

Supporting Information

Azaphilones and *p*-Terphenyls from the Mangrove Endophytic Fungus

Penicillium chermesinum (ZH4-E2) Isolated from the South China Sea

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Figure S1. ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectra of the New Compound (**1**) (CDCl_3)

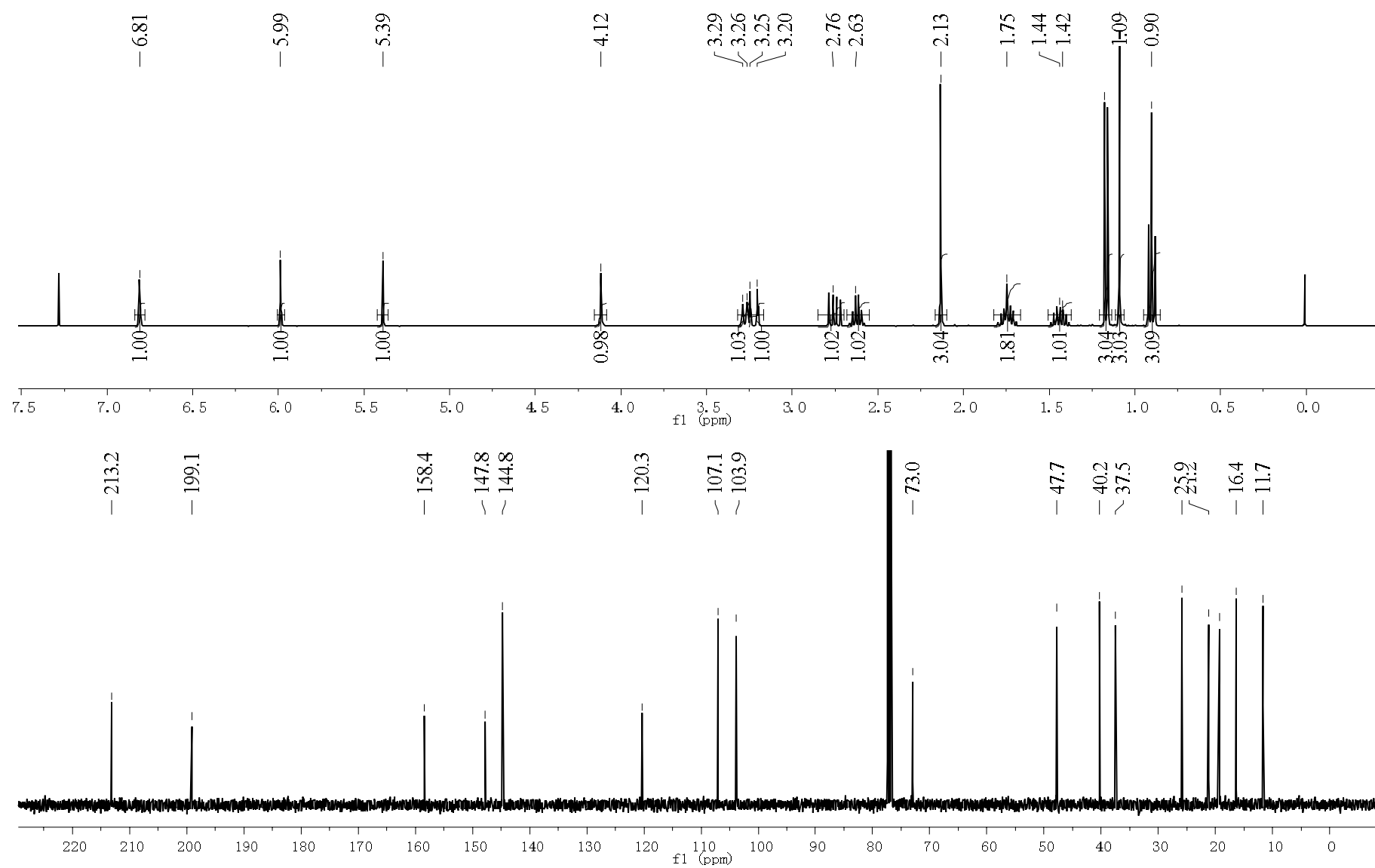


Figure S2. ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectra of the New Compound (1) (**DMSO- d_6**)

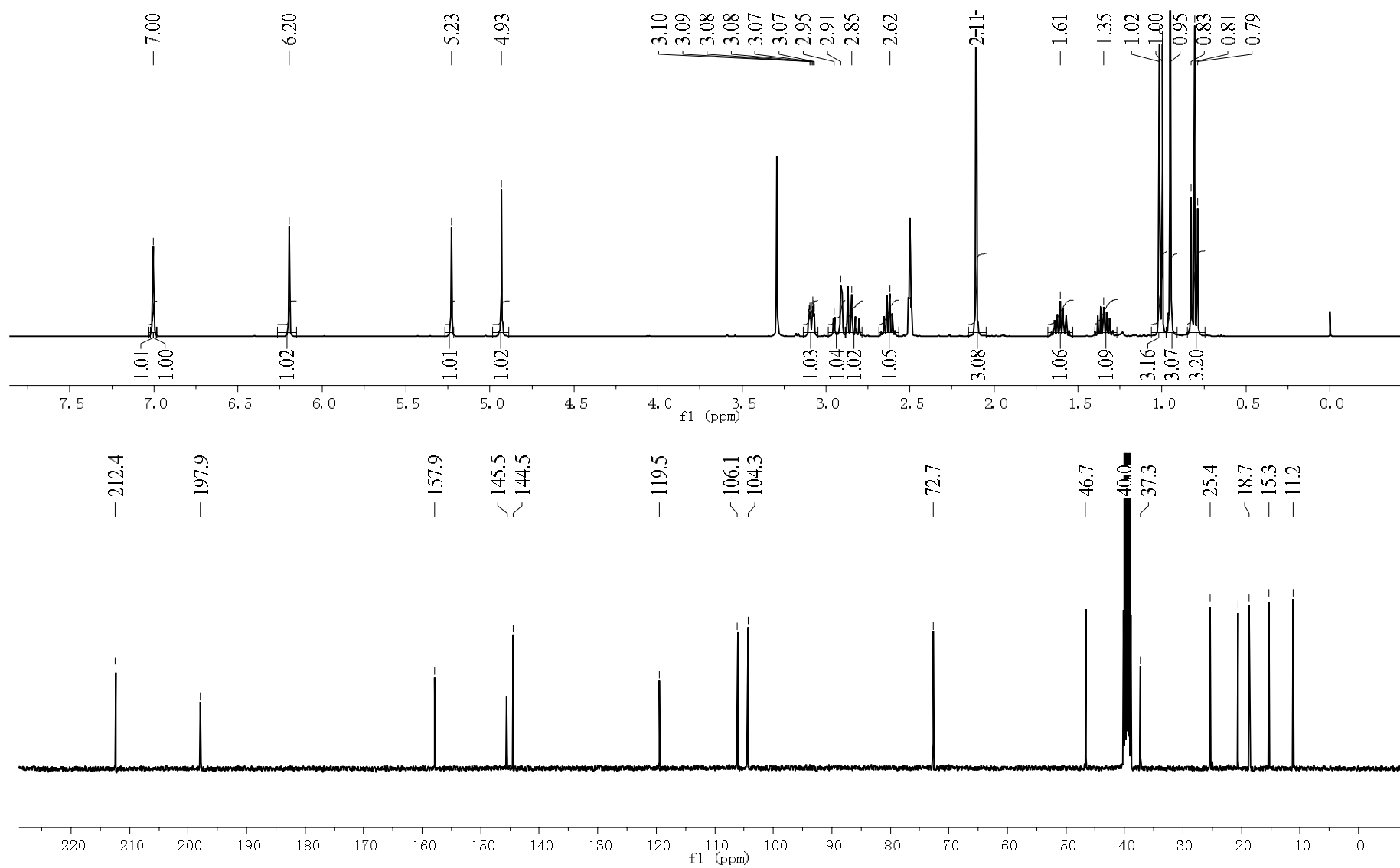


Figure S3. ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectra of the New Compound (**2**) (CDCl_3).

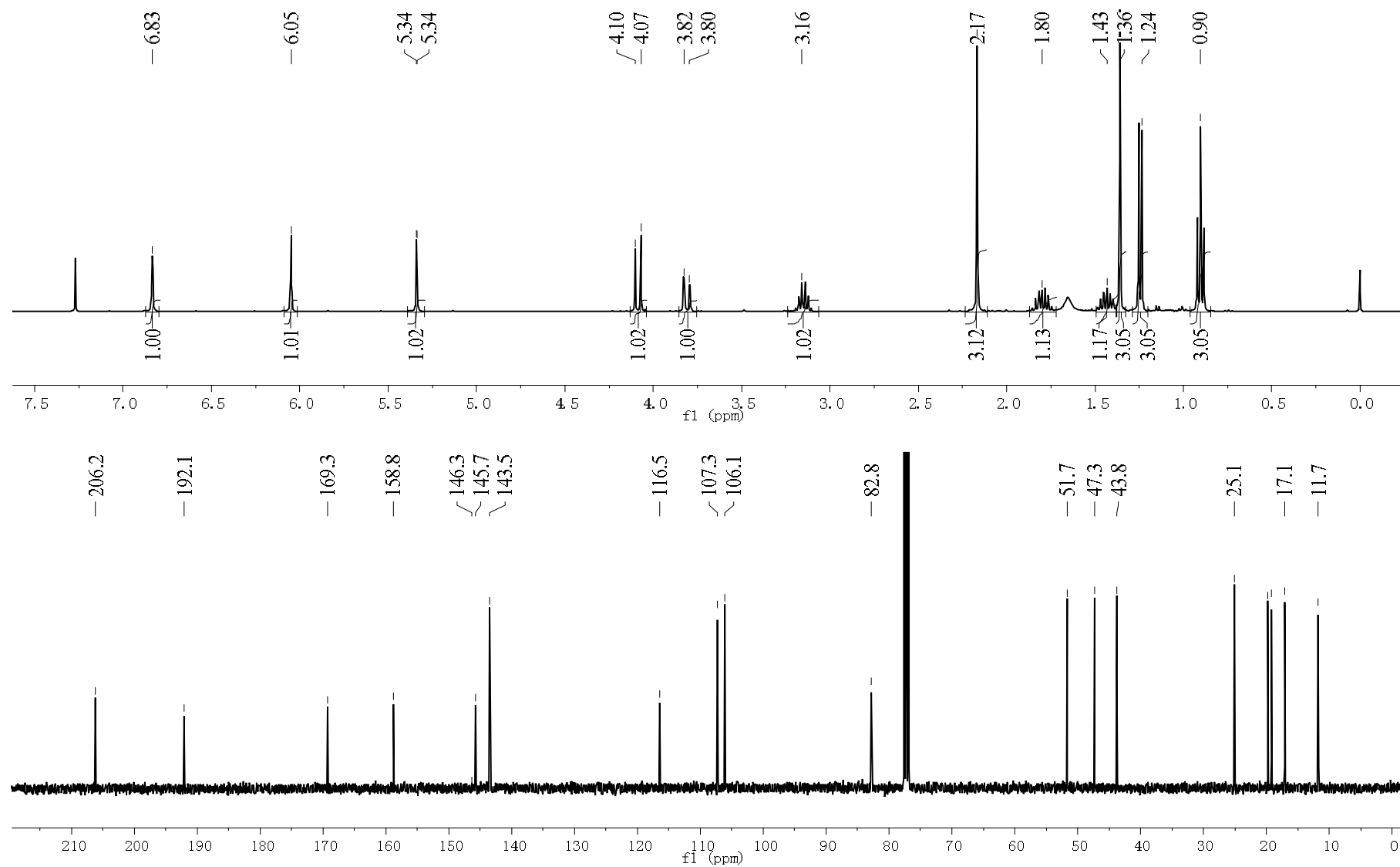


Figure S4. ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectra of the New Compound (**2**) (**DMSO- d_6**).

