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SUPPORTING INFORMATION

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Title: Lyngbyabellins K–N from Two Palmyra Atoll Collections of the Marine Cyanobacterium *Moorea bouillonii*
Author(s): Hyukjae Choi, Emily Mevers, Tara Byrum, Frederick A. Valeriote, William H. Gerwick*

Table S1. NMR Spectroscopic Data for lyngbyabellin L (**2**), 7-*epi*-lyngbyabellin L (**3**), and lyngbyabellin M (**4**) in $CDCl_3$ at 500 MHz (^1H) and 125MHz (^{13}C).

	2				**3**				**4**			
No.	δ_C [ppm]	δ_H [ppm] multi (*J* in Hz)	COSY	HMBC	δ_C [ppm]	δ_H [ppm] multi (*J* in Hz)	COSY	HMBC	δ_C [ppm]	δ_H [ppm] multi (*J* in Hz)	COSY	HMBC
1	174.6				174.6				174.4			
2	42.7	3.31 dq (11.0, 7.3)	3, 9	1, 3, 9	42.6	3.31 dq (11.0, 7.3)	3, 9	1, 3, 9	44.4	2.84 dt (10.8, 6.2)	3, 9	1, 3, 9
3	75.6	5.33 ddd (11.0, 8.4, 3.0)	2, 4a, 4b	1, 2, 5, 10	75.4	5.34 ddd (11.0, 8.2, 3.6)	2, 4a, 4b	1, 2, 5, 10	75.4	3.80 m	2, 3-OH, 4	1, 4, 5
3-OH										5.51 brs	3	
4a	29.9	1.91 m	3, 4b, 5b		30.3	1.95 ddd (14.6, 8.2, 3.6)	3, 4b, 5a, 5b		34.4	1.93 m	3, 4, 5	2, 3, 5, 6
4b		1.72 m	3, 4a, 5a	3, 5, 6		1.67 m	3, 4a, 5a, 5b	3, 5, 6				
5a	20.5	1.61 m	6b	3, 6, 7	21.0	1.63 m	4a, 6a	4, 6, 7	21.5	1.86 m	4, 6	4, 6, 7
5b		1.55 m	4a, 6a	6		1.52 m	4b, 6b, 7	3, 4, 6				
6a	40.1	1.77 m	5b, 6b, 7	4, 5, 7	40.3	1.77 ddd (15.3, 8.3, 4.1)	5a, 7	4, 5, 7	50.0	2.24 m	5, 6, 7	5, 7, 8
6b		1.66 m	5a, 6a, 7	5, 8		1.66 m	5b, 7	5, 8				
7	58.2	4.02 ddq (8.1, 4.0, 6.3)	6a, 8	5	58.5	3.98 ddq (8.4, 4.1, 6.5)	6b, 8		90.8			
8	25.5	1.49 d (6.3)	7	6, 7	25.4	1.49 d (6.5)	7	5, 6	37.7	2.16 s		6, 7
9	15.3	1.30 d (7.3)	2	1, 2, 3	15.1	1.30 d (7.3)	2	1, 2, 3	15.0	1.26 d (7.2)	2	1, 2, 3
10	160.0				160.4				161.8			
11	145.7				145.9				147.6			
12	128.3	8.15 s		10, 11, 13	128.2	8.14 s		10, 11, 13	128.2	8.16 s		10, 11, 13
13	169.7				169.2				171.2			
14	70.1	5.35 m	15a, 15b	13	70.0	5.33 m	15a, 15b	13	70.30	5.41 brd (8.3)	14-OH, 15a, 15b	13, 15
14-OH		6.25 brs				6.24 brs				6.68 brs	14	
15a	69.9	4.76 dd (11.4, 2.2)	14	14, 16	69.4	4.76 dd (11.5, 1.8)	14	14, 16	70.26	4.95 dd (11.2, 2.3)	14, 15b	13, 16
15b		4.58 dd (11.4, 2.9)	14	13, 14		4.57 dd (11.5, 2.6)	14	13, 14		4.30 dd (11.2, 9.1)	14, 15a	13, 14, 16
16	160.8				160.7				161.7			
17	146.1				145.5				145.9			
18	128.9	8.16 s		16, 17, 19	128.9	8.16 s		16, 17, 19	129.2	8.30 s		16, 17, 19
19	169.9				169.7				170.5			
20	77.6	5.51 d (5.5)	21	1, 19, 21, 22, 23	77.4	5.51 d (5.7)	21	1, 19, 21, 22, 23	77.5	5.99 d (3.6)	21	1, 19, 21, 22, 23
21	34.3	2.30 m	20, 22, 23	19, 20, 22, 23	34.8	2.32 td (13.4, 6.7)	20, 22, 23	19, 20, 22, 23	34.4	2.33 m	20, 22, 23	
22	19.2	1.04 d (6.8)	21	20, 21, 23	19.0	1.03 d (6.8)	21	20, 21, 23	19.5	1.13 d (6.9)	21	20, 21, 23
23	17.4	1.06 d (6.7)	21	20, 21, 22	17.3	1.07 d (6.7)	21	20, 21, 22	16.8	0.98 d (6.9)	21	20, 21, 22
24									61.8	4.42 q (7.1)	25	10, 25
25									14.7	1.41 t (7.1)	24	24

Figure S1. HR ESITOFMS of lyngbyabellin K (**1**).

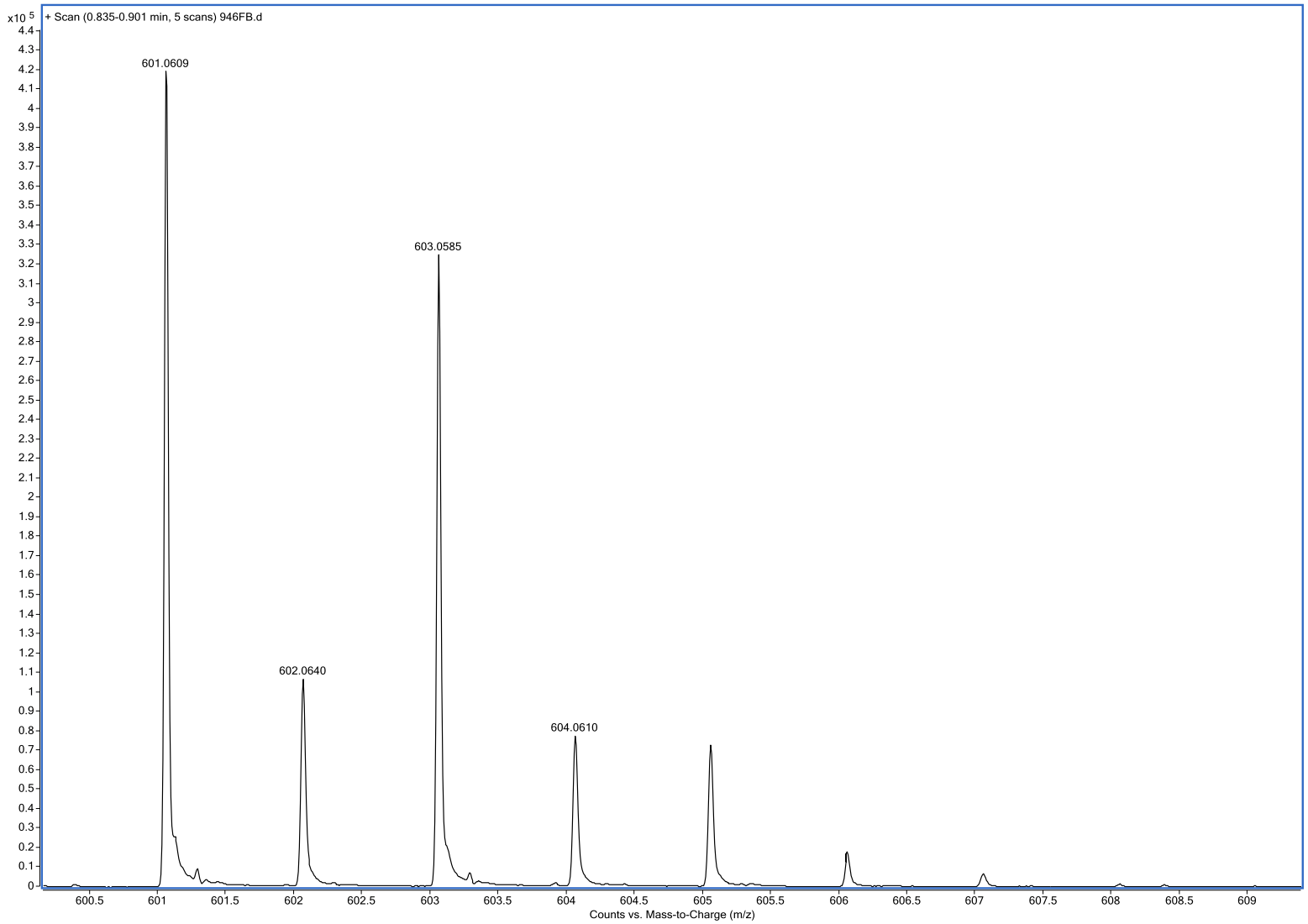


Figure S2. ^{1}H NMR spectrum of lyngbyabellin K (**1**) (recorded in $CDCl_3$ at 500 MHz).

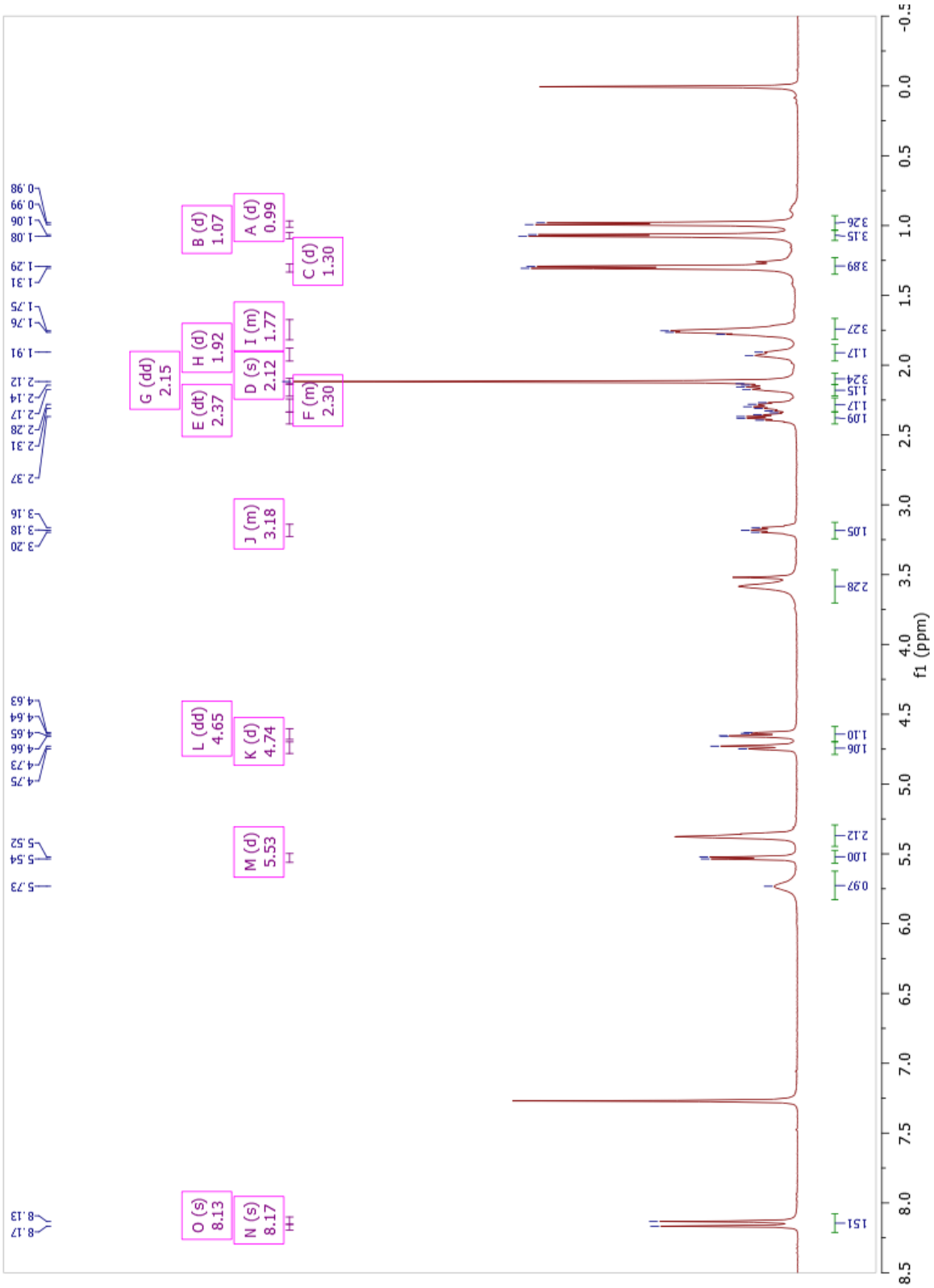


Figure S3. ^{13}C NMR spectrum of lyngbyabellin K (**1**) (recorded in $CDCl_3$ at 125 MHz).

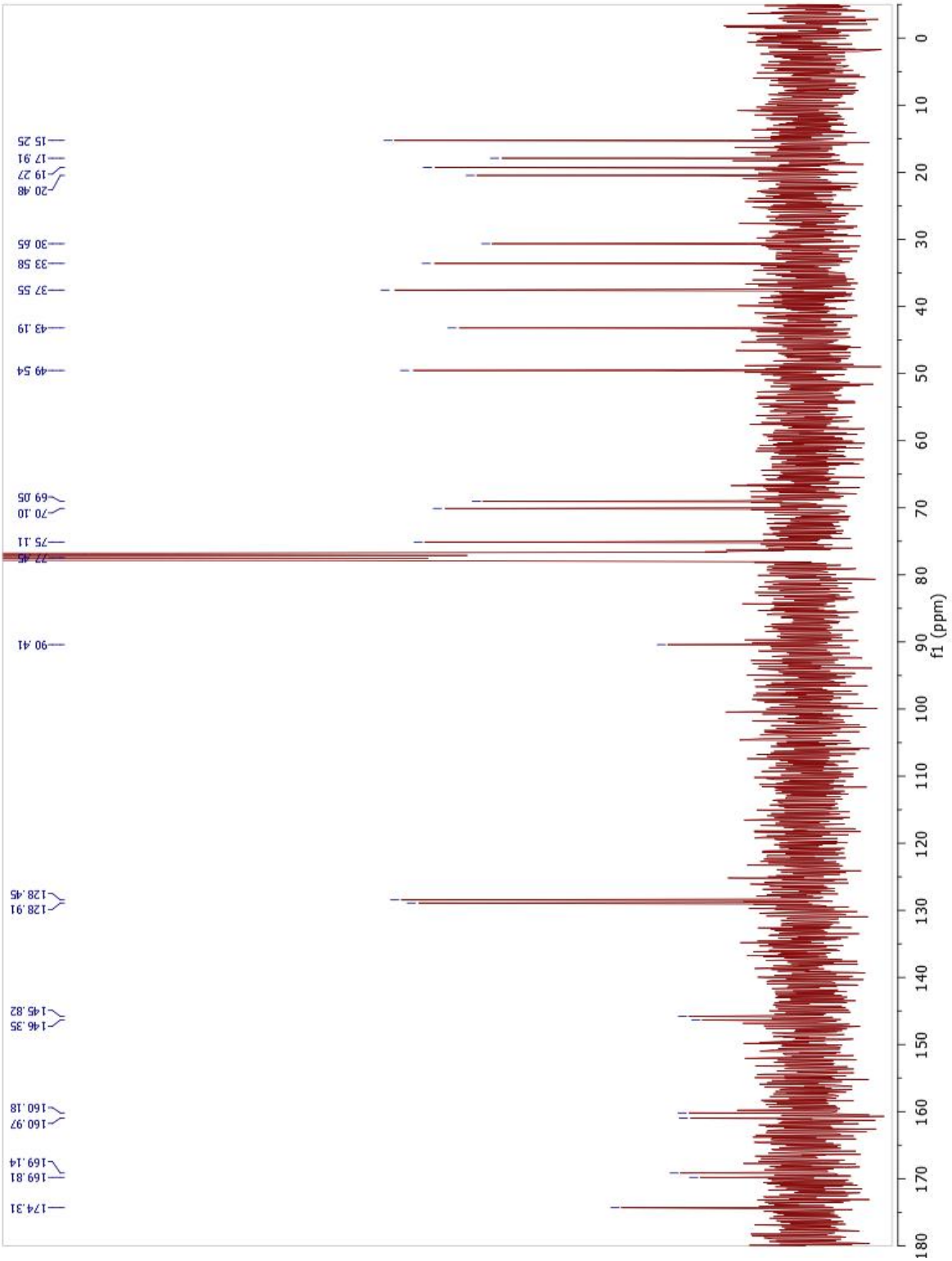


Figure S4. gHSQC spectrum of lyngbyabellin K (**1**) (recorded in $CDCl_3$ at 500 MHz).

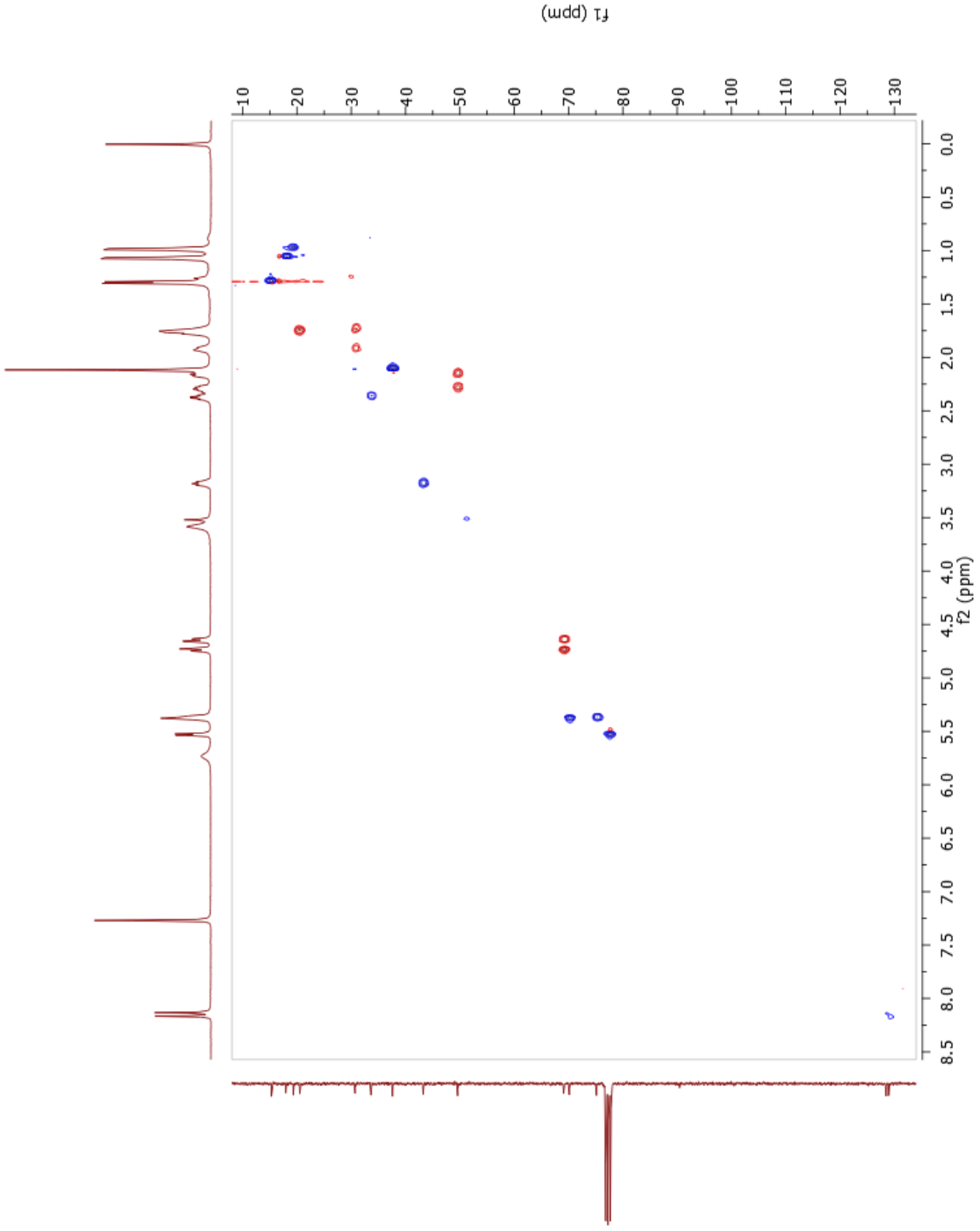


Figure S5. gCOSY spectrum of lyngbyabellin K (**1**) (recorded in $CDCl_3$ at 500 MHz).

