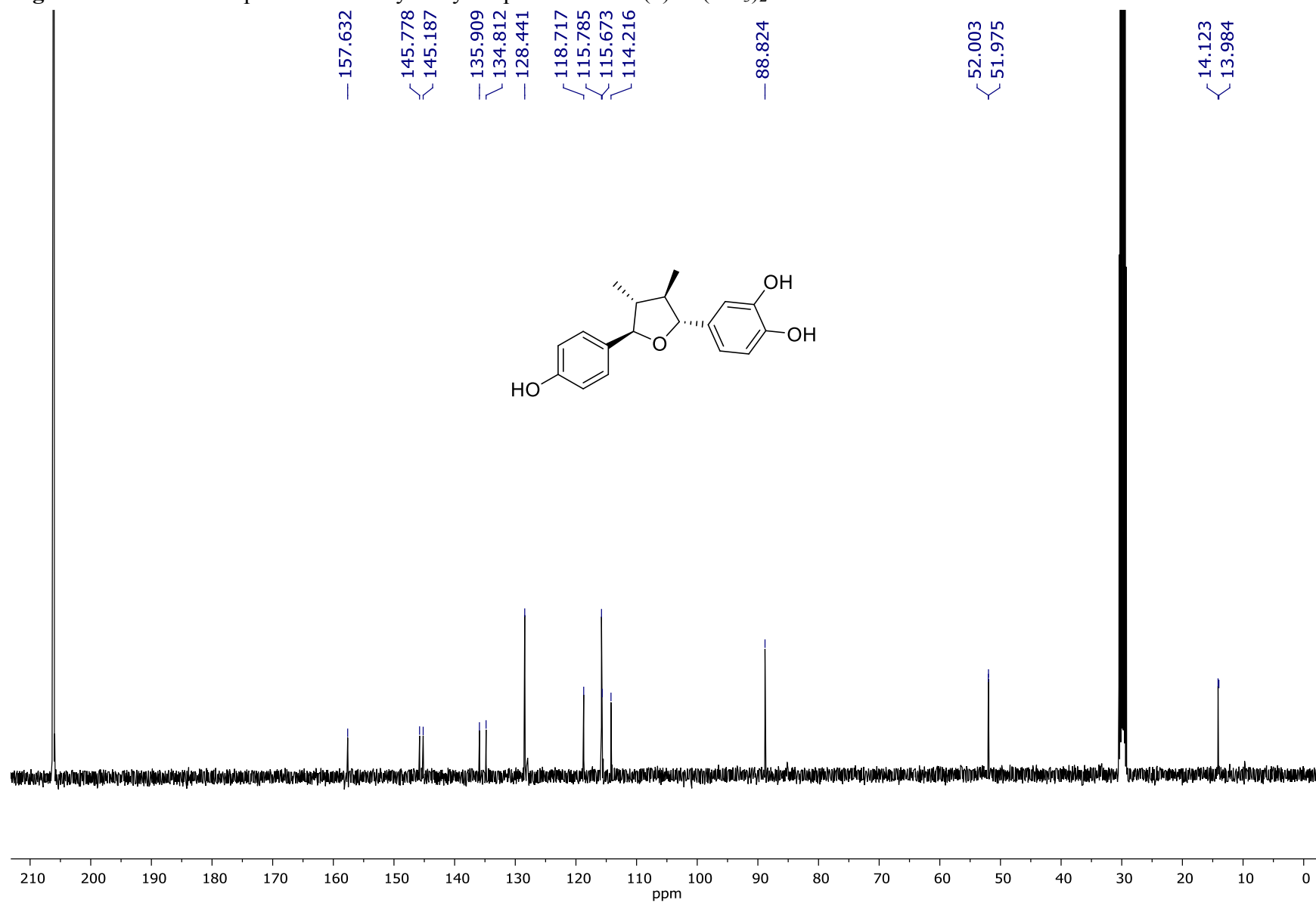


Figure S28. ^{13}C DEPT-135 NMR spectrum of 3'-hydroxy-4-epi-larreatricin (**7**) in $(\text{CD}_3)_2\text{CO}$

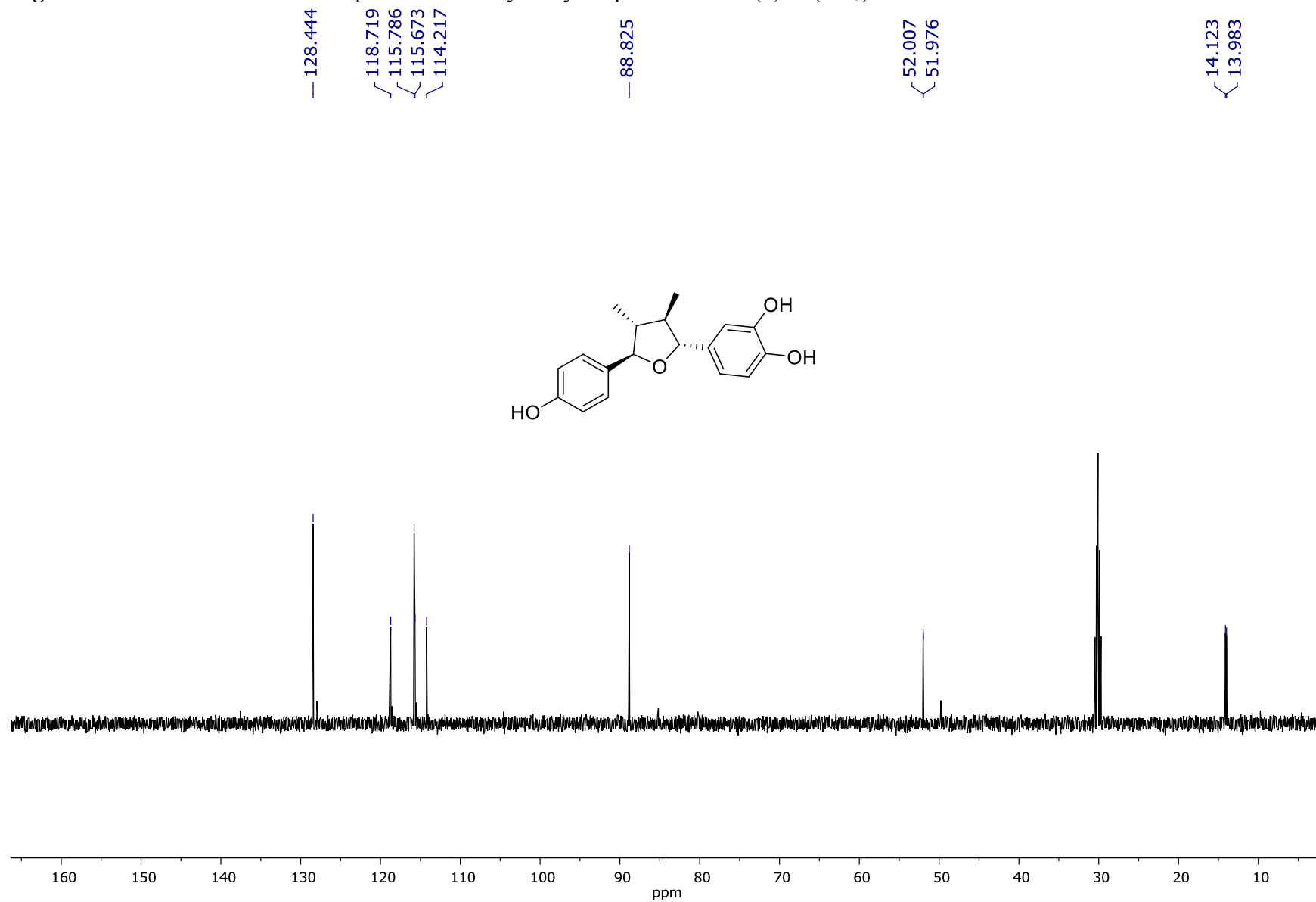


Figure S29. ^{13}C DEPT-90 NMR spectrum of 3'-hydroxy-4-epi-larreatricin (**7**) in $(\text{CD}_3)_2\text{CO}$

