Supporting Information

Serinocyclins A and B, Cyclic Heptapeptides from *Metarhizium anisopliae*

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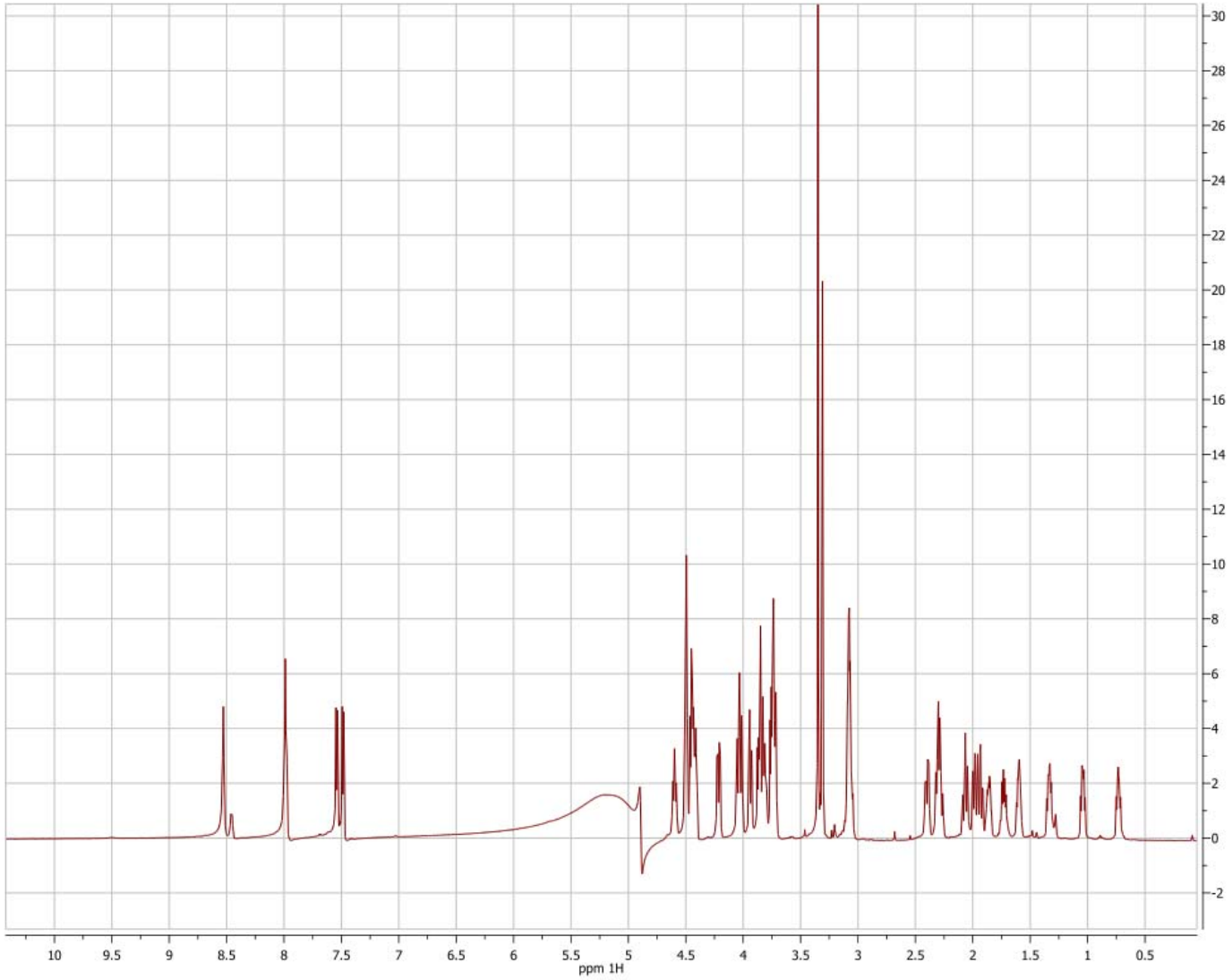


Figure S2. ^{1}H NMR spectrum of **1** (with solvent presaturation): amide region

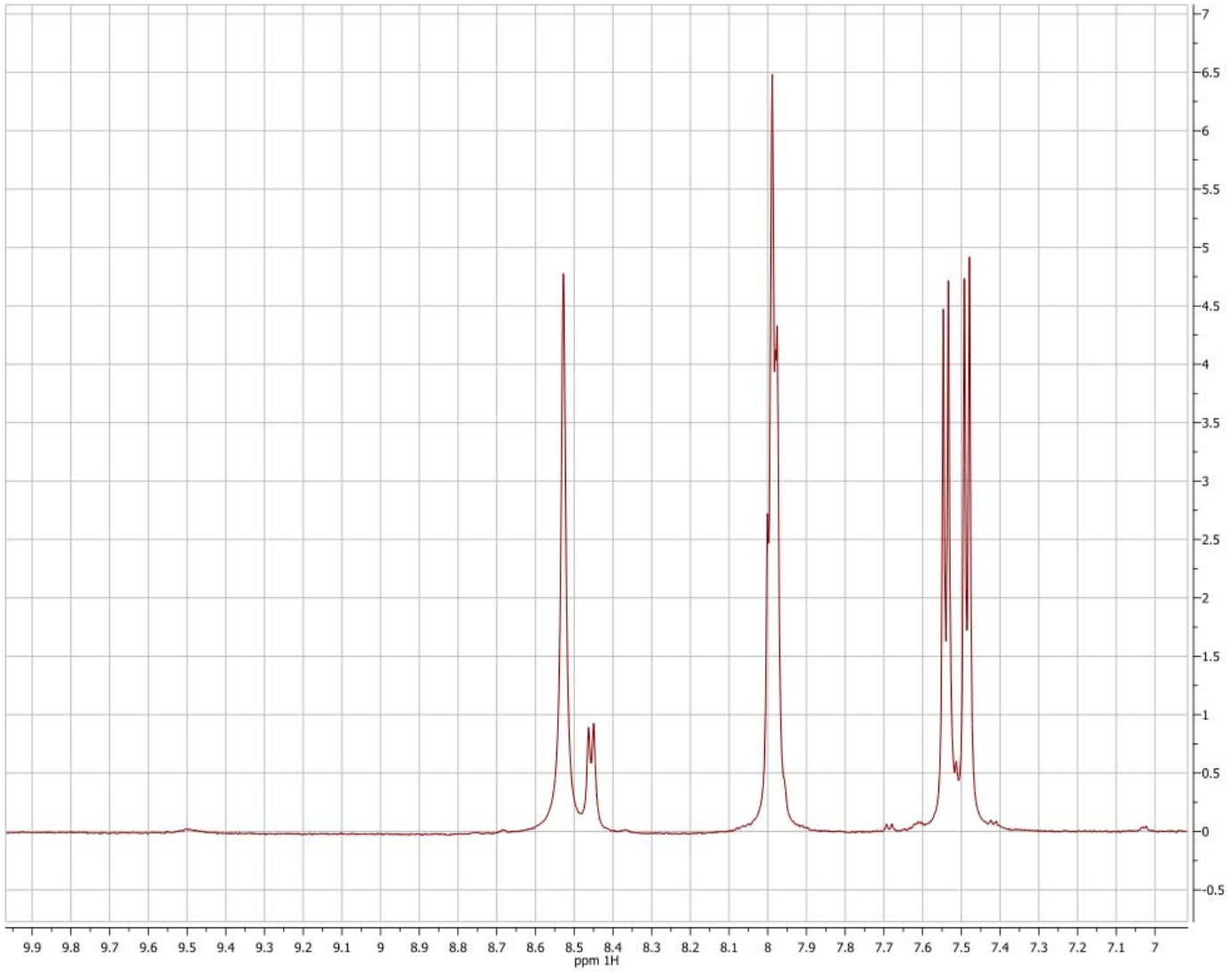


Figure S3. ^{1}H NMR spectrum of **1** (without solvent presaturation)

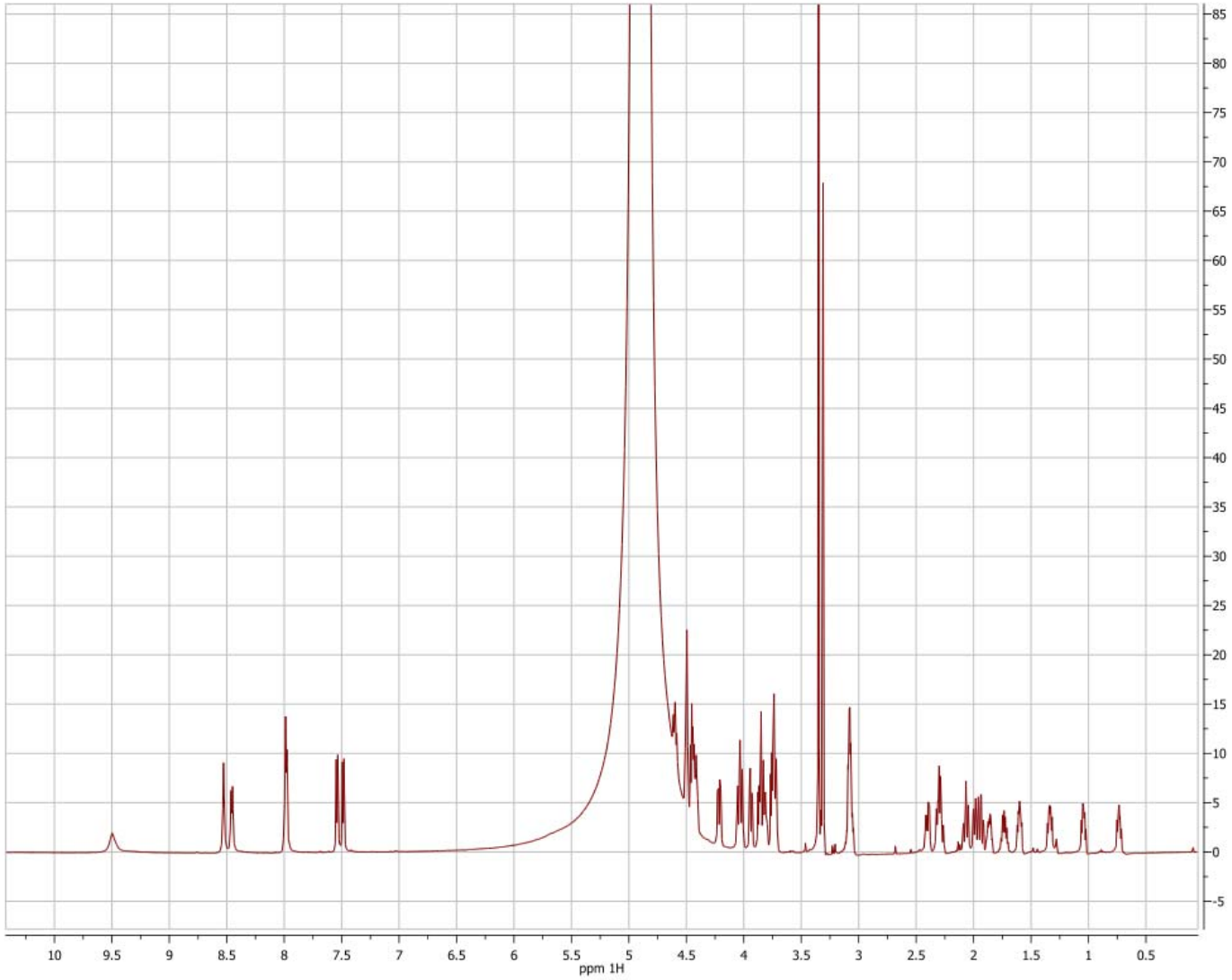


Figure S4. ^{1}H NMR spectrum of **1** (without solvent presaturation): amide region

