Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supplementary Information

Unusual Anti-inflammatory Meroterpenoids from the Marine Sponge *Dactylospongia* sp.

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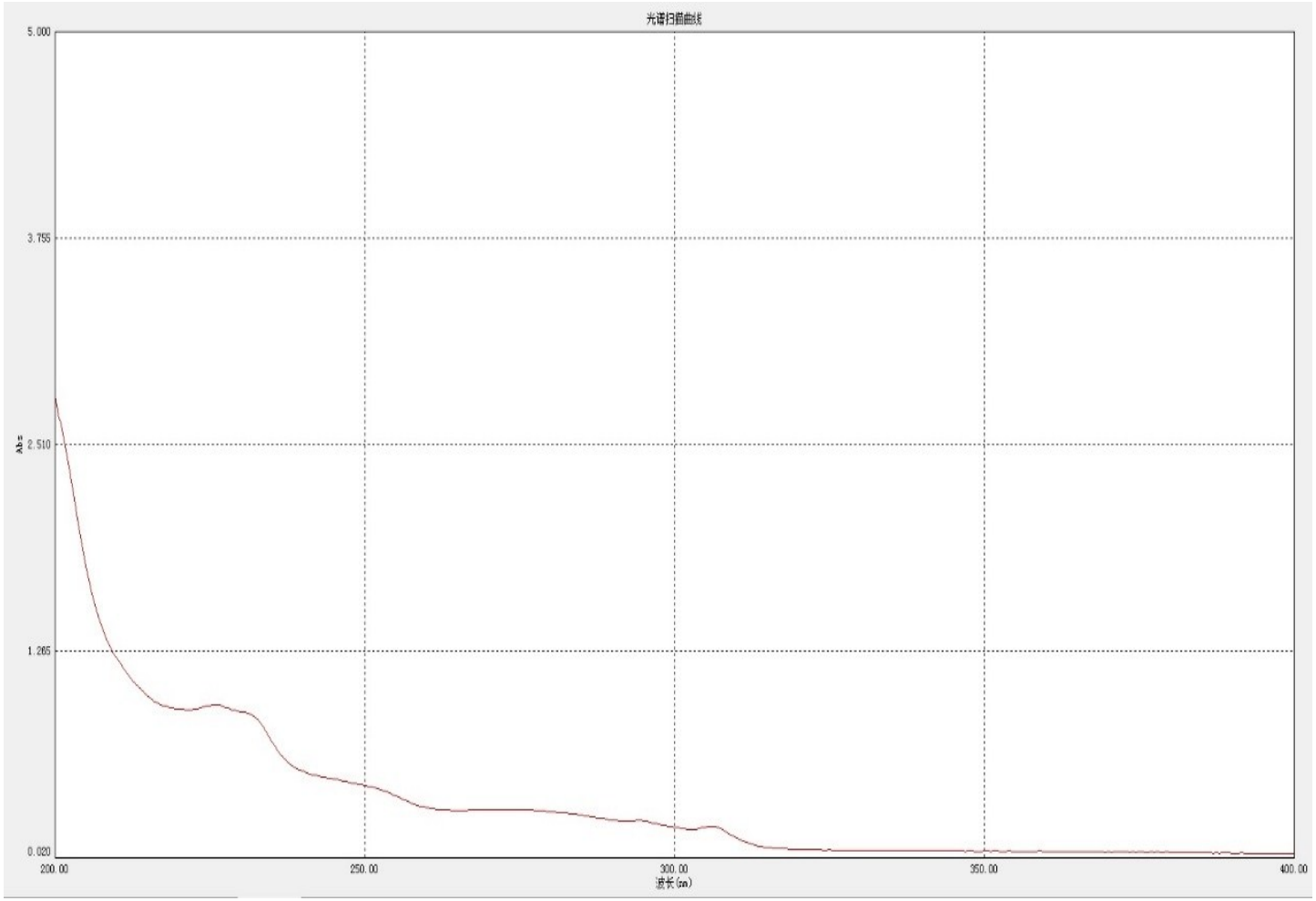
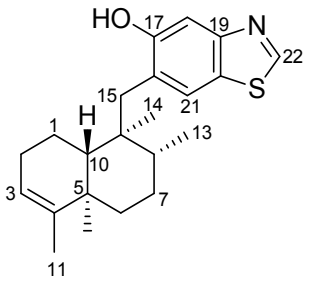
Figure S105. HSQC spectrum of Compound **10** in $CDCl_3$.

Figure S106. NOESY spectrum of Compound **10** in $CDCl_3$.

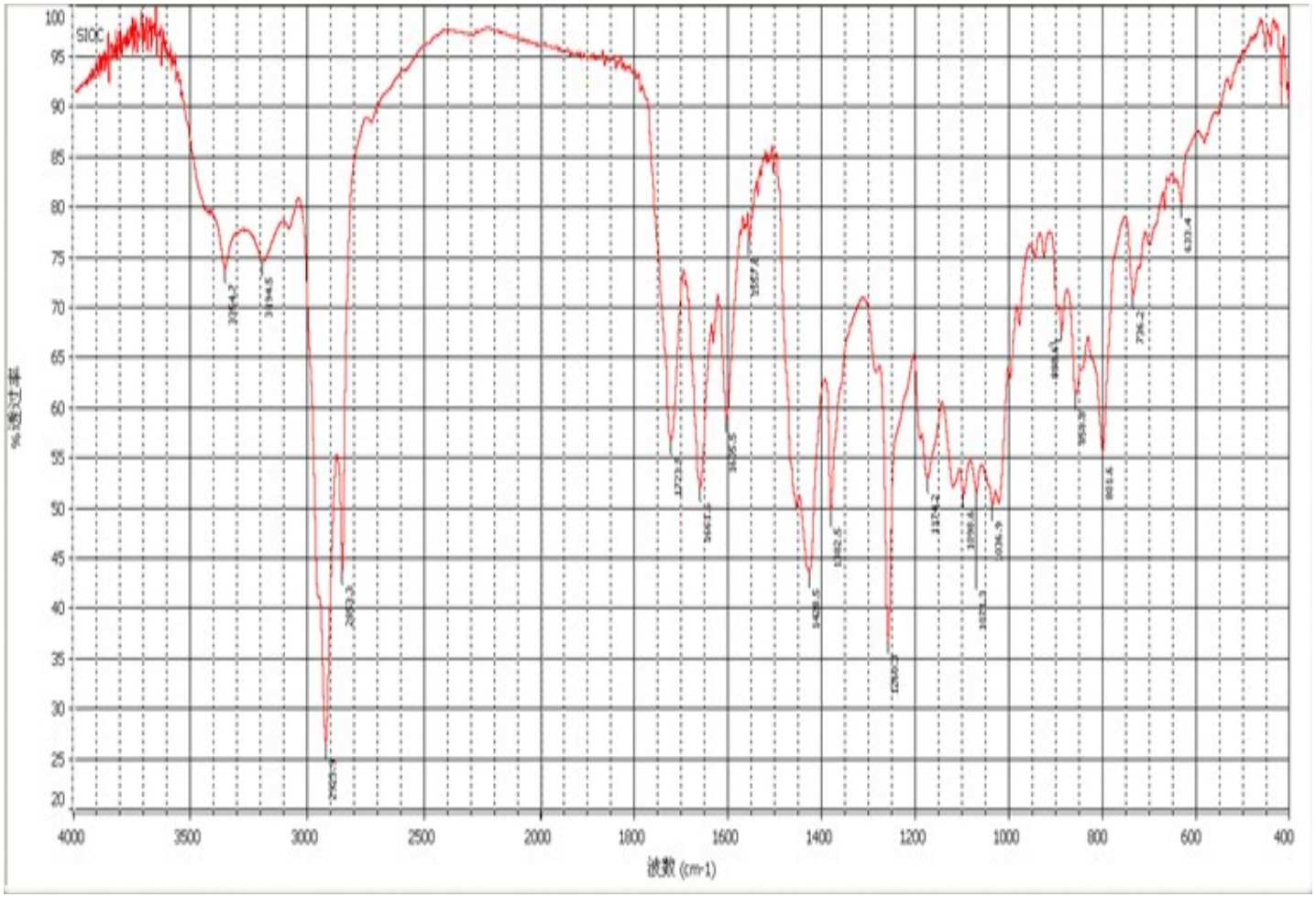
Figure S107. CD spectrum of Compound **10** in MeOH.

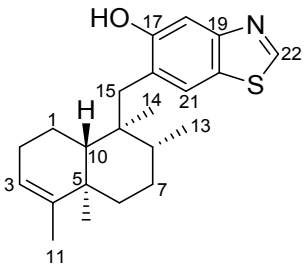




Dactylospongin A (**1**)

Figure S1. UV spectrum of Compound 1 in MeOH.



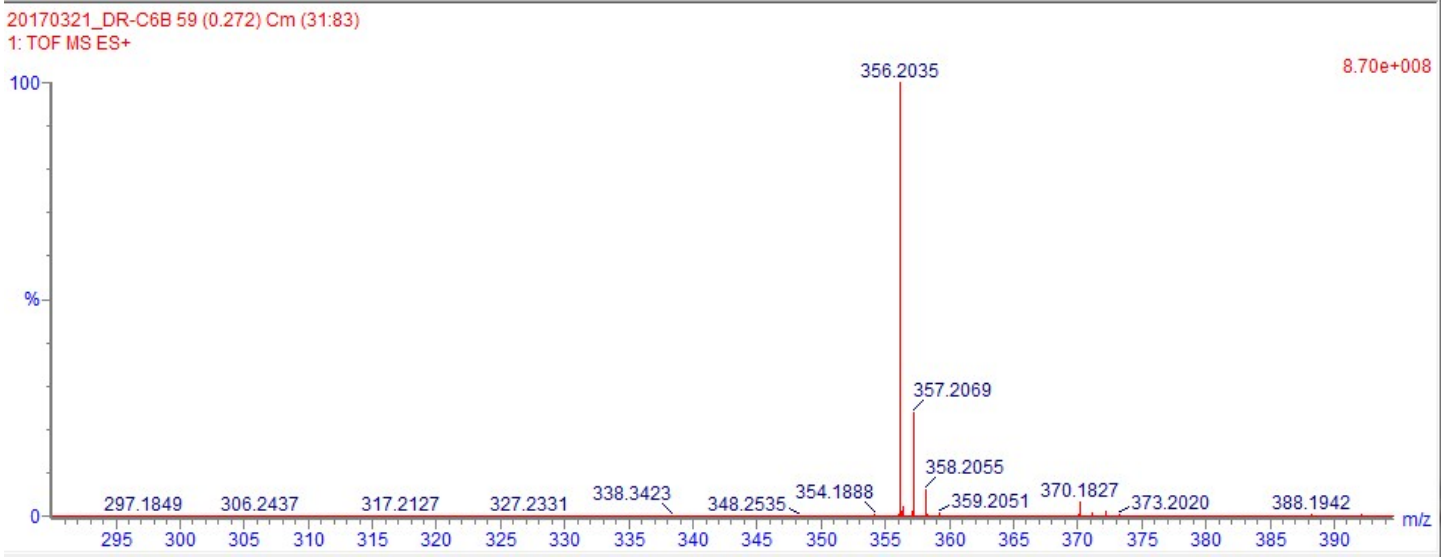


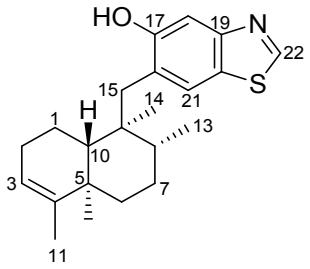
Dactylospongin A (**1**)

Figure S2. IR spectrum of Compound **1**.

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
2613 formula(e) evaluated with 8 results within limits (up to 50 closest results for each mass)
Elements Used:

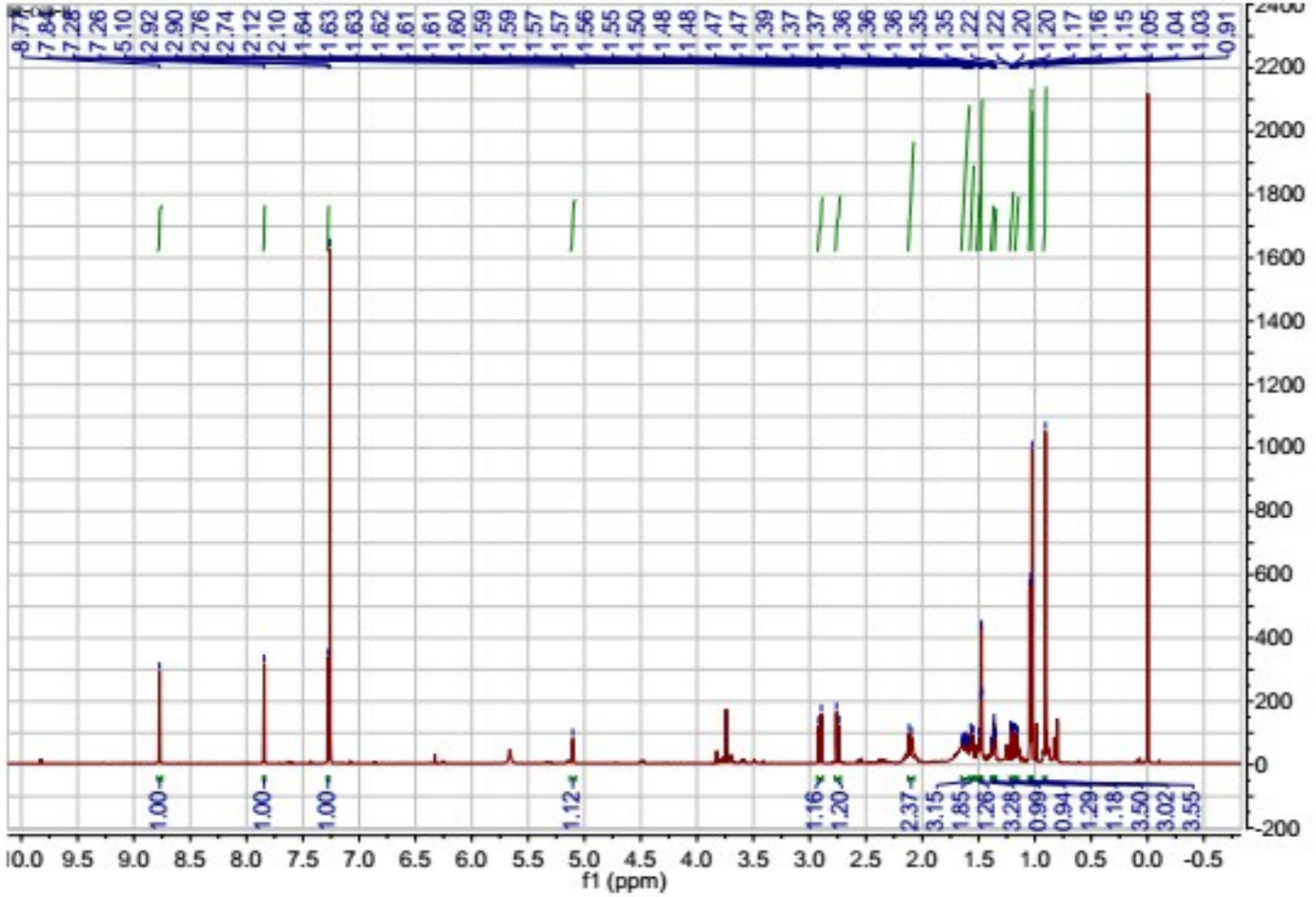
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	S
356.2035	356.2048	-1.3	-3.6	8.5	C22 H30 N O S	3466.6	0.087	91.71	22	30	1	1	1
	356.2008	2.7	7.6	4.5	C17 H30 N3 O3 S	3469.1	2.539	7.90	17	30	3	3	1
	356.2014	2.1	5.9	13.5	C25 H26 N O	3472.9	6.352	0.17	25	26	1	1	
	356.2046	-1.1	-3.1	5.5	C14 H26 N7 O4	3473.5	6.964	0.09	14	26	7	4	
	356.2033	0.2	0.6	0.5	C13 H30 N3 O8	3473.8	7.226	0.07	13	30	3	8	
	356.2006	2.9	8.1	1.5	C9 H26 N9 O6	3474.7	8.189	0.03	9	26	9	6	
	356.2042	-0.7	-2.0	-0.5	C14 H34 N3 O3 S2	3475.2	8.697	0.02	14	34	3	3	2
	356.2015	2.0	5.6	0.5	C10 H30 N9 O S2	3475.9	9.381	0.01	10	30	9	1	2

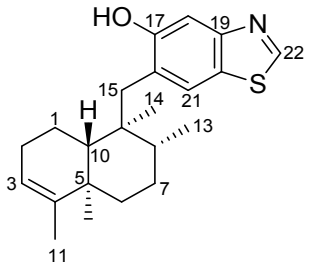




Dactylospongin A (**1**)

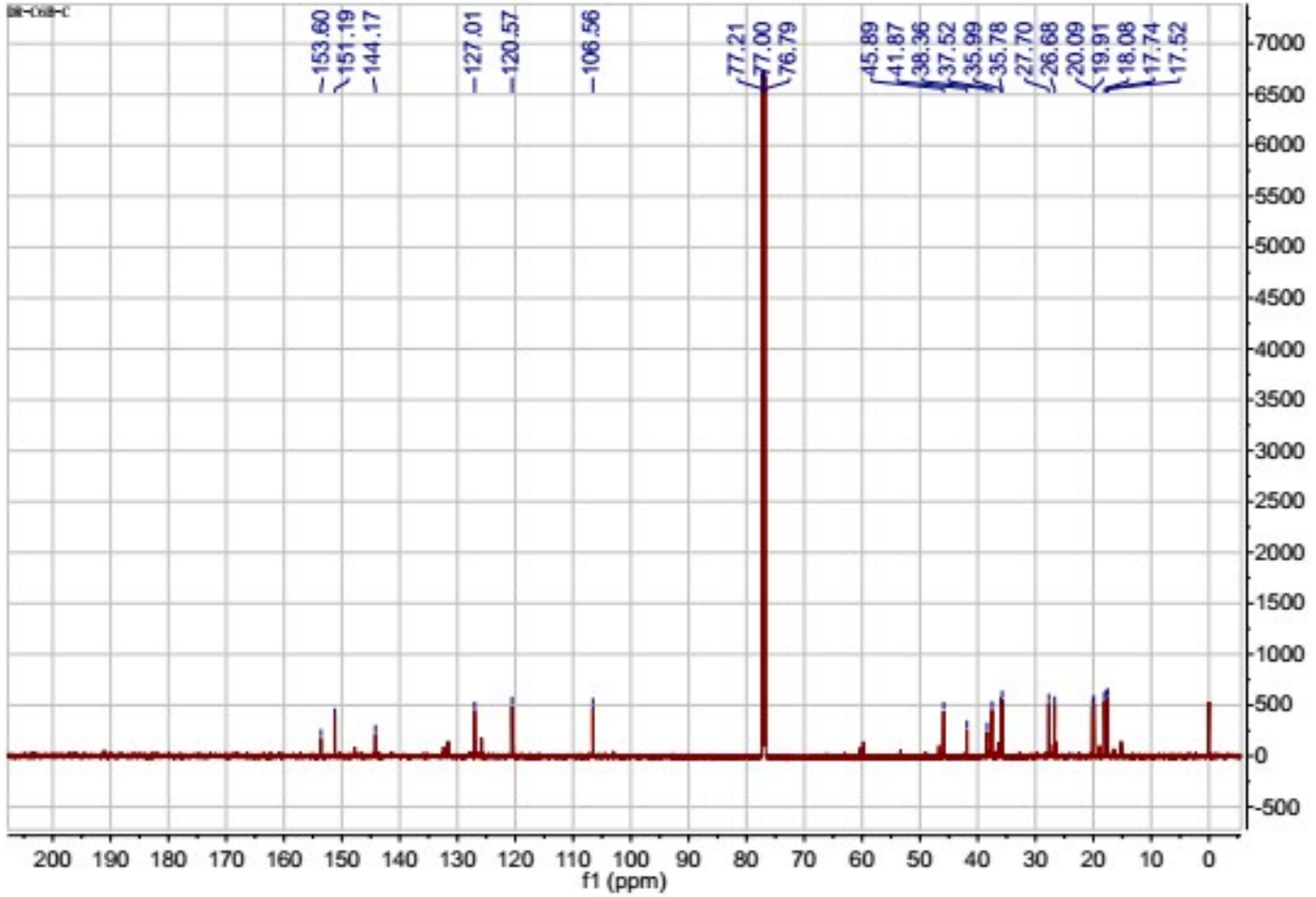
Figure S3. HRESIMS spectrum of Compound **1.**

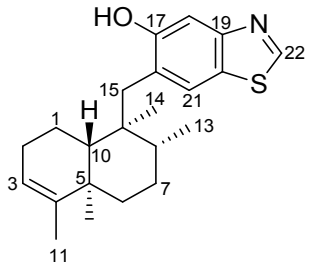




Dactylospongin A (**1**)

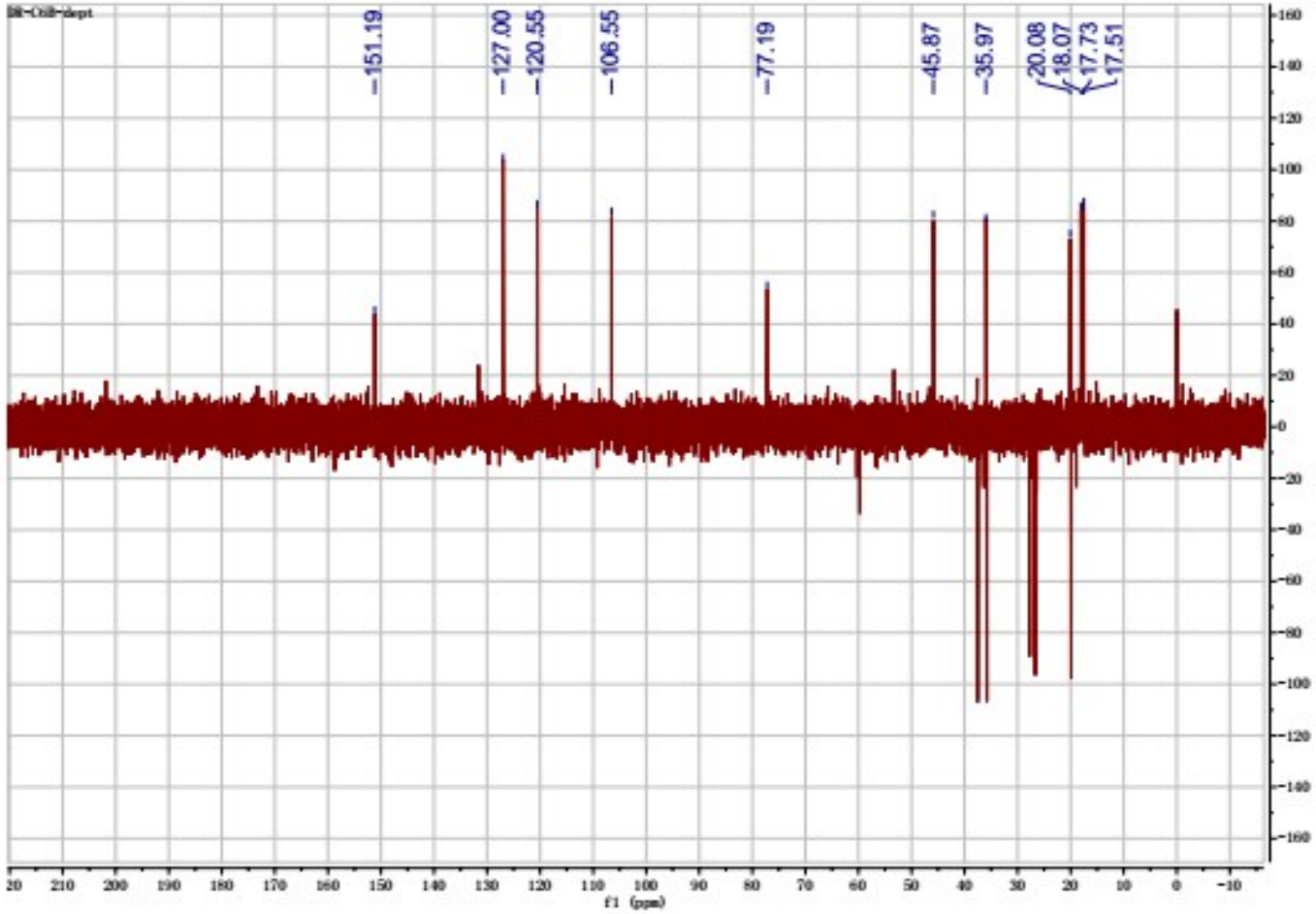
Figure S4. ^{1}H NMR spectrum of Compound **1** in $CDCl_3$.

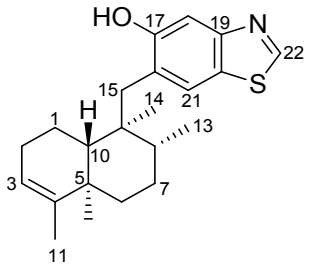




Dactylospongin A (**1**)

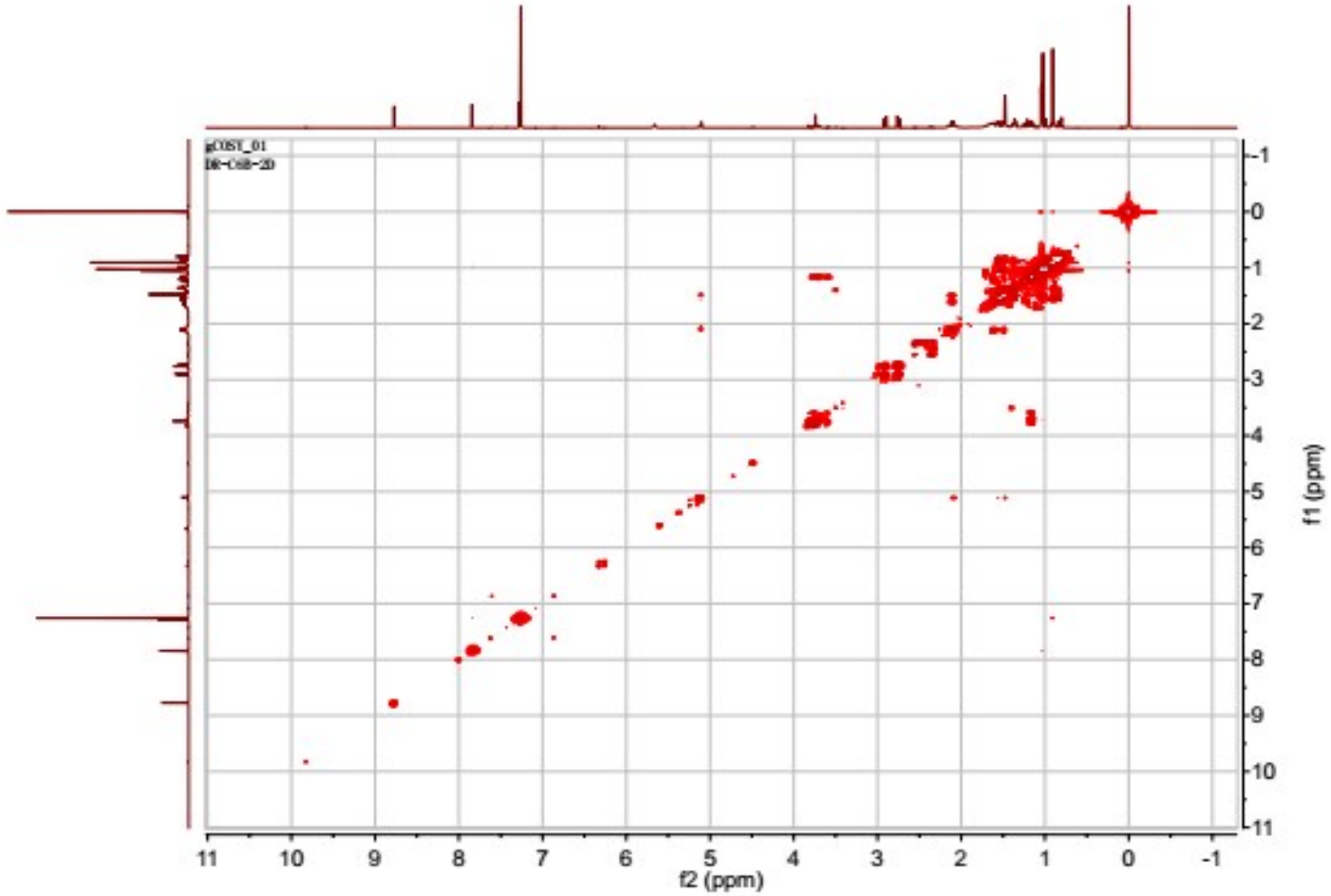
Figure S5. ^{13}C NMR spectrum of Compound **1** in $CDCl_3$.

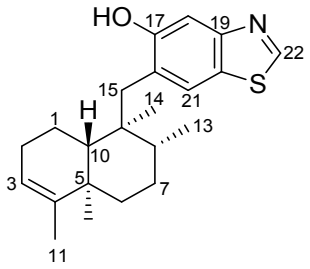




Dactylospongin A (**1**)

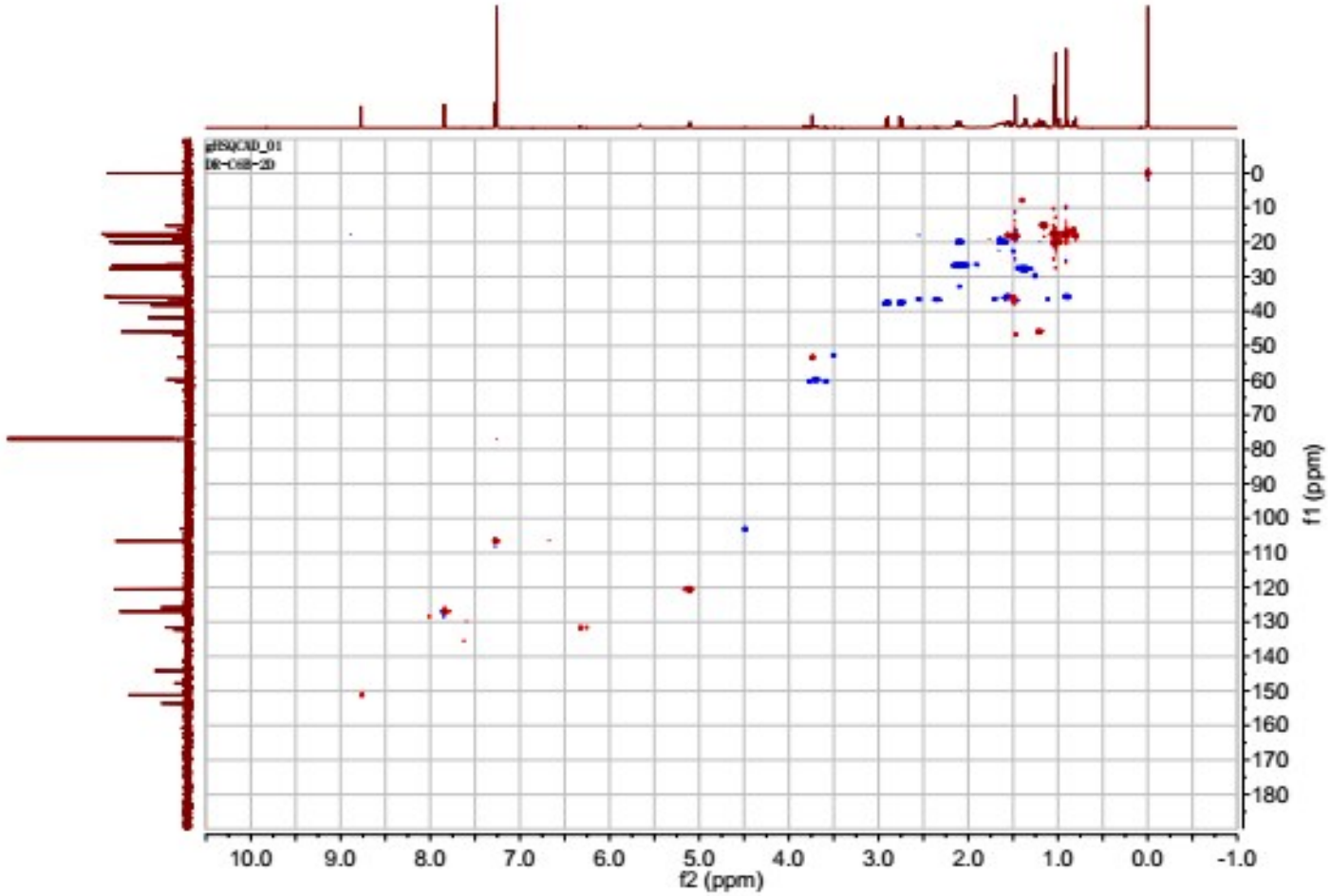
Figure S6. DEPT135 spectrum of Compound **1** in $CDCl_3$.

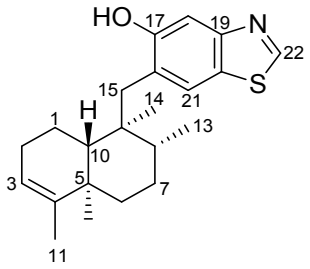




Dactylospongin A (**1**)

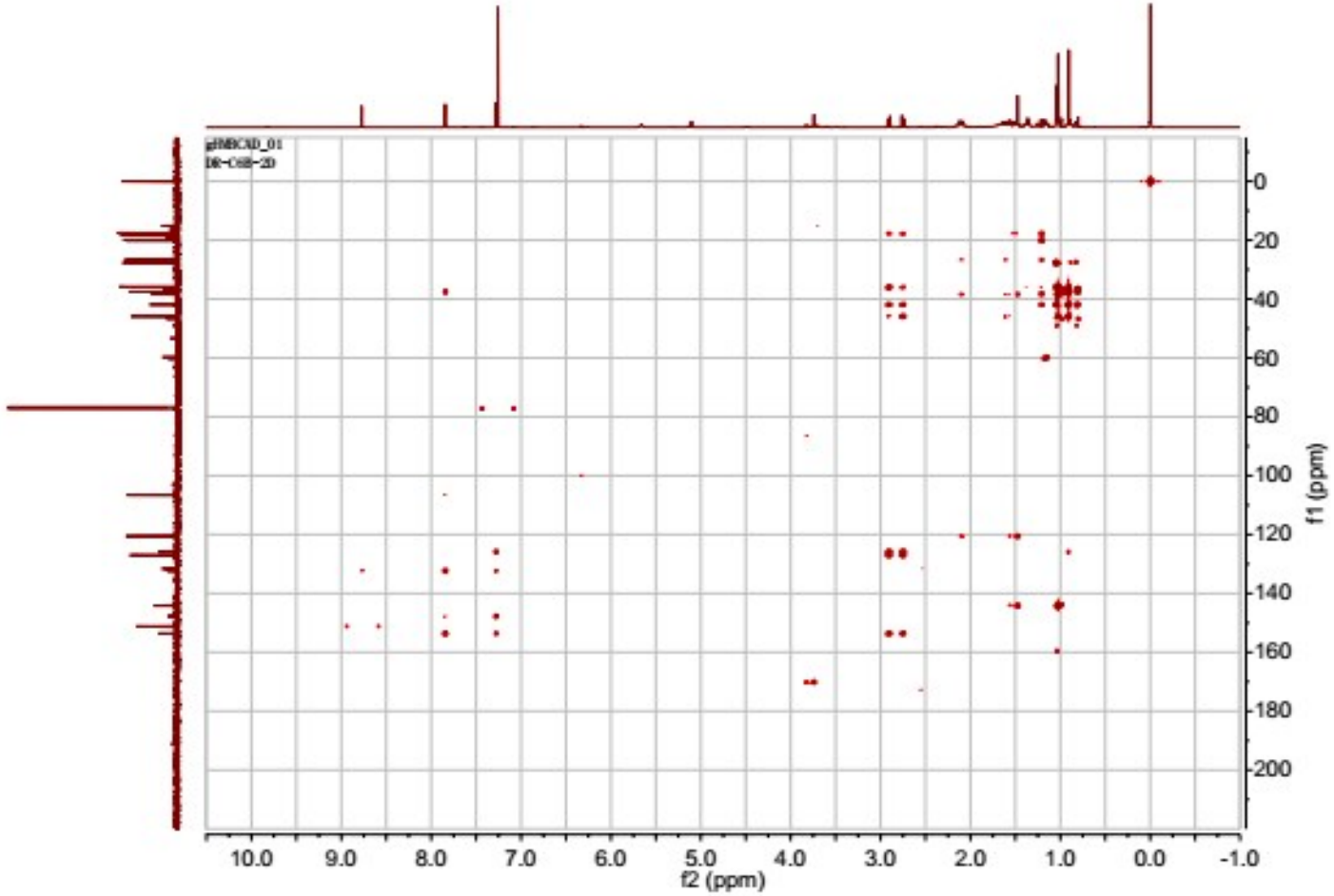
Figure S7. ^{1}H-^{1}H COSY spectrum of Compound **1** in $CDCl_3$.