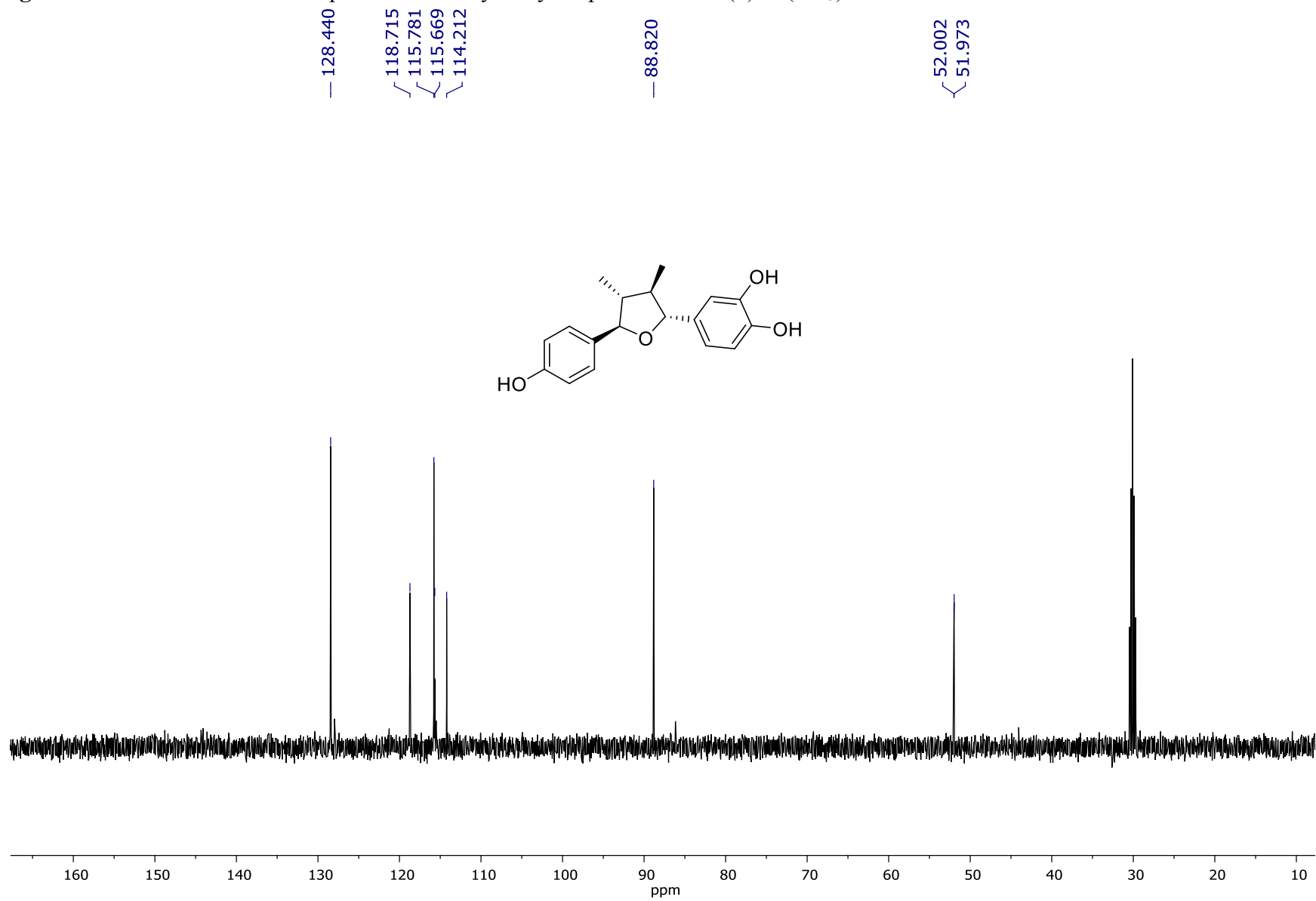


Figure S30. HMQC NMR spectrum of 3'-hydroxy-4-epi-larreatricin (**7**) in (CD₃)₂CO

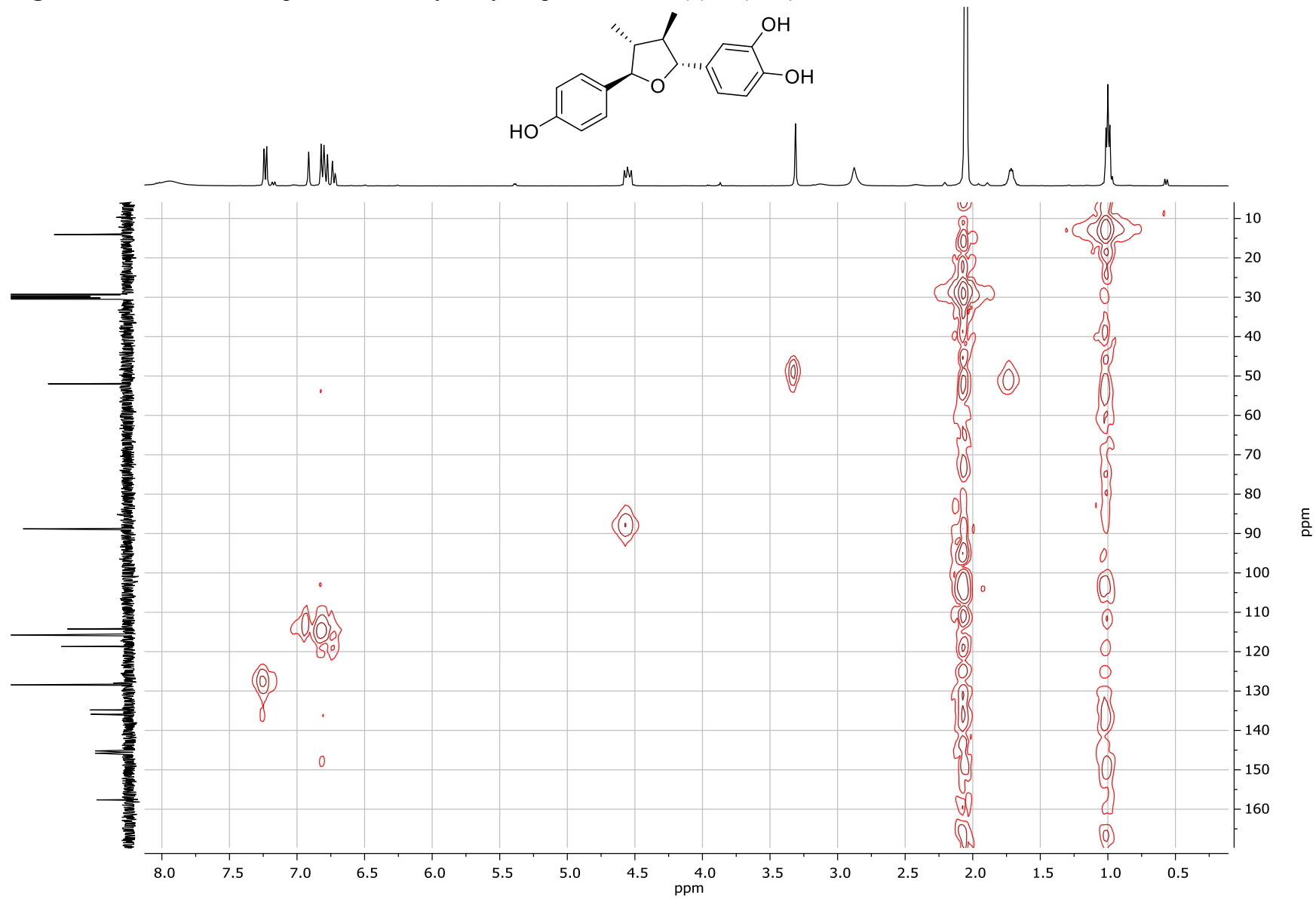


Figure S31. ^1H NMR spectrum of (7R, 7'R)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8R, 8'S)-8, 8'-dimethyltetrahydrofuran (**8**) in $(\text{CD}_3)_2\text{CO}$