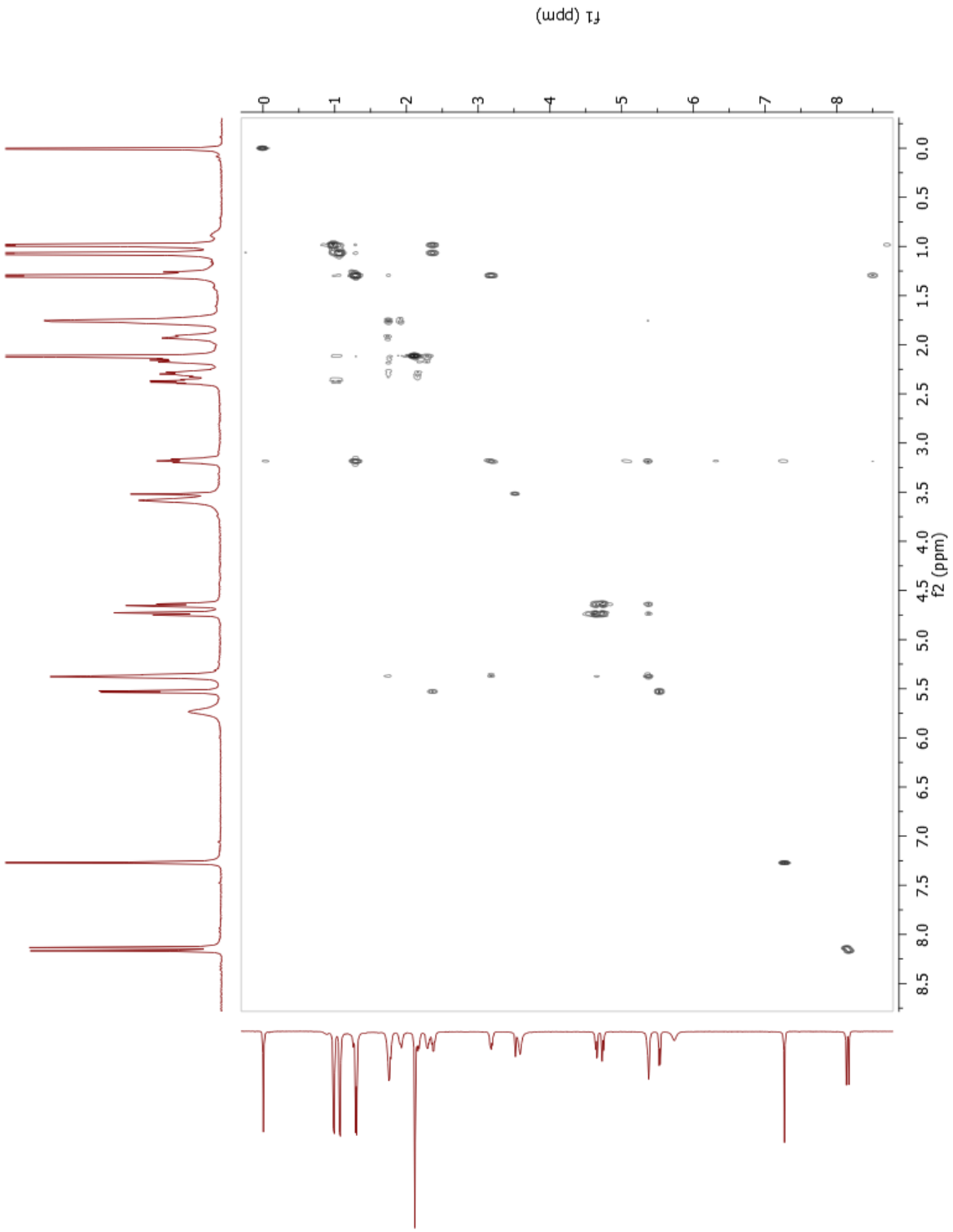


Figure S6. gHMBC spectrum of lyngbyabellin K (**1**) (recorded in $CDCl_3$ at 500 MHz).

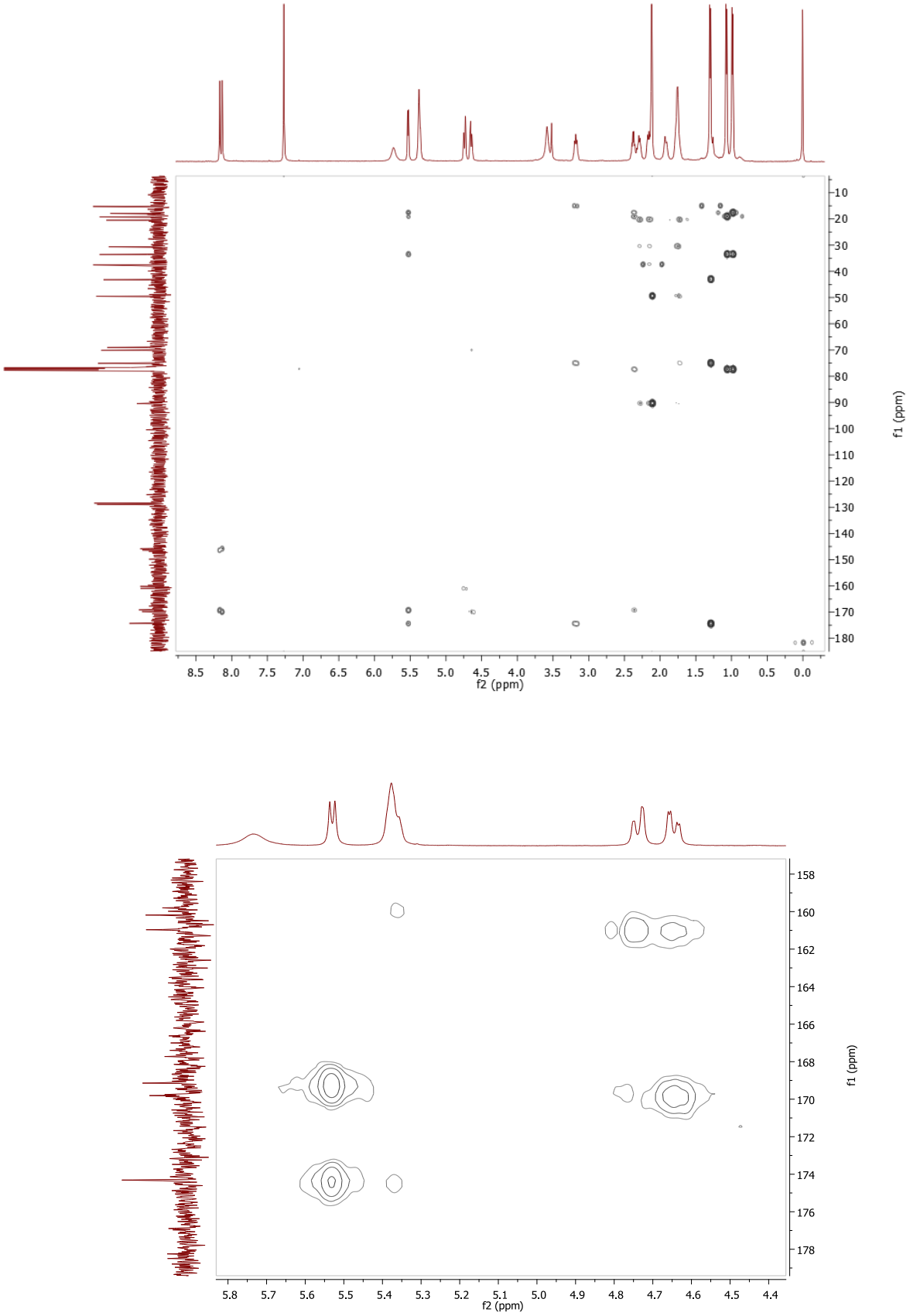


Figure S7. ORTEP representation of lyngbyabellin K (**1**).

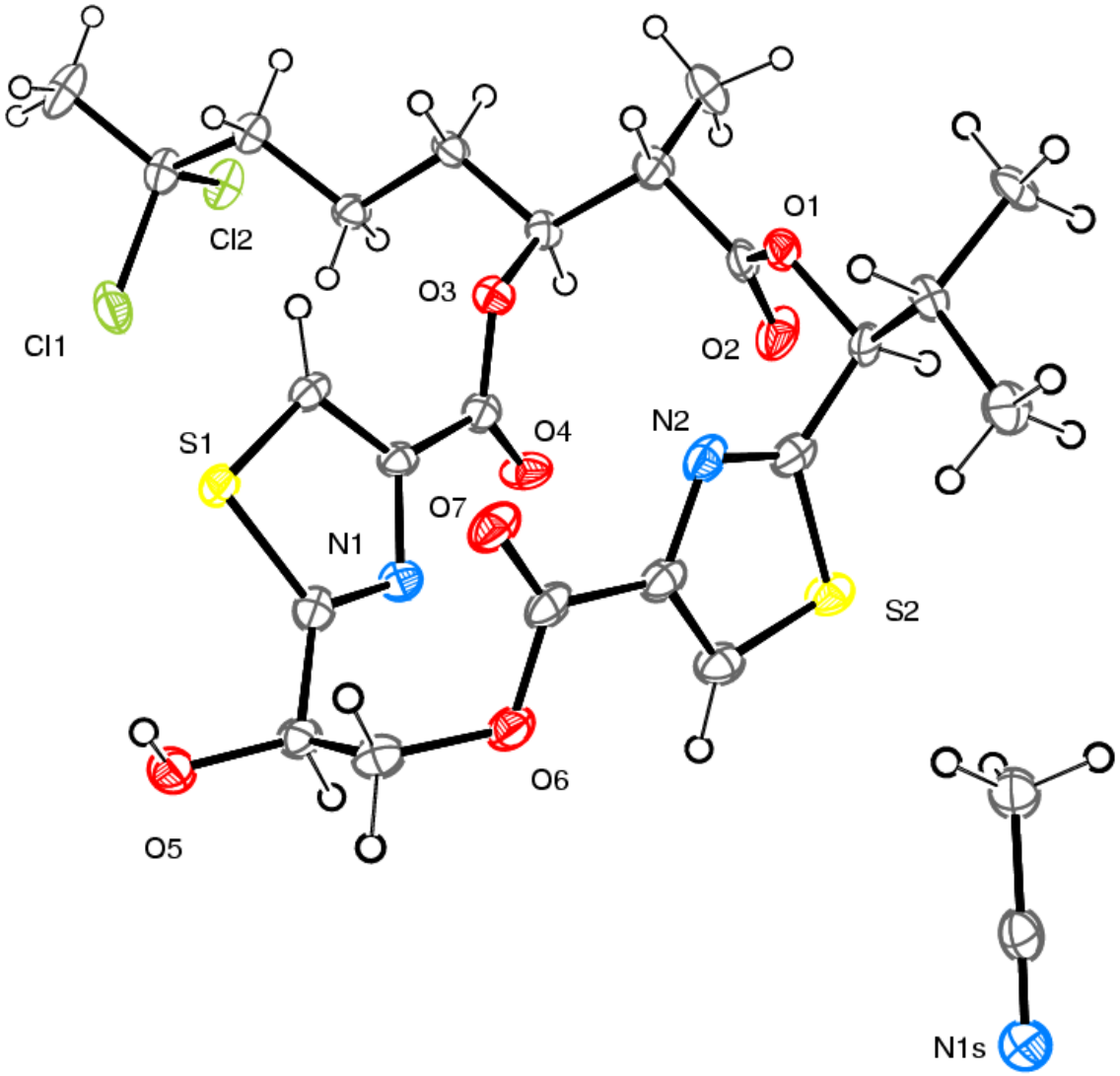


Table S2. Crystal data and structure refinement for lyngbyabellin K (**1**).

Empirical formula	C25 H31 Cl2 N3 O7 S2	
Formula weight	620.55	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 10.6419(8) Å	α= 90°
	b = 5.8776(5) Å	β= 101.928(6)°
	c = 23.859(2) Å	γ = 90°
Volume	1460.1(2) $Å^3$	
Z	2	
Density (calculated)	1.411 Mg/m^3	
Absorption coefficient	3.744 mm^{-1}	
F(000)	648	
Crystal size	0.21 x 0.11 x 0.05 mm^3	
Crystal color, habit	Colorless Needle	
Theta range for data collection	1.89 to 67.67°	
Index ranges	-12<=h<=12, -6<=k<=6, -27<=l<=10	
Reflections collected	7218	
Independent reflections	4362 [R(int) = 0.0358]	
Completeness to theta = 67.50°	90.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8349 and 0.5069	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4362 / 1 / 388	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0626, wR2 = 0.1586	
R indices (all data)	R1 = 0.0721, wR2 = 0.1655	
Absolute structure parameter	-0.02(2)	
Extinction coefficient	not measured	
Largest diff. peak and hole	0.680 and -0.368 $e.Å^{-3}$	

Figure S8. HR ESITOFMS of lyngbyabellin L (**2**).

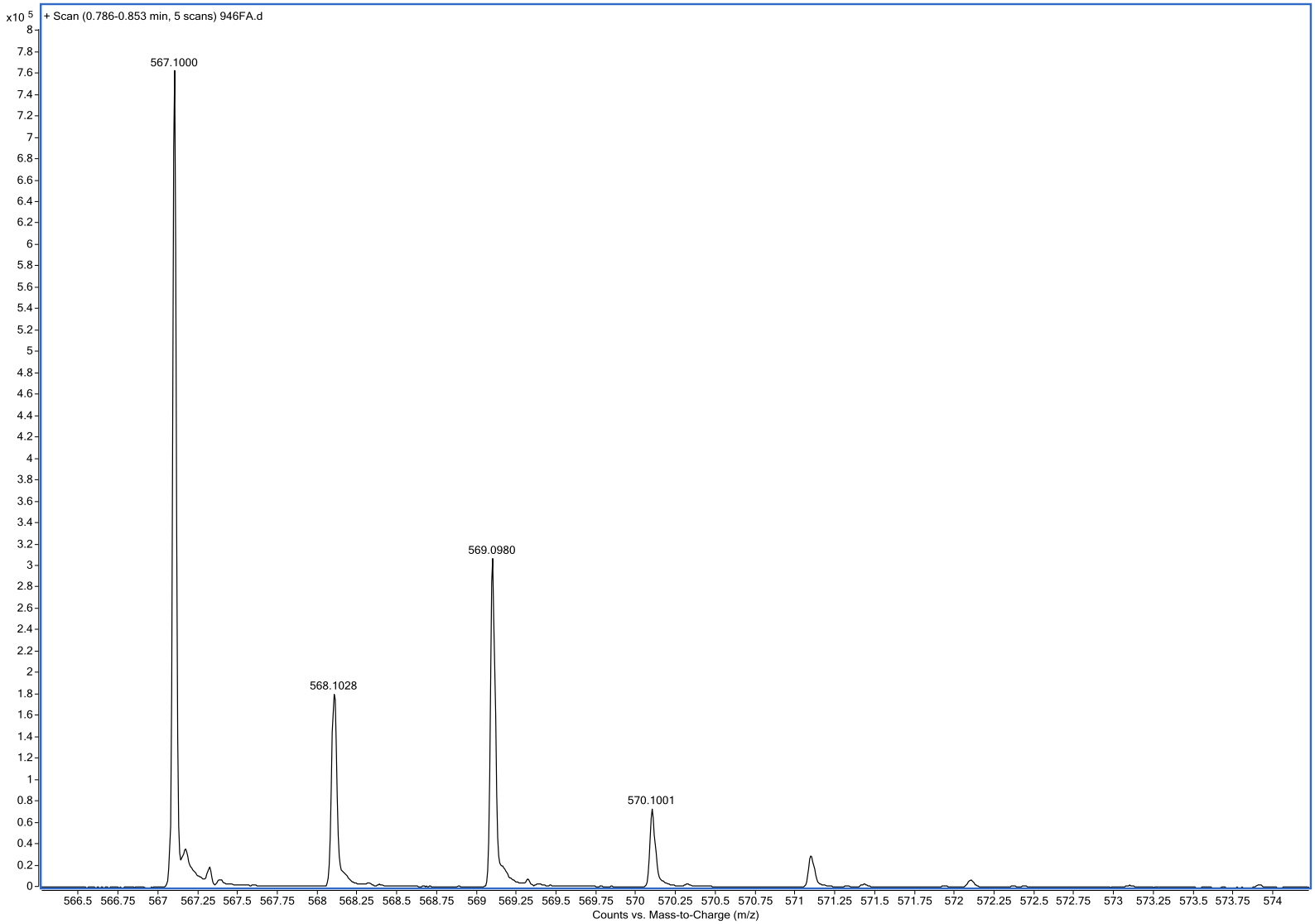


Figure S9. ^{1}H NMR spectrum of lyngbyabellin L (**2**) (recorded in $CDCl_3$ at 500 MHz).

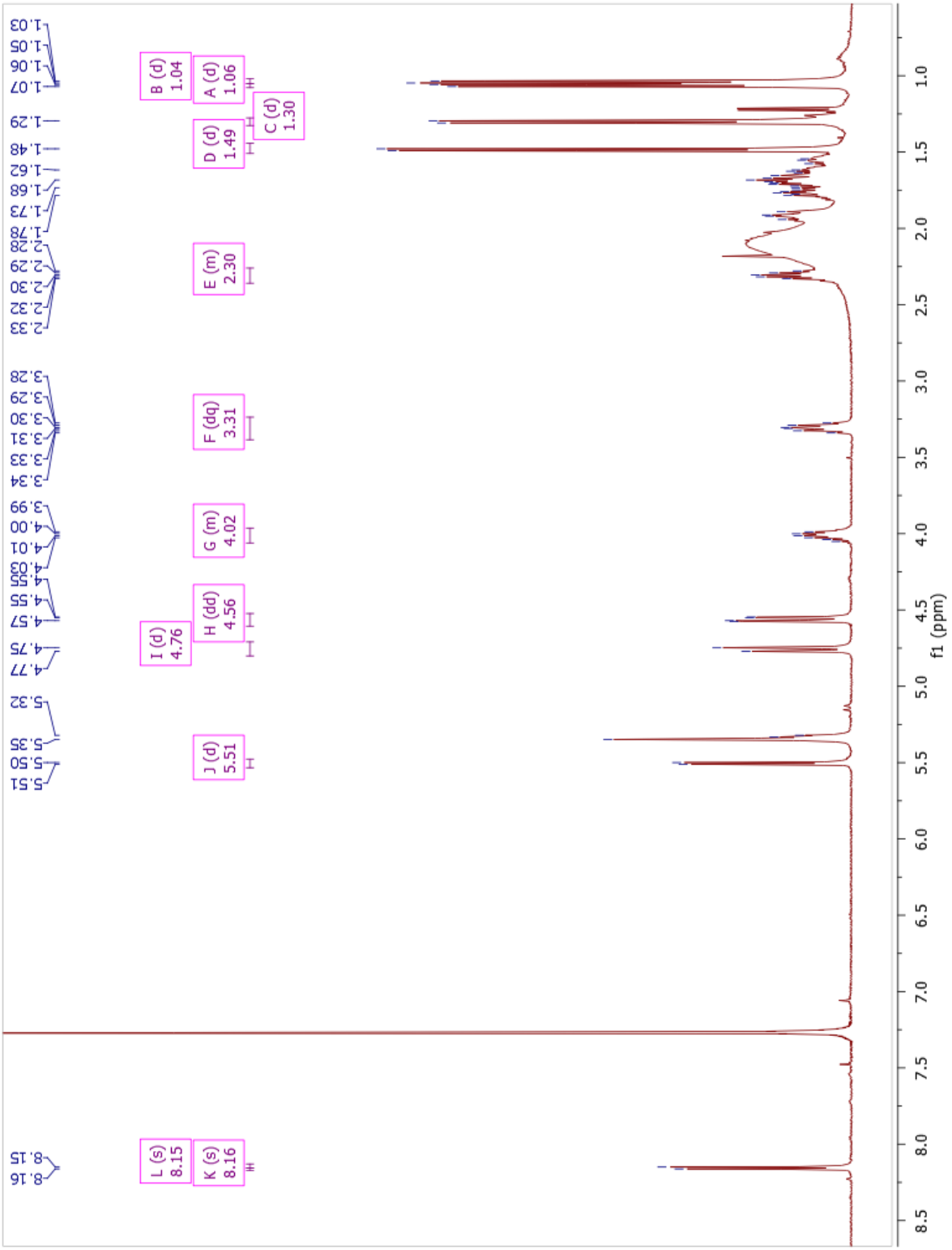


Figure S10. ^{13}C NMR spectrum of lyngbyabellin L (**2**) (recorded in $CDCl_3$ at 125 MHz).