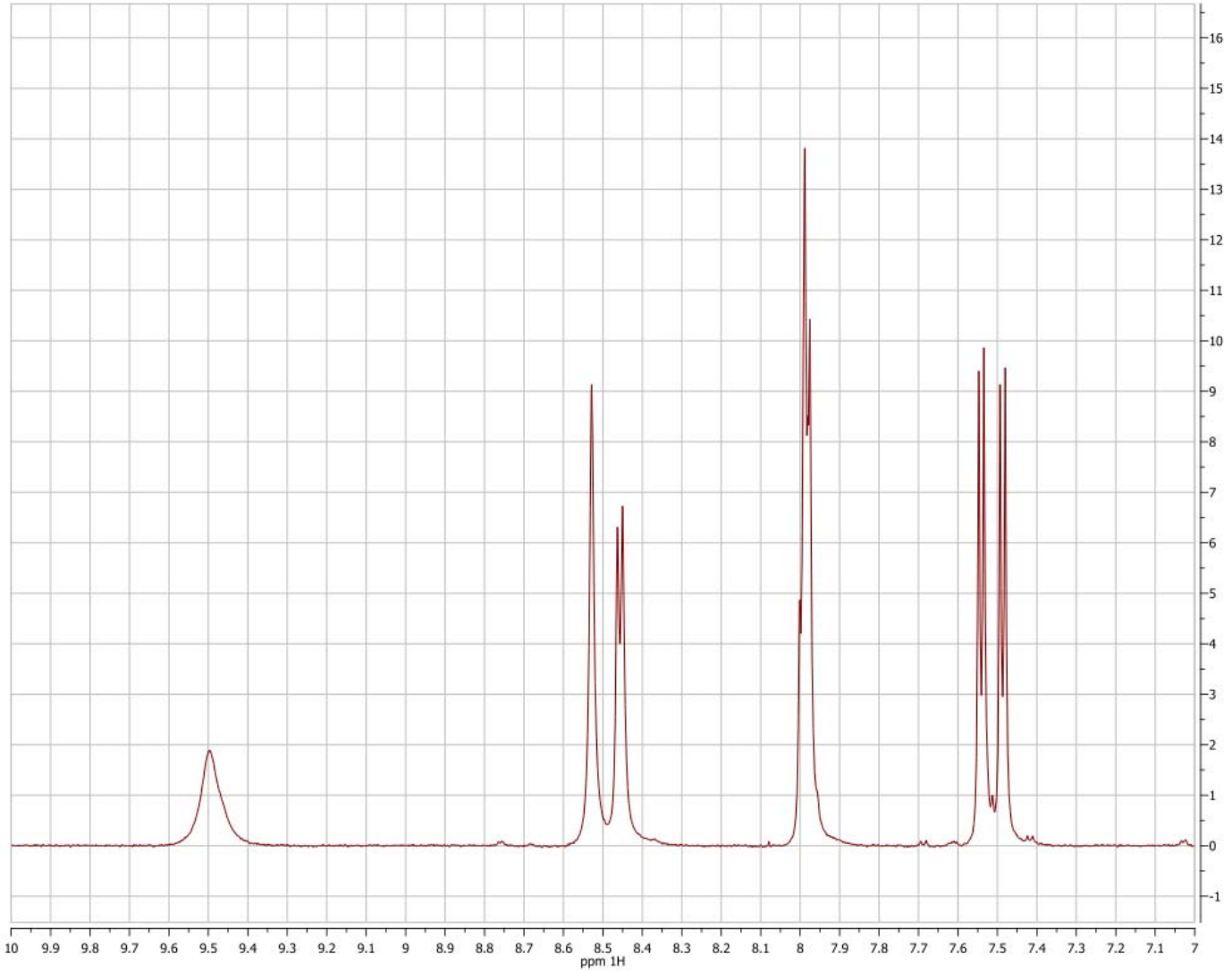


Figure S5. ^{13}C NMR spectrum of **1**

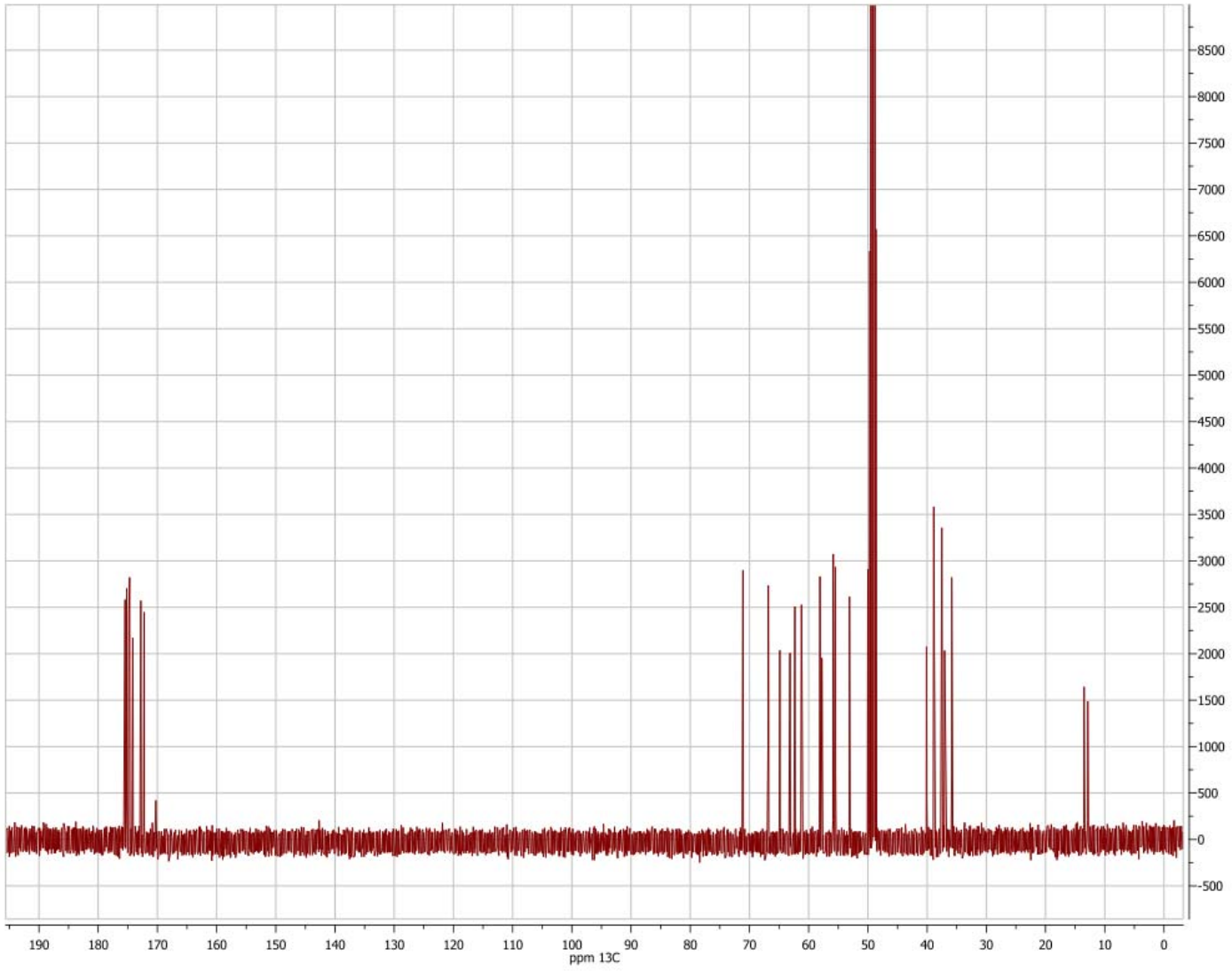


Figure S6. ^{13}C NMR spectrum of **1**: carbonyl region

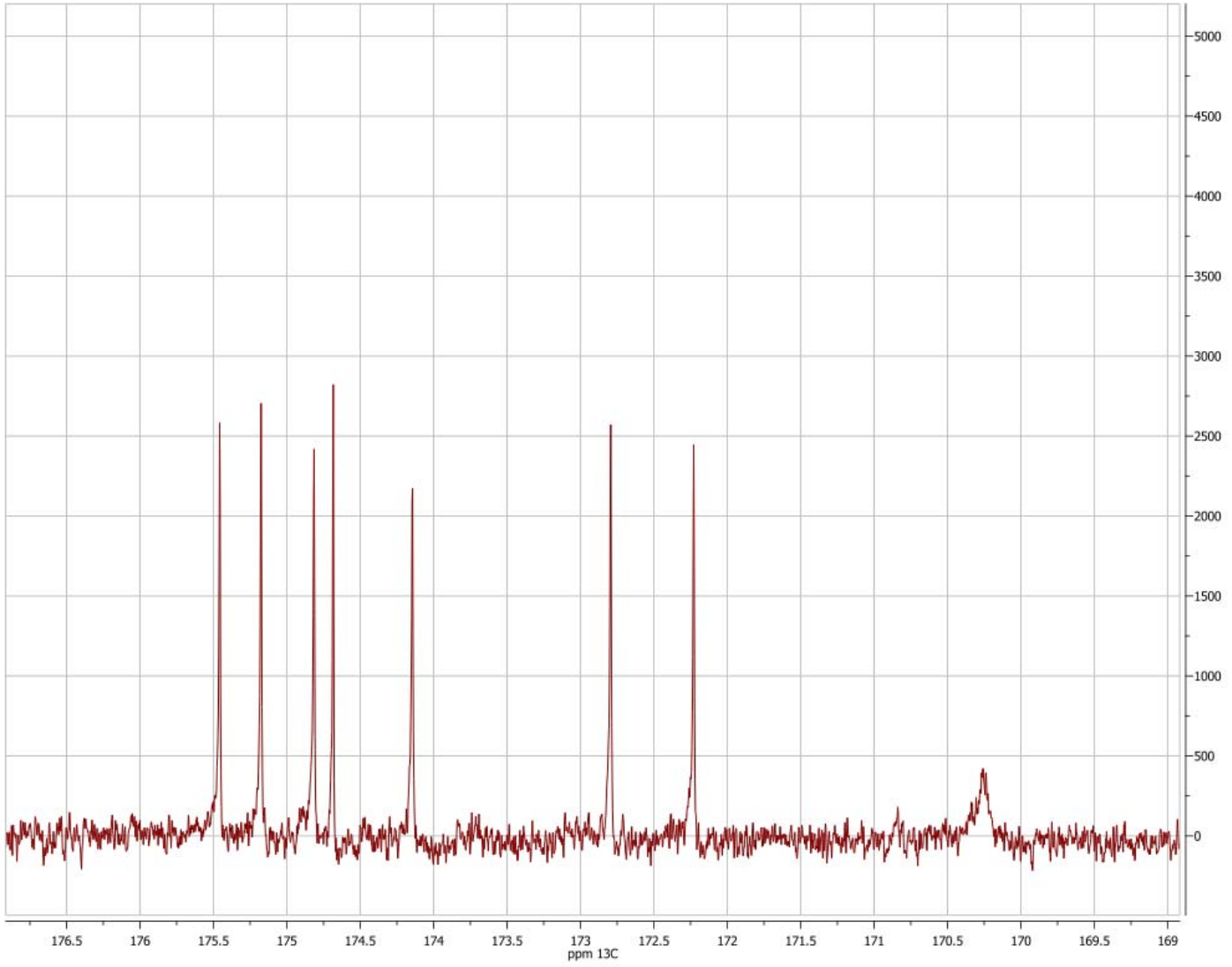


Figure S7. ^{13}C NMR spectrum of **1**: detail 1 of sp^3 region, detail 1

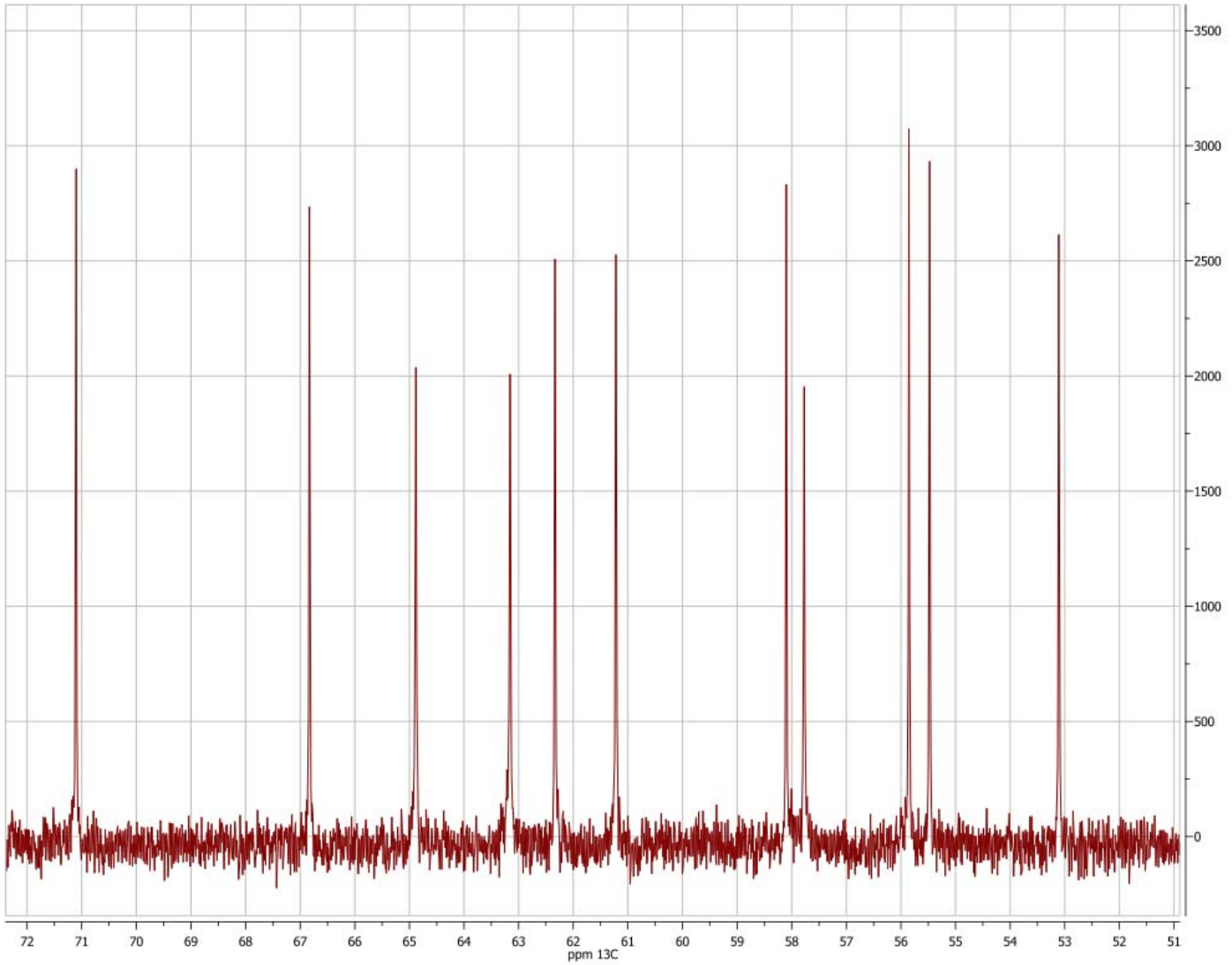