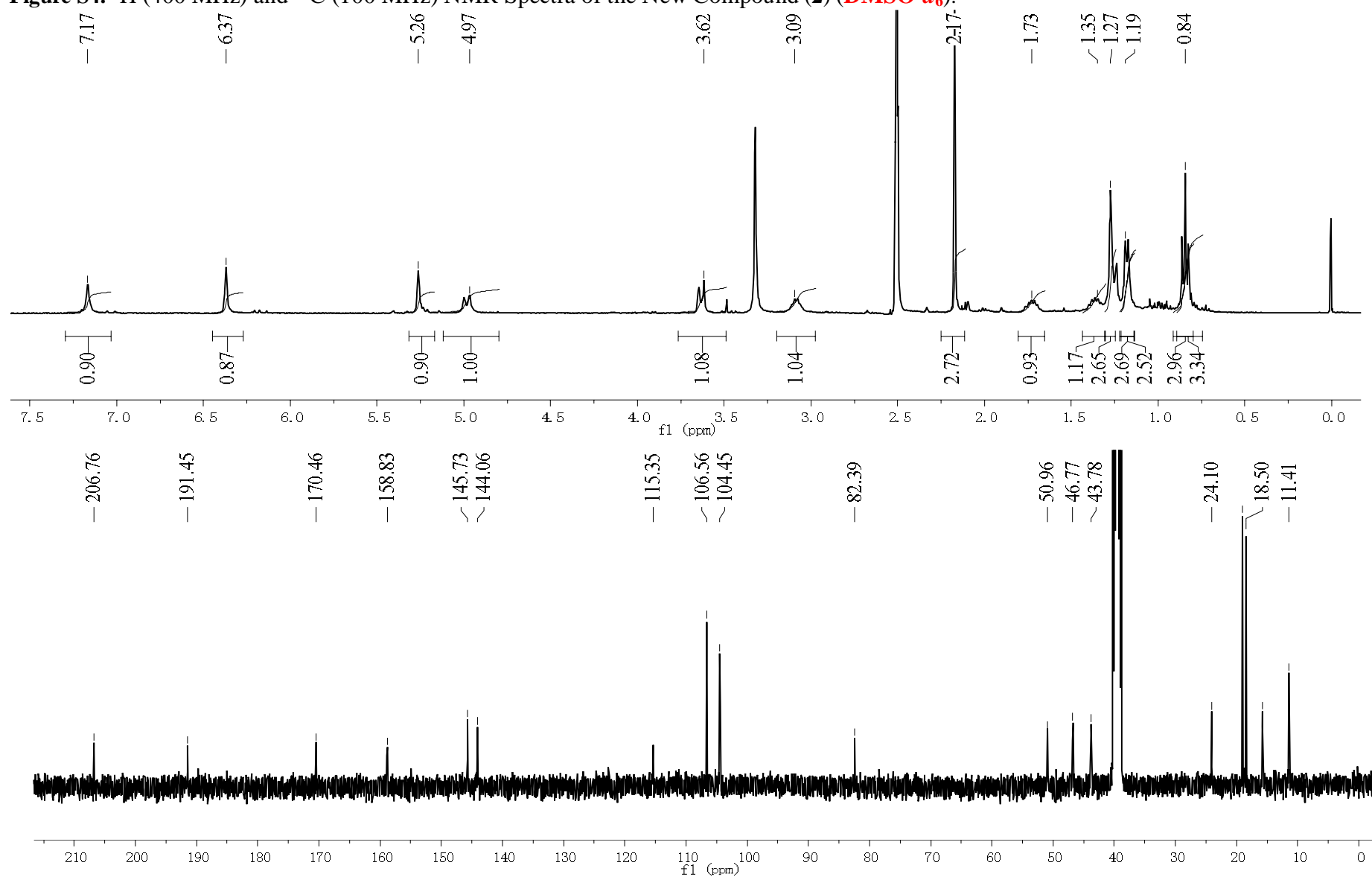


Figure S5. ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectra of the New Compound (**3**) (**DMSO- d_6**)

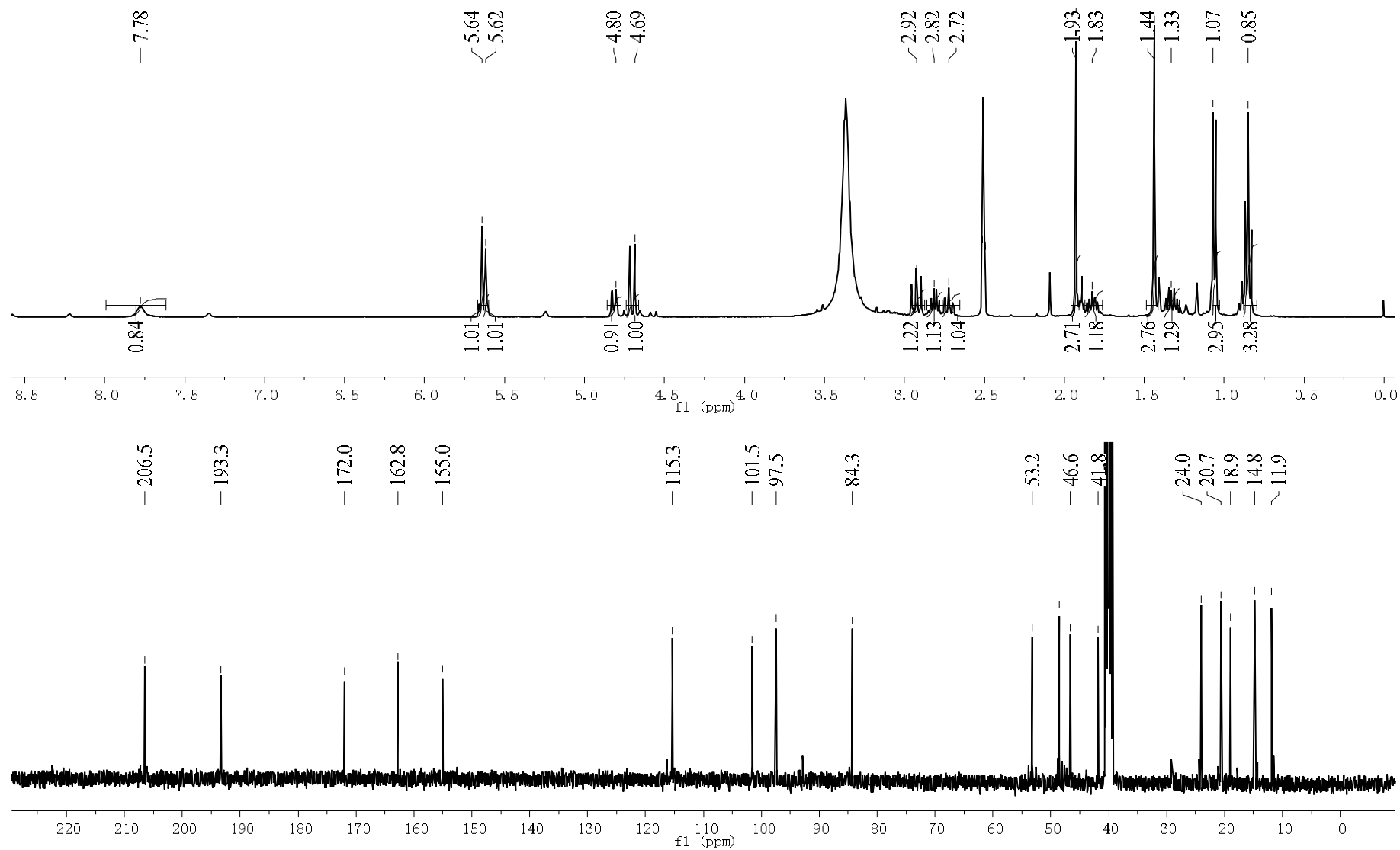


Figure S6. ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectra of the New Compound (**4**) (**Acetone- d_6**)