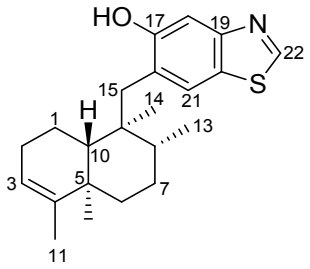




Dactylospongin A (**1**)

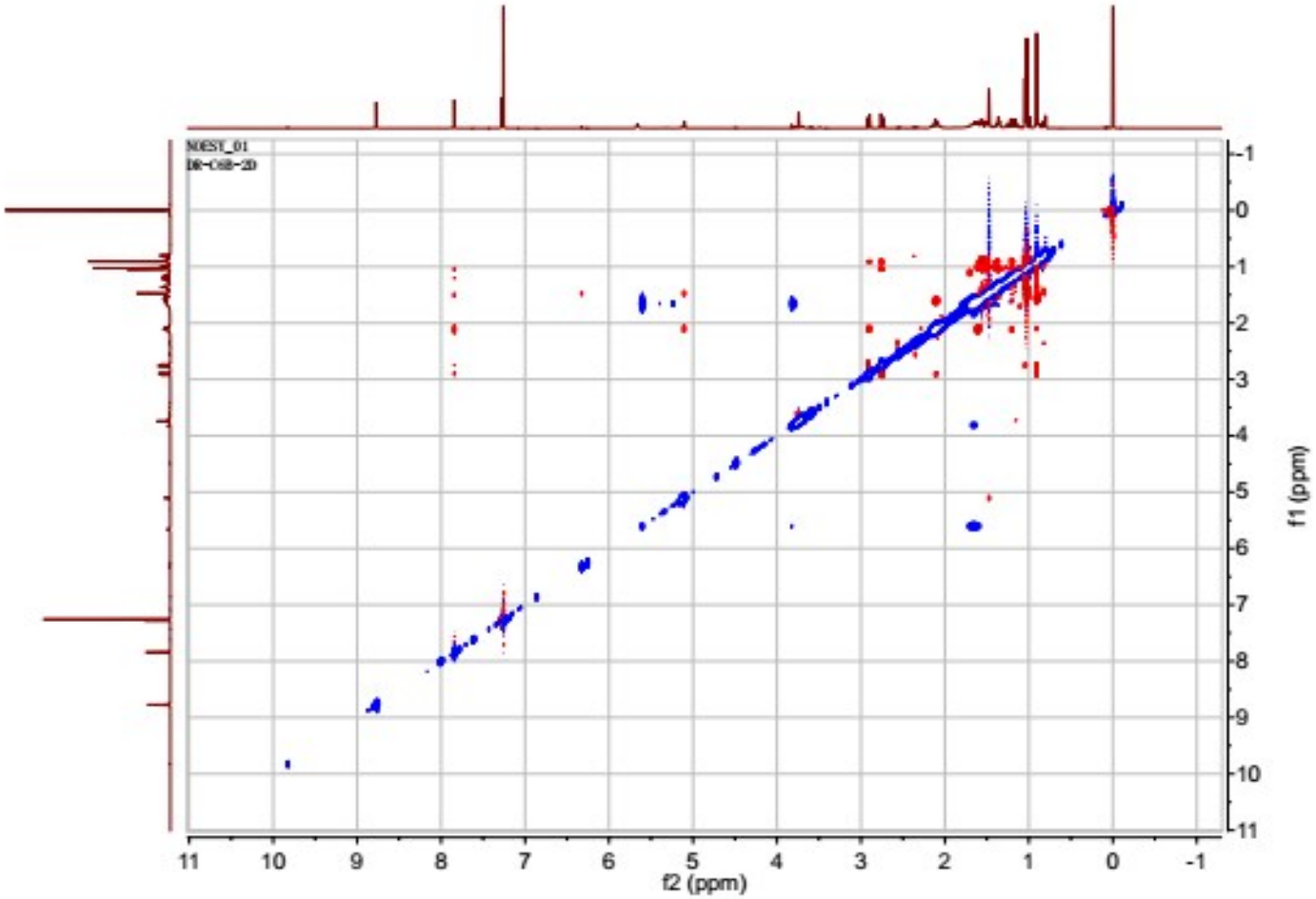
Figure S8. HSQC spectrum of Compound **1** in $CDCl_3$.

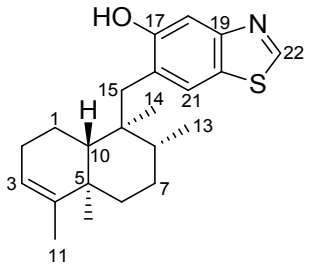




Dactylospongin A (**1**)

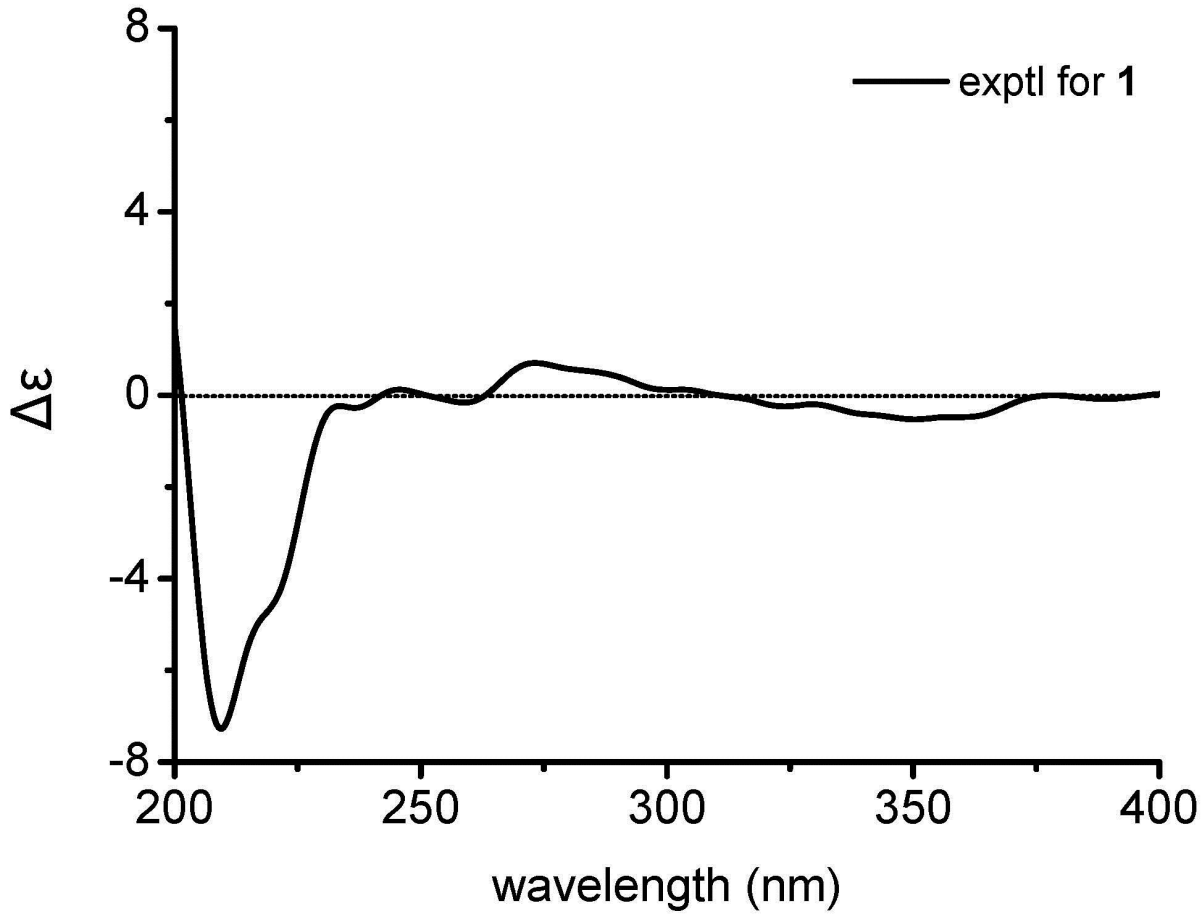
Figure S9. HMBC spectrum of Compound **1** in $CDCl_3$.

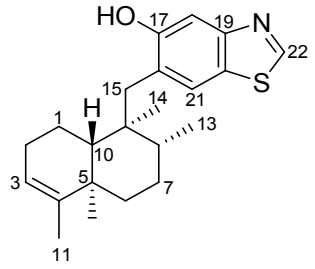




Dactylospongin A (**1**)

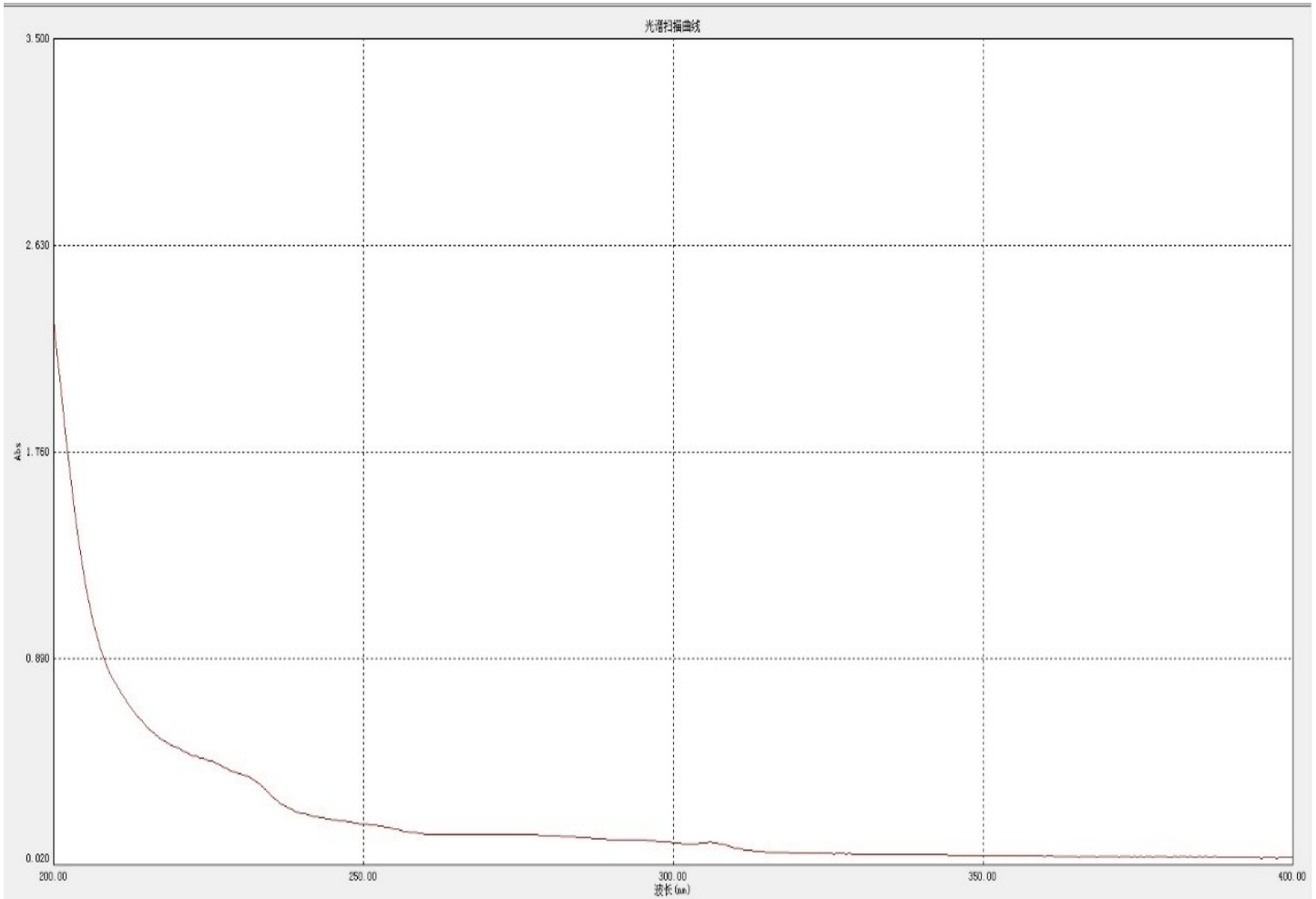
Figure S10. NOESY spectrum of Compound **1** in $CDCl_3$.

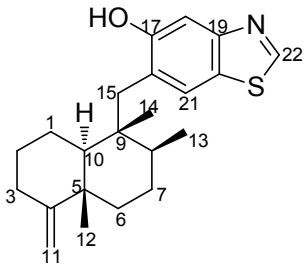




Dactylospongin A (**1**)

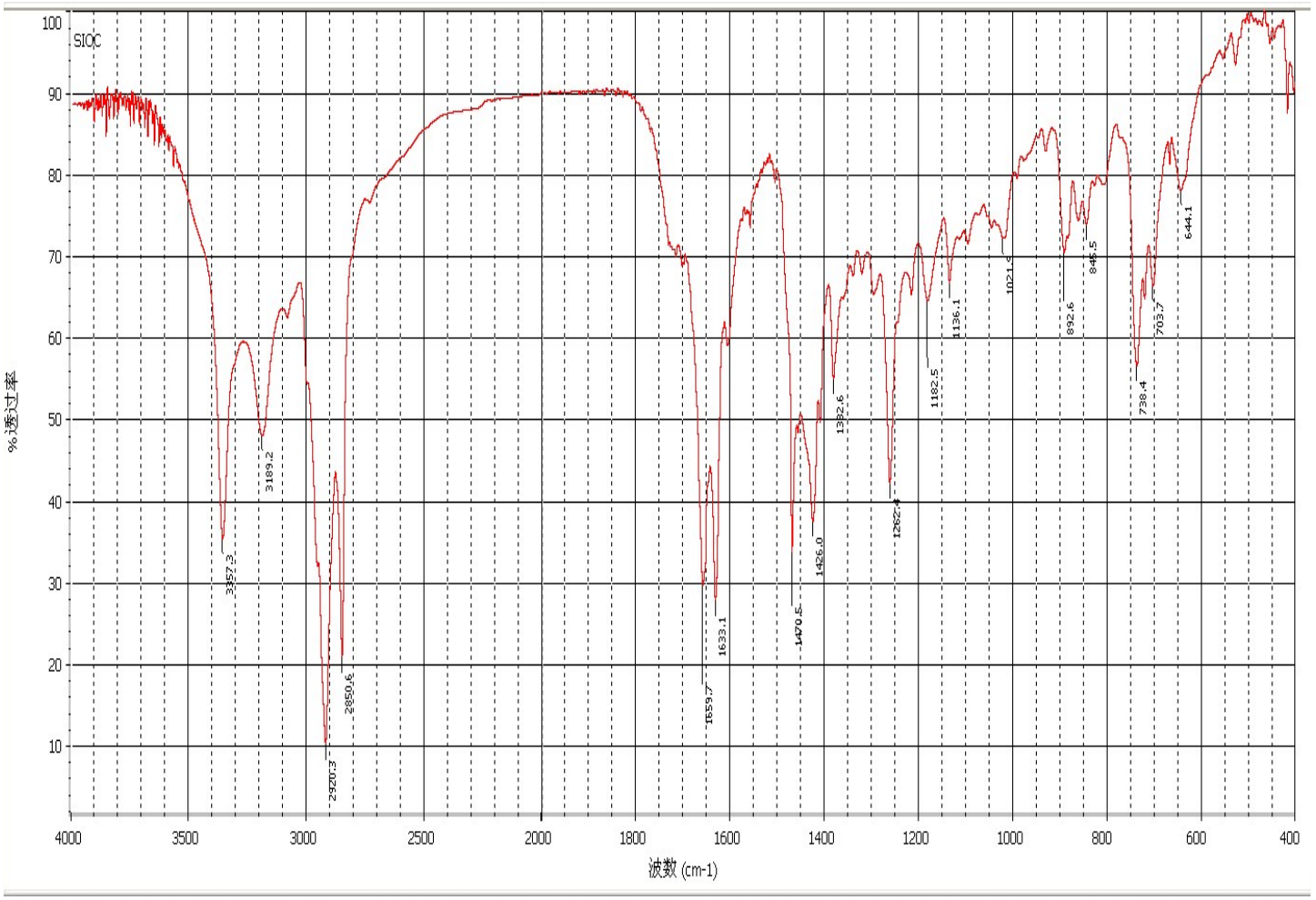
Figure S11. CD Spectrum of Compound **1** in MeOH.

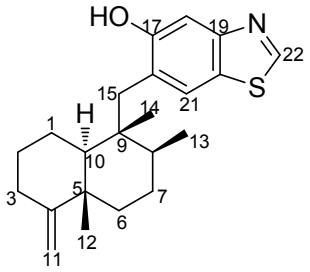




Dactylospongin B (2)

Figure S12. UV spectrum of Compound **2** in MeOH.





Dactylospongin B (2)

Figure S13. IR spectrum of Compound **2**.

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

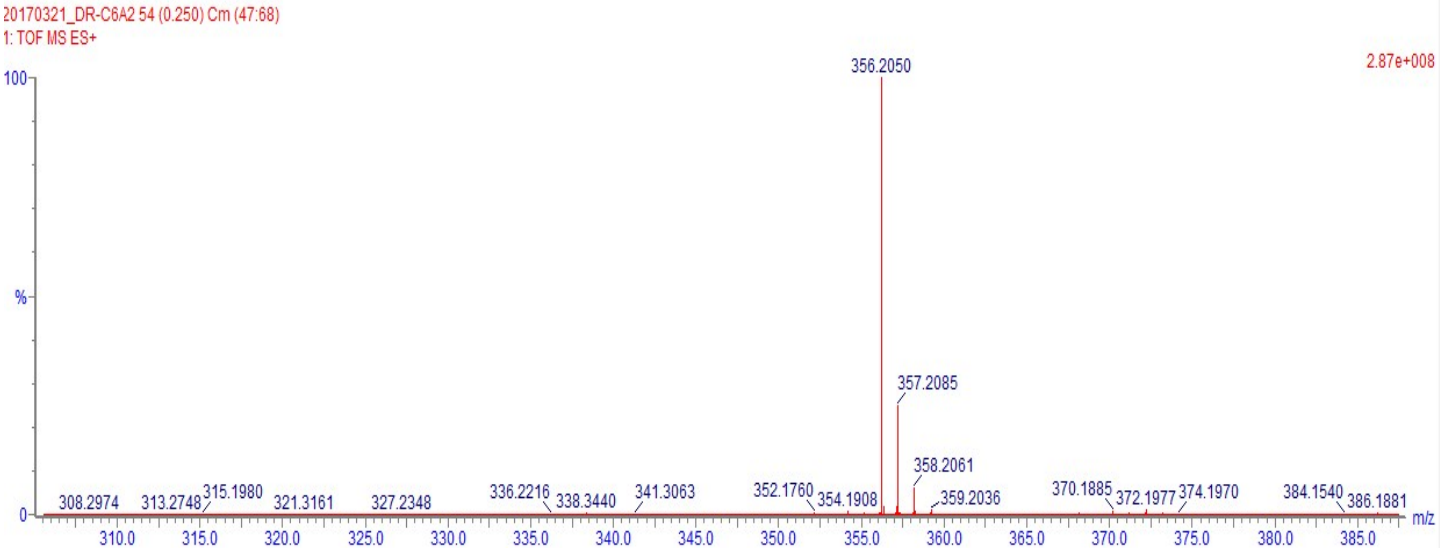
Number of isotope peaks used for i-FIT = 3

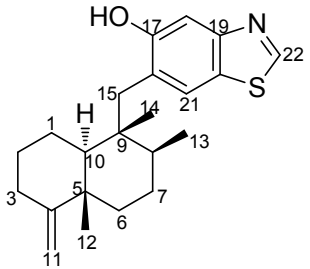
Monoisotopic Mass, Even Electron Ions

4156 formula(e) evaluated with 7 results within limits (up to 50 closest results for each mass)

Elements Used:

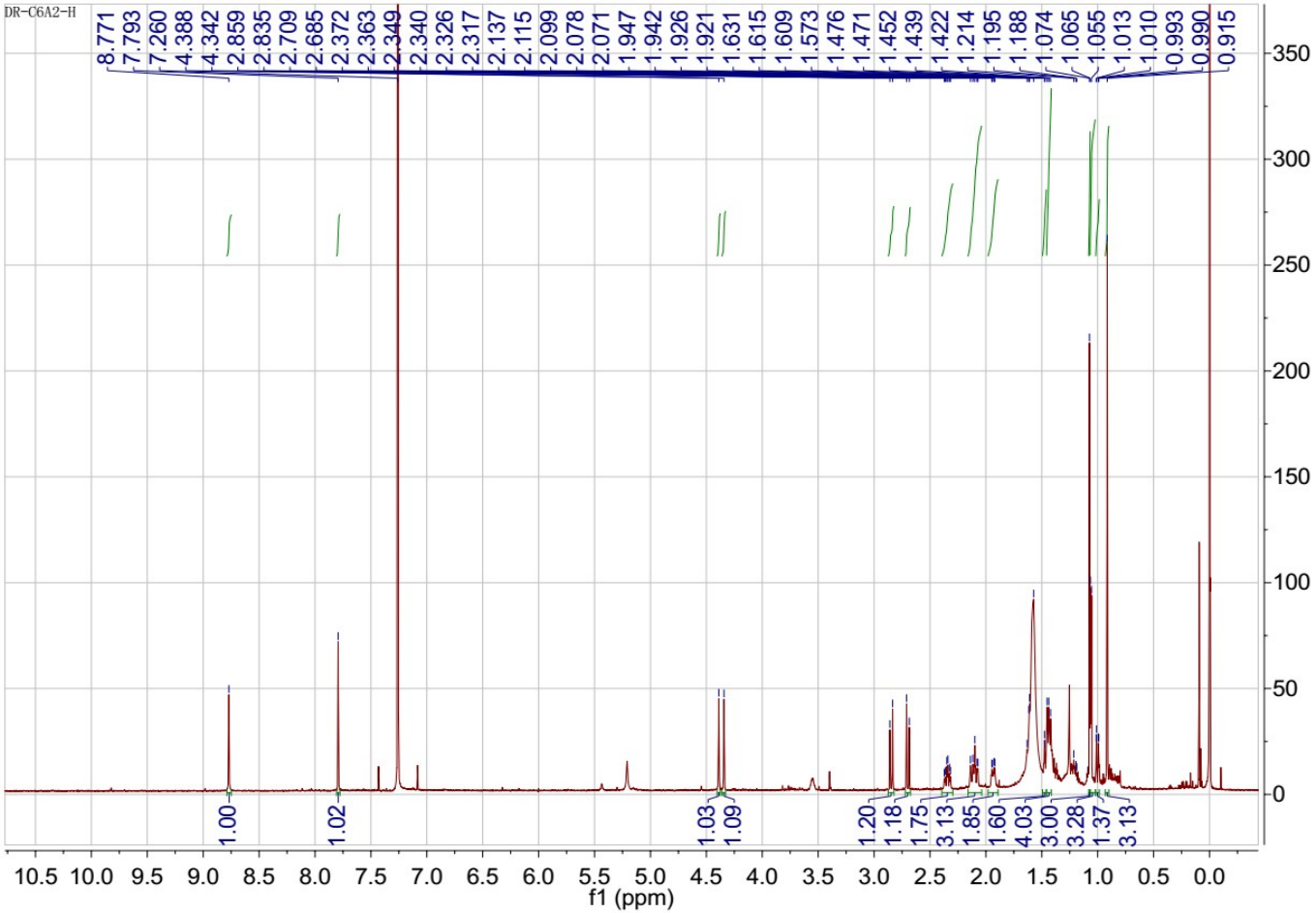
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Na	S
356.2050	356.2048	0.2	0.6	8.5	C22 H30 N O S	3159.0	0.000	99.98	22	30	1	1		1
	356.2058	-0.8	-2.2	0.5	C17 H35 N O Na S2	3168.8	9.785	0.01	17	35	1	1	1	2
	356.2062	-1.2	-3.4	6.5	C17 H27 N5 O2 Na	3169.4	10.408	0.00	17	27	5	2	1	
	356.2049	0.1	0.3	1.5	C16 H31 N O6 Na	3169.5	10.509	0.00	16	31	1	6	1	
	356.2042	0.8	2.2	-0.5	C14 H34 N3 O3 S2	3169.6	10.612	0.00	14	34	3	3		2
	356.2046	0.4	1.1	5.5	C14 H26 N7 O4	3169.4	10.426	0.00	14	26	7	4		
	356.2033	1.7	4.8	0.5	C13 H30 N3 O8	3169.8	10.808	0.00	13	30	3	8		

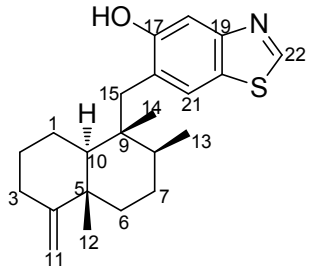




Dactylospongin B (2)

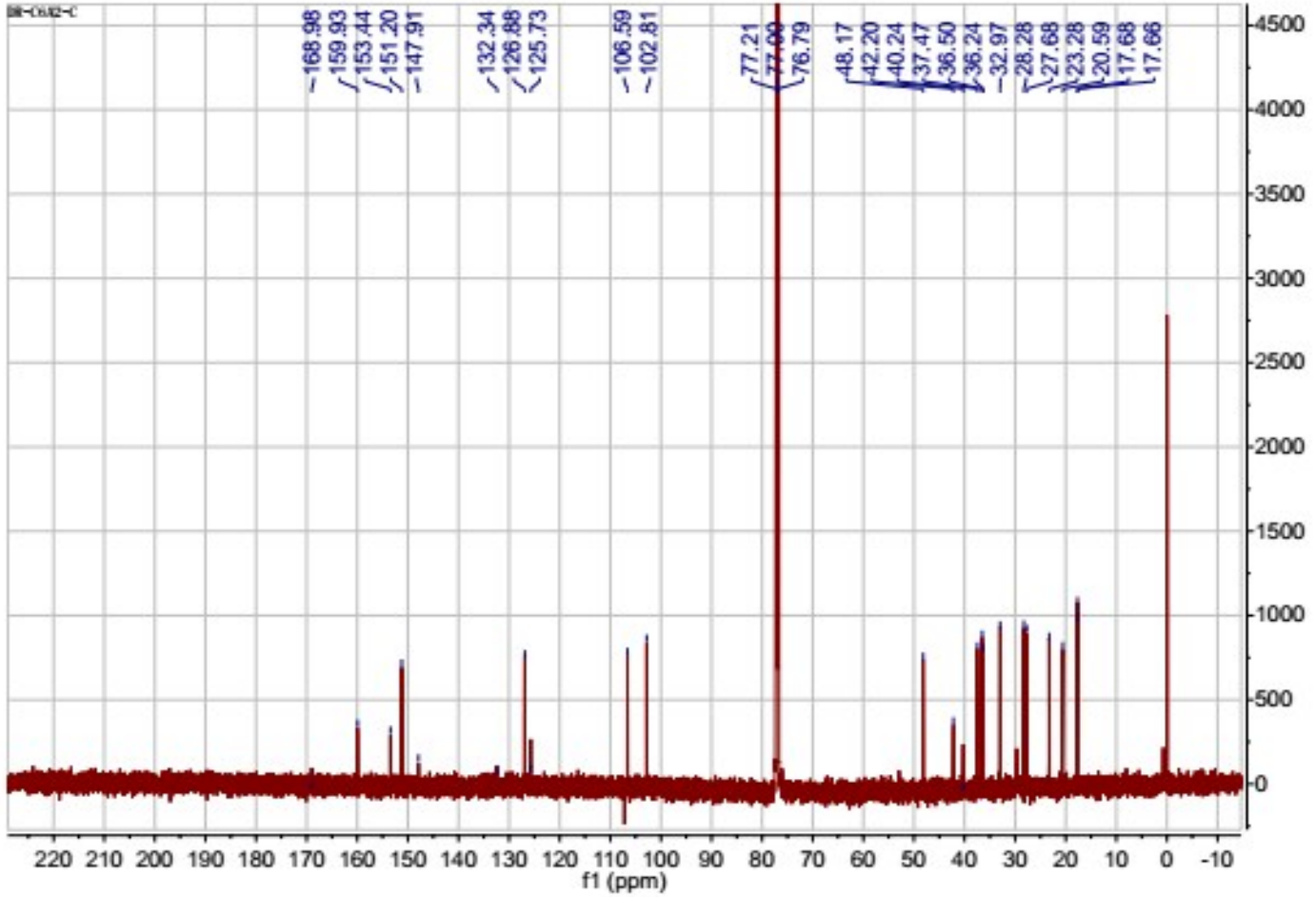
Figure S14. HRESIMS spectrum of Compound **2**.

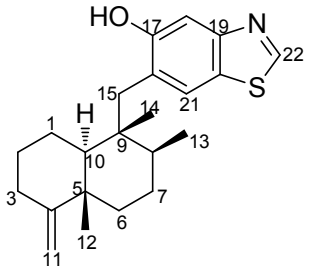




Dactylospongin B (2)

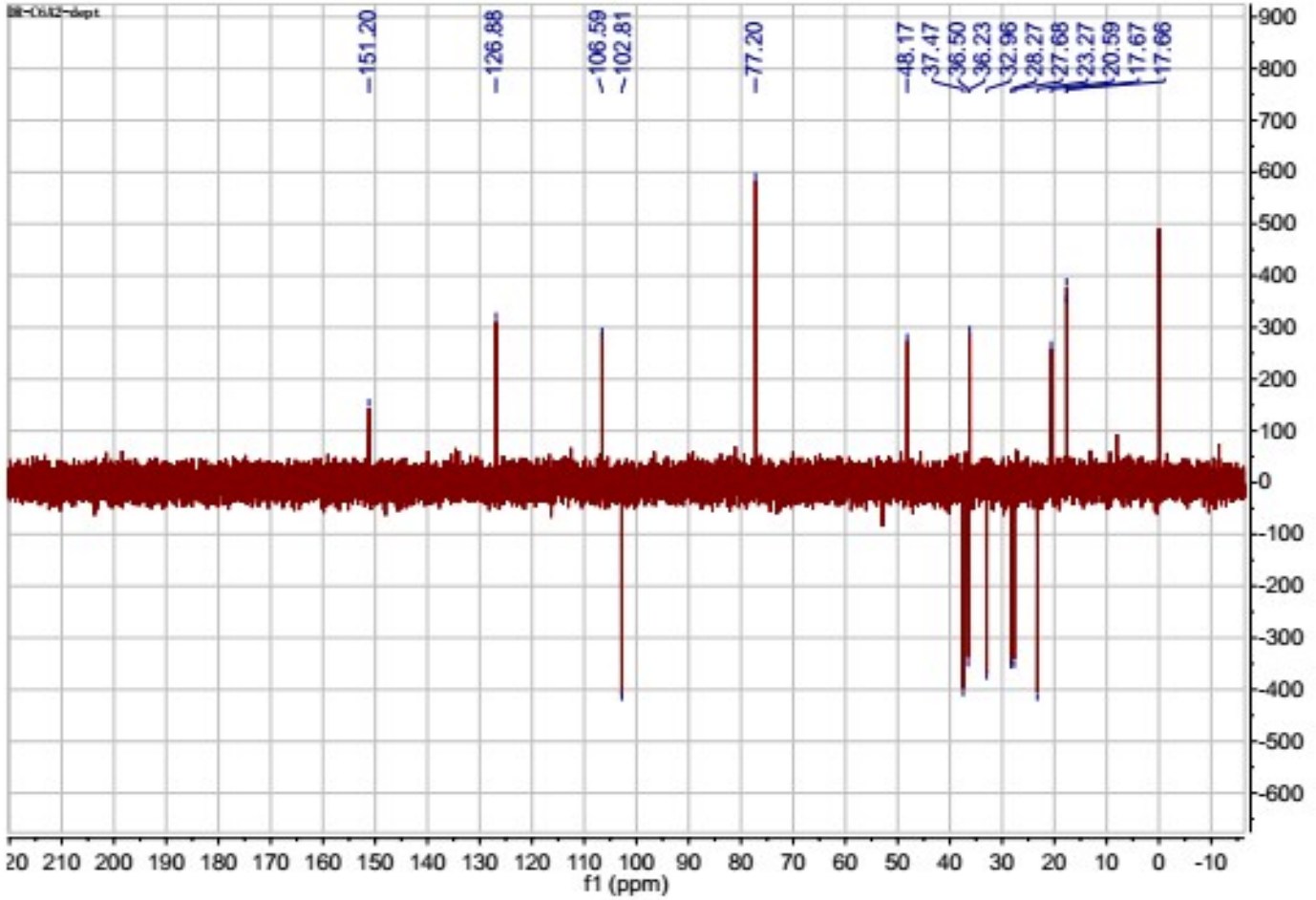
Figure S15. ^{1}H NMR spectrum of Compound **2** in $CDCl_3$.

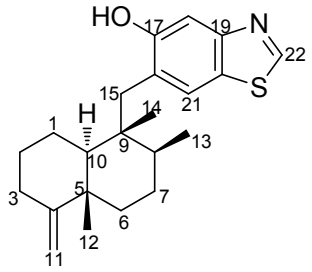




Dactylospongin B (2)

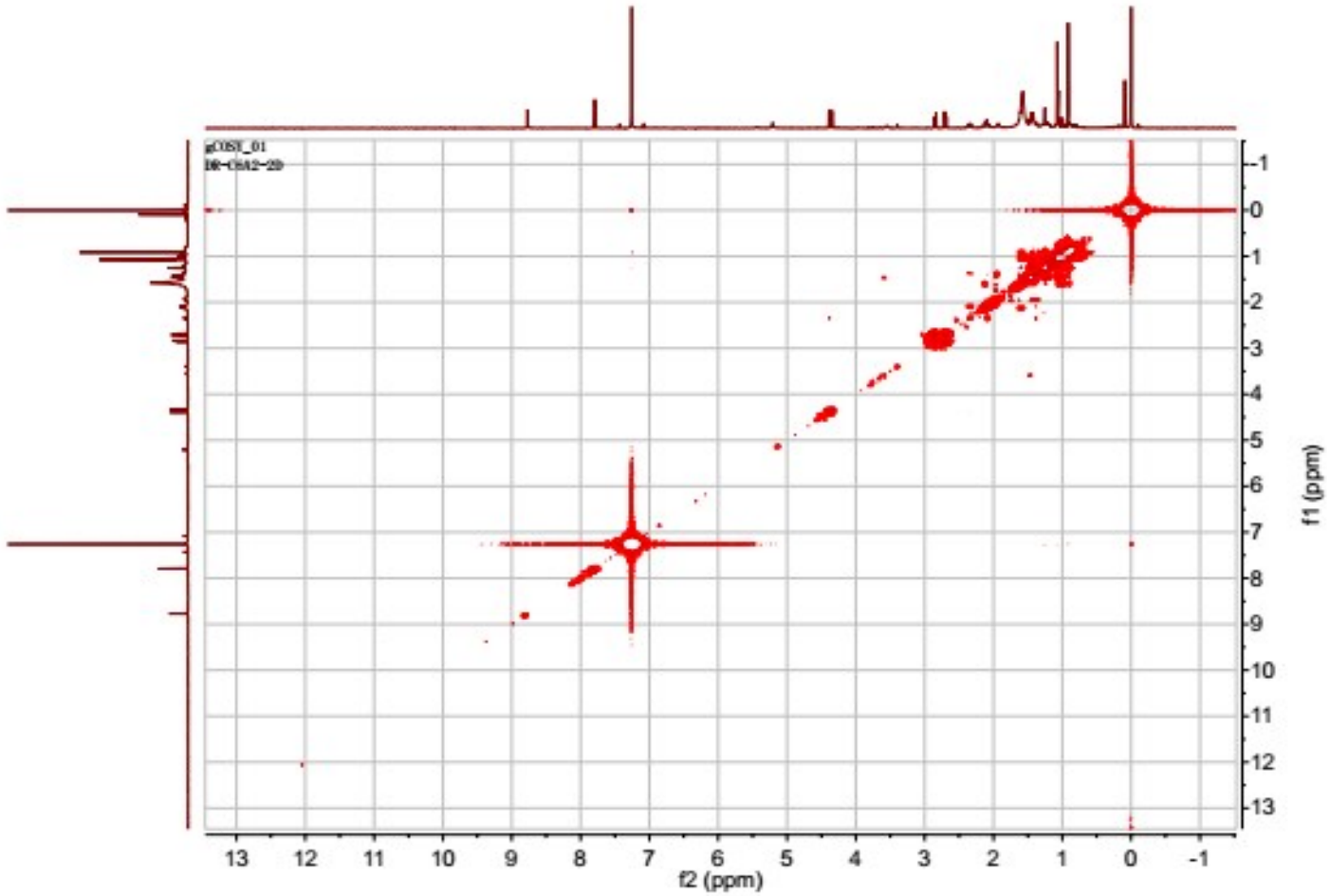
Figure S16. ^{13}C NMR spectrum of Compound **2** in $CDCl_3$.