Figure S8. ^{13}C NMR spectrum of **1**: detail 2 of sp^3 region

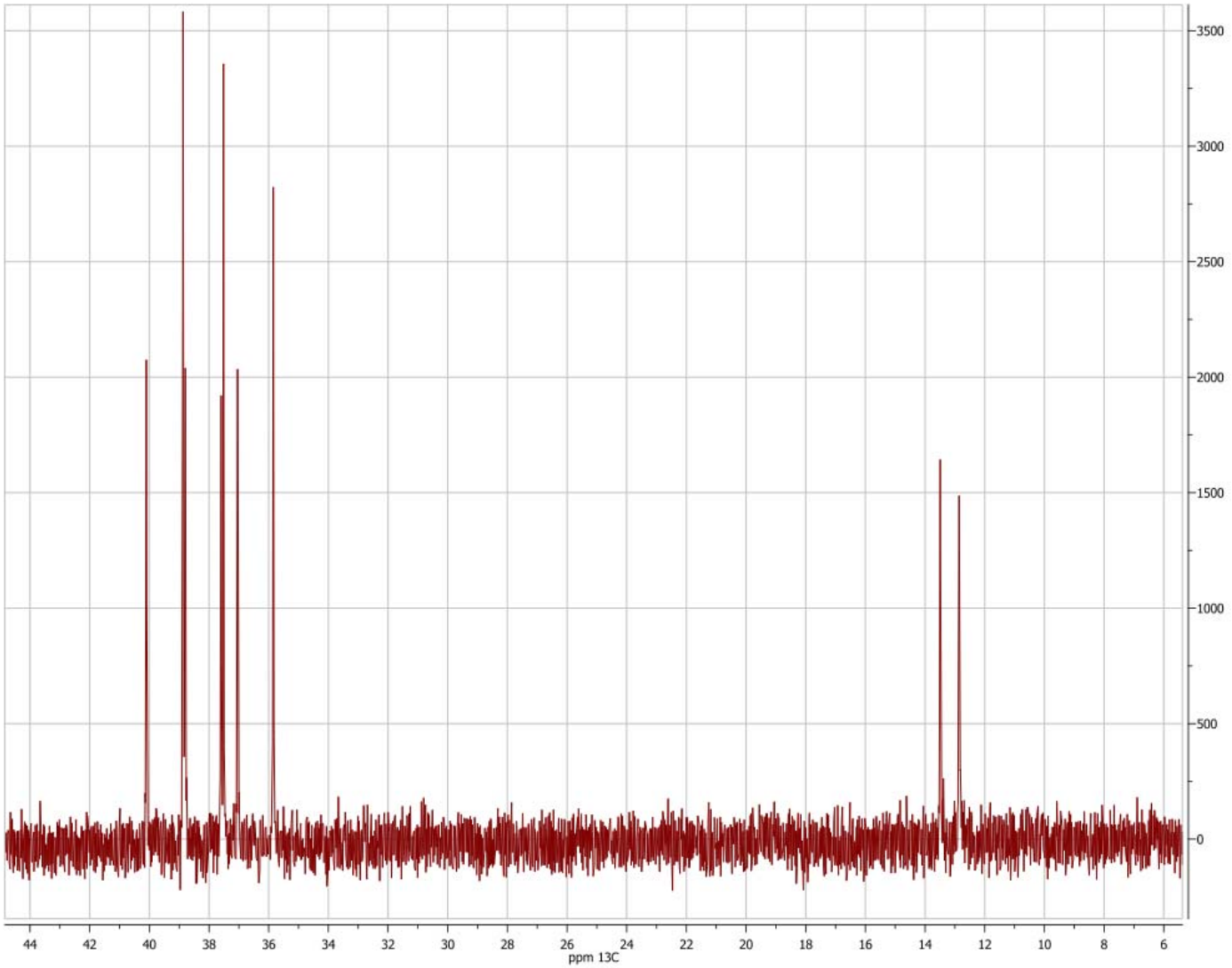


Figure S9. ^{13}C NMR spectrum of **1**: detail 3 of sp^3 region

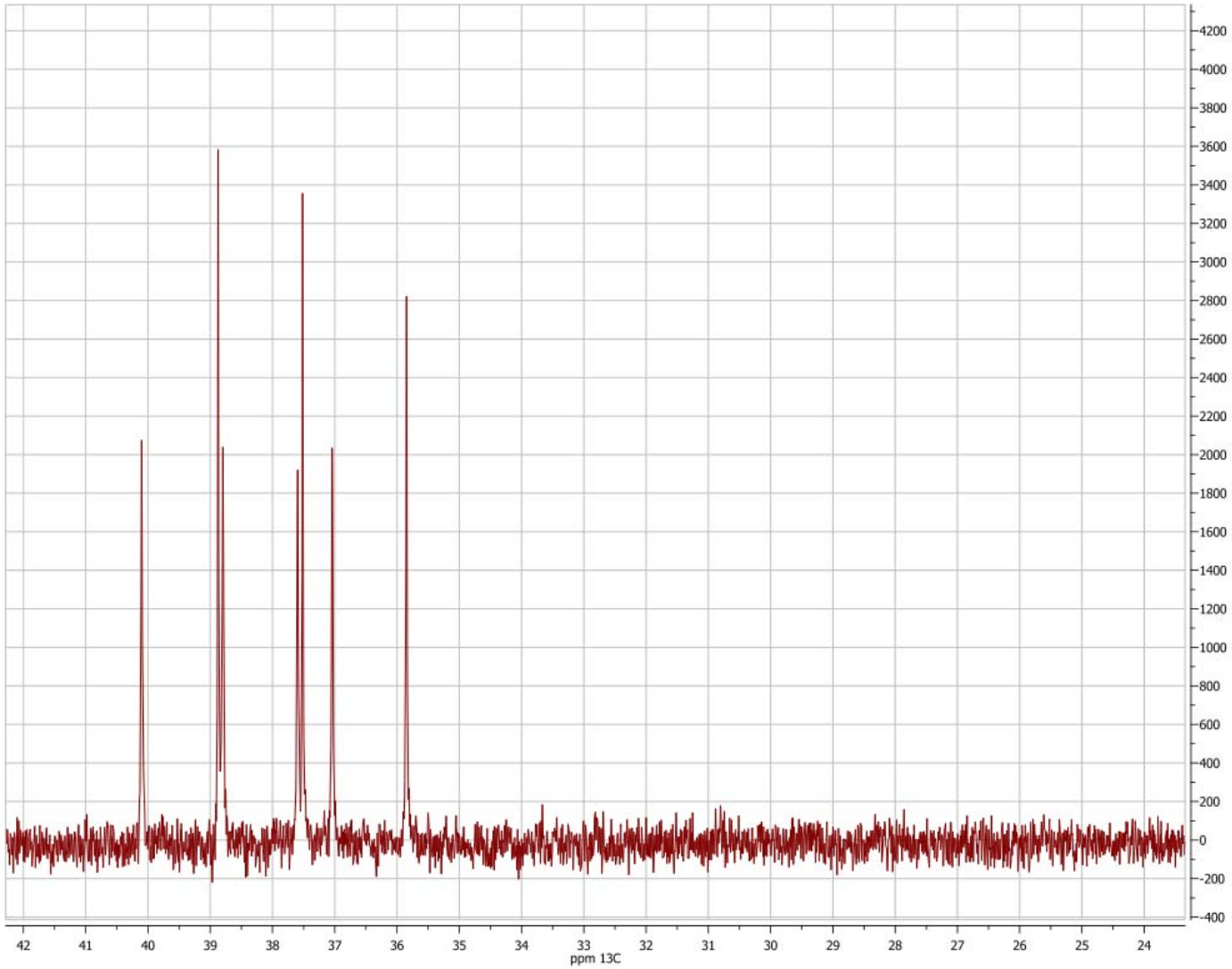


Figure S10. dqCOSY spectrum of **1**

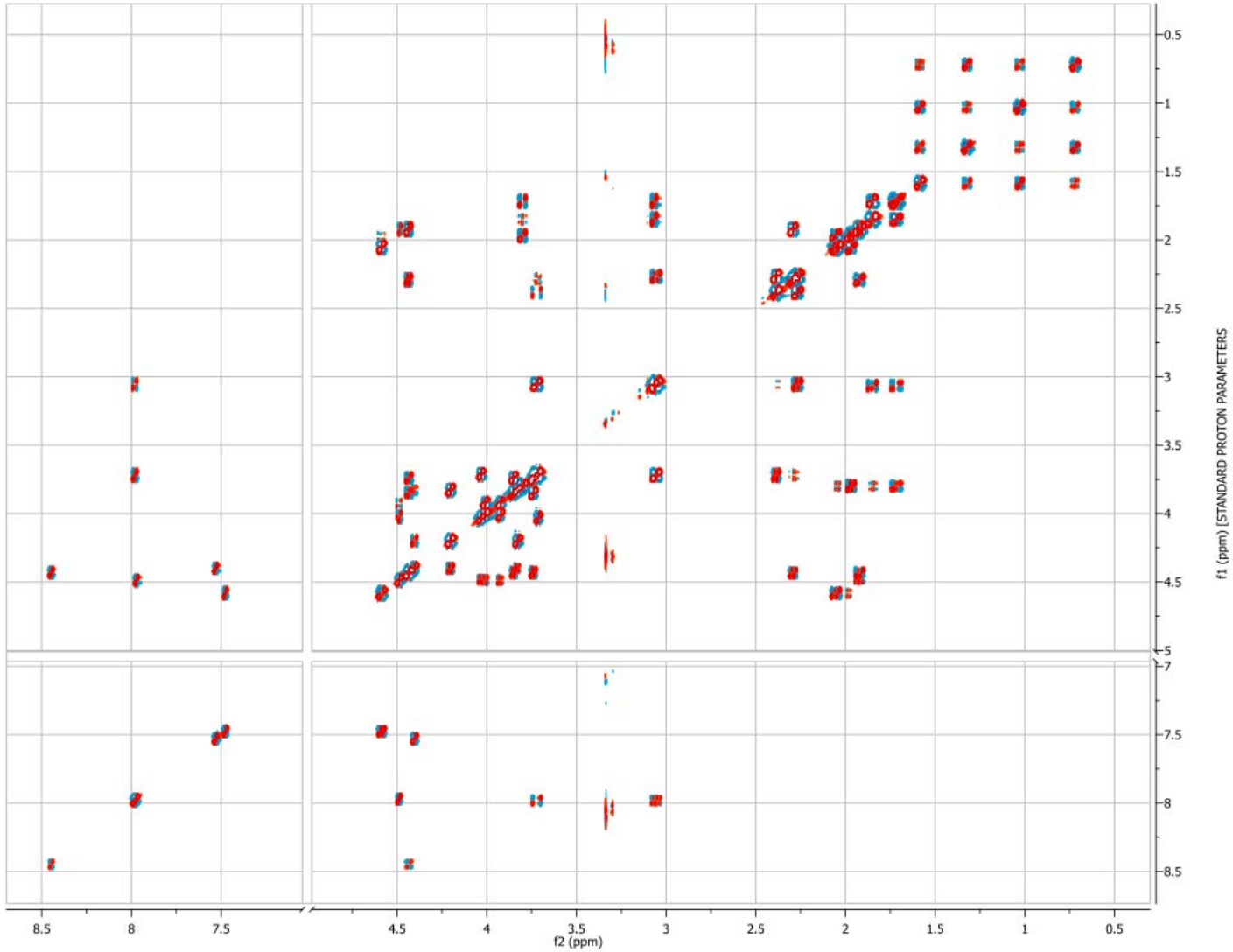


Figure S11. ^{1}H NMR spectrum of **2** (with solvent presaturation)