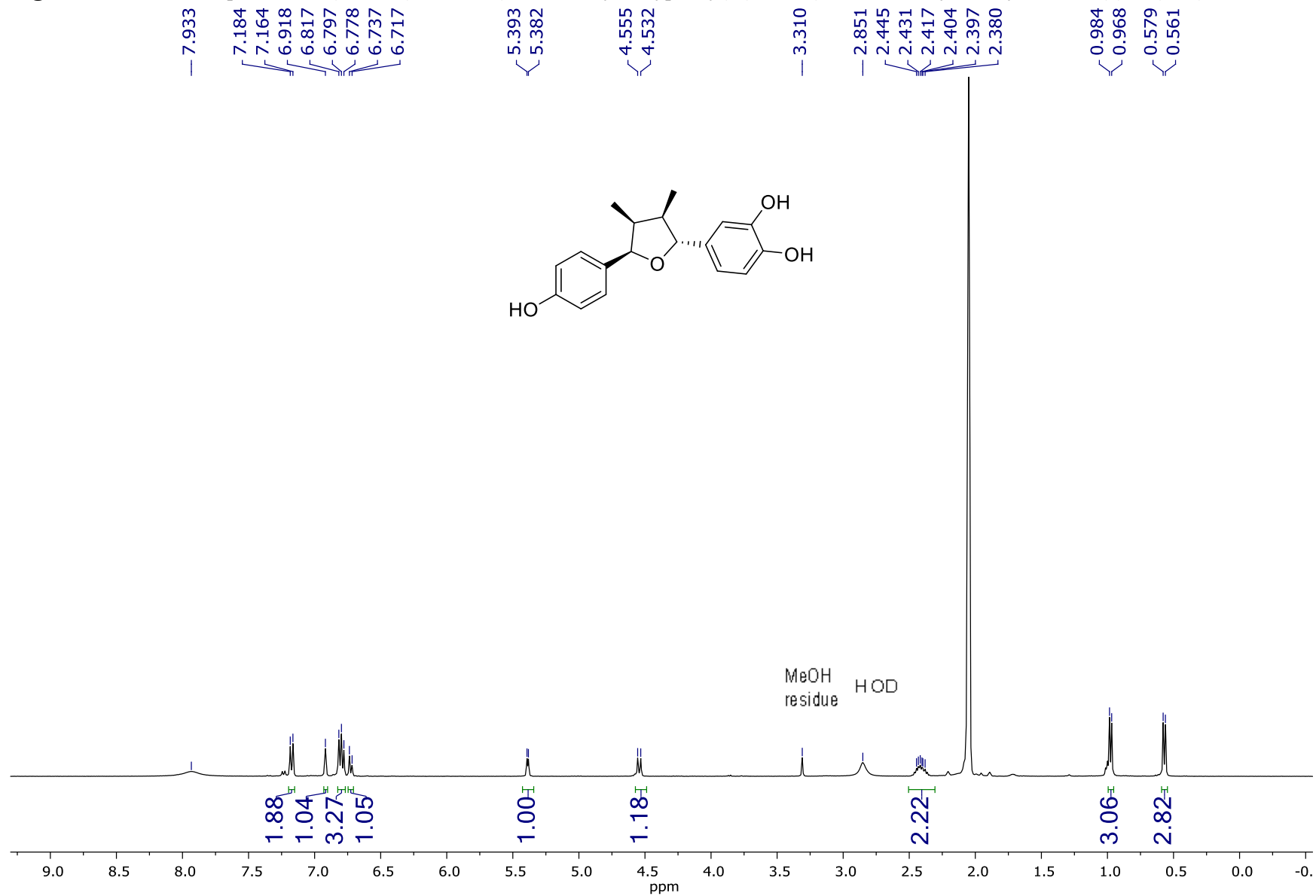


Figure S32. ^{13}C NMR spectrum of (7R, 7'R)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8R, 8'S)-8, 8'-dimethyltetrahydrofuran (**8**) in $(\text{CD}_3)_2\text{CO}$

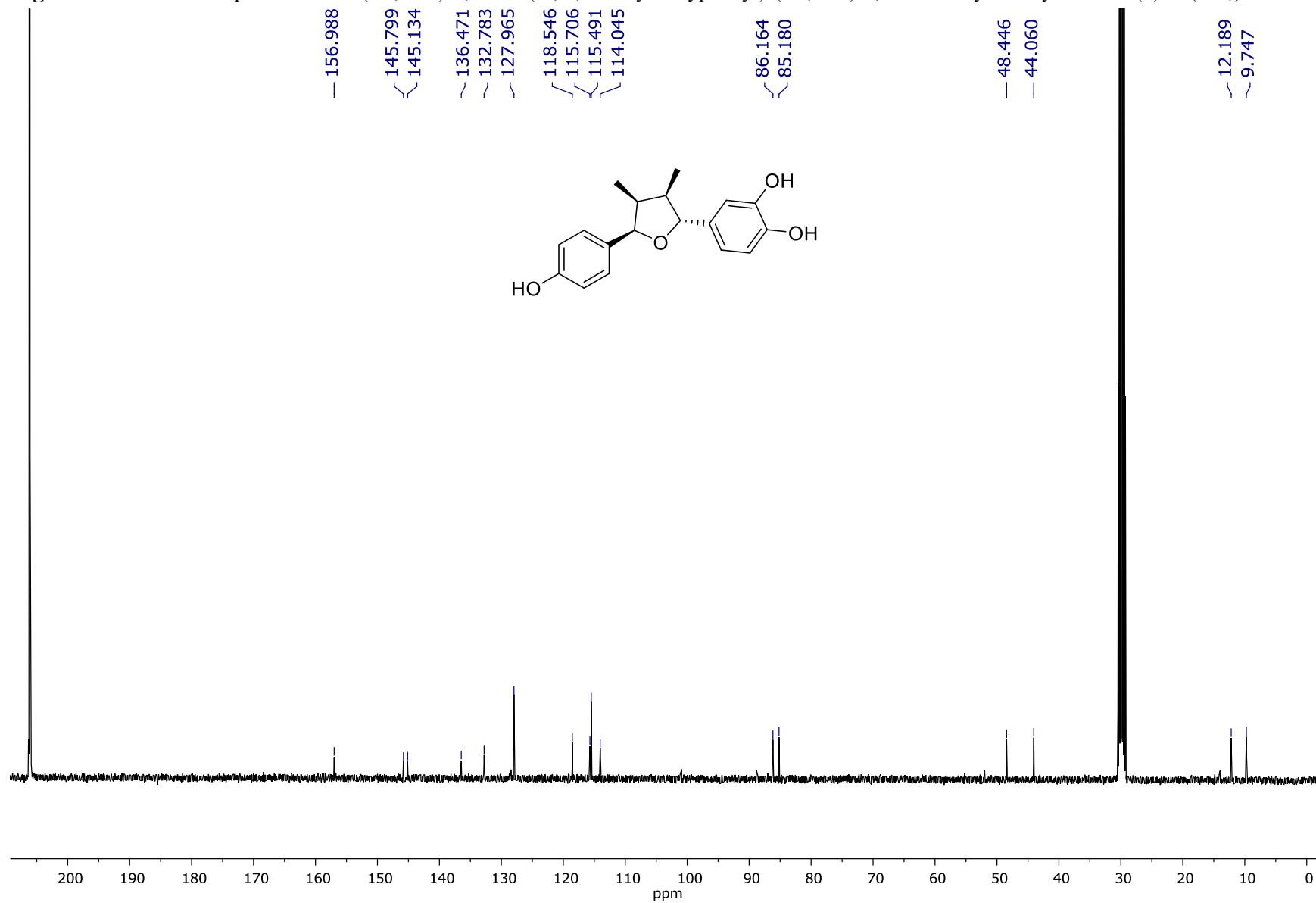


Figure S33. ^{13}C DEPT-135 NMR spectrum of (7R, 7'R)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8R, 8'S)-8, 8'-dimethyltetrahydrofuran (**8**) in $(\text{CD}_3)_2\text{CO}$