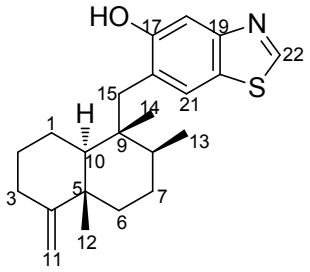




Dactylospongin B (2)

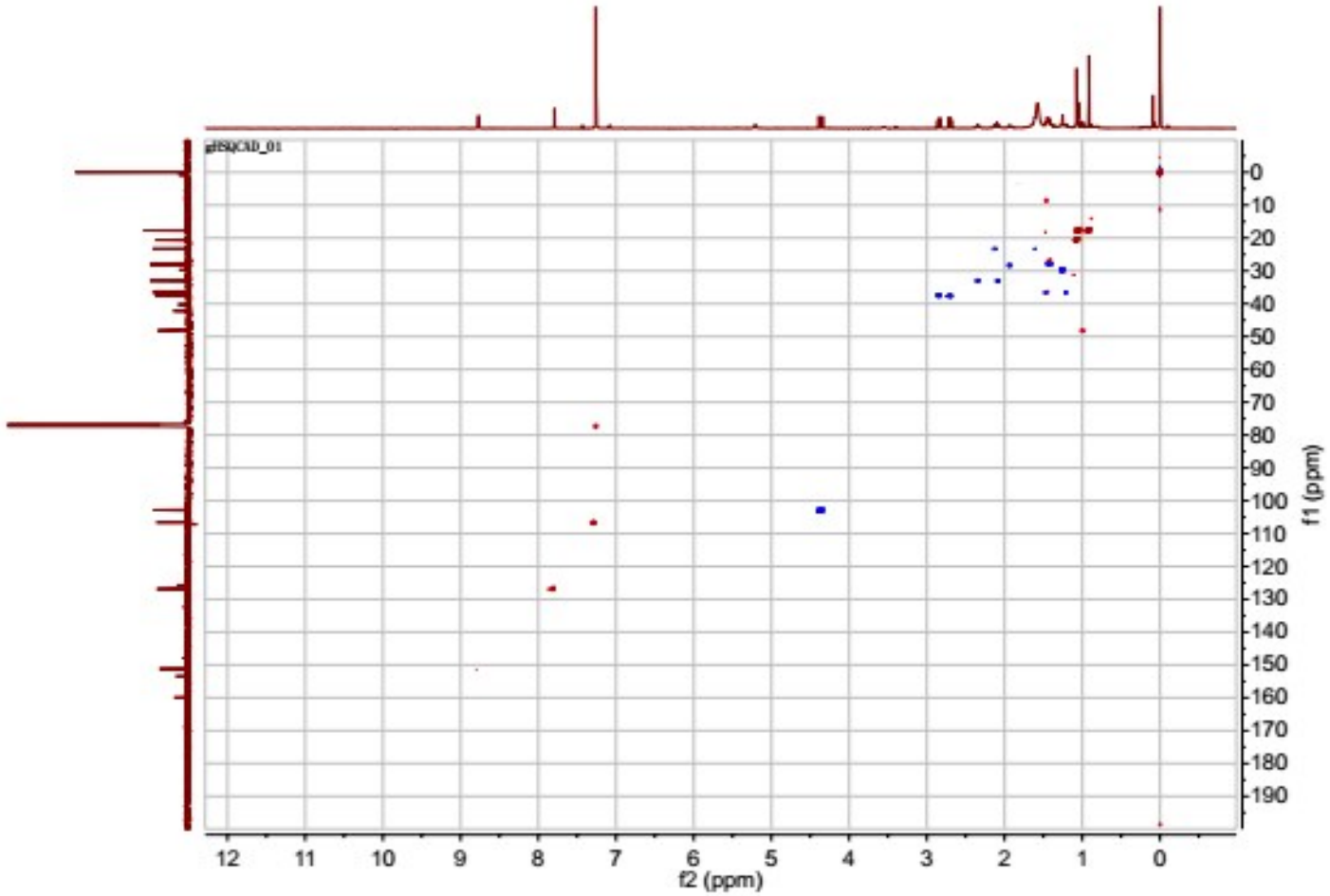
Figure S17. DEPT135 spectrum of Compound **2** in $CDCl_3$.

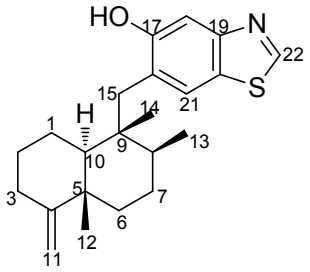




Dactylospongin B (2)

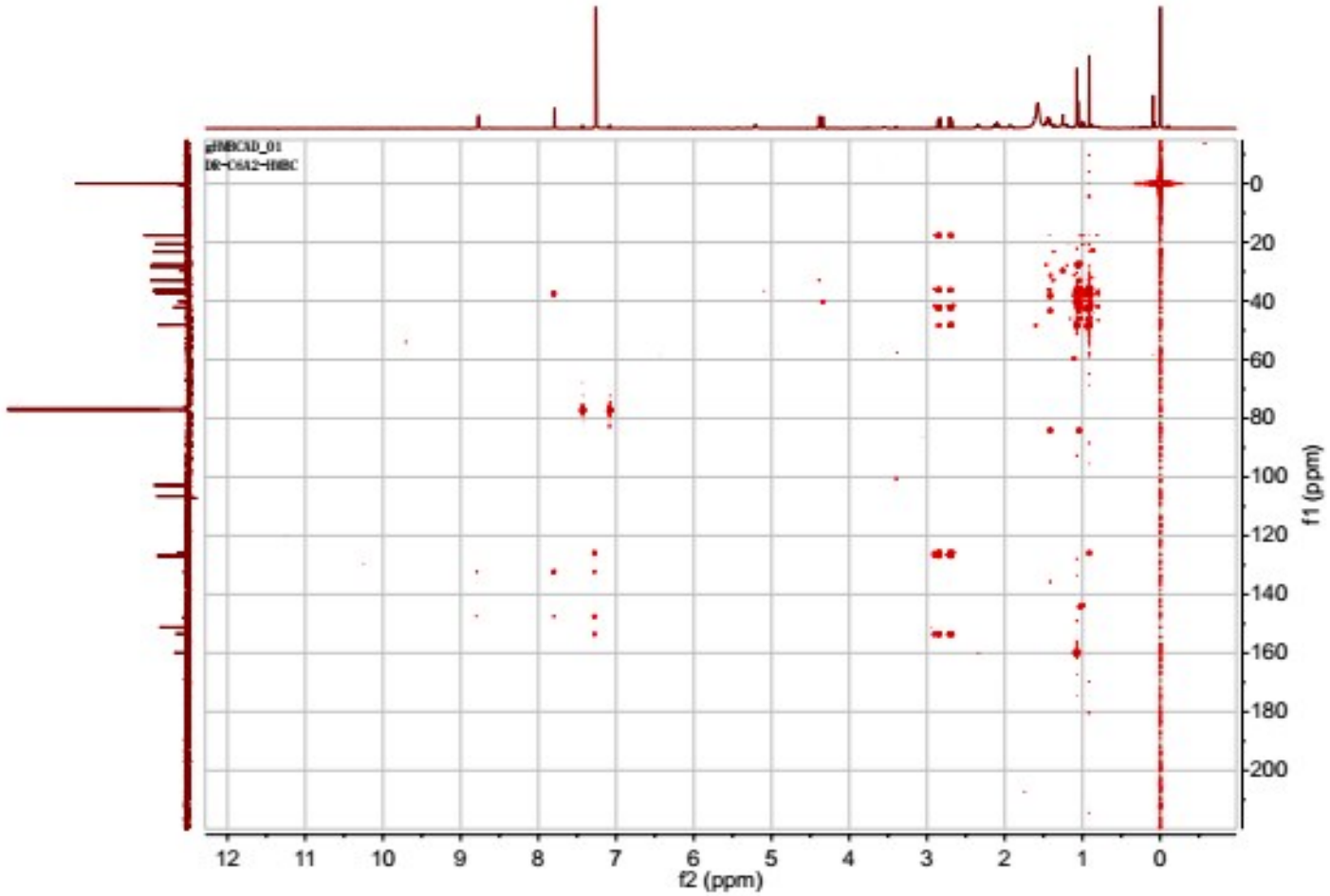
Figure S18. ^{1}H-^{1}H COSY spectrum of Compound **2** in $CDCl_3$.

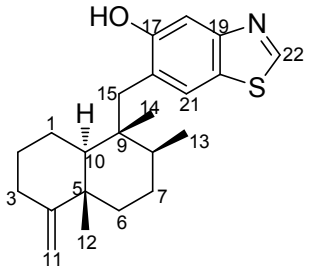




Dactylospongin B (2)

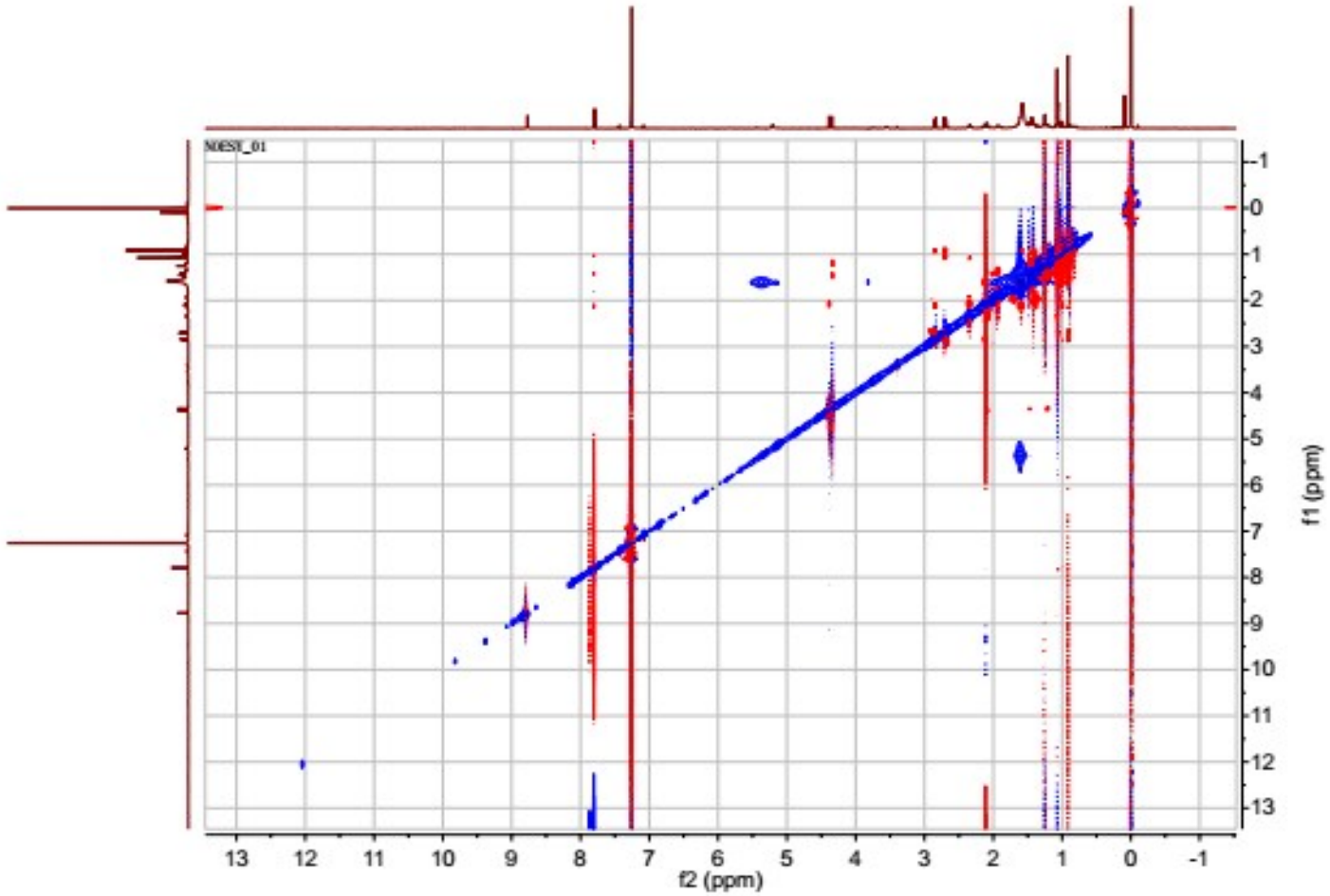
Figure S19. HSQC spectrum of Compound **2** in $CDCl_3$.

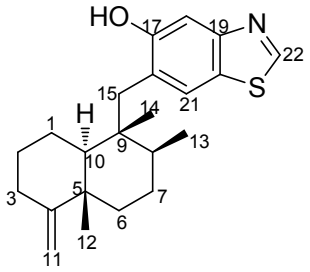




Dactylospongin B (2)

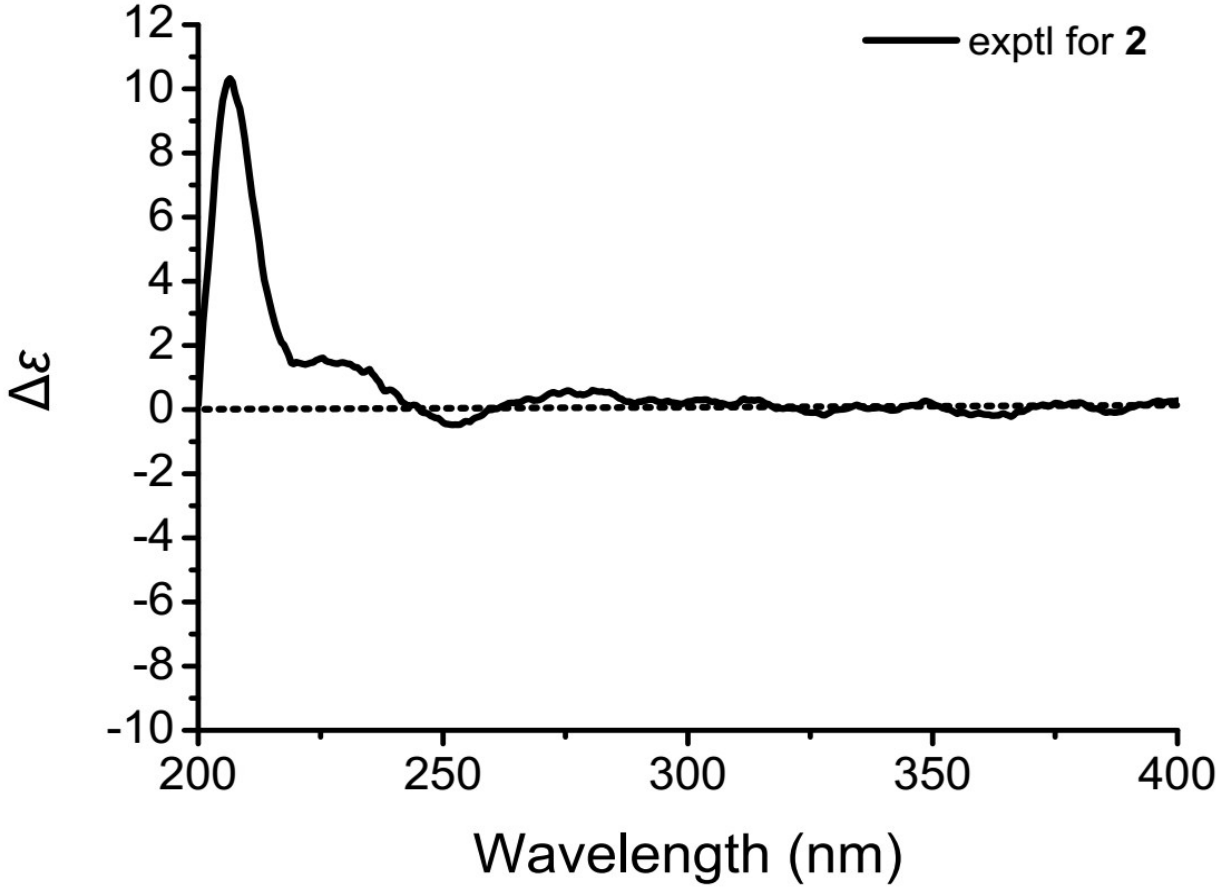
Figure S20. HMBC spectrum of Compound **2** in $CDCl_3$.

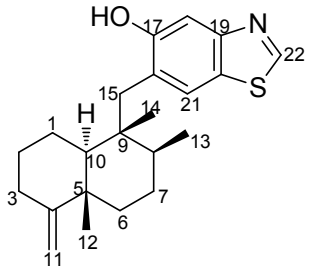




Dactylospongin B (2)

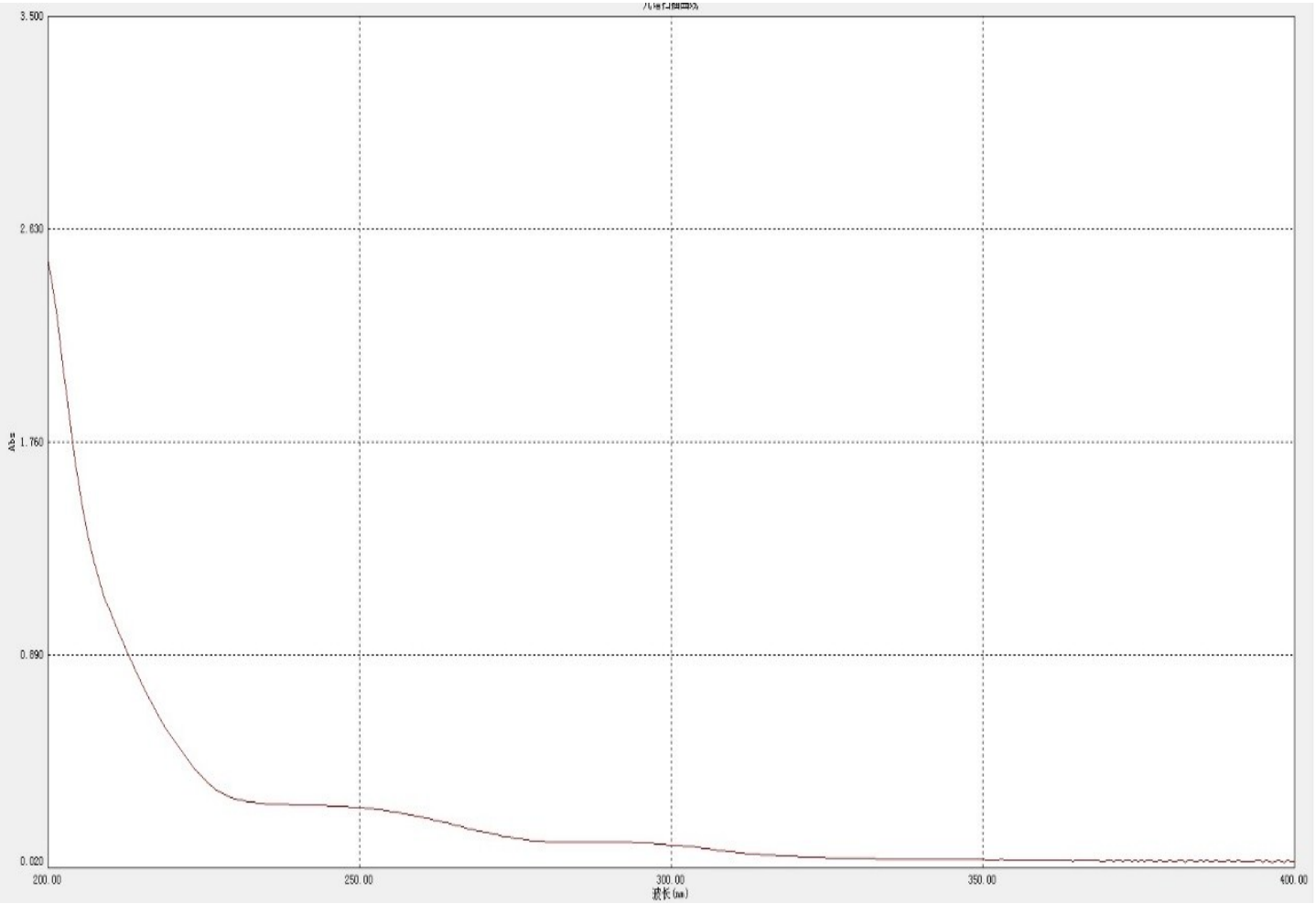
Figure S21. NOESY spectrum of Compound **2** in $CDCl_3$.

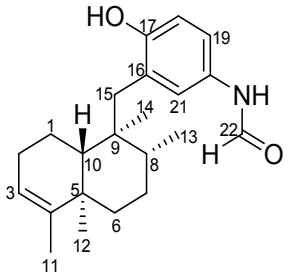




Dactylospongin B (2)

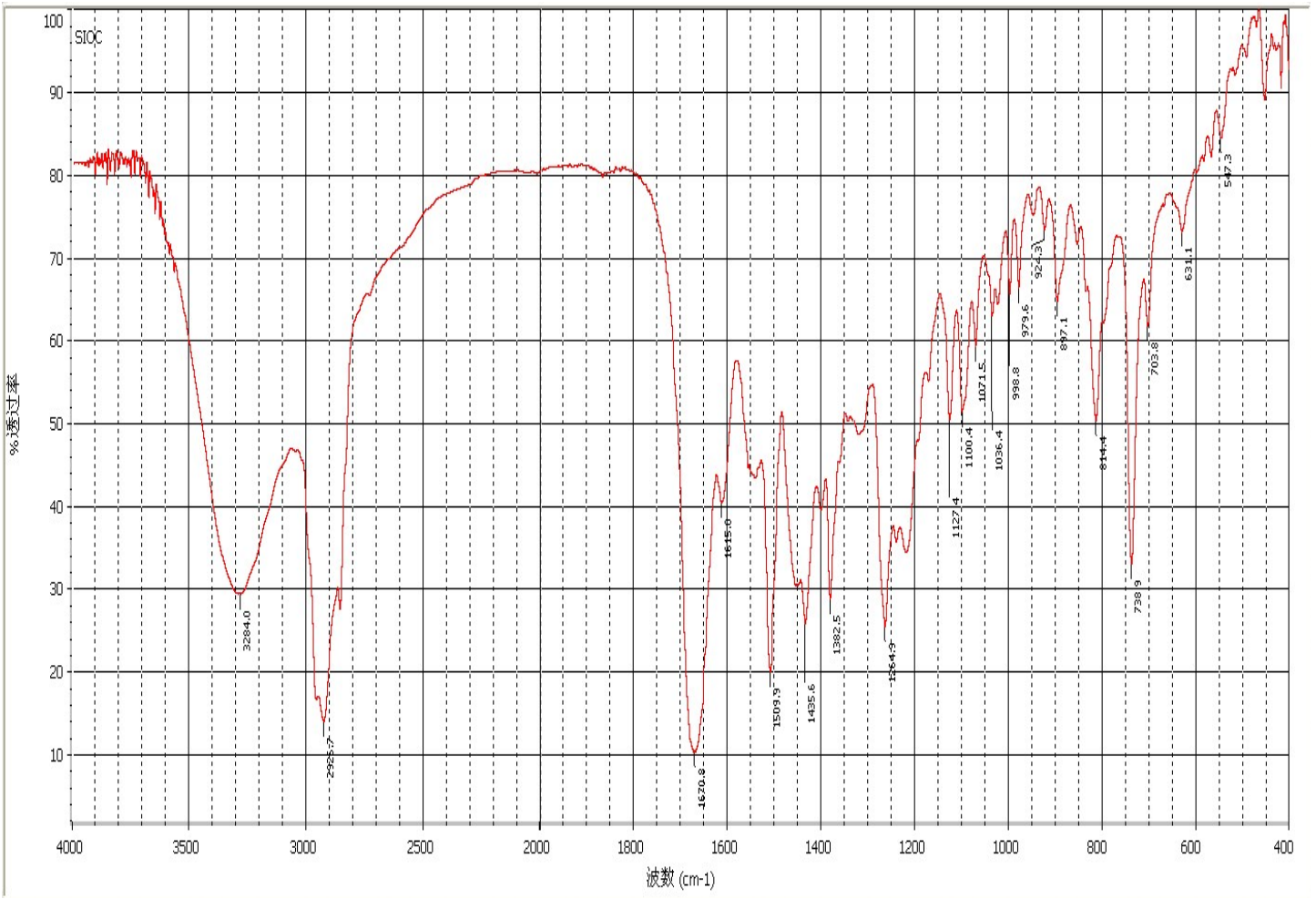
Figure S22. CD spectrum of Compound **2** in MeOH.

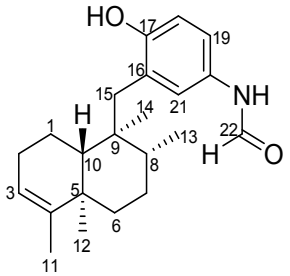




Actylospongin C (**3**)

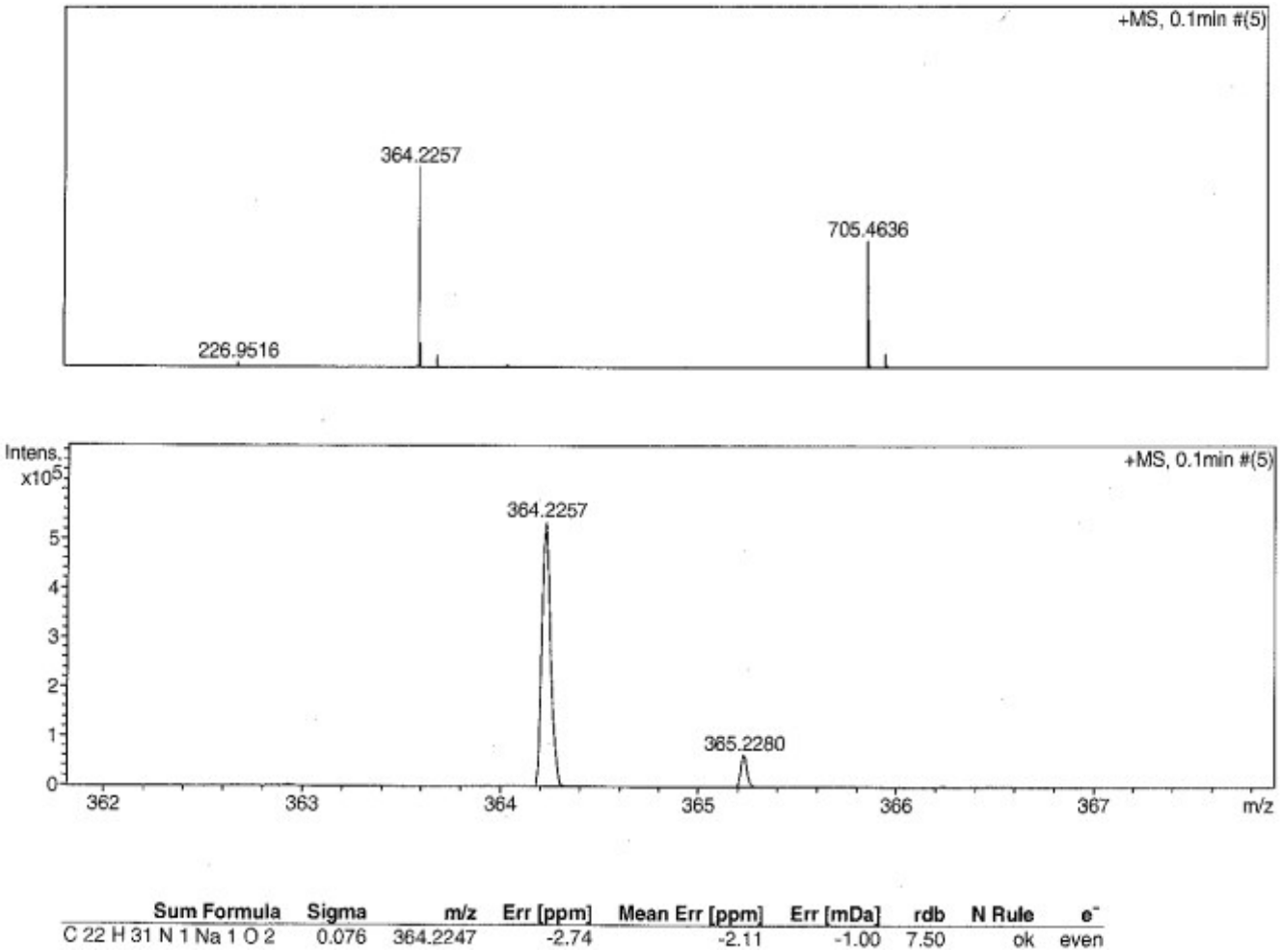
Figure S23. UV spectrum of Compound **3** in MeOH.



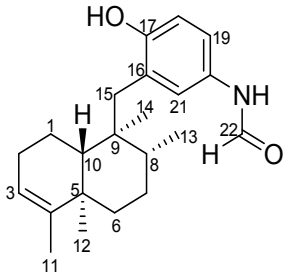


Actylospongin C (**3**)

Figure S24. IR spectrum of Compound **3**.

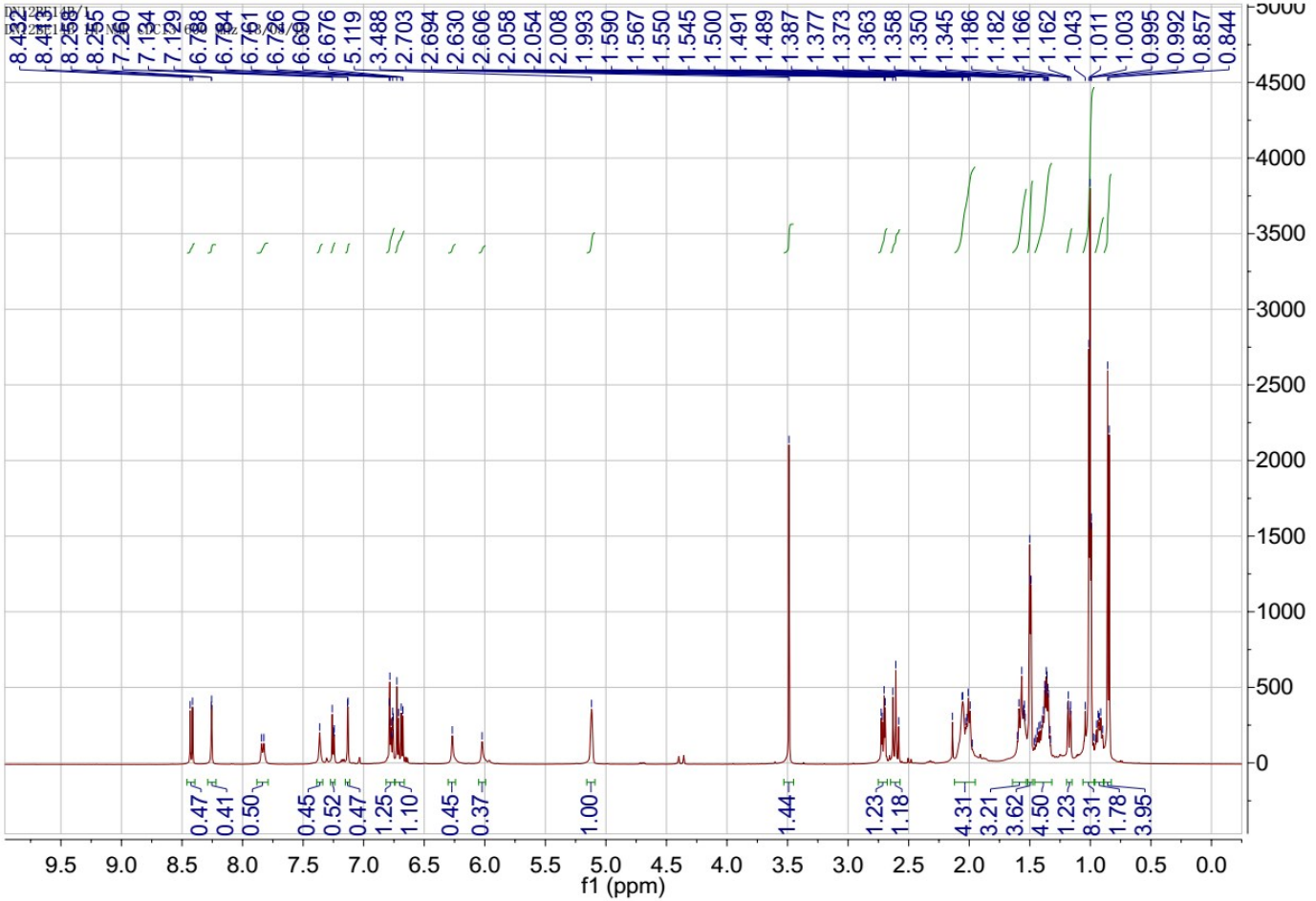


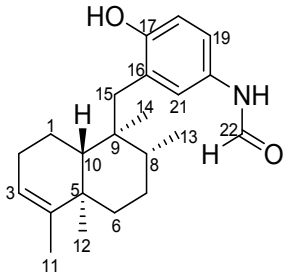
Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 22 H 31 N 1 Na 1 O 2	0.076	364.2247	-2.74	-2.11	-1.00	7.50	ok	even



Actylospongin C (**3**)

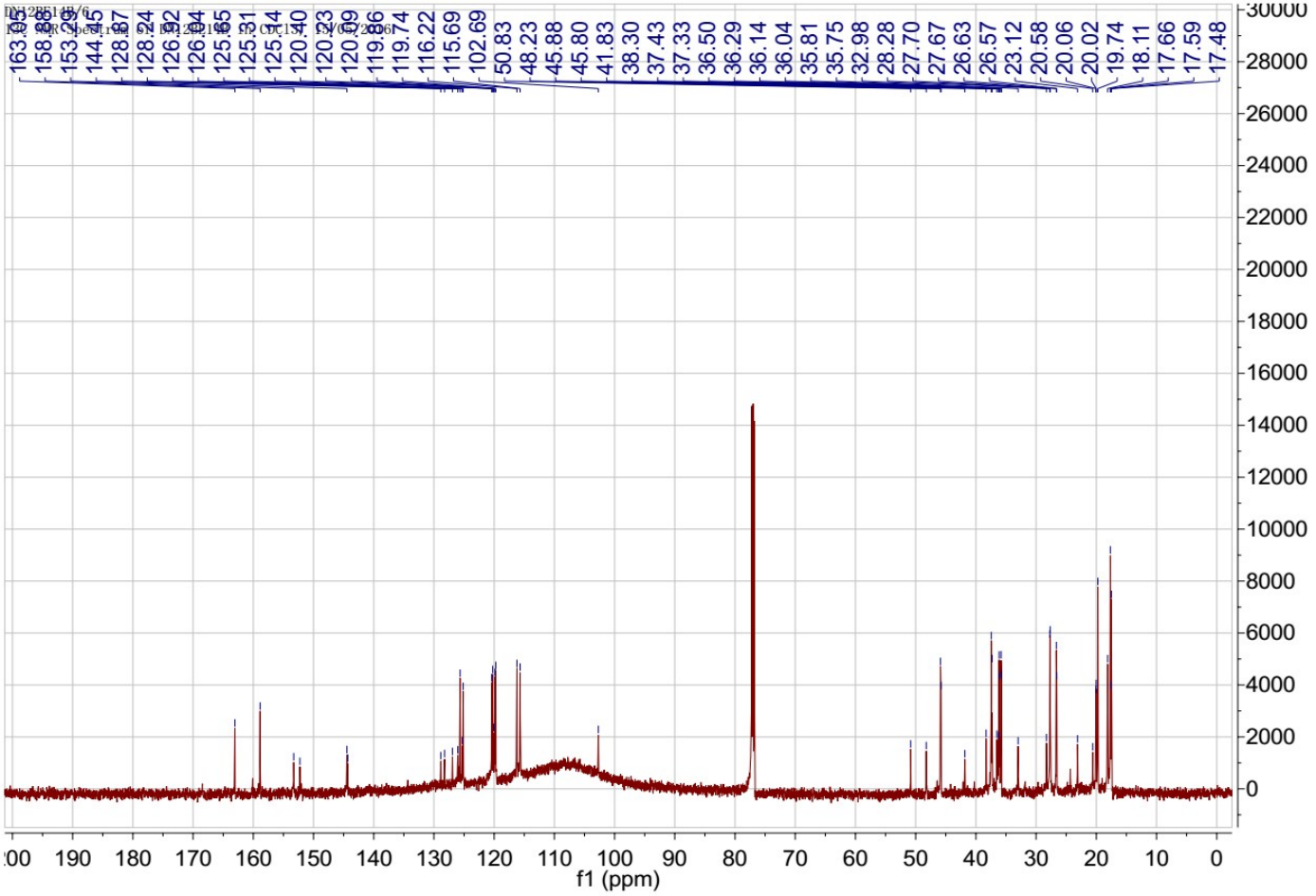
Figure S25. HRESIMS spectrum of Compound **3**.