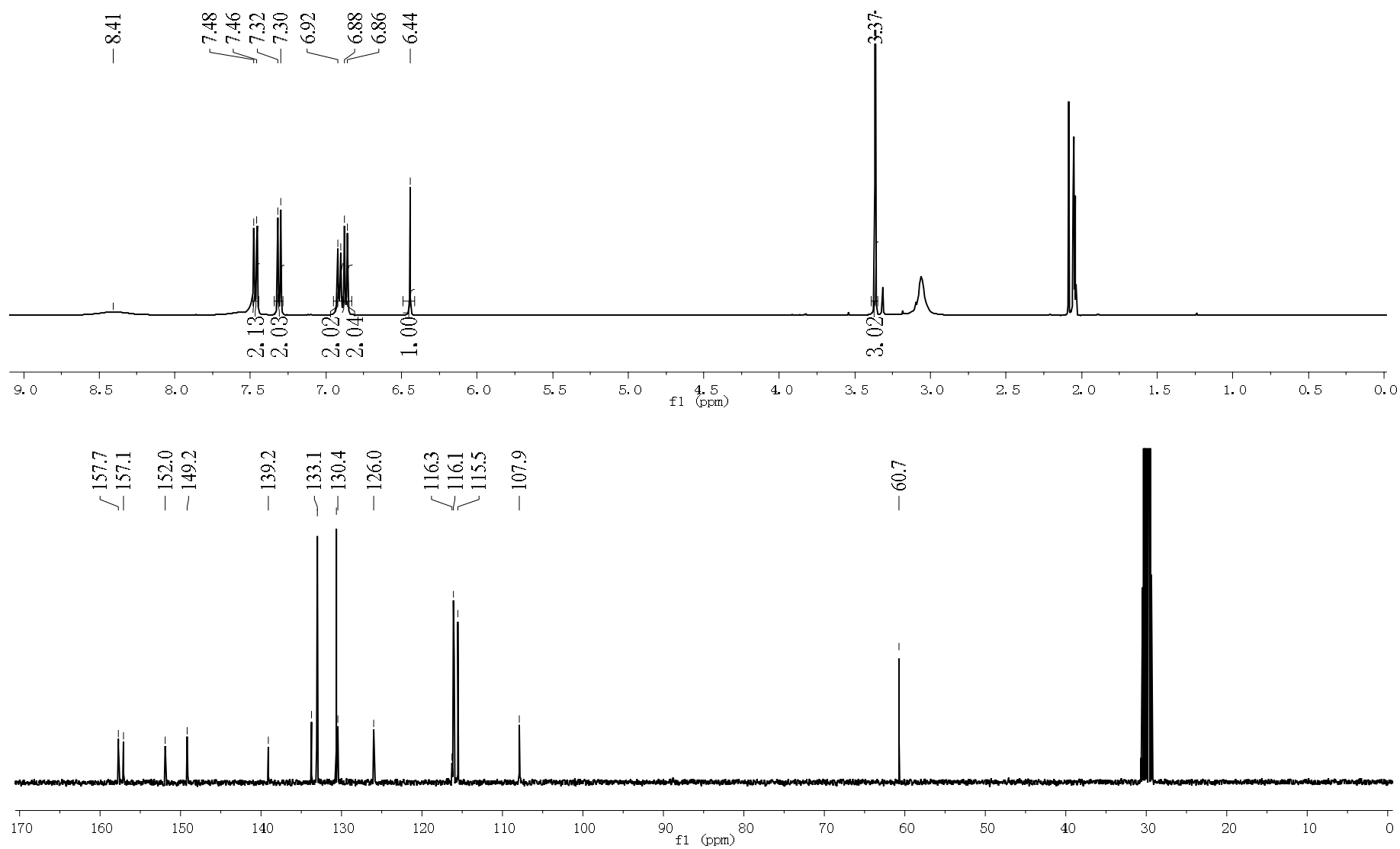


Figure S7. ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectra of the New Compound (**5**) (**DMSO- d_6**)

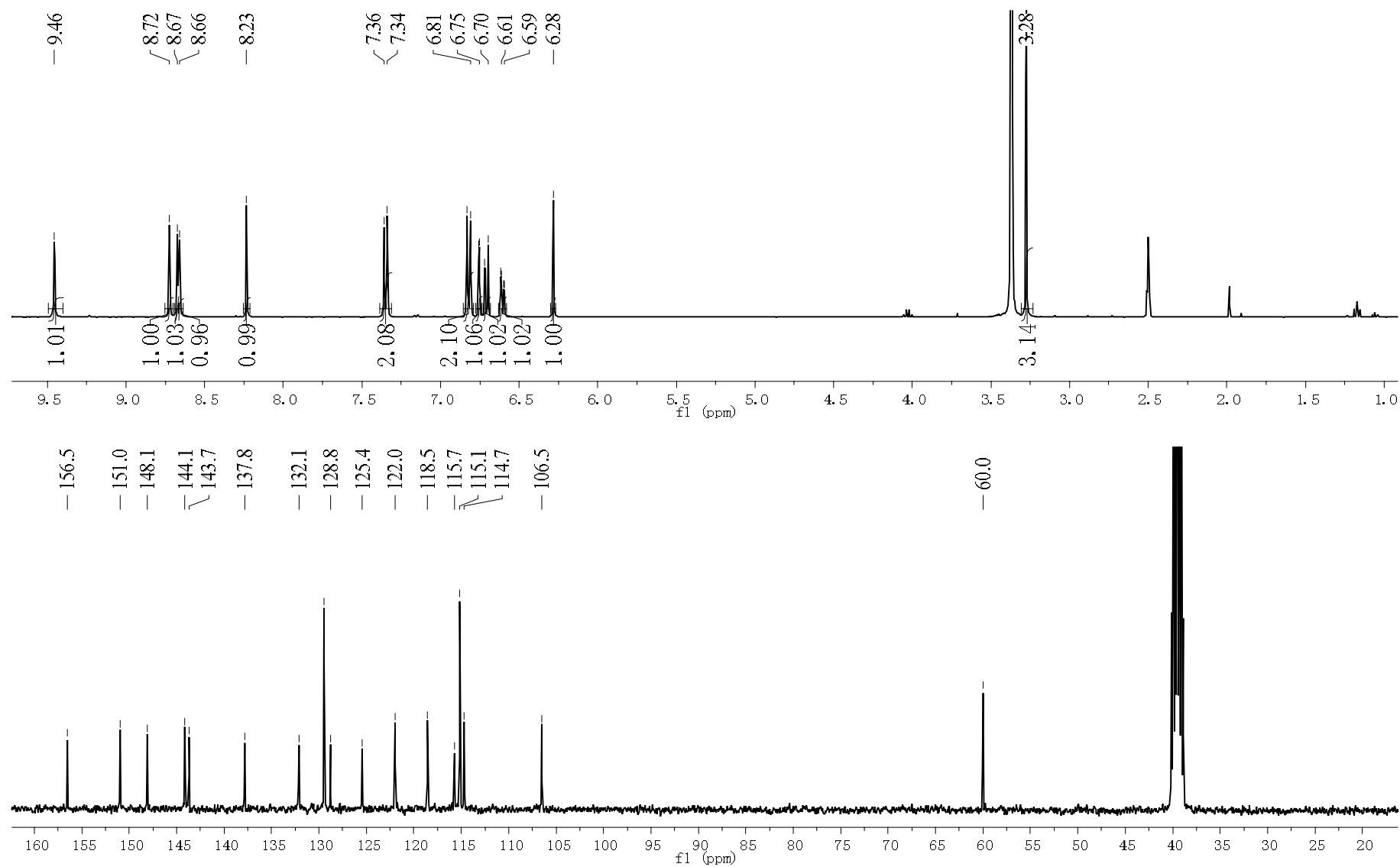


Figure S8. ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectra of the New Compound (7) (**Acetone- d_6**)

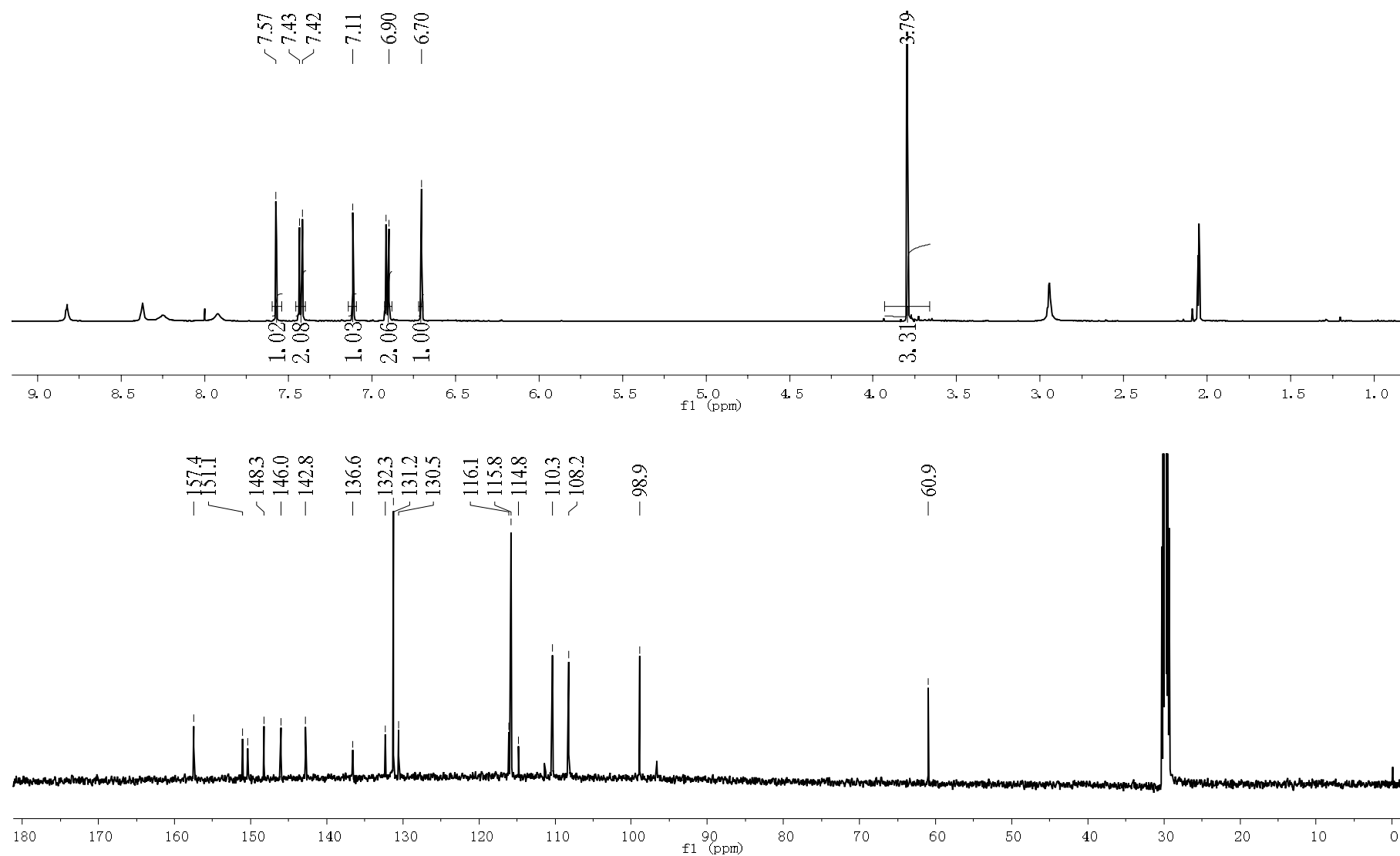


Figure S9. NOESY Spectrum of the New Compound **2** (400 MHz, CDCl₃)

