

*Supporting Information for*

## **Antibacterial Meroterpenoids, Merochlorins G–J from the Marine Bacterium**

***Streptomyces* sp.**

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CA 92093-0204, USA

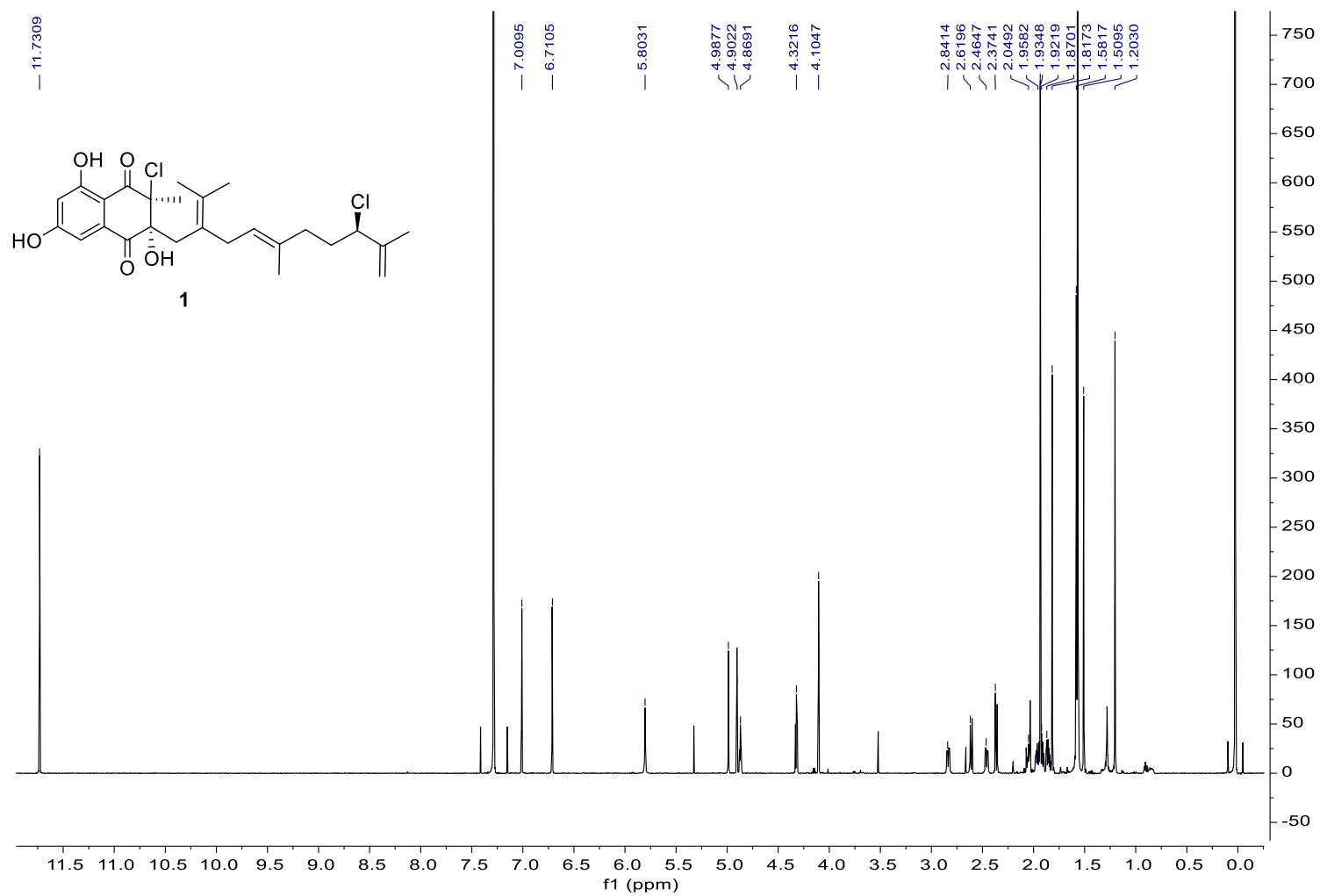
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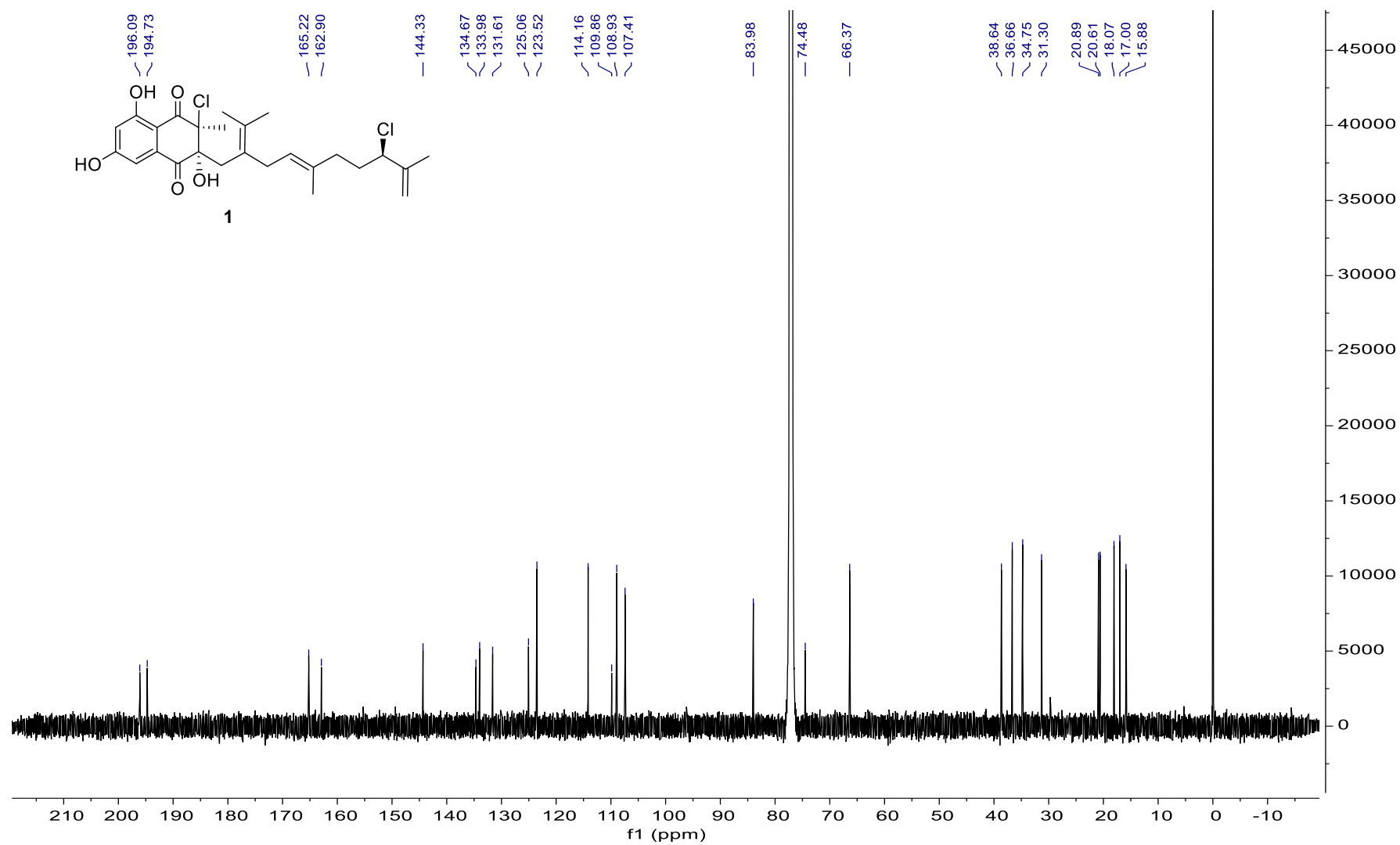
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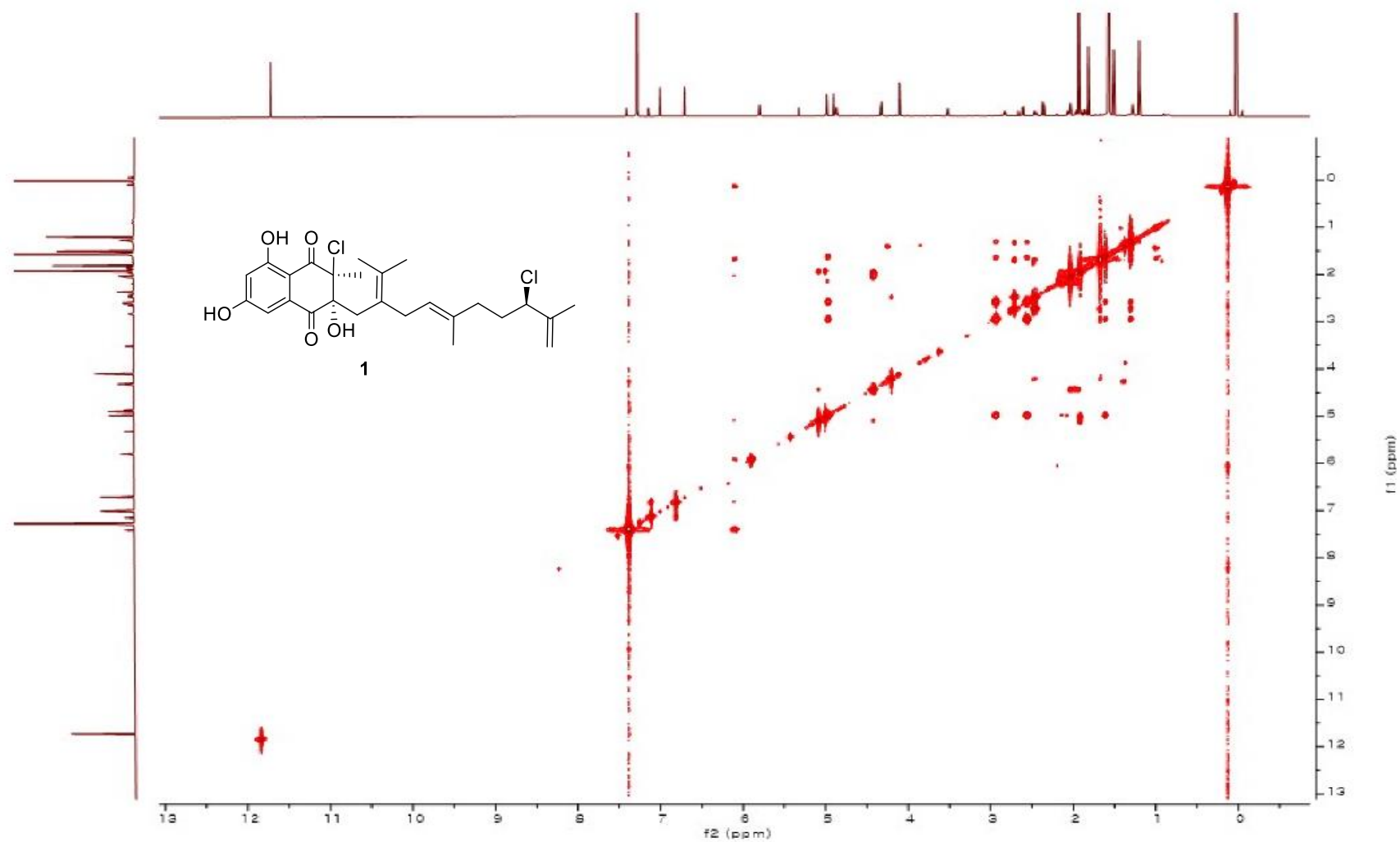
**Figure S1.**  $^1\text{H}$  NMR Spectrum of Merochlorin G (**1**) in  $\text{CDCl}_3$



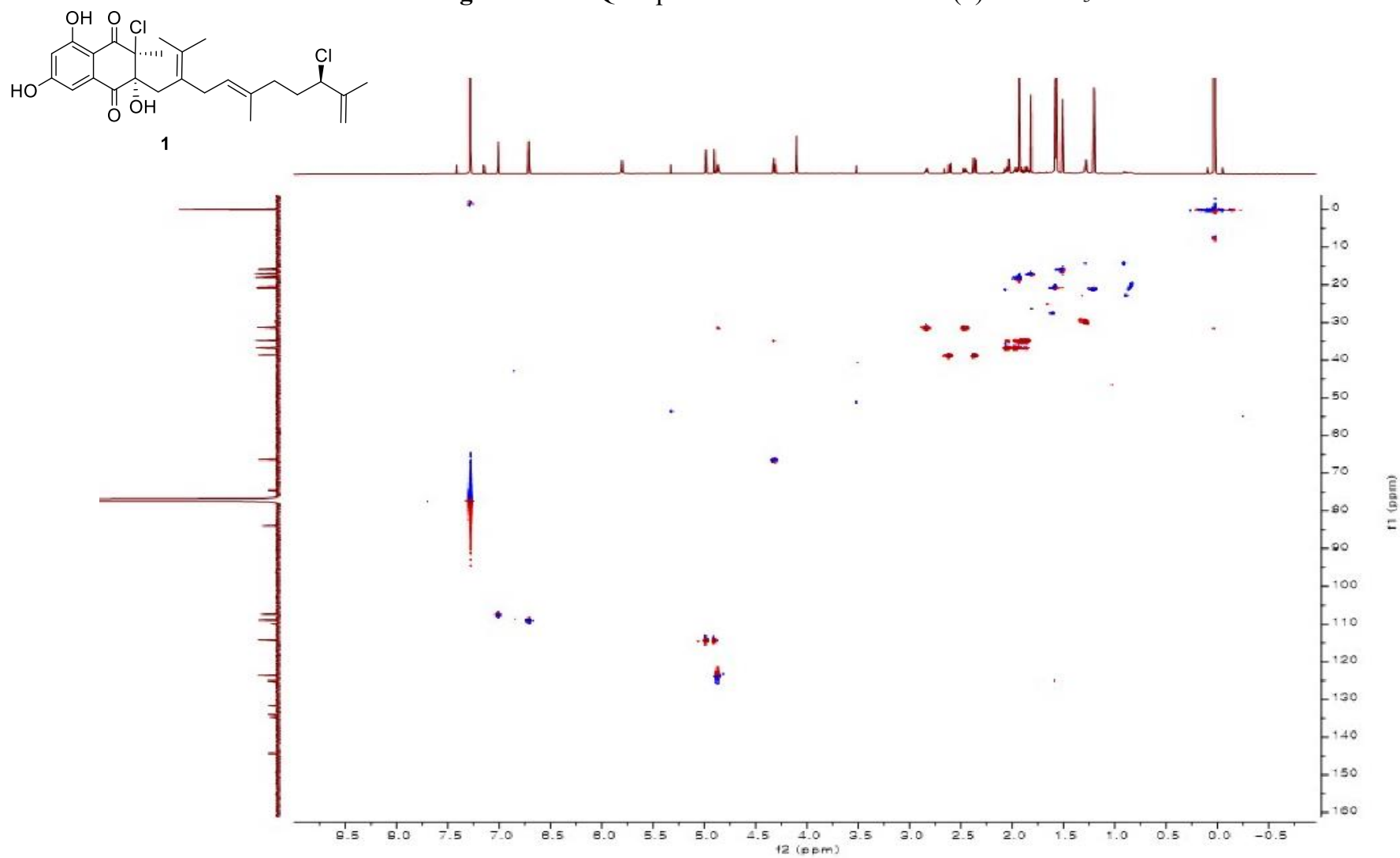
**Figure S2.**  $^{13}\text{C}$  NMR Spectrum of Merochlorin G (**1**) in  $\text{CDCl}_3$



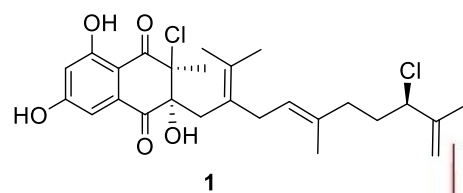
**Figure S3.** COSY Spectrum of Merochlorin G (**1**) in CDCl<sub>3</sub>