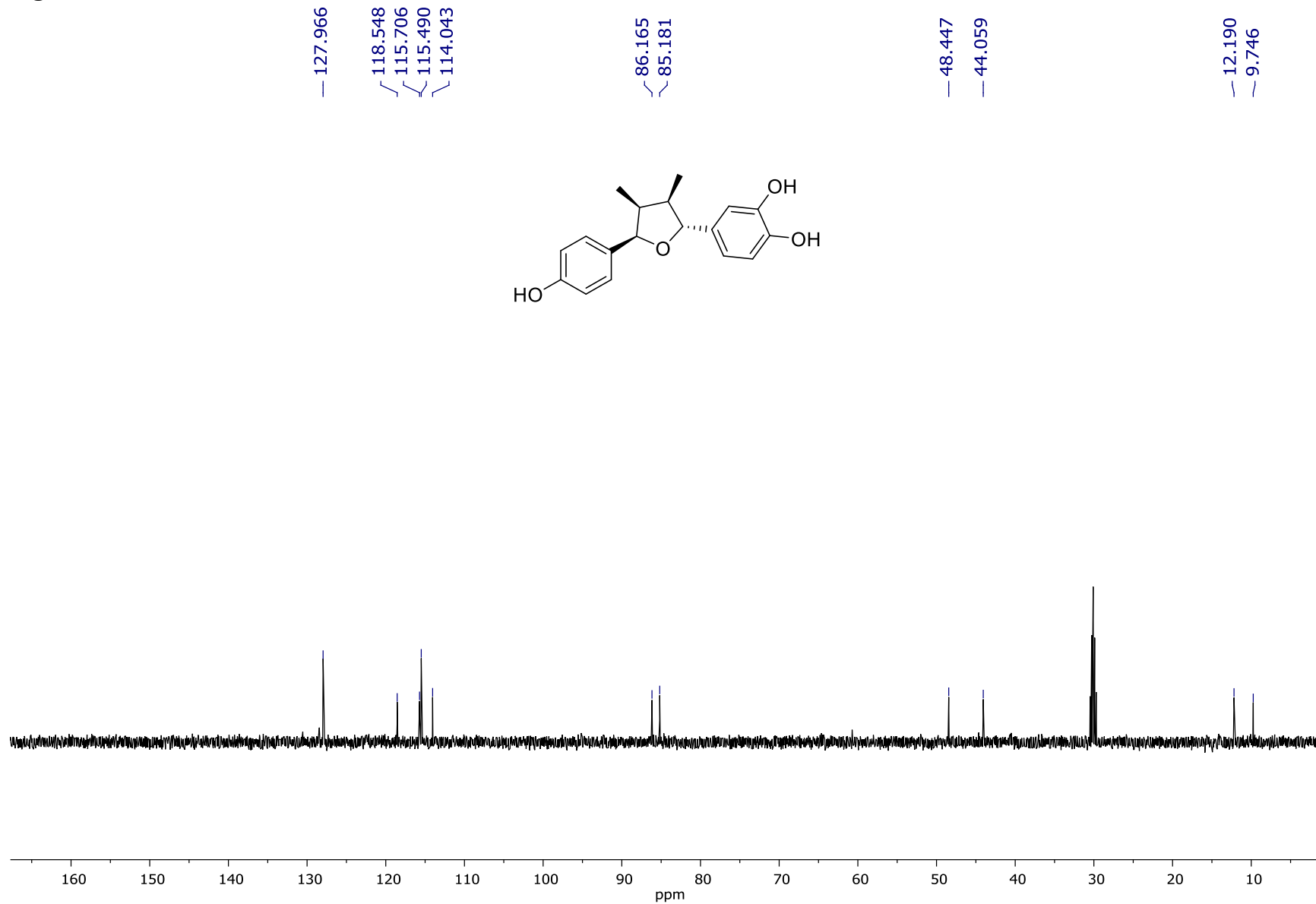


Figure S34. ^{13}C DEPT-90 NMR spectrum of (7R, 7'R)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8R, 8'S)-8, 8'-dimethyltetrahydrofuran (**8**) in $(\text{CD}_3)_2\text{CO}$

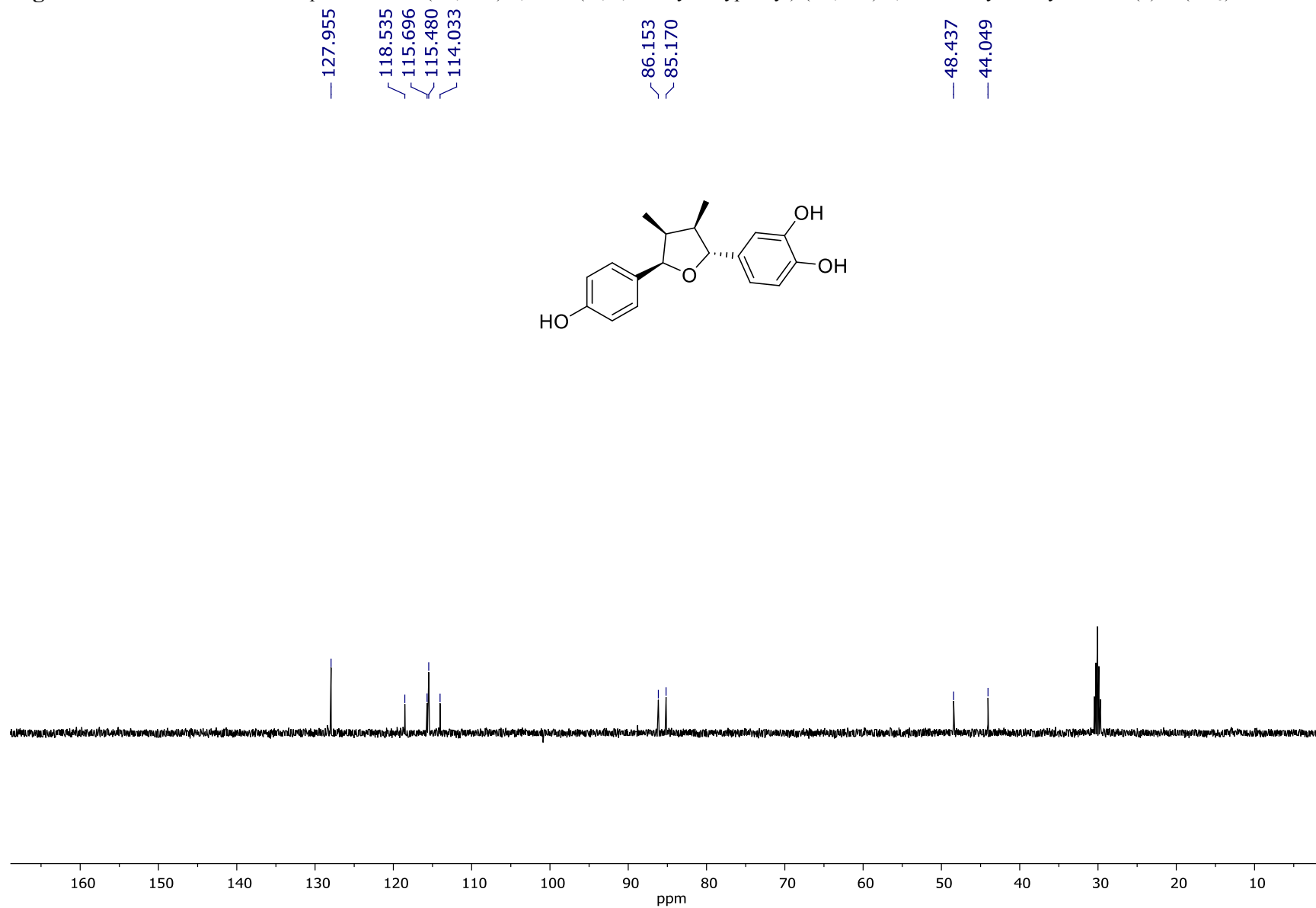


Figure S35. HMQC NMR spectrum of (7R, 7'R)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8R, 8'S)-8, 8'-dimethyltetrahydrofuran (**8**) in (CD₃)₂CO