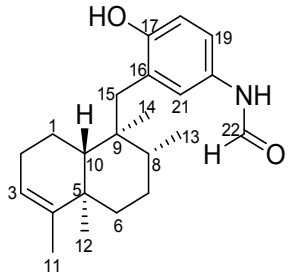




Actylospongin C (**3**)

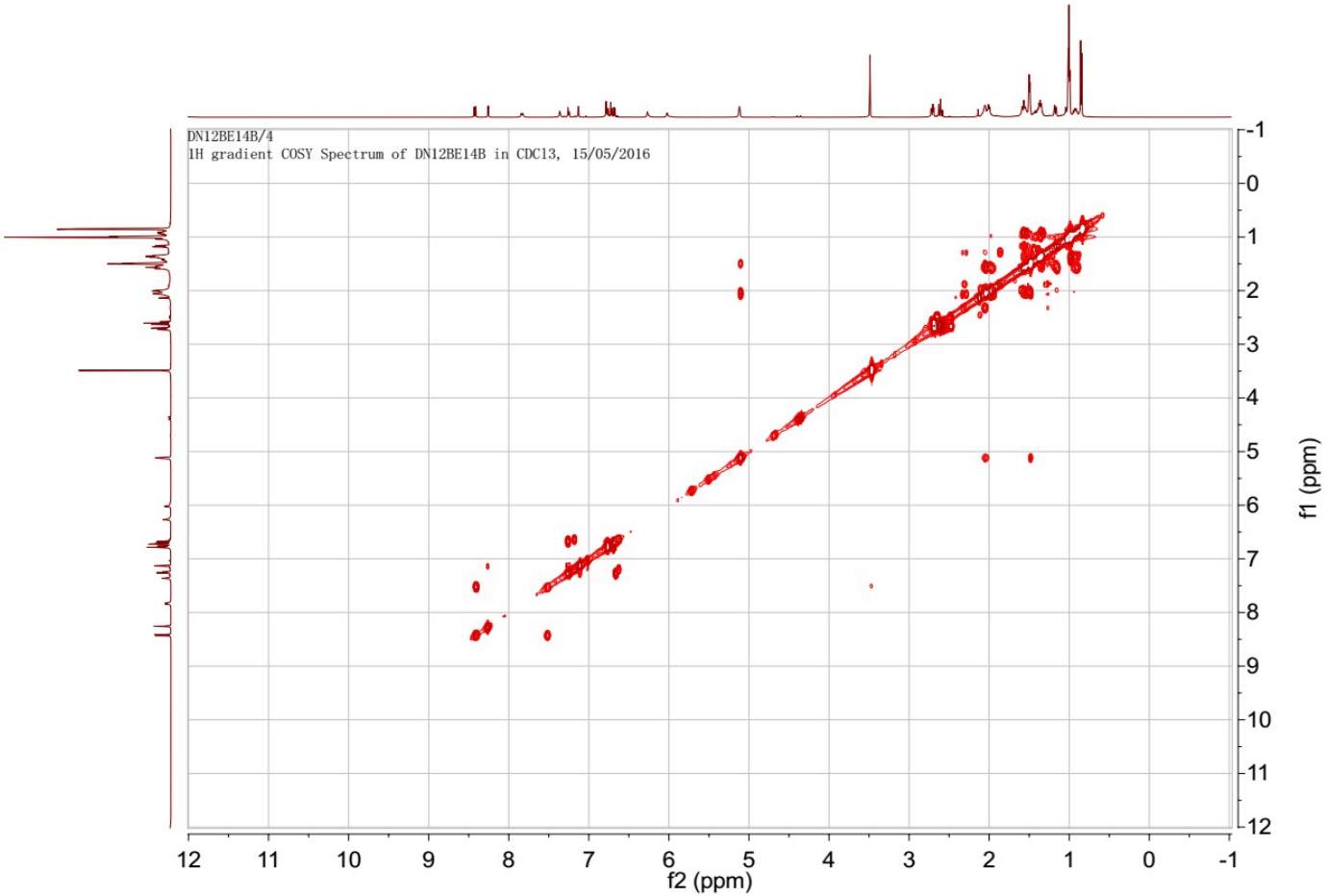
Figure S26. ^{1}H NMR spectrum of Compound **3** in $CDCl_3$.

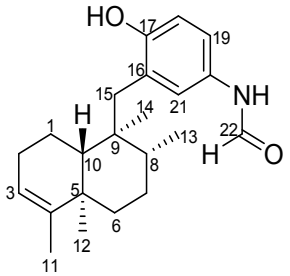




Actylospongin C (**3**)

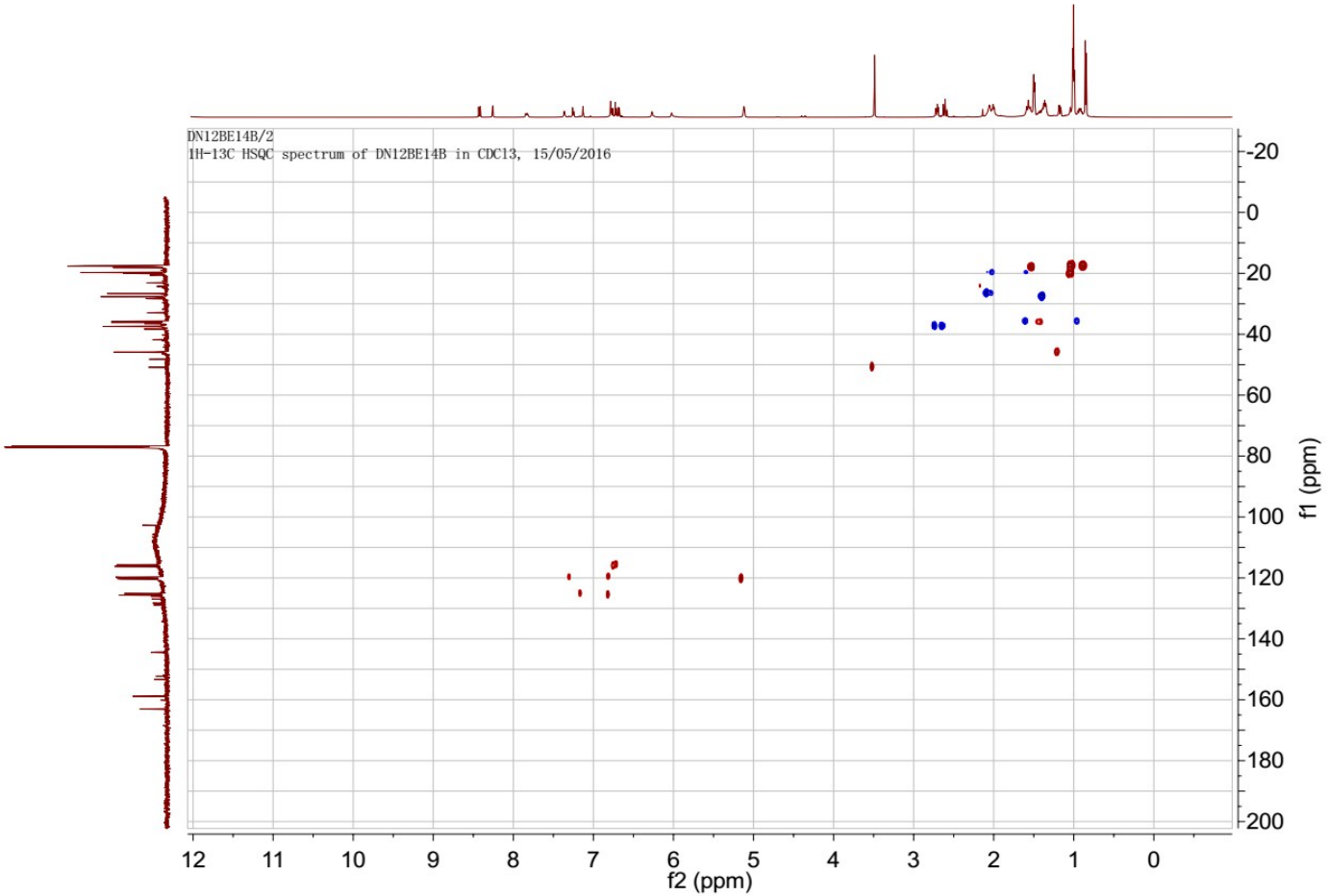
Figure S27. ^{13}C NMR spectrum of Compound **3** in $CDCl_3$.

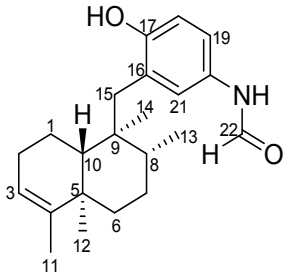




Actylospongin C (**3**)

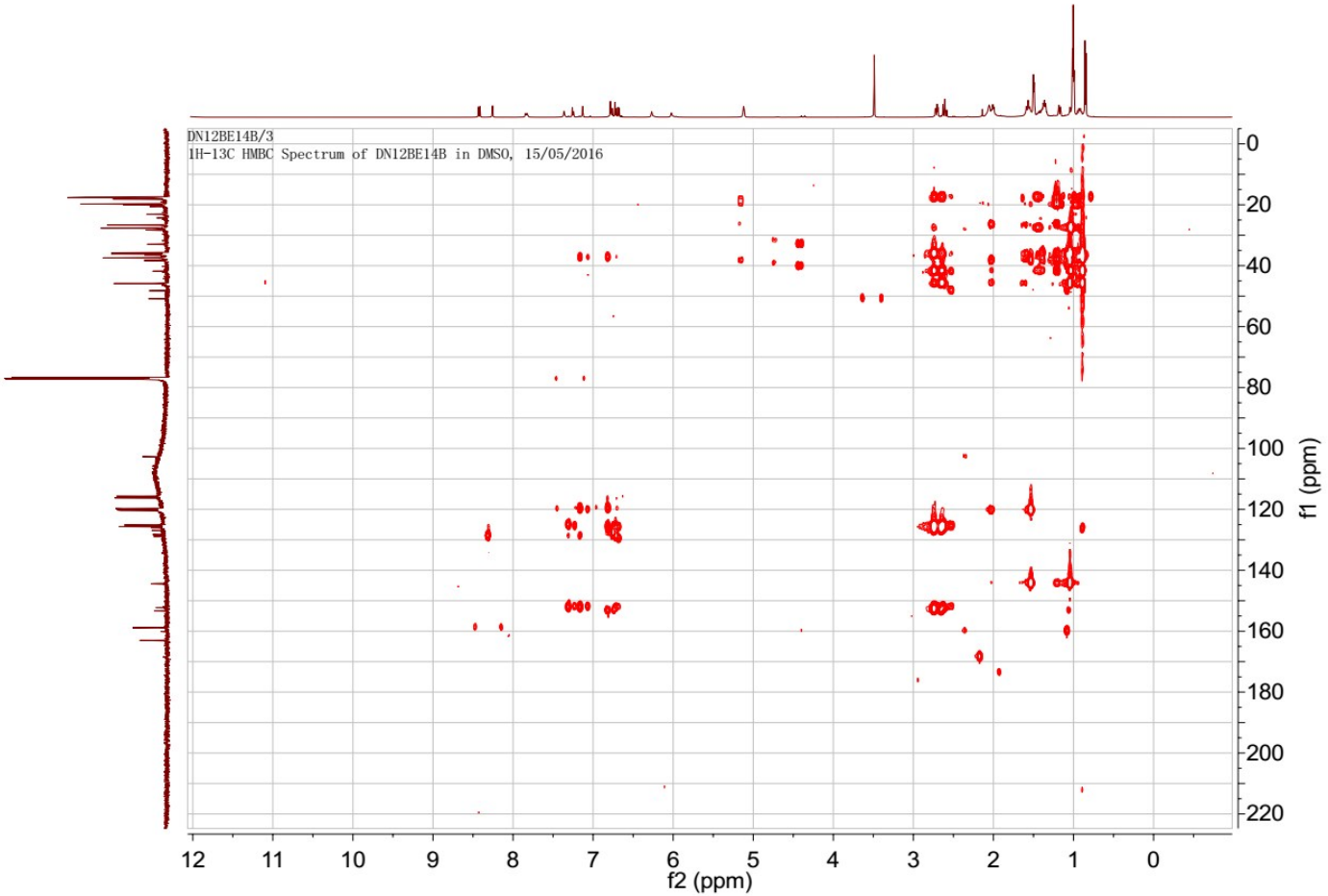
Figure S28. ^{1}H-^{1}H COSY spectrum of Compound **3** in $CDCl_3$.

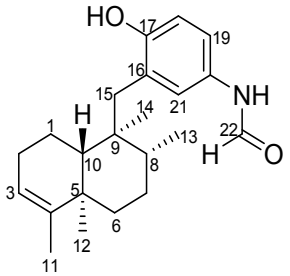




Actylospongin C (**3**)

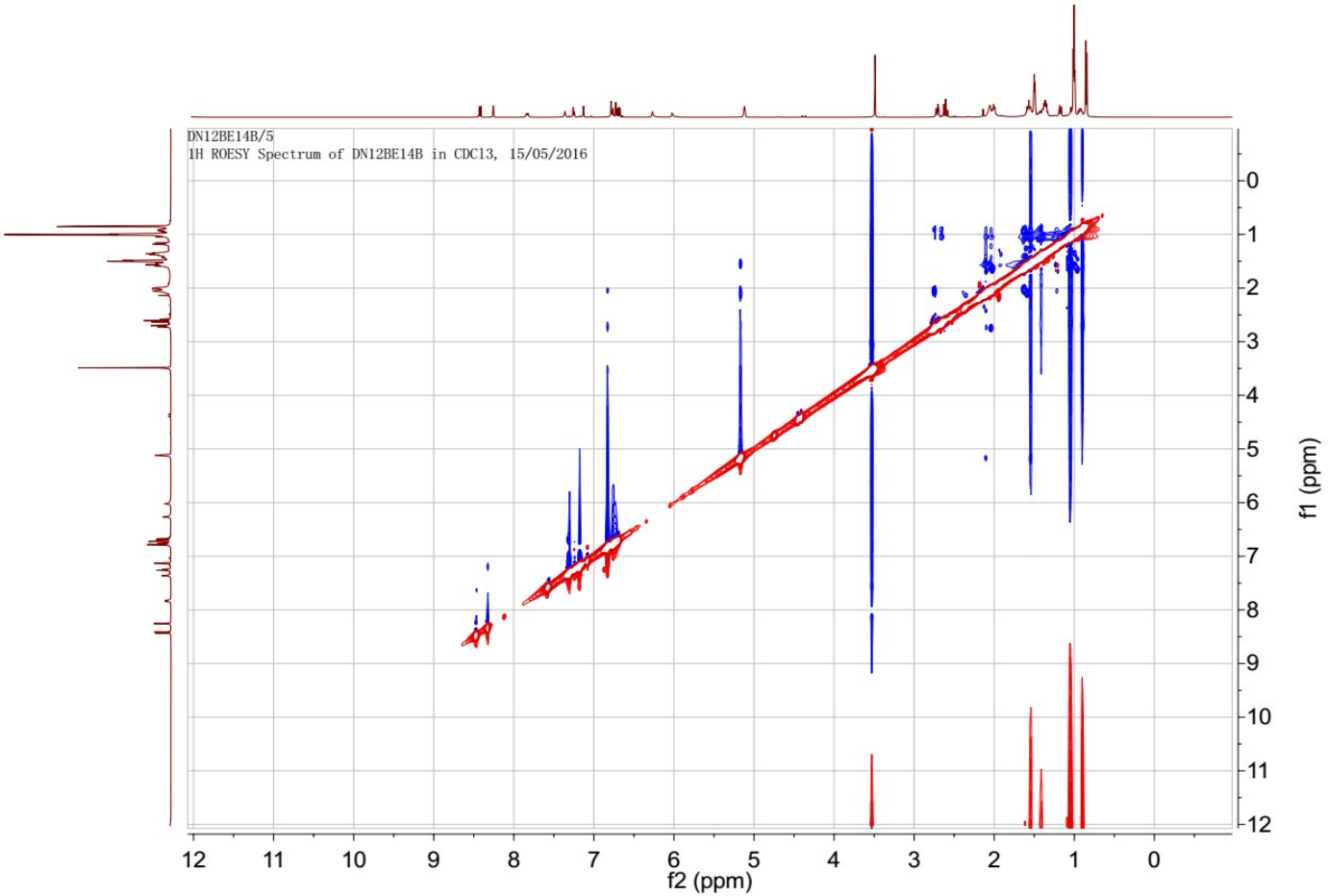
Figure S29. HSQC spectrum of Compound **3** in $CDCl_3$.

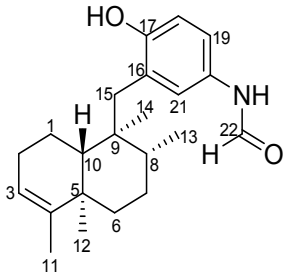




Actylospongin C (**3**)

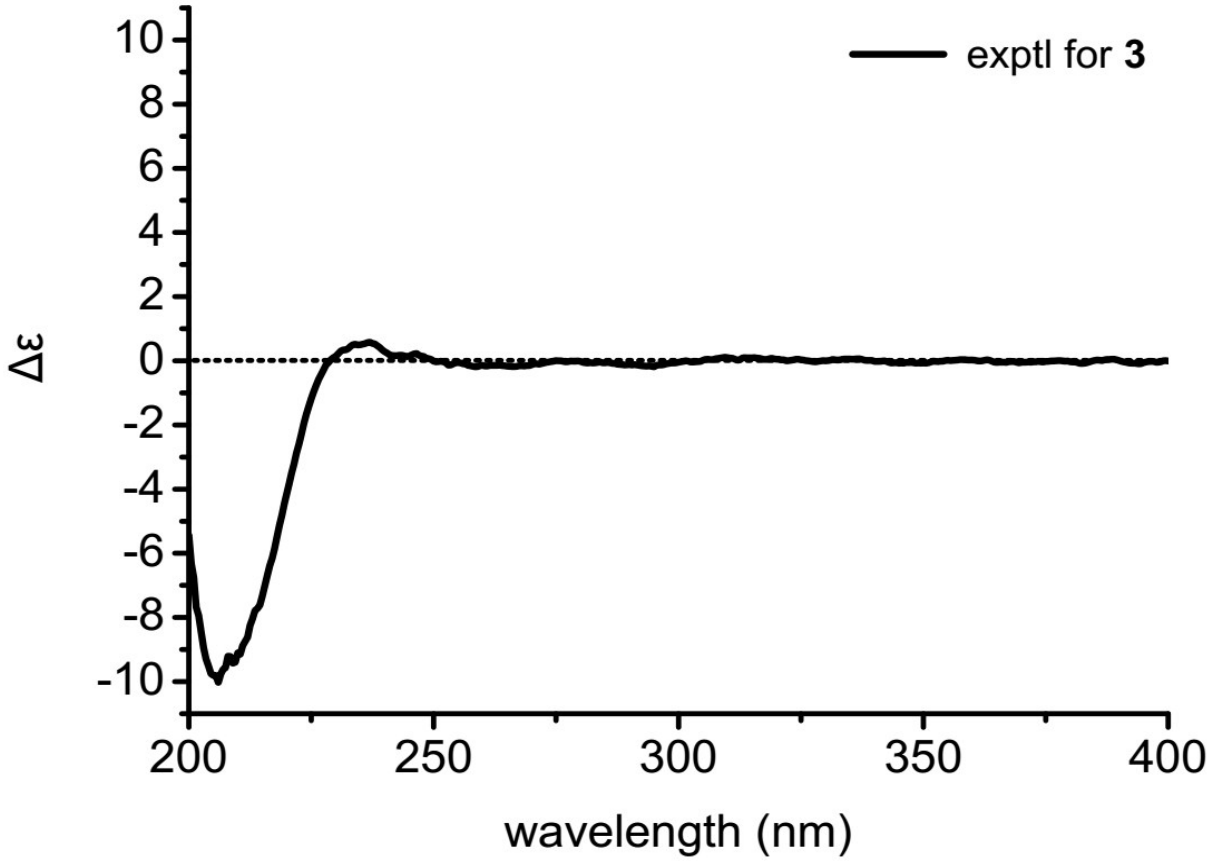
Figure S30. HMBC spectrum of Compound **3** in $CDCl_3$.

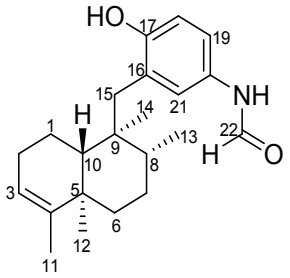




Actylospongin C (**3**)

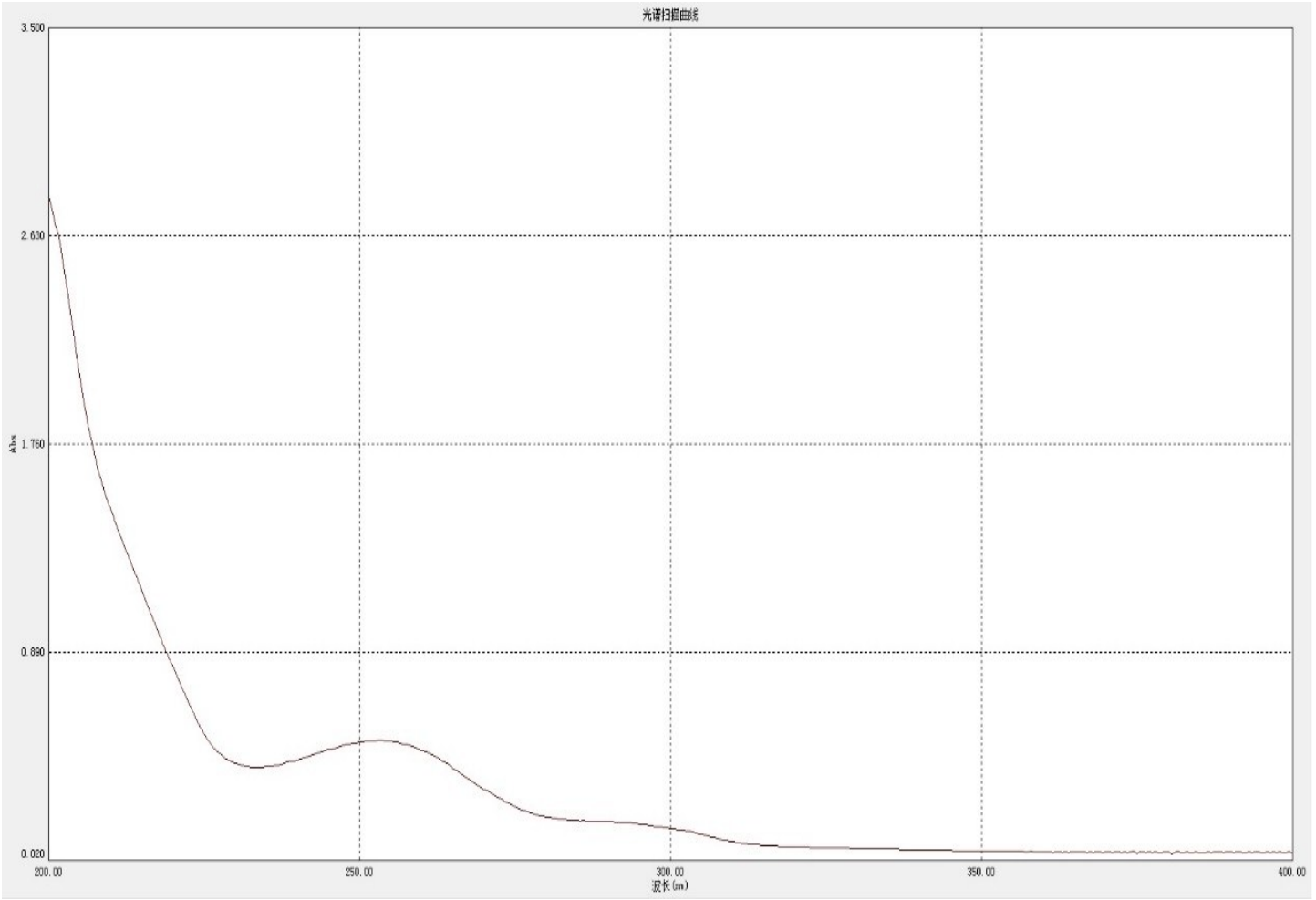
Figure S31. NOESY spectrum of Compound **3** in $CDCl_3$.

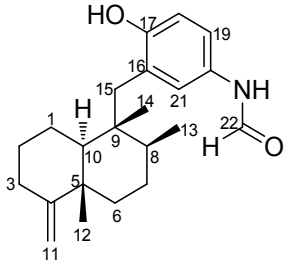




Actylospongin C (**3**)

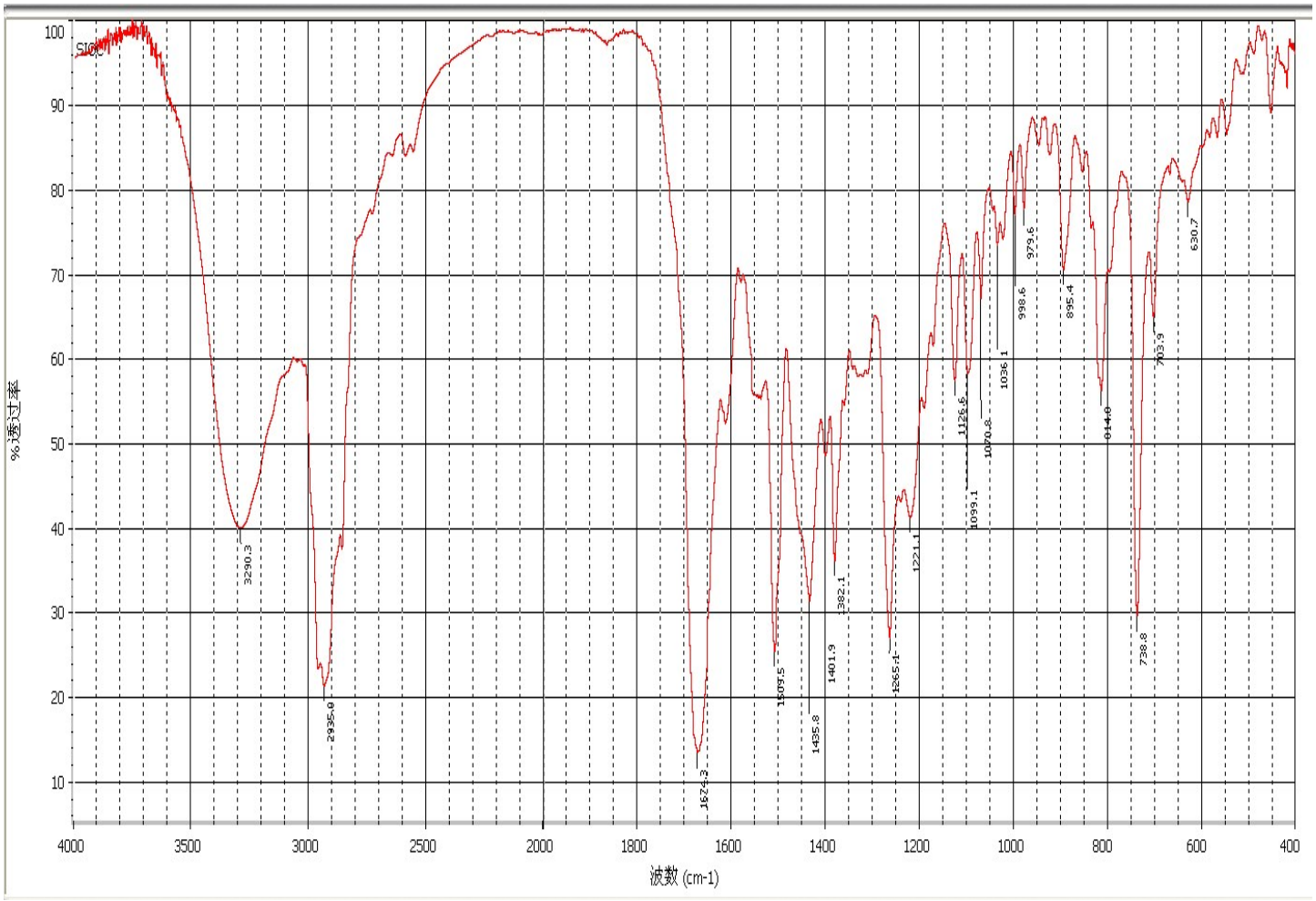
Figure S32. CD spectrum of Compound **3** in MeOH.

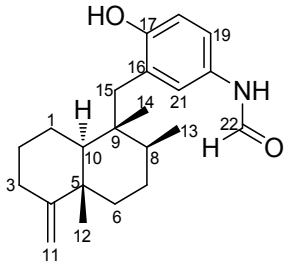




Dactylospongin D (**4**)

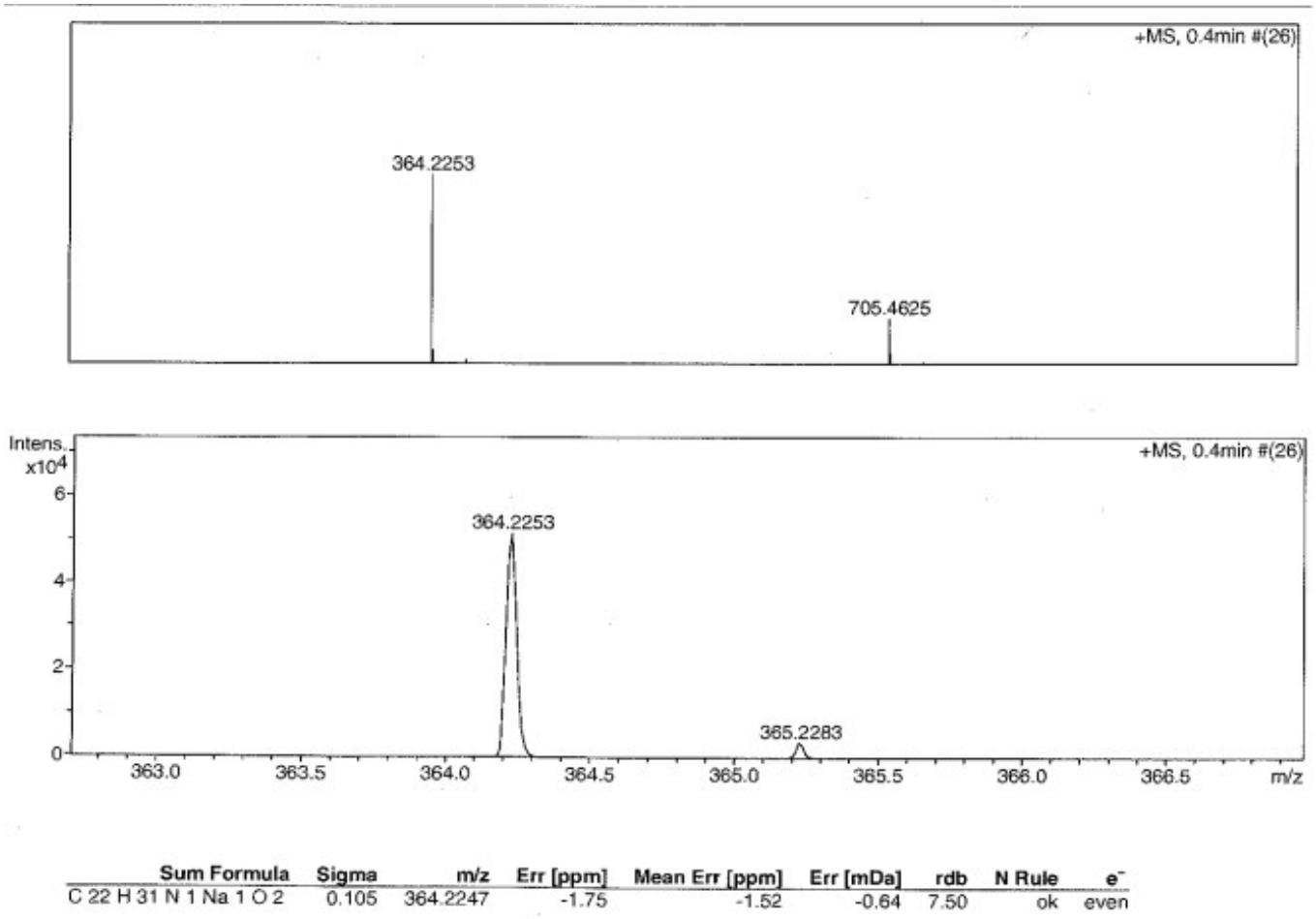
Figure S33. UV spectrum of Compound **4** in MeOH.



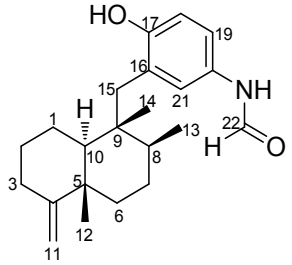


Dactylospongin D (**4**)

Figure S34. IR spectrum of Compound **4**.

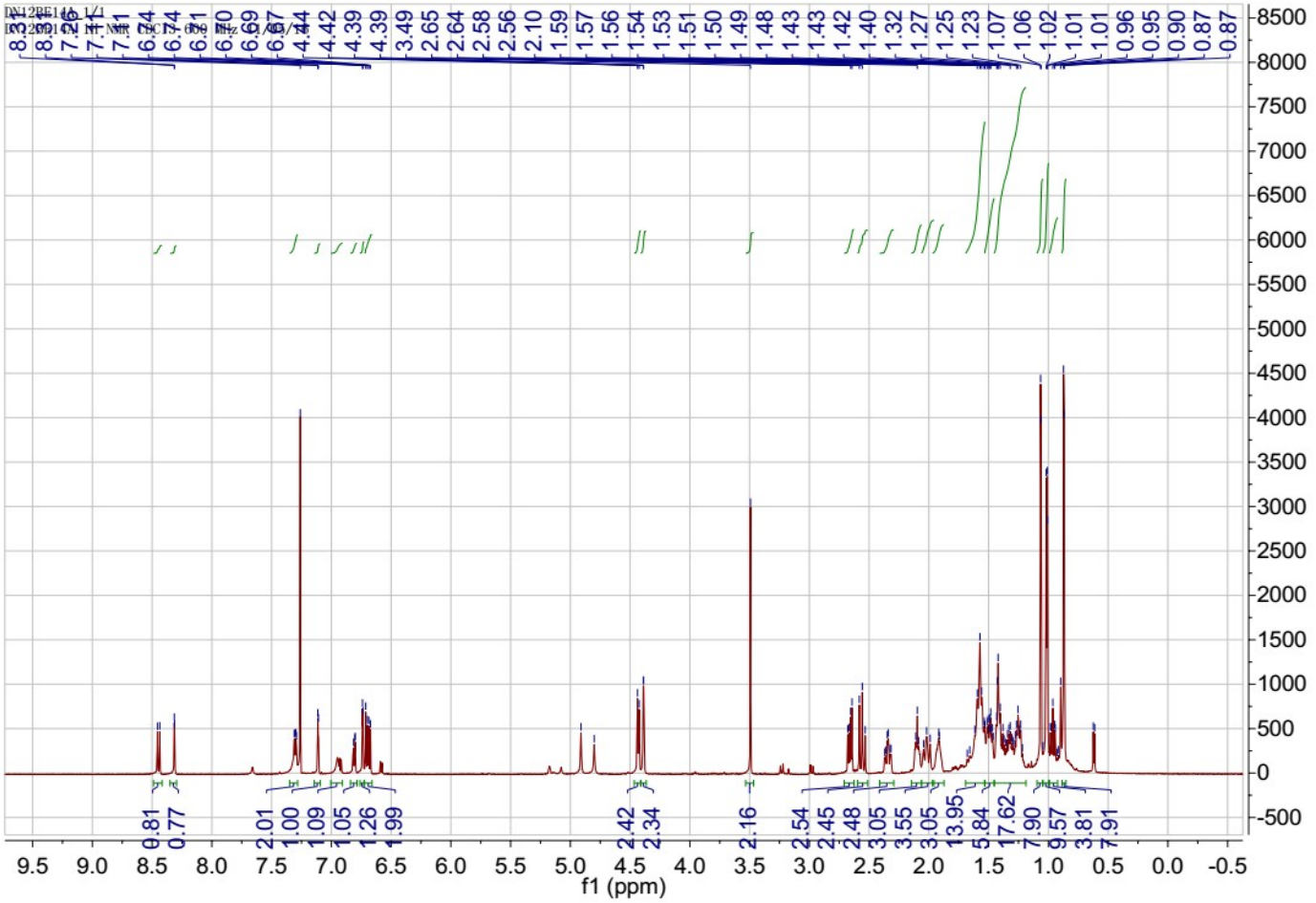


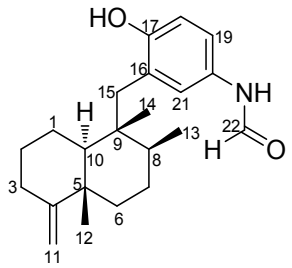
Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 22 H 31 N 1 Na 1 O 2	0.105	364.2247	-1.75	-1.52	-0.64	7.50	ok	even



Dactylospongin D (**4**)

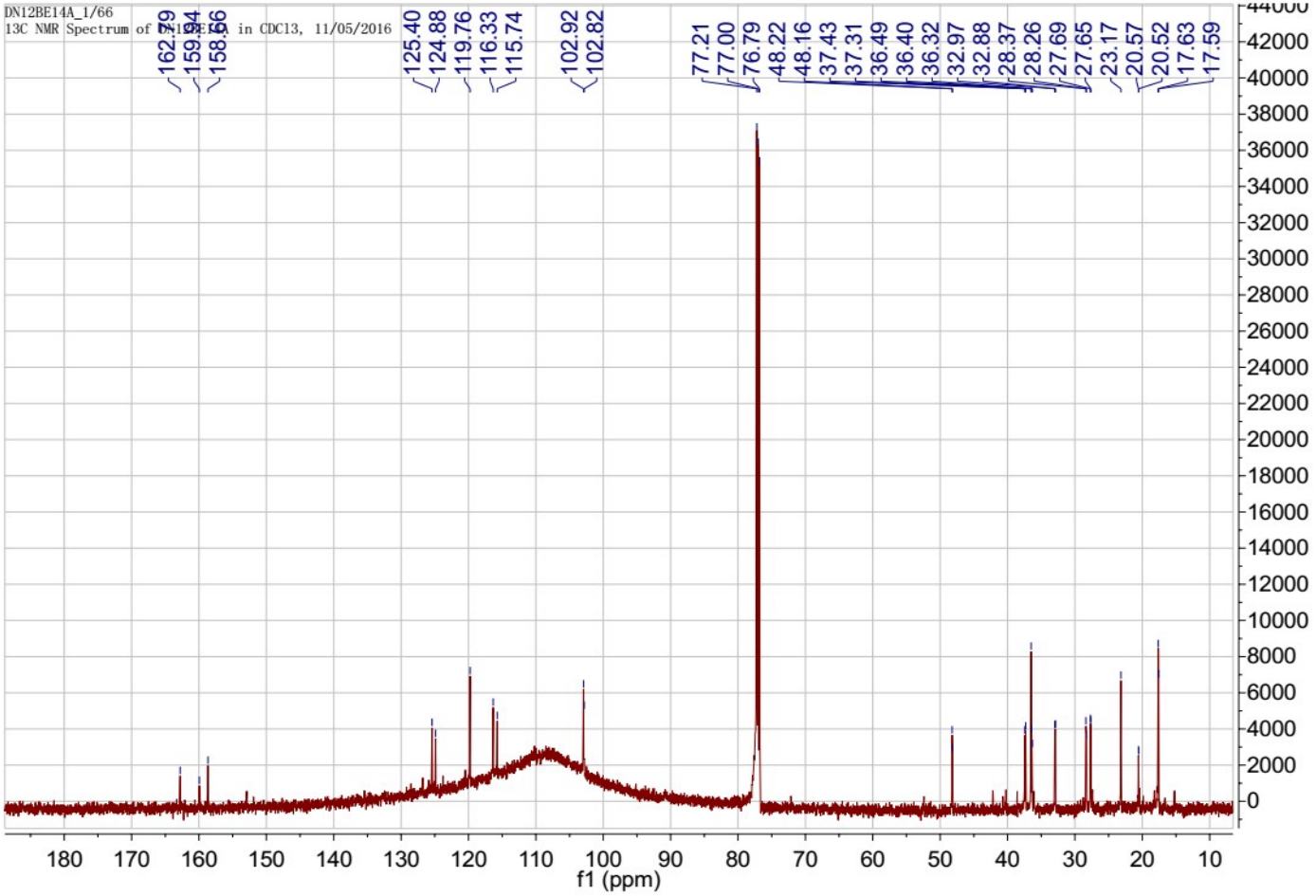
Figure S35. HRESIMS spectrum of Compound **4**.