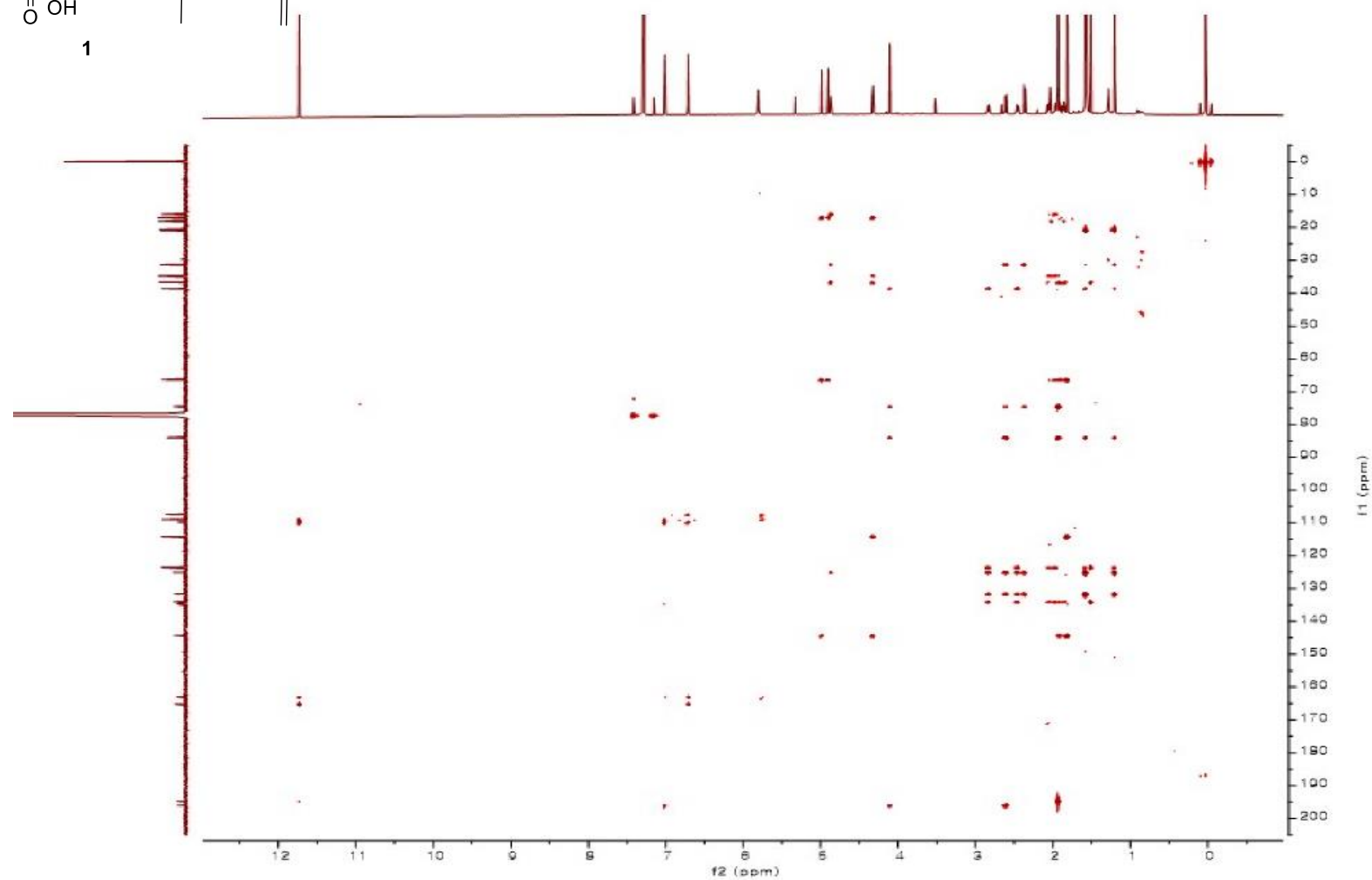
**Figure S4.** HSQC Spectrum of Merochlorin G (**1**) in CDCl<sub>3</sub>

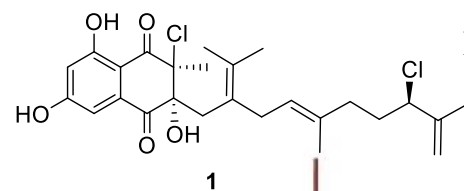




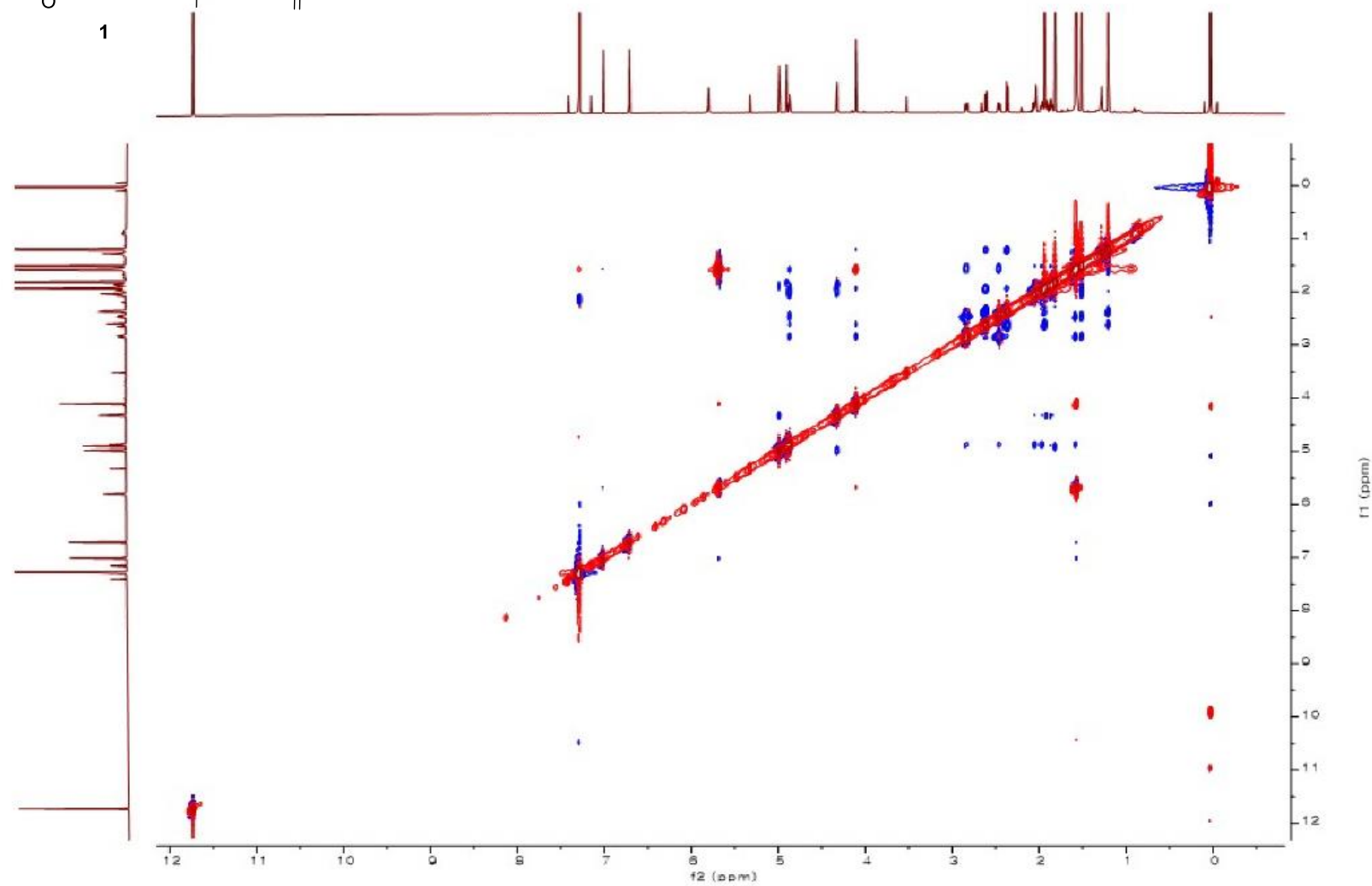


**Figure S5.** HMBC Spectrum of Merochlorin G (**1**) in CDCl<sub>3</sub>

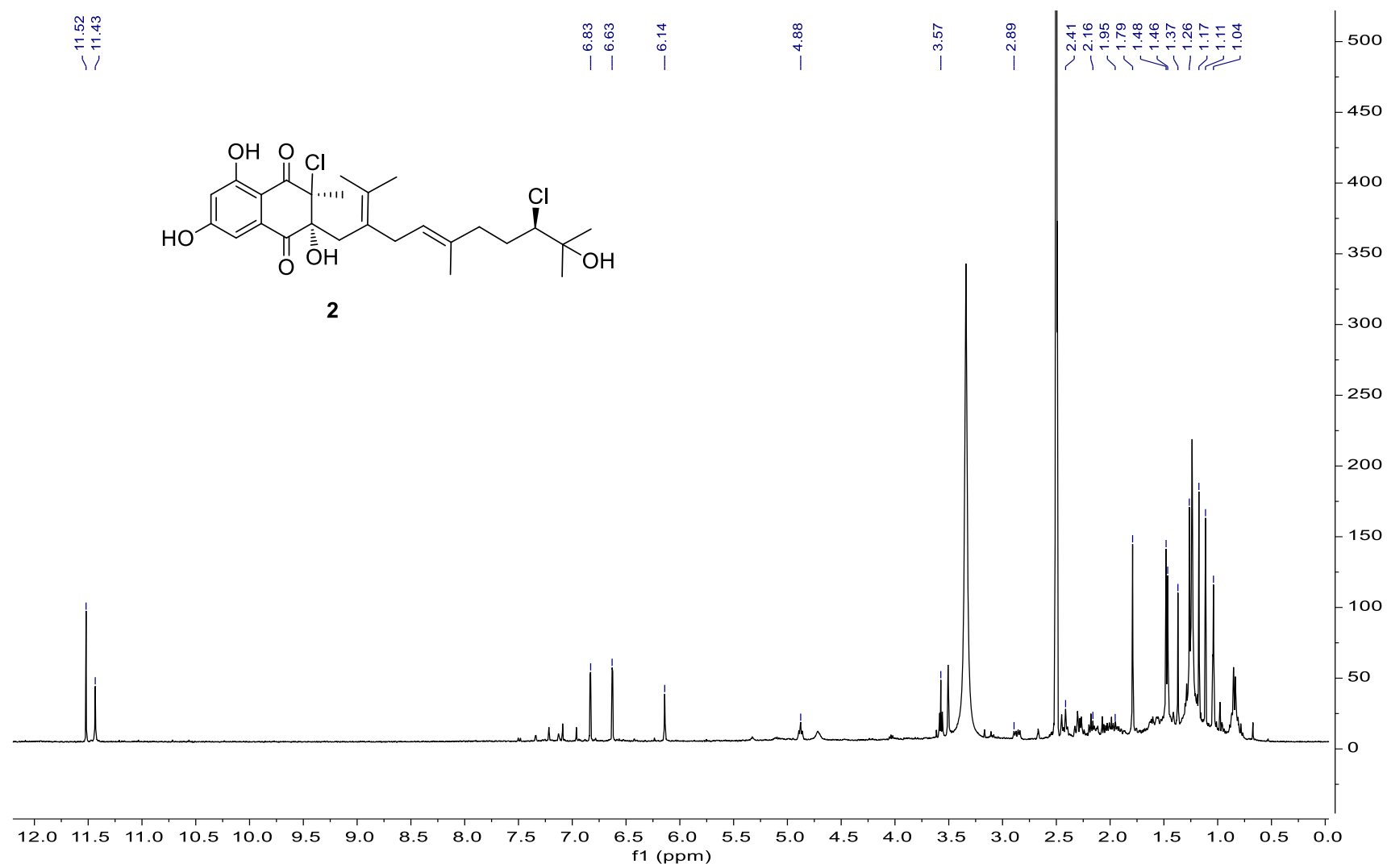




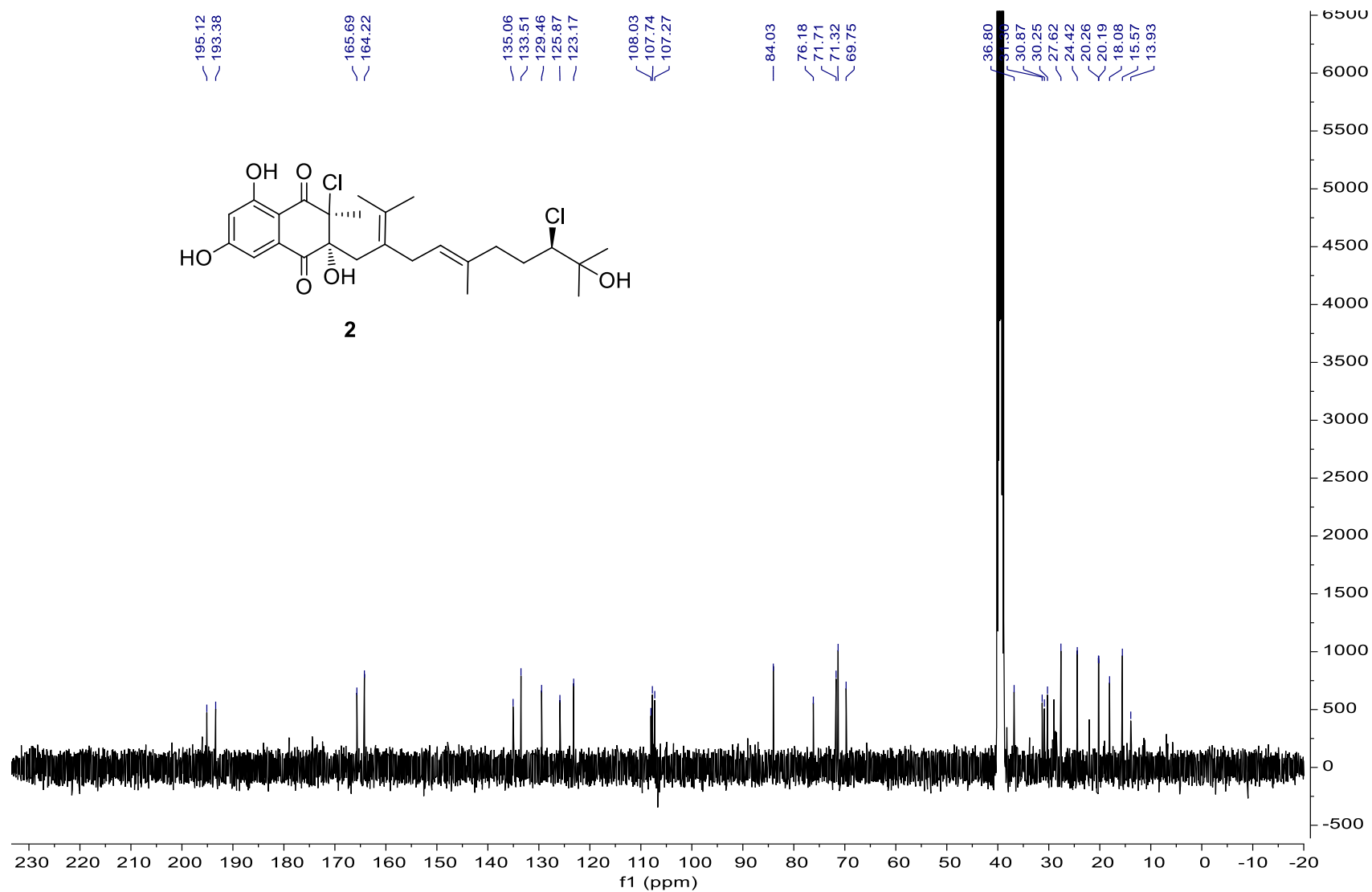
**Figure S6.** NOESY Spectrum of Merochlorin G (**1**) in CDCl<sub>3</sub>



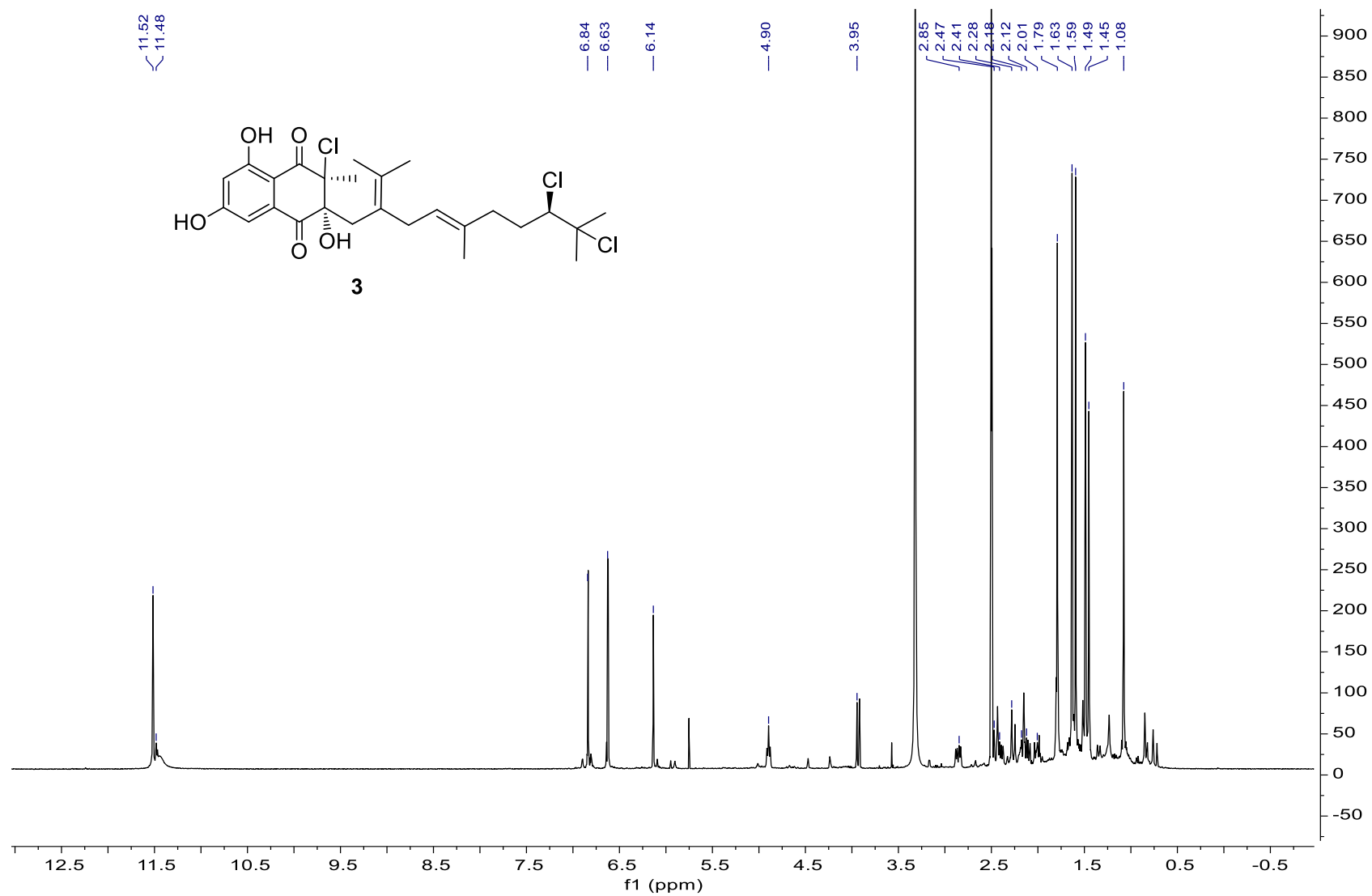
**Figure S7.**  $^1\text{H}$  NMR Spectrum of Merochlorin H (**2**) in  $\text{DMSO-}d_6$