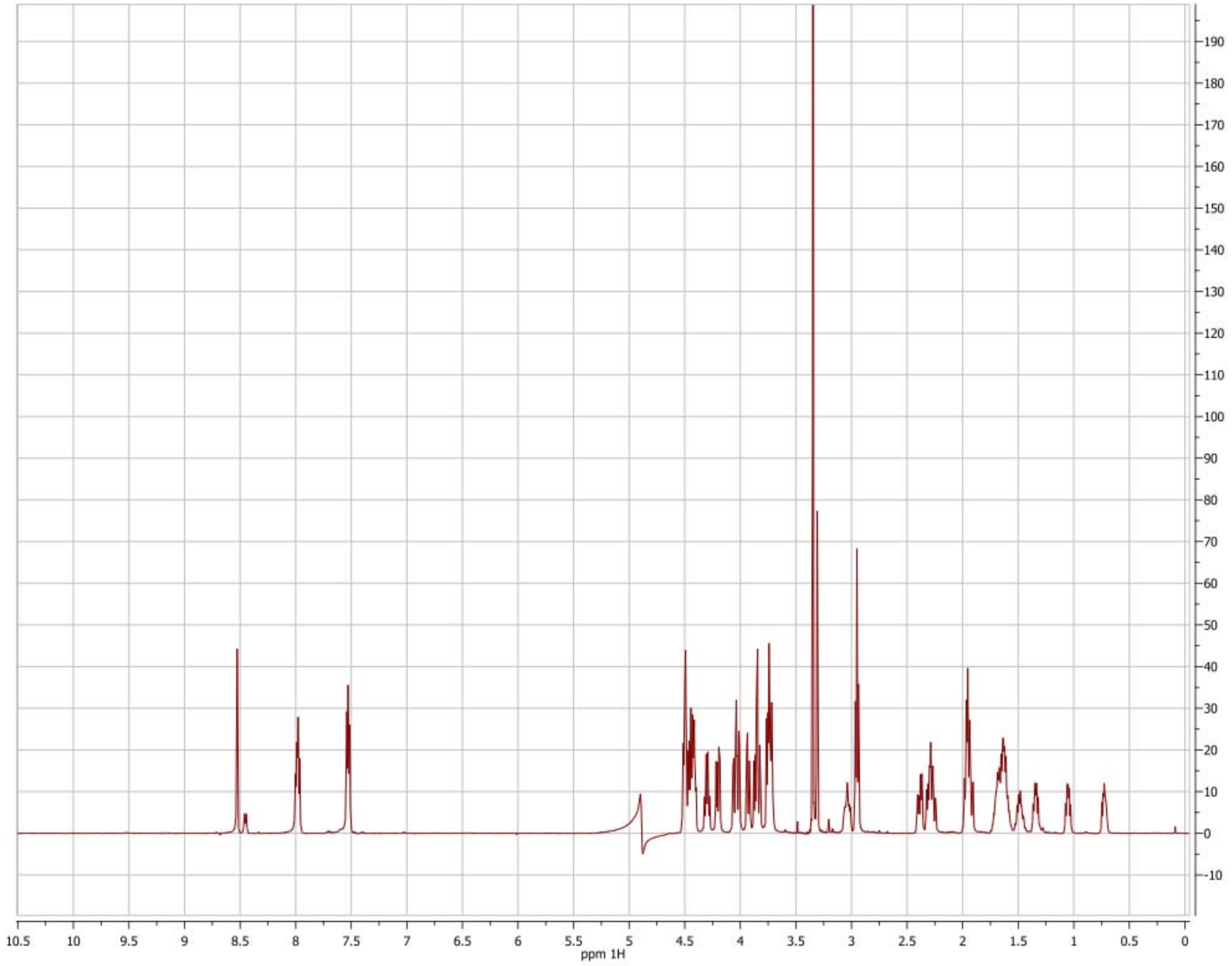


Figure S12. ^{1}H NMR spectrum of **2** (with solvent presaturation): amide region

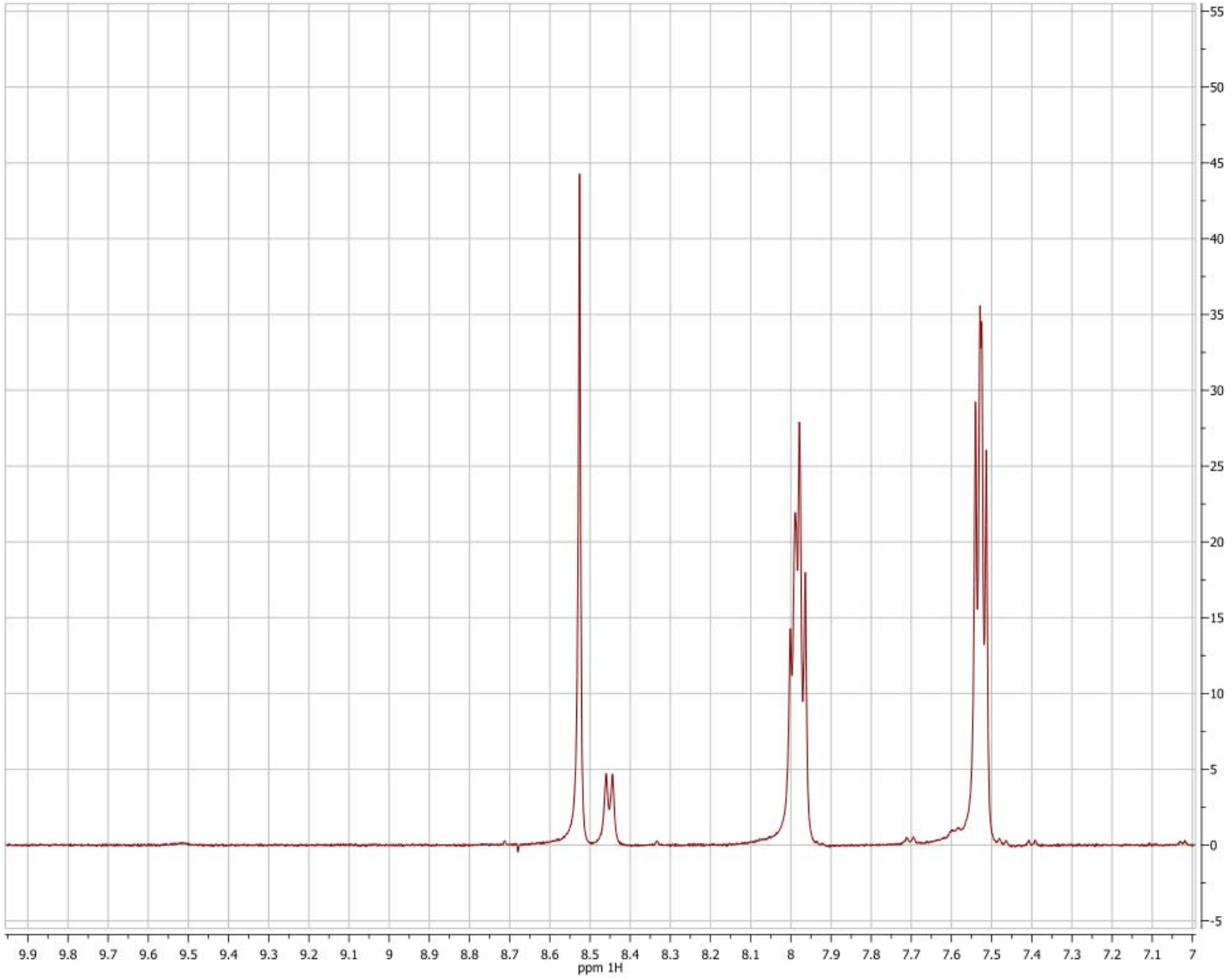


Figure S13. ^{1}H NMR spectrum of **2** (without solvent presaturation)

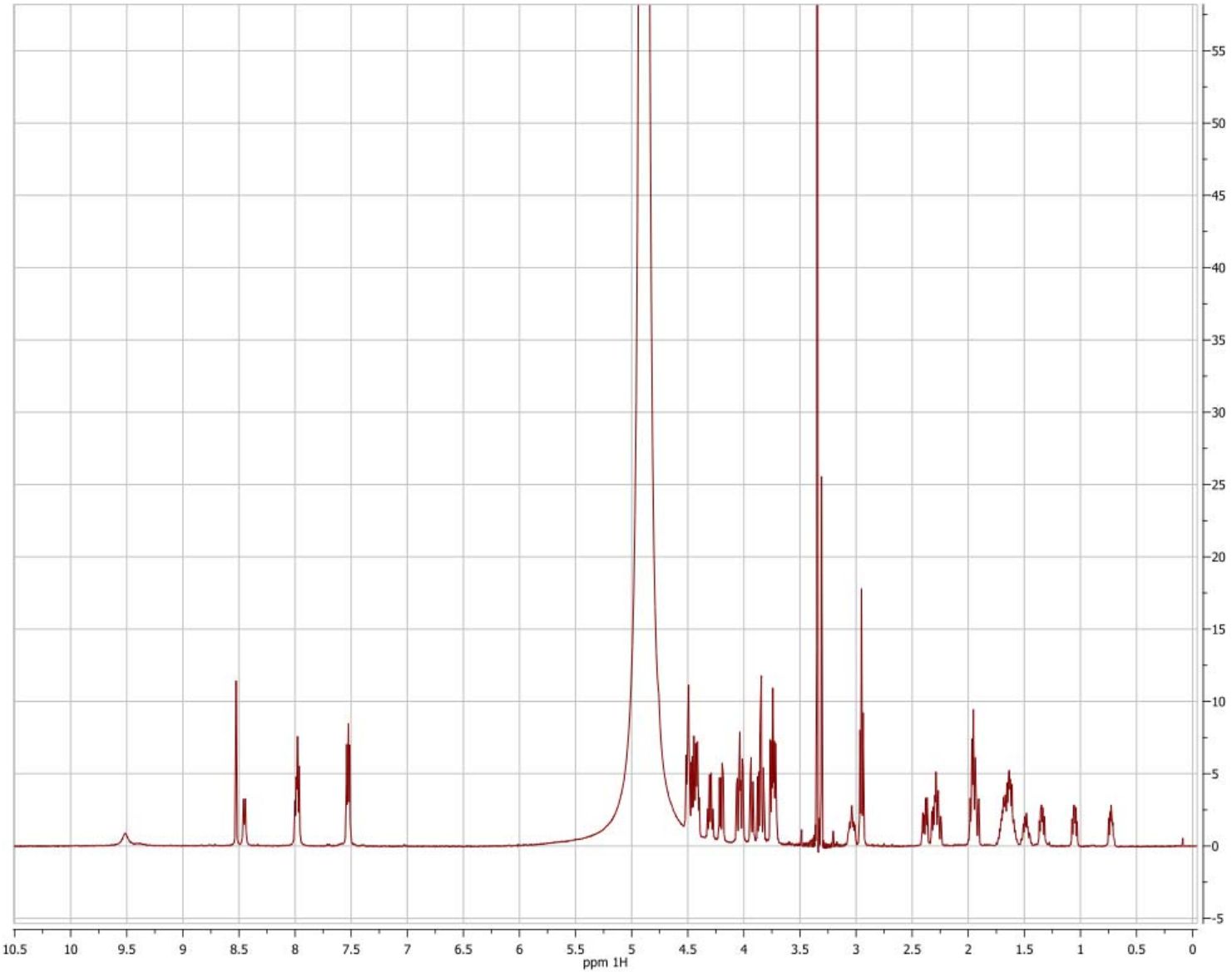


Figure S14. ^{1}H NMR spectrum of **2** (without solvent presaturation): amide region