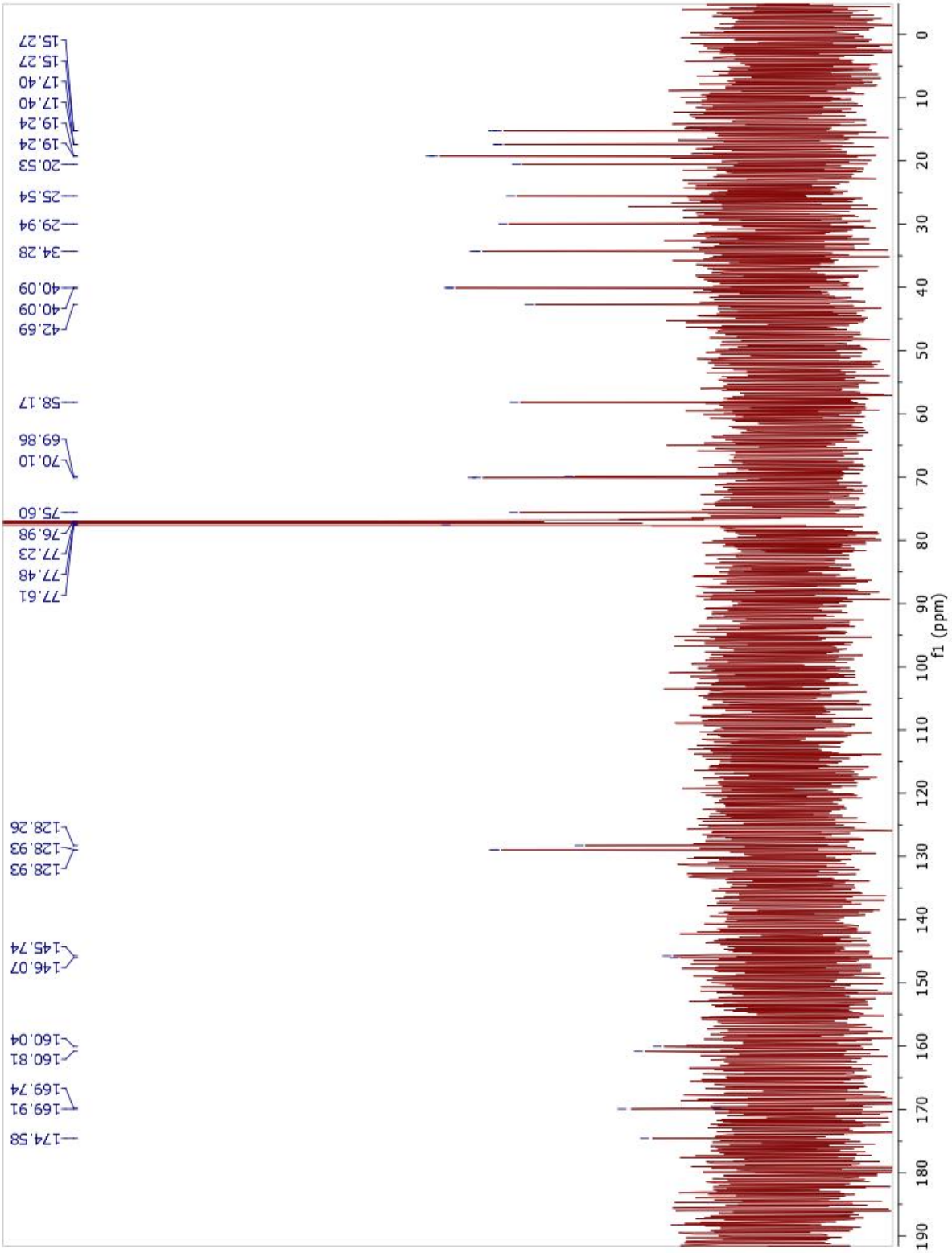


Figure S11. gHSQC spectrum of lyngbyabellin L (**2**) (recorded in $CDCl_3$ at 500 MHz).

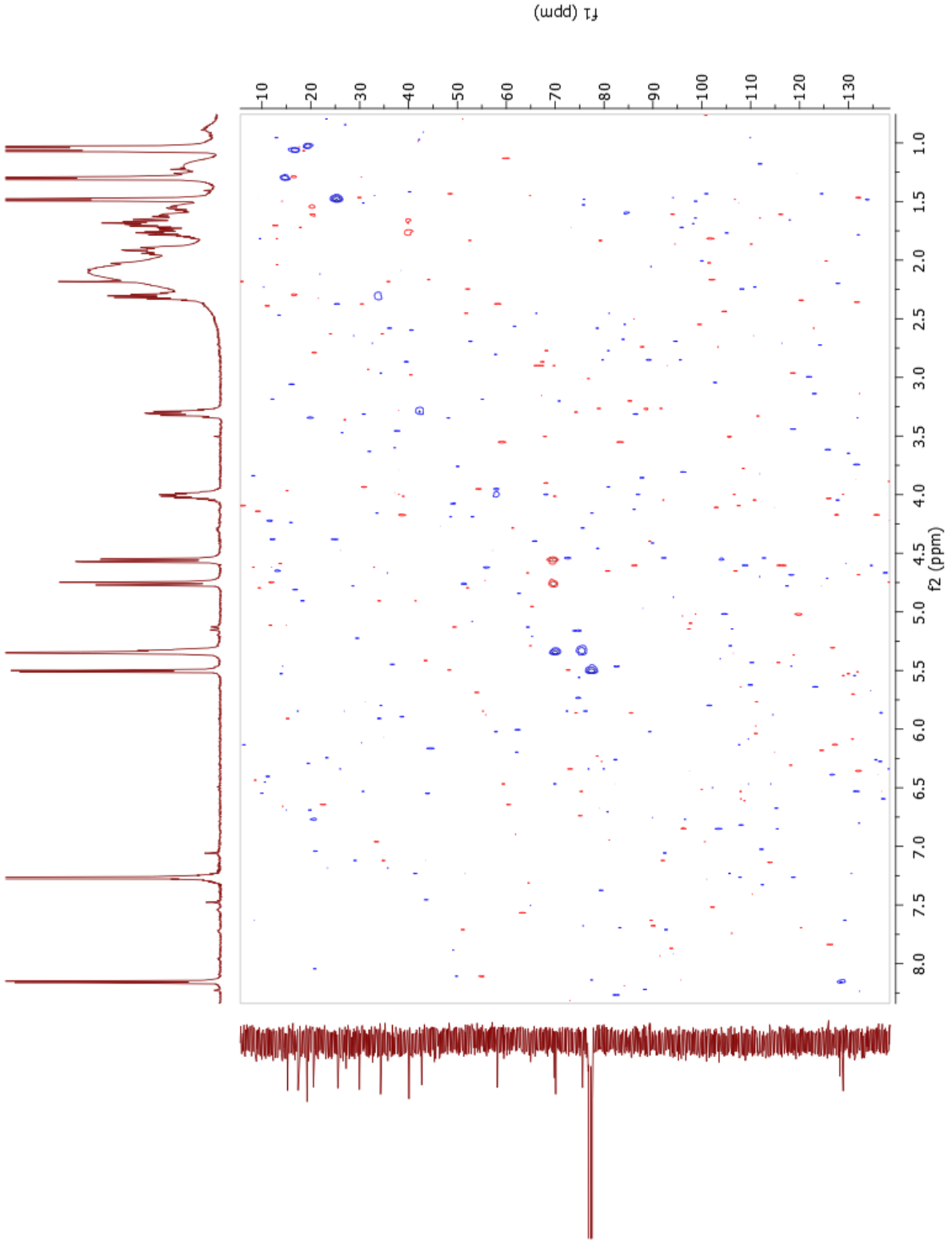


Figure S12. gCOSY spectrum of lyngbyabellin L (**2**) (recorded in $CDCl_3$ at 500 MHz).

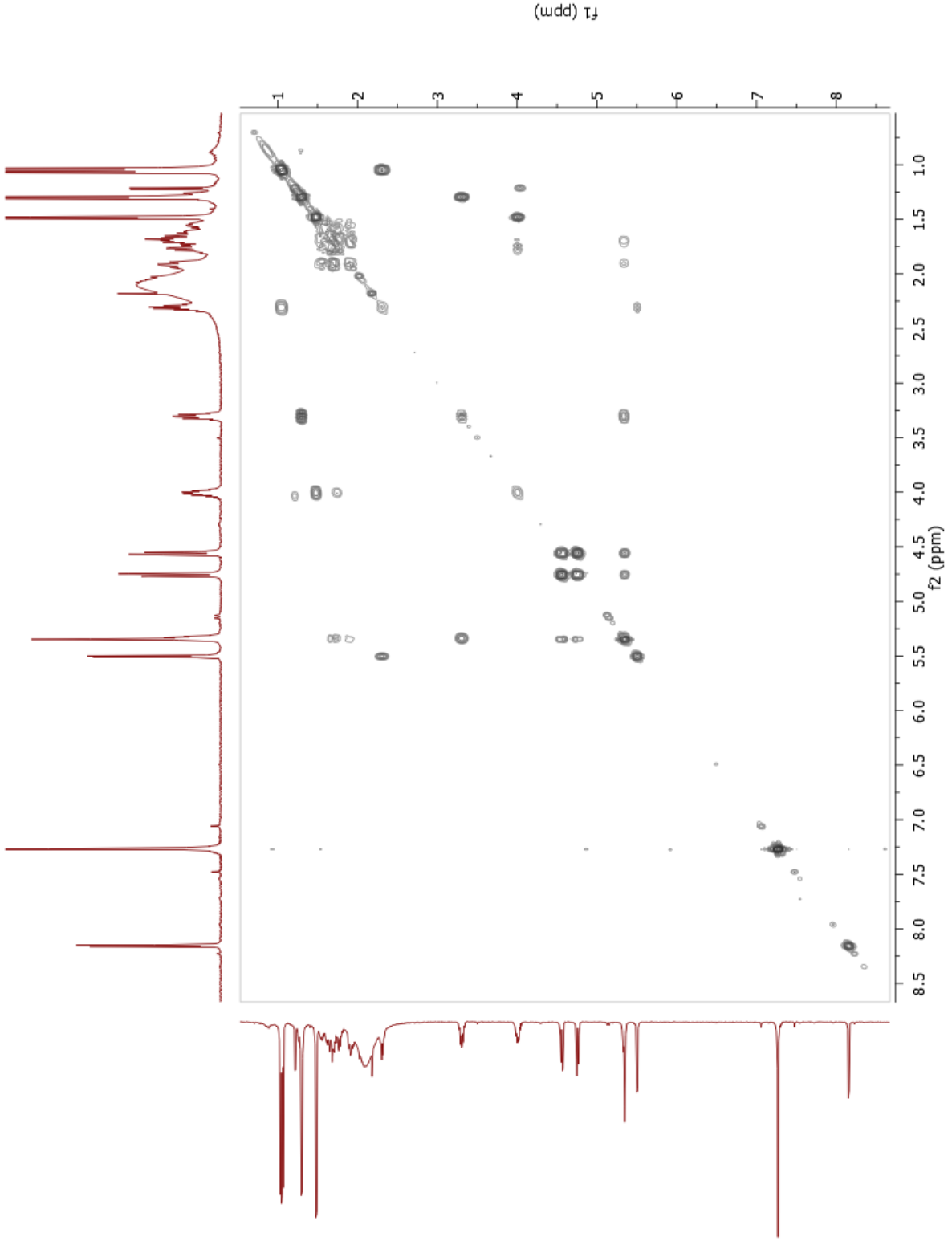


Figure S13. gHMBC spectrum of lyngbyabellin L (**2**) (recorded in $CDCl_3$ at 500 MHz)

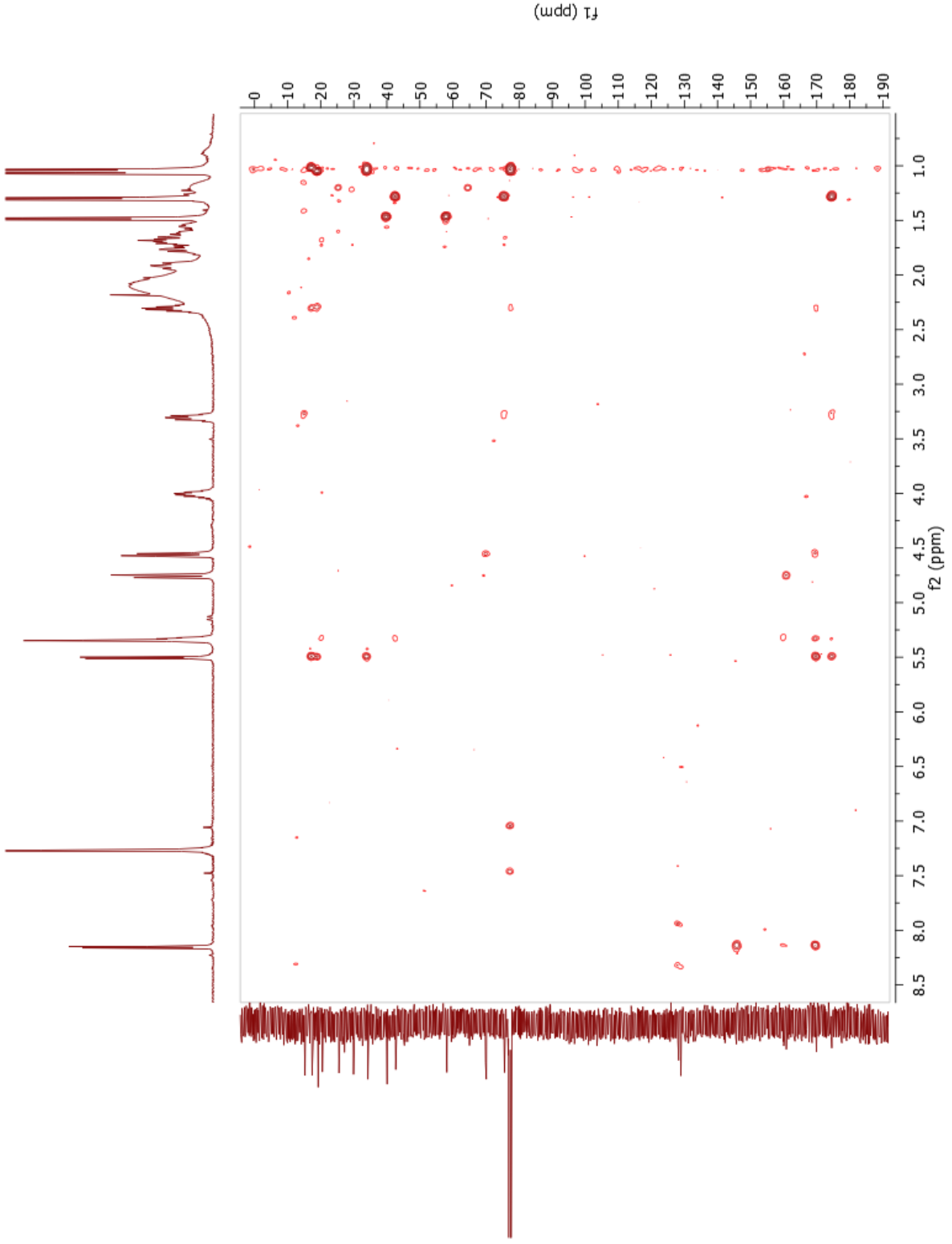


Figure S14. DQF-COSY spectrum of lyngbyabellin L (**2**) (recorded in $CDCl_3$ at 600 MHz)

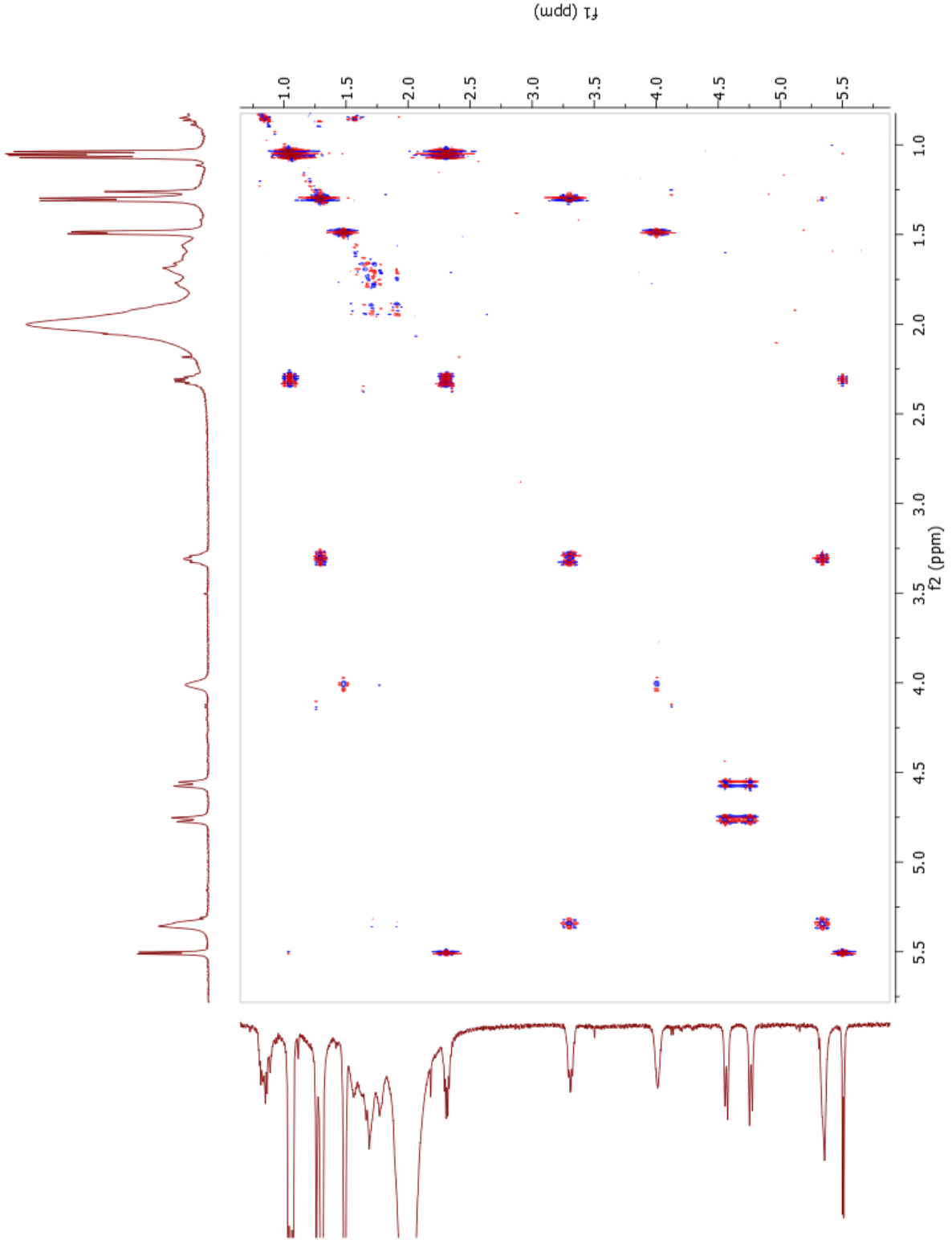


Figure S15. NOESY spectrum of lyngbyabellin L (**2**) (recorded in $CDCl_3$ at 600 MHz)