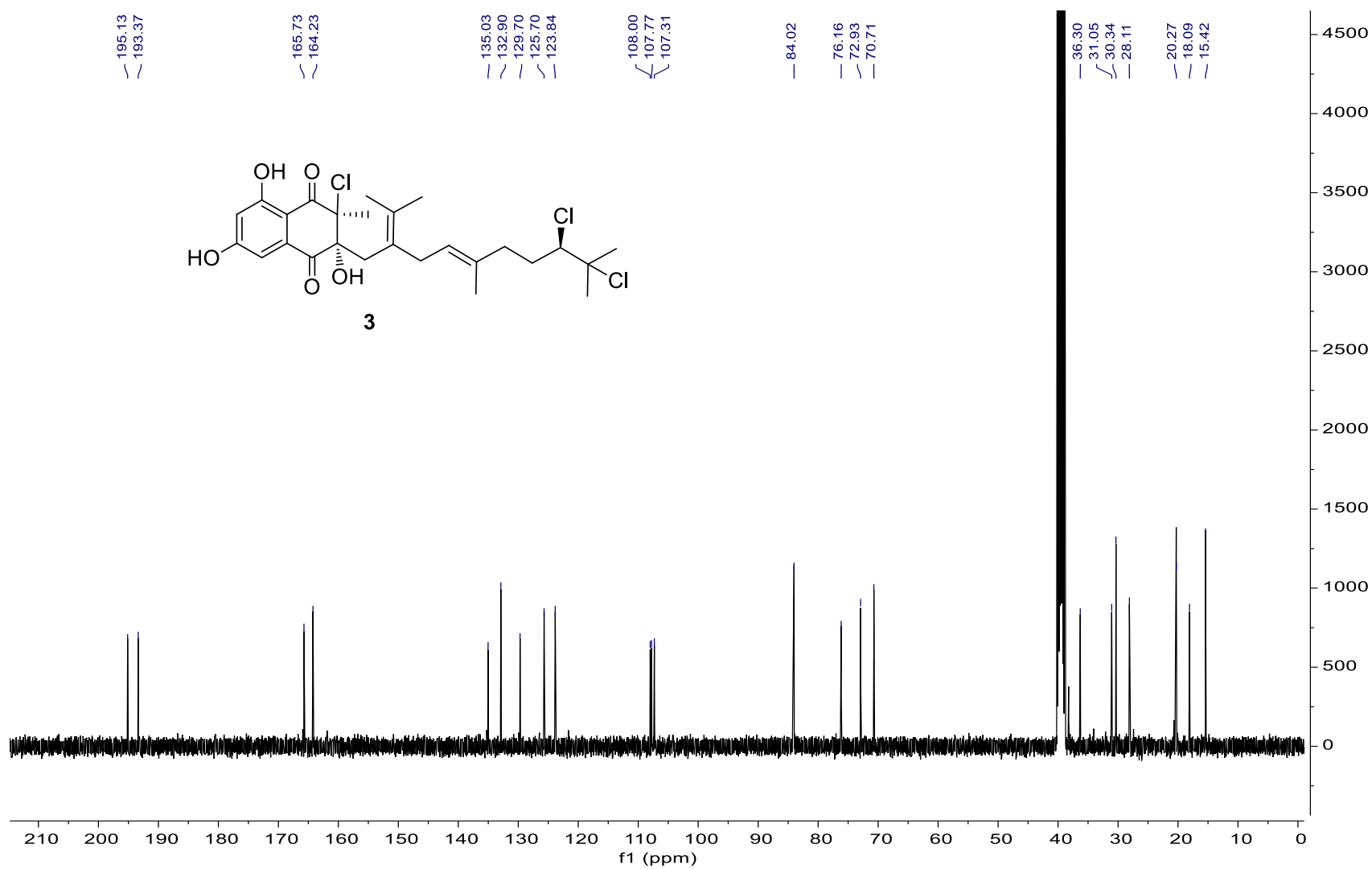
**Figure S8.**  $^{13}\text{C}$  NMR Spectrum of Merochlorin H (**2**) in  $\text{DMSO-}d_6$



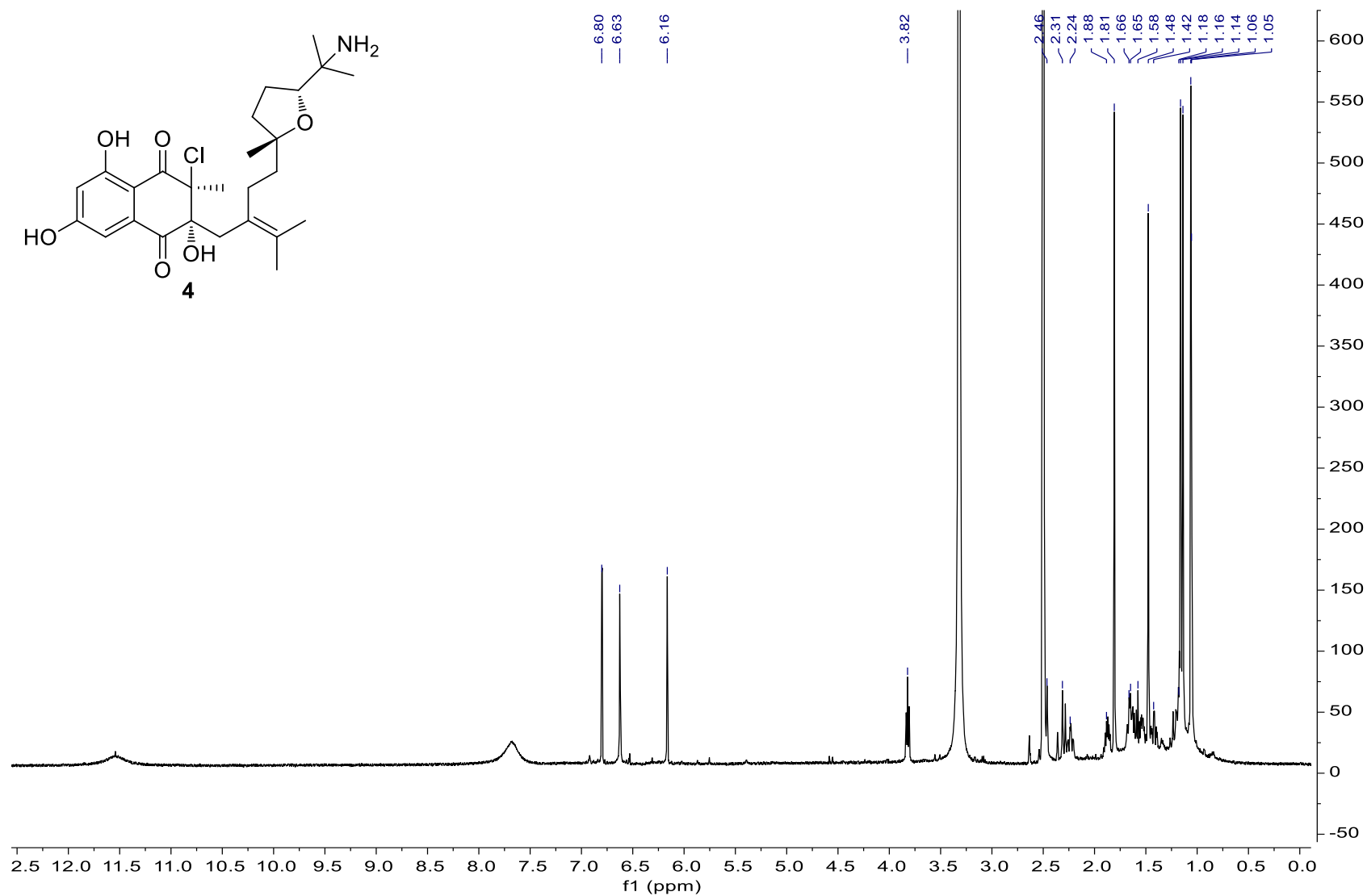
**Figure S9.**  $^1\text{H}$  NMR Spectrum of Merochlorin I (**3**) in  $\text{DMSO-}d_6$



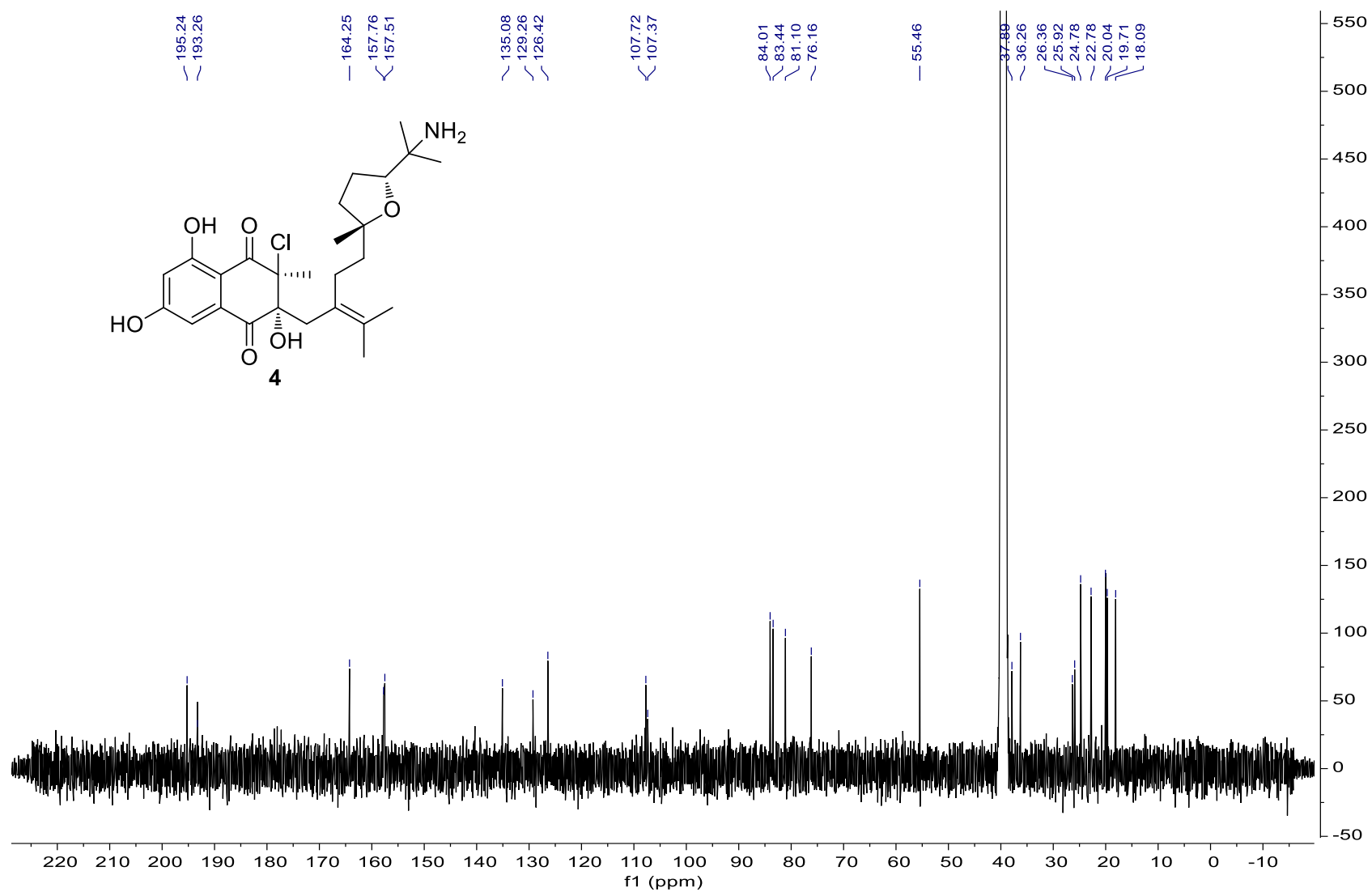
**Figure S10.**  $^{13}\text{C}$  NMR Spectrum of Merochlorin I (**3**) in  $\text{DMSO-}d_6$