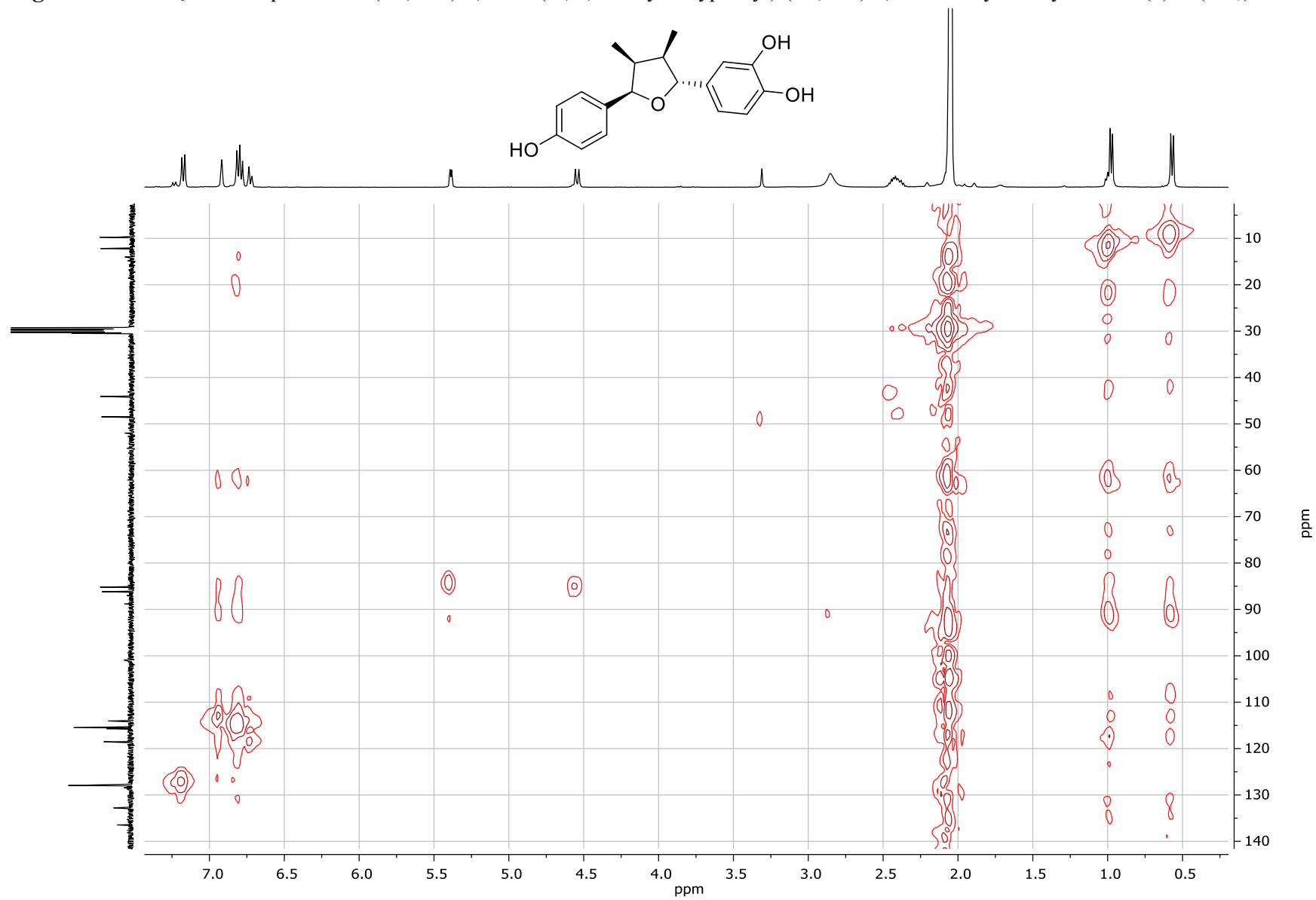


Figure S36. HMBC NMR spectrum of of (7R, 7'R)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8R, 8'S)-8, 8'-dimethyltetrahydrofuran (**8**) in (CD₃)₂CO

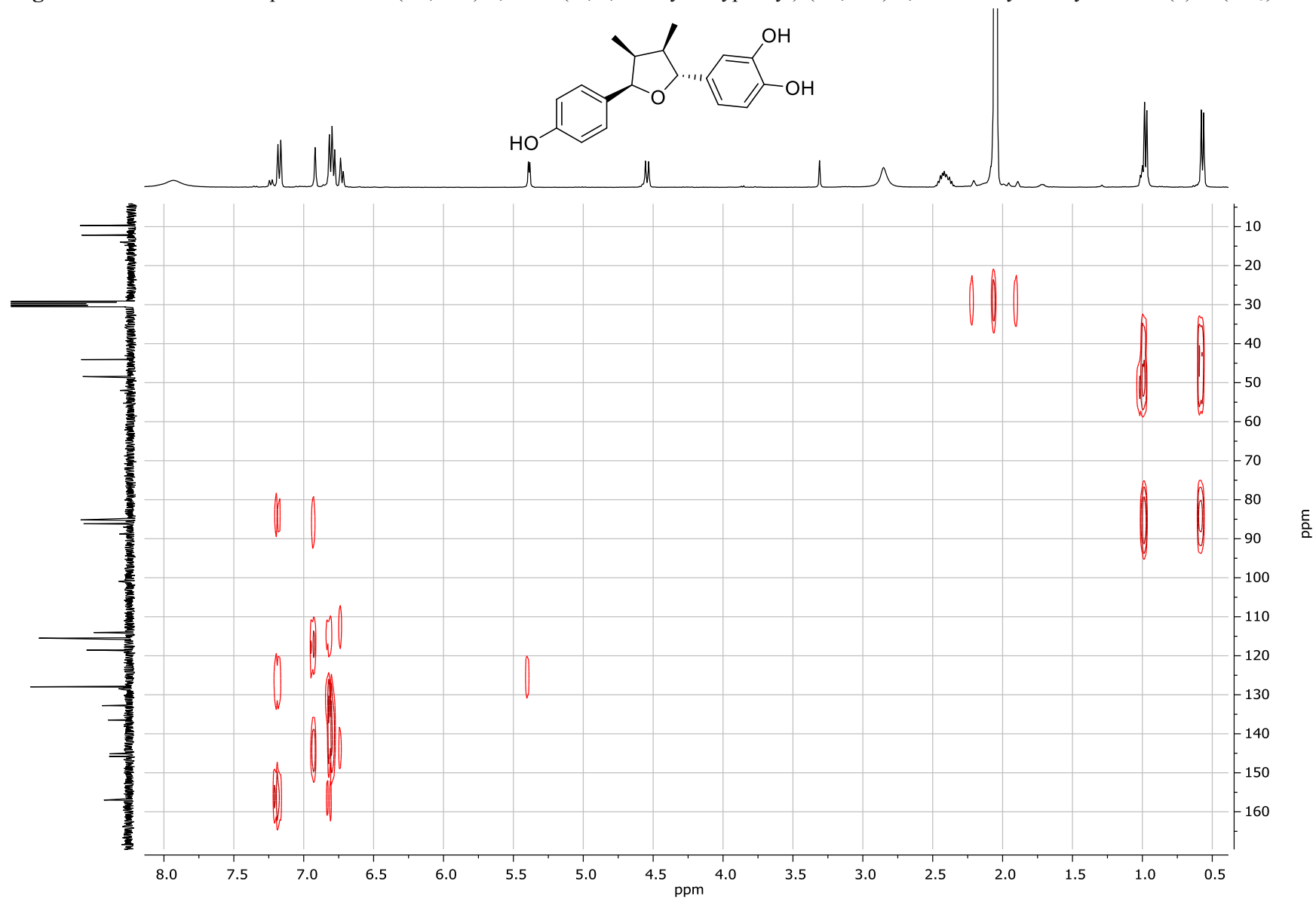


Figure S37. NOESY NMR spectrum of of (7R, 7'R)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8R, 8'S)-8, 8'-dimethyltetrahydrofuran (**8**) in (CD₃)₂CO