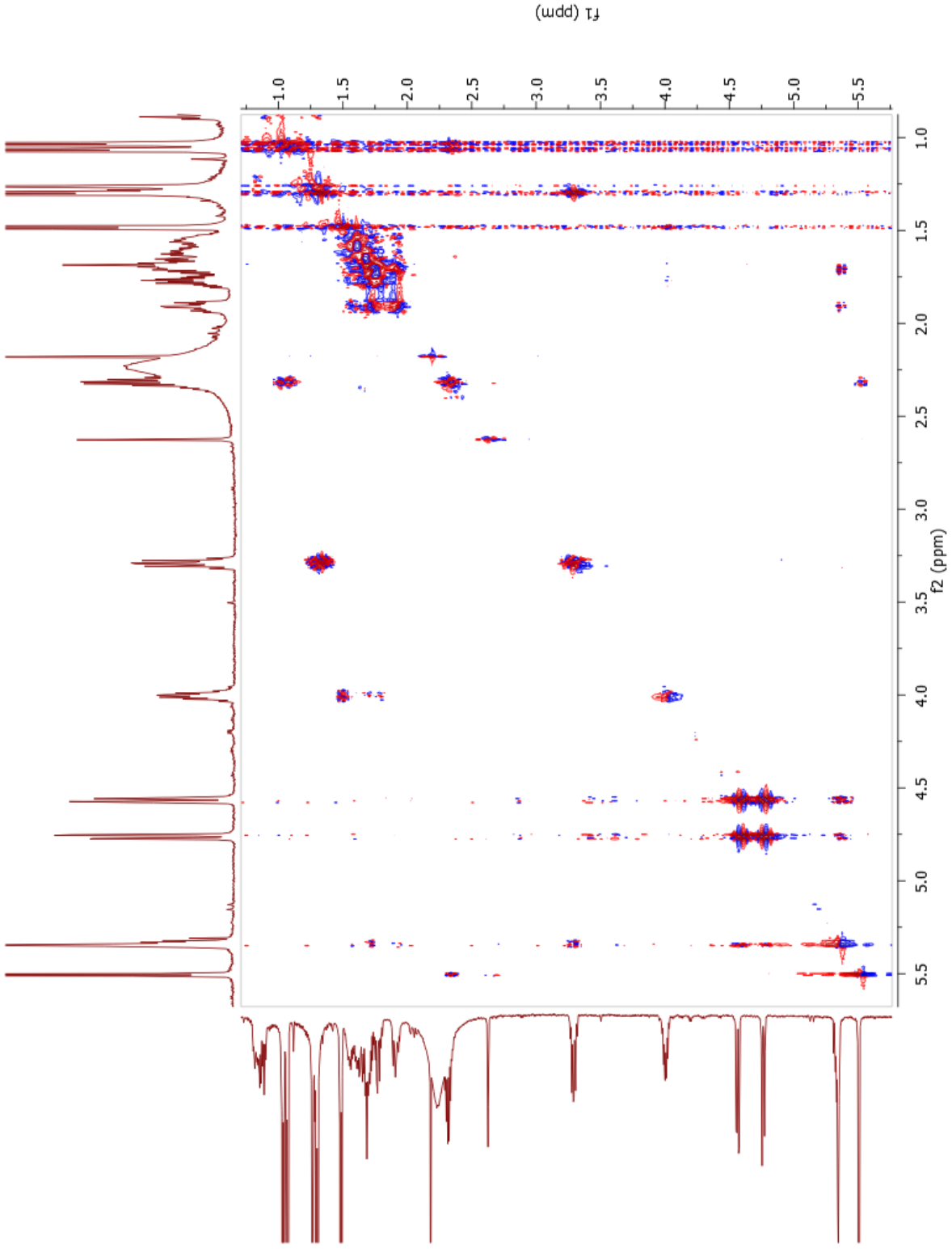
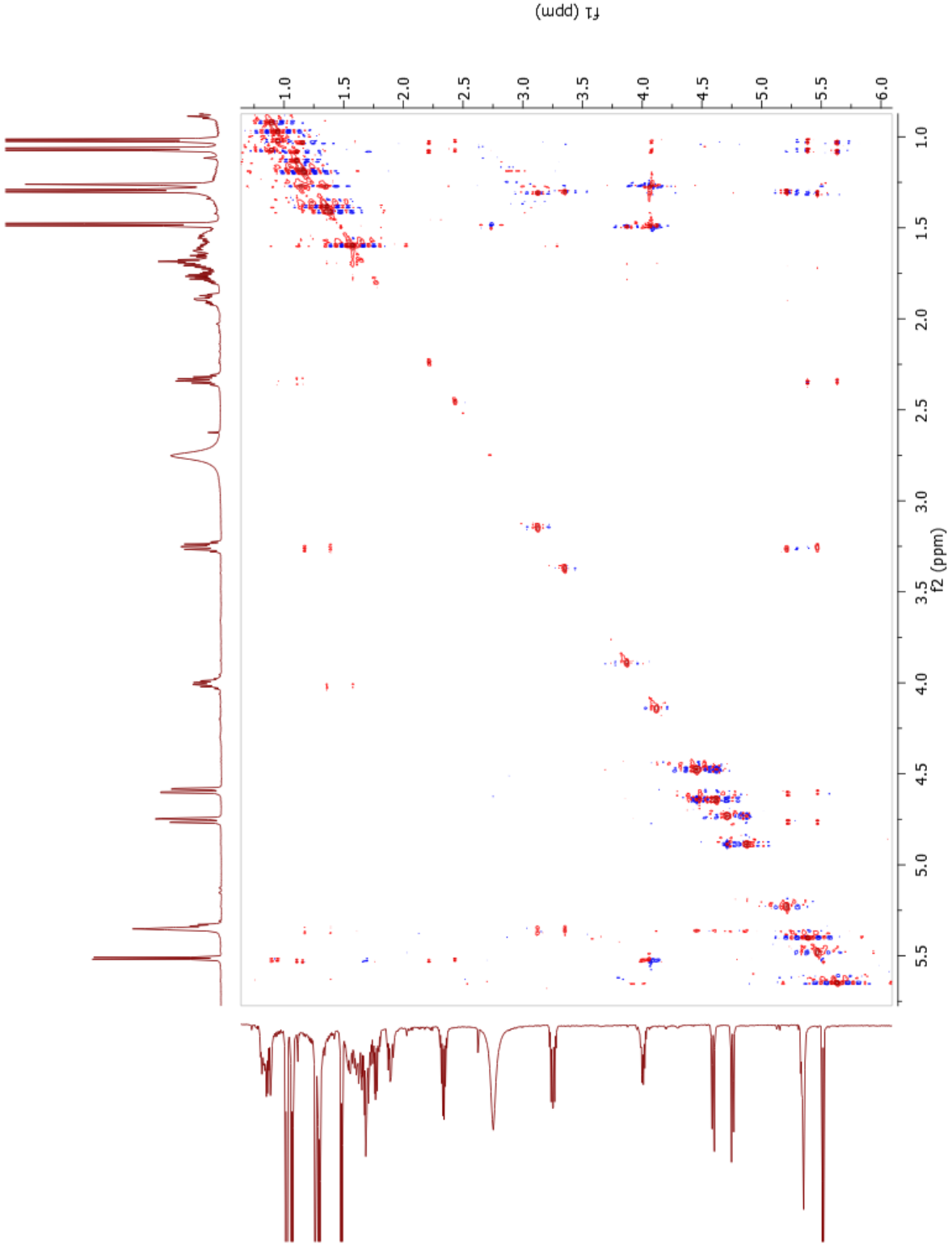


Figure S16. HETLOC spectrum of lyngbyabellin L (**2**) (recorded in $CDCl_3$ at 600 MHz)



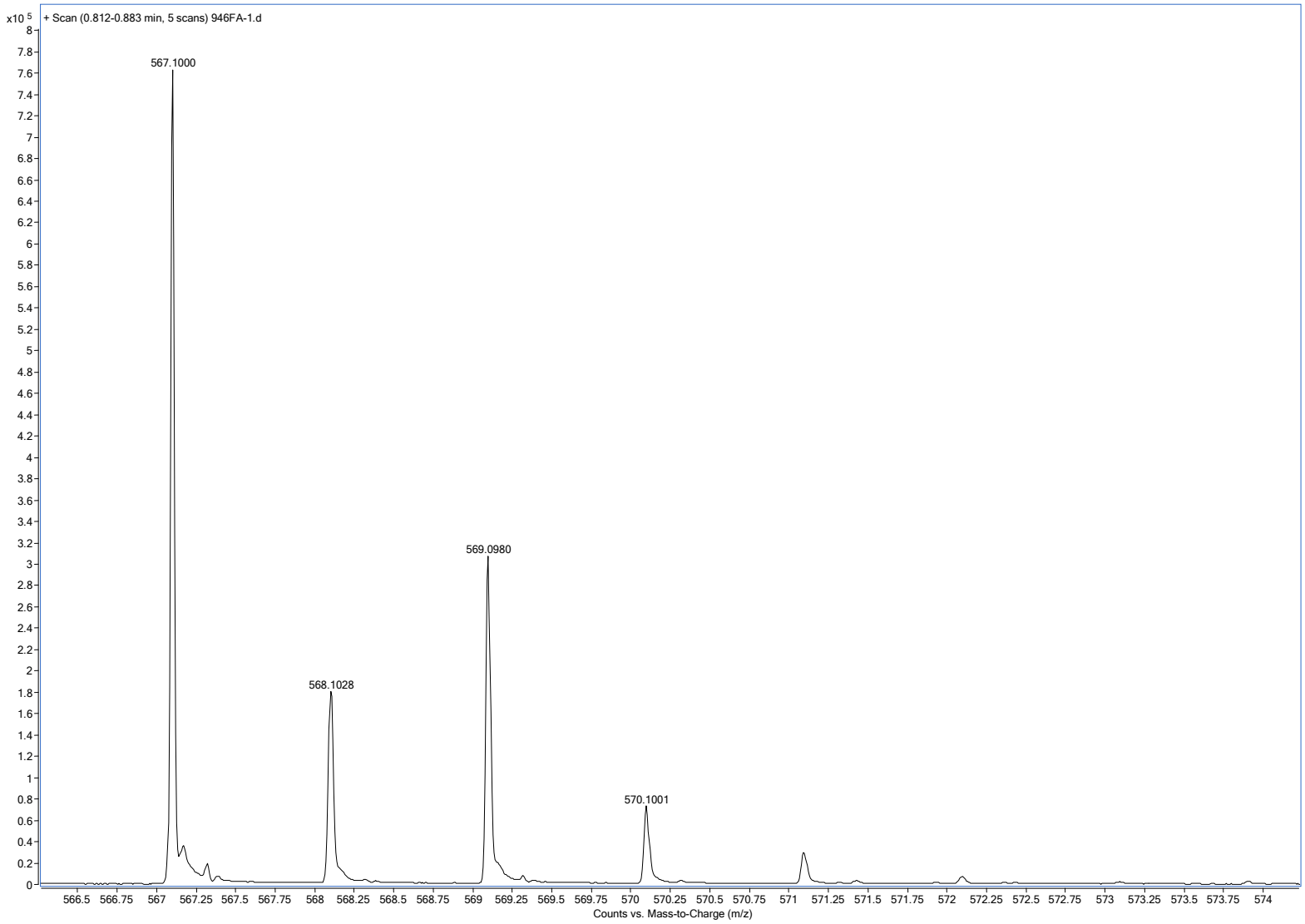


Figure S17. HR ESITOFMS of 7-*epi*-lyngbyabellin L (**3**).

Figure S18. ^{1}H NMR spectrum of 7-*epi*-lyngbyabellin L (**3**) (recorded in $CDCl_3$ at 500 MHz).

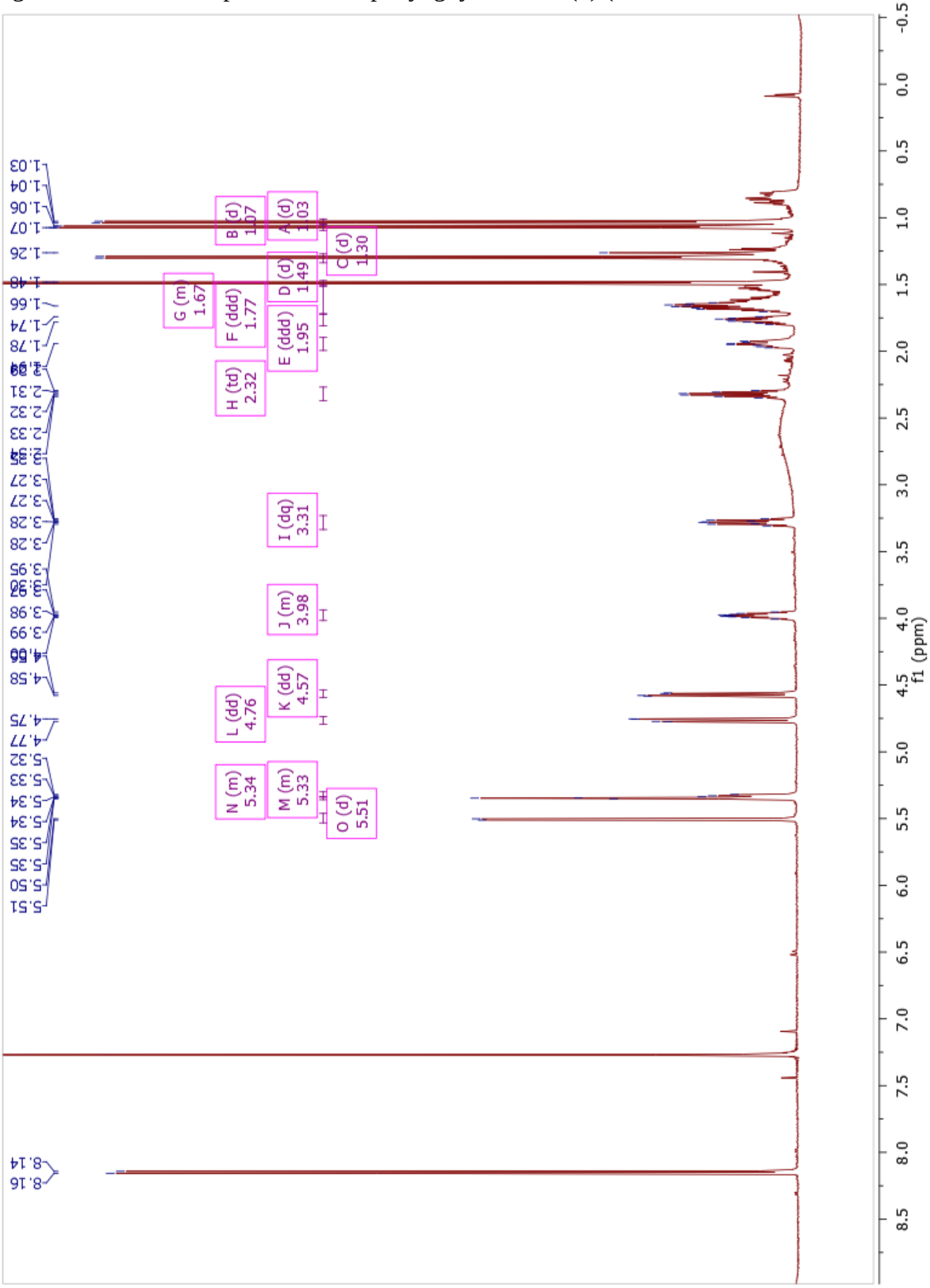


Figure S19. ^{13}C NMR spectrum of 7-*epi*-lyngbyabellin L (**3**) (recorded in $CDCl_3$ at 125 MHz).

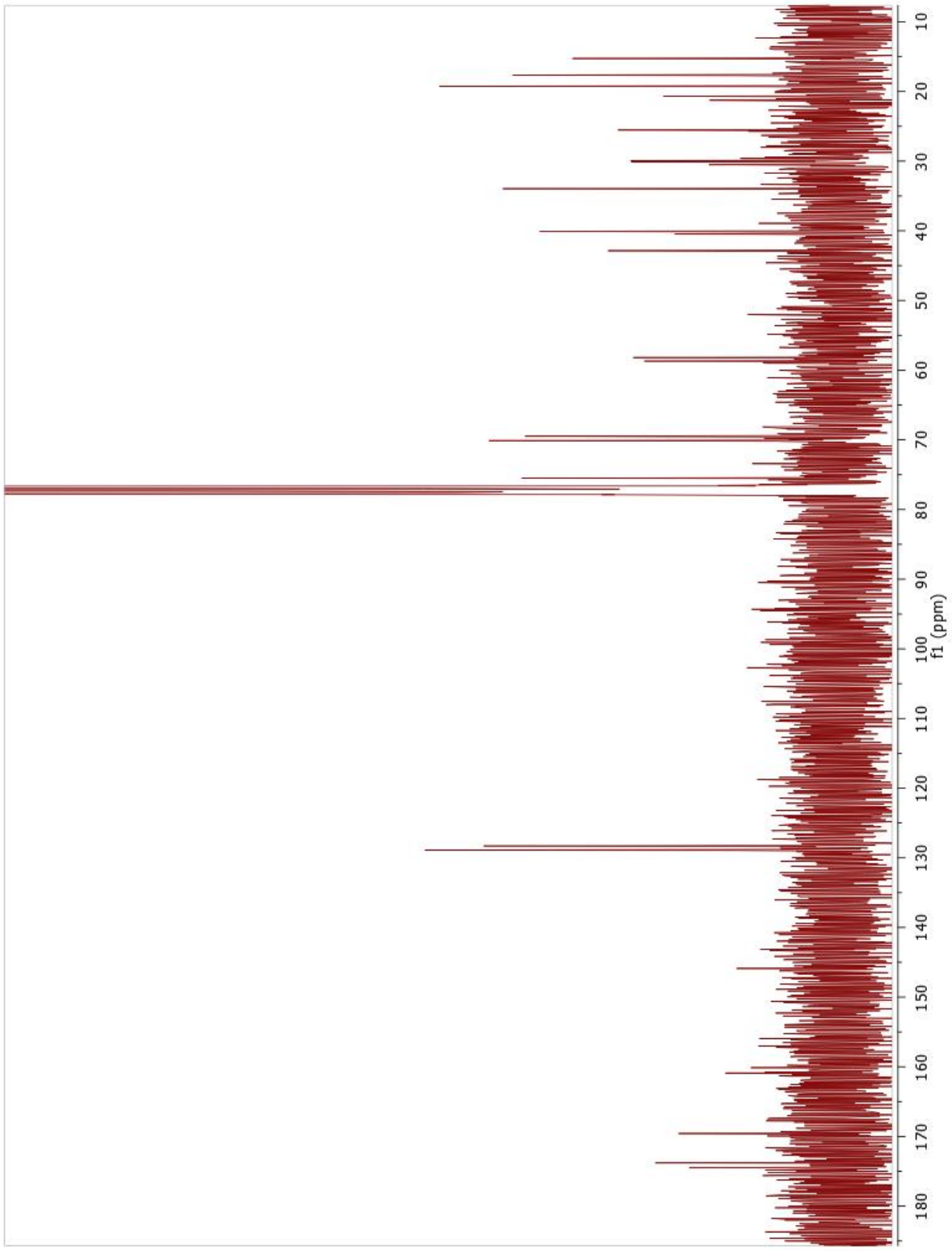


Figure S20. gHSQC spectrum of 7-*epi*-lyngbyabellin L (**3**) (recorded in $CDCl_3$ at 500 MHz).