**Figure S11.**  $^1\text{H}$  NMR Spectrum of Merochlorin J (**4**) in  $\text{DMSO}-d_6$

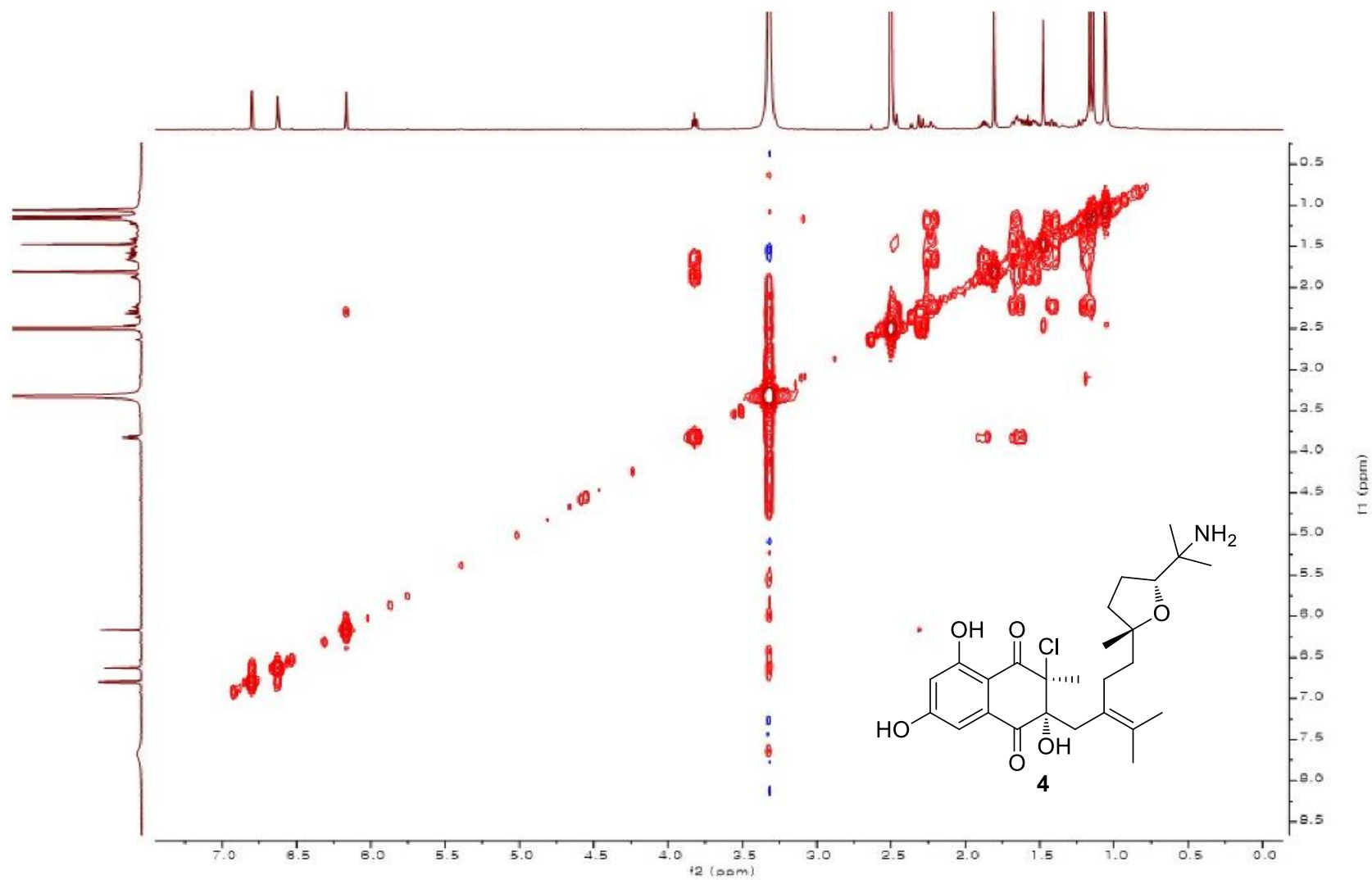


**Figure S12.**  $^{13}\text{C}$  NMR Spectrum of Merochlorin J (**4**) in  $\text{DMSO}-d_6$

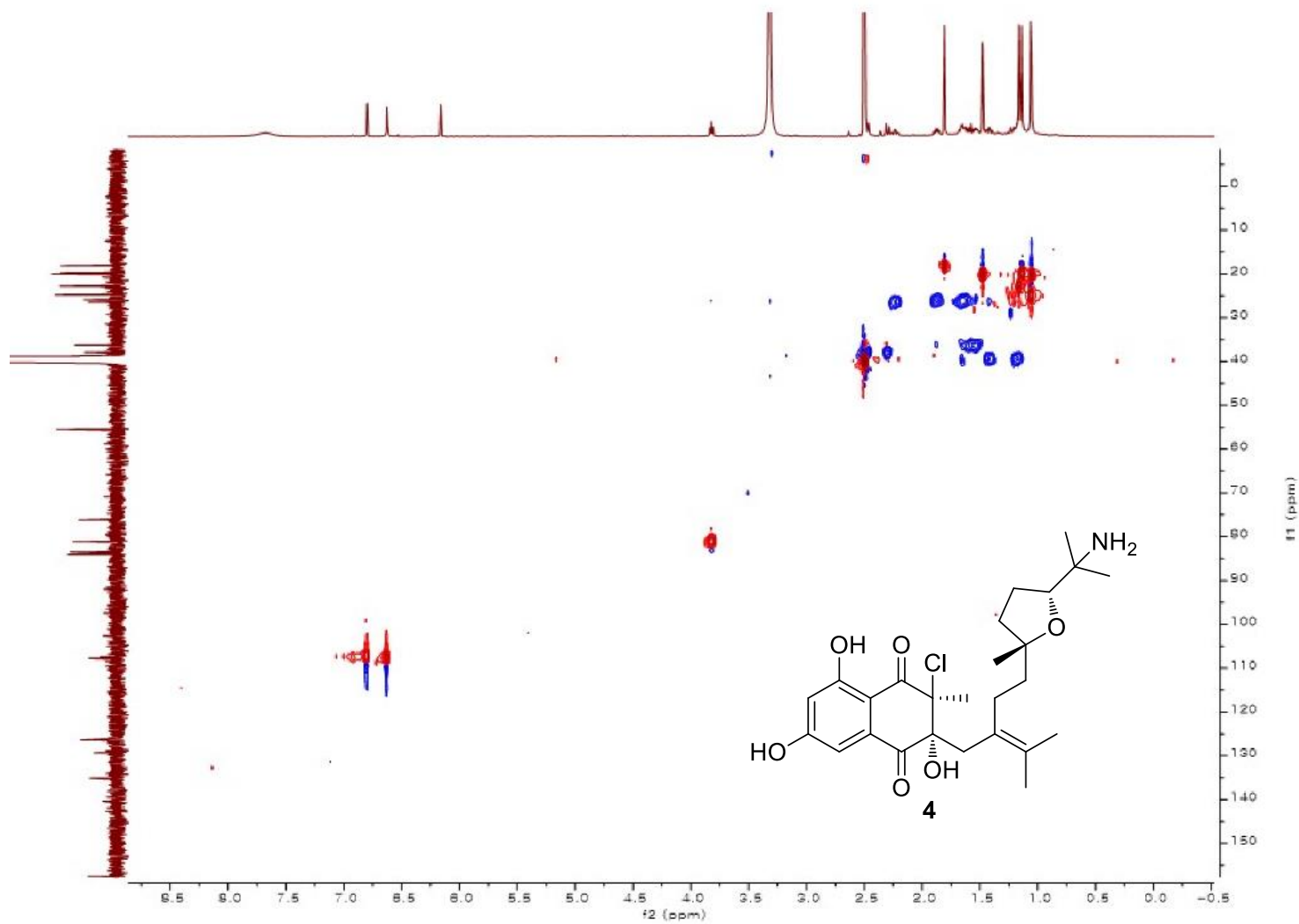




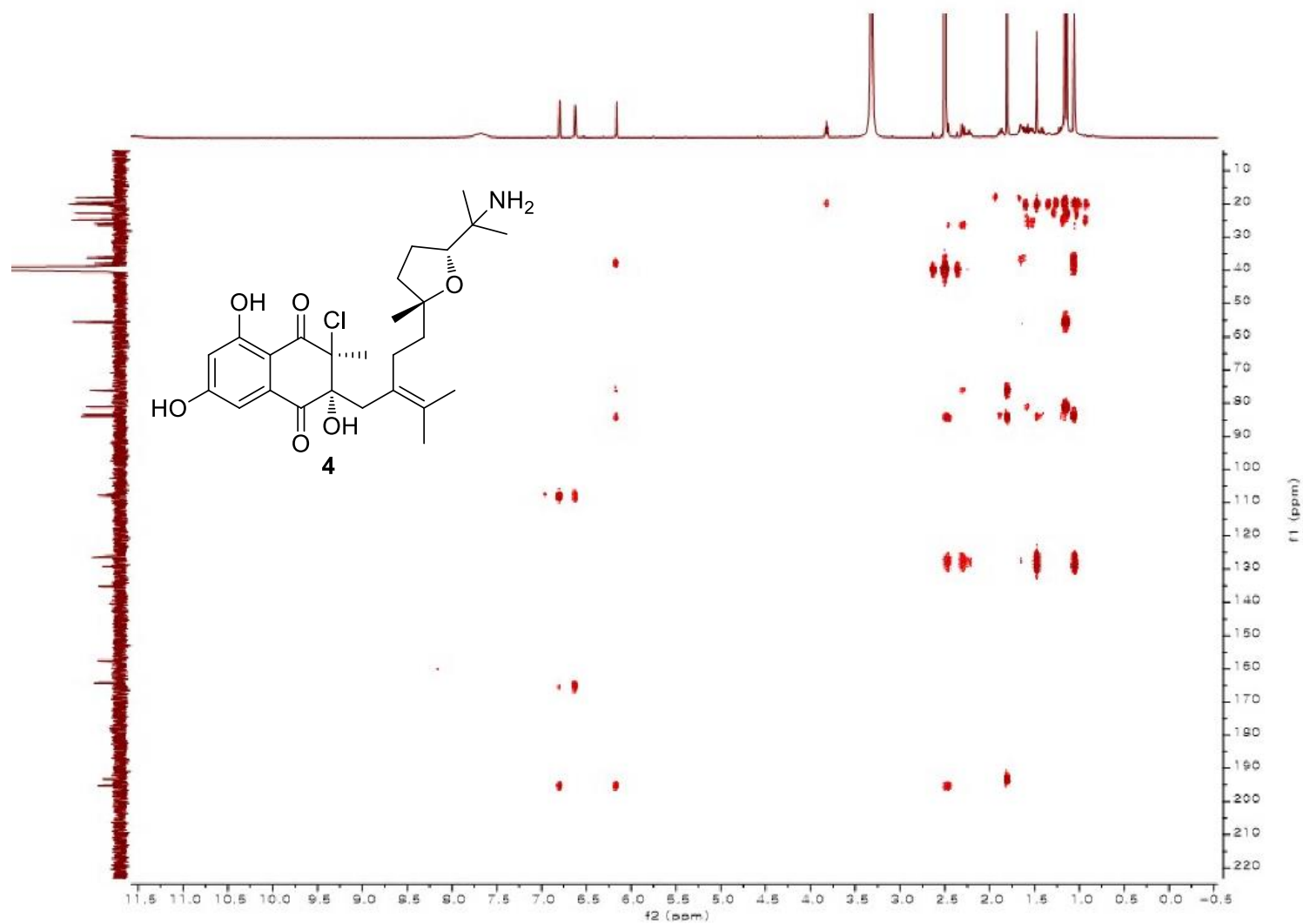
**Figure S13.** COSY Spectrum of Merochlorin J (**4**) in DMSO-*d*<sub>6</sub>



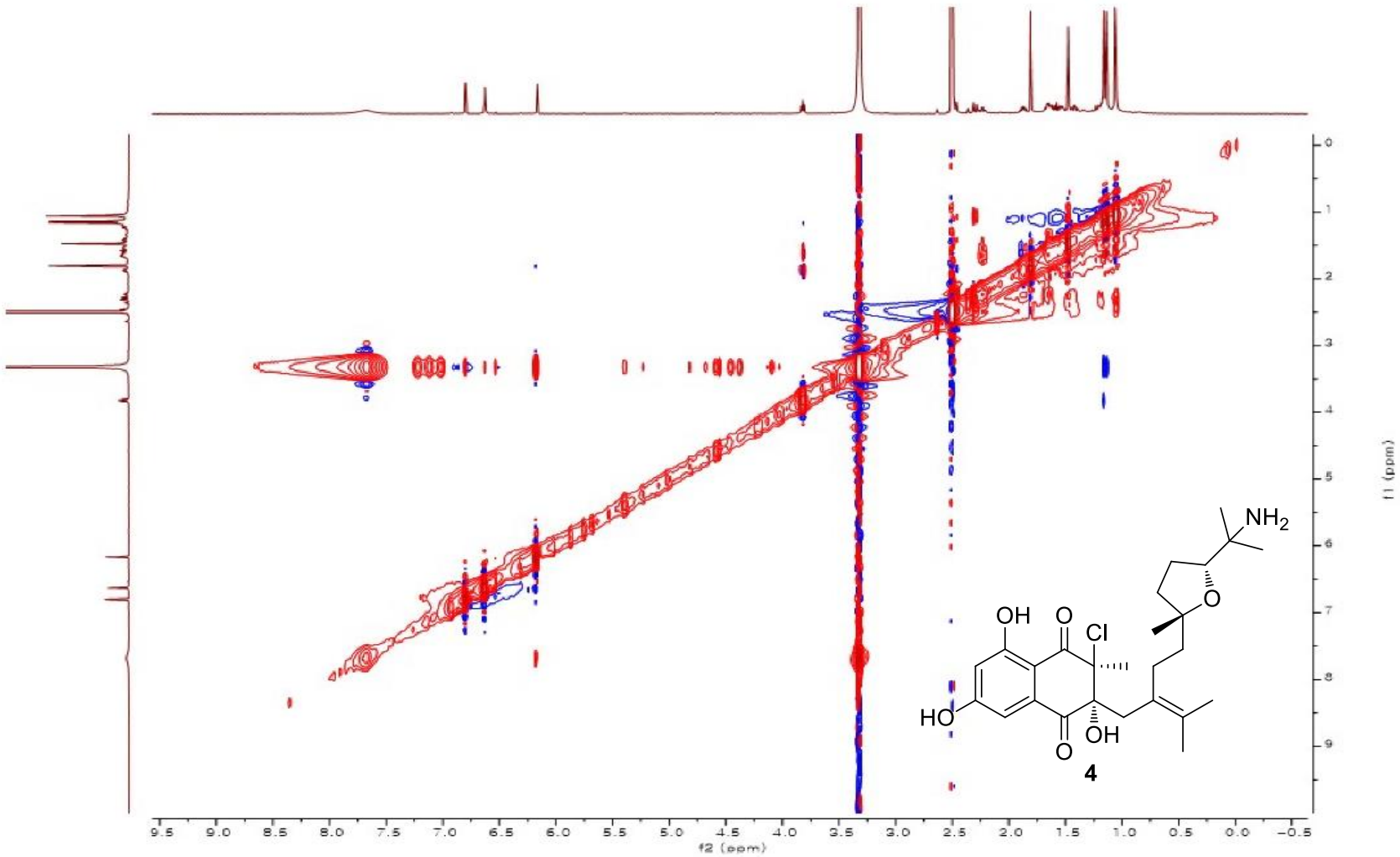
**Figure S14.** HSQC Spectrum of Merochlorin J (**4**) in DMSO-*d*<sub>6</sub>



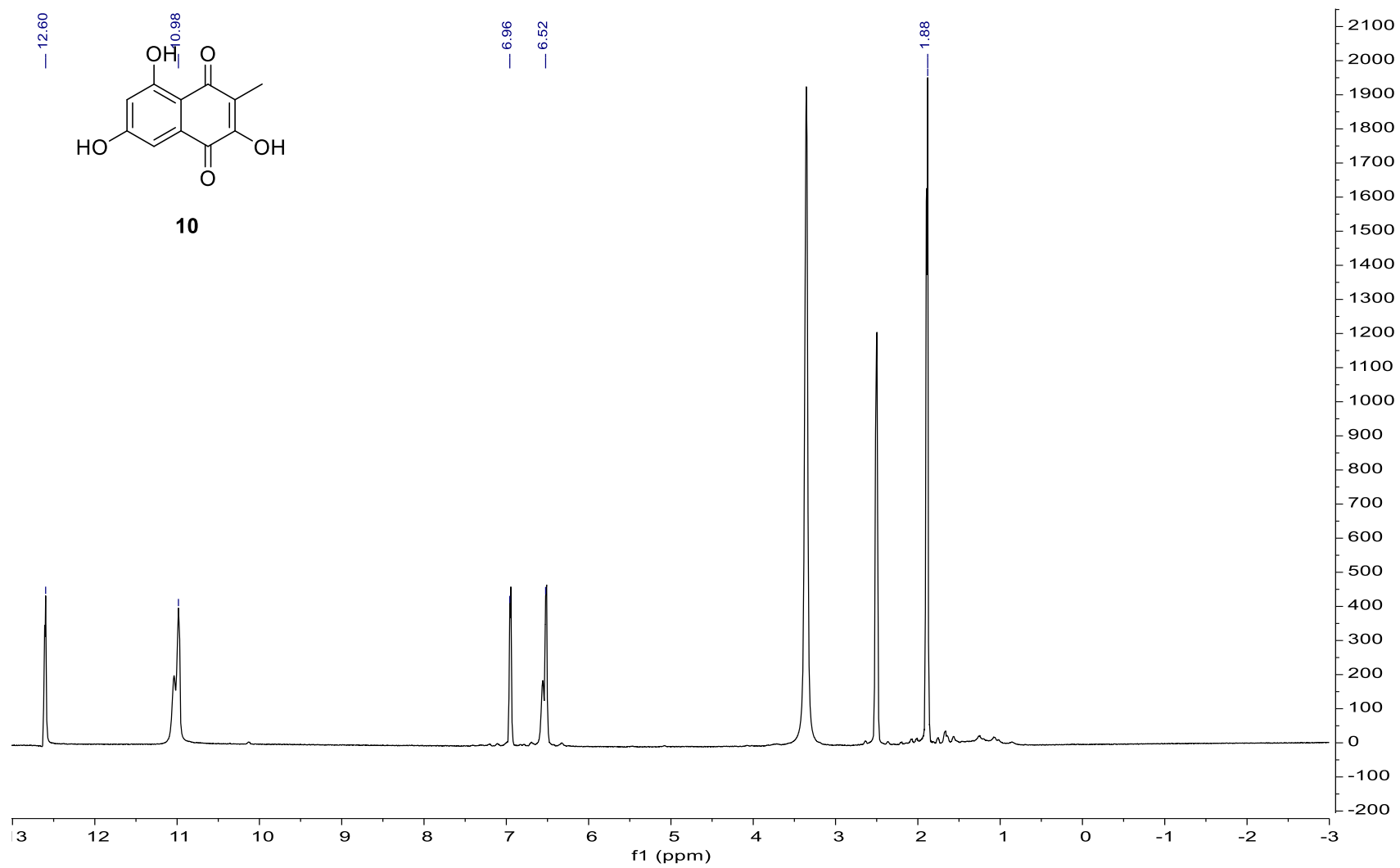
**Figure S15.** HMBC Spectrum of Merochlorin J (**4**) in DMSO-*d*<sub>6</sub>