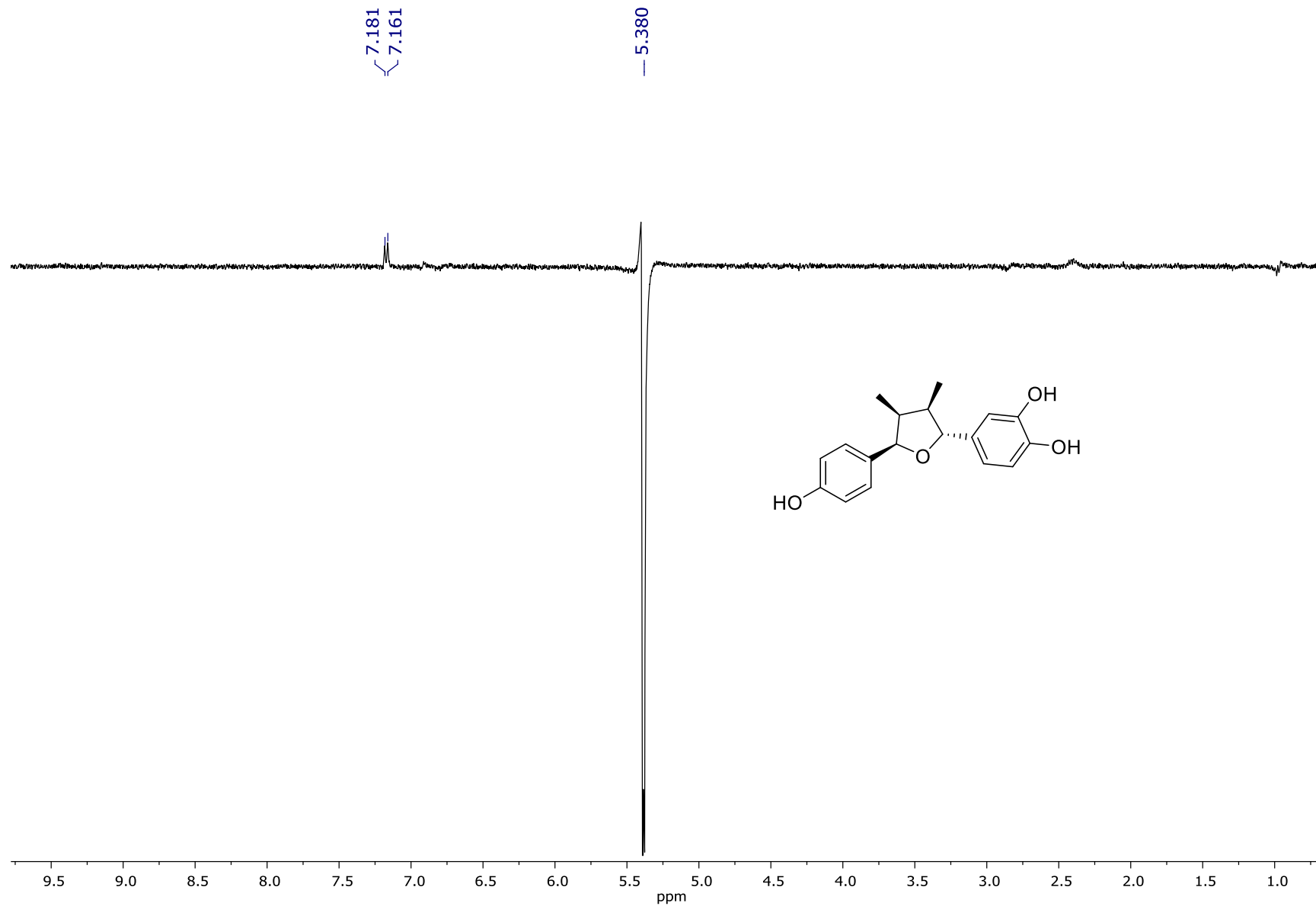


Figure S38. NOESY NMR spectrum of of (7R, 7'R)-7, 7'-bis(4', 3, 4-trihydroxyphenyl)-(8R, 8'S)-8, 8'-dimethyltetrahydrofuran (**8**) in (CD₃)₂CO

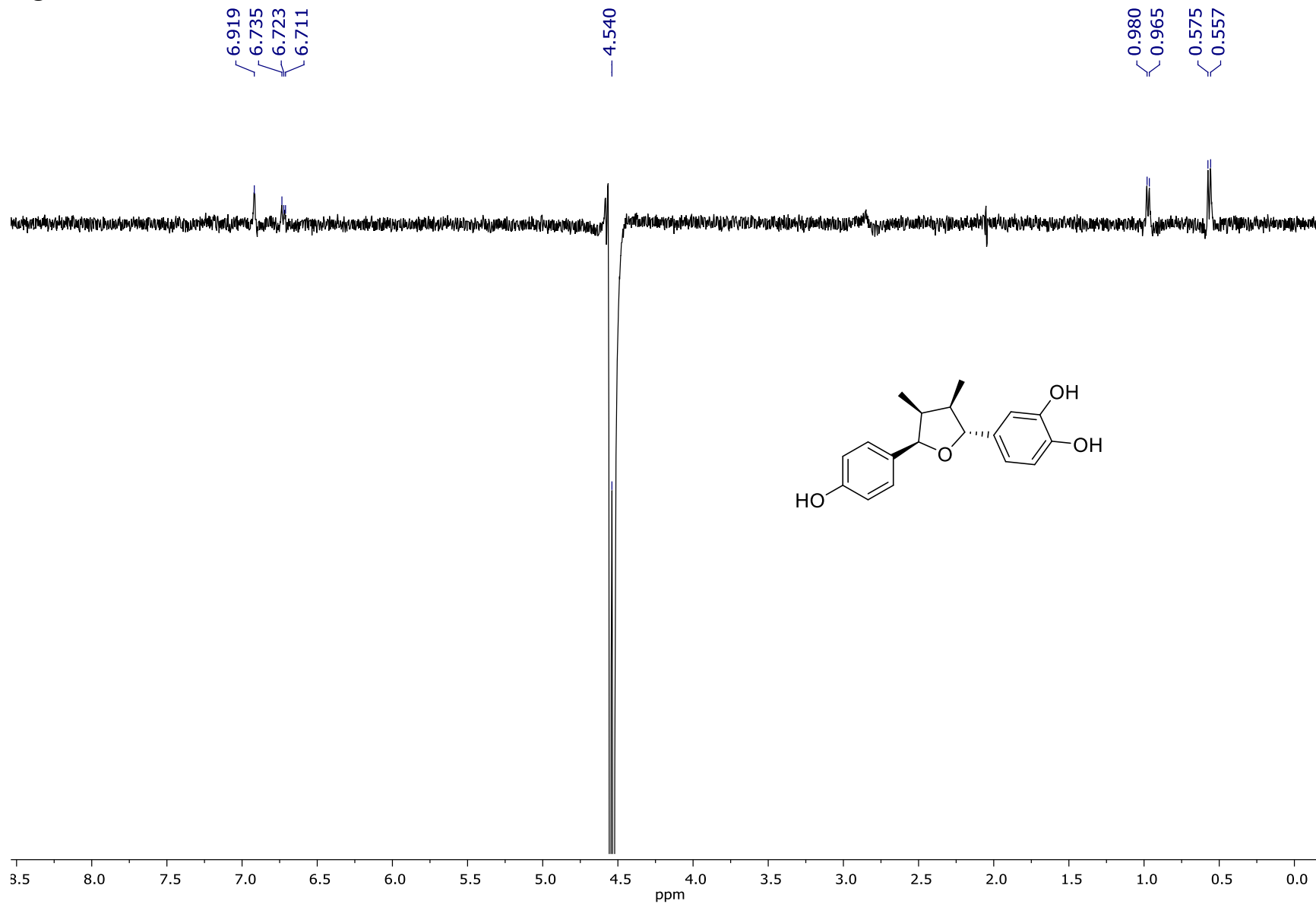


Figure S39. ^1H NMR spectrum of 3-methoxy-6, 7, 4'-trihydroxyflavone (**9**) in CDCl_3 and CD_3OD

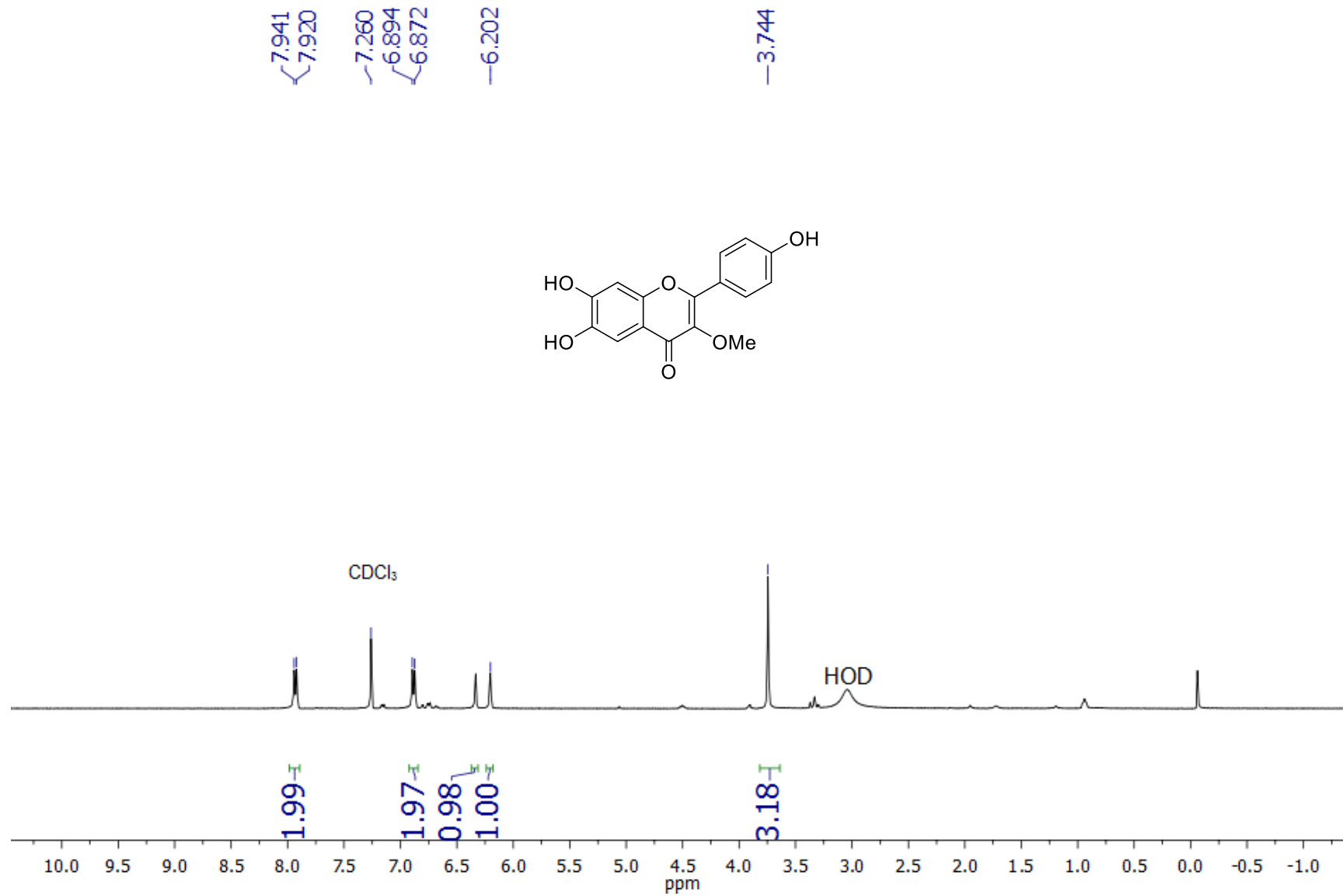


Figure S40. ^{13}C NMR spectrum of 3-methoxy-6, 7, 4'-trihydroxyflavone (**9**) in CDCl_3 and CD_3OD