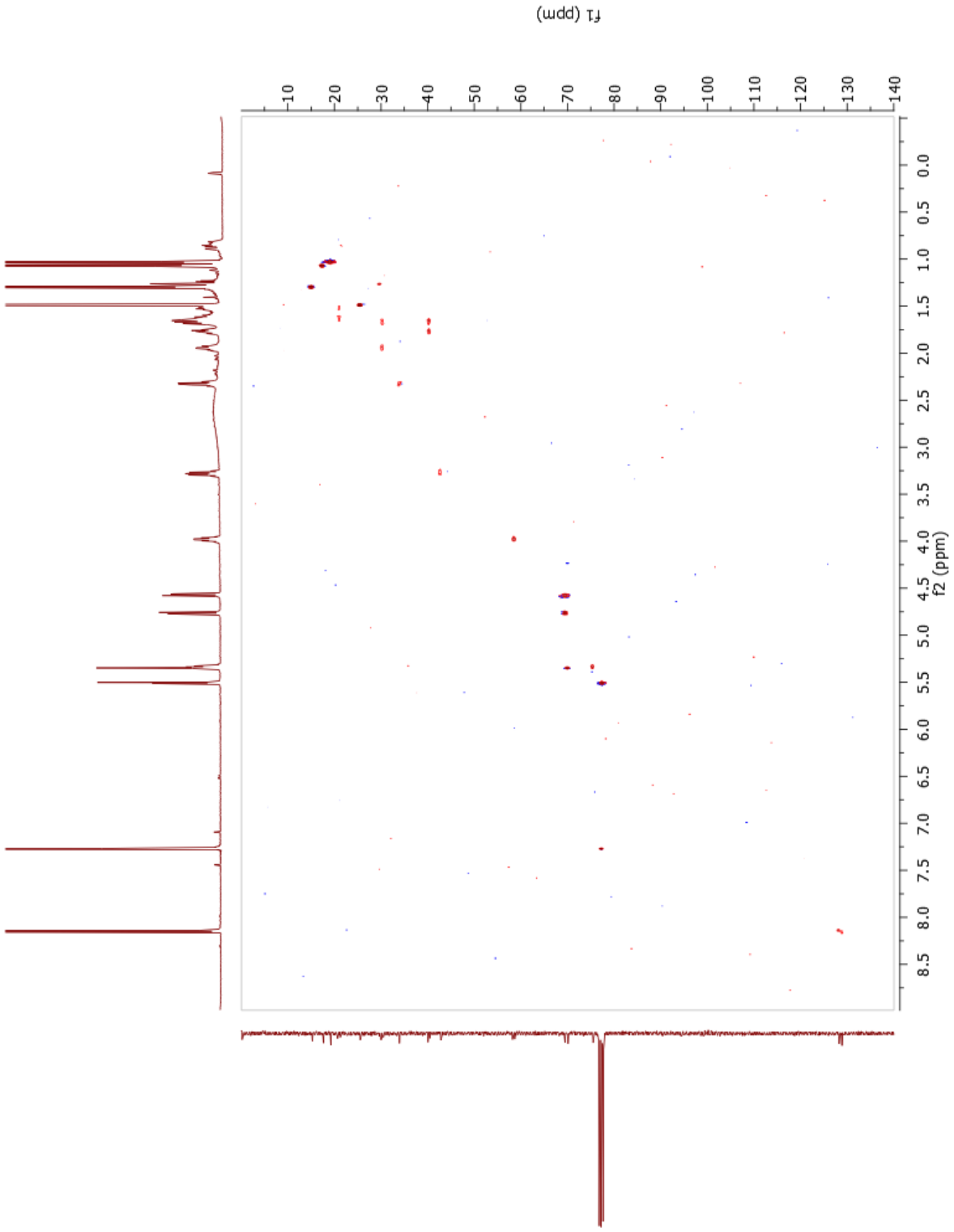


Figure S21. gCOSY spectrum of 7-*epi*-lyngbyabellin L (**3**) (recorded in $CDCl_3$ at 500 MHz).

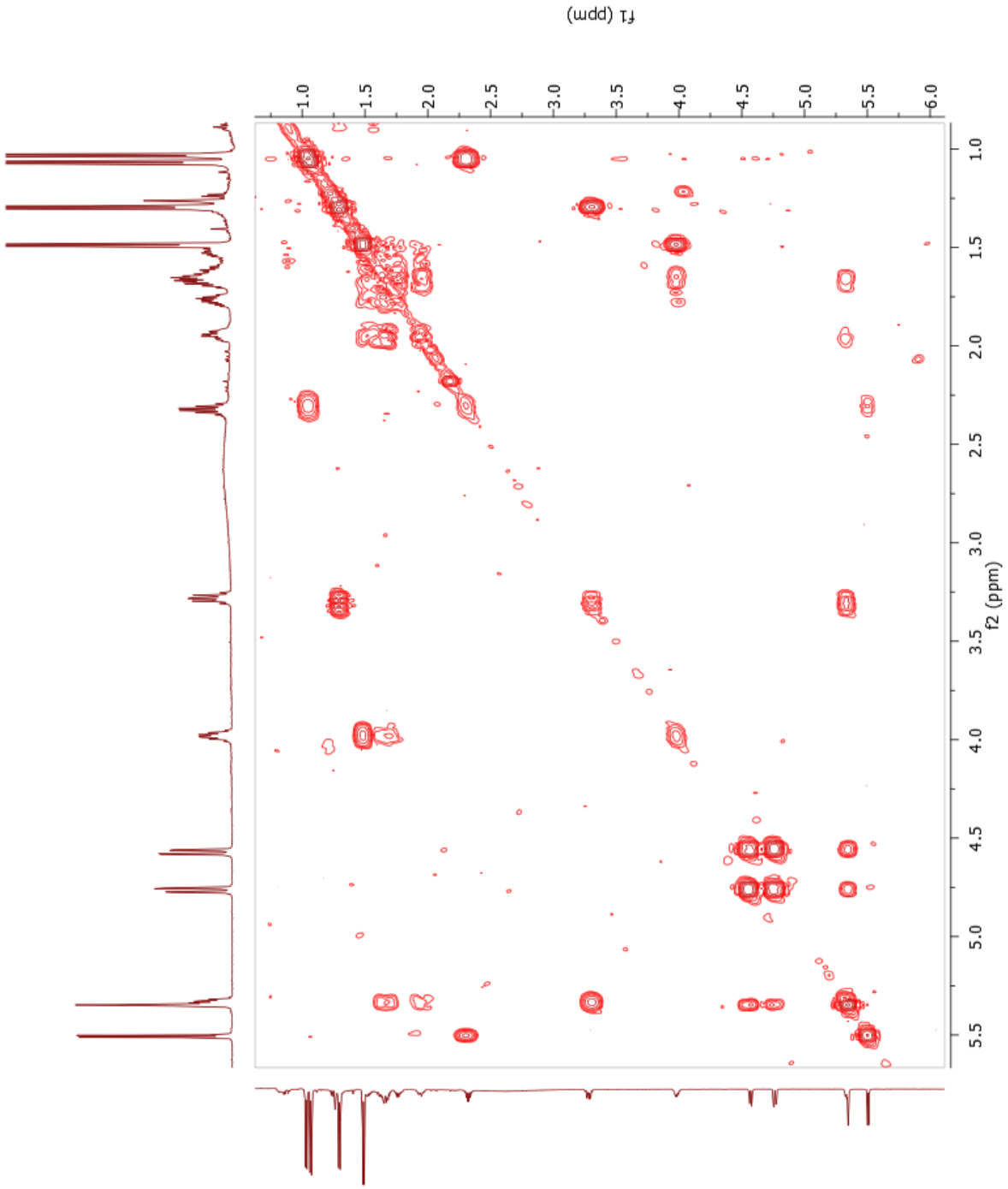


Figure S22. gHMBC spectrum of 7-*epi*-lyngbyabellin L (**3**) (recorded in $CDCl_3$ at 500 MHz).

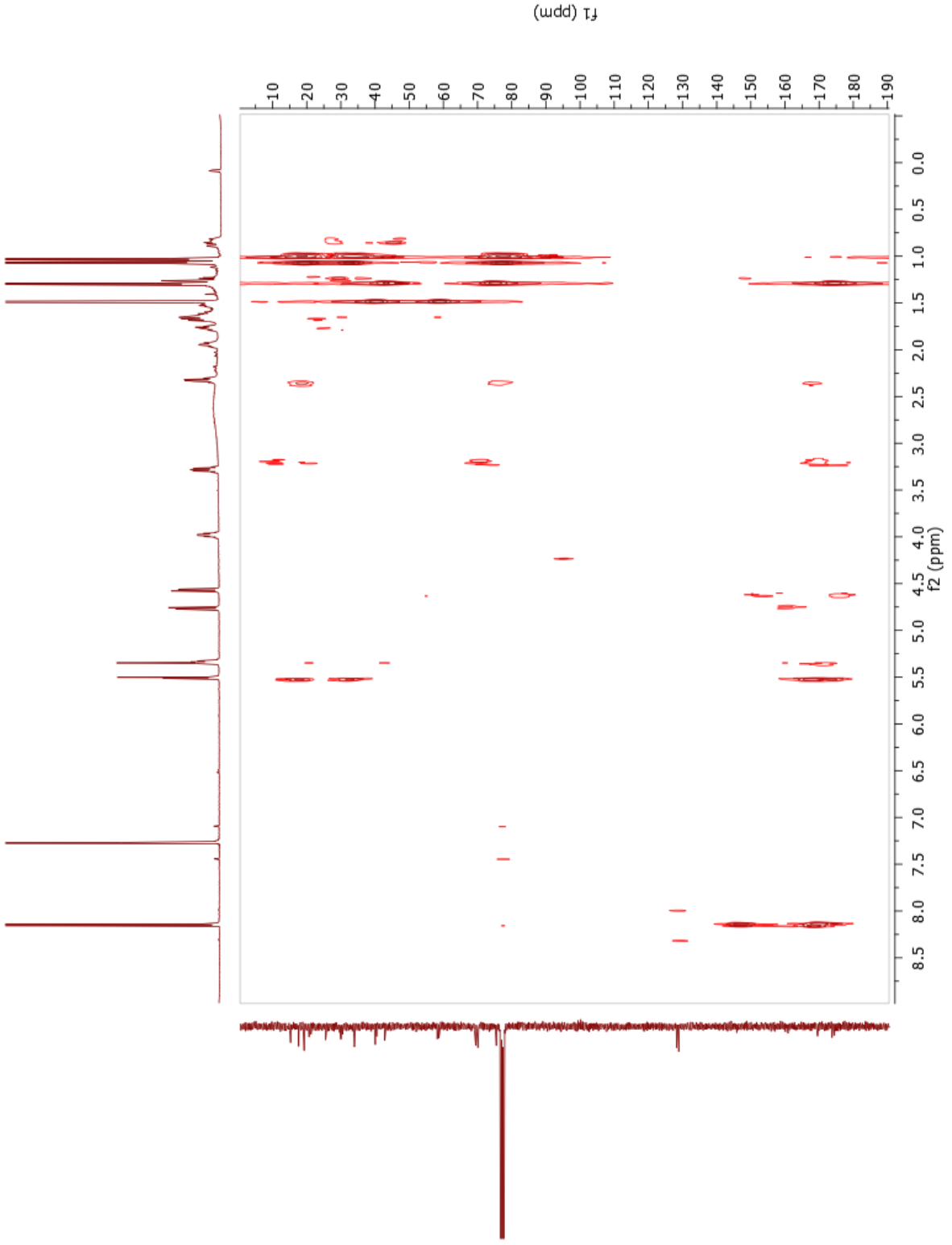


Figure S23. DQF-COSY spectrum of 7-*epi*-lyngbyabellin L (**3**) (recorded in $CDCl_3$ at 600 MHz).

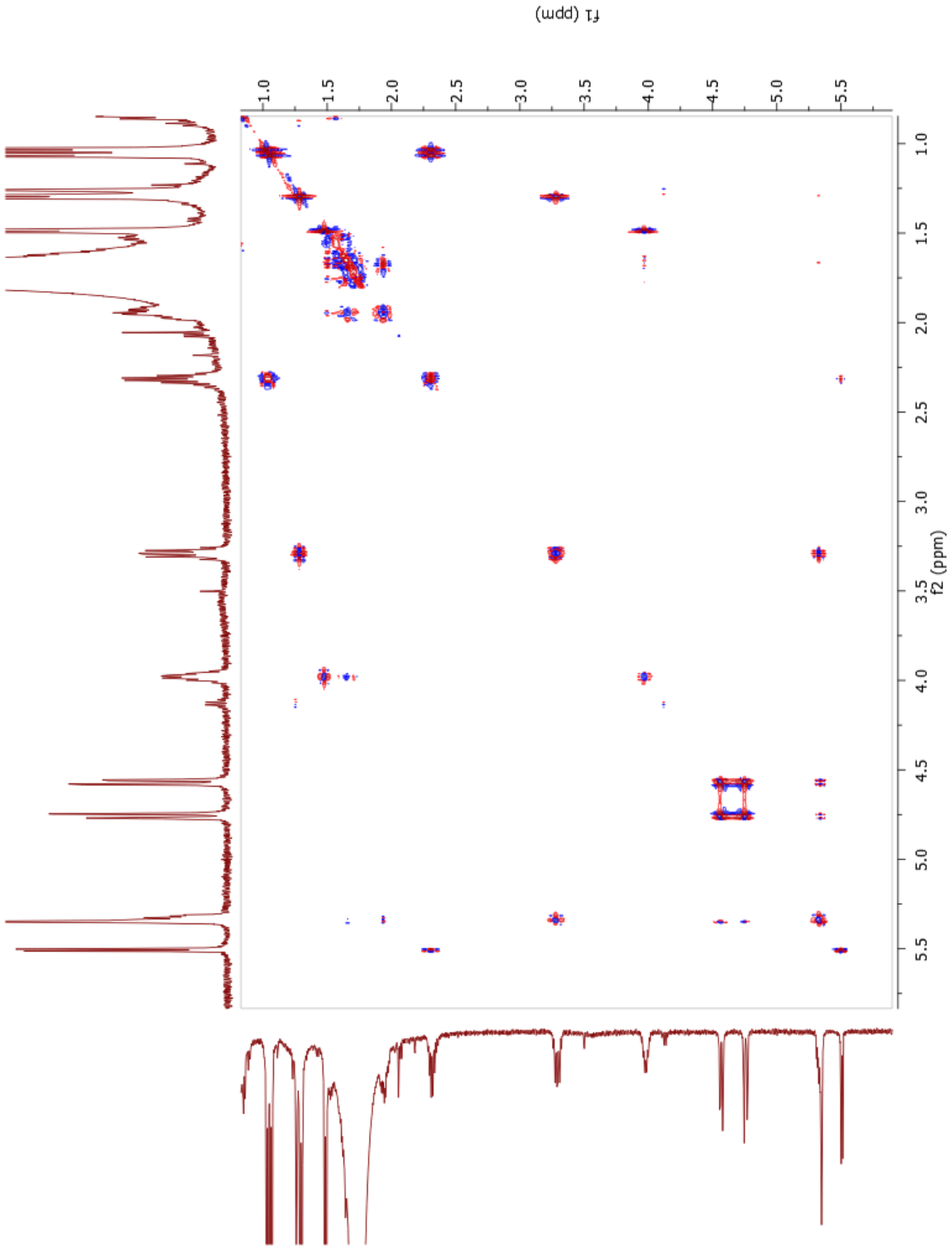


Figure S24. NOESY spectrum of 7-*epi*-lyngbyabellin L (**3**) (recorded in $CDCl_3$ at 600 MHz).

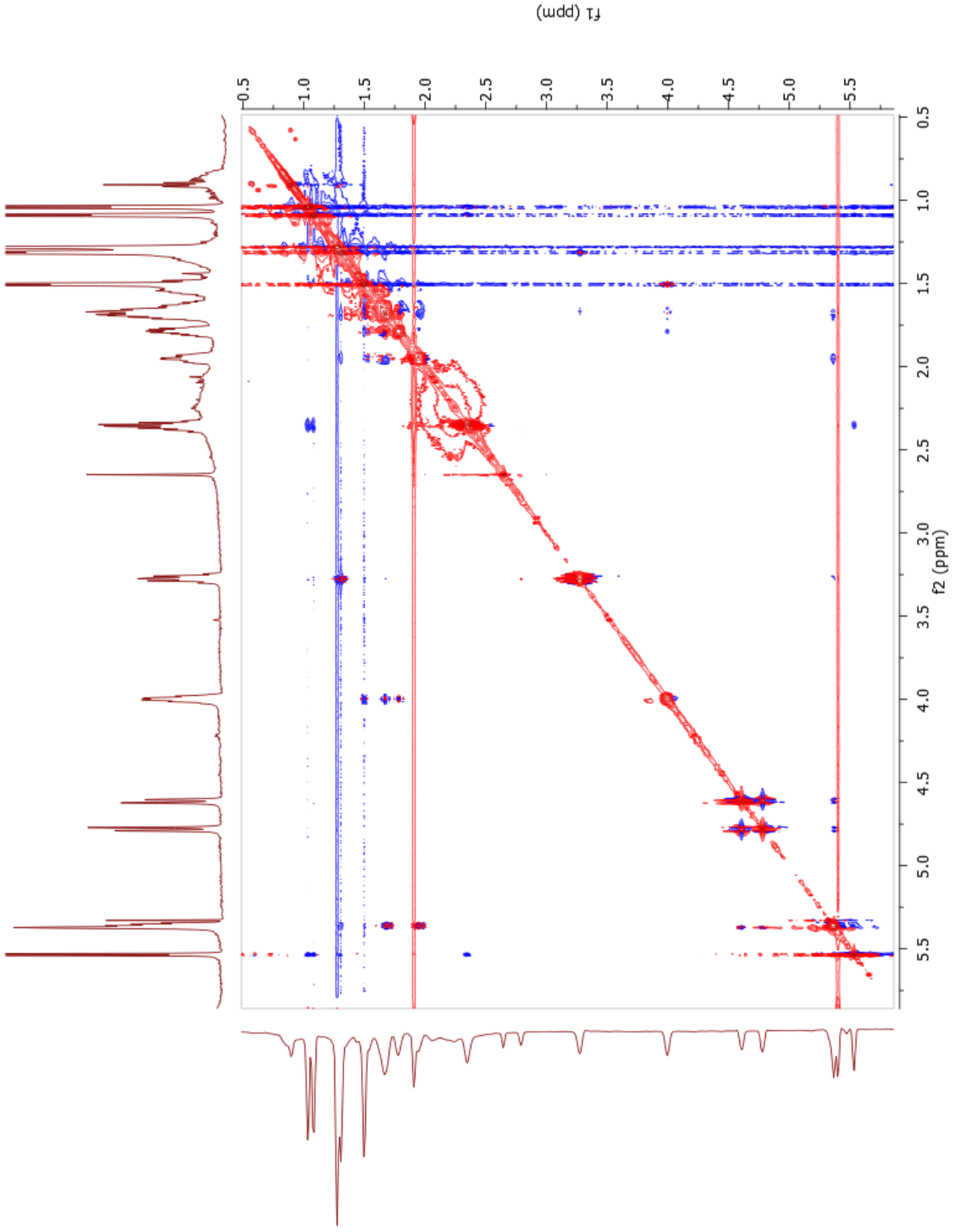


Figure S25. HR ESITOFMS of lyngbyabellin M (**4**).