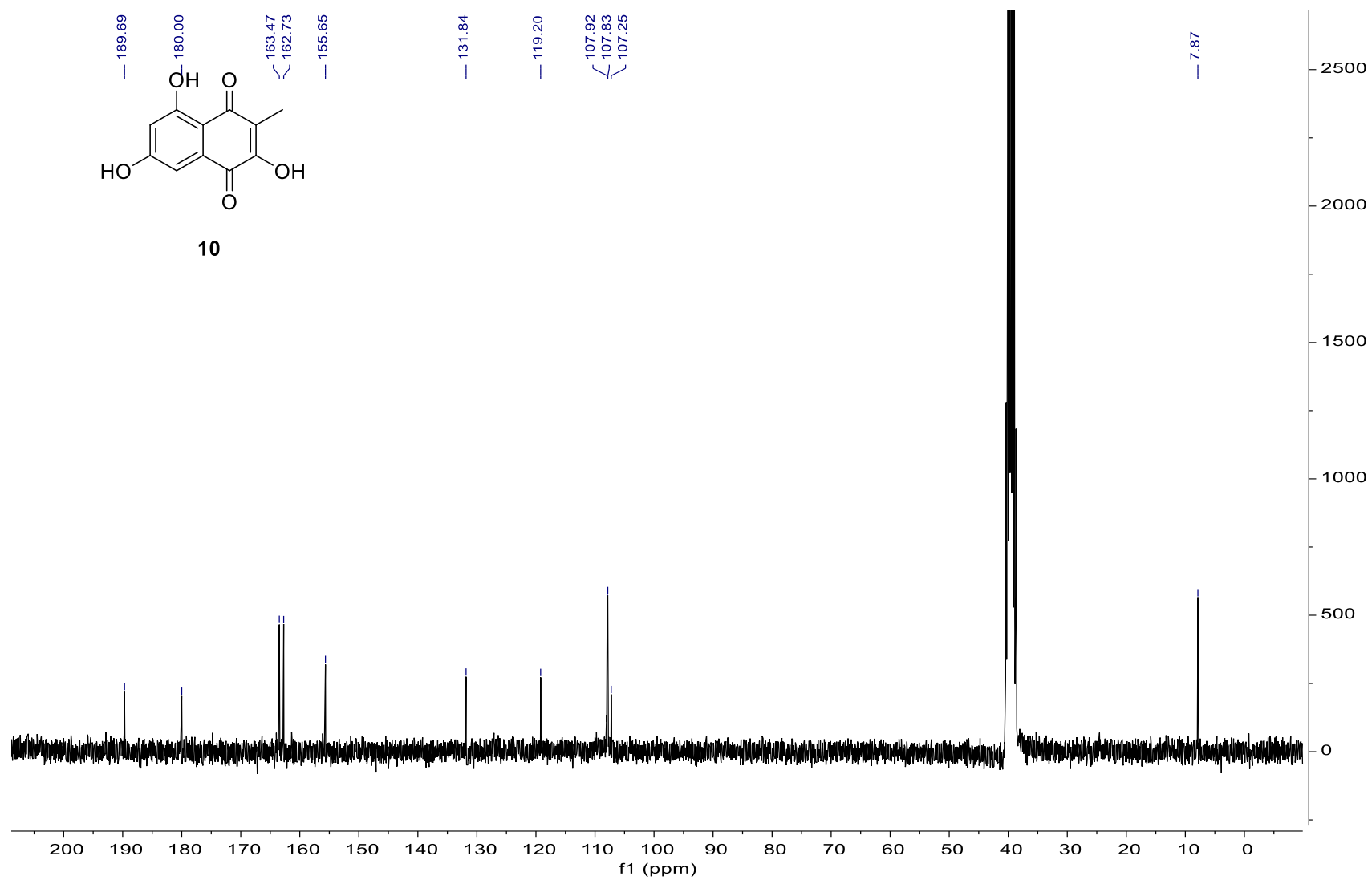
**Figure S16.** NOESY Spectrum of Merochlorin J (**4**) in DMSO-*d*<sub>6</sub>



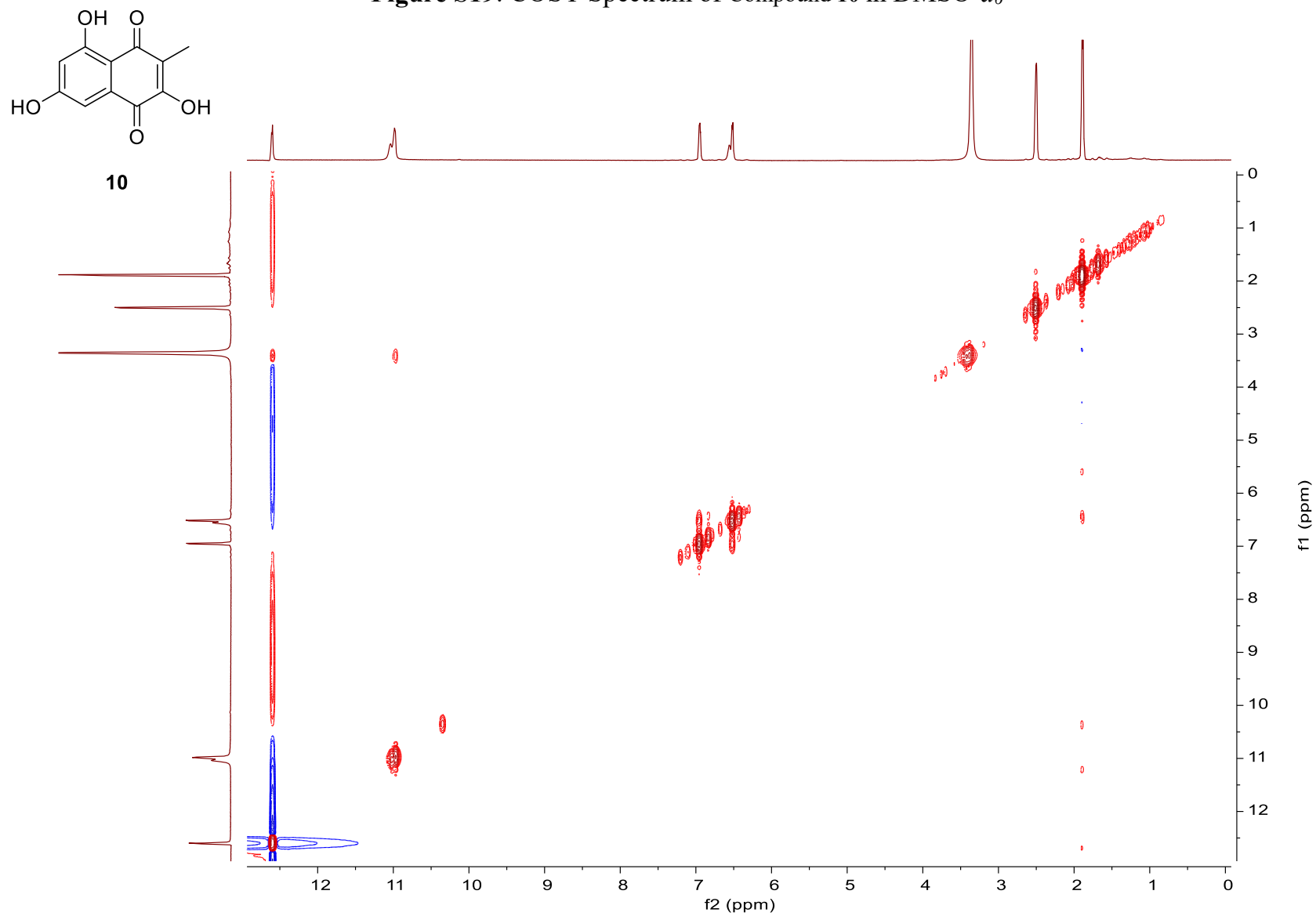
**Figure S17.**  $^1\text{H}$  NMR Spectrum of Compound **10** in  $\text{DMSO}-d_6$

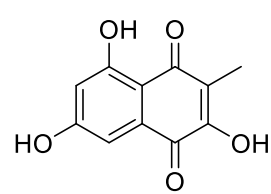


**Figure S18.**  $^{13}\text{C}$  NMR Spectrum of Compound **10** in  $\text{DMSO-}d_6$



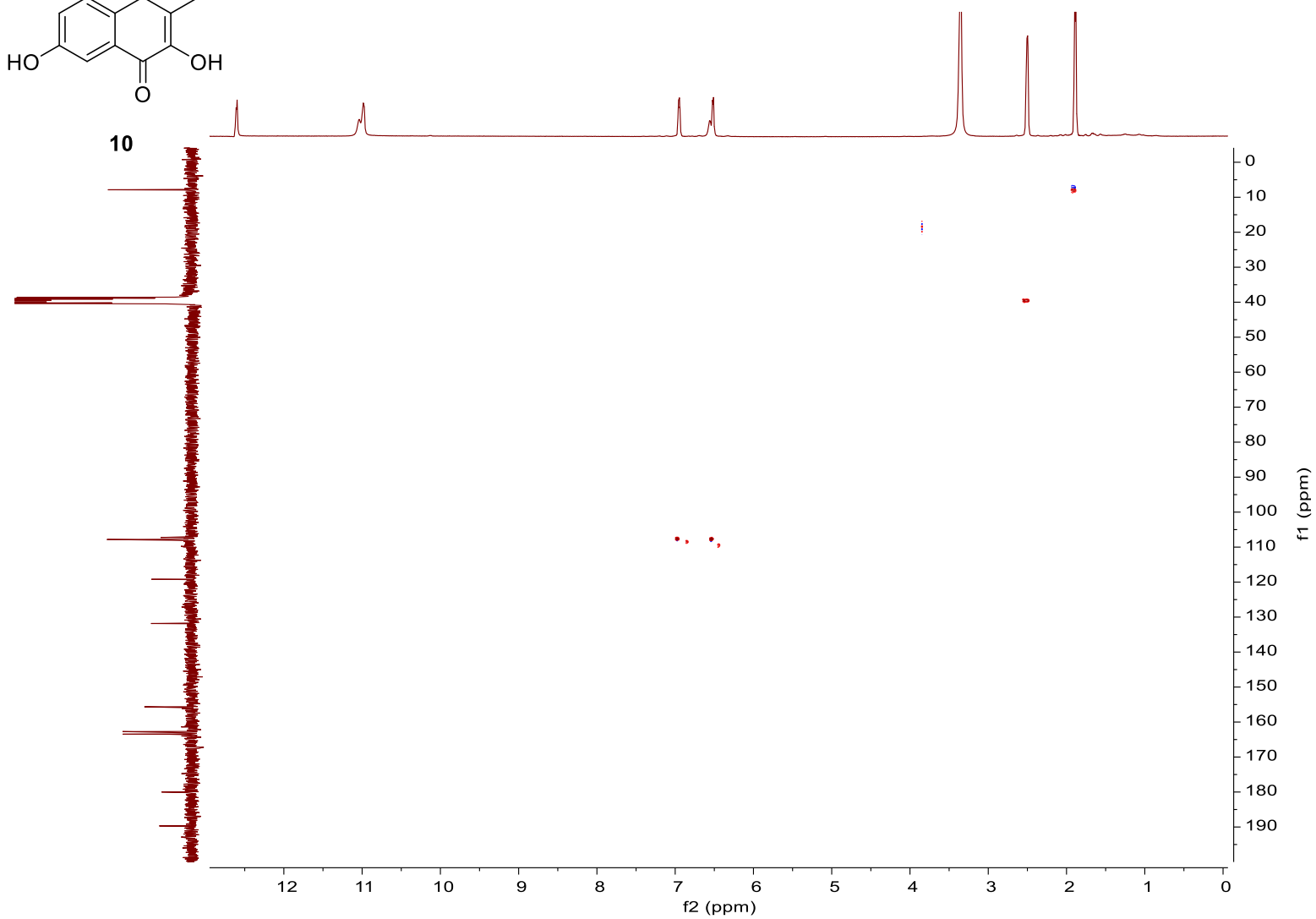
**Figure S19.** COSY Spectrum of Compound **10** in DMSO- $d_6$





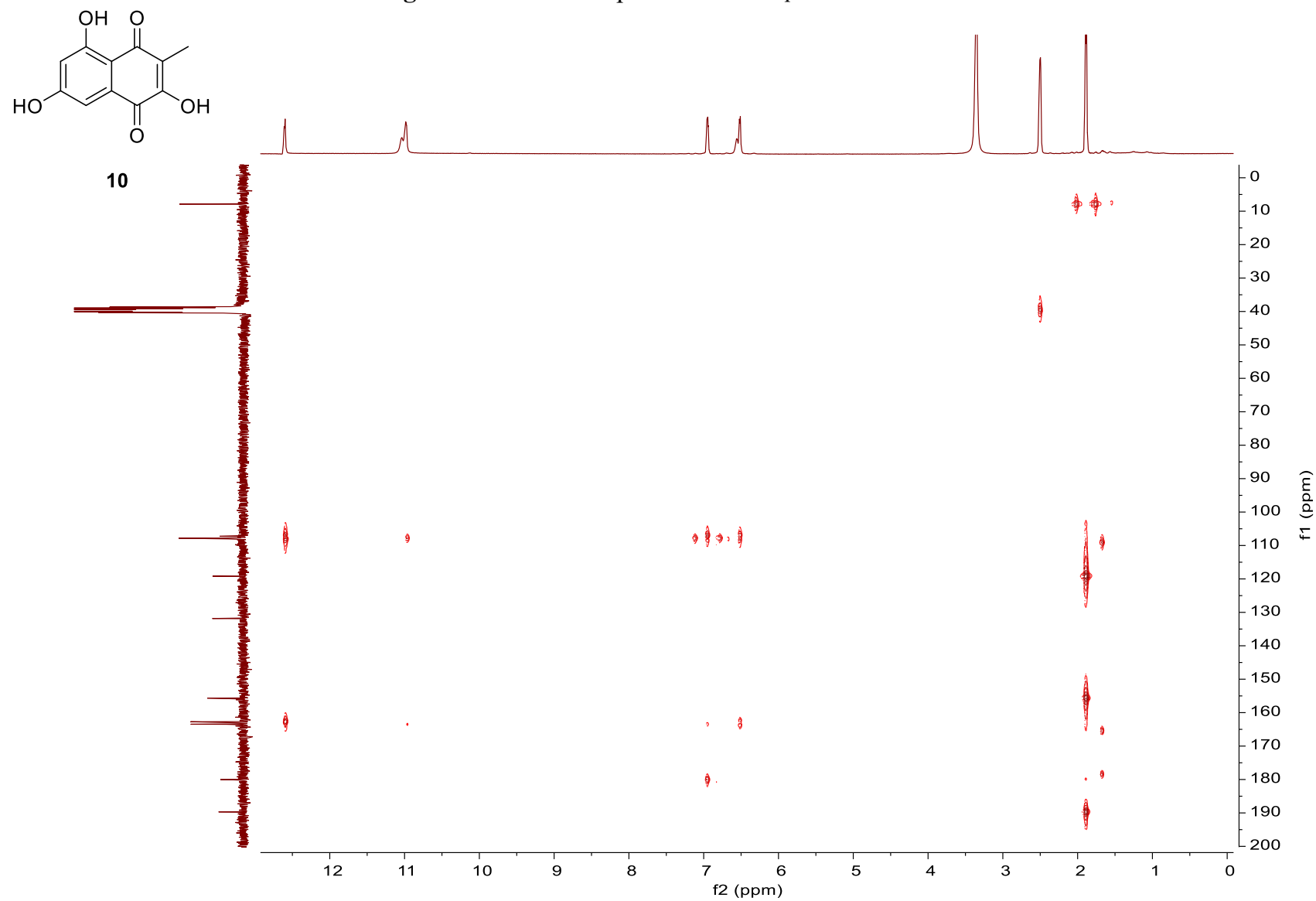
**10**

**Figure S20.** HSQC Spectrum of Compound **10** in DMSO- $d_6$





**Figure S21.** HMBC Spectrum of Compound **10** in DMSO- $d_6$



**Figure S22.** DP4 analysis of NMR calculation of Merochlorin G (1)

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[instructions](#)  
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[step 2](#)  
[step 3](#)  
[step 4](#)  
[applet source code](#)

[Other NMR](#)  
[parameters:](#)  
[CP3](#)

Assignment of stereochemistry and structure using NMR and DP4

Please select version of database to use:  
☐ DP4-original  
☒ DP4-database2

Select probability distribution:  
☒ t distribution (recommended)  
☐ normal distribution

13C Calc:  
C1,C2,C3,C4,C5,C6,C9,C10,C11,C12,C16,C17,C18  
108.16,159.57,108.16,135.65,112.43,163.43,203.6  
107.97,159.78,108.45,135.77,112.4,163.42,203.56

1H Calc:  
H34,H35,H38,H39,H40,H41,H42,H43,H44,H45,H4  
5.73,6.41,2.86,2.71,2.05,2.16,2.48,4.68,1.04,1.09,1  
5.68,6.43,2.74,2.72,1.96,1.91,2.49,4.68,1.17,1.14,1

13C Expt:  
108.9(C1), 162.9(C2), 107.4(C3), 134.7(C4), 109.9

1H Expt:  
6.71(H34), 7.01(H35), 5.8(H38), 2.61(H39), 2.37(H

Results of DP4 using both carbon and proton data:  
Isomer 1: 86.6%  
Isomer 2: 13.4%

Results of DP4 using the carbon data only:  
Isomer 1: 58.3%  
Isomer 2: 41.7%

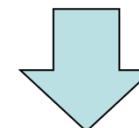
Results of DP4 using the proton data only:  
Isomer 1: 82.2%  
Isomer 2: 17.8%