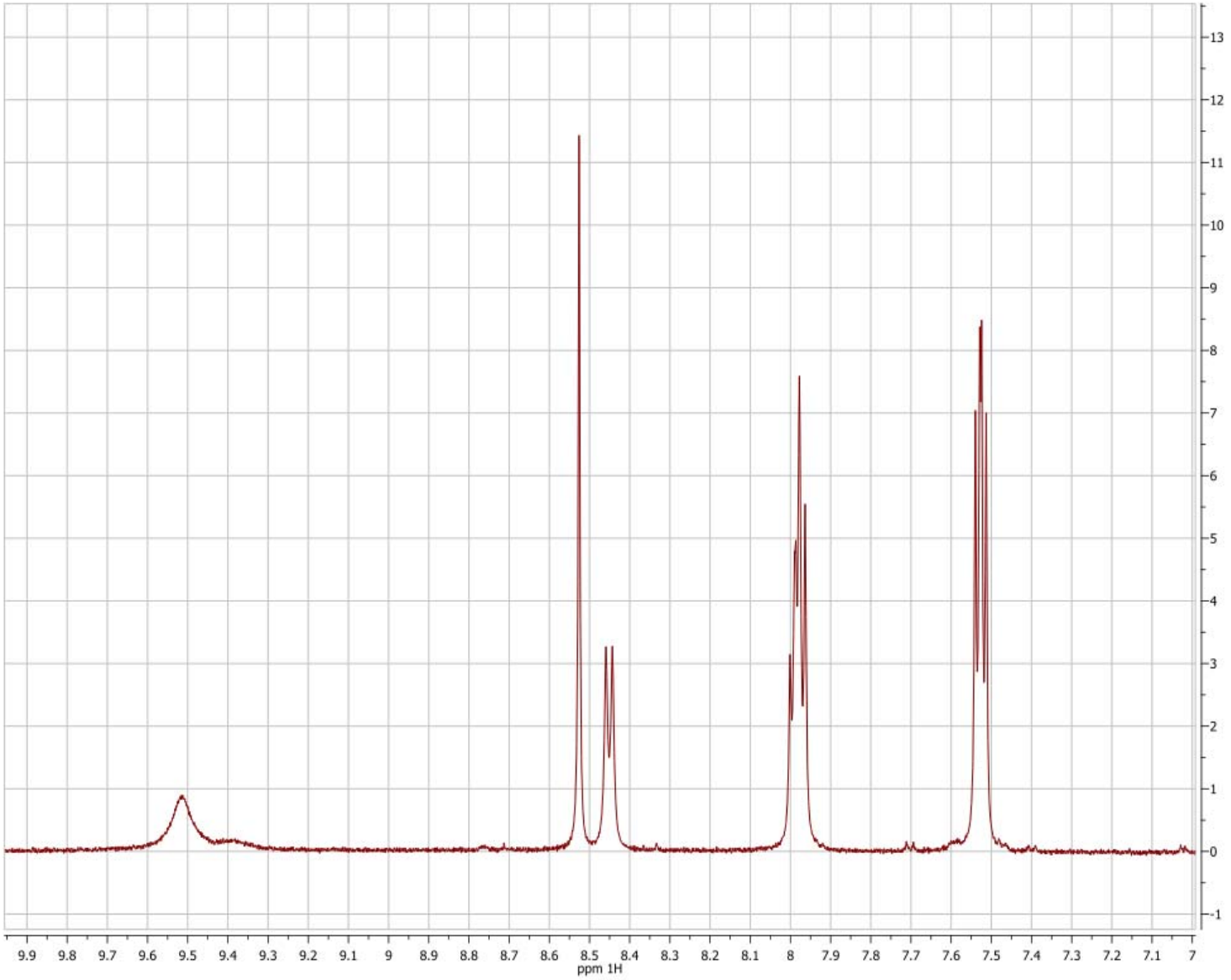


Figure S15. ^{13}C NMR spectrum of **2**

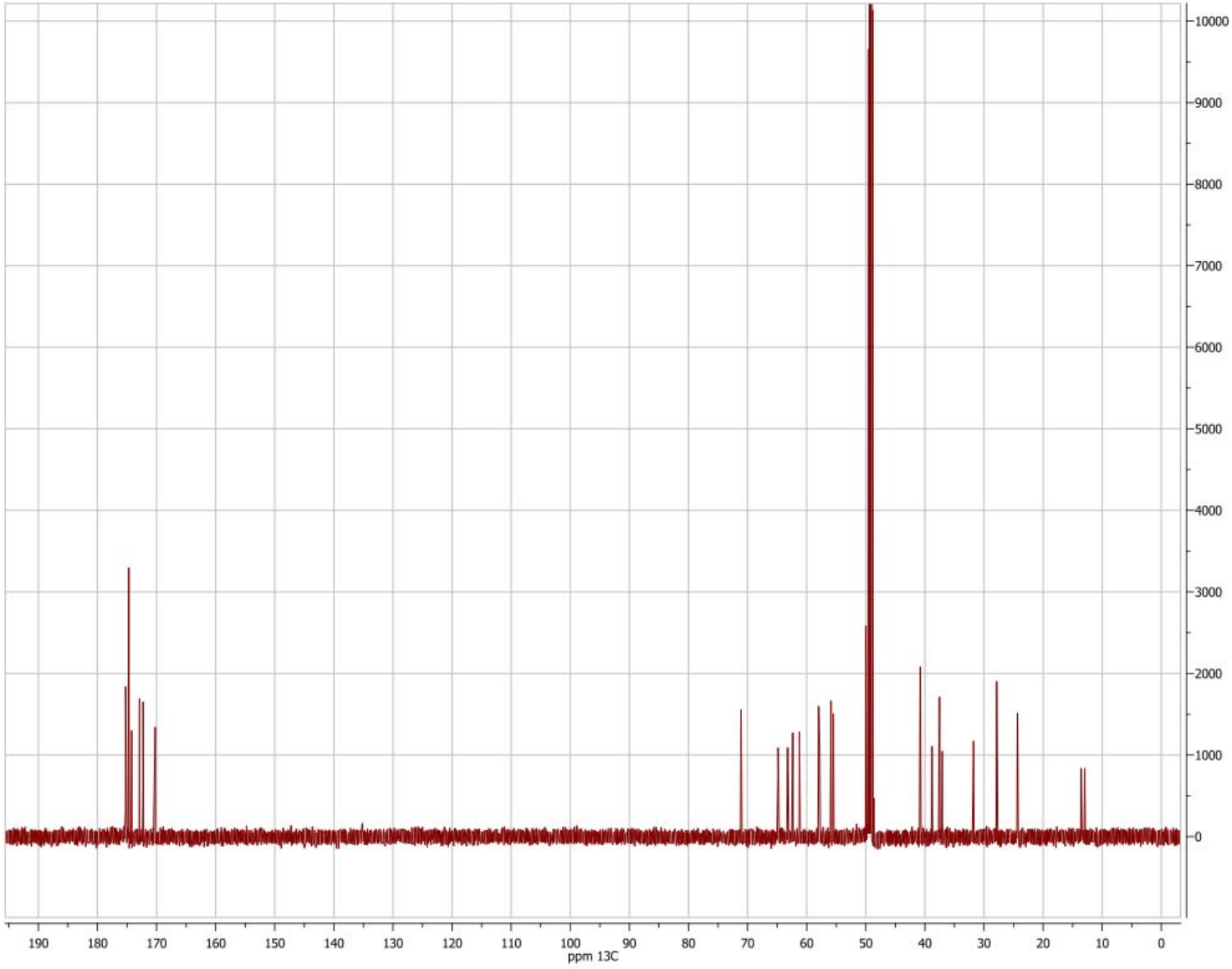


Figure S16. ^{13}C NMR spectrum of **2**: carbonyl region

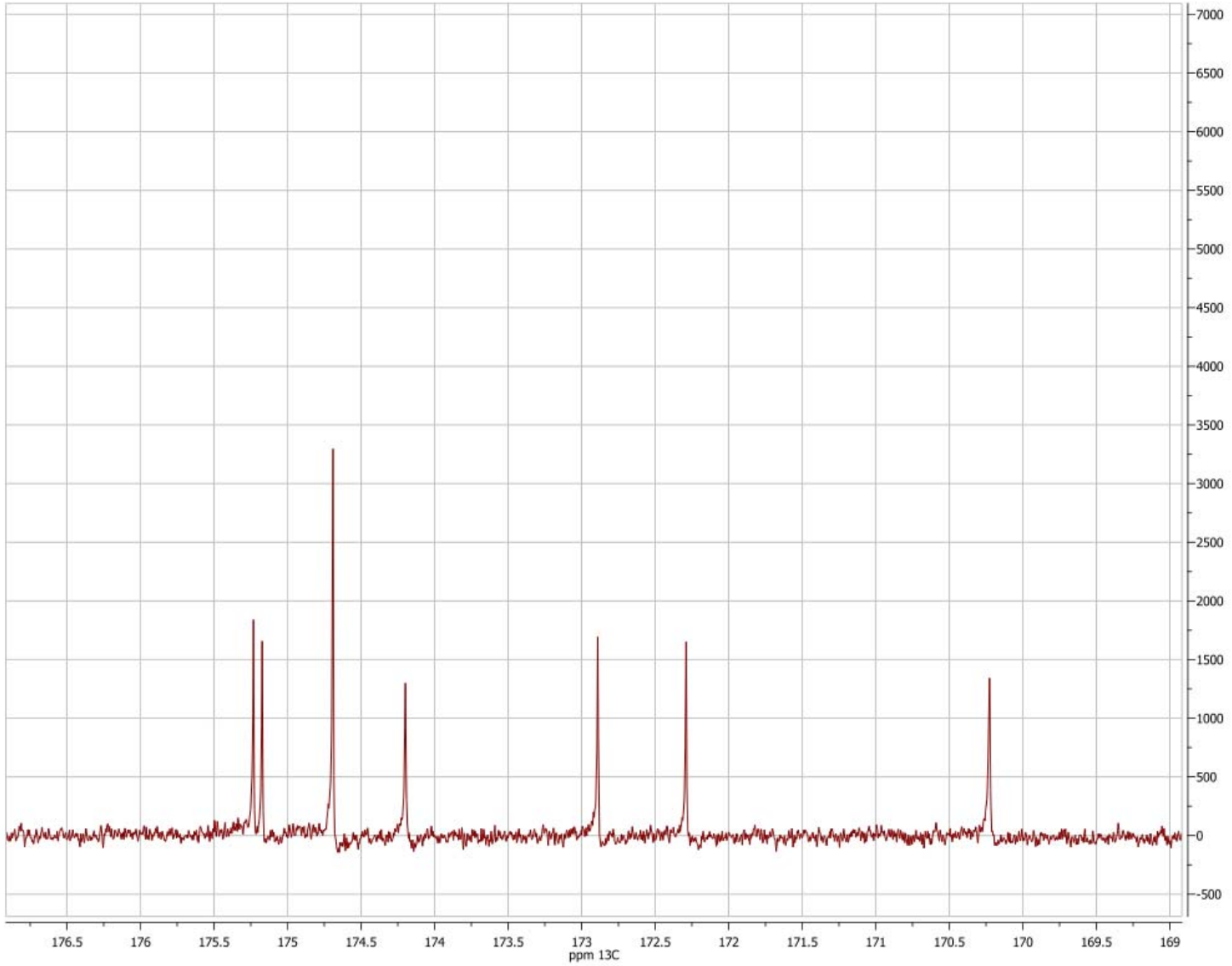


Figure S17. ^{13}C NMR spectrum of **2**: detail 1 of sp^3 region

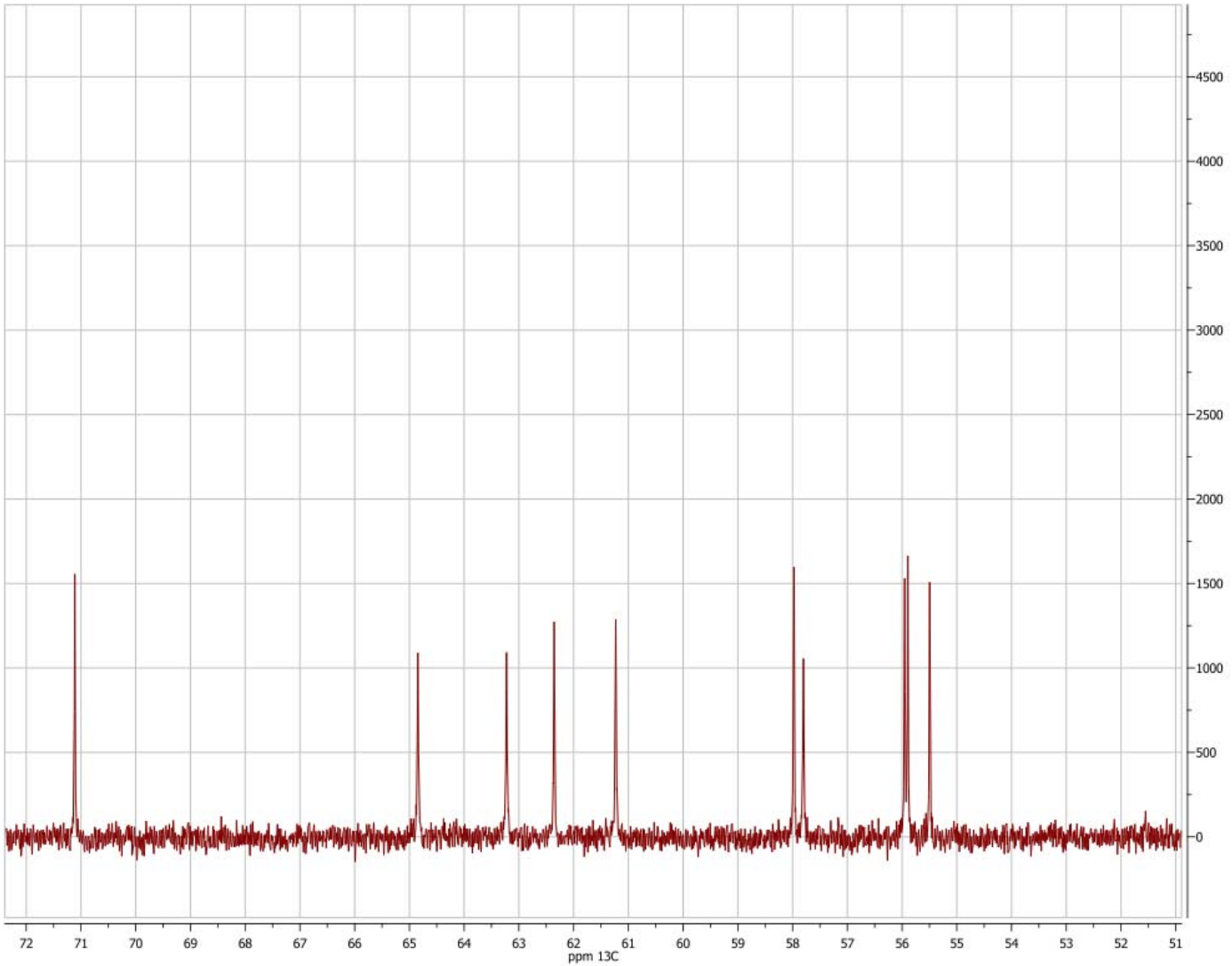


Figure S18. ^{13}C NMR spectrum of **2**: detail 2 of sp^3 region

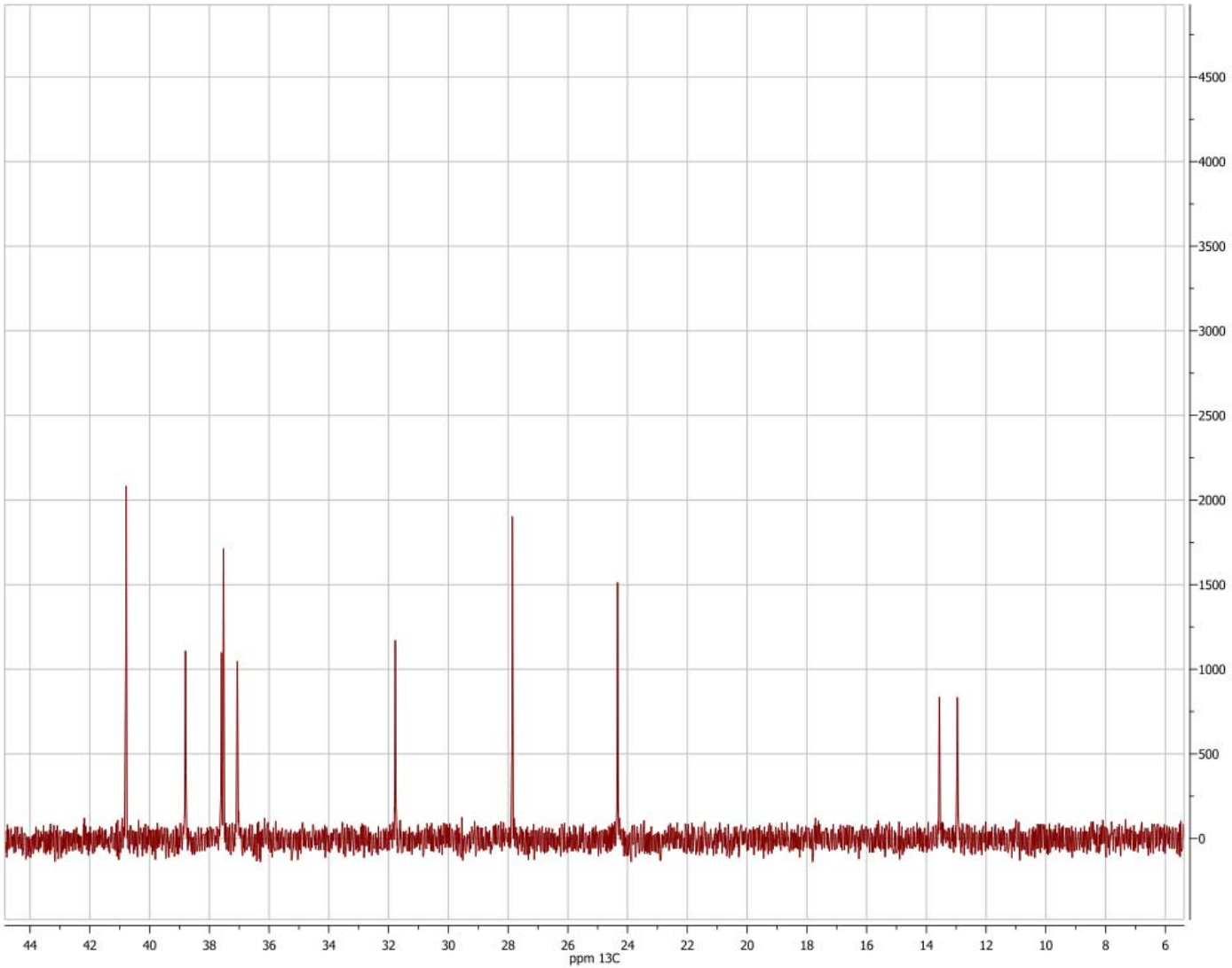


Figure S19. ^{13}C NMR spectrum of **2**: detail 3 of sp^3 region

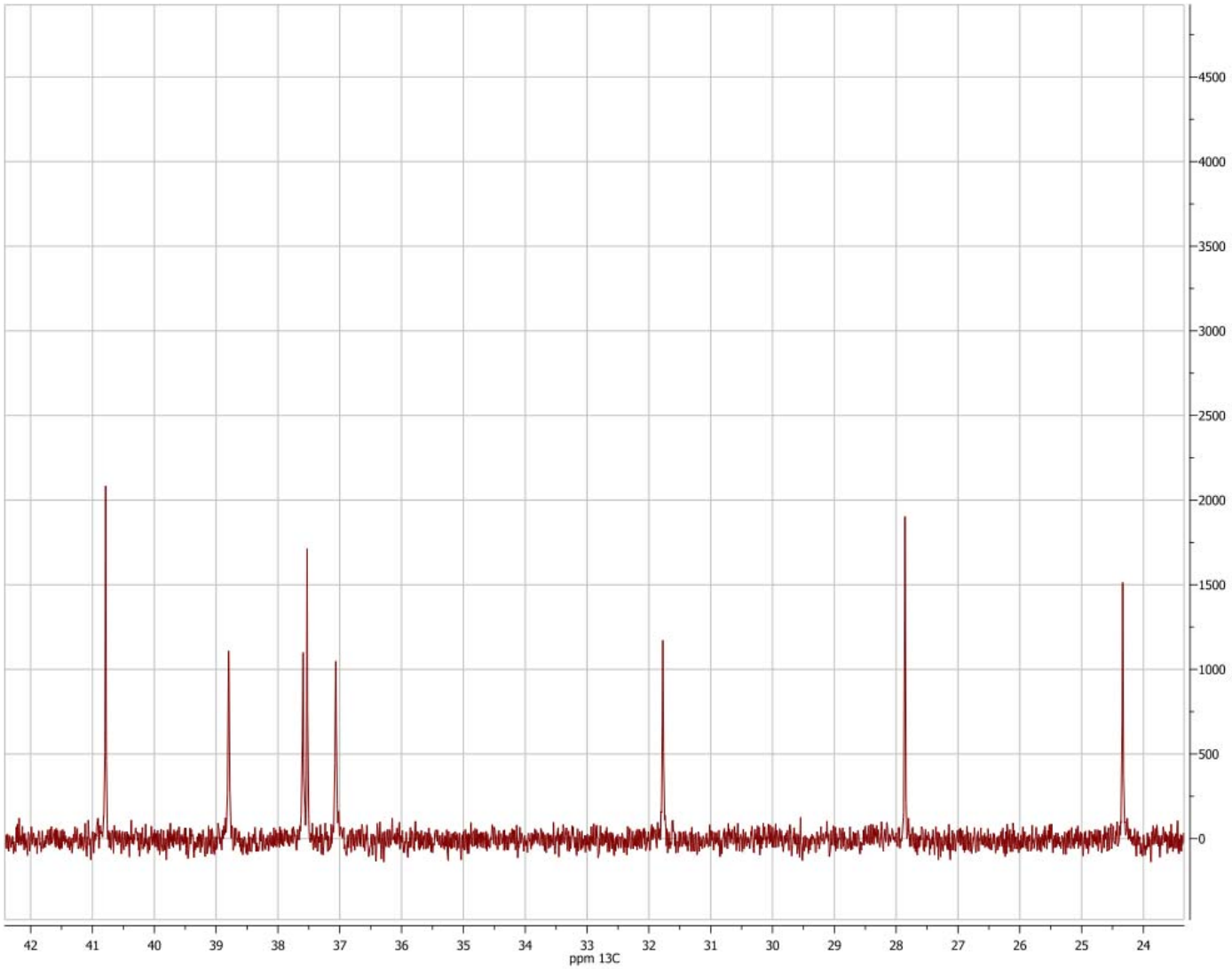


Figure S20. gCOSY spectrum of **2**

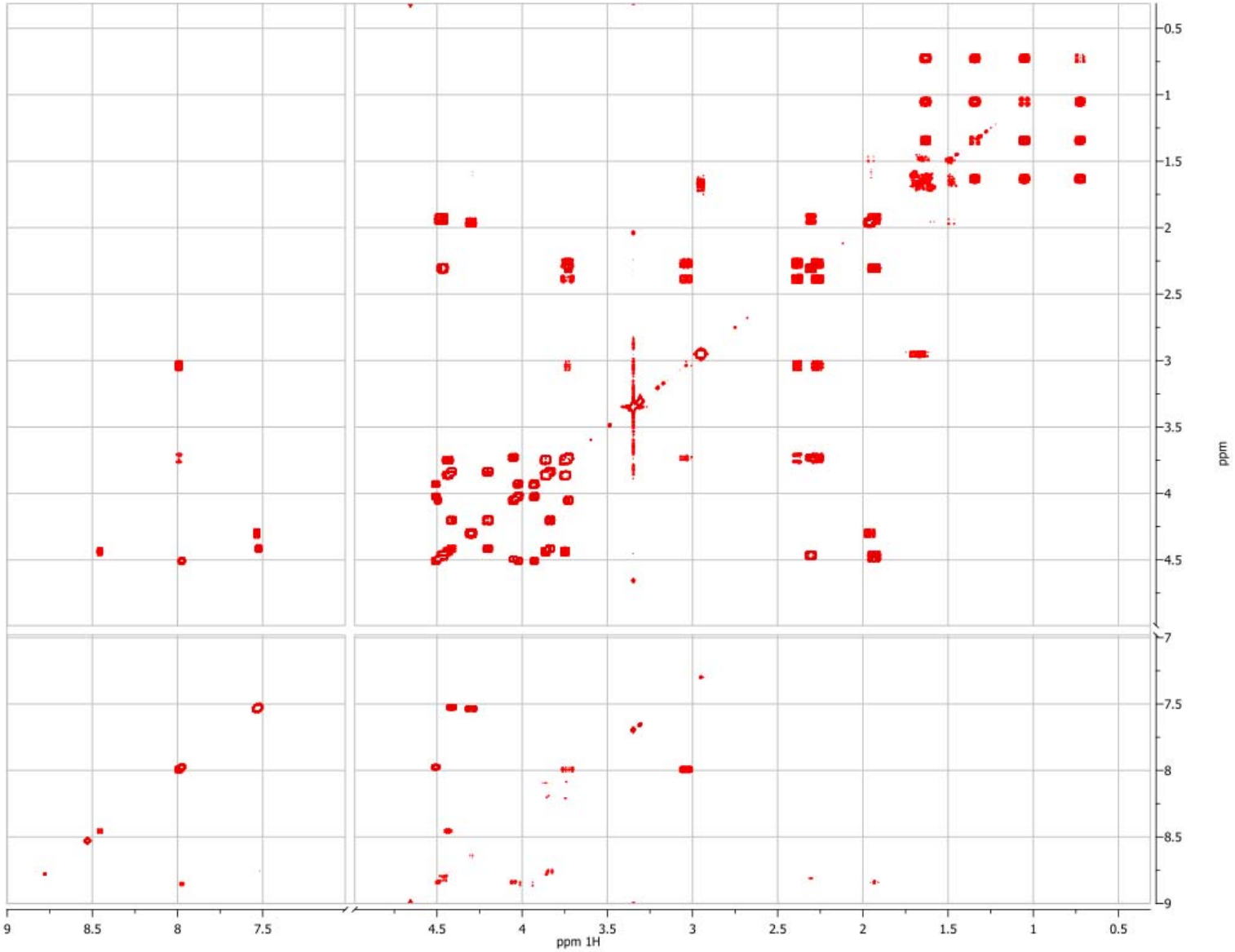


Figure S21. Probit plot for effect of **1** on swimming in *Aedes aegypti* larvae.

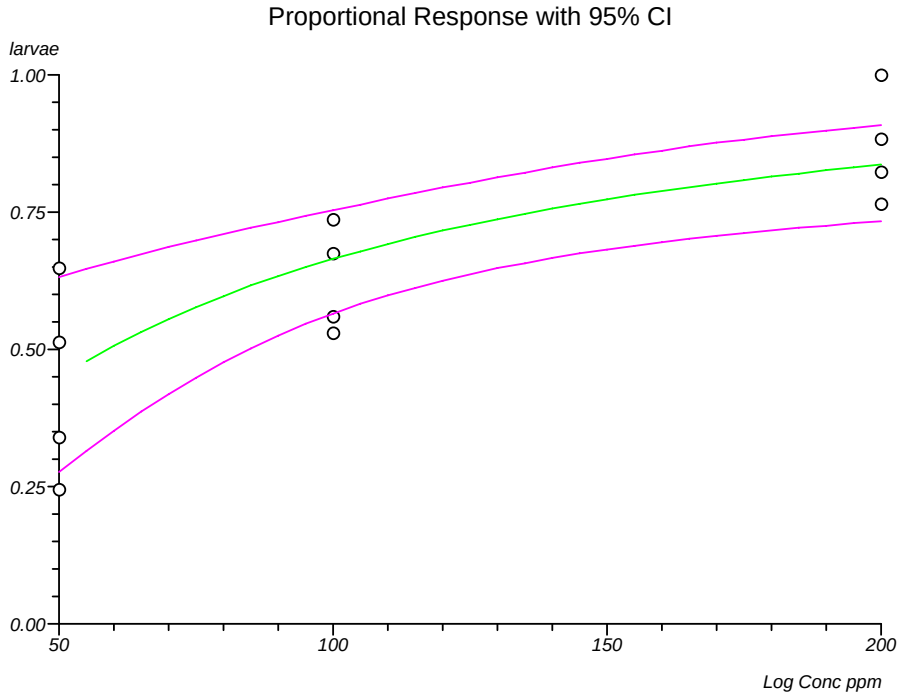
constant = -3.254389
slope = 1.839706

Median * Dose = 58.745268
Confidence interval (No Heterogeneity) = 25.950352 to 82.289173

* Dose for centile 90 = 292.132408
Confidence interval (No Heterogeneity) = 177.678738 to 1548.854659

Chi² (heterogeneity of deviations from model) = 6.405153 (10 df) P = 0.7802

t for slope = 3.362501 (10 df) P = 0.0072



Probit analysis - further statistics

Iterations = 3

Sxx = 3.366044
Sxy = 6.192533
Syy = 17.797591

Variance of B = 0.191735
Standard error of B without heterogeneity = 0.547124

Estimated natural response rate (C) = 0.05303
Variance of B = without heterogeneity
Standard error of B 0.036348 = 1

Figure S22. Comparison of tracks of tail, center, and head from serinocyclin A-treated and untreated *Aedes aegypti* larvae. Using a high-speed digital camera (Redlake®) mounted on a compound microscope, videographs were acquired for 2.0 sec at 250 frames/sec of third instar *A. aegypti* larvae swimming in wells of a 24-well plate ca. 16 mm in diameter. Tracks shown were traced by hand by advancing frame-by-frame and marking the position in each frame of (A) the larval tail, the center, (B) first abdominal segment, and (C) the head. Tracks on the left side each panel are from a single untreated larva and those on the right are from a single larva treated with serinocylin A at 100 ppm. The line separating treated from untreated tracks is a 1 cm scale bar. Arrows indicate "forward" progress (i.e. in the direction of the tail).