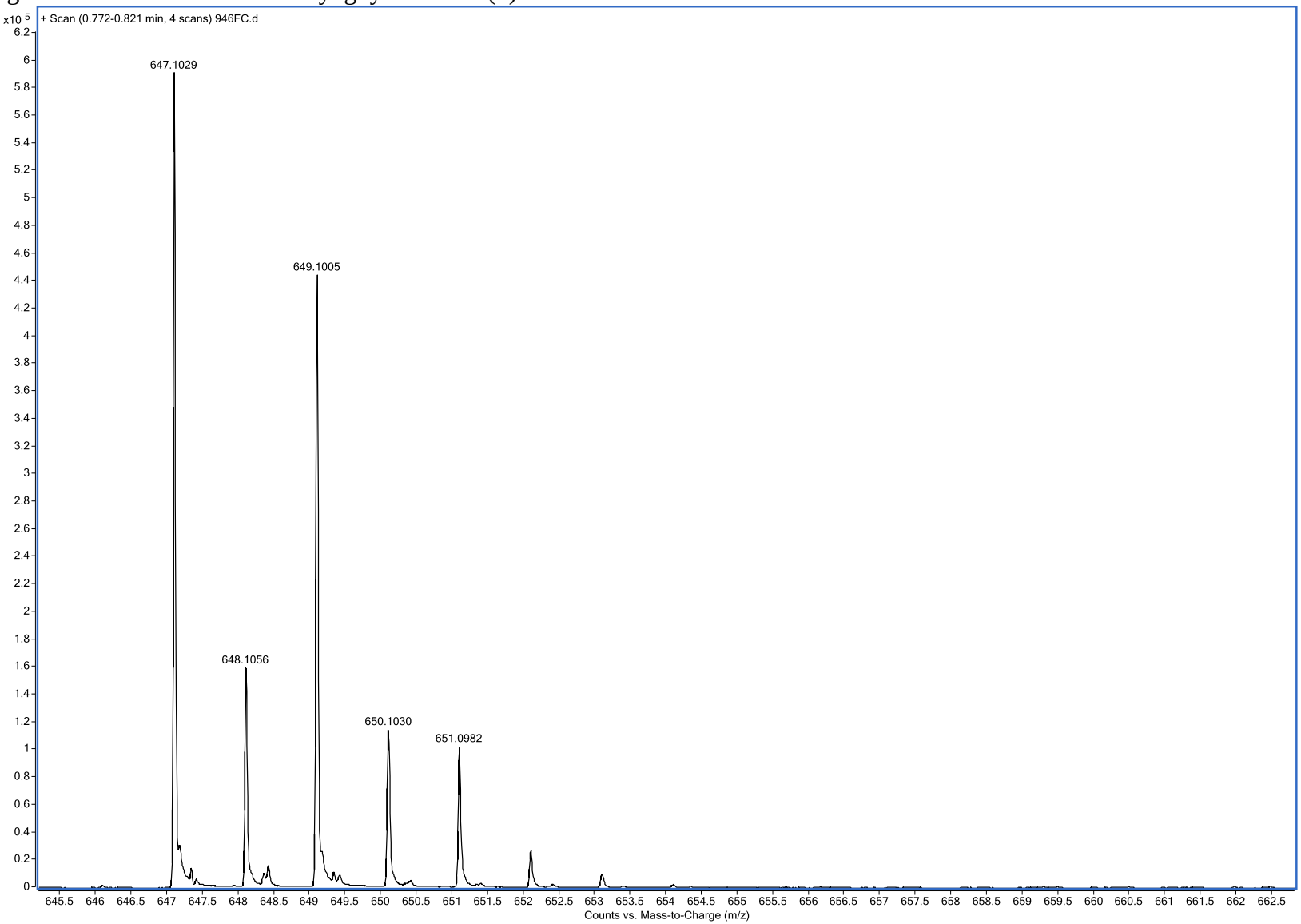


Figure S26. ^{1}H NMR spectrum of lyngbyabellin M (**4**) (recorded in $CDCl_3$ at 500 MHz).

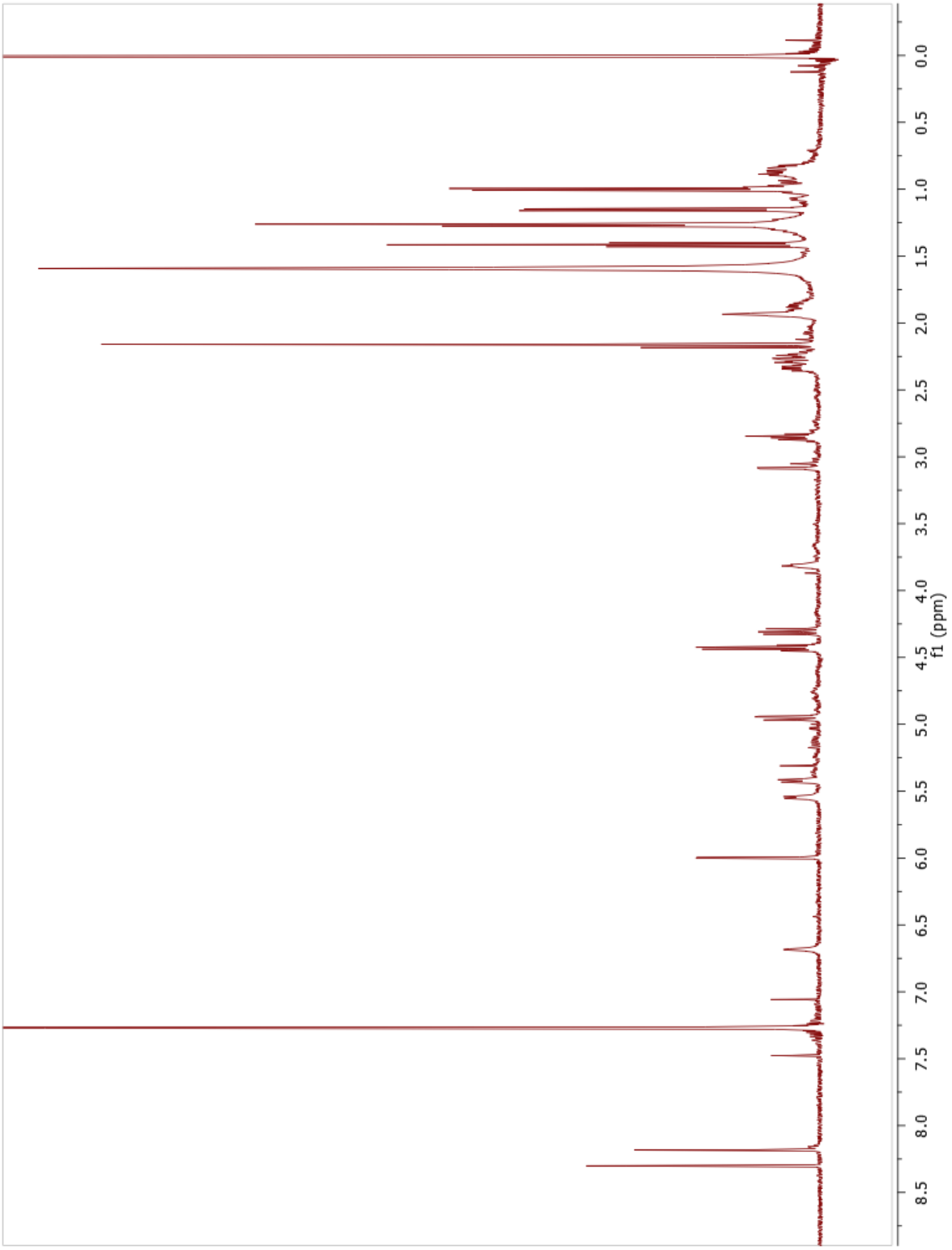


Figure S27. ^{13}C NMR spectrum of lyngbyabellin M (**4**) (recorded in $CDCl_3$ at 125 MHz).

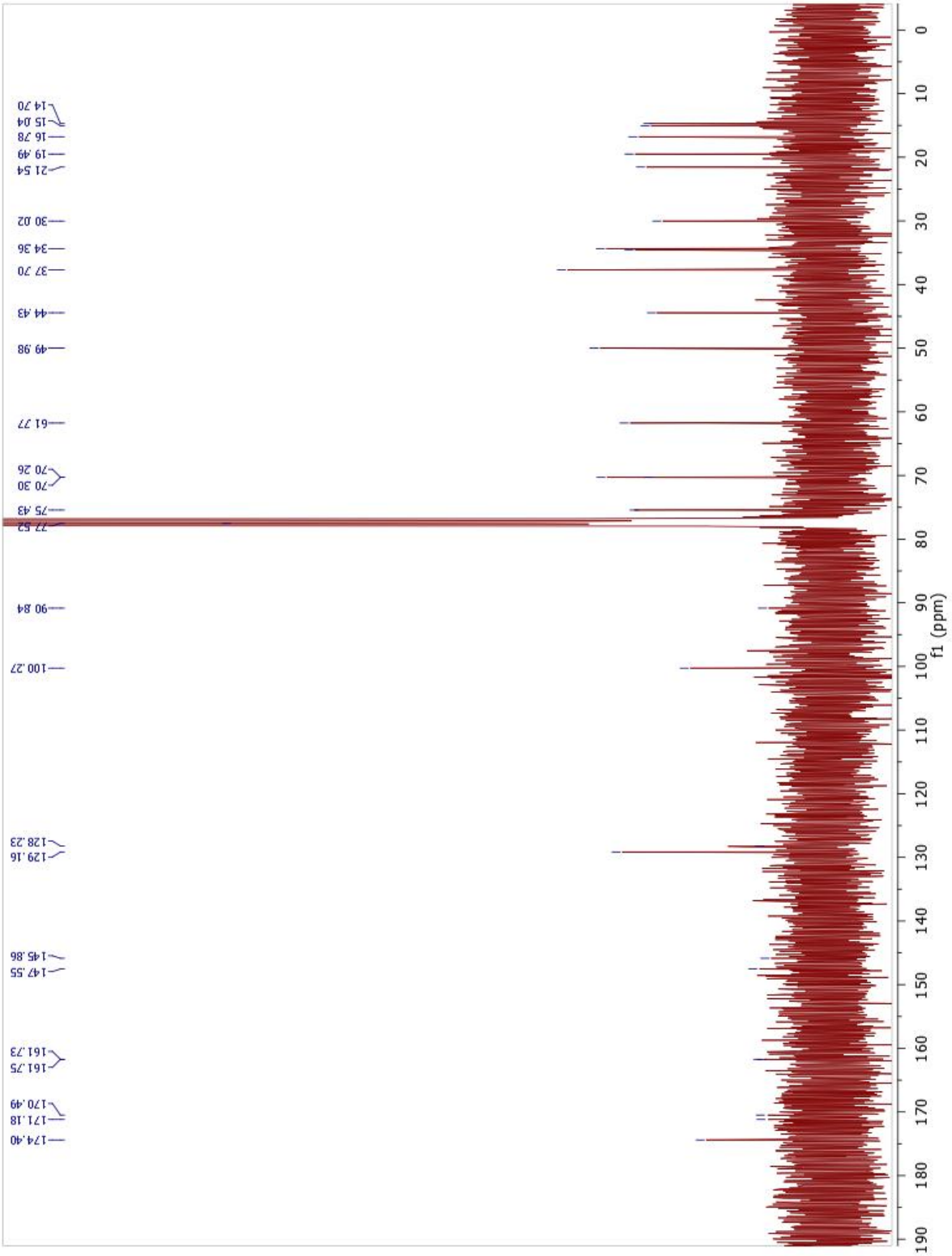


Figure S28. gHSQC spectrum of lyngbyabellin M (**4**) (recorded in $CDCl_3$ at 600 MHz).

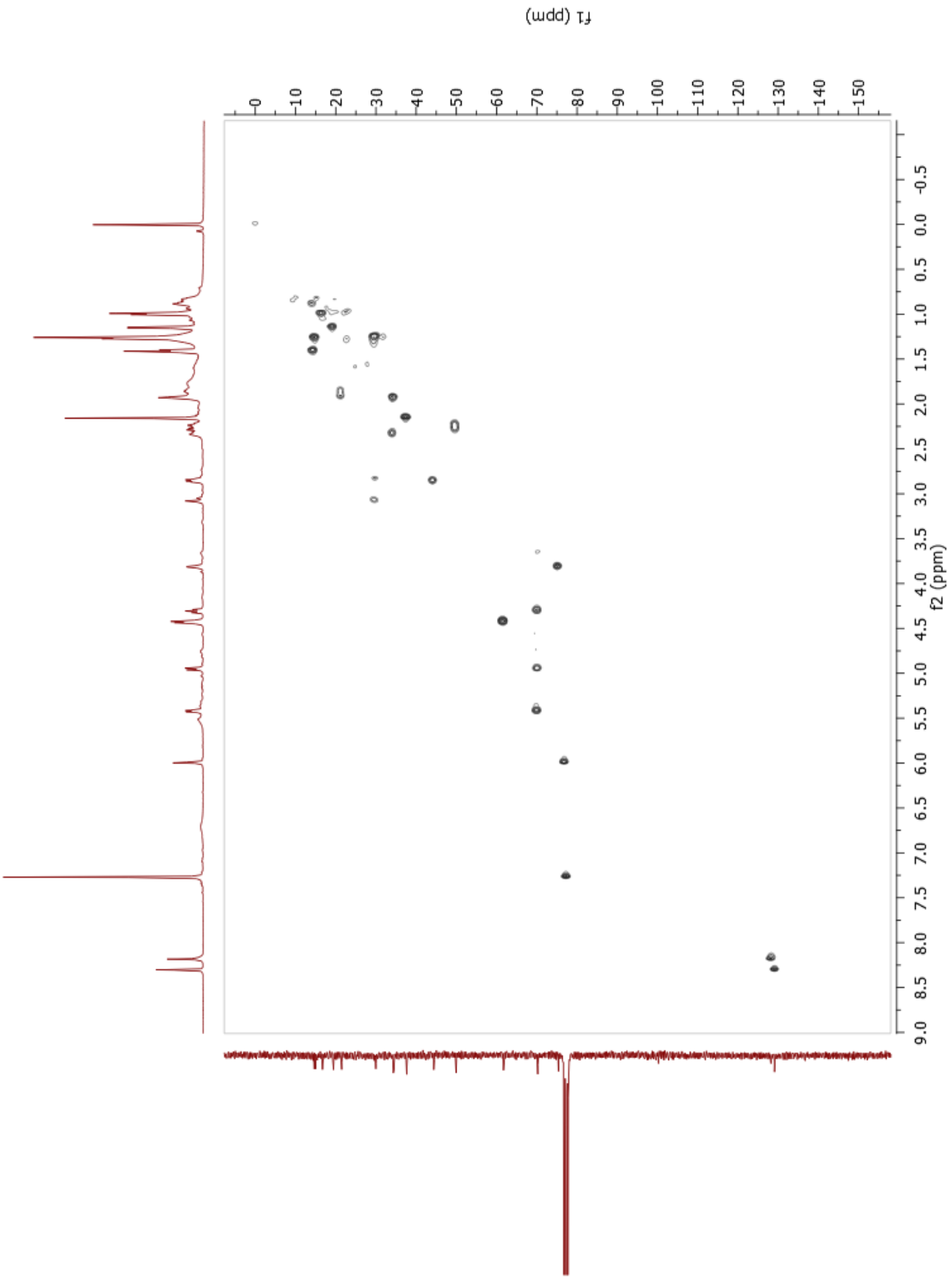


Figure S29. gCOSY spectrum of lyngbyabellin M (**4**) (recorded in $CDCl_3$ at 500 MHz).

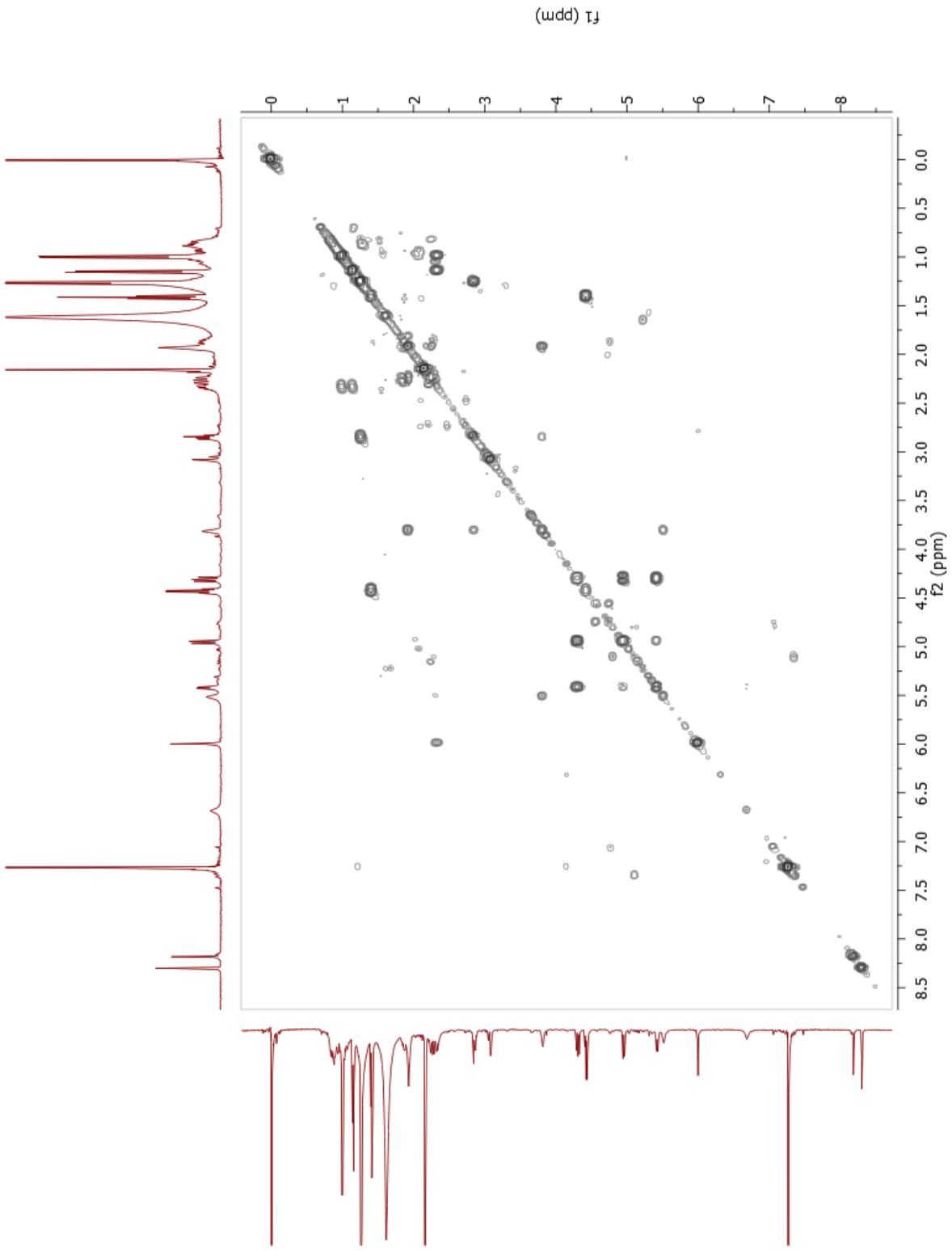


Figure S30. gHMBC spectrum of lyngbyabellin M (**4**) (recorded in $CDCl_3$ at 500 MHz).

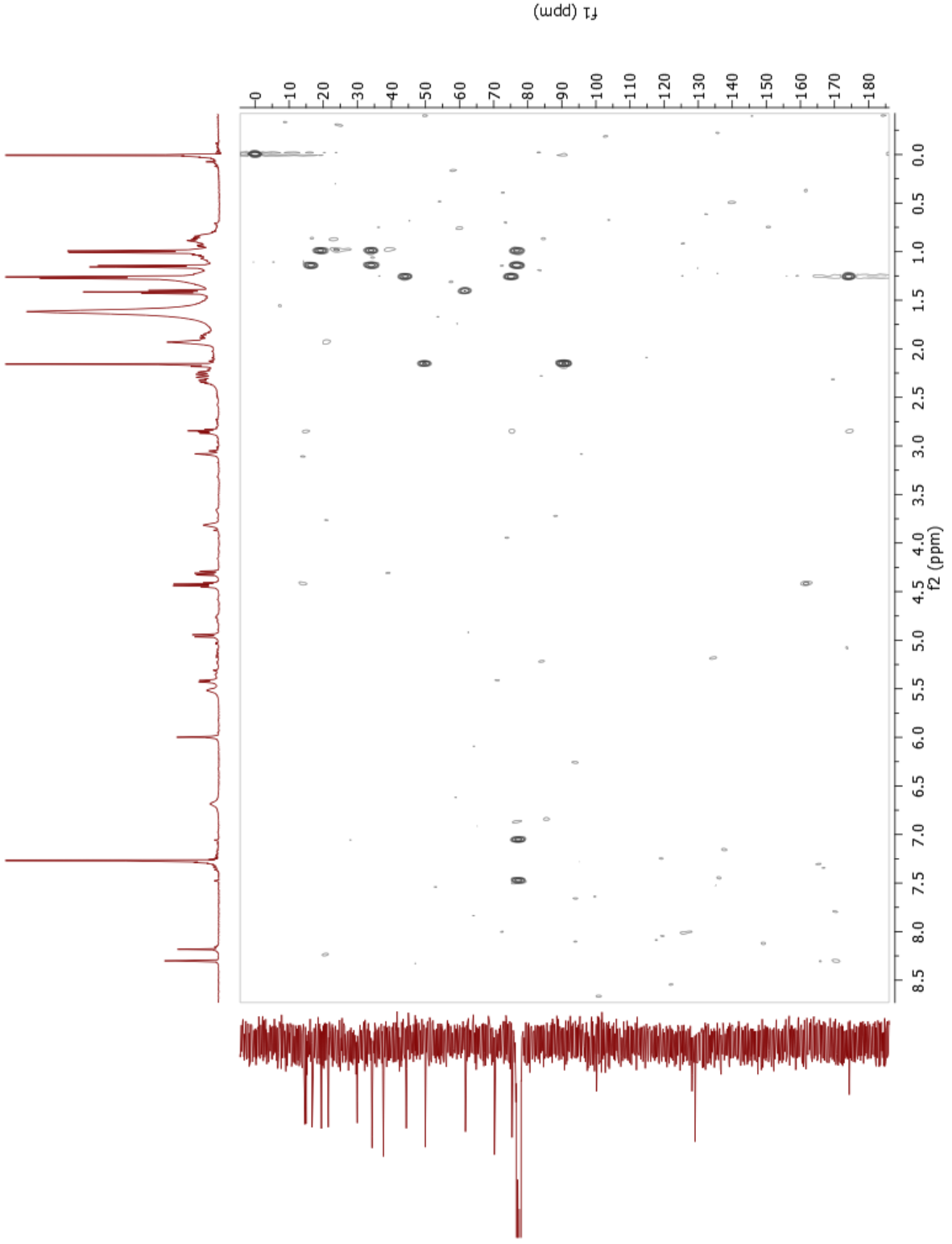


Figure S31. ^{1}H NMR spectrum of 3,14-di-*S*-MTPA ester of lyngbyabellin M **(6)** (recorded in $CDCl_3$ at 600 MHz).