(c) Jonathan M Goodman and Steven G Smith

[How to use this applet](#)

Assigning Stereochemistry to Single Diastereoisomers by GIAO NMR Calculation: The DP4 Probability  
S. G. Smith and J. M. Goodman *J. Am. Chem. Soc.* 2010, **132**, 12946-12959  
DOI: [10.1021/ja105035r](https://doi.org/10.1021/ja105035r)

	18R	18S
<sup>13</sup> C data	58.3%	41.7%
<sup>1</sup> H data	82.2%	17.8%
Total	86.6%	13.4%



**NMR data match 86.6%**  
**18R configuration**

**Figure S23.** DP4 analysis of NMR calculation of Merochlorin J (4)

Results of DP4 using both carbon and proton data:

Isomer 1: 100.0%

Isomer 2: 0.0%

Isomer 3: 0.0%

Isomer 4: 0.0%

Results of DP4 using the carbon data only:

Isomer 1: 0.8%

Isomer 2: 10.4%

Isomer 3: 87.7%

Isomer 4: 1.1%

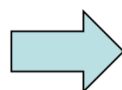
Results of DP4 using the proton data only:

Isomer 1: 100.0%

Isomer 2: 0.0%

Isomer 3: 0.0%

Isomer 4: 0.0%



	<b>15<i>R</i>,18<i>R</i></b>	<b>15<i>R</i>,18<i>S</i></b>	<b>15<i>S</i>,18<i>R</i></b>	<b>15<i>S</i>,18<i>S</i></b>
<sup>13</sup> C data	0.8%	10.4%	87.7%	1.1%
<sup>1</sup> H data	100.0%	0.0%	0.0%	0.0%
Total	100.0%	0.0%	0.0%	0.0%

Results of DP4 using both carbon and proton data:

Isomer 1: 100.0%

Isomer 2: 0.0%

Isomer 3: 0.0%

Isomer 4: 0.0%

Results of DP4 using the carbon data only:

Isomer 1: 2.8%

Isomer 2: 69.5%

Isomer 3: 26.9%

Isomer 4: 0.8%

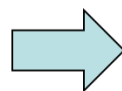
Results of DP4 using the proton data only:

Isomer 1: 100.0%

Isomer 2: 0.0%

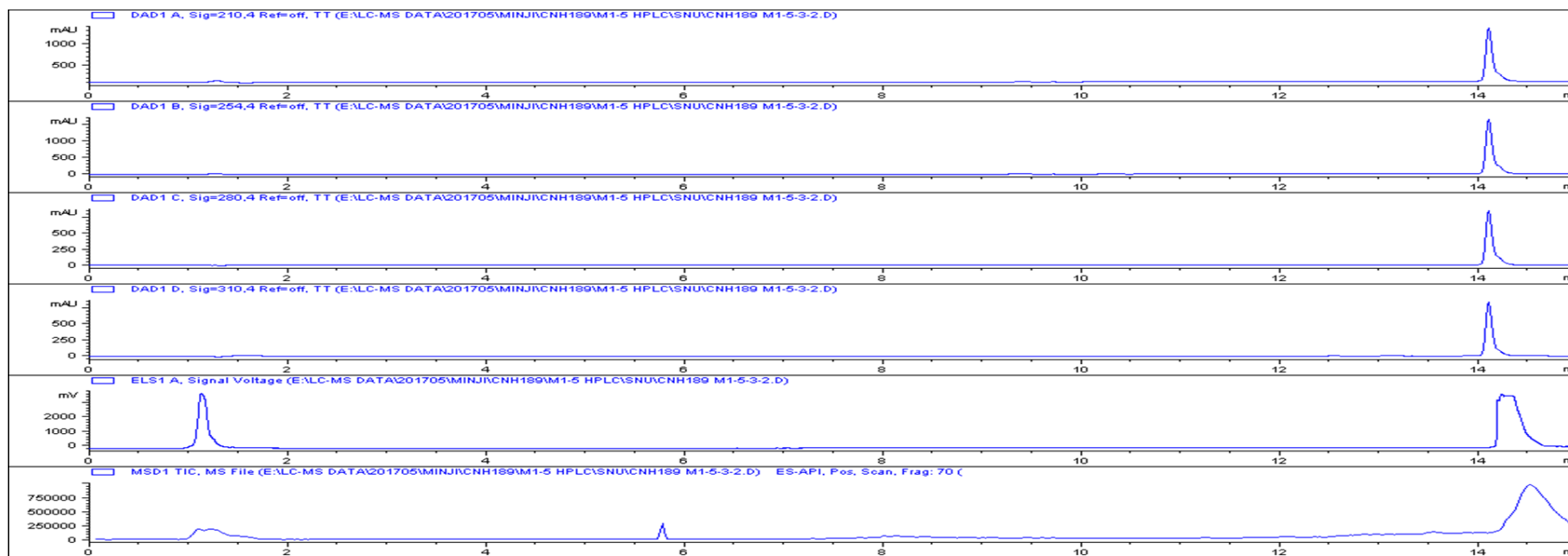
Isomer 3: 0.0%

Isomer 4: 0.0%

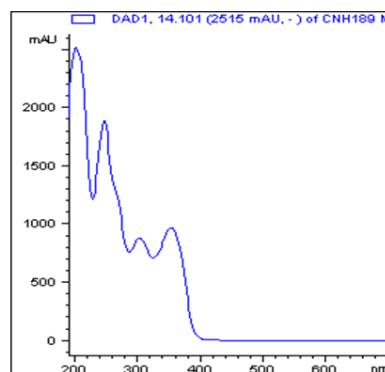


	<b>15<i>R</i>,18<i>R</i></b>	<b>15<i>R</i>,18<i>S</i></b>	<b>15<i>S</i>,18<i>R</i></b>	<b>15<i>S</i>,18<i>S</i></b>
<sup>13</sup> C data	2.8%	69.5%	26.9%	0.8%
<sup>1</sup> H data	100.0%	0.0%	0.0%	0.0%
Total	100.0%	0.0%	0.0%	0.0%

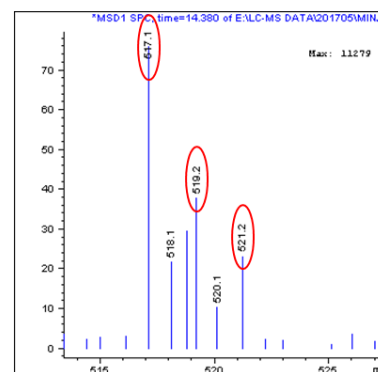
Figure S24. LRMS spectrum of Merochlorins G (1)



UV

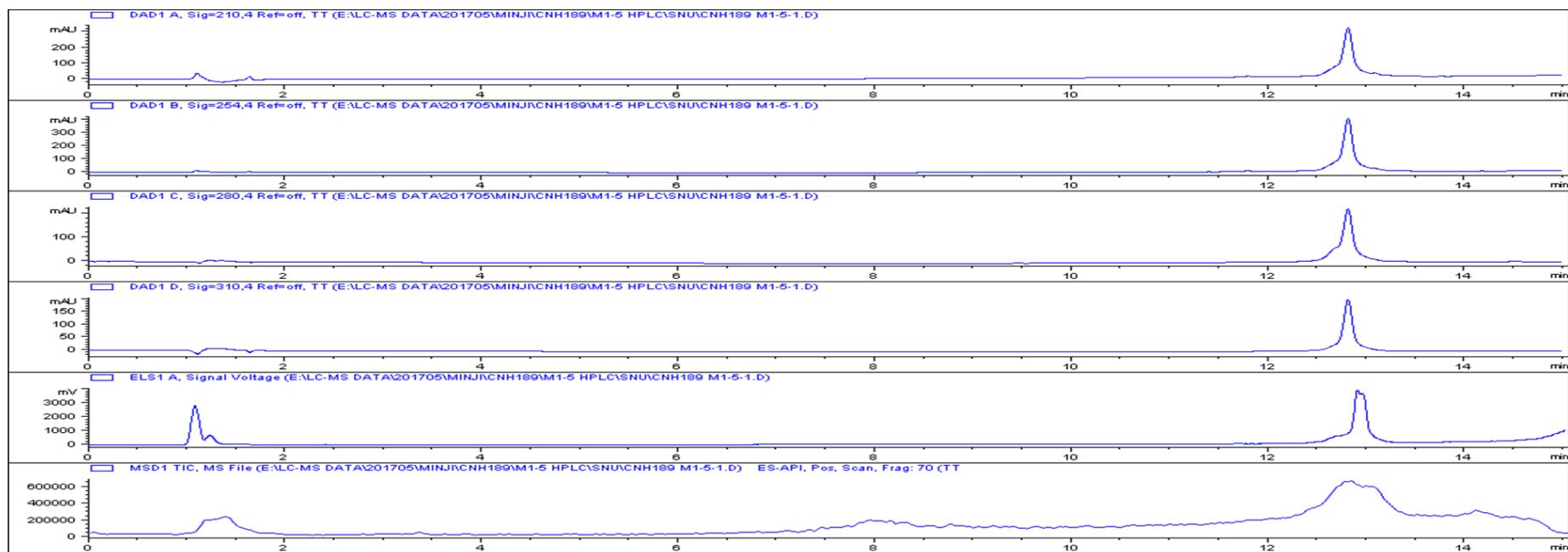


MS

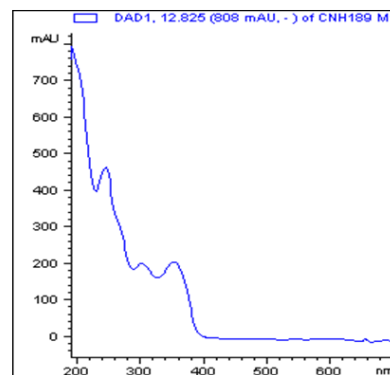


2 Cl ratio = 9:6:1

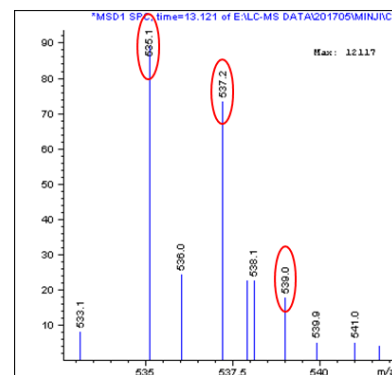
Figure S25. LRMS spectrum of Merochlorins H (2)



UV

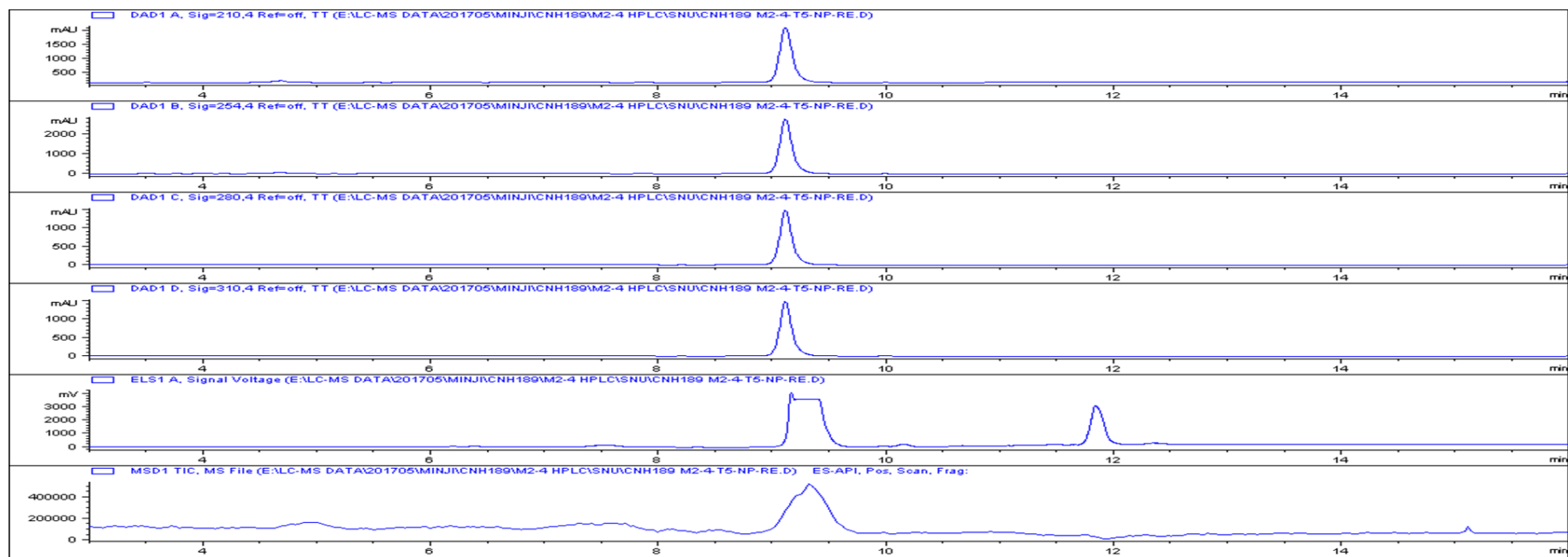


MS

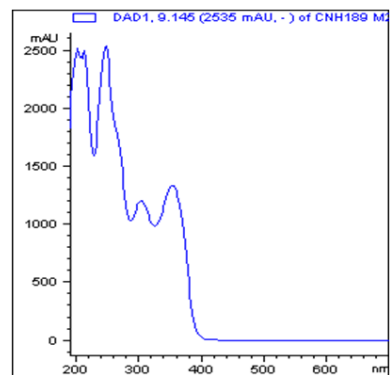


2 Cl ratio = 9:6:1

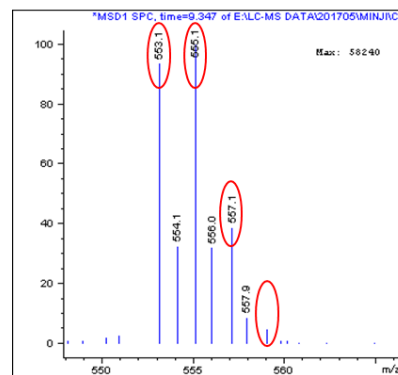
Figure S26. LRMS spectrum of Merochlorins I (3)



UV

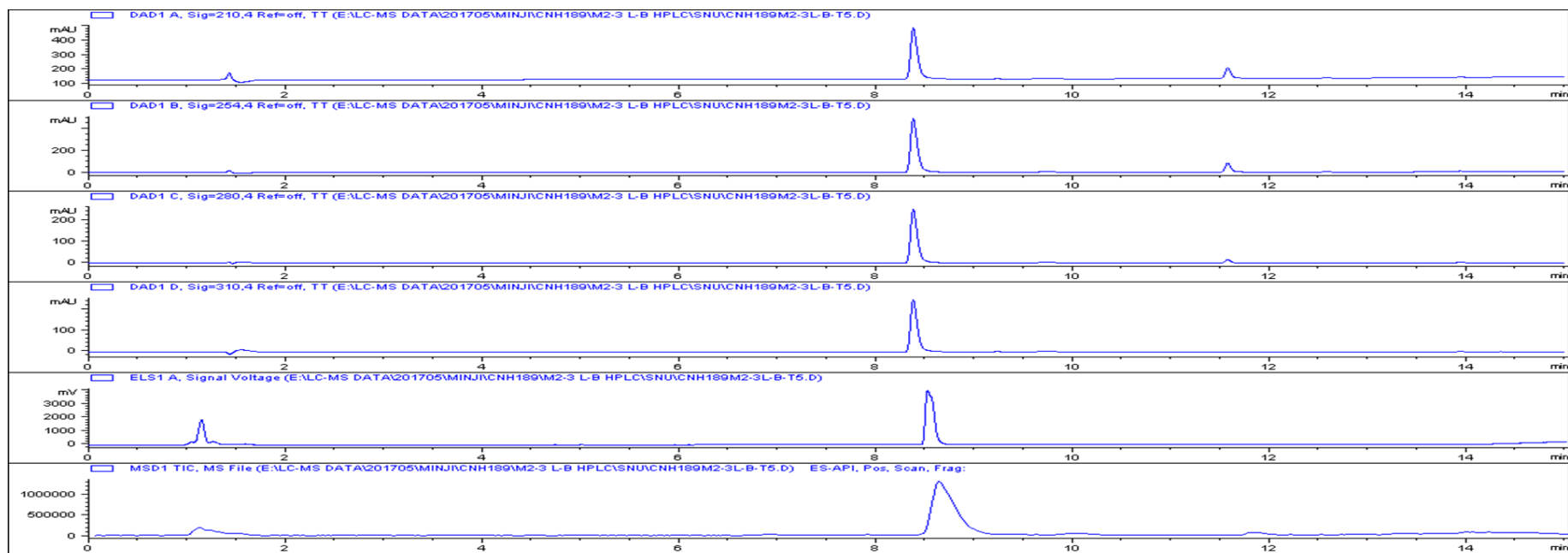


MS

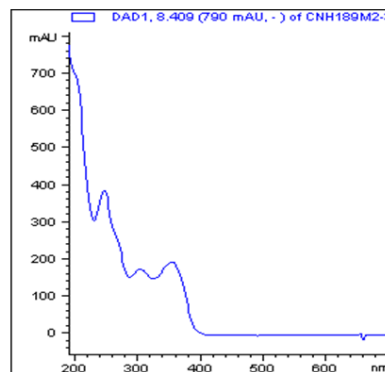


3 Cl ratio = 27:27:9:1

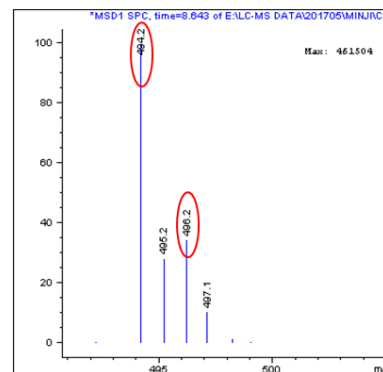
Figure S27. LRMS spectrum of Merochlorins J (4)