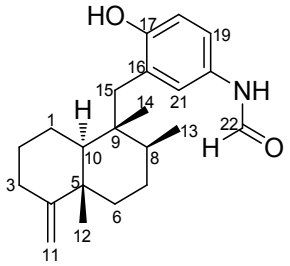




Dactylospongin D (**4**)

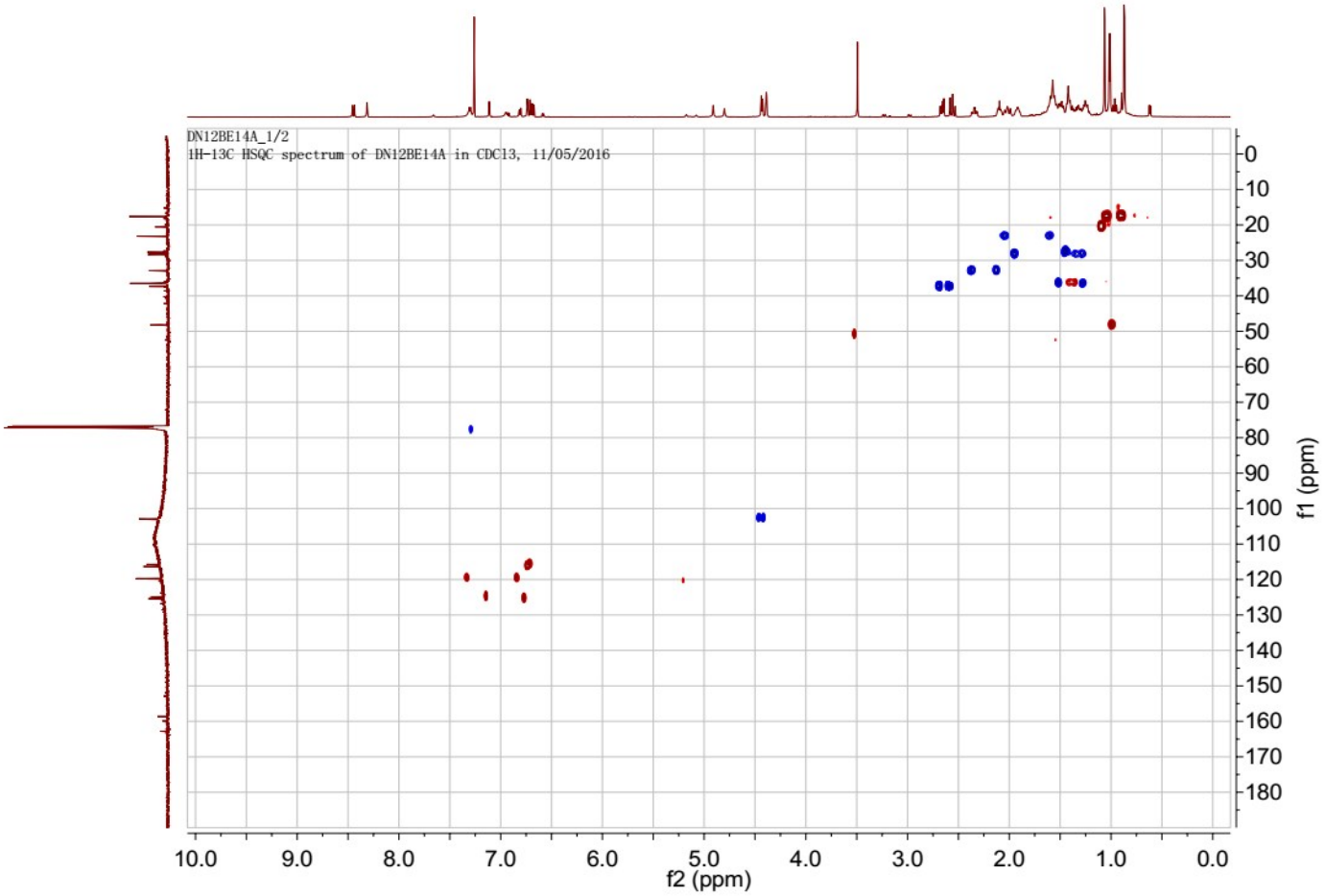
Figure S36. ^{1}H NMR spectrum of Compound **4** in $CDCl_3$.

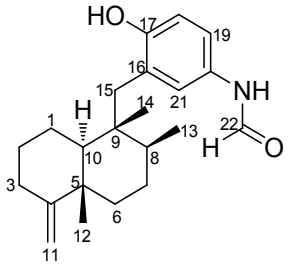




Dactylospongin D (**4**)

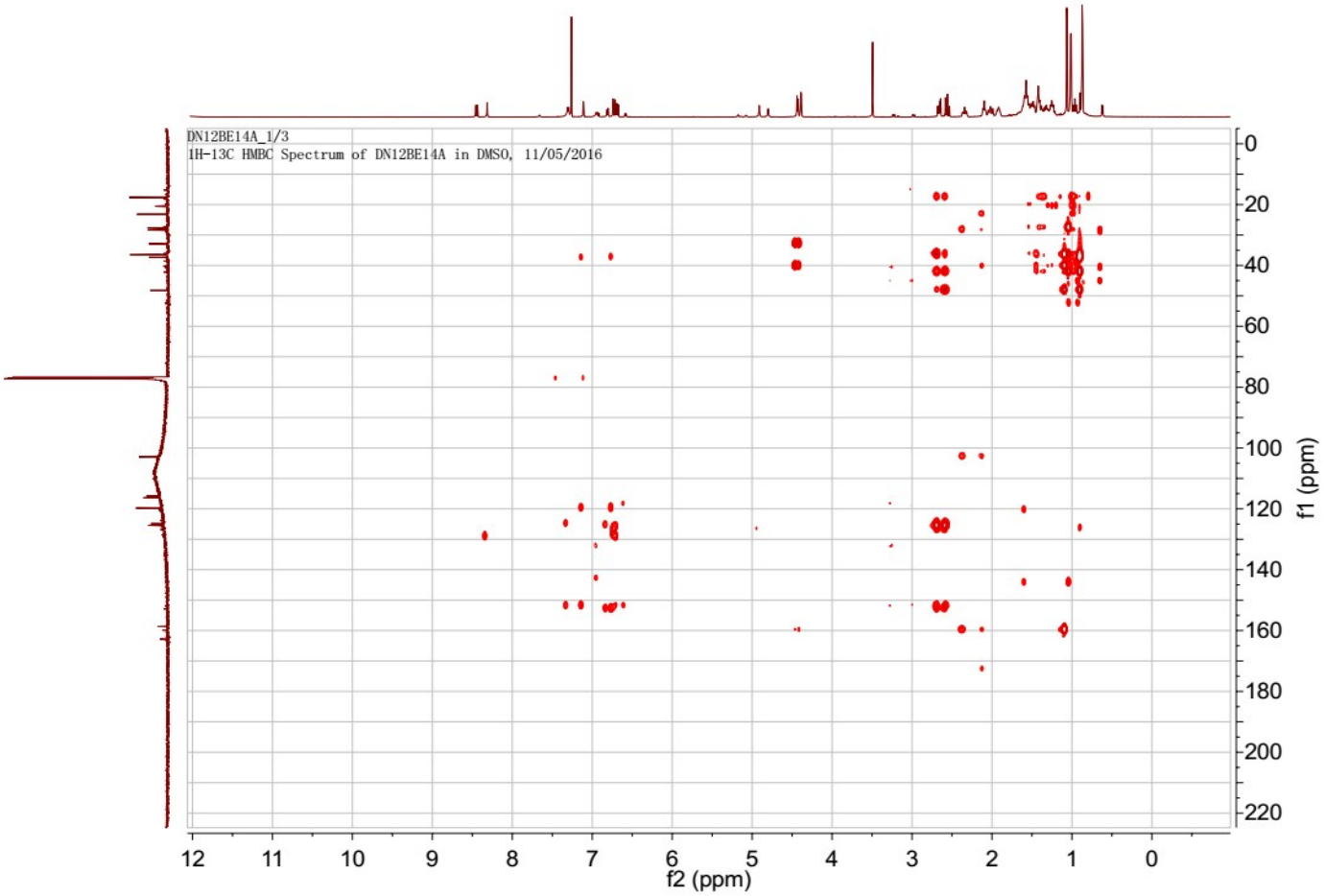
Figure S37. ^{13}C NMR spectrum of Compound **4** in $CDCl_3$.

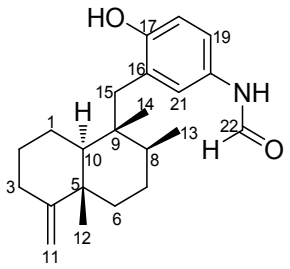




Dactylospongin D (**4**)

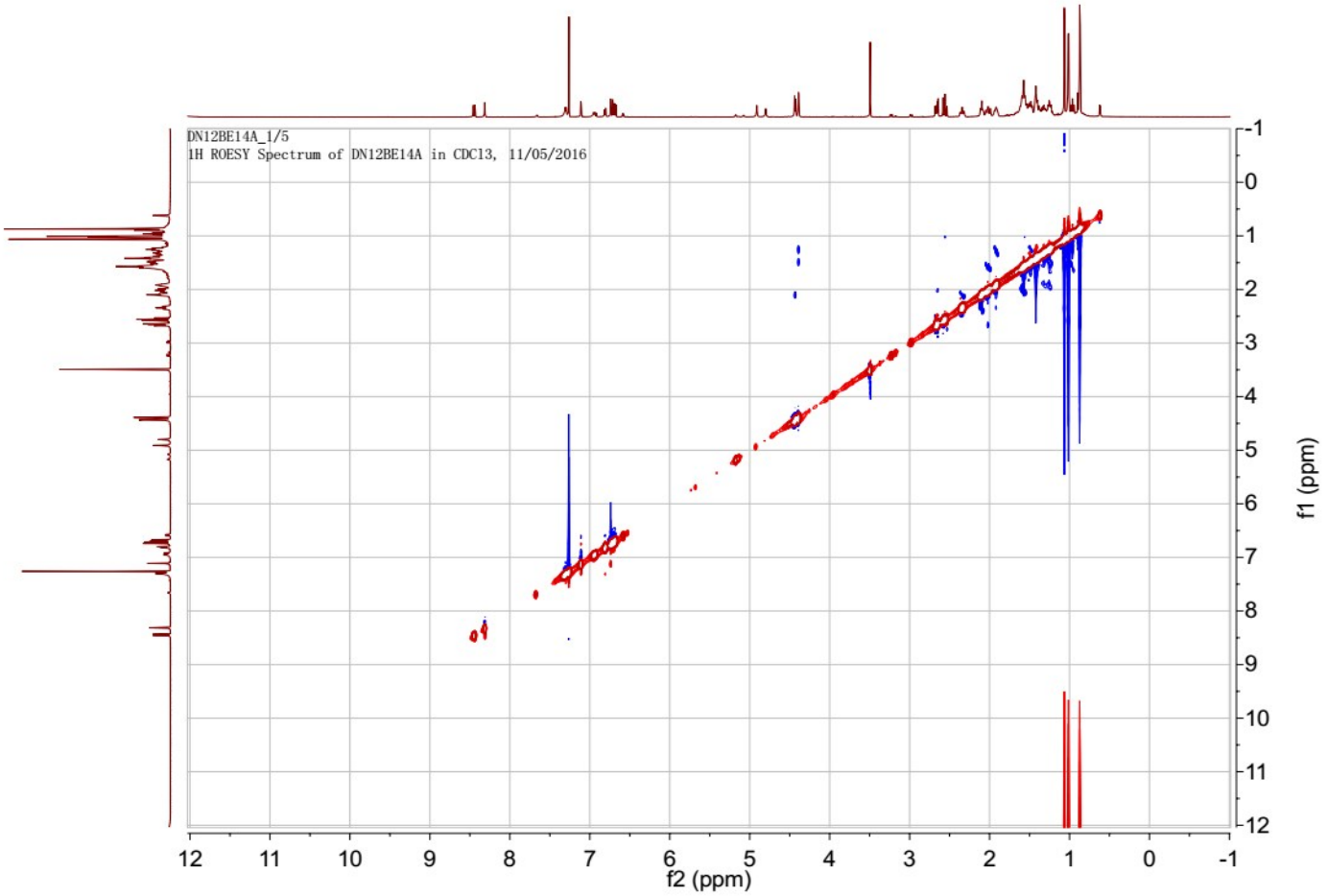
Figure S38. HSQC spectrum of Compound **4** in $CDCl_3$.

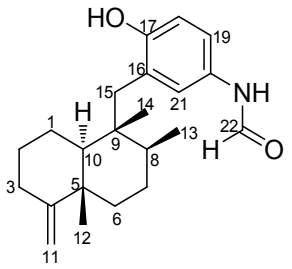




Dactylospongin D (**4**)

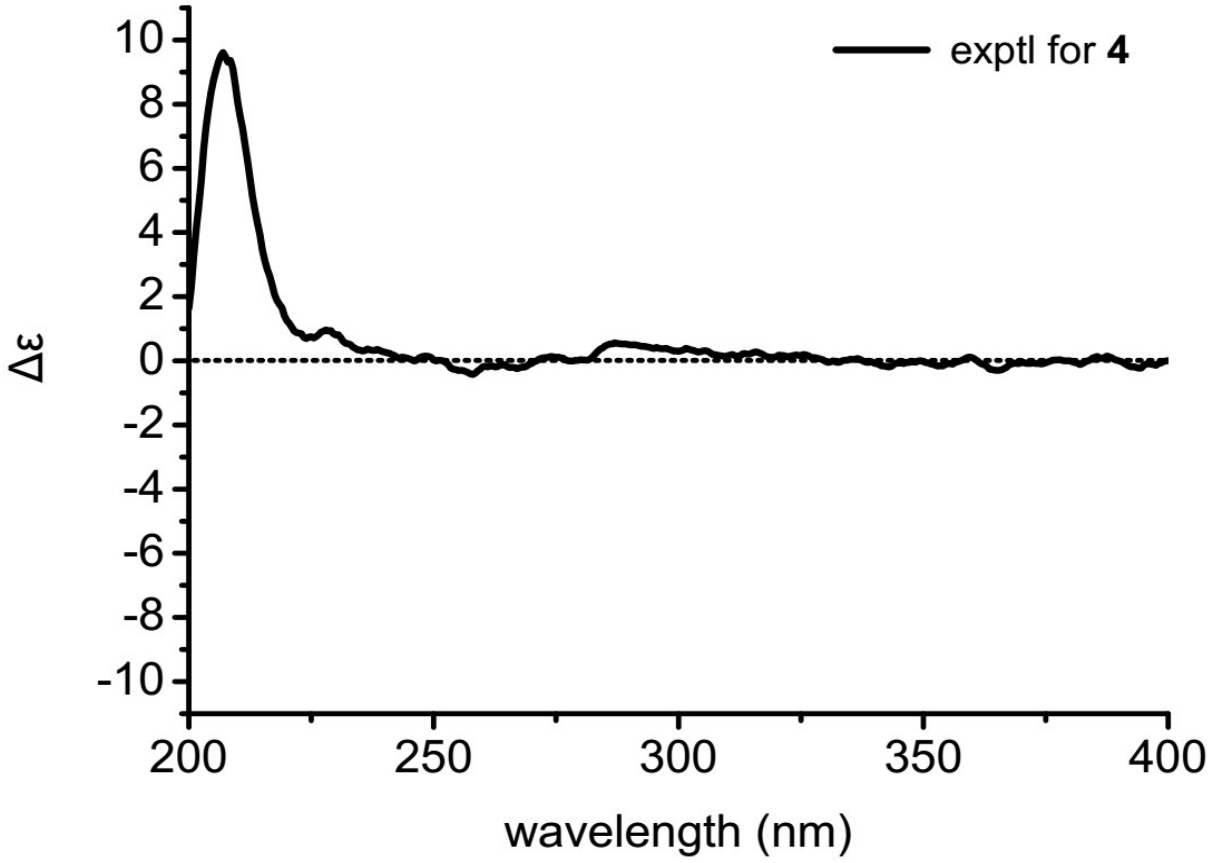
Figure S39. HMBC spectrum of Compound **4** in $CDCl_3$.

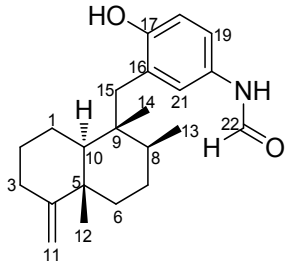




Dactylospongin D (**4**)

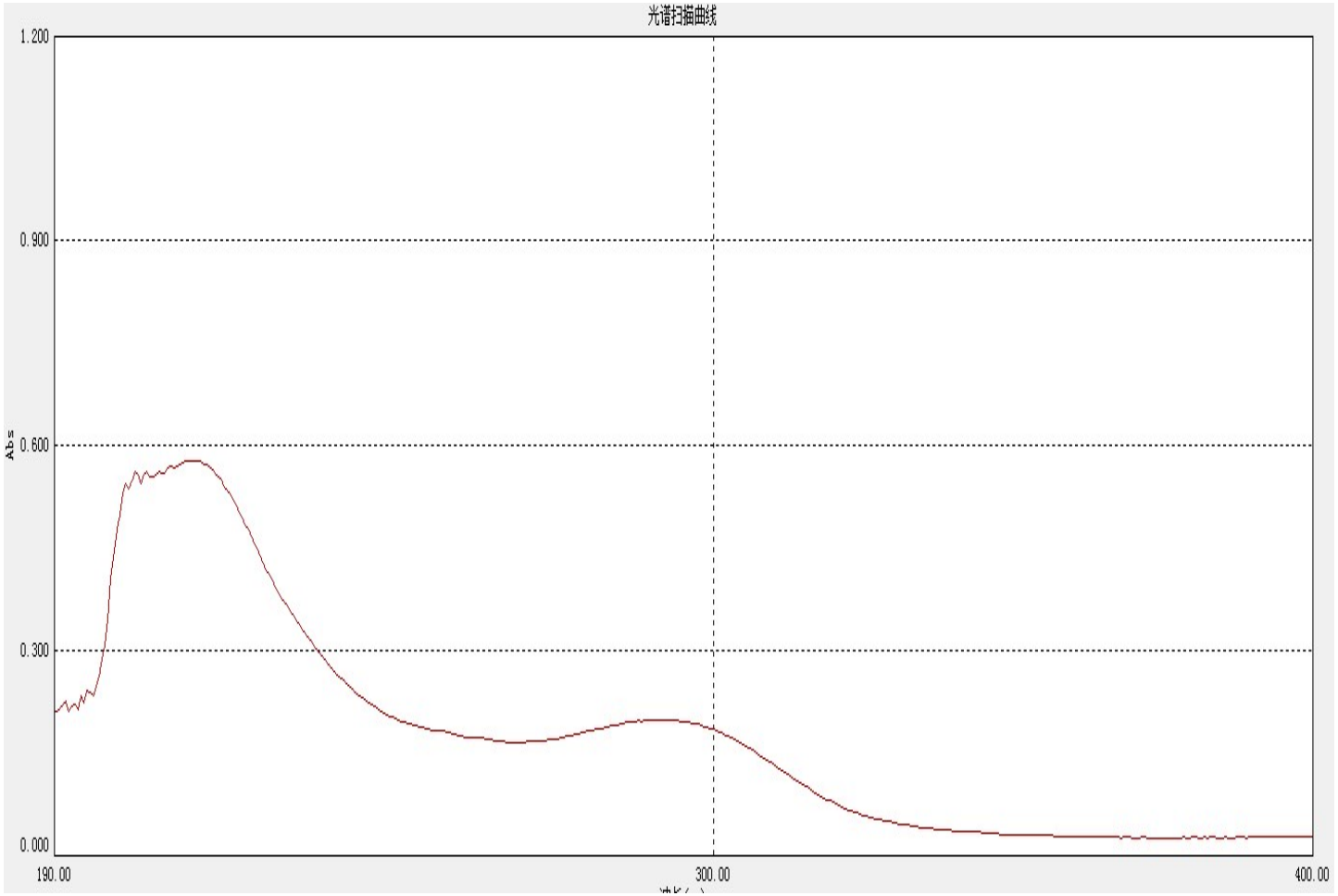
Figure S40. NOESY spectrum of Compound **4** in $CDCl_3$.

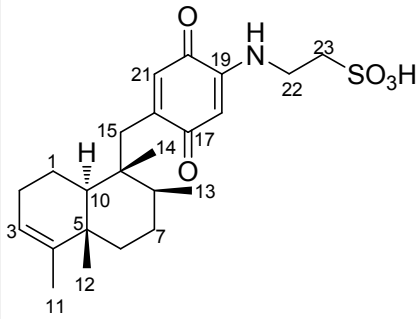




Dactylospongin D (**4**)

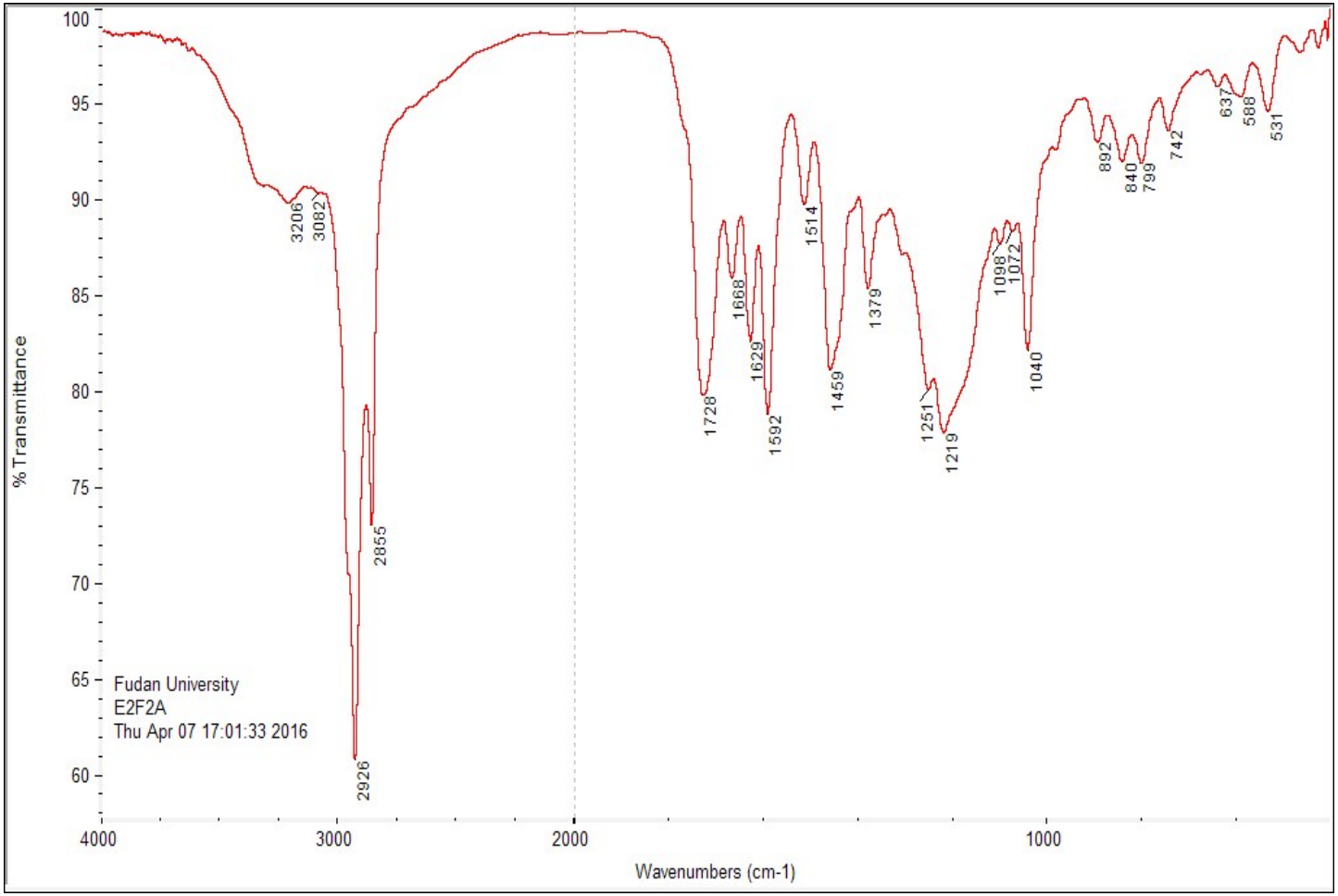
Figure S41. CD spectrum of Compound **4** in MeOH.

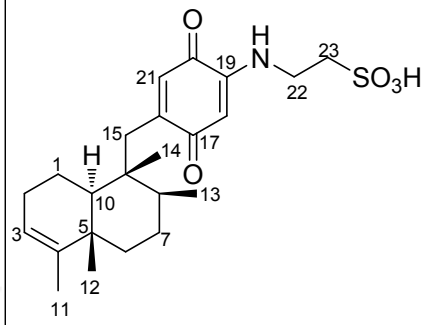




Ent-melemeleone B (**5**)

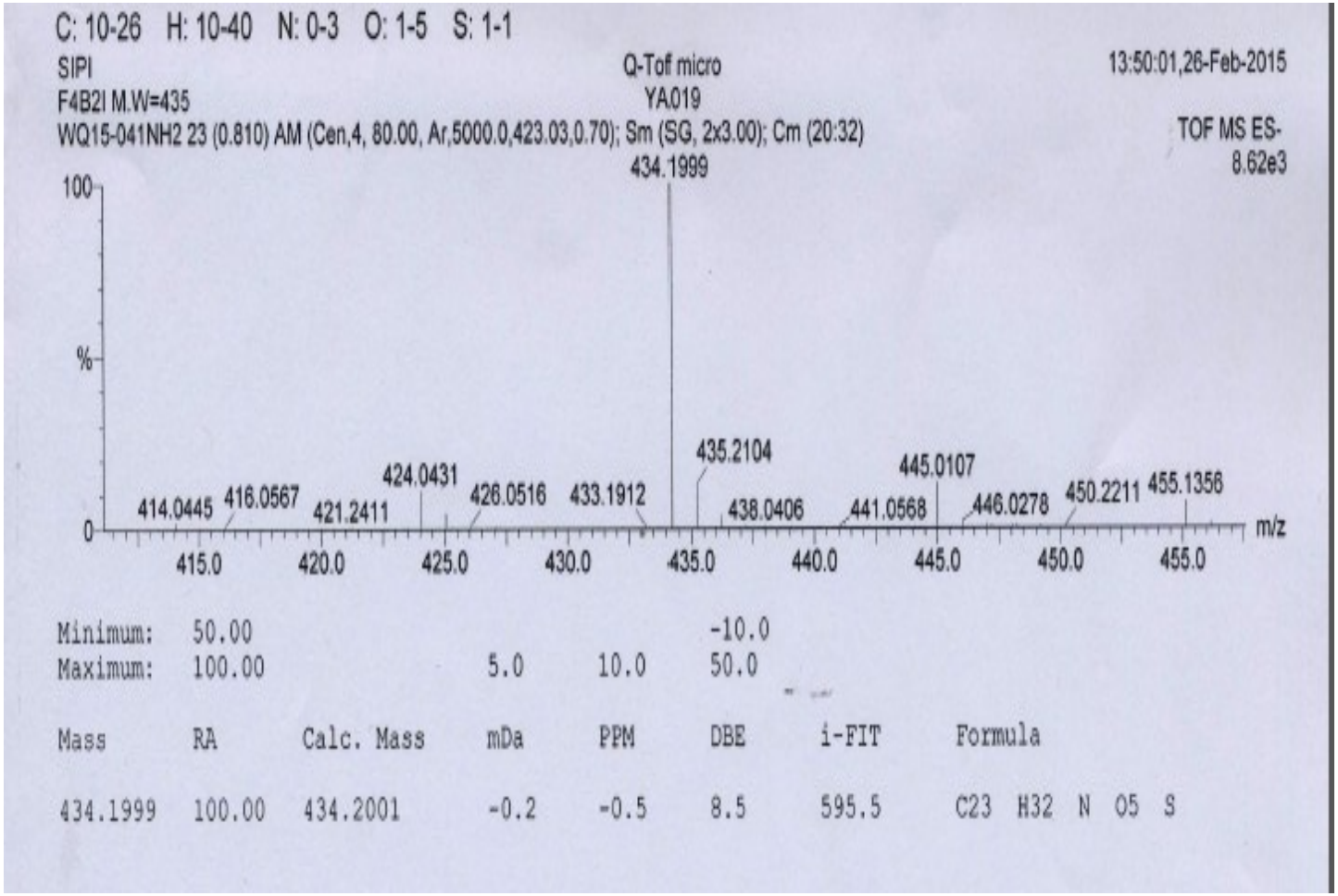
Figure S42. UV spectrum of Compound **5** in MeOH.

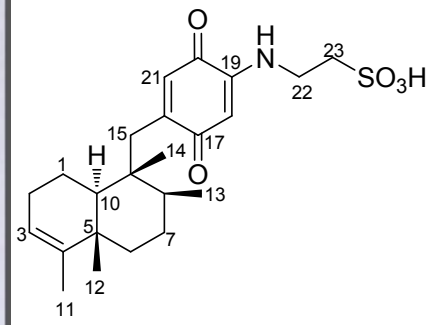




Ent-melemeleone B (**5**)

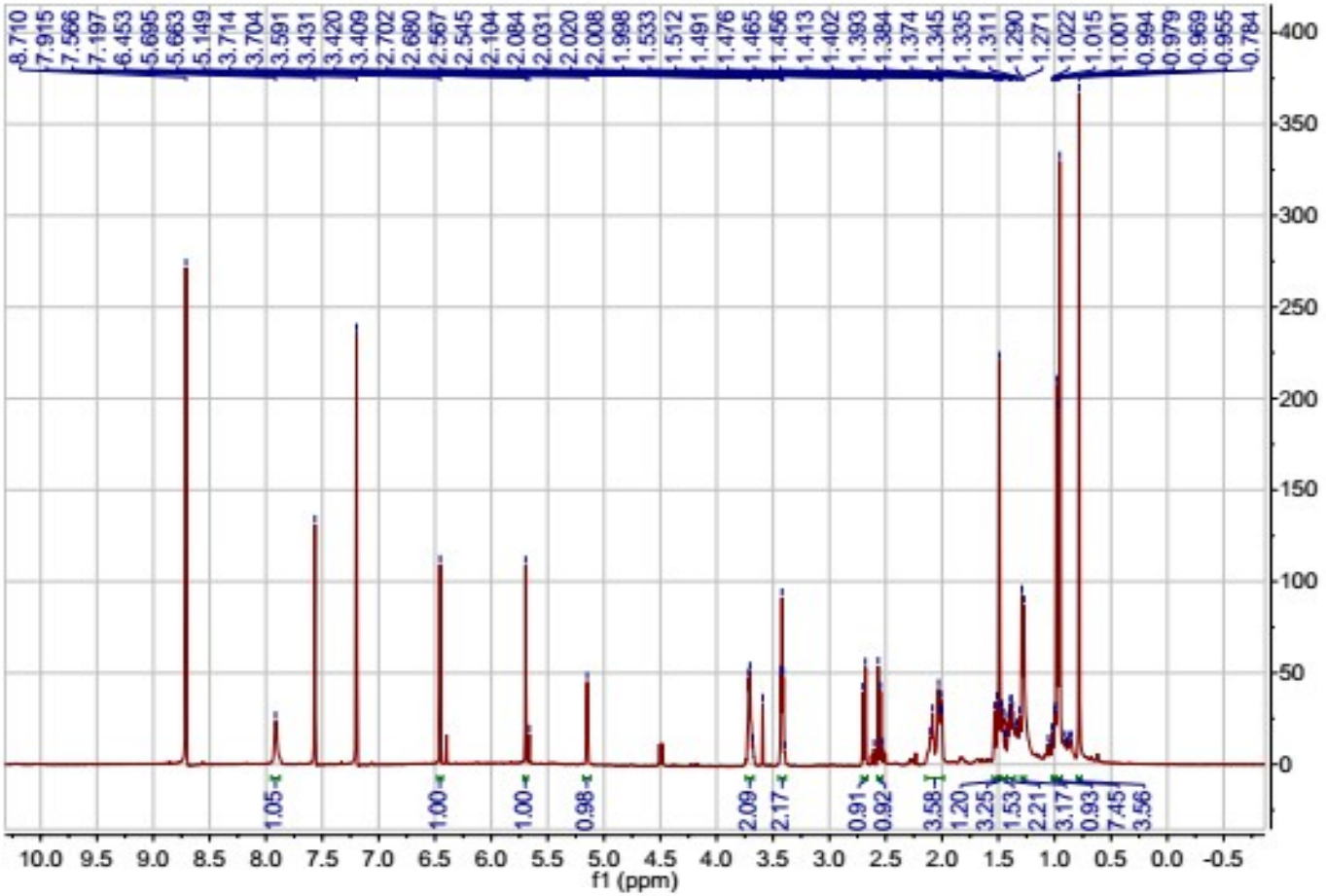
Figure S43. IR spectrum of Compound **5**.