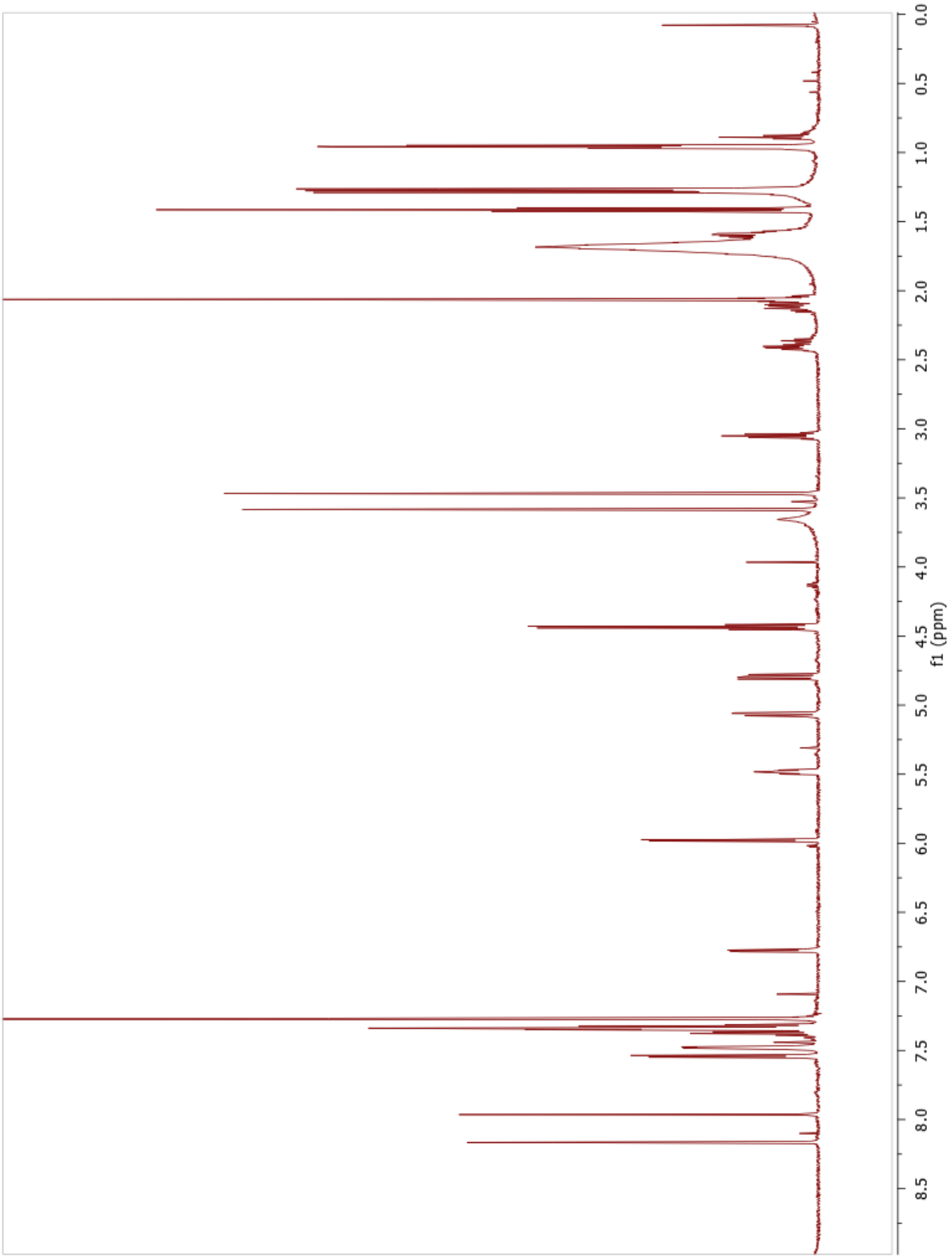


Figure S32. ^{1}H NMR spectrum of 3,14-di-*R*-MTPA ester of lyngbyabellin M **(7)** (recorded in $CDCl_3$ at 600 MHz).

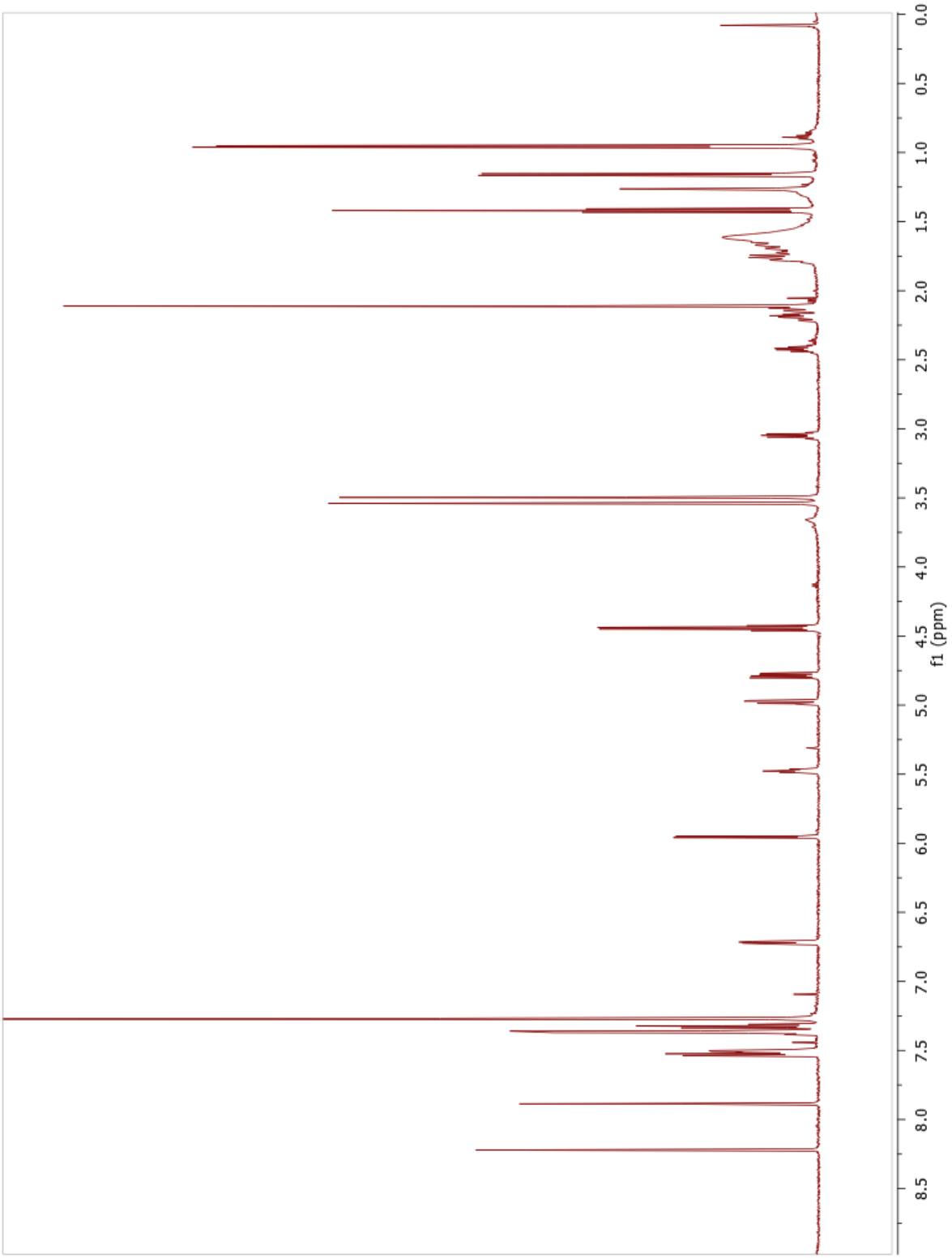


Figure S33. HR ESITOFMS of lyngbyabellin N (**5**).

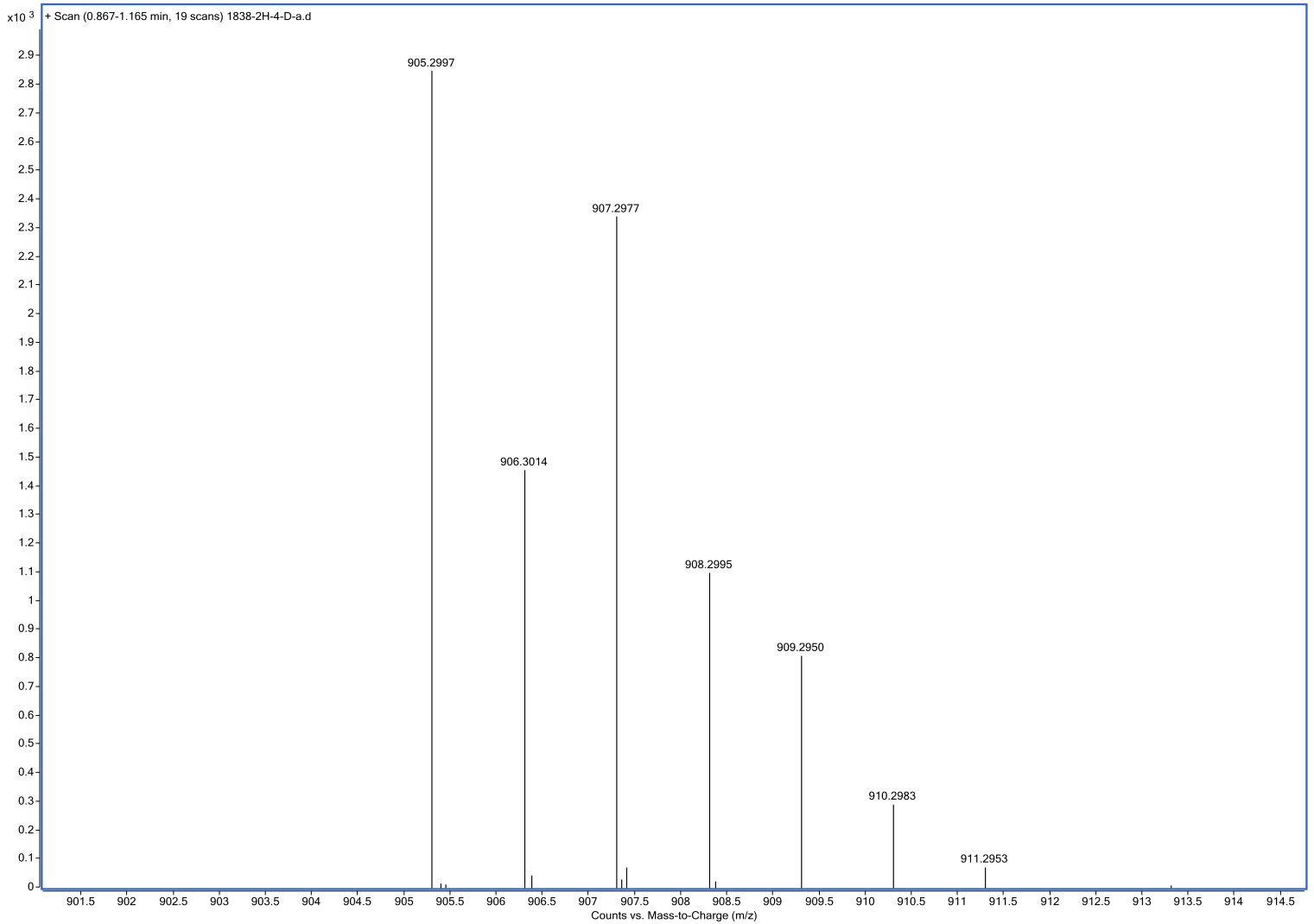


Figure S34. ^{1}H NMR spectrum of lyngbyabellin N (**5**) (recorded in d_6-DMSO at 500 MHz)

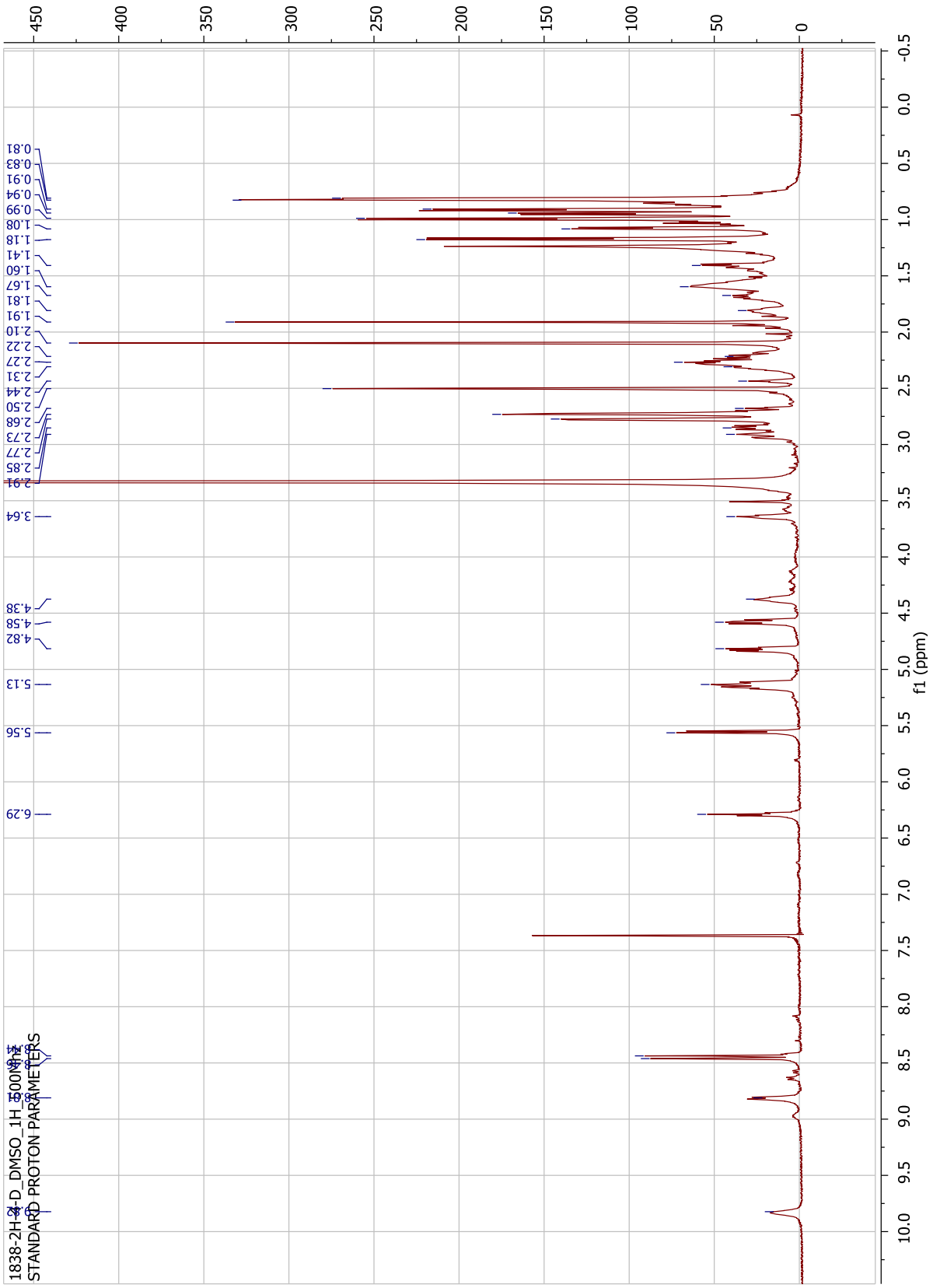


Figure S35. ^{13}C NMR spectrum of lyngbyabellin N (**5**) (recorded in d_6-DMSO at 75 MHz)

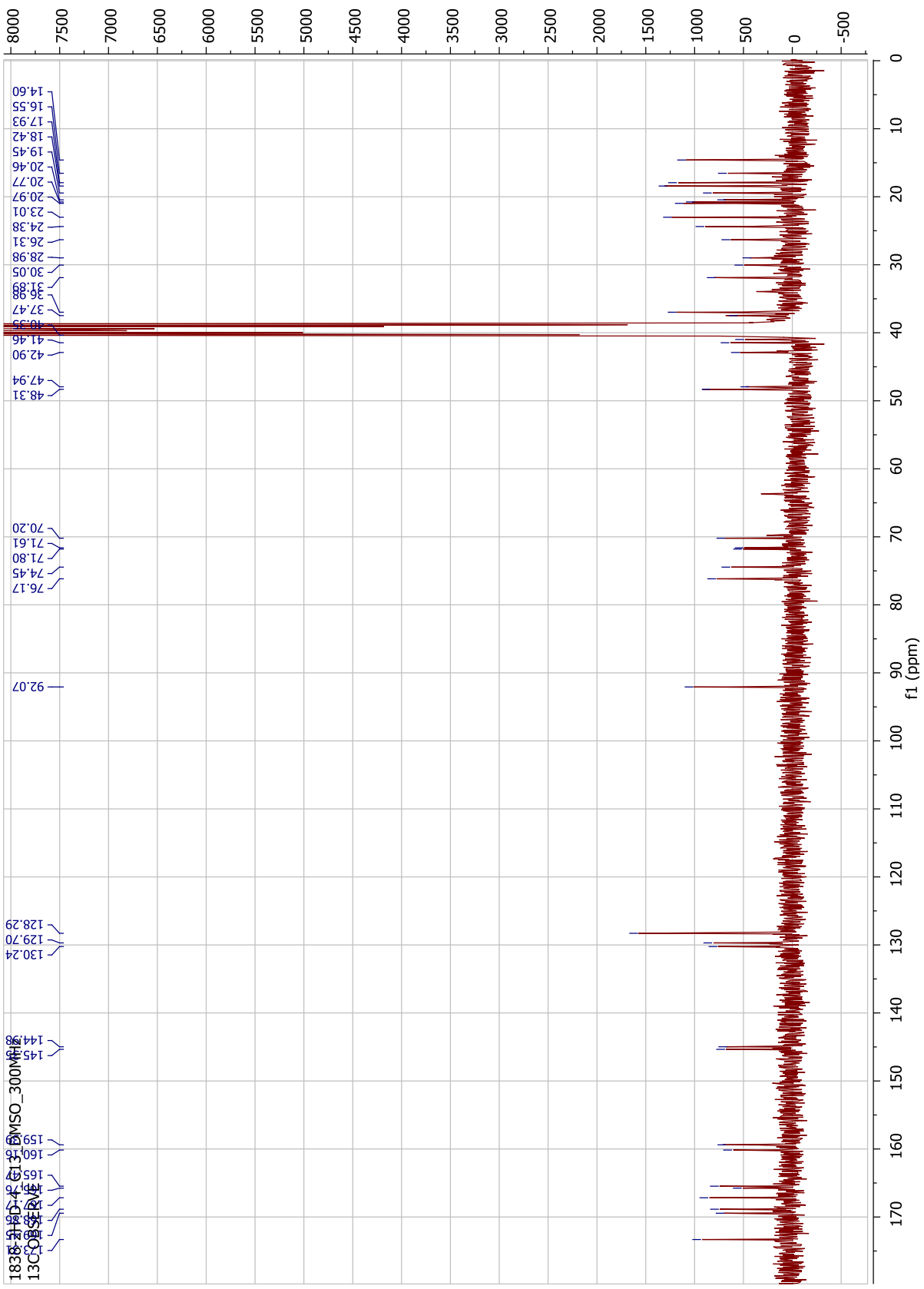


Figure S36. gHSQC spectrum of lyngbyabellin N (**5**) (recorded in d_6-DMSO at 500 MHz)