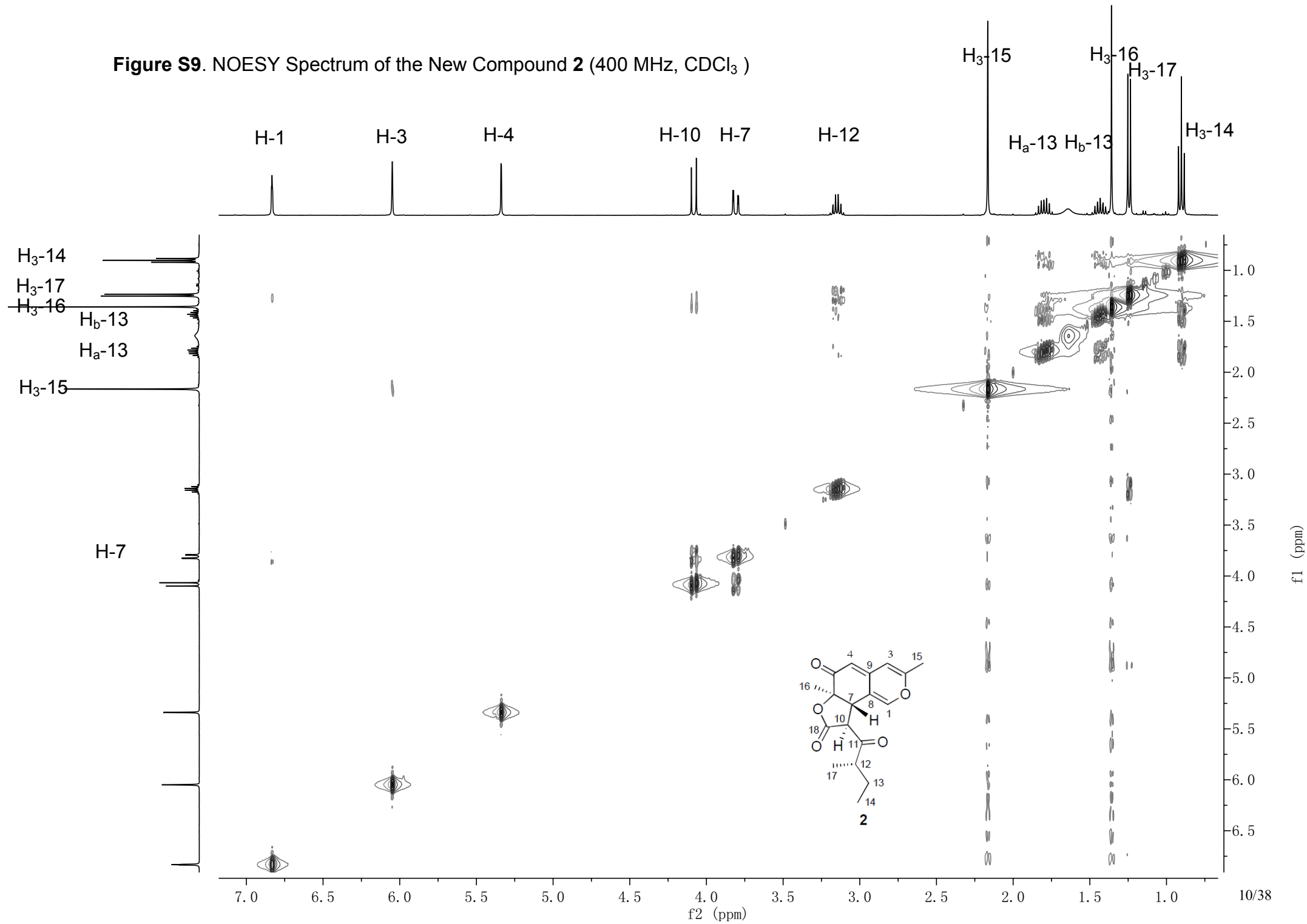


Figure S10. NOESY Spectrum of the New Compound **3** (500 MHz, DMSO- d_6)

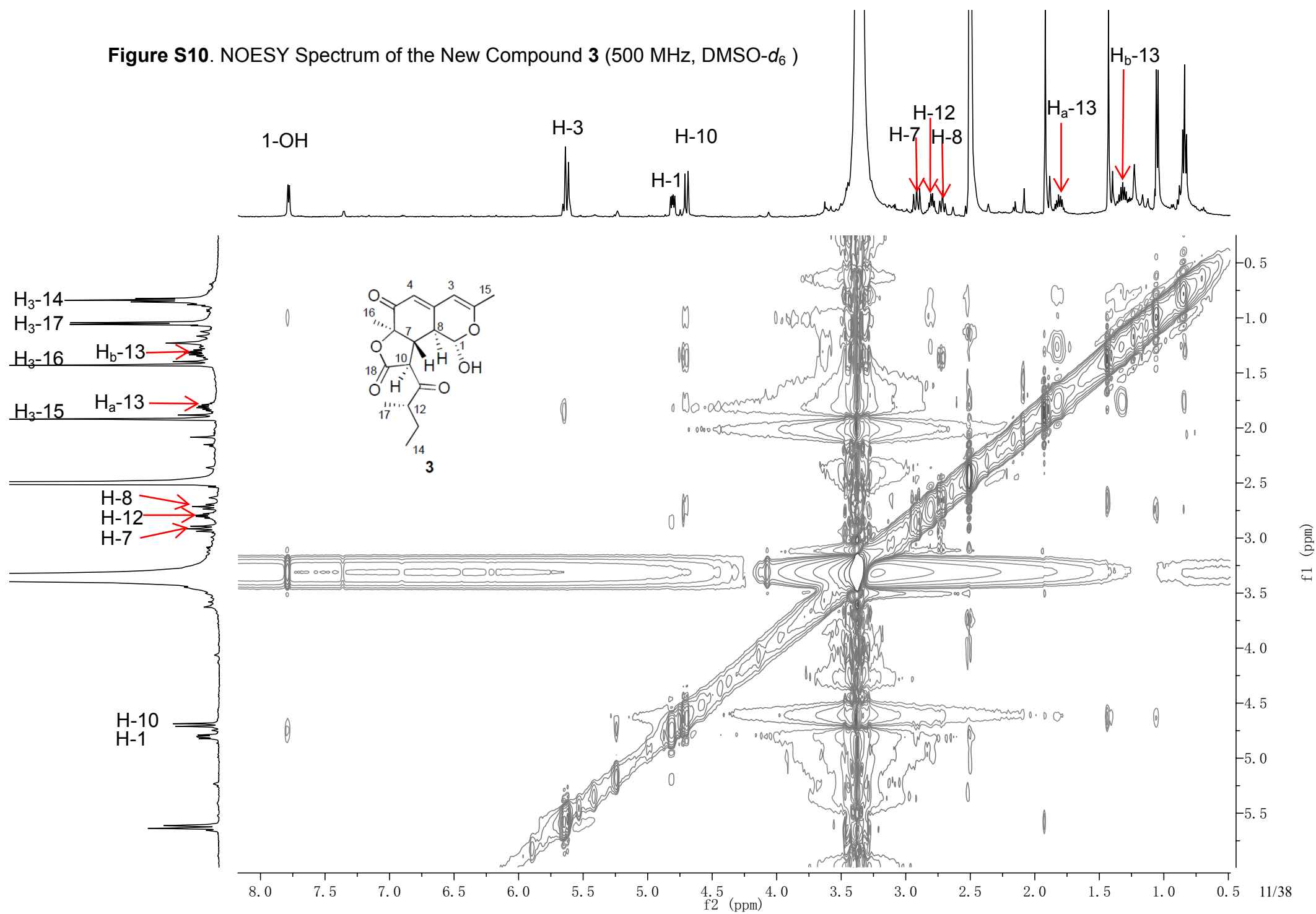


Table S1. Comparison of ^1H and ^{13}C NMR Spectroscopic Data for **2** and Monochaetin ^a (CDCl_3)

Position	Chermesinone B (2) ^b		Monochaetin ^c		$\Delta \delta_{\text{C}}$	$\Delta \delta_{\text{H}}$
	δ_{C}	δ_{H} mult. (<i>J</i> in Hz)	δ_{C}	δ_{H} mult. (<i>J</i> in Hz)		
1	143.5, CH	6.83, s	143.3, CH	6.79, dd (1.9, 1.3)	0.2	0.04
2	158.8, C		158.5, C		0.3	
3	107.3, CH	6.05, s	107.0, CH	6.02, q (< 0.4)	0.3	0.03
4	106.1, CH	5.34, d (0.8)	105.7, CH	5.29, d (1.3)	0.4	0.05
5	192.1, C		191.8, C		0.3	
6	82.8, C		82.6, C		0.2	
7	43.8, CH	3.81, dd (12.9, 1.9)	43.7, CH	3.76, dd (12.8, 1.9)	0.1	0.05
8	116.5, C		116.2, C		0.3	
9	145.7, C		145.5, C		0.2	
10	51.7, CH	4.09, d (12.9)	52.1, CH	4.05, d (12.8)	0.6	0.04
11	206.2, C		205.9, C		0.3	
12	47.3, CH	3.15, m	46.7, CH	3.19, qdd (6.7, 7.4, 5.4)	0.6	-0.04
13	25.1, CH ₂	1.80, m	26.3, CH ₂	1.81, qdd (7.4, 13.0, 5.4)	-1.2	-0.01
		1.43, m		1.48, qdd (7.4, 13.0, 7.4)		
14	11.7, CH ₃	0.90, t (7.4)	11.5, CH ₃	0.97, t (7.4)	0.2	-0.07
15	19.8, CH ₃	2.17, s	19.5, CH ₃	2.13, d (< 0.4)	0.3	0.05
16	19.1, CH ₃	1.36, s	18.9, CH ₃	1.32, s	0.2	0.04
17	17.1, CH₃	1.24, d (7.1)	14.4, CH₃	1.11, d (6.7)	2.7	0.13
18	169.3, C		169.1, C		0.2	

^a Steyn, P. S.; Vleggaar, R. *J. Chem. Soc. Perkin. Trans. I* **1986**, *11*, 1975–1976.^b ^1H at 400 MHz, ^{13}C at 100MHz.^c ^1H at 500 MHz, ^{13}C at 125MHz.

Table S2. ^1H (400 MHz) and ^{13}C (100 MHz) NMR Spectroscopic Data for **1** and **2** ($\text{DMSO-}d_6$)

Position	Chermesinone A (1)		Chermesinone B (2)	
	δ_{C} , type	δ_{H} mult. (J in Hz)	δ_{C} , type	δ_{H} mult. (J in Hz)
1	144.5, CH	7.00, d (1.4)	144.1, CH	7.17, s
2	157.9, C		158.8, C	
3	106.1, CH	6.20, s	106.6, CH	6.37, s
4	104.3, CH	5.23, d (1.1)	104.5, CH	5.26, d (0.8)
5	197.9, C		191.5, C	
6	72.7, C		82.4, C	
7	40.0, CH	3.08, ddd (9.0, 2.8, 1.8)	43.8, CH	3.62, m
8	119.5, C		115.4, C	
9	145.5, C		145.7, C	
10	37.3, CH_2	3.22, dd (18.0, 3.0) 2.85, dd (18.0, 9.0)	50.9, CH	4.98, d (12.8)
11	212.4, C		206.8, C	
12	46.7, CH	2.62, m	46.8, CH	3.09, m
13	25.4, CH_2	1.61, 1.35, m	24.1, CH_2	1.73, 1.35, m
14	11.2, CH_3	0.81, t (7.4)	11.4, CH_3	0.84, t (7.4)
15	18.7, CH_3	2.11, d (0.5)	19.1, CH_3	2.17, s
16	20.6, CH_3	0.95, s	18.5, CH_3	1.27, s
17	15.3, CH_3	1.01, d (6.0)	15.8, CH_3	1.18, d (6.7)
18			170.5, C	

3. Crystal Data for 1

Table S3. Crystal Data and Structure Refinement for jl_9_110127_2 (Compound 1)