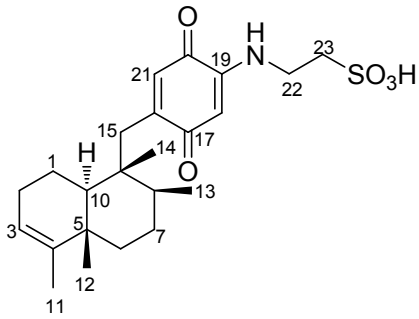




Ent-melemeleone B (**5**)

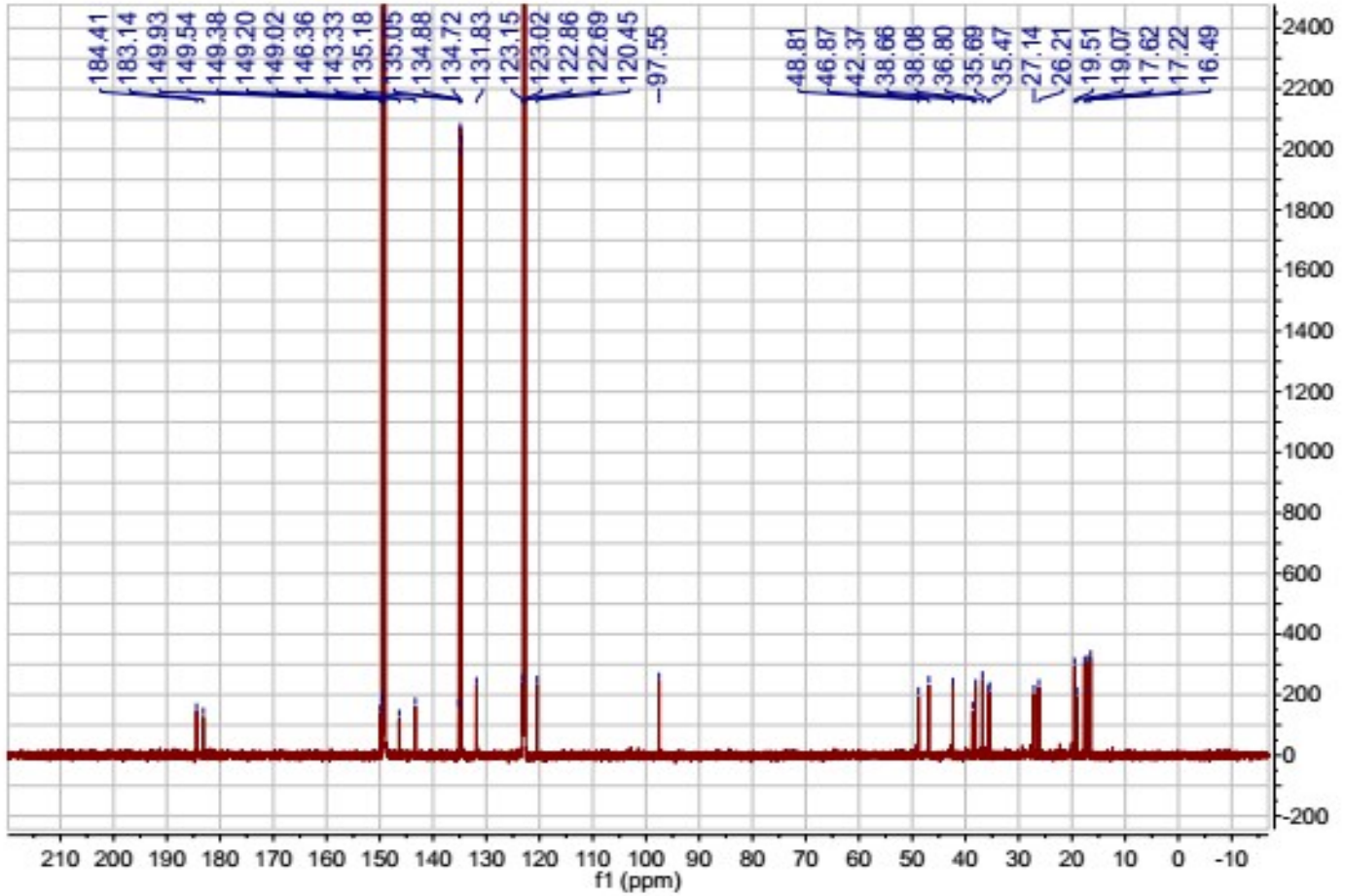
Figure S44. HRESIMS spectrum of Compound **5**.

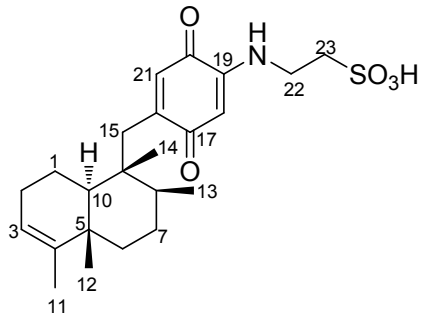




Ent-melemeleone B (**5**)

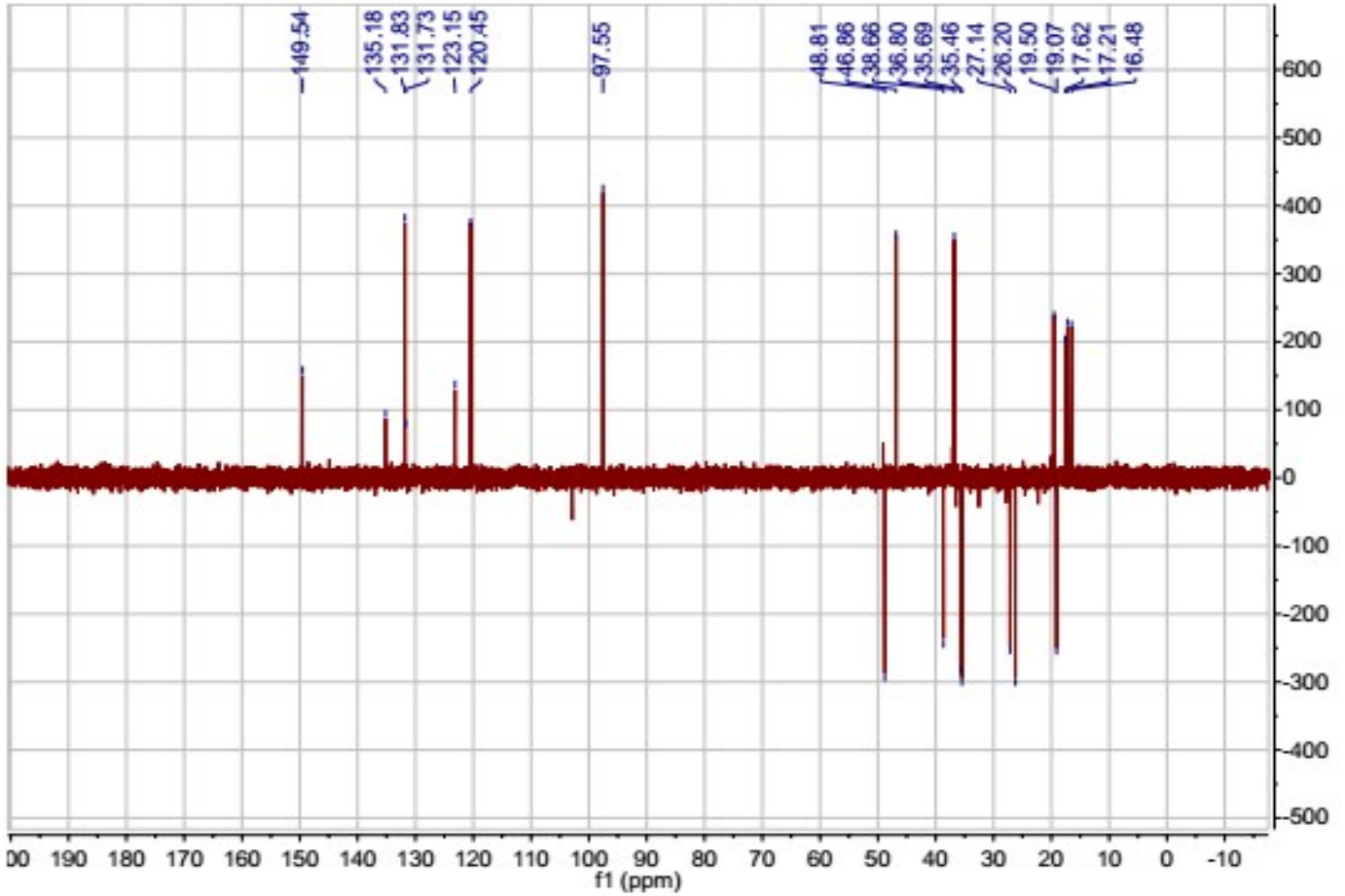
Figure S45. ^{1}H NMR spectrum of Compound **5** in Pyr-d_5.

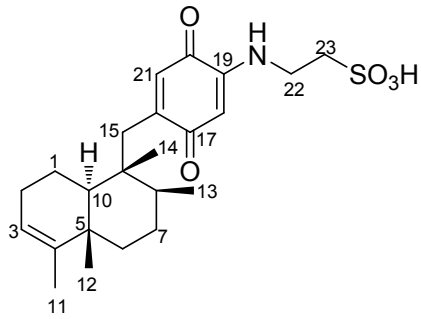




Ent-melemeleone B (**5**)

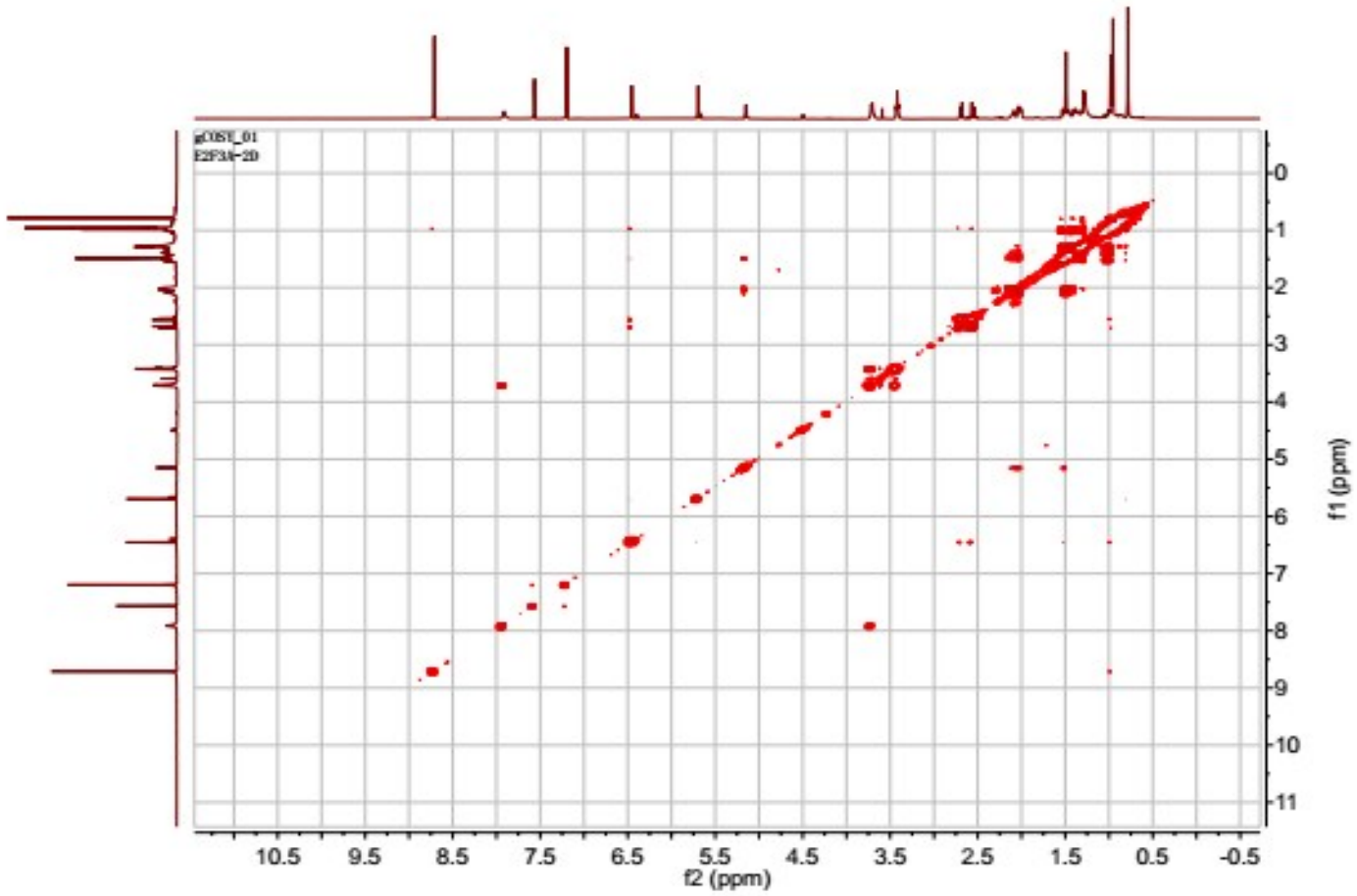
Figure S46. ^{13}C NMR spectrum of Compound **5** in Pyr-d_5.

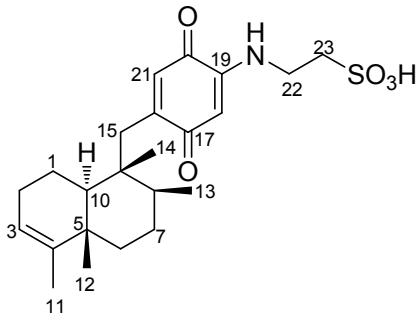




Ent-melemeleone B (**5**)

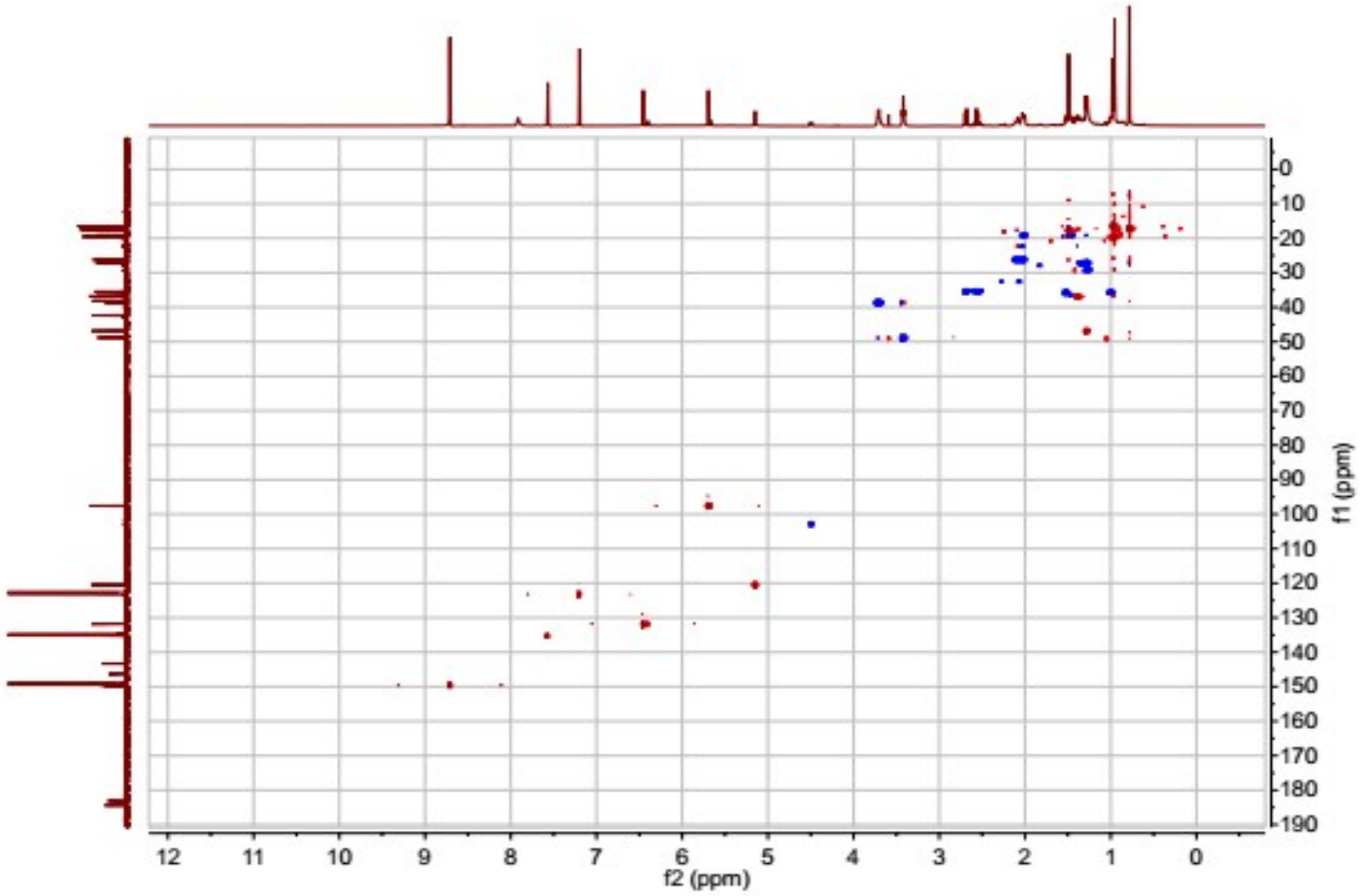
Figure S47. DEPT135 spectrum of Compound **5** in Pyr-d_5.

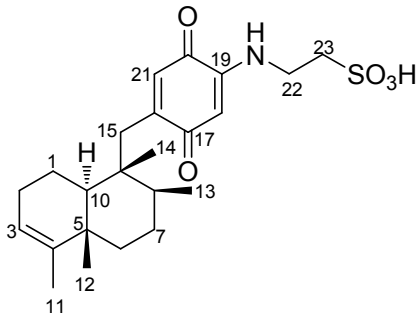




Ent-melemeleone B (**5**)

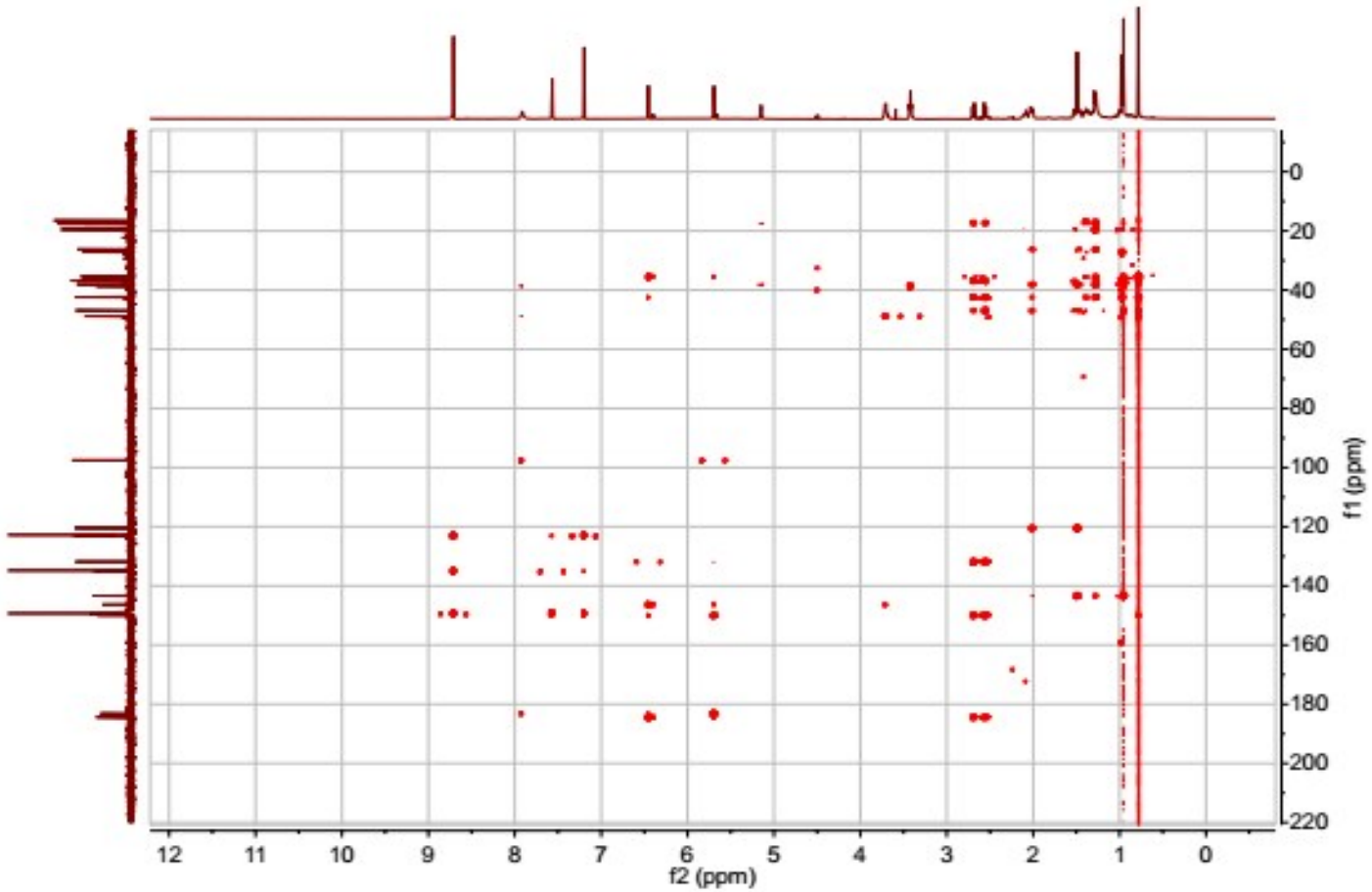
Figure S48. ^{1}H-^{1}H COSY spectrum of Compound **5** in Pyr-d_5.

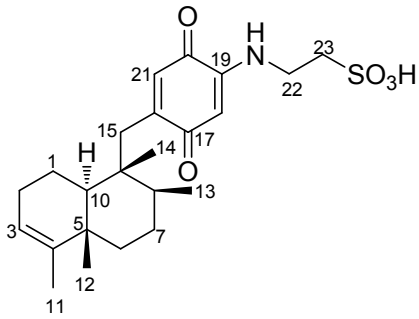




Ent-melemeleone B (**5**)

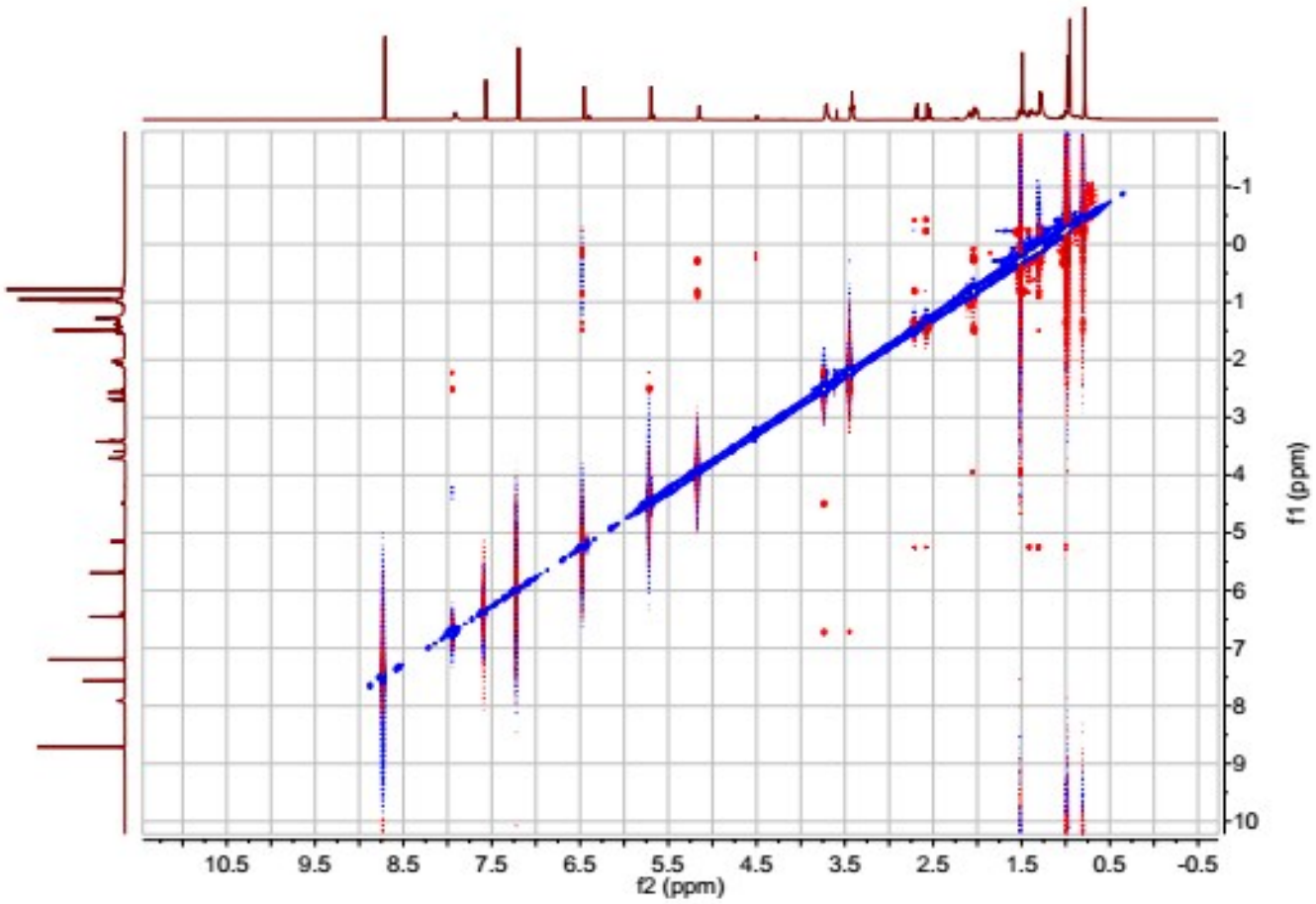
Figure S49. HSQC spectrum of Compound **5** in Pyr-d_5.

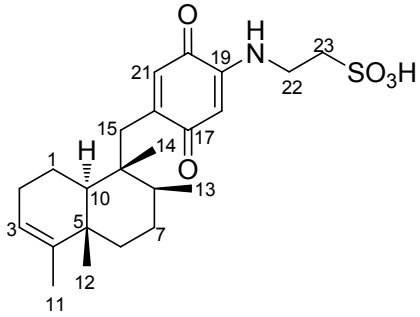




Ent-melemeleone B (**5**)

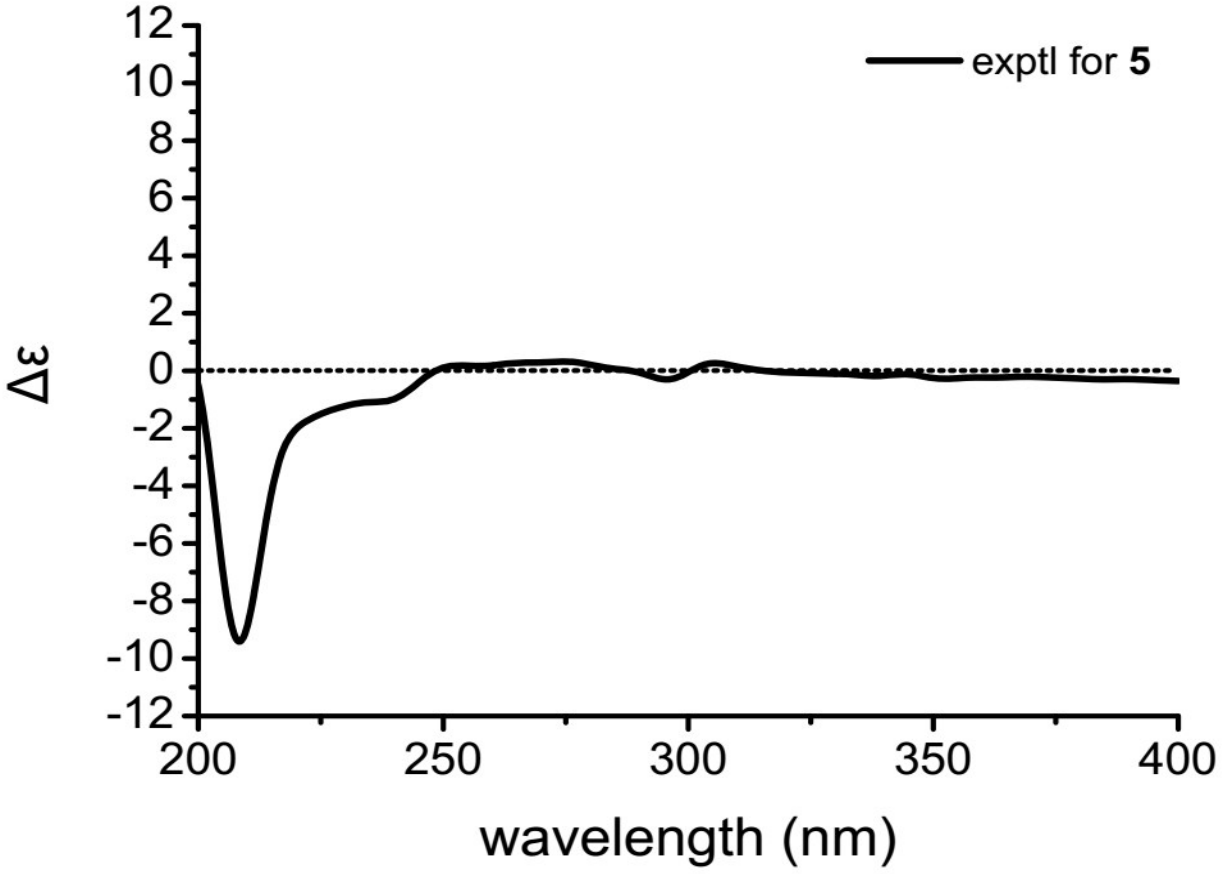
Figure S50. HMBC spectrum of Compound **5** in Pyr-d_5.

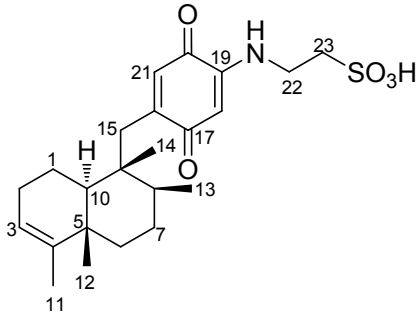




Ent-melemeleone B (**5**)

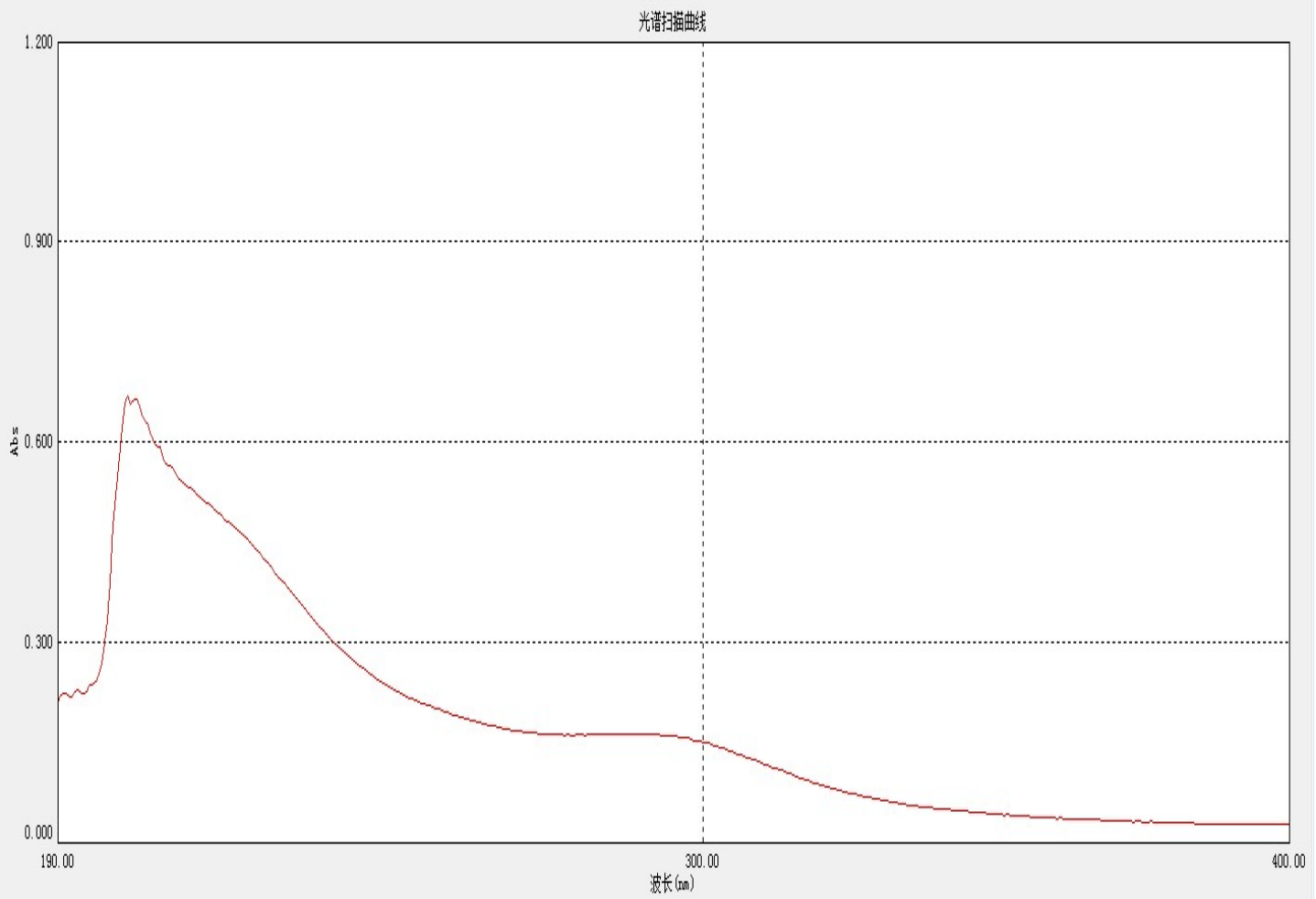
Figure S51. NOESY spectrum of Compound **5** in Pyr-d_5.

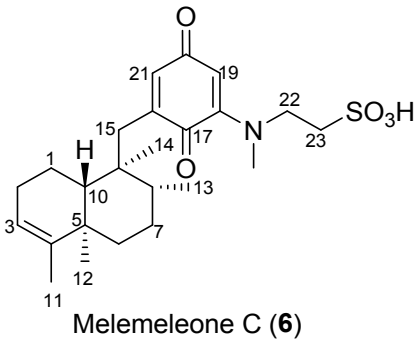




Ent-melemeleone B (**5**)

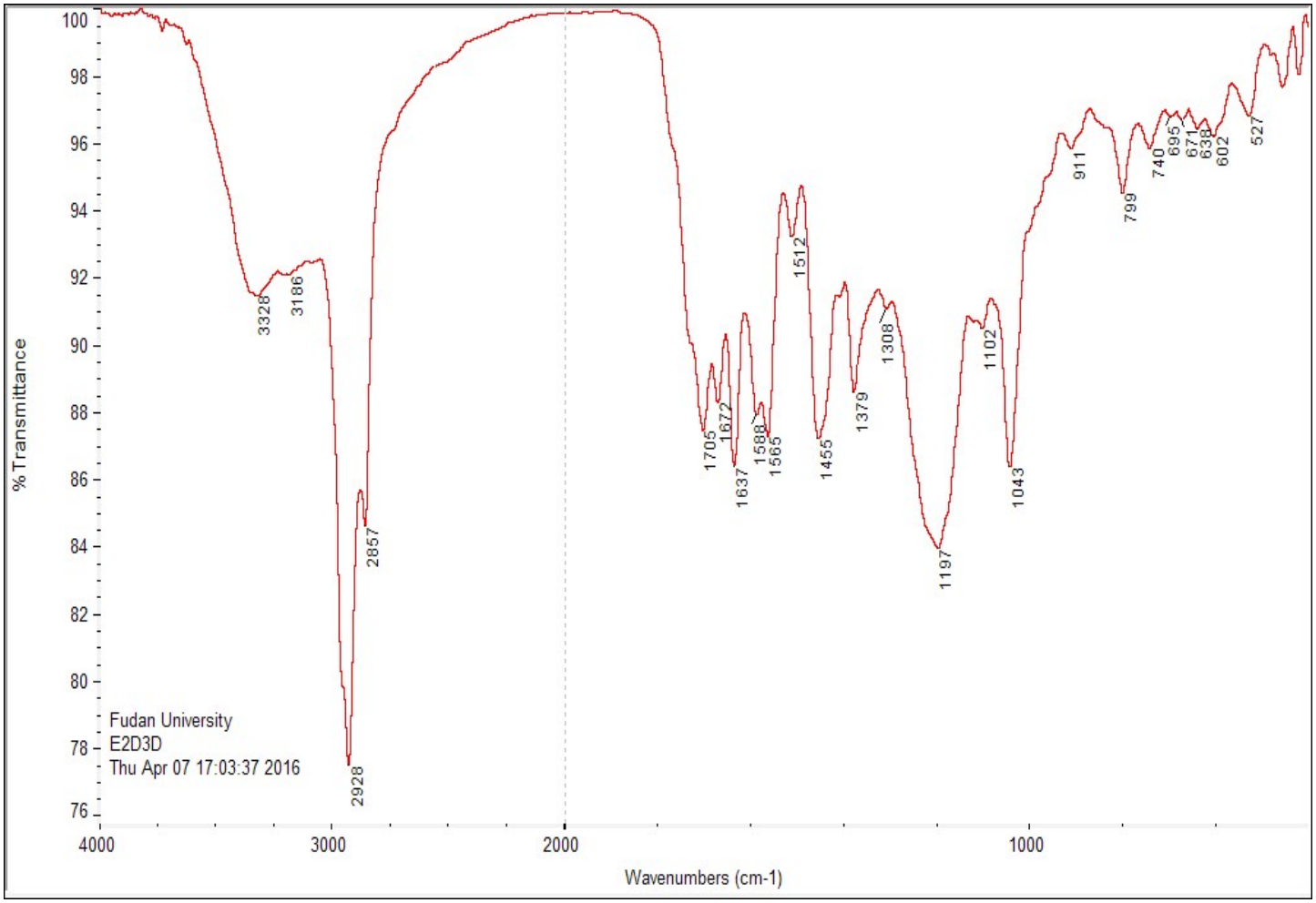
Figure S52. CD spectrum of Compound **5** in MeOH.