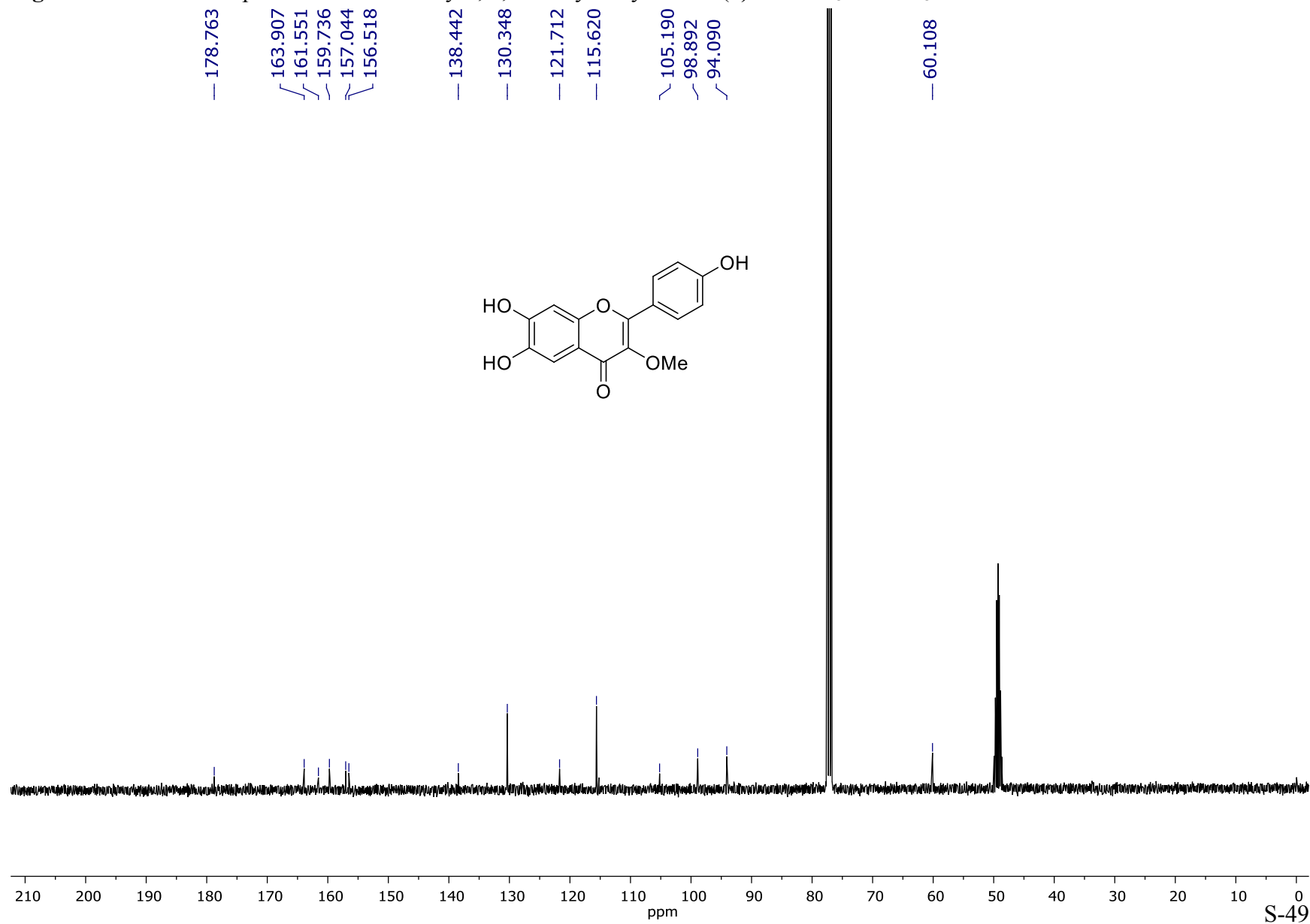


Figure S41. ^{13}C DEPT-135 NMR spectrum of 3-methoxy-6, 7, 4'-trihydroxyflavone (**9**) in CDCl_3 and CD_3OD

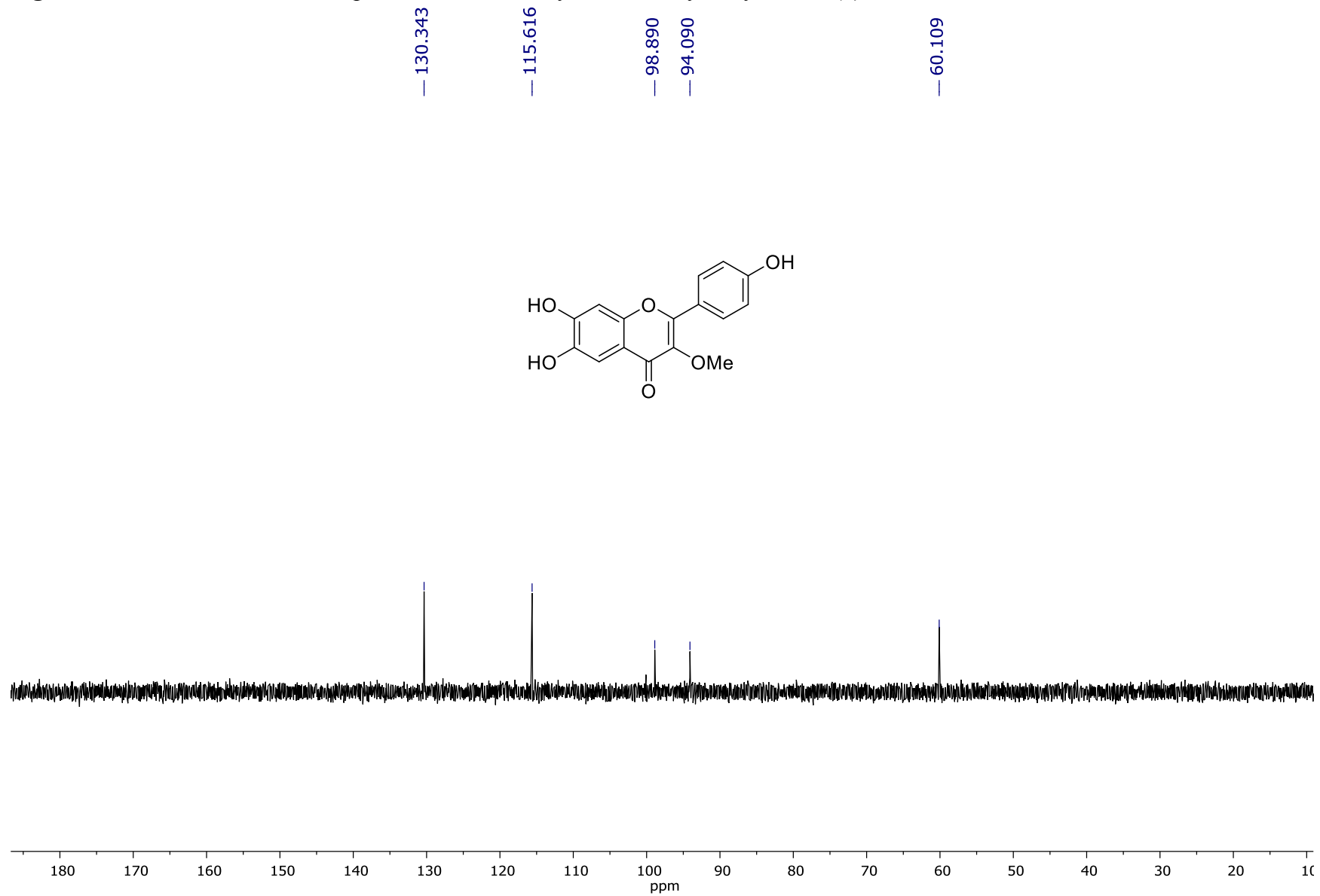


Figure S42. ^{13}C DEPT-90 NMR spectrum of 3-methoxy-6, 7, 4'-trihydroxyflavone (**9**) in CDCl_3 and CD_3OD