Identification code	jl_9_110127_2
Empirical formula	C17 H22 O4
Formula weight	290.35
Temperature	123(2) K
Wavelength	1.5418 Å
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 5.88250(10) Å alpha = 90 deg. b = 8.9553(2) Å beta = 100.6710(10) deg. c = 14.63630(15) Å gamma = 90 deg.
Volume	757.70(2) Å ³
Z, Calculated density	2, 1.273 Mg/m ³
Absorption coefficient	0.728 mm ⁻¹
F(000)	312
Crystal size	0.25 x 0.20 x 0.10 mm
Theta range for data collection	3.07 to 68.64 deg.
Limiting indices	-7<=h<=7, -10<=k<=10, -17<=l<=17
Reflections collected / unique	14768 / 2777 [R(int) = 0.0311]
Completeness to theta = 68.64	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9307 and 0.8389
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2777 / 0 / 195
Goodness-of-fit on F ²	1.077
Final R indices [I>2sigma(I)]	R1 = 0.0308, wR2 = 0.0744
R indices (all data)	R1 = 0.0344, wR2 = 0.0772
Absolute structure parameter	0.07(2)
Largest diff. peak and hole	0.107 and -0.188 e.Å ⁻³

Table S4. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for jl_9_110127_2 (Compound **1**)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	5453(3)	6009(2)	7609(1)	24(1)
C(2)	4440(3)	4077(2)	6530(1)	27(1)
C(3)	6161(3)	4460(2)	6094(1)	29(1)
C(4)	7615(3)	5731(2)	6383(1)	25(1)
C(5)	9271(3)	6225(2)	5910(1)	28(1)
C(6)	10513(3)	7574(2)	6171(1)	29(1)
C(7)	9759(2)	8553(2)	6923(1)	26(1)
C(8)	9031(2)	7568(2)	7684(1)	22(1)
C(9)	7244(2)	6449(2)	7235(1)	22(1)
C(10)	8345(3)	8485(2)	8470(1)	25(1)
C(11)	8343(2)	7618(2)	9362(1)	23(1)
C(12)	7150(3)	8357(2)	10080(1)	27(1)
C(13)	7797(3)	7630(2)	11038(1)	33(1)
C(14)	10295(3)	7854(2)	11509(1)	41(1)
C(15)	2831(3)	2797(2)	6308(1)	37(1)
C(16)	7811(3)	9588(2)	6451(1)	31(1)
C(17)	4514(3)	8302(2)	9737(1)	37(1)
O(1)	3984(2)	4878(1)	7270(1)	28(1)
O(2)	12106(2)	8046(1)	5802(1)	38(1)
O(3)	11710(2)	9428(1)	7346(1)	33(1)
O(4)	9239(2)	6395(1)	9487(1)	30(1)

Table S5. Bond Lengths [Å] and Angles [deg] for jl_9_110127_2 (Compound 1)

C(1)-C(9)	1.334(2)
C(1)-O(1)	1.3637(18)
C(1)-H(1)	0.9500
C(2)-C(3)	1.337(2)
C(2)-O(1)	1.3670(19)
C(2)-C(15)	1.484(2)
C(3)-C(4)	1.439(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.368(2)
C(4)-C(9)	1.455(2)
C(5)-C(6)	1.427(2)
C(5)-H(5)	0.9500
C(6)-O(2)	1.2398(19)
C(6)-C(7)	1.535(2)
C(7)-O(3)	1.4320(18)
C(7)-C(16)	1.536(2)
C(7)-C(8)	1.541(2)
C(8)-C(9)	1.512(2)
C(8)-C(10)	1.527(2)
C(8)-H(8)	1.0000
C(10)-C(11)	1.520(2)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-O(4)	1.2144(19)
C(11)-C(12)	1.519(2)
C(12)-C(13)	1.529(2)
C(12)-C(17)	1.540(2)
C(12)-H(12)	1.0000
C(13)-C(14)	1.517(2)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800

O(3)-H(3A)	0.8400
C(9)-C(1)-O(1)	124.42(14)
C(9)-C(1)-H(1)	117.8
O(1)-C(1)-H(1)	117.8
C(3)-C(2)-O(1)	121.35(14)
C(3)-C(2)-C(15)	127.06(15)
O(1)-C(2)-C(15)	111.60(13)
C(2)-C(3)-C(4)	121.62(14)
C(2)-C(3)-H(3)	119.2
C(4)-C(3)-H(3)	119.2
C(5)-C(4)-C(3)	123.18(14)
C(5)-C(4)-C(9)	121.62(14)
C(3)-C(4)-C(9)	115.19(13)
C(4)-C(5)-C(6)	121.04(14)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
O(2)-C(6)-C(5)	124.27(15)
O(2)-C(6)-C(7)	117.38(15)
C(5)-C(6)-C(7)	118.28(13)
O(3)-C(7)-C(6)	107.90(12)
O(3)-C(7)-C(16)	109.58(14)
C(6)-C(7)-C(16)	108.21(13)
O(3)-C(7)-C(8)	108.01(12)
C(6)-C(7)-C(8)	110.29(13)
C(16)-C(7)-C(8)	112.75(12)
C(9)-C(8)-C(10)	115.10(12)
C(9)-C(8)-C(7)	109.23(12)
C(10)-C(8)-C(7)	112.58(12)
C(9)-C(8)-H(8)	106.5
C(10)-C(8)-H(8)	106.5
C(7)-C(8)-H(8)	106.5
C(1)-C(9)-C(4)	118.47(14)
C(1)-C(9)-C(8)	123.78(13)
C(4)-C(9)-C(8)	117.57(12)
C(11)-C(10)-C(8)	114.55(13)
C(11)-C(10)-H(10A)	108.6
C(8)-C(10)-H(10A)	108.6
C(11)-C(10)-H(10B)	108.6
C(8)-C(10)-H(10B)	108.6
H(10A)-C(10)-H(10B)	107.6
O(4)-C(11)-C(12)	122.17(14)
O(4)-C(11)-C(10)	121.33(13)
C(12)-C(11)-C(10)	116.50(13)
C(11)-C(12)-C(13)	112.37(13)
C(11)-C(12)-C(17)	109.09(12)

C(13)-C(12)-C(17)	110.51(13)
C(11)-C(12)-H(12)	108.3
C(13)-C(12)-H(12)	108.3
C(17)-C(12)-H(12)	108.3
C(14)-C(13)-C(12)	114.61(14)
C(14)-C(13)-H(13A)	108.6
C(12)-C(13)-H(13A)	108.6
C(14)-C(13)-H(13B)	108.6
C(12)-C(13)-H(13B)	108.6
H(13A)-C(13)-H(13B)	107.6
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(2)-C(15)-H(15A)	109.5
C(2)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(2)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(7)-C(16)-H(16A)	109.5
C(7)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(7)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(12)-C(17)-H(17A)	109.5
C(12)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(12)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(1)-O(1)-C(2)	118.31(12)
C(7)-O(3)-H(3A)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S6. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for jl_9_110127_2 (Compound 1)

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(1)	26(1)	25(1)	21(1)	-3(1)	3(1)	-2(1)
C(2)	33(1)	26(1)	21(1)	-1(1)	-1(1)	0(1)
C(3)	37(1)	28(1)	21(1)	-3(1)	3(1)	3(1)
C(4)	27(1)	26(1)	20(1)	3(1)	3(1)	5(1)
C(5)	32(1)	32(1)	20(1)	2(1)	9(1)	5(1)
C(6)	26(1)	37(1)	23(1)	8(1)	5(1)	4(1)
C(7)	24(1)	29(1)	25(1)	2(1)	5(1)	-4(1)
C(8)	23(1)	23(1)	21(1)	2(1)	4(1)	2(1)
C(9)	24(1)	23(1)	20(1)	2(1)	3(1)	3(1)
C(10)	26(1)	23(1)	25(1)	0(1)	5(1)	-2(1)
C(11)	22(1)	23(1)	23(1)	-2(1)	1(1)	-3(1)
C(12)	32(1)	23(1)	27(1)	-1(1)	7(1)	-1(1)
C(13)	43(1)	32(1)	25(1)	-2(1)	12(1)	0(1)
C(14)	56(1)	37(1)	28(1)	2(1)	-1(1)	-8(1)
C(15)	45(1)	31(1)	34(1)	-4(1)	2(1)	-8(1)
C(16)	34(1)	29(1)	30(1)	6(1)	7(1)	1(1)
C(17)	32(1)	42(1)	38(1)	-1(1)	13(1)	4(1)
O(1)	30(1)	28(1)	26(1)	-3(1)	6(1)	-6(1)
O(2)	34(1)	53(1)	32(1)	7(1)	15(1)	-4(1)
O(3)	28(1)	39(1)	33(1)	1(1)	8(1)	-12(1)
O(4)	38(1)	28(1)	25(1)	1(1)	6(1)	6(1)

Table S7. Hydrogen Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for jl_9_110127_2 (Compound **1**)

	x	y	z	U(eq)
H(1)	5182	6517	8149	29
H(3)	6432	3878	5582	34
H(5)	9599	5660	5401	33
H(8)	10430	6980	7967	27
H(10A)	9427	9336	8609	30
H(10B)	6778	8900	8252	30
H(12)	7637	9428	10137	32
H(13A)	6781	8040	11446	39
H(13B)	7488	6545	10973	39
H(14A)	11317	7355	11147	62
H(14B)	10534	7427	12136	62
H(14C)	10648	8924	11549	62
H(15A)	3244	2225	5792	56
H(15B)	1244	3169	6130	56
H(15C)	2943	2152	6855	56
H(16A)	7409	10290	6910	46
H(16B)	6449	8991	6190	46
H(16C)	8331	10145	5951	46
H(17A)	4134	8739	9113	55
H(17B)	3742	8871	10163	55
H(17C)	3988	7262	9715	55
H(3A)	12690	9448	6995	50

Table S8. Torsion Angles [deg] for jl_9_110127_2 (Compound **1**)

O(1)-C(2)-C(3)-C(4)	-0.1(2)
C(15)-C(2)-C(3)-C(4)	-179.66(15)
C(2)-C(3)-C(4)-C(5)	-174.70(15)
C(2)-C(3)-C(4)-C(9)	6.8(2)
C(3)-C(4)-C(5)-C(6)	173.85(14)
C(9)-C(4)-C(5)-C(6)	-7.7(2)
C(4)-C(5)-C(6)-O(2)	176.43(15)
C(4)-C(5)-C(6)-C(7)	-6.8(2)
O(2)-C(6)-C(7)-O(3)	-27.44(18)
C(5)-C(6)-C(7)-O(3)	155.60(13)
O(2)-C(6)-C(7)-C(16)	91.05(16)
C(5)-C(6)-C(7)-C(16)	-85.91(16)
O(2)-C(6)-C(7)-C(8)	-145.20(14)
C(5)-C(6)-C(7)-C(8)	37.84(18)
O(3)-C(7)-C(8)-C(9)	-170.58(12)
C(6)-C(7)-C(8)-C(9)	-52.89(15)
C(16)-C(7)-C(8)-C(9)	68.20(16)
O(3)-C(7)-C(8)-C(10)	60.25(16)
C(6)-C(7)-C(8)-C(10)	177.95(11)
C(16)-C(7)-C(8)-C(10)	-60.97(16)
O(1)-C(1)-C(9)-C(4)	3.0(2)
O(1)-C(1)-C(9)-C(8)	-172.00(14)
C(5)-C(4)-C(9)-C(1)	173.38(15)
C(3)-C(4)-C(9)-C(1)	-8.1(2)
C(5)-C(4)-C(9)-C(8)	-11.3(2)
C(3)-C(4)-C(9)-C(8)	167.24(13)
C(10)-C(8)-C(9)-C(1)	-15.5(2)
C(7)-C(8)-C(9)-C(1)	-143.22(15)
C(10)-C(8)-C(9)-C(4)	169.51(12)
C(7)-C(8)-C(9)-C(4)	41.74(17)
C(9)-C(8)-C(10)-C(11)	72.15(16)
C(7)-C(8)-C(10)-C(11)	-161.78(12)
C(8)-C(10)-C(11)-O(4)	13.4(2)
C(8)-C(10)-C(11)-C(12)	-166.10(12)
O(4)-C(11)-C(12)-C(13)	16.3(2)
C(10)-C(11)-C(12)-C(13)	-164.23(12)
O(4)-C(11)-C(12)-C(17)	-106.65(16)
C(10)-C(11)-C(12)-C(17)	72.86(16)
C(11)-C(12)-C(13)-C(14)	67.68(18)
C(17)-C(12)-C(13)-C(14)	-170.21(15)
C(9)-C(1)-O(1)-C(2)	4.0(2)
C(3)-C(2)-O(1)-C(1)	-5.5(2)
C(15)-C(2)-O(1)-C(1)	174.13(13)