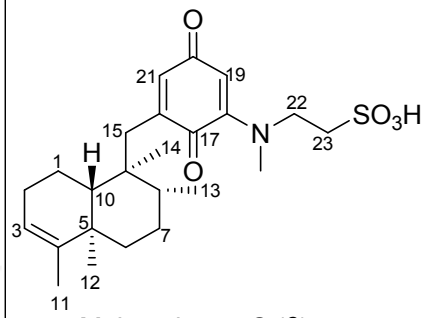




Melemeleone C (**6**)

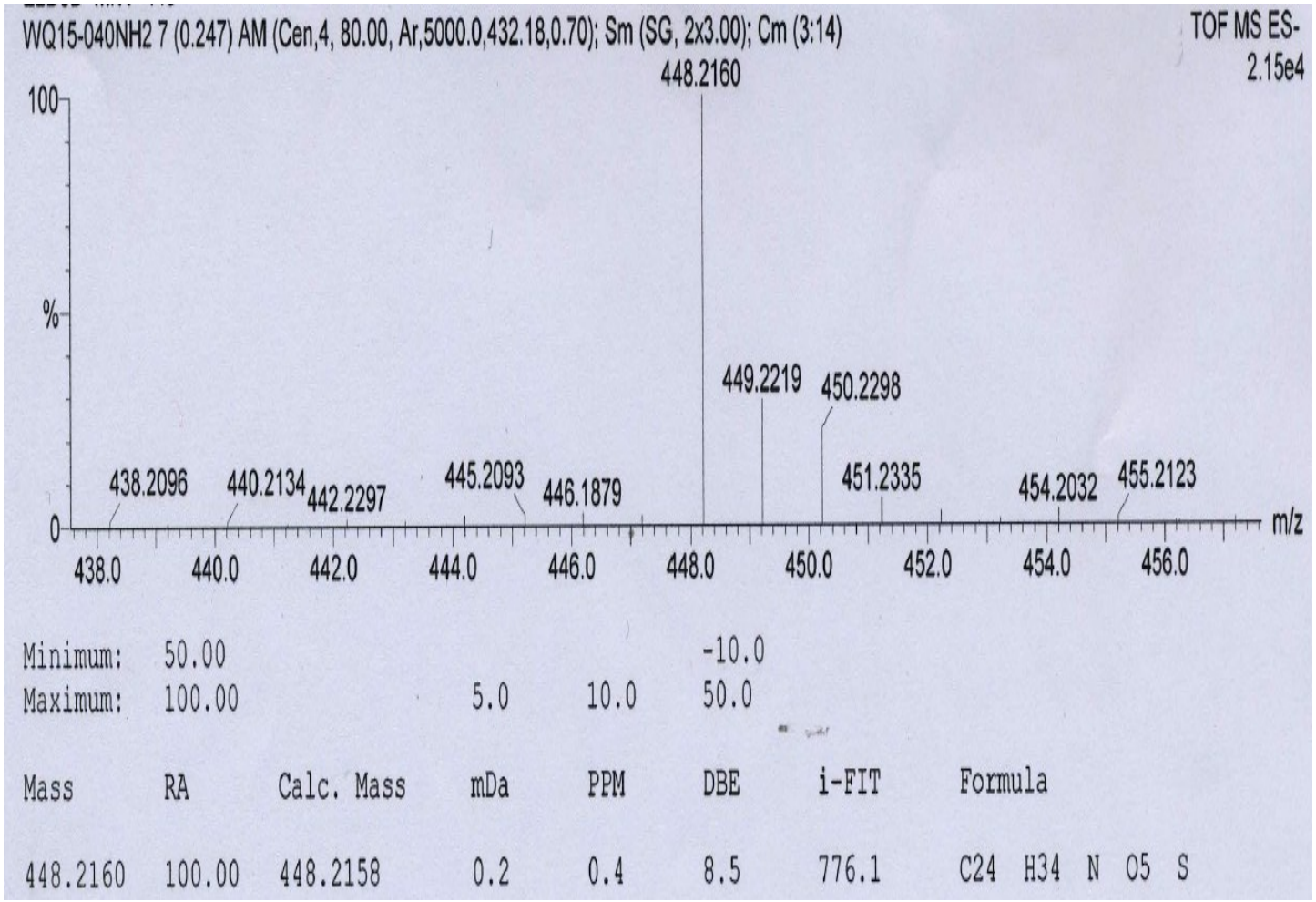
Figure S53. UV spectrum of Compound **6** in MeOH.

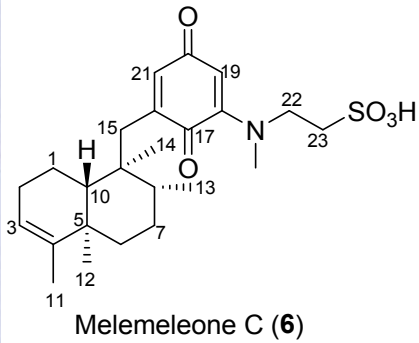




Melemeleone C (**6**)

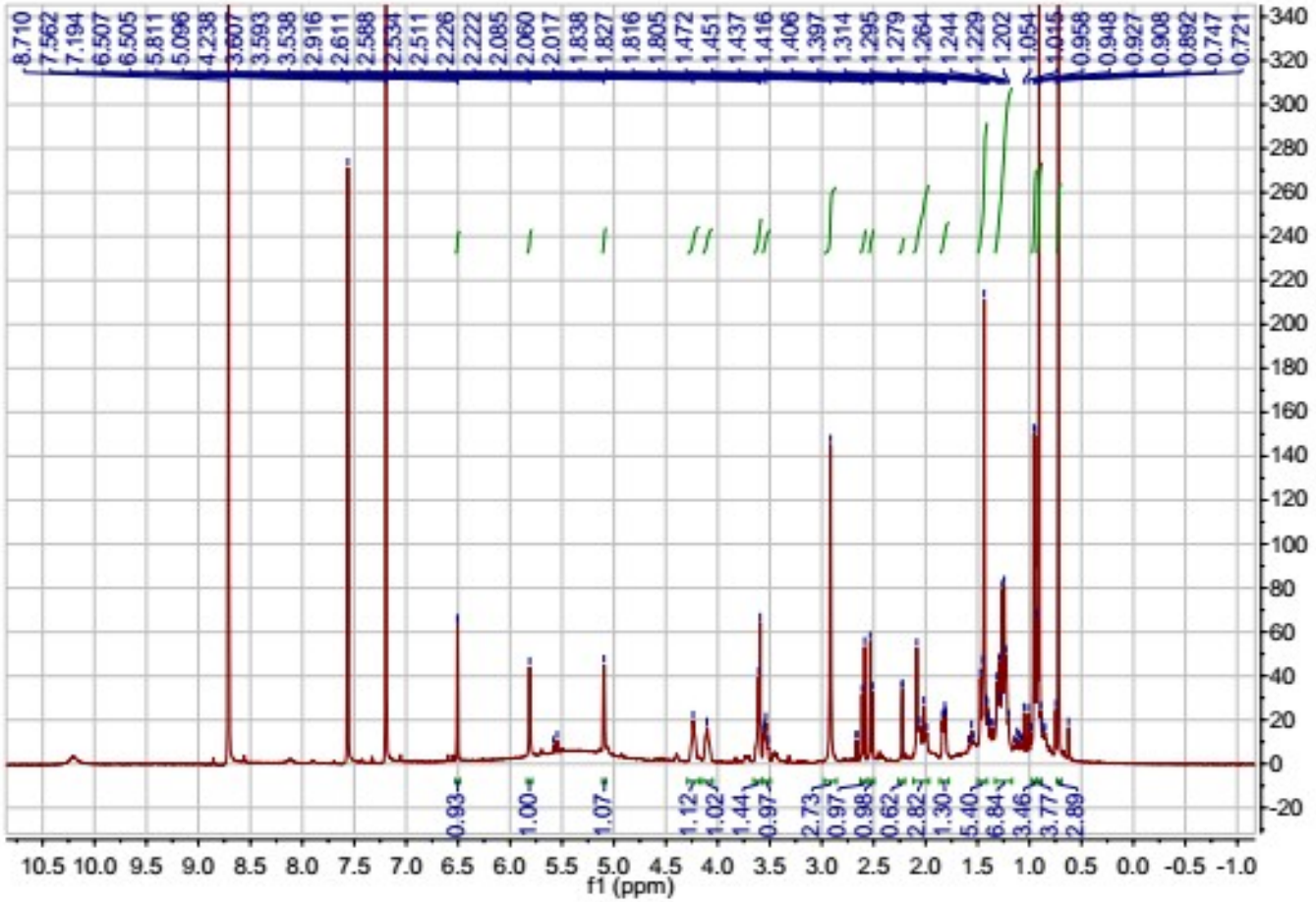
Figure S54. IR spectrum of Compound **6**.

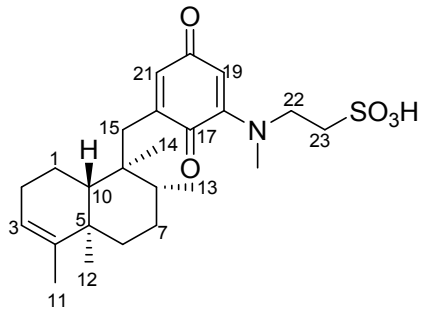




Melemeleone C (**6**)

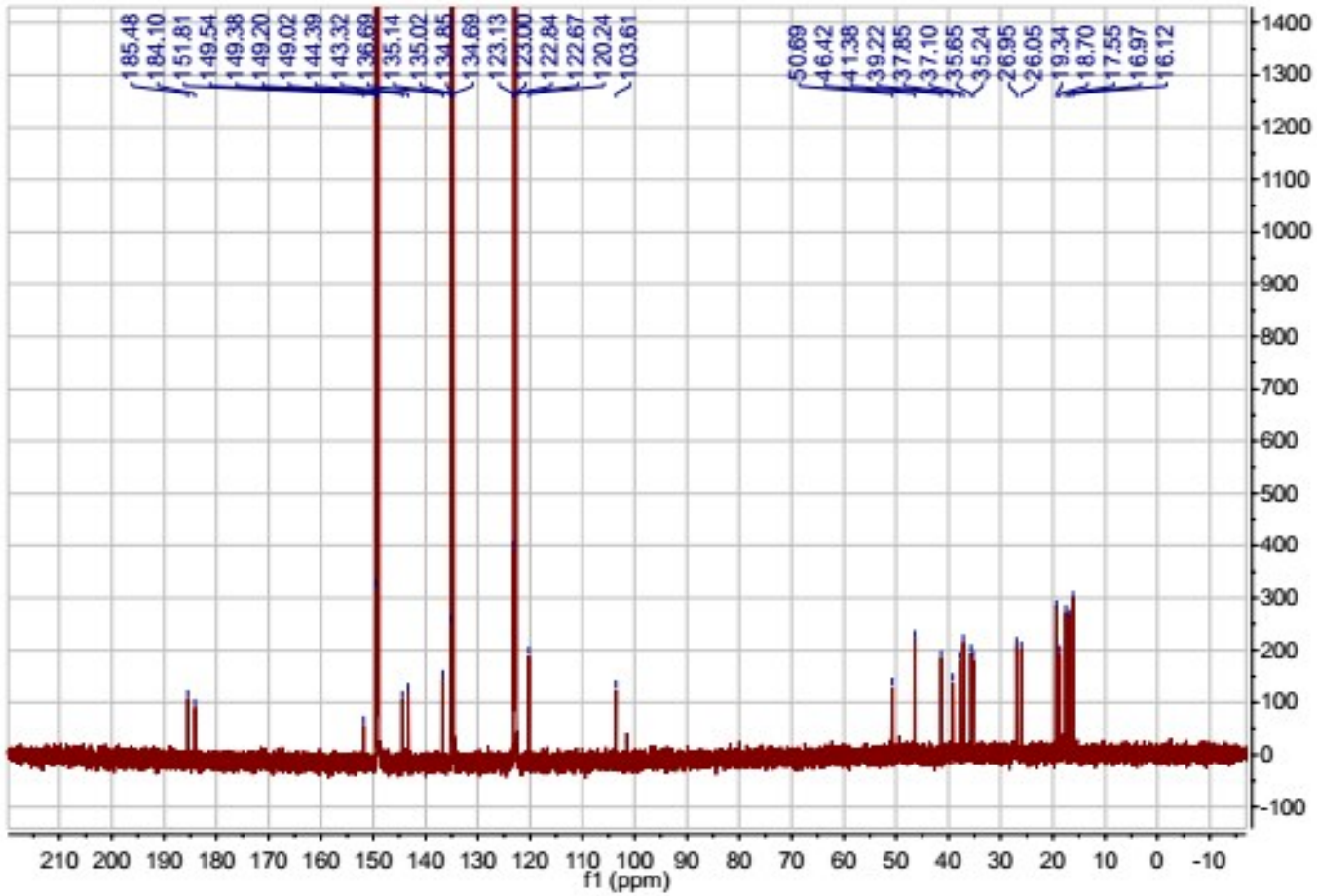
Figure S55. HRESIMS spectrum of Compound **6**.

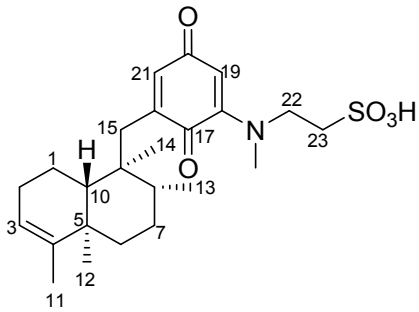




Melemeleone C (**6**)

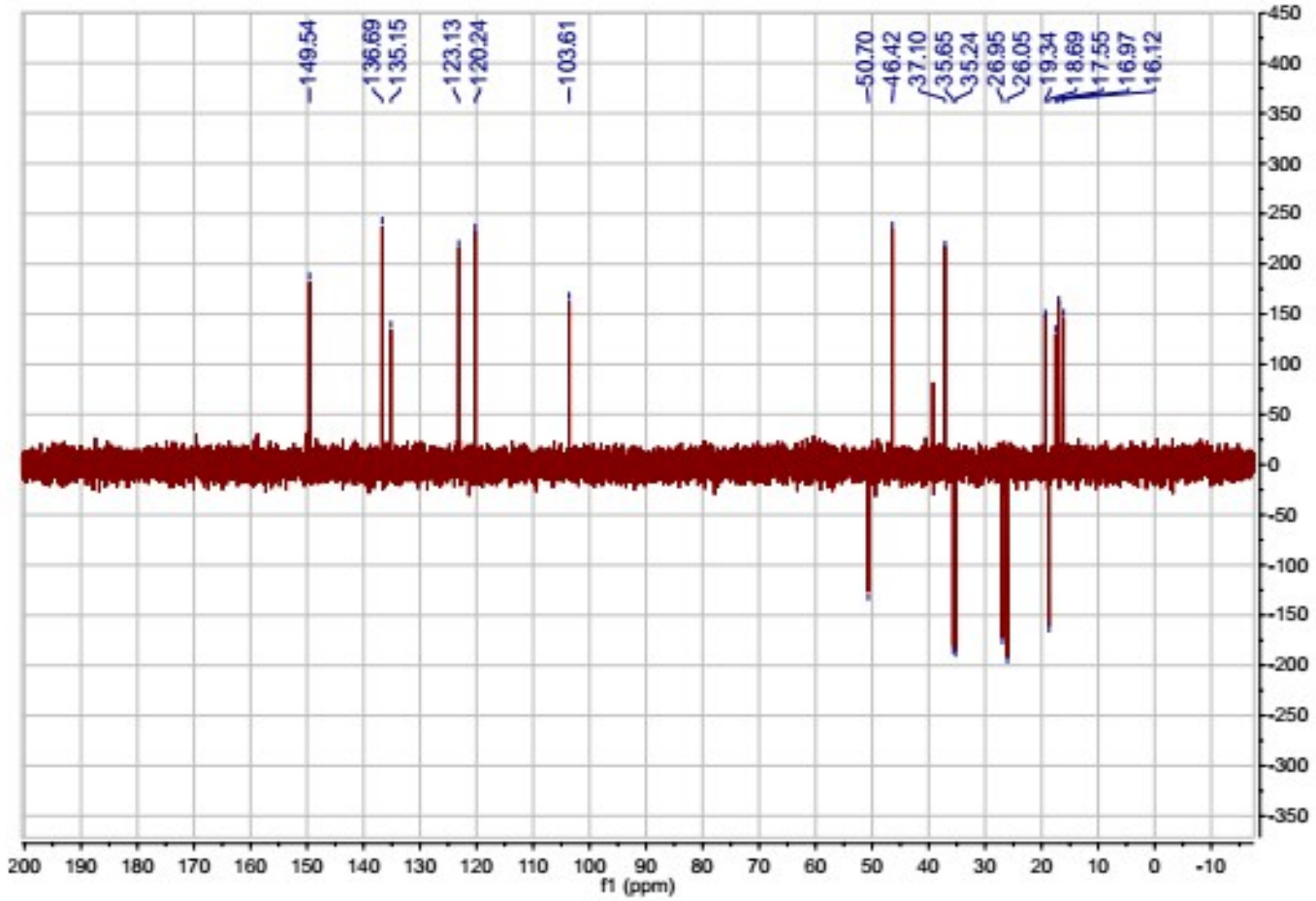
Figure S56. ^{1}H NMR spectrum of Compound **6** in Pyr-d_5.

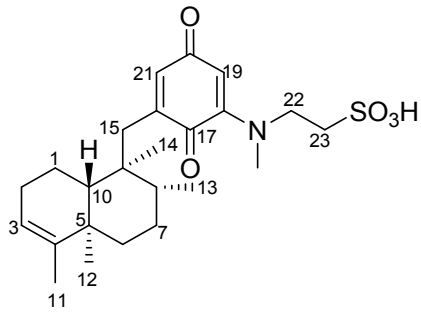




Melemeleone C (**6**)

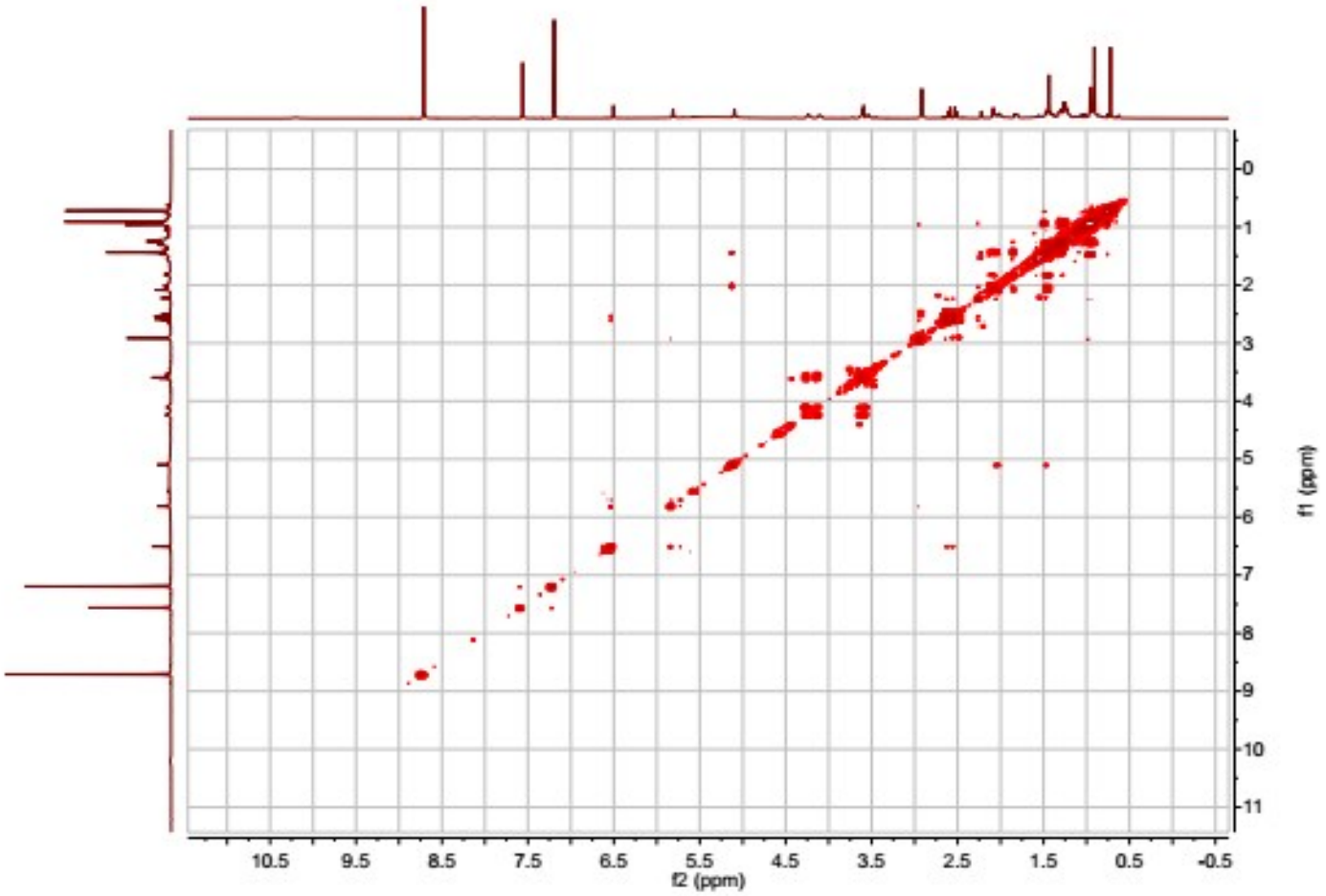
Figure S57. ^{13}C NMR spectrum of Compound **6** in Pyr-d_5.

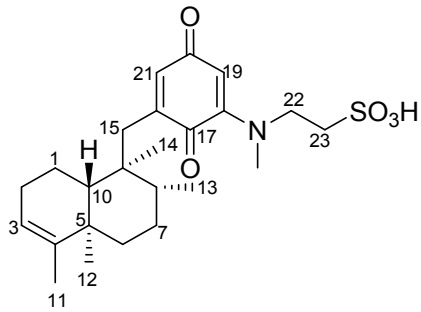




Melemeleone C (**6**)

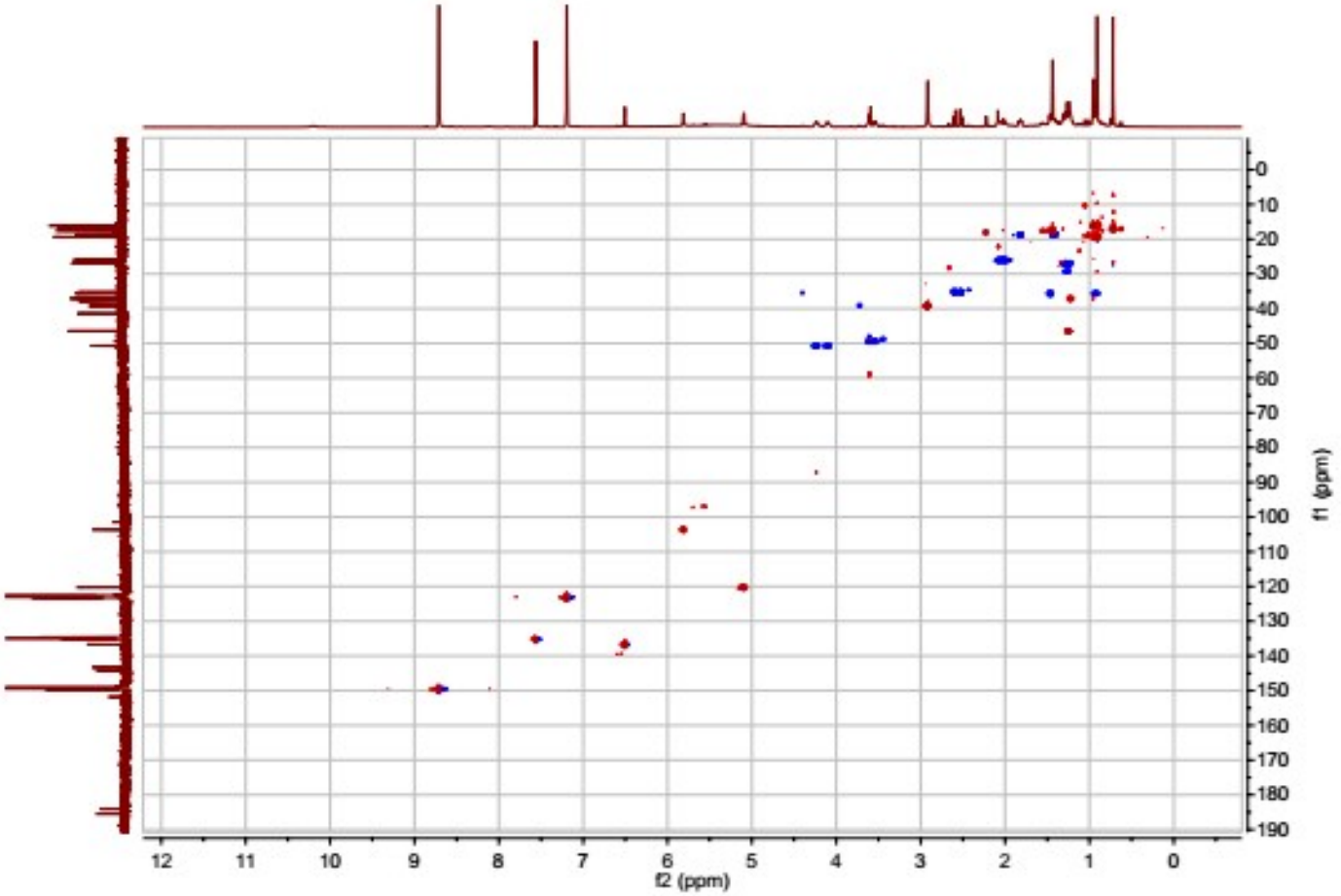
Figure S58. DEPT135 spectrum of Compound **6** in Pyr-d_5.

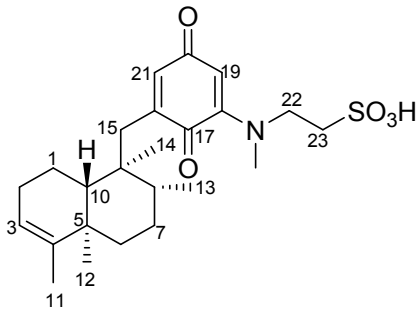




Melemeleone C (**6**)

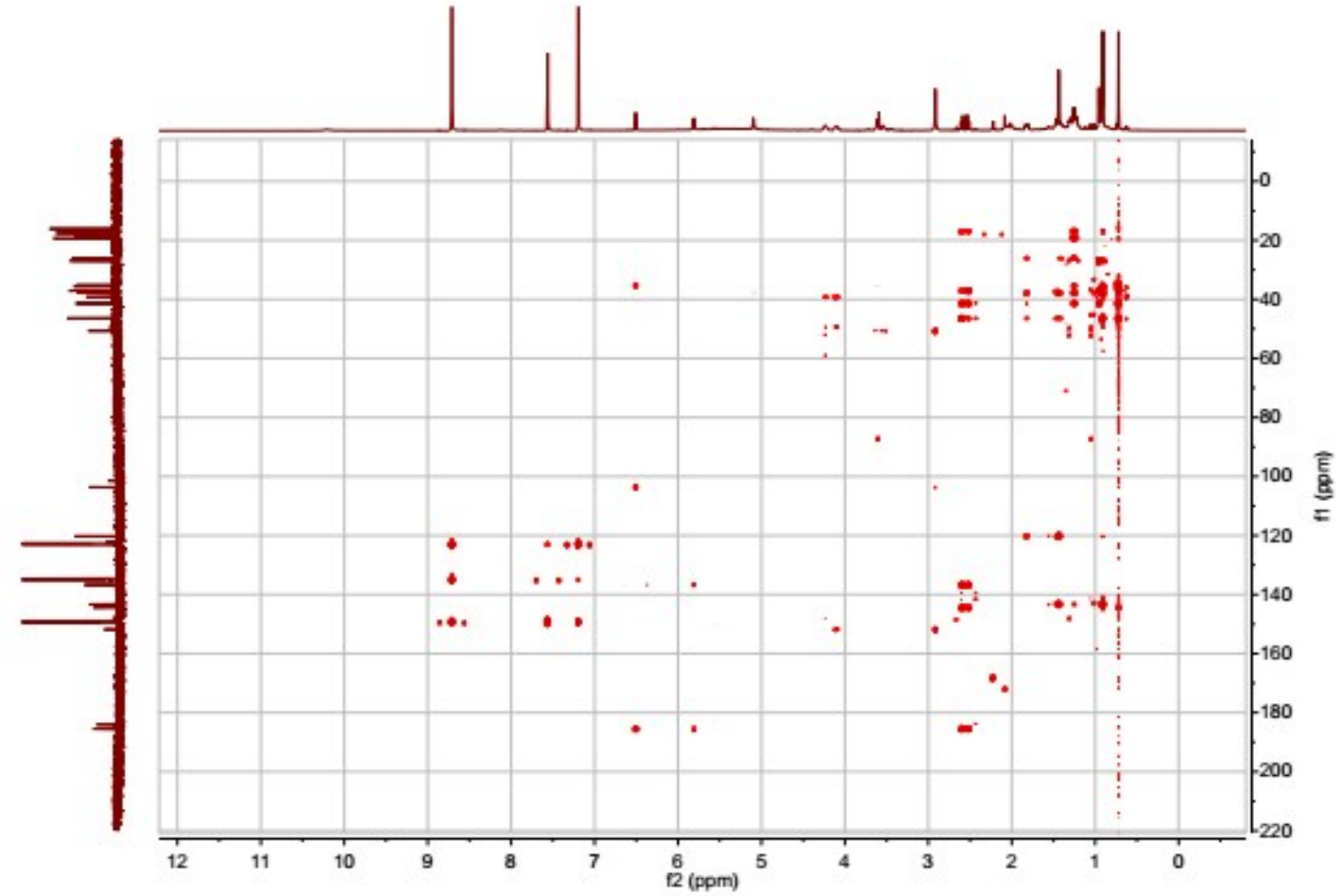
Figure S59. ^{1}H-^{1}H COSY spectrum of Compound **6** in Pyr-d_5.

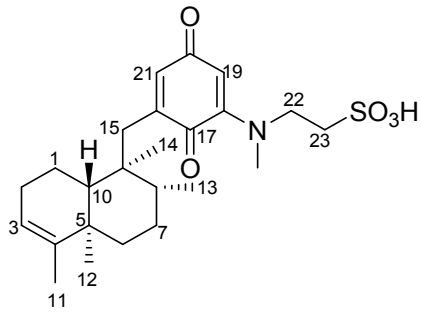




Melemeleone C (**6**)

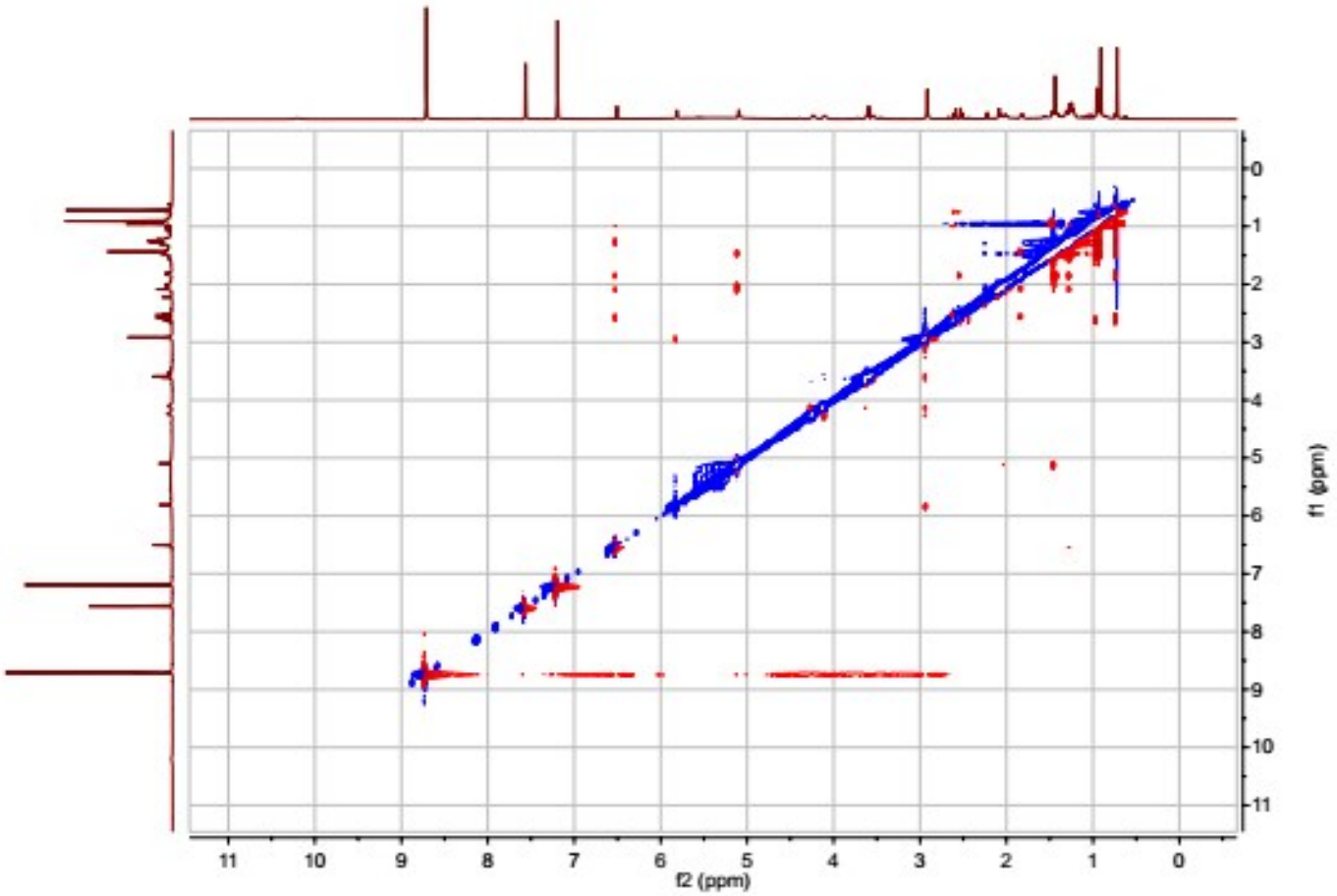
Figure S60. HSQC spectrum of Compound **6** in Pyr-d_5.