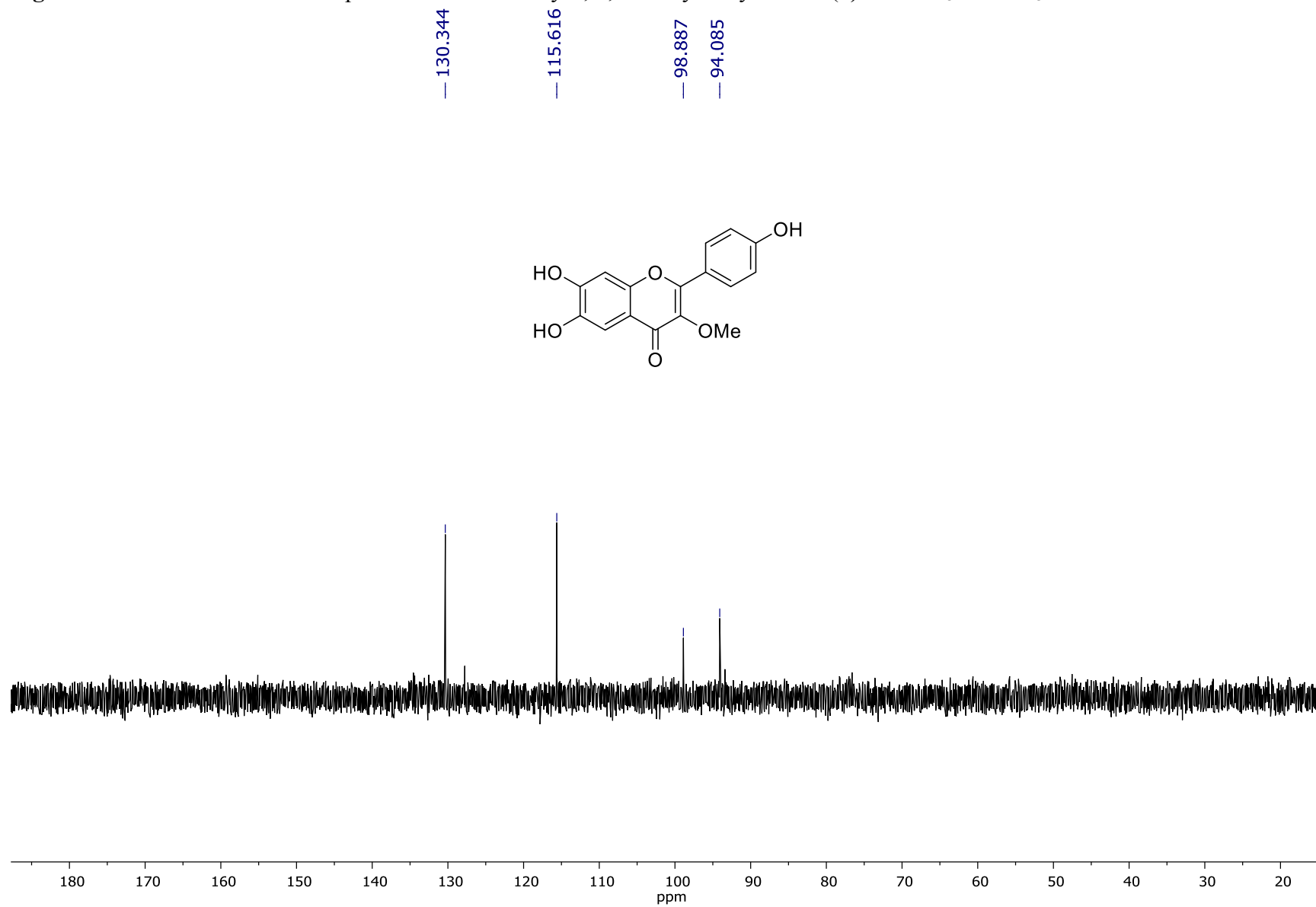


Figure S43. HMQC NMR spectrum of 3-methoxy-6, 7, 4'-trihydroxyflavone (**9**) in CDCl₃ and CD₃OD

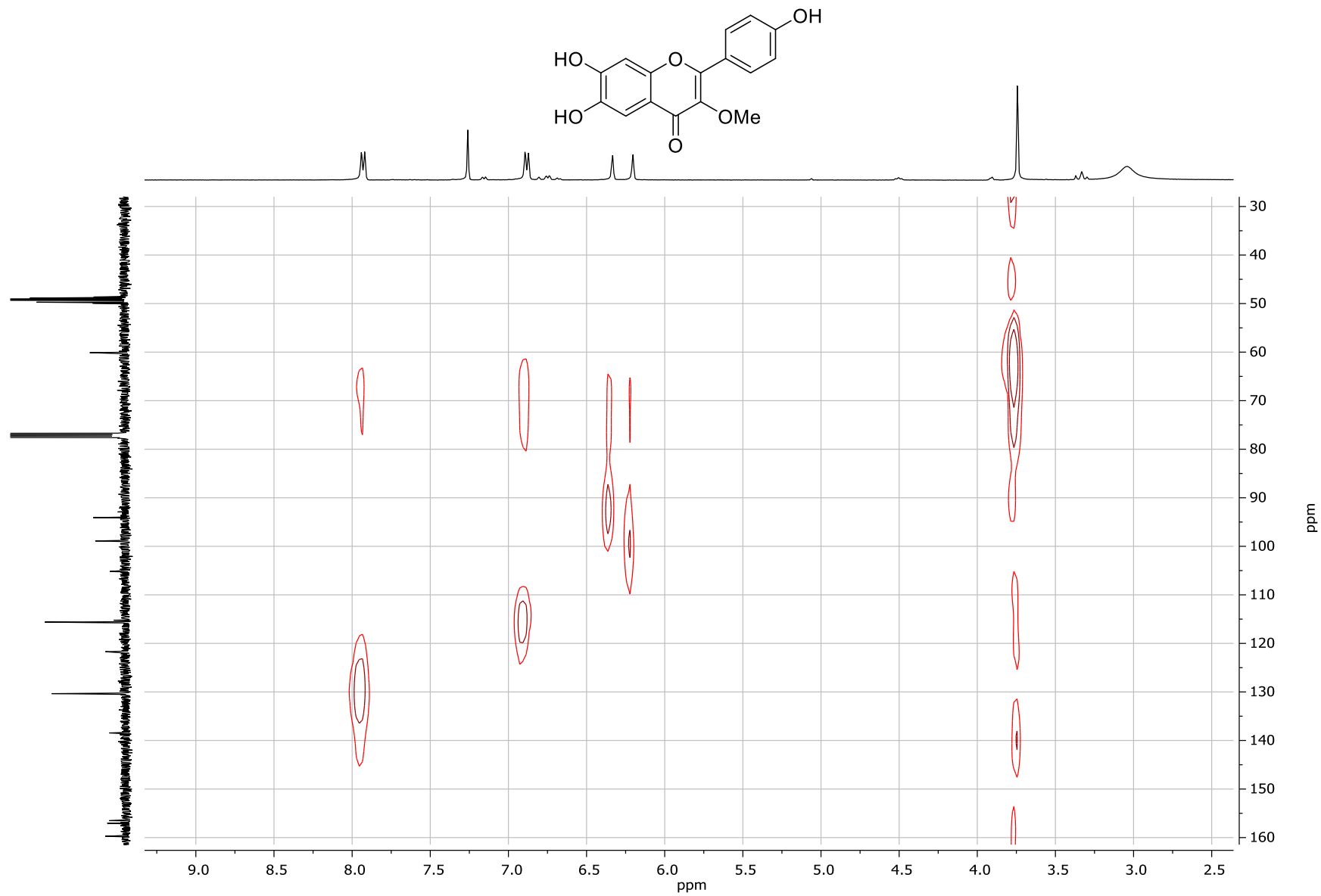


Figure S44. HMBC NMR spectrum of 3-methoxy-6, 7, 4'-trihydroxyflavone (**9**) in CDCl₃ and CD₃OD