Symmetry transformations used to generate equivalent atoms:

Table S9. Hydrogen Bonds [Å and deg.] for jl_9_110127_2 (Compound **1**)

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3A)...O(2)	0.84	2.13	2.6242(17)	117.7

Symmetry transformations used to generate equivalent atoms:

4. Crystal Data for 4

Table S10. Crystal Data and Structure Refinement for L (Compound 4)

Identification code	L
Empirical formula	$2(\text{C}_{19}\text{H}_{16}\text{O}_5) \cdot 3\text{H}_2\text{O}$
Formula weight	702.68
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 8.2934(12) Å alpha = 109.717(5) deg. b = 15.048(2) Å beta = 103.493(4) deg. c = 15.381(3) Å gamma = 98.942(4) deg.
Volume	1698.6(4) Å ³
Z, Calculated density	4, 1.374 Mg/m ³
Absorption coefficient	0.104 mm ⁻¹
F(000)	740
Crystal size	0.19 x 0.14 x 0.10 mm
Theta range for data collection	3.02 to 25.99 deg.
Limiting indices	-10 ≤ h ≤ 10, -15 ≤ k ≤ 18, -18 ≤ l ≤ 18
Reflections collected / unique	12833 / 6581 [R(int) = 0.0641]
Completeness to theta = 25.99	98.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9894 and 0.9810
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6581 / 0 / 469
Goodness-of-fit on F ²	1.058
Final R indices [I > 2sigma(I)]	R1 = 0.0666, wR2 = 0.1514
R indices (all data)	R1 = 0.1386, wR2 = 0.2213
Extinction coefficient	0.0098(18)
Largest diff. peak and hole	0.421 and -0.435 e.Å ⁻³

Table S11. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for L (Compound **4**)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(4A)	6470(5)	8987(3)	5234(3)	36(1)
C(5A)	6083(6)	9406(3)	6083(3)	40(1)
C(6A)	4882(5)	8861(3)	6319(3)	40(1)
C(1A)	4013(5)	7898(3)	5714(3)	33(1)
C(2A)	4427(5)	7485(3)	4866(3)	41(1)
C(3A)	5641(6)	8019(3)	4624(3)	43(1)
C(1B)	2760(5)	7342(3)	6016(3)	33(1)
C(2B)	991(5)	7080(3)	5576(3)	35(1)
C(3B)	-140(5)	6574(3)	5892(3)	35(1)
C(4B)	441(5)	6293(3)	6654(3)	32(1)
C(5B)	2218(5)	6572(3)	7120(3)	34(1)
C(6B)	3320(5)	7084(3)	6803(3)	35(1)
C(1C)	-701(5)	5700(3)	6978(3)	33(1)
C(2C)	-2252(5)	5875(3)	7093(3)	33(1)
C(3C)	-3297(5)	5300(3)	7378(3)	36(1)
C(4C)	-2829(5)	4512(3)	7545(3)	35(1)
C(5C)	-1276(5)	4334(3)	7458(3)	37(1)
C(6C)	-242(5)	4920(3)	7175(3)	35(1)
C(7B)	-2702(6)	5427(3)	4730(3)	52(1)
O(1A)	7650(4)	9492(2)	4964(2)	44(1)
O(4B)	5050(3)	7339(2)	7316(2)	40(1)
O(2B)	332(4)	7350(2)	4818(2)	46(1)
O(5C)	-3869(4)	3906(2)	7798(2)	49(1)
O(3B)	-1884(3)	6407(2)	5414(2)	42(1)
O(2W)	1323(4)	8610(2)	3863(2)	53(1)
O(3W)	3024(4)	7823(2)	2324(2)	50(1)
C(4)	7334(5)	5999(3)	11195(3)	34(1)
C(3)	7615(6)	6992(3)	11550(3)	42(1)
C(2)	8439(5)	7526(3)	11122(3)	39(1)
C(1)	8983(5)	7061(3)	10334(3)	32(1)
C(6)	8754(5)	6055(3)	10016(3)	35(1)
C(5)	7921(5)	5516(3)	10429(3)	39(1)
C(1')	9694(5)	7618(3)	9813(3)	31(1)
C(2')	8612(5)	7976(3)	9241(3)	32(1)
C(3')	9224(5)	8478(3)	8723(3)	30(1)
C(4')	10931(5)	8627(3)	8737(3)	32(1)
C(5')	12021(5)	8262(3)	9300(3)	33(1)

C(6')	11390(5)	7768(3)	9813(3)	34(1)
C(1")	11605(5)	9226(3)	8247(3)	31(1)
C(2")	10735(5)	9119(3)	7303(3)	34(1)
C(3")	11355(5)	9710(3)	6880(3)	36(1)
C(4")	12869(5)	10440(3)	7386(3)	35(1)
C(5")	13752(5)	10573(3)	8317(3)	35(1)
C(6")	13122(5)	9971(3)	8741(3)	35(1)
C(7')	8078(6)	9810(3)	8704(3)	48(1)
O(1)	6464(4)	5467(2)	11602(2)	46(1)
O(4')	12524(4)	7426(2)	10362(2)	43(1)
O(2')	6932(3)	7845(2)	9226(2)	40(1)
O(5")	13554(4)	11041(2)	6988(2)	41(1)
O(3')	8050(3)	8817(2)	8180(2)	34(1)
O(1W)	4380(4)	6479(2)	9337(2)	54(1)

Table S12. Bond Lengths [Å] and Angles [deg] for L (Compound **4**)

C(4A)-O(1A)	1.372(4)
C(4A)-C(5A)	1.381(5)
C(4A)-C(3A)	1.394(6)
C(5A)-C(6A)	1.383(5)
C(5A)-H(5D)	0.9500
C(6A)-C(1A)	1.392(6)
C(6A)-H(6B)	0.9500
C(1A)-C(2A)	1.391(5)
C(1A)-C(1B)	1.488(5)
C(2A)-C(3A)	1.387(6)
C(2A)-H(2C)	0.9500
C(3A)-H(3B)	0.9500
C(1B)-C(6B)	1.394(5)
C(1B)-C(2B)	1.394(5)
C(2B)-O(2B)	1.382(5)
C(2B)-C(3B)	1.391(5)
C(3B)-C(4B)	1.385(5)
C(3B)-O(3B)	1.400(5)
C(4B)-C(5B)	1.405(5)
C(4B)-C(1C)	1.483(5)
C(5B)-C(6B)	1.382(5)
C(5B)-H(5F)	0.9500
C(6B)-O(4B)	1.387(5)
C(1C)-C(2C)	1.392(5)
C(1C)-C(6C)	1.392(6)
C(2C)-C(3C)	1.375(5)
C(2C)-H(2D)	0.9500
C(3C)-C(4C)	1.387(6)
C(3C)-H(3C)	0.9500
C(4C)-O(5C)	1.372(5)
C(4C)-C(5C)	1.383(6)
C(5C)-C(6C)	1.379(5)
C(5C)-H(5G)	0.9500
C(6C)-H(6C)	0.9500
C(7B)-O(3B)	1.433(5)
C(7B)-H(7D)	0.9800
C(7B)-H(7E)	0.9800
C(7B)-H(7F)	0.9800
O(1A)-H(1A)	0.8406
O(4B)-H(4A)	0.8400
O(2B)-H(2E)	0.8400

O(5C)-H(5H)	0.8400
O(2W)-H(2G)	0.8557
O(2W)-H(2F)	0.8516
O(3W)-H(3D)	0.7487
O(3W)-H(3F)	0.7809
C(4)-C(3)	1.367(6)
C(4)-O(1)	1.386(4)
C(4)-C(5)	1.397(5)
C(3)-C(2)	1.394(6)
C(3)-H(3)	0.9500
C(2)-C(1)	1.394(5)
C(2)-H(2)	0.9500
C(1)-C(6)	1.392(5)
C(1)-C(1')	1.487(5)
C(6)-C(5)	1.384(5)
C(6)-H(6)	0.9500
C(5)-H(5)	0.9500
C(1')-C(6')	1.389(5)
C(1')-C(2')	1.403(5)
C(2')-O(2')	1.370(4)
C(2')-C(3')	1.394(5)
C(3')-C(4')	1.392(5)
C(3')-O(3')	1.402(4)
C(4')-C(5')	1.407(5)
C(4')-C(1'')	1.481(5)
C(5')-C(6')	1.385(5)
C(5')-H(5A)	0.9500
C(6')-O(4')	1.391(5)
C(1'')-C(6'')	1.399(5)
C(1'')-C(2'')	1.404(5)
C(2'')-C(3'')	1.372(5)
C(2'')-H(2A)	0.9500
C(3'')-C(4'')	1.389(6)
C(3'')-H(3A)	0.9500
C(4'')-O(5'')	1.376(4)
C(4'')-C(5'')	1.379(5)
C(5'')-C(6'')	1.388(5)
C(5'')-H(5B)	0.9500
C(6'')-H(6A)	0.9500
C(7')-O(3')	1.433(5)
C(7')-H(7A)	0.9800
C(7')-H(7B)	0.9800
C(7')-H(7C)	0.9800
O(1)-H(1)	0.8397