UV



MS



1 Cl ratio = 3:1

Figure S28. HRMS spectrum of Merochlorin G (1)

[ Elemental Composition ]				Date : 22-Feb-2018 14:22		Page: 1
Data : FAB-Q485						
Sample: CNH189.494B						
Note : m-NBA						
Inlet : Direct				Ion Mode : FAB+		
RT : 2.70 min				Scan#: (121,130)		
Elements : C 100/0, H 100/0, Cl 3/1(35Cl 3/0, 37Cl 3/0), O 10/0, Na 1/0						
Mass Tolerance : 20ppm, 5mmu if m/z < 250, 10mmu if m/z > 500						
Unsaturation (U.S.) : -0.5 - 30.0						
Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition		
517.1517	2.9	+5.3 / +2.8	21.5	C 35 H 27 35Cl 2		
		-3.8 / -2.0	26.5	C 38 H 24 37Cl		
		+11.1 / +5.8	13.5	C 30 H 32 35Cl 37Cl 2 O		
		+9.6 / +4.9	12.5	C 29 H 32 35Cl 3 O 2		
		+0.4 / +0.2	17.5	C 32 H 29 35Cl 37Cl O 2		
		-10.3 / -5.3	21.5	C 34 H 26 35Cl O 3		
		+6.2 / +3.2	9.5	C 27 H 34 37Cl 3 O 3		
		+4.7 / +2.4	8.5	C 26 H 34 35Cl 2 37Cl O 4		
		-4.5 / -2.3	13.5	C 29 H 31 37Cl 2 O 4		
		-6.0 / -3.1	12.5	C 28 H 31 35Cl 2 O 5		
		-15.2 / -7.8	17.5	C 31 H 28 37Cl O 5		
		+19.2 / +9.9	17.5	C 30 H 26 35Cl O 6		
		-0.2 / -0.1	4.5	C 23 H 36 35Cl 37Cl 2 O 6		
		-1.8 / -0.9	3.5	C 22 H 36 35Cl 3 O 7		
		-10.9 / -5.7	8.5	C 25 H 33 35Cl 37Cl O 7		
		+14.3 / +7.4	13.5	C 27 H 28 37Cl O 8		
		-5.1 / -2.6	0.5	C 20 H 38 37Cl 3 O 8		
		-6.7 / -3.5	-0.5	C 19 H 38 35Cl 2 37Cl O 9		
		-15.8 / -8.2	4.5	C 22 H 35 37Cl 2 O 9		
		-17.4 / -9.0	3.5	C 21 H 35 35Cl 2 O 10		
		+18.6 / +9.6	4.5	C 21 H 33 35Cl 37Cl O 10		
		+10.0 / +5.2	18.5	C 33 H 28 35Cl 2 Na		
		+0.8 / +0.4	23.5	C 36 H 25 37Cl Na		
		-18.6 / -9.6	10.5	C 29 H 35 37Cl 3 Na		
		+15.8 / +8.2	10.5	C 28 H 33 35Cl 37Cl 2 O Na		
		+14.2 / +7.4	9.5	C 27 H 33 35Cl 3 O 2 Na		
		+5.1 / +2.6	14.5	C 30 H 30 35Cl 37Cl O 2 Na		
		-5.6 / -2.9	18.5	C 32 H 27 35Cl O 3 Na		
		+10.9 / +5.6	6.5	C 25 H 35 37Cl 3 O 3 Na		
		+9.3 / +4.8	5.5	C 24 H 35 35Cl 2 37Cl O 4 Na		
		+0.2 / +0.1	10.5	C 27 H 32 37Cl 2 O 4 Na		
		-1.4 / -0.7	9.5	C 26 H 32 35Cl 2 O 5 Na		
		-10.5 / -5.4	14.5	C 29 H 29 37Cl O 5 Na		
		+4.4 / +2.3	1.5	C 21 H 37 35Cl 37Cl 2 O 6 Na		
		+2.9 / +1.5	0.5	C 20 H 37 35Cl 3 O 7 Na		
		-6.3 / -3.2	5.5	C 23 H 34 35Cl 37Cl O 7 Na		
		-17.0 / -8.8	9.5	C 25 H 31 35Cl O 8 Na		
		+19.0 / +9.8	10.5	C 25 H 29 37Cl O 8 Na		
		-11.2 / -5.8	1.5	C 20 H 36 37Cl 2 O 9 Na		
		-12.7 / -6.6	0.5	C 19 H 36 35Cl 2 O 10 Na		



Figure S29. HRMS spectrum of Merochlorin H (2)

[ Elemental Composition ]				Date : 22-Feb-2018 14:08		Page: 1
Data : FAB-Q484						
Sample: CNH189.512						
Note : m-NBA						
Inlet : Direct				Ion Mode : FAB+		
RT : 5.13 min				Scan#: (222,254)		
Elements : C 100/0, H 100/0, Cl 3/1(35Cl 3/0, 37Cl 3/0), O 10/0, Na 1/0						
Mass Tolerance : 20ppm, 5mmu if m/z < 250, 10mmu if m/z > 500						
Unsaturation (U.S.) : -0.5 - 30.0						
Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition		
535.1627	4.1	-18.6 / -10.0	15.5	C 33 H 34 35Cl 3		
		+16.2 / +8.6	16.5	C 33 H 32 35Cl 2 37Cl		
		+7.3 / +3.9	21.5	C 36 H 29 37Cl 2		
		+5.8 / +3.1	20.5	C 35 H 29 35Cl 2 O		
		-3.0 / -1.6	25.5	C 38 H 26 37Cl O		
		+11.4 / +6.1	12.5	C 30 H 34 35Cl 37Cl 2 O 2		
		+9.9 / +5.3	11.5	C 29 H 34 35Cl 3 O 3		
		+1.1 / +0.6	16.5	C 32 H 31 35Cl 37Cl O 3		
		-9.3 / -5.0	20.5	C 34 H 28 35Cl O 4		
		+6.7 / +3.6	8.5	C 27 H 36 37Cl 3 O 4		
		+5.2 / +2.8	7.5	C 26 H 36 35Cl 2 37Cl O 5		
		-3.6 / -1.9	12.5	C 29 H 33 37Cl 2 O 5		
		-5.2 / -2.8	11.5	C 28 H 33 35Cl 2 O 6		
		-14.0 / -7.5	16.5	C 31 H 30 37Cl O 6		
		+0.5 / +0.2	3.5	C 23 H 38 35Cl 37Cl 2 O 7		
		-1.1 / -0.6	2.5	C 22 H 38 35Cl 3 O 8		
		-9.9 / -5.3	7.5	C 25 H 35 35Cl 37Cl O 8		
		+14.5 / +7.8	12.5	C 27 H 30 37Cl O 9		
		-4.3 / -2.3	-0.5	C 20 H 40 37Cl 3 O 9		
		-14.6 / -7.8	3.5	C 22 H 37 37Cl 2 O 10		
		-14.1 / -7.5	12.5	C 31 H 35 35Cl 3 Na		
		+11.8 / +6.3	18.5	C 34 H 30 37Cl 2 Na		
		+10.3 / +5.5	17.5	C 33 H 30 35Cl 2 O Na		
		+1.5 / +0.8	22.5	C 36 H 27 37Cl O Na		
		-17.3 / -9.3	9.5	C 29 H 37 37Cl 3 O Na		
		+15.9 / +8.5	9.5	C 28 H 35 35Cl 37Cl 2 O 2 Na		
		+14.4 / +7.7	8.5	C 27 H 35 35Cl 3 O 3 Na		
		+5.6 / +3.0	13.5	C 30 H 32 35Cl 37Cl O 3 Na		
		-4.8 / -2.5	17.5	C 32 H 29 35Cl O 4 Na		
		+11.2 / +6.0	5.5	C 25 H 37 37Cl 3 O 4 Na		
		+9.7 / +5.2	4.5	C 24 H 37 35Cl 2 37Cl O 5 Na		
		+0.9 / +0.5	9.5	C 27 H 34 37Cl 2 O 5 Na		
		-0.7 / -0.4	8.5	C 26 H 34 35Cl 2 O 6 Na		
		-9.5 / -5.1	13.5	C 29 H 31 37Cl O 6 Na		
		+5.0 / +2.7	0.5	C 21 H 39 35Cl 37Cl 2 O 7 Na		
		+3.4 / +1.8	-0.5	C 20 H 39 35Cl 3 O 8 Na		
		-5.4 / -2.9	4.5	C 23 H 36 35Cl 37Cl O 8 Na		
		-15.7 / -8.4	8.5	C 25 H 33 35Cl O 9 Na		
		-10.1 / -5.4	0.5	C 20 H 38 37Cl 2 O 10 Na		

Figure S30. HRMS spectrum of Merochlorin I (3)