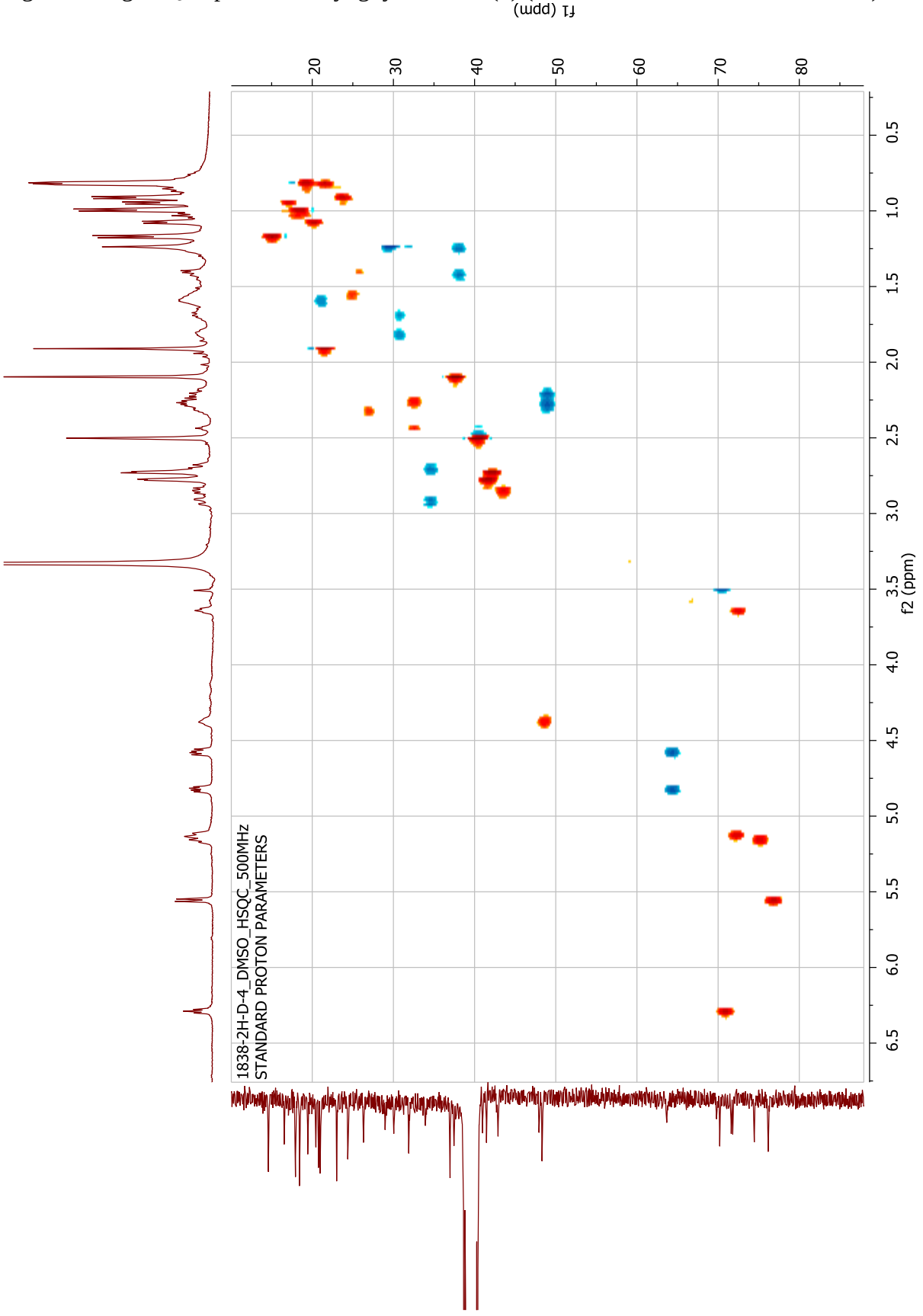


Figure S37. gCOSY spectrum of lyngbyabellin N (**5**) (recorded in d_6-DMSO at 500 MHz)

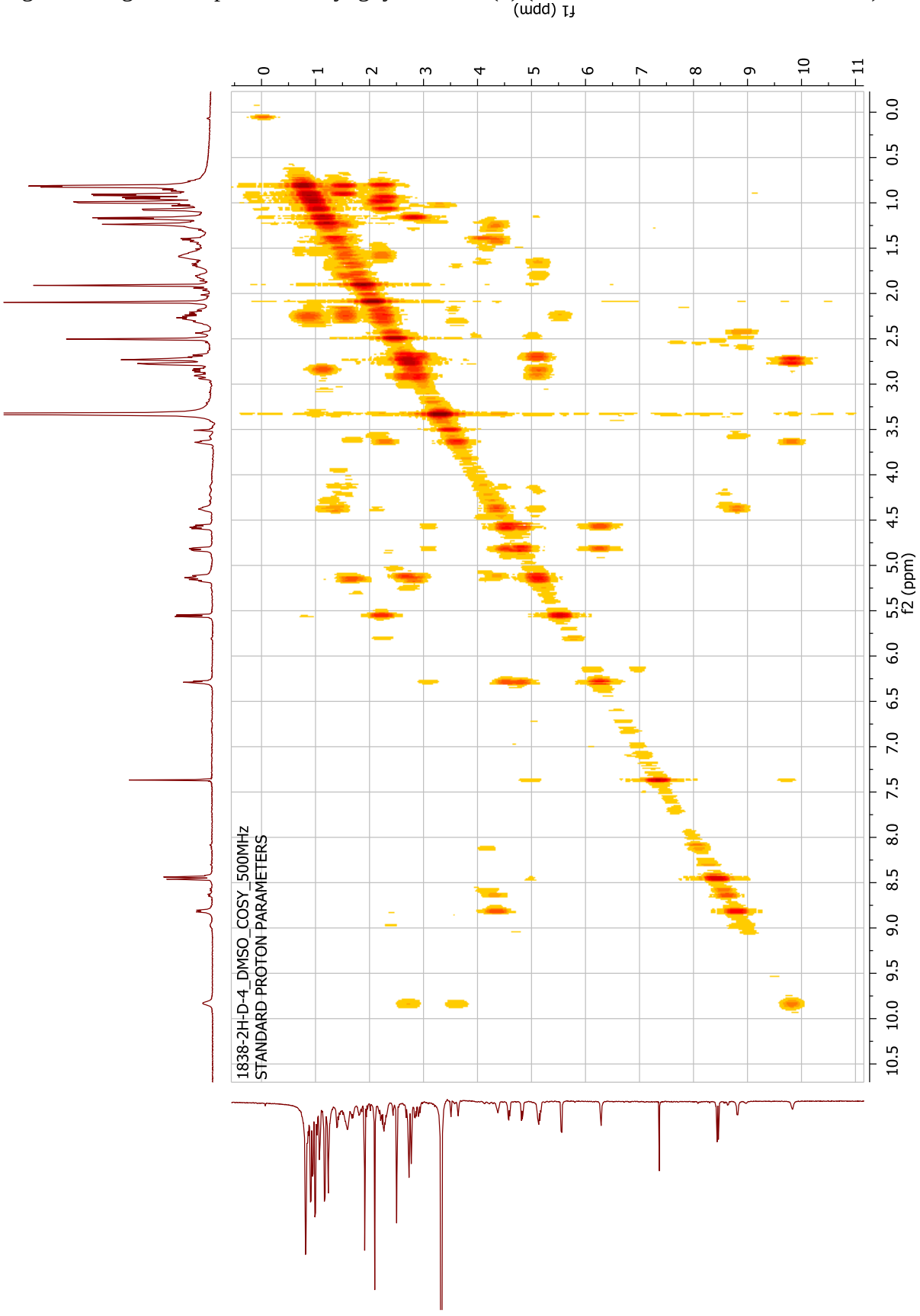


Figure S38. gHMBC spectrum of lyngbyabellin N (**5**) (recorded in d_6-DMSO at 500 MHz)

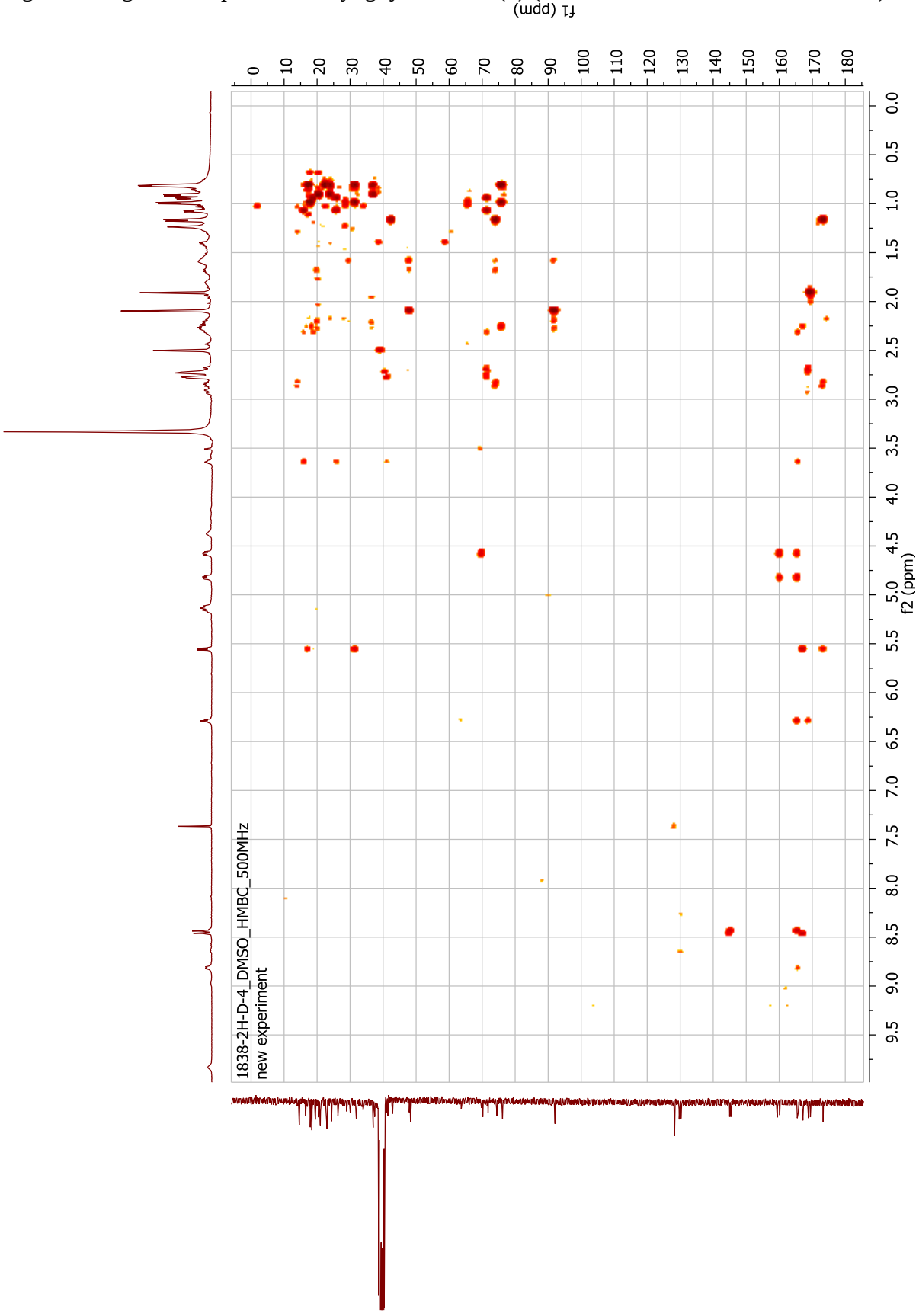


Figure S39. TOCSY spectrum of lyngbyabellin N (**5**) (recorded in d_6-DMSO at 500 MHz)

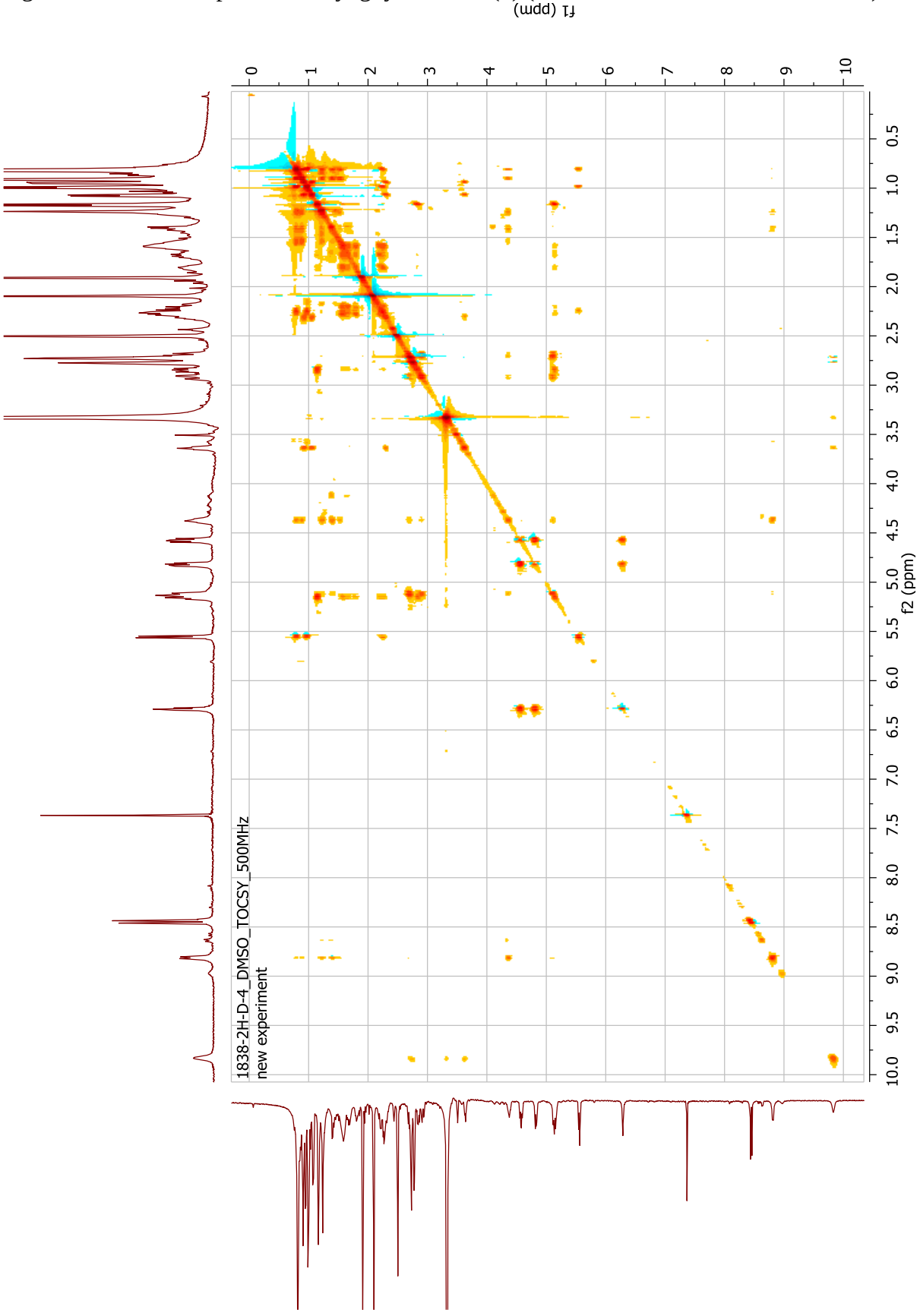


Figure S40. ^{1}H NMR spectrum of lyngbyabellin N (**5**) (recorded in $CDCl_3$ at 500 MHz)

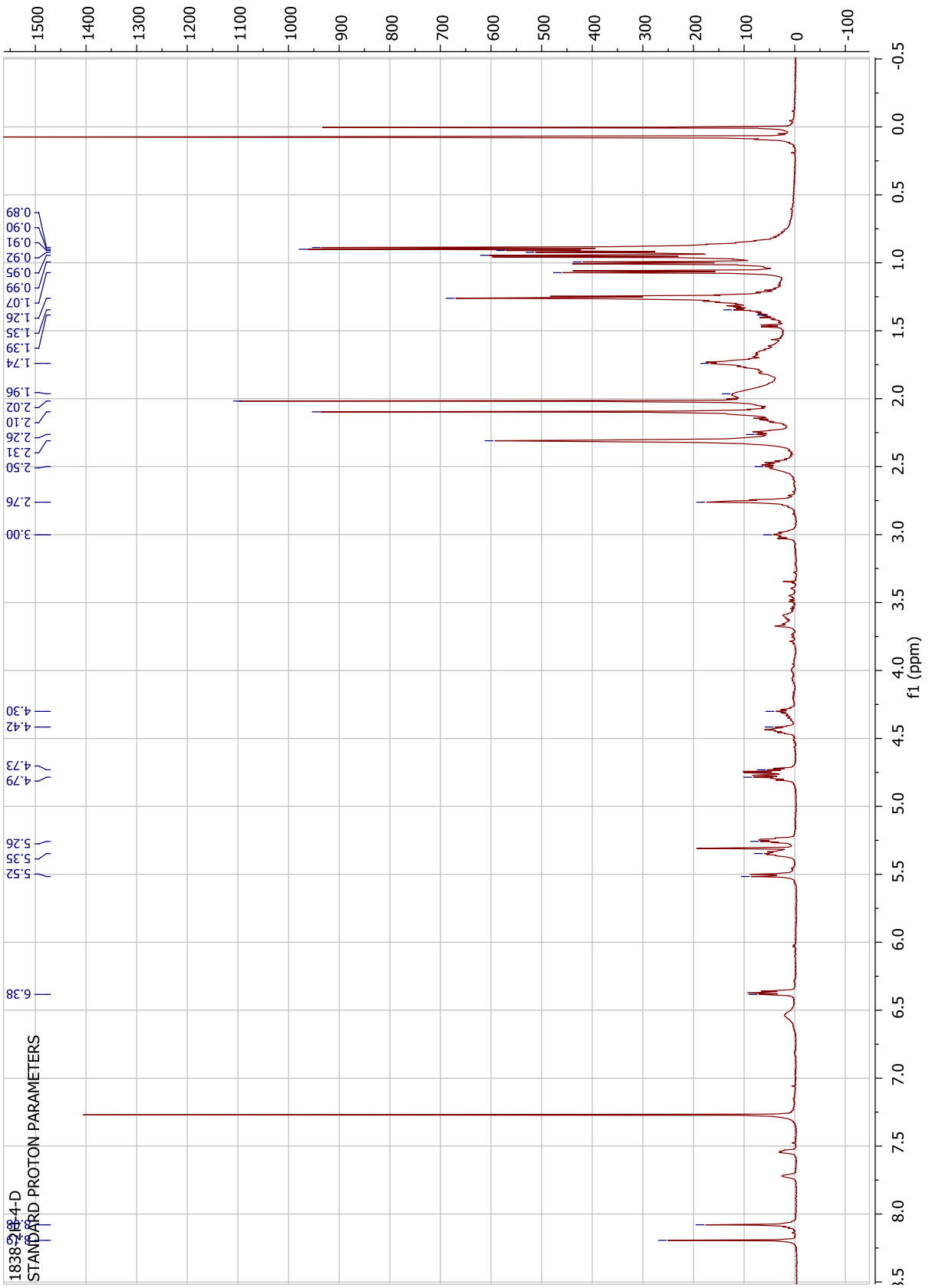


Figure S41. ^{13}C NMR spectrum of lyngbyabellin N (**5**) (recorded in $CDCl_3$ at 75 MHz)