O(4')-H(4)	0.8400
O(2')-H(2B)	0.8400
O(5'')-H(5C)	0.8400
O(1W)-H(1D)	0.8535
O(1W)-H(1C)	0.8659
O(1A)-C(4A)-C(5A)	122.2(4)
O(1A)-C(4A)-C(3A)	118.2(3)
C(5A)-C(4A)-C(3A)	119.6(4)
C(4A)-C(5A)-C(6A)	119.7(4)
C(4A)-C(5A)-H(5D)	120.1
C(6A)-C(5A)-H(5D)	120.1
C(5A)-C(6A)-C(1A)	121.9(4)
C(5A)-C(6A)-H(6B)	119.0
C(1A)-C(6A)-H(6B)	119.0
C(2A)-C(1A)-C(6A)	117.6(4)
C(2A)-C(1A)-C(1B)	122.8(4)
C(6A)-C(1A)-C(1B)	119.5(3)
C(3A)-C(2A)-C(1A)	121.2(4)
C(3A)-C(2A)-H(2C)	119.4
C(1A)-C(2A)-H(2C)	119.4
C(2A)-C(3A)-C(4A)	120.0(4)
C(2A)-C(3A)-H(3B)	120.0
C(4A)-C(3A)-H(3B)	120.0
C(6B)-C(1B)-C(2B)	115.9(4)
C(6B)-C(1B)-C(1A)	120.4(4)
C(2B)-C(1B)-C(1A)	123.7(3)
O(2B)-C(2B)-C(3B)	118.8(4)
O(2B)-C(2B)-C(1B)	119.3(3)
C(3B)-C(2B)-C(1B)	121.9(4)
C(4B)-C(3B)-C(2B)	121.5(4)
C(4B)-C(3B)-O(3B)	123.0(3)
C(2B)-C(3B)-O(3B)	115.5(3)
C(3B)-C(4B)-C(5B)	117.3(3)
C(3B)-C(4B)-C(1C)	123.6(3)
C(5B)-C(4B)-C(1C)	119.1(3)
C(6B)-C(5B)-C(4B)	120.3(4)
C(6B)-C(5B)-H(5F)	119.8
C(4B)-C(5B)-H(5F)	119.8
C(5B)-C(6B)-O(4B)	116.2(3)
C(5B)-C(6B)-C(1B)	123.0(4)
O(4B)-C(6B)-C(1B)	120.7(3)
C(2C)-C(1C)-C(6C)	116.9(4)
C(2C)-C(1C)-C(4B)	123.2(4)

C(6C)-C(1C)-C(4B)	119.9(4)
C(3C)-C(2C)-C(1C)	121.7(4)
C(3C)-C(2C)-H(2D)	119.1
C(1C)-C(2C)-H(2D)	119.1
C(2C)-C(3C)-C(4C)	120.1(4)
C(2C)-C(3C)-H(3C)	119.9
C(4C)-C(3C)-H(3C)	119.9
O(5C)-C(4C)-C(5C)	119.0(4)
O(5C)-C(4C)-C(3C)	121.5(4)
C(5C)-C(4C)-C(3C)	119.4(4)
C(6C)-C(5C)-C(4C)	119.6(4)
C(6C)-C(5C)-H(5G)	120.2
C(4C)-C(5C)-H(5G)	120.2
C(5C)-C(6C)-C(1C)	122.2(4)
C(5C)-C(6C)-H(6C)	118.9
C(1C)-C(6C)-H(6C)	118.9
O(3B)-C(7B)-H(7D)	109.5
O(3B)-C(7B)-H(7E)	109.5
H(7D)-C(7B)-H(7E)	109.5
O(3B)-C(7B)-H(7F)	109.5
H(7D)-C(7B)-H(7F)	109.5
H(7E)-C(7B)-H(7F)	109.5
C(4A)-O(1A)-H(1A)	112.2
C(6B)-O(4B)-H(4A)	109.5
C(2B)-O(2B)-H(2E)	109.5
C(4C)-O(5C)-H(5H)	109.5
C(3B)-O(3B)-C(7B)	114.8(3)
H(2G)-O(2W)-H(2F)	109.0
H(3D)-O(3W)-H(3F)	103.3
C(3)-C(4)-O(1)	119.6(4)
C(3)-C(4)-C(5)	120.6(4)
O(1)-C(4)-C(5)	119.8(4)
C(4)-C(3)-C(2)	119.8(4)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(3)-C(2)-C(1)	120.9(4)
C(3)-C(2)-H(2)	119.5
C(1)-C(2)-H(2)	119.5
C(6)-C(1)-C(2)	118.1(4)
C(6)-C(1)-C(1')	121.0(3)
C(2)-C(1)-C(1')	120.8(4)
C(5)-C(6)-C(1)	121.4(4)
C(5)-C(6)-H(6)	119.3
C(1)-C(6)-H(6)	119.3

C(6)-C(5)-C(4)	119.1(4)
C(6)-C(5)-H(5)	120.4
C(4)-C(5)-H(5)	120.4
C(6')-C(1')-C(2')	116.6(3)
C(6')-C(1')-C(1)	123.4(4)
C(2')-C(1')-C(1)	119.9(3)
O(2')-C(2')-C(3')	120.2(3)
O(2')-C(2')-C(1')	118.3(3)
C(3')-C(2')-C(1')	121.5(3)
C(4')-C(3')-C(2')	121.1(4)
C(4')-C(3')-O(3')	121.5(3)
C(2')-C(3')-O(3')	117.4(3)
C(3')-C(4')-C(5')	117.8(3)
C(3')-C(4')-C(1'')	120.8(4)
C(5')-C(4')-C(1'')	121.2(3)
C(6')-C(5')-C(4')	120.3(4)
C(6')-C(5')-H(5A)	119.9
C(4')-C(5')-H(5A)	119.9
C(5')-C(6')-C(1')	122.8(4)
C(5')-C(6')-O(4')	117.9(3)
C(1')-C(6')-O(4')	119.3(3)
C(6'')-C(1'')-C(2'')	117.0(4)
C(6'')-C(1'')-C(4')	120.2(3)
C(2'')-C(1'')-C(4')	122.7(3)
C(3'')-C(2'')-C(1'')	121.5(4)
C(3'')-C(2'')-H(2A)	119.2
C(1'')-C(2'')-H(2A)	119.2
C(2'')-C(3'')-C(4'')	120.3(4)
C(2'')-C(3'')-H(3A)	119.9
C(4'')-C(3'')-H(3A)	119.9
O(5'')-C(4'')-C(5'')	117.8(3)
O(5'')-C(4'')-C(3'')	122.4(4)
C(5'')-C(4'')-C(3'')	119.8(4)
C(4'')-C(5'')-C(6'')	119.7(4)
C(4'')-C(5'')-H(5B)	120.2
C(6'')-C(5'')-H(5B)	120.2
C(5'')-C(6'')-C(1'')	121.7(4)
C(5'')-C(6'')-H(6A)	119.1
C(1'')-C(6'')-H(6A)	119.1
O(3')-C(7')-H(7A)	109.5
O(3')-C(7')-H(7B)	109.5
H(7A)-C(7')-H(7B)	109.5
O(3')-C(7')-H(7C)	109.5
H(7A)-C(7')-H(7C)	109.5

H(7B)-C(7')-H(7C)	109.5
C(4)-O(1)-H(1)	113.8
C(6')-O(4')-H(4)	109.5
C(2')-O(2')-H(2B)	109.5
C(4'')-O(5'')-H(5C)	109.5
C(3')-O(3')-C(7')	112.2(3)
H(1D)-O(1W)-H(1C)	109.1

Symmetry transformations used to generate equivalent atoms:

Table S13. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for L (Compound **4**)

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hka^*b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(4A)	33(2)	41(2)	40(2)	25(2)	13(2)	6(2)
C(5A)	50(3)	34(2)	43(2)	19(2)	21(2)	7(2)
C(6A)	49(3)	34(2)	45(2)	21(2)	25(2)	8(2)
C(1A)	36(2)	31(2)	39(2)	19(2)	17(2)	8(2)
C(2A)	47(3)	42(2)	39(2)	20(2)	20(2)	5(2)
C(3A)	53(3)	39(2)	42(2)	18(2)	23(2)	10(2)
C(1B)	38(2)	30(2)	34(2)	17(2)	12(2)	5(2)
C(2B)	38(2)	36(2)	34(2)	21(2)	11(2)	6(2)
C(3B)	28(2)	42(2)	37(2)	18(2)	12(2)	6(2)
C(4B)	34(2)	33(2)	32(2)	15(2)	13(2)	6(2)
C(5B)	35(2)	37(2)	39(2)	24(2)	14(2)	10(2)
C(6B)	32(2)	32(2)	41(2)	16(2)	12(2)	5(2)
C(1C)	35(2)	33(2)	33(2)	14(2)	13(2)	9(2)
C(2C)	33(2)	32(2)	38(2)	16(2)	15(2)	9(2)
C(3C)	33(2)	41(2)	40(2)	18(2)	19(2)	10(2)
C(4C)	38(2)	37(2)	36(2)	19(2)	17(2)	8(2)
C(5C)	39(2)	36(2)	47(2)	23(2)	21(2)	12(2)
C(6C)	32(2)	41(2)	43(2)	22(2)	19(2)	11(2)
C(7B)	44(3)	52(3)	46(3)	14(2)	8(2)	-3(2)
O(1A)	48(2)	48(2)	45(2)	27(1)	22(1)	3(1)
O(4B)	28(2)	48(2)	47(2)	28(1)	8(1)	2(1)
O(2B)	39(2)	60(2)	51(2)	38(2)	12(1)	11(2)
O(5C)	52(2)	44(2)	69(2)	30(2)	41(2)	12(2)
O(3B)	29(2)	50(2)	49(2)	26(2)	7(1)	6(1)
O(2W)	64(2)	48(2)	57(2)	30(2)	26(2)	9(2)
O(3W)	48(2)	53(2)	58(2)	32(2)	21(2)	7(2)
C(4)	32(2)	41(2)	46(2)	29(2)	20(2)	10(2)
C(3)	53(3)	36(2)	46(2)	20(2)	28(2)	13(2)
C(2)	47(3)	34(2)	46(2)	19(2)	25(2)	9(2)
C(1)	38(2)	31(2)	34(2)	17(2)	17(2)	6(2)
C(6)	42(2)	36(2)	39(2)	20(2)	25(2)	12(2)
C(5)	44(2)	29(2)	48(2)	17(2)	20(2)	9(2)
C(1')	33(2)	30(2)	33(2)	15(2)	15(2)	8(2)
C(2')	33(2)	27(2)	37(2)	14(2)	17(2)	5(2)
C(3')	34(2)	30(2)	34(2)	19(2)	13(2)	11(2)
C(4')	35(2)	32(2)	33(2)	15(2)	16(2)	7(2)
C(5')	33(2)	33(2)	41(2)	20(2)	18(2)	9(2)

C(6')	38(2)	36(2)	38(2)	22(2)	15(2)	14(2)
C(1'')	31(2)	36(2)	38(2)	20(2)	21(2)	11(2)
C(2'')	33(2)	37(2)	36(2)	18(2)	15(2)	7(2)
C(3'')	34(2)	44(2)	34(2)	20(2)	11(2)	6(2)
C(4'')	38(2)	39(2)	43(2)	25(2)	24(2)	12(2)
C(5'')	32(2)	39(2)	39(2)	20(2)	14(2)	2(2)
C(6'')	33(2)	39(2)	39(2)	22(2)	15(2)	9(2)
C(7')	60(3)	41(3)	51(3)	22(2)	18(2)	23(2)
O(1)	50(2)	42(2)	62(2)	32(2)	31(2)	11(1)
O(4')	48(2)	55(2)	44(2)	32(2)	22(1)	23(2)
O(2')	32(2)	50(2)	45(2)	28(2)	14(1)	8(1)
O(5'')	49(2)	42(2)	43(2)	27(1)	22(1)	6(1)
O(3')	36(2)	32(2)	38(1)	19(1)	11(1)	7(1)
O(1W)	40(2)	68(2)	74(2)	41(2)	29(2)	18(2)