Page: 1

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[ Elemental Composition ]
Data : FAB-Q995
Sample: CNH189 M2-4 T5
Note : m-NBA
Inlet : Direct
RT : 4.16 min
Elements : C 100/0, H 100/0, Cl 4/2(35Cl 4/0, 37Cl 4/0), O 10/0, Na 1/0
Mass Tolerance : 20ppm, 5mmu if m/z < 250, 10mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 50.0
Date : 15-Jun-2018 18:12
Ion Mode : FAB+
Scan#: (181,205)

```

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
553.1281	0.6	+4.3 / +2.4	20.5	C 35 H 28 35Cl 3
		-4.2 / -2.3	25.5	C 38 H 25 35Cl 37Cl
		+11.2 / +6.2	13.5	C 31 H 33 37Cl 4
		+9.8 / +5.4	12.5	C 30 H 33 35Cl 2 37Cl 2 O
		+1.2 / +0.7	17.5	C 33 H 30 37Cl 3 O
		+8.3 / +4.6	11.5	C 29 H 33 35Cl 4 O 2
		-0.2 / -0.1	16.5	C 32 H 30 35Cl 2 37Cl O 2
		-8.8 / -4.9	21.5	C 35 H 27 37Cl 2 O 2
		-10.3 / -5.7	20.5	C 34 H 27 35Cl 2 O 3
		+5.2 / +2.9	8.5	C 27 H 35 35Cl 37Cl 3 O 3
		+3.7 / +2.1	7.5	C 26 H 35 35Cl 3 37Cl O 4
		-4.8 / -2.7	12.5	C 29 H 32 35Cl 37Cl 2 O 4
		-6.3 / -3.5	11.5	C 28 H 32 35Cl 3 O 5
		-14.8 / -8.2	16.5	C 31 H 29 35Cl 37Cl O 5
		+0.6 / +0.3	4.5	C 24 H 37 37Cl 4 O 5
		+17.3 / +9.6	16.5	C 30 H 27 35Cl 2 O 6
		-0.9 / -0.5	3.5	C 23 H 37 35Cl 2 37Cl 2 O 6
		-9.4 / -5.2	8.5	C 26 H 34 37Cl 3 O 6
		-2.3 / -1.3	2.5	C 22 H 37 35Cl 4 O 7
		-10.9 / -6.0	7.5	C 25 H 34 35Cl 2 37Cl O 7
		+12.8 / +7.1	12.5	C 27 H 29 35Cl 37Cl O 8
		-5.4 / -3.0	-0.5	C 20 H 39 35Cl 37Cl 3 O 8
		-15.4 / -8.5	3.5	C 22 H 36 35Cl 37Cl 2 O 9
		-16.9 / -9.4	2.5	C 21 H 36 35Cl 3 O 10
		+16.7 / +9.2	3.5	C 21 H 34 35Cl 2 37Cl O 10
		+8.2 / +4.5	8.5	C 24 H 31 37Cl 2 O 10
		+8.7 / +4.8	17.5	C 33 H 29 35Cl 3 Na
		+0.1 / +0.1	22.5	C 36 H 26 35Cl 37Cl Na
		-18.0 / -10.0	9.5	C 29 H 36 35Cl 37Cl 3 Na
		+15.6 / +8.6	10.5	C 29 H 34 37Cl 4 Na
		+14.1 / +7.8	9.5	C 28 H 34 35Cl 2 37Cl 2 O Na
		+5.6 / +3.1	14.5	C 31 H 31 37Cl 3 O Na
		+12.6 / +7.0	8.5	C 27 H 34 35Cl 4 O 2 Na
		+4.1 / +2.3	13.5	C 30 H 31 35Cl 2 37Cl O 2 Na
		-4.4 / -2.5	18.5	C 33 H 28 37Cl 2 O 2 Na
		-5.9 / -3.3	17.5	C 32 H 28 35Cl 2 O 3 Na
		+9.5 / +5.3	5.5	C 25 H 36 35Cl 37Cl 3 O 3 Na
		+8.1 / +4.5	4.5	C 24 H 36 35Cl 3 37Cl O 4 Na
		-0.5 / -0.3	9.5	C 27 H 33 35Cl 37Cl 2 O 4 Na
		-1.9 / -1.1	8.5	C 26 H 33 35Cl 3 O 5 Na
		-10.5 / -5.8	13.5	C 29 H 30 35Cl 37Cl O 5 Na
		+5.0 / +2.7	1.5	C 22 H 38 37Cl 4 O 5 Na
		+3.5 / +1.9	0.5	C 21 H 38 35Cl 2 37Cl 2 O 6 Na
		-5.0 / -2.8	5.5	C 24 H 35 37Cl 3 O 6 Na
		+2.0 / +1.1	-0.5	C 20 H 38 35Cl 4 O 7 Na
		-6.5 / -3.6	4.5	C 23 H 35 35Cl 2 37Cl O 7 Na
		-15.1 / -8.3	9.5	C 26 H 32 37Cl 2 O 7 Na
		-16.5 / -9.1	8.5	C 25 H 32 35Cl 2 O 8 Na
		+17.1 / +9.5	9.5	C 25 H 30 35Cl 37Cl O 8 Na
		-11.1 / -6.1	0.5	C 20 H 37 35Cl 37Cl 2 O 9 Na
		-12.6 / -6.9	-0.5	C 19 H 37 35Cl 3 O 10 Na
		+12.5 / +6.9	5.5	C 22 H 32 37Cl 2 O 10 Na

Figure S31. HRMS spectrum of Merochlorin J (4)

[ Elemental Composition ]  
 Date : 03-Apr-2018 13:20  
 Sample: CNH189.493-T4  
 Note : m-NBA  
 Inlet : Direct  
 RT : 0.82 min  
 Elements : C 100/0, H 100/0, Cl 2/0(35Cl 2/0, 37Cl 2/0), N 10/0, O 10/0  
 Mass Tolerance : 20ppm, 5mmu if m/z < 250, 10mmu if m/z > 500  
 Unsaturation (U.S.) : 5.0 - 20.0

Ion Mode : FAB+  
 Scan#: (26,51)

Observed m/z	Int%	Err(ppm / mmu)	U.S.	Composition
494.2311	100.0	-2.1 / -1.0	13.0	C 32 H 38 35Cl 37Cl
		-14.3 / -7.1	12.5	C 31 H 38 35Cl 2 N
		+11.2 / +5.5	13.0	C 30 H 36 35Cl 2 N 2
		+1.6 / +0.8	18.0	C 33 H 33 37Cl N 2
		-10.6 / -5.2	17.5	C 32 H 33 35Cl N 3
		+14.9 / +7.4	18.0	C 31 H 31 35Cl N 4
		-1.8 / -0.9	10.0	C 25 H 36 37Cl 2 N 6
		-14.0 / -6.9	9.5	C 24 H 36 35Cl 37Cl N 7
		+11.5 / +5.7	10.0	C 23 H 34 35Cl 37Cl N 8
		-0.7 / -0.3	9.5	C 22 H 34 35Cl 2 N 9
		-10.2 / -5.1	14.5	C 25 H 31 37Cl N 9
		+15.2 / +7.5	15.0	C 24 H 29 37Cl N 10
		-13.3 / -6.6	17.0	C 34 H 35 35Cl O
		+12.2 / +6.0	17.5	C 33 H 33 35Cl N O
		-4.5 / -2.2	9.5	C 27 H 38 37Cl 2 N 3 O
		-16.7 / -8.2	9.0	C 26 H 38 35Cl 37Cl N 4 O
		+8.8 / +4.3	9.5	C 25 H 36 35Cl 37Cl N 5 O
		-3.4 / -1.7	9.0	C 24 H 36 35Cl 2 N 6 O
		-13.0 / -6.4	14.0	C 27 H 33 37Cl N 6 O
		+12.5 / +6.2	14.5	C 26 H 31 37Cl N 7 O
		+0.3 / +0.1	14.0	C 25 H 31 35Cl N 8 O
		+4.0 / +2.0	19.0	C 26 H 26 N 10 O
		-16.4 / -8.1	6.0	C 19 H 36 37Cl 2 N 10 O
		-7.2 / -3.6	9.0	C 29 H 40 37Cl 2 O 2
		-19.4 / -9.6	8.5	C 28 H 40 35Cl 37Cl N O 2
		+18.2 / +9.0	9.5	C 28 H 38 37Cl 2 N O 2
		+6.1 / +3.0	9.0	C 27 H 38 35Cl 37Cl N 2 O 2
		-6.1 / -3.0	8.5	C 26 H 38 35Cl 2 N 3 O 2
		-15.7 / -7.8	13.5	C 29 H 35 37Cl N 3 O 2
		+19.3 / +9.5	9.0	C 25 H 36 35Cl 2 N 4 O 2
		+9.8 / +4.8	14.0	C 28 H 33 37Cl N 4 O 2
		-2.4 / -1.2	13.5	C 27 H 33 35Cl N 5 O 2
		+11.3 / +0.6	18.5	C 28 H 28 N 7 O 2
		-19.1 / -9.4	5.5	C 21 H 38 37Cl 2 N 7 O 2
		+6.4 / +3.2	6.0	C 20 H 36 37Cl 2 N 8 O 2
		-5.8 / -2.9	5.5	C 19 H 36 35Cl 37Cl N 9 O 2
		-18.0 / -8.9	5.0	C 18 H 36 35Cl 2 N 10 O 2
		+19.6 / +9.7	6.0	C 18 H 34 35Cl 37Cl N 10 O 2
		-8.8 / -4.4	8.0	C 28 H 40 35Cl 2 O 3
		-18.4 / -9.1	13.0	C 31 H 37 37Cl O 3
		+16.6 / +8.2	8.5	C 27 H 38 35Cl 2 N O 3
		+7.0 / +3.5	13.5	C 30 H 35 37Cl N O 3
		-5.1 / -2.5	13.0	C 29 H 35 35Cl N 2 O 3
		-1.4 / -0.7	18.0	C 30 H 30 N 4 O 3
		+3.7 / +1.8	5.5	C 22 H 38 37Cl 2 N 5 O 3
		-8.5 / -4.2	5.0	C 21 H 38 35Cl 37Cl N 6 O 3
		+16.9 / +8.4	5.5	C 20 H 36 35Cl 37Cl N 7 O 3
		+4.7 / +2.3	5.0	C 19 H 36 35Cl 2 N 8 O 3
		-4.8 / -2.4	10.0	C 22 H 33 37Cl N 8 O 3
		-17.0 / -8.4	9.5	C 21 H 33 35Cl N 9 O 3
		+8.4 / +4.2	10.0	C 20 H 31 35Cl N 10 O 3
		+17.6 / +8.7	13.0	C 30 H 35 35Cl O 4
		-4.2 / -2.1	17.5	C 32 H 32 N O 4
		+0.9 / +0.5	5.0	C 24 H 40 37Cl 2 N 2 O 4
		+14.2 / +7.0	5.0	C 22 H 38 35Cl 37Cl N 4 O 4

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[ Elemental Composition ]

-7.5 / -3.7	9.5	C 24 H 35 37Cl N 5 O 4
-19.7 / -9.8	9.0	C 23 H 35 35Cl N 6 O 4
+17.9 / +8.8	10.0	C 23 H 33 37Cl N 6 O 4
+5.7 / +2.8	9.5	C 22 H 33 35Cl N 7 O 4
-16.0 / -7.9	14.0	C 24 H 30 N 8 O 4
+9.4 / +4.7	14.5	C 23 H 28 N 9 O 4
-10.3 / -5.1	9.0	C 26 H 37 37Cl N 2 O 5
+15.2 / +7.5	9.5	C 25 H 35 37Cl N 3 O 5
+3.0 / +1.5	9.0	C 24 H 35 35Cl N 4 O 5
-18.7 / -9.3	13.5	C 26 H 32 N 5 O 5
+6.7 / +3.3	14.0	C 25 H 30 N 6 O 5
+3.3 / +1.6	6.0	C 17 H 33 37Cl N 10 O 5
+12.5 / +6.2	9.0	C 27 H 37 37Cl O 6
+0.3 / +0.1	8.5	C 26 H 37 35Cl N O 6
+4.0 / +2.0	13.5	C 27 H 32 N 3 O 6
+0.6 / +0.3	5.5	C 19 H 35 37Cl N 7 O 6
-11.6 / -5.7	5.0	C 18 H 35 35Cl N 8 O 6
+13.9 / +6.8	5.5	C 17 H 33 35Cl N 9 O 6
-7.9 / -3.9	10.0	C 19 H 30 N 10 O 6
+1.3 / +0.6	13.0	C 29 H 34 O 7
-2.1 / -1.0	5.0	C 21 H 37 37Cl N 4 O 7
+11.1 / +5.5	5.0	C 19 H 35 35Cl N 6 O 7
-10.6 / -5.2	9.5	C 21 H 32 N 7 O 7
+14.8 / +7.3	10.0	C 20 H 30 N 8 O 7
-13.3 / -6.6	9.0	C 23 H 34 N 4 O 8
+12.1 / +6.0	9.5	C 22 H 32 N 5 O 8
-16.0 / -7.9	8.5	C 25 H 36 N O 9
+9.4 / +4.6	9.0	C 24 H 34 N 2 O 9
-2.5 / -1.2	5.5	C 16 H 32 N 9 O 9
-5.2 / -2.6	5.0	C 18 H 34 N 6 O 10

Page: 2

Figure S32. HRMS spectrum of Compound 10

[ Mass Spectrum ]

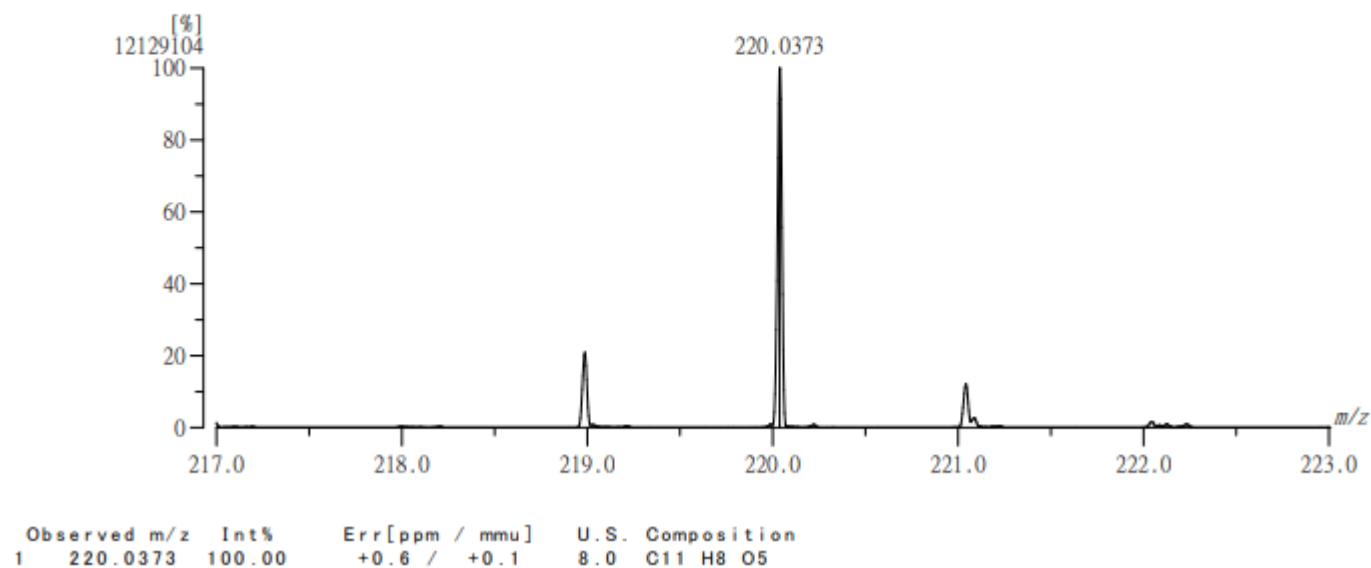
Date : EI-A768 Date : 25-May-2021 14:53

RT : 1.03 min Scan# : (51,60)

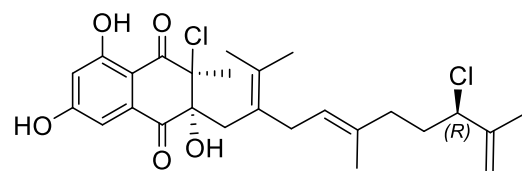
Elements : C 100/0, H 100/0, O 10/0

Mass Tolerance : 10ppm, 5mmu if  $m/z < 500$ , 10mmu if  $m/z > 1000$

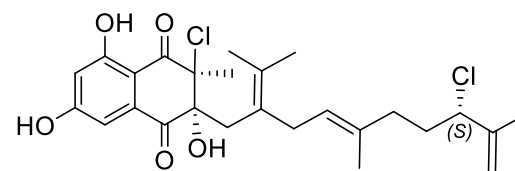
Unsaturation (U.S.) : -0.5 - 20.0



**Figure S33.** Simulated conformer models of two possible diastereomers of **1** (18*R*, 18*S*)

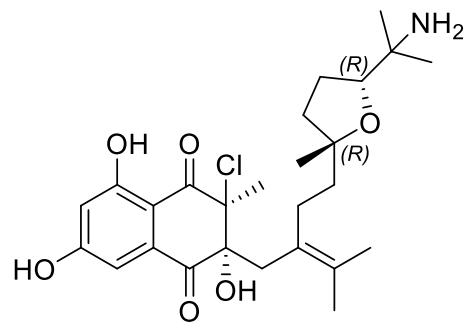


Diastereomer 1 (18*R*)

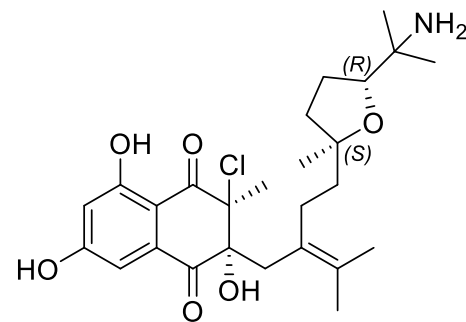


Diastereomer 2 (18*S*)

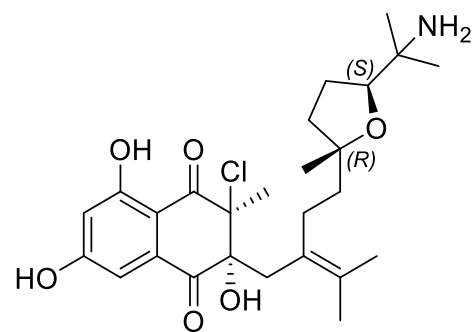
**Figure S34.** Simulated conformer models of four possible diastereomers of **4** (15*R*/18*R*, 15*R*/18*S*, 15*S*/18*R*, and 15*S*/18*S*)



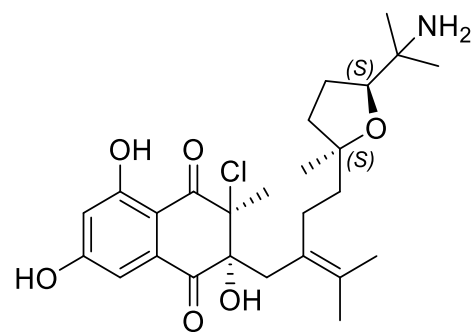
Diastereomer 1 (15*R*/18*R*)



Diastereomer 2 (15*R*/18*S*)



Diastereomer 3 (15*S*/18*R*)



Diastereomer 4 (15*S*/18*S*)

**Table S1.** Experimental (Exp.) and calculated (Cal.) chemical shift values (CS,  $\delta$ ) of merochlorin G (**1**)

Number	Atom	calculated 18 <i>R</i>	calculated 18 <i>S</i>	experimental
1	c	108.16	107.97	108.9
2	c	159.57	159.78	162.9
3	c	108.16	108.45	107.4
4	c	135.65	135.77	134.7
5	c	112.43	112.4	109.9
6	c	163.43	163.42	165.3
9	c	203.67	203.5	195.1
10	c	89.71	89.48	84
11	c	86.76	86.36	74.5
12	c	200.54	201.1	194.7
16	c	47.96	47.54	38.6
17	c	132.19	132.08	131.6
18	c	38.26	38.4	31.3
19	c	130.26	130.52	123.5
20	c	137.59	138.27	134
22	c	137.66	138.47	125.1
23	c	25.3	25.26	20.6
24	c	25.52	25.6	20.9
25	c	42.54	43.81	36.6
26	c	20.92	20.27	18.1
27	c	38.71	39.35	34.8
28	c	65.66	66.75	66.4
29	c	148.71	149.75	144.3

30	c	26.11	25.65	17
32	c	116.44	116.23	114.2
33	c	31.86	31.99	15.9

**Table S2.** Experimental (Exp.) and calculated (Cal.) chemical shift values (CS,  $\delta$ ) of merochlorin J (**4**)

Number	Atom	15 <i>R</i> /18 <i>R</i>	15 <i>R</i> /18 <i>S</i>	15 <i>S</i> /18 <i>R</i>	15 <i>S</i> /18 <i>S</i>	experimental
1	c	112.9	113.67	111.18	113.16	107.7
2	c	165.02	163.53	165.74	165.26	164.1
3	c	110.42	113.85	108.91	109.53	107.2
4	c	135.27	135.75	135.7	135.54	134.9
5	c	110.41	111.33	109.25	110.05	107.8
6	c	166.57	163.95	166.75	166.66	165.2
7	c	203.08	203.22	203.88	202.65	195.3
8	c	88.89	89.23	88.6	89.18	84
9	c	91.95	87.46	92.44	91.74	76.1
10	c	197.14	199.27	197.43	197.46	193.6
15	c	35.16	33.01	33.85	34.79	18.1
17	c	48.89	48.77	44.52	48.75	37.9
18	c	130.88	132.69	131.53	130.58	126.4
20	c	140.95	139.64	140.77	140.89	129.2
21	c	35.26	34.4	33.55	35.31	26.3
22	c	26.89	25.88	26.16	27.14	20



23	c	28.69	27.65	27.08	28.8	20
24	c	45.84	45.39	47.81	46.01	39.7
25	c	85.48	84.72	86.23	85.87	83.4
27	c	88.78	88.85	87.2	88.08	81
28	c	33.45	31.99	33.48	31.36	25.9
29	c	40.48	38.69	47.77	42.57	36.3
30	c	34.35	35.84	33.14	31.59	24.7
31	c	56.02	56.17	56.78	56.55	55.5
32	c	35.05	32.38	31.62	36.4	19.7
33	c	30.62	31.58	31.68	29.91	22.8
35	h	5.98	5.95	6.05	6.12	6.62
36	h	6.42	6.54	6.21	6.12	6.81
39	h	0.76	0.73	0.77	0.82	1.81
40	h	1.39	1.25	1.45	1.35	1.81
41	h	2.33	2.13	2.29	2.29	1.81
42	h	3.22	3.24	3.28	3.32	2.45
43	h	1.9	1.59	1.69	1.51	2.31
44	h	2.99	2.6	2.98	3.04	6.16
45	h	1.25	0.99	1.34	0.9	2.23
46	h	1.71	1.56	1.98	2.04	1.65
47	h	1.35	1.43	1.45	1.65	1.05
48	h	1.6	1.26	1.17	1.4	1.05
49	h	1.43	1.11	1.7	1.49	1.05
50	h	2.02	2.18	2.54	1.47	1.47

51	h	1.32	1.09	1.21	1.76	1.47
52	h	1.67	1.28	1.28	1.91	1.47
53	h	1.12	0.93	0.94	1.33	1.42
54	h	1.31	1.07	0.96	0.89	1.17
55	h	3.4	3.69	3.62	3.53	3.98
56	h	1.55	1.38	1.32	1.65	1.88
57	h	1.36	1.25	1.35	1.4	1.64
58	h	1.33	1.11	1.54	1.19	1.56
59	h	1.73	1.67	1.4	0.96	1.56
60	h	0.86	0.77	0.62	0.64	1.06
61	h	1.3	0.87	1.01	1.26	1.06
62	h	0.8	0.5	1.33	1.03	1.06
63	h	1.22	0.71	0.87	0.99	1.14
64	h	0.99	1.08	1.48	1.28	1.14
65	h	0.92	0.63	0.82	0.99	1.14
66	h	1.15	0.34	0.6	1.06	1.16
67	h	1.31	1.26	1.41	1.04	1.16
68	h	0.95	0.83	1.05	0.72	1.16