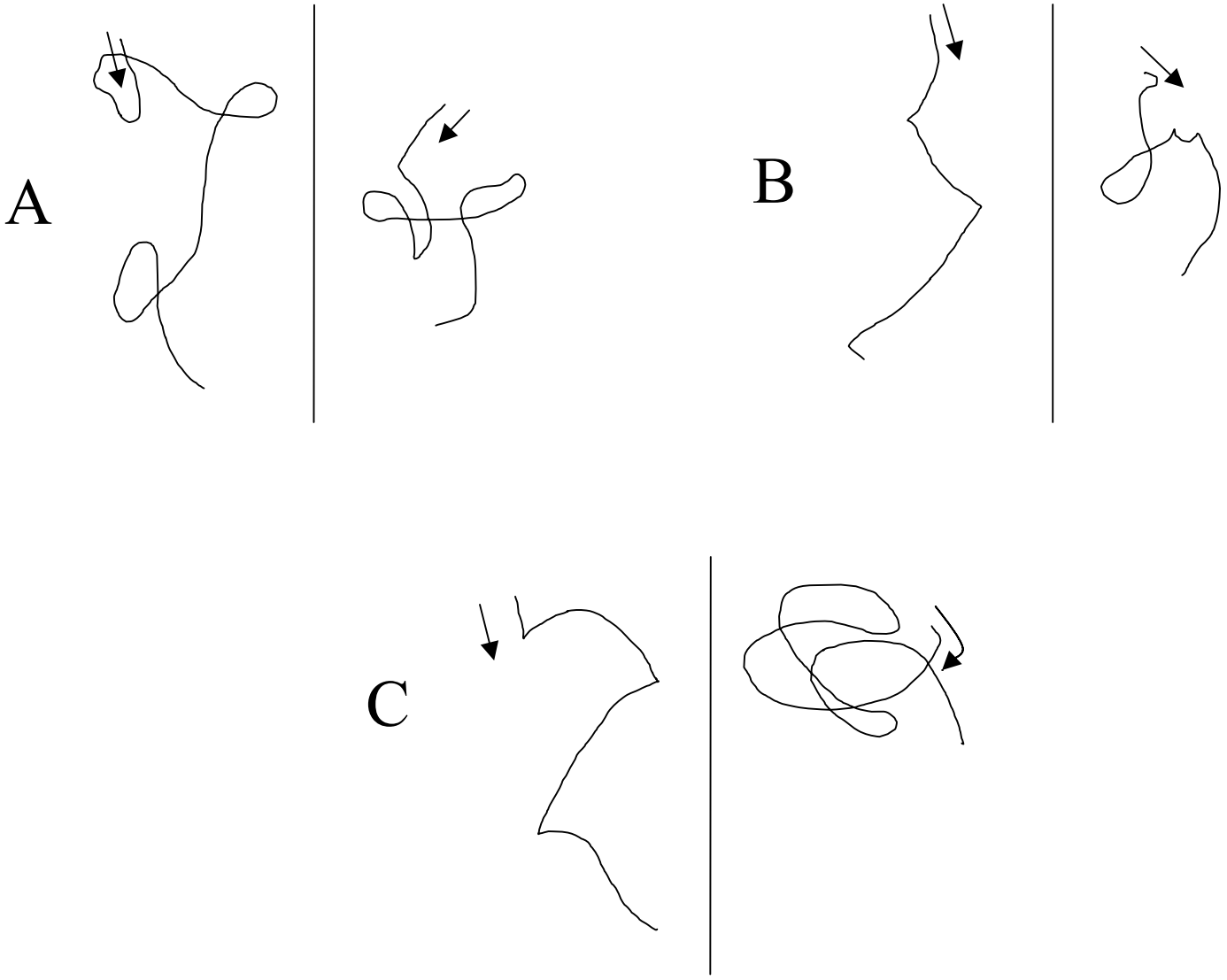


Table S1. Crystal data and structure refinement for **1**.

Compound name	Serinocyclin A
Empirical formula	C27 H45 N8 O12 (plus 3 H_2O molecules and 1 formate ion)
Formula weight	673.71
Temperature	100(5) K
Wavelength	0.9179 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 9.193(10) Å b = 16.074(10) Å c = 11.852(10) Å α = 90° β = 97.4(5)° γ = 90°
Cell volume	1737(3) $Å^3$
Z	2
Density (calculated)	1.466 Mg/m^3
Absorption coefficient	0.122 mm^{-1}
F(000)	812
Crystal size	0.06 x 0.06 x 0.003 mm^3
θ range for data collection	2.24 to 27.31° (limiting resolution 1.0 Å)
Index ranges	-9<=h<=8, 0<=k<=15, 0<=l<=10
Reflections collected	5536
Independent reflections	1670 (1600 used for refinement, 70 as a test set for R(free))
R(merge)	0.058
Completeness	88.8%
Absorption correction	Order 6 spherical harmonics, in SCALA
Refinement method	Full-matrix least squares on F^2
Data / restraints / parameters	1600 / 94 / 475
Goodness-of-fit on F^2	1.342
Final R values (all data)	R1 = 0.0889, wR2 = 0.2426, R1(free) = 0.1371
R values (I > 2sigma(I))	R1 = 0.0868, wR2 = 0.2394, R1(free) = 0.1354
Absolute structure parameter	-2.1(35)
Largest DF map peak and hole	0.47, -0.37 $e^-/Å^3$

Table S2. Crystal data: Atomic coordinates (fractional cell) and equivalent isotropic displacement parameters (Å^2) for **1**.

	x	y	z	U(eq)	U(iso)	Occupancy
Residue 1, Acc						
N_1	0.6930(9)	-0.0534(6)	0.5120(8)	0.034(2)		
CA_1	0.7169(11)	-0.0001(6)	0.4197(10)	0.037(3)		
C_1	0.6233(12)	0.0764(6)	0.4092(9)	0.039(3)		
O_1	0.6762(9)	0.1470(5)	0.3968(7)	0.039(2)		
CB1_1	0.8697(14)	0.0083(9)	0.3858(13)	0.050(4)		
CB2_1	0.7551(13)	-0.0397(8)	0.3132(10)	0.045(3)		
Residue 2, Hyp						
N_2	0.4814(9)	0.0668(5)	0.4139(8)	0.035(2)		
CA_2	0.3822(11)	0.1401(5)	0.4040(10)	0.033(3)		
C_2	0.4163(11)	0.2045(7)	0.4948(10)	0.037(3)		
O_2	0.3776(10)	0.2777(5)	0.4780(7)	0.050(2)		
CB_2	0.2299(12)	0.1009(6)	0.4032(12)	0.049(4)		
CG_2	0.2481(12)	0.0201(7)	0.3376(11)	0.050(4)		
OD1_2	0.2422(10)	0.0403(7)	0.2211(9)	0.069(3)		
CD2_2	0.3961(12)	-0.0104(7)	0.3928(11)	0.044(3)		
Residue 3, Ser1						
N_3	0.4912(10)	0.1793(6)	0.5941(8)	0.038(3)		
CA_3	0.5409(12)	0.2383(7)	0.6856(9)	0.038(3)		
C_3	0.6928(11)	0.2719(6)	0.6822(10)	0.036(3)		
O_3	0.7381(9)	0.3264(6)	0.7517(8)	0.056(2)		
CB_3	0.515(2)	0.2088(10)	0.8011(12)	0.079(5)		
OG_3	0.548(2)	0.1256(11)	0.8212(14)	0.147(7)		
Residue 4, HyLys						
N_4	0.7720(9)	0.2467(6)	0.6017(9)	0.041(3)		
CA_4	0.9180(10)	0.2783(7)	0.5913(9)	0.041(3)		
C_4	1.0382(11)	0.2282(8)	0.6612(9)	0.038(3)		
O_4	1.1610(9)	0.2600(5)	0.6837(8)	0.048(2)		
CB_4	0.9496(10)	0.2782(8)	0.4663(8)	0.038(3)		
CG_4	0.8420(12)	0.3273(7)	0.3849(8)	0.038(3)		
OD1_4	0.8468(9)	0.4125(5)	0.4247(8)	0.046(2)		
CD2_4	0.8747(16)	0.3240(7)	0.2650(9)	0.054(4)		
CE_4a	0.886(4)	0.2400(14)	0.2102(17)		0.031(9)	0.39(2)
NZ_4a	0.800(5)	0.235(2)	0.093(2)		0.065(11)	0.39(2)
CE_4b	0.802(4)	0.2451(17)	0.2041(18)		0.079(9)	0.61(2)
NZ_4b	0.868(3)	0.2433(14)	0.0889(15)		0.071(8)	0.61(2)
Residue 5, β-Ala						
N_5	1.0093(10)	0.1515(7)	0.6903(10)	0.046(3)		
C_5	0.9986(14)	0.0722(11)	0.9265(11)	0.064(4)		
O_5	0.8791(12)	0.1114(7)	0.9196(10)	0.071(3)		
CA_5	1.1317(15)	0.1096(11)	0.8849(11)	0.064(4)		
CB_5	1.1164(13)	0.0975(8)	0.7547(11)	0.050(4)		

Table S2 (continued).

	x	y	z	U(eq)	U(iso)	Occupancy
Residue 6, Ser2						
N_6	1.0077(11)	-0.0045(7)	0.9698(9)	0.053(3)		
CA_6	0.8820(12)	-0.0486(8)	1.0055(10)	0.055(4)		
C_6	0.8005(12)	-0.0963(9)	0.9052(10)	0.055(4)		
O_6	0.7931(17)	-0.1710(7)	0.9033(10)	0.097(4)		
CB_6	0.9337(16)	-0.1082(9)	1.1031(10)	0.068(5)		
OG_6	1.0427(16)	-0.1611(9)	1.0742(10)	0.108(5)		
Residue 7, Ser3						
N_7	0.7424(10)	-0.0482(7)	0.8219(8)	0.047(3)		
CA_7	0.6788(10)	-0.0821(7)	0.7122(9)	0.040(3)		
C_7	0.7077(10)	-0.0229(8)	0.6182(11)	0.042(4)		
O_7	0.7410(9)	0.0518(5)	0.6398(7)	0.048(2)		
CB_7	0.5122(11)	-0.0965(8)	0.7067(11)	0.047(3)		
OG_7	0.4308(9)	-0.0203(7)	0.6945(9)	0.070(3)		
Solvent species: water						
O_8	0.586(2)	0.0968(15)	0.0565(16)	0.161(8)		
O_9	0.423(4)	0.217(3)	0.106(3)	0.272(18)		
O_10	1.113(3)	0.1815(19)	0.141(2)	0.208(11)		
Solvent species: formate						
O1_11a	0.706(3)	0.3970(15)	0.025(2)		0.062(9)	0.39(2)
C_11a	0.687(4)	0.471(2)	-0.048(3)		0.083(14)	0.39(2)
O2_11a	0.535(3)	0.474(2)	-0.108(3)		0.094(13)	0.39(2)
O1_11b	0.606(4)	0.3292(15)	0.030(3)		0.133(11)	0.61(2)
C_11b	0.589(2)	0.4145(13)	-0.0231(17)		0.046(6)	0.61(2)
O2_11b	0.581(6)	0.487(2)	0.057(4)		0.23(2)	0.61(2)

Table S3. Anisotropic displacement parameters (Å^2) for **1**.