Table S14. Hydrogen Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for L (Compound **4**)

	x	y	z	U(eq)
H(5D)	6641	10066	6503	49
H(6B)	4643	9153	6910	47
H(2C)	3869	6825	4446	50
H(3B)	5907	7724	4041	51
H(5F)	2665	6407	7657	41
H(2D)	-2599	6406	6972	40
H(3C)	-4341	5443	7461	43
H(5G)	-923	3810	7593	44
H(6C)	817	4788	7112	42
H(7D)	-2584	4975	5060	77
H(7E)	-2161	5266	4214	77
H(7F)	-3921	5368	4447	77
H(1A)	8001	10086	5334	66
H(4A)	5603	7701	7115	60
H(2E)	-686	7374	4780	69
H(5H)	-4724	4121	7874	74
H(2G)	1835	8387	3445	80
H(2F)	1226	8232	4164	80
H(3D)	3253	7345	2235	75
H(3F)	3894	8188	2431	75
H(3)	7251	7317	12087	50
H(2)	8631	8216	11370	47
H(6)	9177	5731	9505	42
H(5)	7752	4827	10195	46
H(5A)	13194	8355	9328	40
H(2A)	9692	8626	6949	41
H(3A)	10746	9619	6238	43
H(5B)	14786	11073	8667	42
H(6A)	13737	10068	9384	41
H(7A)	9217	10232	8856	72
H(7B)	7820	9869	9308	72
H(7C)	7217	10009	8306	72
H(1)	6236	4860	11301	68
H(4)	12293	7488	10879	64
H(2B)	6324	7821	8694	60
H(5C)	13140	10781	6380	61
H(1D)	5402	6835	9528	81
H(1C)	3779	6798	9655	81

Table S15. Torsion Angles [deg] for L (Compound **4**)

O(1A)-C(4A)-C(5A)-C(6A)	-180.0(4)
C(3A)-C(4A)-C(5A)-C(6A)	0.1(6)
C(4A)-C(5A)-C(6A)-C(1A)	-1.3(7)
C(5A)-C(6A)-C(1A)-C(2A)	1.8(6)
C(5A)-C(6A)-C(1A)-C(1B)	178.7(4)
C(6A)-C(1A)-C(2A)-C(3A)	-1.1(6)
C(1B)-C(1A)-C(2A)-C(3A)	-178.0(4)
C(1A)-C(2A)-C(3A)-C(4A)	0.0(7)
O(1A)-C(4A)-C(3A)-C(2A)	-179.4(4)
C(5A)-C(4A)-C(3A)-C(2A)	0.5(7)
C(2A)-C(1A)-C(1B)-C(6B)	108.8(5)
C(6A)-C(1A)-C(1B)-C(6B)	-68.0(5)
C(2A)-C(1A)-C(1B)-C(2B)	-73.8(6)
C(6A)-C(1A)-C(1B)-C(2B)	109.4(5)
C(6B)-C(1B)-C(2B)-O(2B)	177.1(4)
C(1A)-C(1B)-C(2B)-O(2B)	-0.4(6)
C(6B)-C(1B)-C(2B)-C(3B)	-1.3(6)
C(1A)-C(1B)-C(2B)-C(3B)	-178.8(4)
O(2B)-C(2B)-C(3B)-C(4B)	-179.3(4)
C(1B)-C(2B)-C(3B)-C(4B)	-0.9(6)
O(2B)-C(2B)-C(3B)-O(3B)	-1.7(6)
C(1B)-C(2B)-C(3B)-O(3B)	176.8(4)
C(2B)-C(3B)-C(4B)-C(5B)	2.3(6)
O(3B)-C(3B)-C(4B)-C(5B)	-175.1(4)
C(2B)-C(3B)-C(4B)-C(1C)	-176.0(4)
O(3B)-C(3B)-C(4B)-C(1C)	6.5(6)
C(3B)-C(4B)-C(5B)-C(6B)	-1.6(6)
C(1C)-C(4B)-C(5B)-C(6B)	176.9(4)
C(4B)-C(5B)-C(6B)-O(4B)	179.1(4)
C(4B)-C(5B)-C(6B)-C(1B)	-0.7(6)
C(2B)-C(1B)-C(6B)-C(5B)	2.1(6)
C(1A)-C(1B)-C(6B)-C(5B)	179.7(4)
C(2B)-C(1B)-C(6B)-O(4B)	-177.7(4)
C(1A)-C(1B)-C(6B)-O(4B)	-0.1(6)
C(3B)-C(4B)-C(1C)-C(2C)	-44.4(6)
C(5B)-C(4B)-C(1C)-C(2C)	137.2(4)
C(3B)-C(4B)-C(1C)-C(6C)	135.0(4)
C(5B)-C(4B)-C(1C)-C(6C)	-43.4(5)
C(6C)-C(1C)-C(2C)-C(3C)	-0.7(6)
C(4B)-C(1C)-C(2C)-C(3C)	178.8(4)
C(1C)-C(2C)-C(3C)-C(4C)	-1.0(6)
C(2C)-C(3C)-C(4C)-O(5C)	-177.8(4)

C(2C)-C(3C)-C(4C)-C(5C)	2.5(6)
O(5C)-C(4C)-C(5C)-C(6C)	178.0(4)
C(3C)-C(4C)-C(5C)-C(6C)	-2.3(6)
C(4C)-C(5C)-C(6C)-C(1C)	0.6(6)
C(2C)-C(1C)-C(6C)-C(5C)	0.9(6)
C(4B)-C(1C)-C(6C)-C(5C)	-178.6(4)
C(4B)-C(3B)-O(3B)-C(7B)	-77.8(5)
C(2B)-C(3B)-O(3B)-C(7B)	104.6(4)
O(1)-C(4)-C(3)-C(2)	-177.9(4)
C(5)-C(4)-C(3)-C(2)	2.4(6)
C(4)-C(3)-C(2)-C(1)	0.0(7)
C(3)-C(2)-C(1)-C(6)	-2.9(6)
C(3)-C(2)-C(1)-C(1')	173.5(4)
C(2)-C(1)-C(6)-C(5)	3.7(6)
C(1')-C(1)-C(6)-C(5)	-172.8(4)
C(1)-C(6)-C(5)-C(4)	-1.4(6)
C(3)-C(4)-C(5)-C(6)	-1.7(6)
O(1)-C(4)-C(5)-C(6)	178.5(4)
C(6)-C(1)-C(1')-C(6')	-69.9(5)
C(2)-C(1)-C(1')-C(6')	113.7(5)
C(6)-C(1)-C(1')-C(2')	106.4(5)
C(2)-C(1)-C(1')-C(2')	-70.0(5)
C(6')-C(1')-C(2')-O(2')	-179.7(3)
C(1)-C(1')-C(2')-O(2')	3.7(5)
C(6')-C(1')-C(2')-C(3')	-1.7(6)
C(1)-C(1')-C(2')-C(3')	-178.3(3)
O(2')-C(2')-C(3')-C(4')	179.3(3)
C(1')-C(2')-C(3')-C(4')	1.3(6)
O(2')-C(2')-C(3')-O(3')	-1.3(5)
C(1')-C(2')-C(3')-O(3')	-179.4(3)
C(2')-C(3')-C(4')-C(5')	-0.6(6)
O(3')-C(3')-C(4')-C(5')	-179.9(3)
C(2')-C(3')-C(4')-C(1'')	-175.3(3)
O(3')-C(3')-C(4')-C(1'')	5.5(6)
C(3')-C(4')-C(5')-C(6')	0.4(6)
C(1'')-C(4')-C(5')-C(6')	175.0(3)
C(4')-C(5')-C(6')-C(1')	-0.8(6)
C(4')-C(5')-C(6')-O(4')	-179.7(4)
C(2')-C(1')-C(6')-C(5')	1.5(6)
C(1)-C(1')-C(6')-C(5')	177.9(4)
C(2')-C(1')-C(6')-O(4')	-179.7(3)
C(1)-C(1')-C(6')-O(4')	-3.2(6)
C(3')-C(4')-C(1'')-C(6'')	130.2(4)
C(5')-C(4')-C(1'')-C(6'')	-44.3(5)

C(3')-C(4')-C(1'')-C(2'')	-46.3(5)
C(5')-C(4')-C(1'')-C(2'')	139.3(4)
C(6'')-C(1'')-C(2'')-C(3'')	0.8(6)
C(4')-C(1'')-C(2'')-C(3'')	177.4(4)
C(1'')-C(2'')-C(3'')-C(4'')	-0.5(6)
C(2'')-C(3'')-C(4'')-O(5'')	179.1(4)
C(2'')-C(3'')-C(4'')-C(5'')	0.0(6)
O(5'')-C(4'')-C(5'')-C(6'')	-178.9(4)
C(3'')-C(4'')-C(5'')-C(6'')	0.2(6)
C(4'')-C(5'')-C(6'')-C(1'')	0.1(6)
C(2'')-C(1'')-C(6'')-C(5'')	-0.6(6)
C(4')-C(1'')-C(6'')-C(5'')	-177.3(4)
C(4')-C(3')-O(3')-C(7')	-85.9(4)
C(2')-C(3')-O(3')-C(7')	94.8(4)

Symmetry transformations used to generate equivalent atoms:

Table S16. Hydrogen Bonds [Å and deg.] for L (Compound **4**)

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(1C)...O(4')#1	0.87	1.82	2.681(4)	176.8
O(1W)-H(1D)...O(2')	0.85	2.07	2.791(4)	141.7
O(5'')-H(5C)...O(1A)#2	0.84	1.89	2.716(4)	166.2
O(2')-H(2B)...O(4B)	0.84	1.95	2.761(4)	161.0
O(4')-H(4)...O(3W)#3	0.84	2.02	2.786(4)	151.2
O(1)-H(1)...O(1W)#4	0.84	1.84	2.680(5)	176.6
O(3W)-H(3F)...O(5'')#2	0.78	2.07	2.822(4)	162.3
O(3W)-H(3D)...O(5C)#5	0.75	2.01	2.755(4)	171.4
O(2W)-H(2F)...O(2B)	0.85	2.07	2.897(4)	164.8
O(2W)-H(2G)...O(3W)	0.86	2.17	3.029(4)	176.9
O(5C)-H(5H)...O(1)#6	0.84	1.90	2.710(4)	162.3
O(4B)-H(4A)...O(3')	0.84	2.27	2.765(4)	118.0
O(1A)-H(1A)...O(2W)#7	0.84	1.84	2.681(4)	177.6

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z #2 -x+2,-y+2,-z+1 #3 x+1,y,z+1
#4 -x+1,-y+1,-z+2 #5 -x,-y+1,-z+1 #6 -x,-y+1,-z+2
#7 -x+1,-y+2,-z+1