	U11	U22	U33	U23	U13	U12
N_1	0.027(5)	0.031(6)	0.045(7)	0.007(5)	0.007(4)	-0.001(5)
CA_1	0.012(6)	0.038(8)	0.061(9)	-0.011(6)	0.005(5)	-0.006(6)
C_1	0.019(7)	0.032(8)	0.063(9)	-0.007(6)	-0.004(5)	-0.007(7)
O_1	0.024(4)	0.029(6)	0.065(6)	-0.001(4)	0.009(4)	0.003(4)
CB1_1	0.028(8)	0.034(8)	0.090(10)	0.002(7)	0.015(7)	0.002(6)
CB2_1	0.044(8)	0.030(8)	0.061(8)	0.000(6)	0.008(6)	0.002(6)
N_2	0.024(6)	0.026(6)	0.055(7)	-0.002(5)	0.000(4)	-0.008(5)
CA_2	0.024(7)	0.028(7)	0.046(8)	0.012(5)	-0.001(5)	0.006(6)
C_2	0.009(6)	0.045(9)	0.057(9)	-0.004(6)	0.008(6)	0.003(6)
O_2	0.054(6)	0.033(6)	0.064(6)	0.004(4)	0.010(4)	0.018(4)
CB_2	0.048(9)	0.022(8)	0.071(9)	-0.006(6)	-0.018(7)	0.004(6)
CG_2	0.042(8)	0.039(8)	0.068(11)	-0.011(6)	0.007(7)	-0.003(6)
OD1_2	0.049(6)	0.087(8)	0.067(8)	-0.017(5)	-0.005(5)	-0.001(5)
CD2_2	0.027(7)	0.051(9)	0.055(8)	-0.010(7)	0.010(6)	0.011(7)
N_3	0.028(6)	0.024(5)	0.061(7)	-0.006(5)	-0.002(5)	-0.003(5)
CA_3	0.036(8)	0.031(8)	0.049(9)	-0.007(6)	0.007(6)	-0.005(6)
C_3	0.022(7)	0.030(8)	0.053(8)	-0.006(6)	-0.009(6)	0.012(6)
O_3	0.039(5)	0.060(7)	0.068(6)	-0.015(5)	0.000(4)	0.000(5)
CB_3	0.085(13)	0.058(13)	0.090(14)	-0.002(9)	0.002(10)	0.008(9)
OG_3	0.144(16)	0.18(2)	0.114(13)	-0.010(12)	-0.014(10)	0.061(15)
N_4	0.021(6)	0.032(6)	0.072(8)	-0.017(5)	0.009(5)	-0.004(5)
CA_4	0.022(7)	0.034(8)	0.065(9)	-0.004(6)	0.002(6)	0.000(6)
C_4	0.015(7)	0.039(9)	0.056(8)	-0.010(6)	-0.014(5)	-0.007(6)
O_4	0.040(6)	0.029(5)	0.073(6)	-0.002(4)	0.007(4)	-0.003(4)
CB_4	0.015(6)	0.044(8)	0.057(9)	-0.006(6)	0.010(5)	-0.009(6)
CG_4	0.026(6)	0.024(8)	0.063(9)	0.008(6)	0.000(6)	-0.002(6)
OD1_4	0.033(5)	0.030(5)	0.075(6)	-0.001(4)	0.007(4) 0	.004(4)
CD2_4	0.052(9)	0.036(8)	0.072(11)	0.004(6)	0.001(7)	-0.002(6)
N_5	0.024(6)	0.025(7)	0.087(8)	-0.003(5)	-0.006(5)	-0.013(5)
C_5	0.042(10)	0.083(14)	0.063(10)	-0.018(9)	-0.002(7)	0.013(10)
O_5	0.067(8)	0.047(6)	0.100(9)	0.008(6)	0.012(6)	0.001(6)
CA_5	0.034(8)	0.081(11)	0.075(12)	0.010(8)	-0.003(7)	-0.006(8)
CB_5	0.029(7)	0.041(9)	0.077(11)	-0.001(7)	-0.002(6)	0.001(6)
N_6	0.042(7)	0.062(9)	0.053(7)	-0.009(6)	-0.005(5)	0.014(6)
CA_6	0.028(7)	0.085(11)	0.051(9)	-0.003(7)	-0.003(6)	0.007(8)
C_6	0.056(9)	0.063(13)	0.043(9)	0.004(8)	-0.001(7)	0.014(8)
O_6	0.174(14)	0.035(8)	0.077(8)	0.005(6)	-0.007(7)	-0.012(7)
CB_6	0.063(10)	0.086(13)	0.052(9)	0.002(8)	-0.002(7)	0.043(10)
OG_6	0.119(11)	0.139(13)	0.069(8)	0.006(8)	0.020(7)	0.064(10)
N_7	0.038(6)	0.041(7)	0.056(7)	-0.001(6)	-0.013(5)	0.007(5)
CA_7	0.024(7)	0.025(7)	0.068(9)	0.005(6)	-0.001(6)	0.006(5)
C_7	0.010(6)	0.047(10)	0.064(11)	0.015(8)	-0.005(6)	-0.002(6)
O_7	0.042(5)	0.034(6)	0.067(6)	0.004(4)	-0.003(4)	-0.012(4)

Table S3 (continued).

	U11	U22	U33	U23	U13	U12
CB_7	0.040(8)	0.059(10)	0.044(8)	0.005(6)	0.007(6)	0.012(7)
OG_7	0.038(5)	0.079(8)	0.089(7)	-0.037(6)	-0.007(5)	-0.001(6)
O_8	0.175(16)	0.18(2)	0.138(14)	-0.024(13)	0.039(12)	0.067(15)
O_9	0.26(3)	0.25(3)	0.29(4)	-0.10(3)	0.00(3)	0.12(3)
O_10	0.29(3)	0.21(3)	0.119(15)	0.003(15)	-0.007(16)	-0.02(2)

Table S4. Chiral amino acid analysis of hydrolyzates of **1** and **2** using the ligand-exchange method.

Amino Acid	Standard t_R[a]	hydrolyzate **1**[b]	hydrolyzate **2**[b]
β-Ala	3.18	+	+
L-Lys	3.18		
D-HyLys[c]	3.40	+	
D-Lys	3.50		+
(2*S*,4*R*)- Hyp (*trans*-4-hydroxy-L-proline)	4.18	+	+
L-Ser	4.36	+	+
D-Ser	4.64	+	+
Acc	5.59	+	+
(2*R*,4*R*)- Hyp (*cis*-4-hydroxy-D-proline)	6.27		
(2*R*,4*S*)- Hyp (*trans*-4-hydroxy-D-proline)	6.27		
(2*S*,4*S*)- Hyp (*cis*-4-hydroxy-L-proline)	9.17		

[a]HPLC retention times (t_R, min) of underivatized amino acids standards (see Experimental section for details).
[b]Presence of amino acids in hydrolyzates of **1** and **2** as confirmed by co-chromatography experiments are indicated (+).
[c]Standards of HyLys isomers were not commercially available. The t_R of the 2*R,S*- isomer was assigned, *a posteriori*, to a peak present in the chromatogram of **1** that was not present in the chromatogram of **2**.

Table S5. Chiral amino acid analysis of hydrolyzates of **1** and **2** using two HPLC methods following derivatization with L-FDAA (Marfey's reagent).

	Method 1[a] standard t_R[c]			Method 2[b] standard t_R[c]	hydrolyzate[d]	
Amino Acid	*m/z*	347 nm[e]	XIC[f]	347 nm	**1**	**2**
(2*S*,4*R*)-Hyp (*trans*-4-hydroxy-L-proline)	382	2.98	3.15	3.08	+	+
(2*R*,4*S*)-Hyp(*trans*-4-hydroxy-D-proline)	382	3.28	3.36	3.61		
L-Ser	356	4.11	4.27	4.92	+	+
(2*R*,4*S*)-HyLys α-derivative[g]	413	5.01	5.21	6.22	+	
L-Lys α-derivative	397	5.83	6.03	7.28		
D-Ser	356	5.83	5.97	7.77	+	+
D-Lys α-derivative	397	7.74	7.81	10.47		+
β-Ala	340	7.74	8.05	10.96	+	+
HyLys ω-derivative[g]	413	9.30	9.49	12.66	+	
Acc	352	11.74	11.87	16.89	+	+
D+L Lys ω-derivatives[h]	397	12.13	12.29	16.89		+

[a]Phenomenex Prodigy column with UV diode array and ESIMS detection (see Experimental section for details).
[b]Phenomenex Luna column with UV single wavelength detection (see Experimental section for details).
[c]HPLC retention times of derivatized standard amino acids using the indicated detection method.
[d]Presence of amino acids in hydrolyzates of **1** and **2** as confirmed by HPLC-ESIMS (Method 1) and co-chromatography experiments (using Method 2) are indicated (+).
[e]Detection by diode array with chromatogram extracted at 347 nm (inline with and prior to ESIMS detection).
[f]Detection by ESIMS in negative ion mode using ion chromatograms extracted from the scan range (*m/z* 180-700) at the *m/z* indicated (inline with and subsequent to diode array detection).
[g]Standards of HyLys isomers were not commercially available. The t_R of the derivatives of the 2*R,S*- isomer were assigned, *a posteriori*, to peaks present in the chromatograms of **1** that were not present in the corresponding chromatograms of **2**.
[h]D+L Lys ω-derivatives do not resolve (see reference 32, p. 3349)

Table S6. NMR spectroscopic data (CD_3OH) for serinocyclin B (**2**)

Unit	position	δ_C[a] (or δ_N[b]), mult	δH[c] (*J* in Hz) [-$\Delta\delta/\Delta T$ ppb/K]	HMBC[d]	NOESY[e]
Acc	NH	126.7, NH	9.52, br s		
	α	37.5, qC			
	β1a	13.6, CH_2	1.63, m	C, N, α, β2	
	β1b		0.73, ddd (10.3, 7.5, 4.8)	C, N, α, β2	NH; β-Ala NH, β2
	β2a	13.0, CH_2	1.34, ddd (10.4, 7.5, 5.6)	C, N, α, β1	Hyp δ2
	β2b		1.05, ddd (10.4, 7.5, 5.6)	C, N, α, β1	Hyp δ2
	C=O	174.7, qC			
Hyp	N	129.1, tN			
	α	62.4, CH	4.45, m	C, N; Acc C	
	β1	38.8, CH_2	2.30, m	N, γ, δ	
	β2		1.92, m	C, α	δ1, Ser1 NH
	γ	71.1, CH	4.49, m	α, δ	β**1**,2
	δ1	57.8, CH_2	4.05, m	Acc C	β2, Ser1 NH
	δ2		3.72, m	α, β, γ	Acc β2a,**b**
	C=O	175.2, qC			
Ser-1	NH	109.8, NH	7.52, d (7.8)	α, β; Hyp C	β1,2; Hyp-β2, δ1
	α	58.0, CH	4.42, m	C, N, β; Lys N	
	β1	63.2, CH_2	4.20, dd (12.0, 5.5)	C, N, α	
	β2		3.84, m	C, N, α	
	C=O	172.9, qC			
Lys	NH	120.5, NH	7.53, d (7.7)	α, β; Ser-1 C	α, β, γ**1**,2, ε; β-Ala NH
	α	56.0, CH	4.30, ddd (7.6, 7.6, 7.6)	C, N, β, γ; Ser-1 C, β-Ala N	β, γ**1**,2
	β	31.8, CH_2	1.92, m	N, γ, δ	β-Ala NH
	γ1	24.3, CH_2	1.61, m	α, δ	
	γ2		1.46, m	α, β, ε	
	δ	27.9, CH_2	1.70, m	β, γ, ε, ε-N	
	ε	40.8, CH_2	2.90, t (7.1)	γ, δ, ε-N	β, γ**1**,2, δ
	ε-NH_3	31.3, NH_3^+		δ, γ, ε-N	
	C=O	174.7, qC			
β-Ala	NH	114.0, NH	7.99, m	β; Lys C	HyLys NH, β; Acc β1b
	β1	37.6, CH_2	3.73, m	C, N, α; Lys C	
	β2		3.04, m	α; Lys C	Acc β1b
	α1	37.1, CH_2	2.38, ddd (9.2, 6.7, 1.6)	C, N, β	Ser-2 NH
	α2		2.27, m	C, N, β; Ser-2 N	
	C=O	175.2, qC			
Ser-2	NH	123.2, NH	8.45, d (8.8)	α	β1,**2**; β-ala α1
	α	55.9, CH	4.44, m	C, β, β-Ala C	
	β1	61.2, CH_2	3.86, m	C, N, α	
	β2		3.75, m	C, N, α	
	C=O	172.3, qC			
Ser-3	NH	115.8, NH	7.97, m	C, β; Ser-2 C	β1,**2**
	α	55.5, CH	4.51, m	C, N, β	
	β1	64.8, CH_2	4.02, dd (11.2, 3.0)	C, N, α[f]	
	β2		3.93, dd (11.2, 2.9)	C, N, α	
	C=O	174.2, qC			

[a]Assigned from ^{13}C (125 mHz).
[b]Assigned from ^{15}N HSQC and ^{15}N HMBC (600 mHz).
[c]500 mHz
[d]Correlations, optimized for 5, 8 Hz (H→^{13}C) and 4, 8 Hz (H→^{15}N), are from proton(s) stated to carbon or nitrogen at indicated position. Correlations to Acc carbons and nitrogens observed at -6 and 4 ºC respectively. Stronger correlation to one member of a geminal pair indicated in bold
[e]Inter-residual correlations are indicated for both partners and, thus, appear twice in column; intra-residual correlations are indicated once.
[f]Weak correlation.