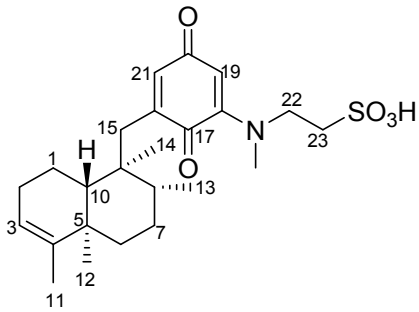




Melemeleone C (**6**)

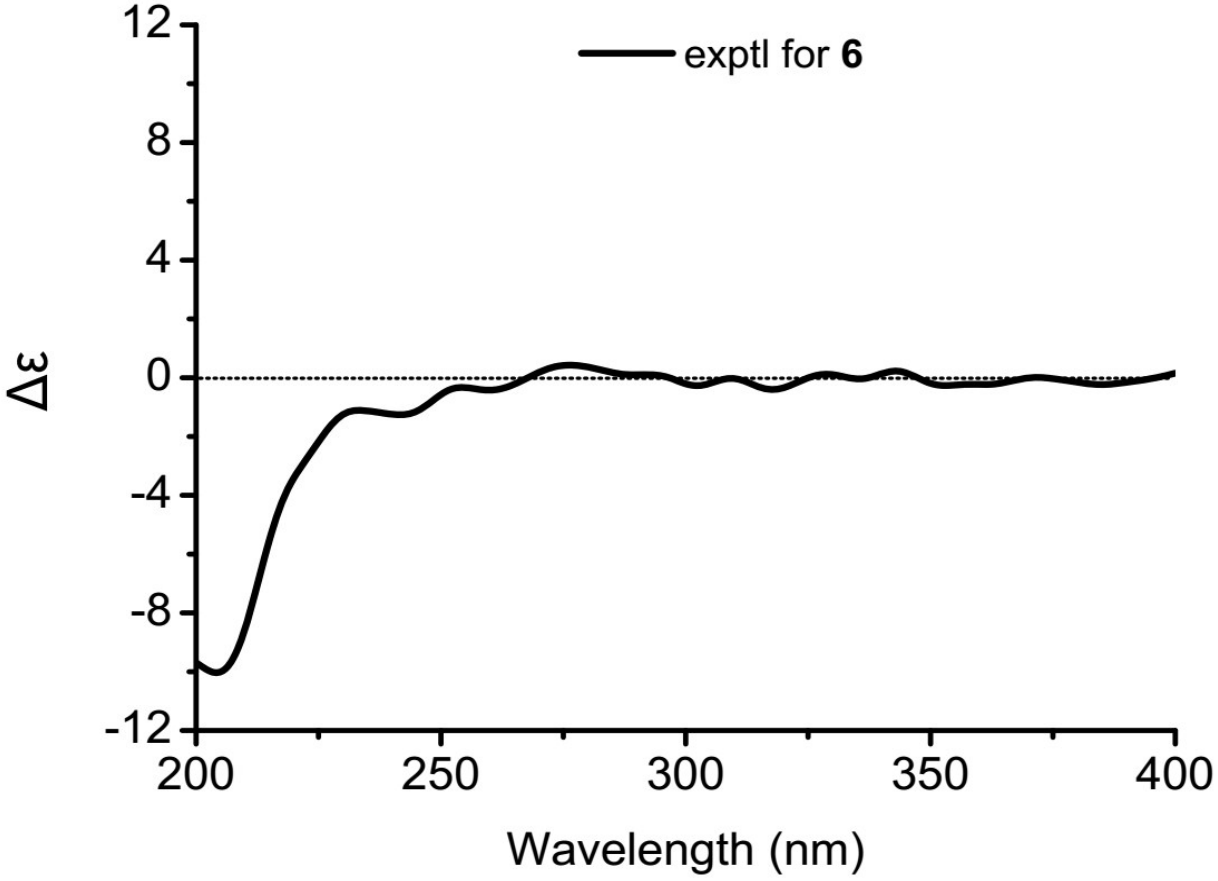
Figure S61. HMBC spectrum of Compound **6** in Pyr-d_5.

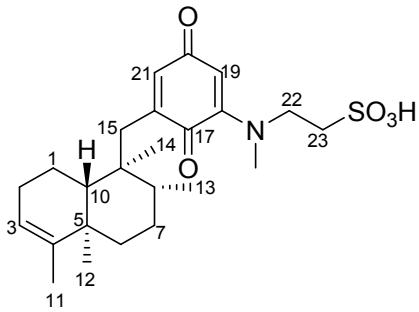




Melemeleone C (**6**)

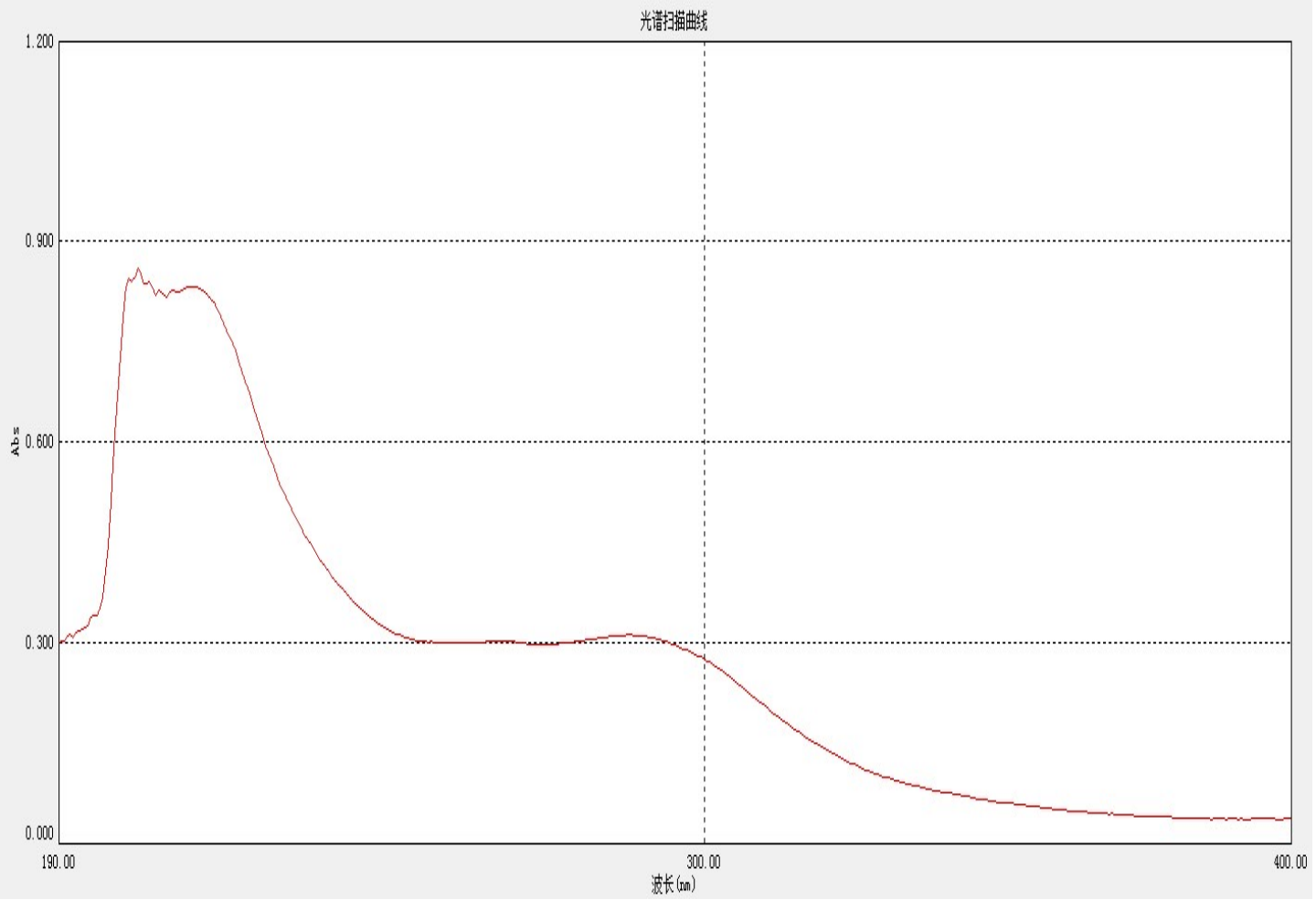
Figure S62. NOESY spectrum of Compound **6** in Pyr-d_5.

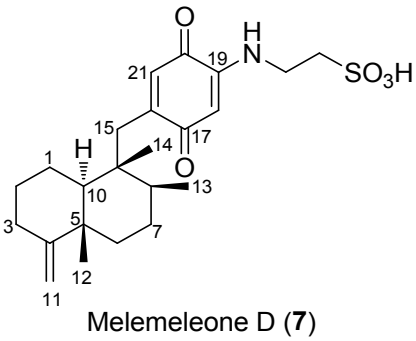




Melemeleone C (**6**)

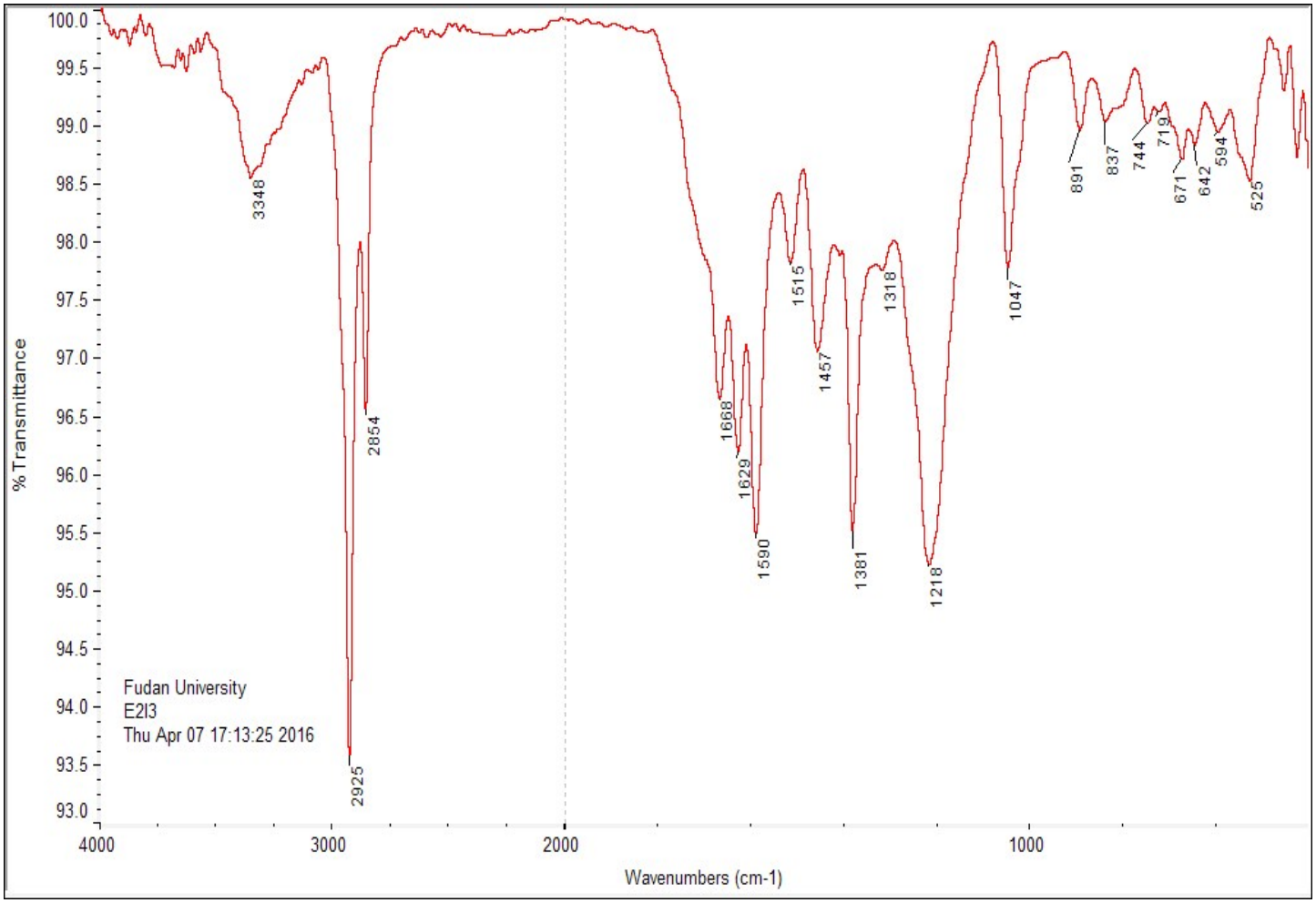
Figure S63. CD spectrum of Compound **6** in MeOH.

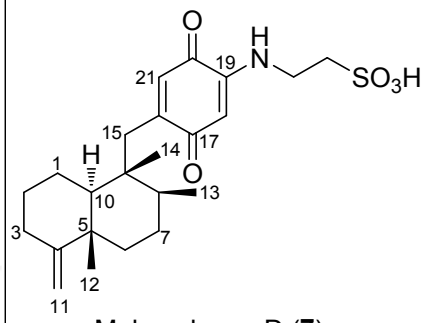




Melemeleone D (**7**)

Figure S64. UV spectrum of Compound **7** in MeOH.



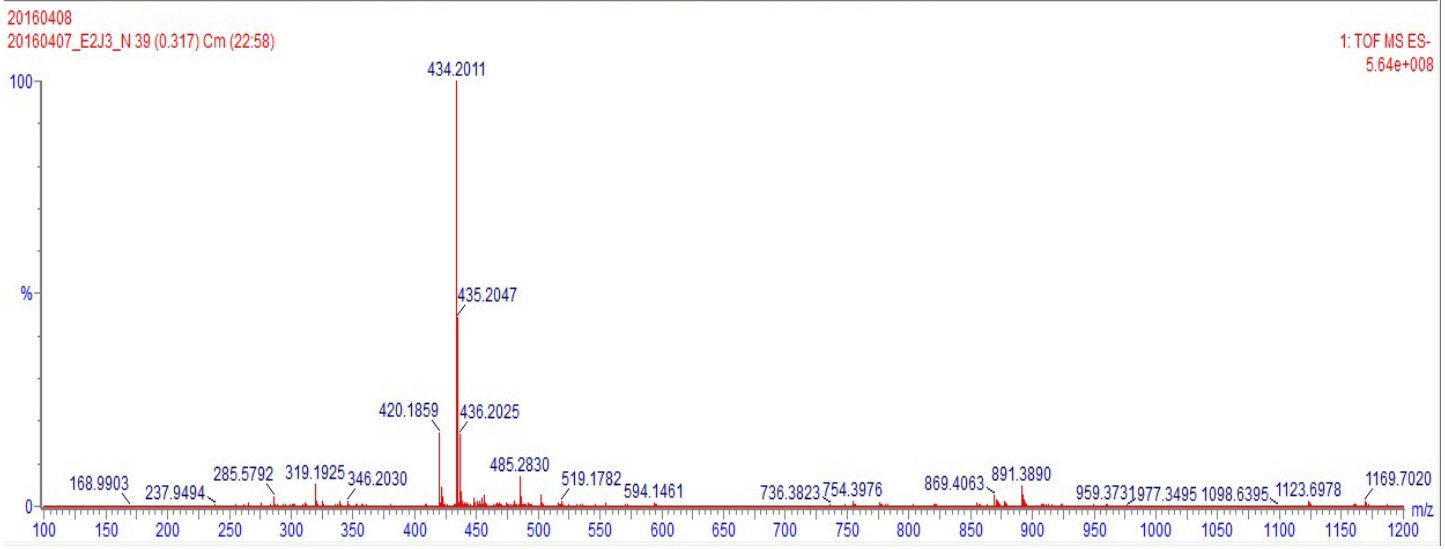


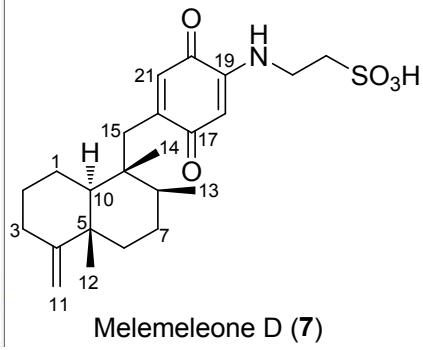
Melemeleone D (**7**)

Figure S65. IR spectrum of Compound **7**.

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
6588 formula(e) evaluated with 43 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:

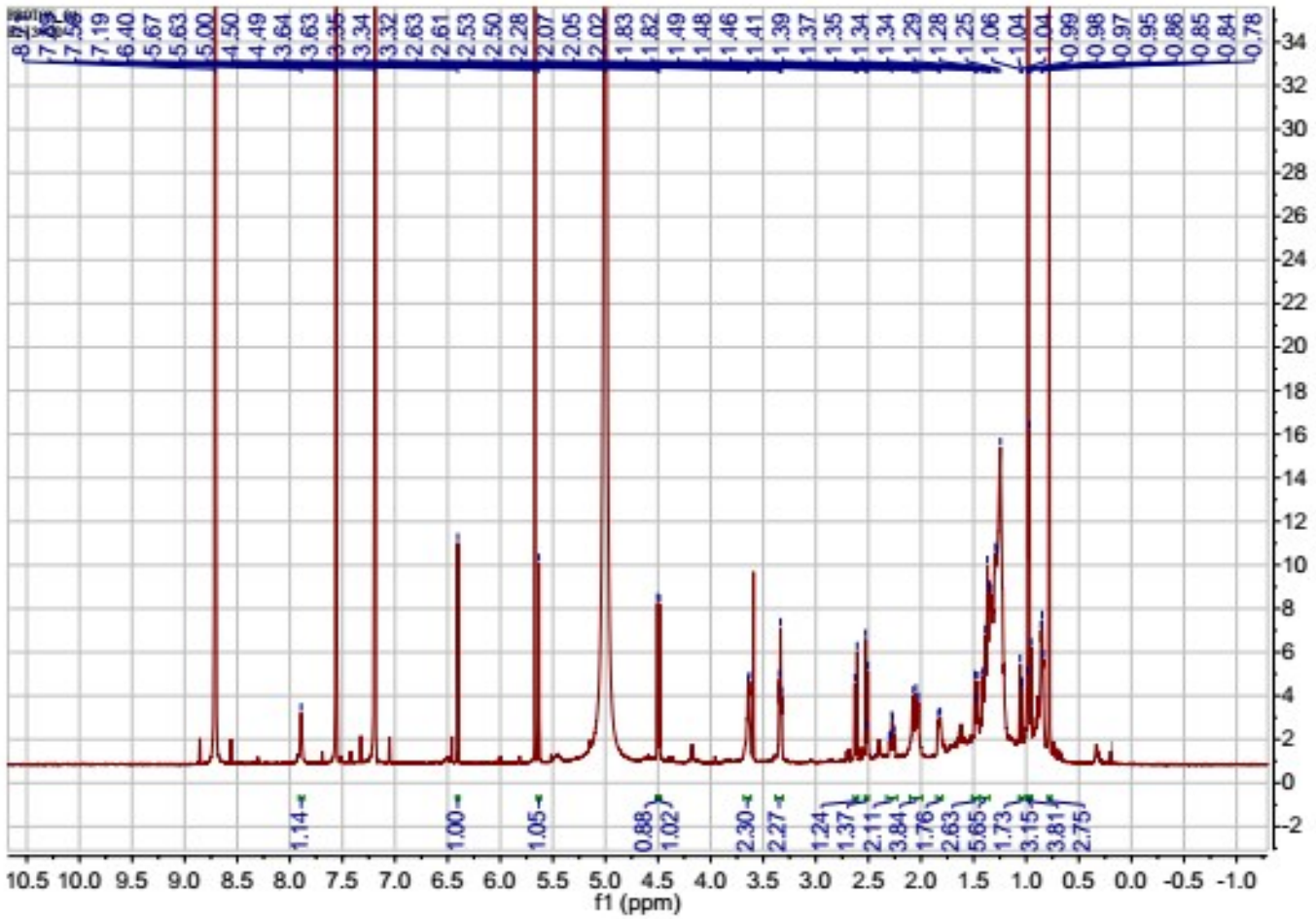
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	S
434.2011	434.2001	1.0	2.3	8.5	C23 H32 N O5 S	2591.8	0.772	46.19	23	32	1	5	1
	434.2015	-0.4	-0.9	13.5	C24 H28 N5 O S	2591.9	0.825	43.84	24	28	5	1	1
	434.1976	3.5	8.1	12.5	C27 H32 N S2	2593.9	2.837	5.86	27	32	1		2
	434.2010	0.1	0.2	7.5	C24 H36 N S3	2596.0	4.954	0.71	24	36	1		3
	434.1974	3.7	8.5	9.5	C19 H28 N7 O3 S	2596.0	4.973	0.69	19	28	7	3	1
	434.2060	-4.9	-11.3	-0.5	C16 H36 N O10 S	2596.2	5.148	0.58	16	36	1	10	1
	434.2048	-3.7	-8.5	8.5	C21 H32 N5 O S2	2596.3	5.204	0.55	21	32	5	1	2
	434.2035	-2.4	-5.5	3.5	C20 H36 N O5 S2	2596.5	5.403	0.45	20	36	1	5	2

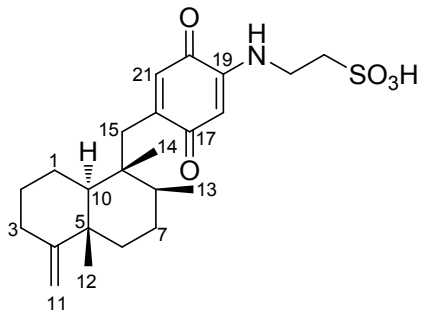




Melemeleone D (**7**)

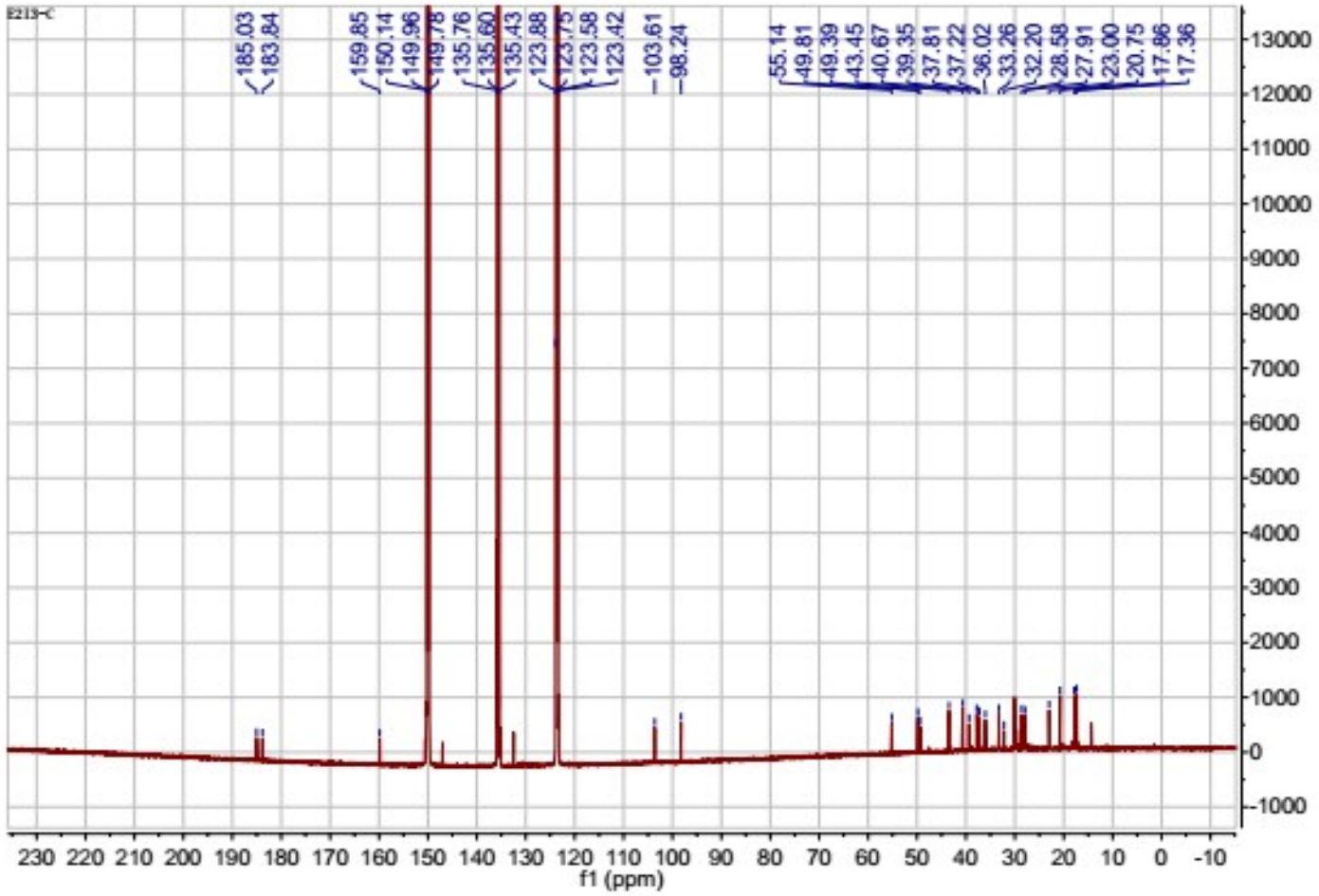
Figure S66. HRESIMS spectrum of Compound **7**.

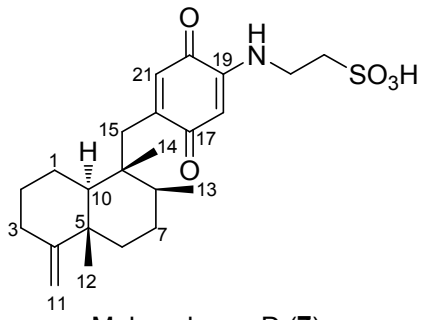




Melemeleone D (**7**)

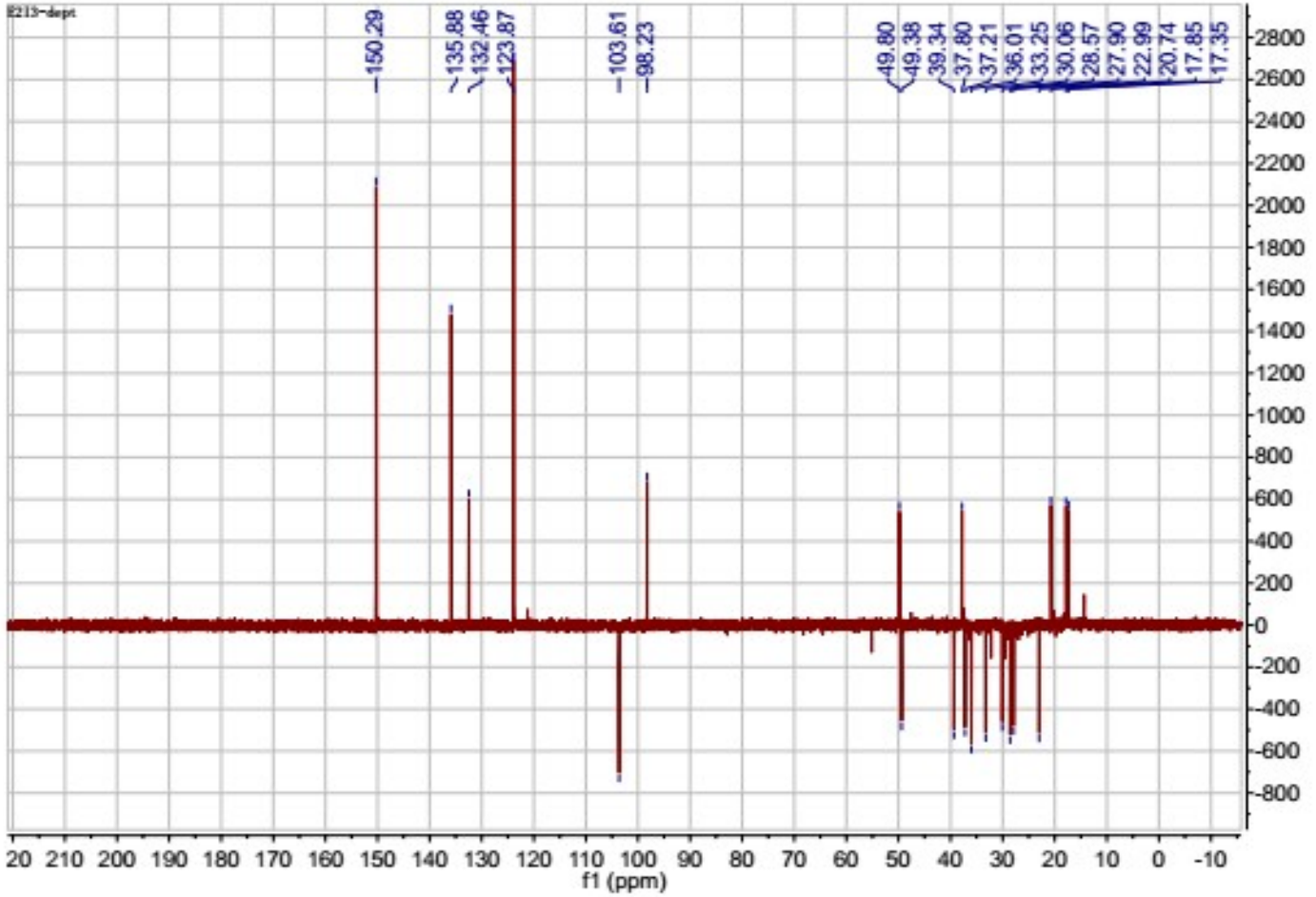
Figure S67. ^{1}H NMR spectrum of Compound **7** in Pyr-d_5.

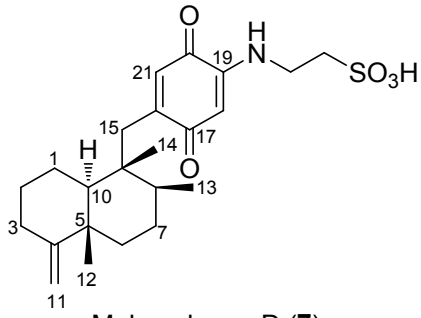




Melemeleone D (**7**)

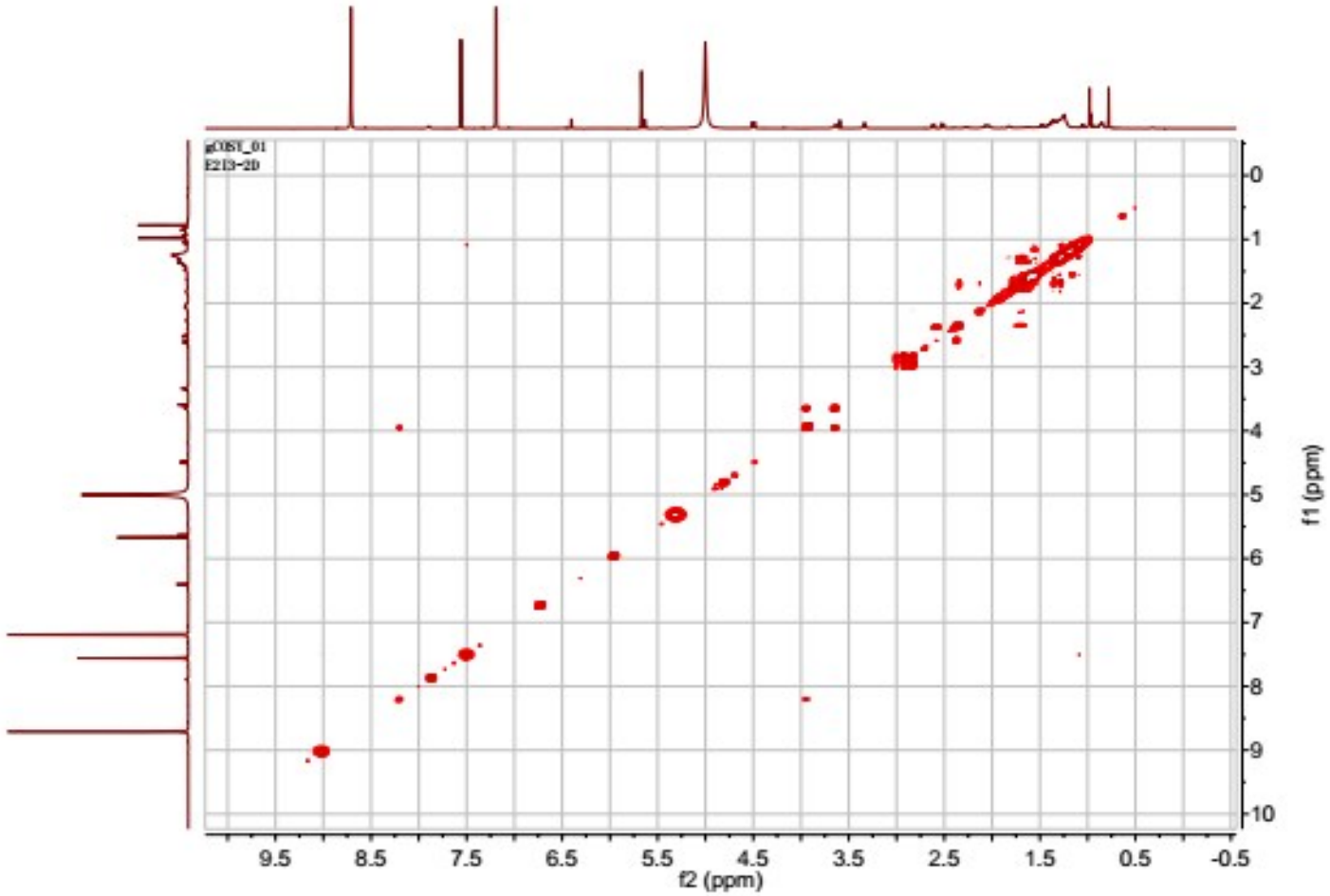
Figure S68. ^{13}C NMR spectrum of Compound **7** in Pyr-d_5.

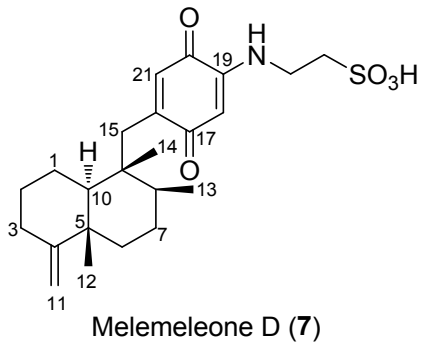




Melemeleone D (**7**)

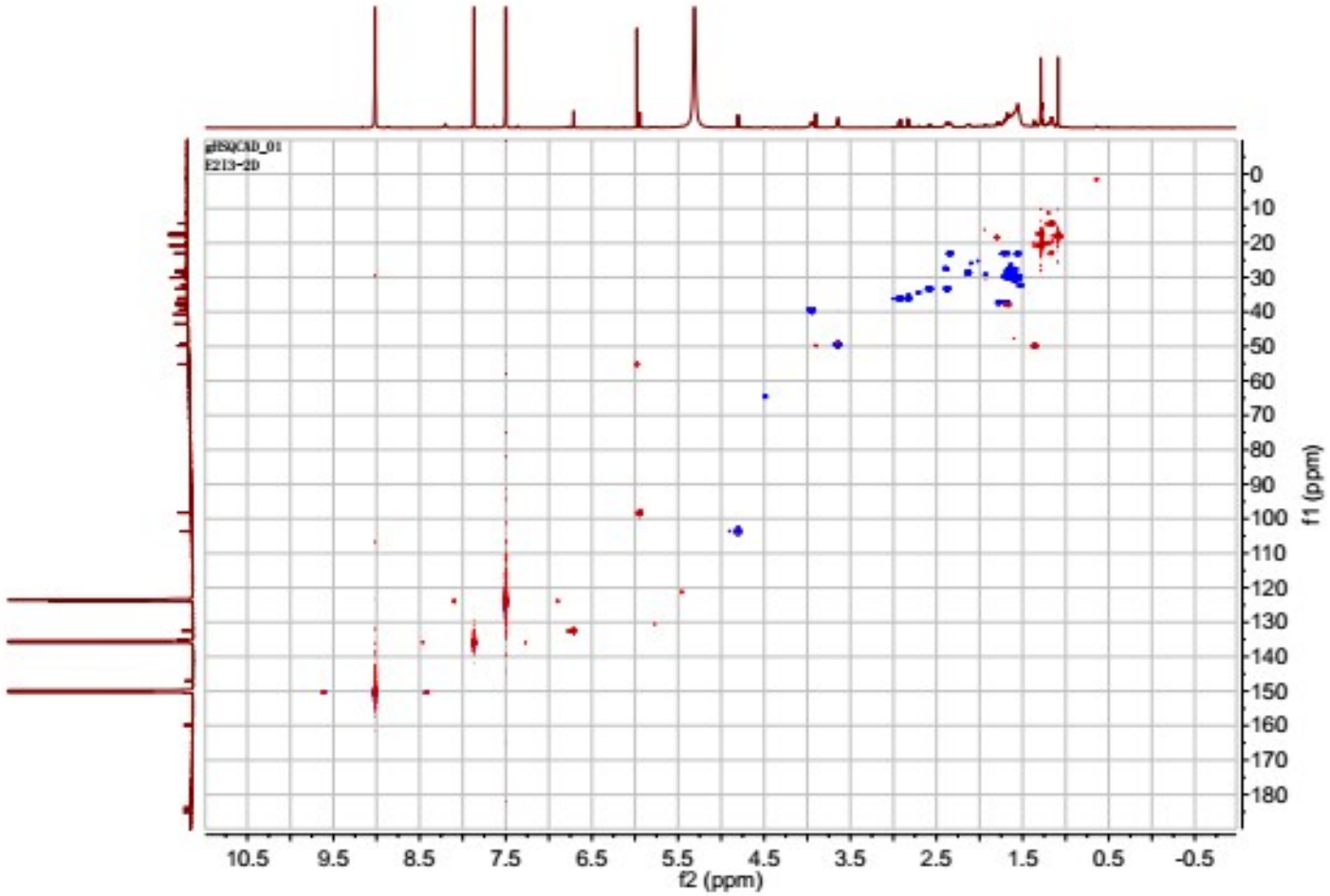
Figure S69. DEPT135 spectrum of Compound **7** in Pyr-d_5.

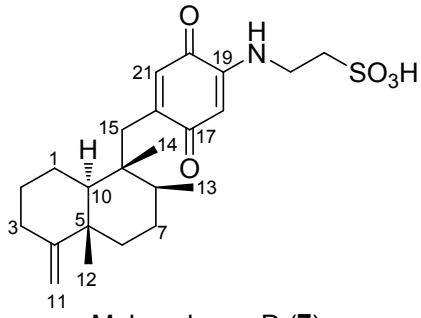




Melemeleone D (**7**)

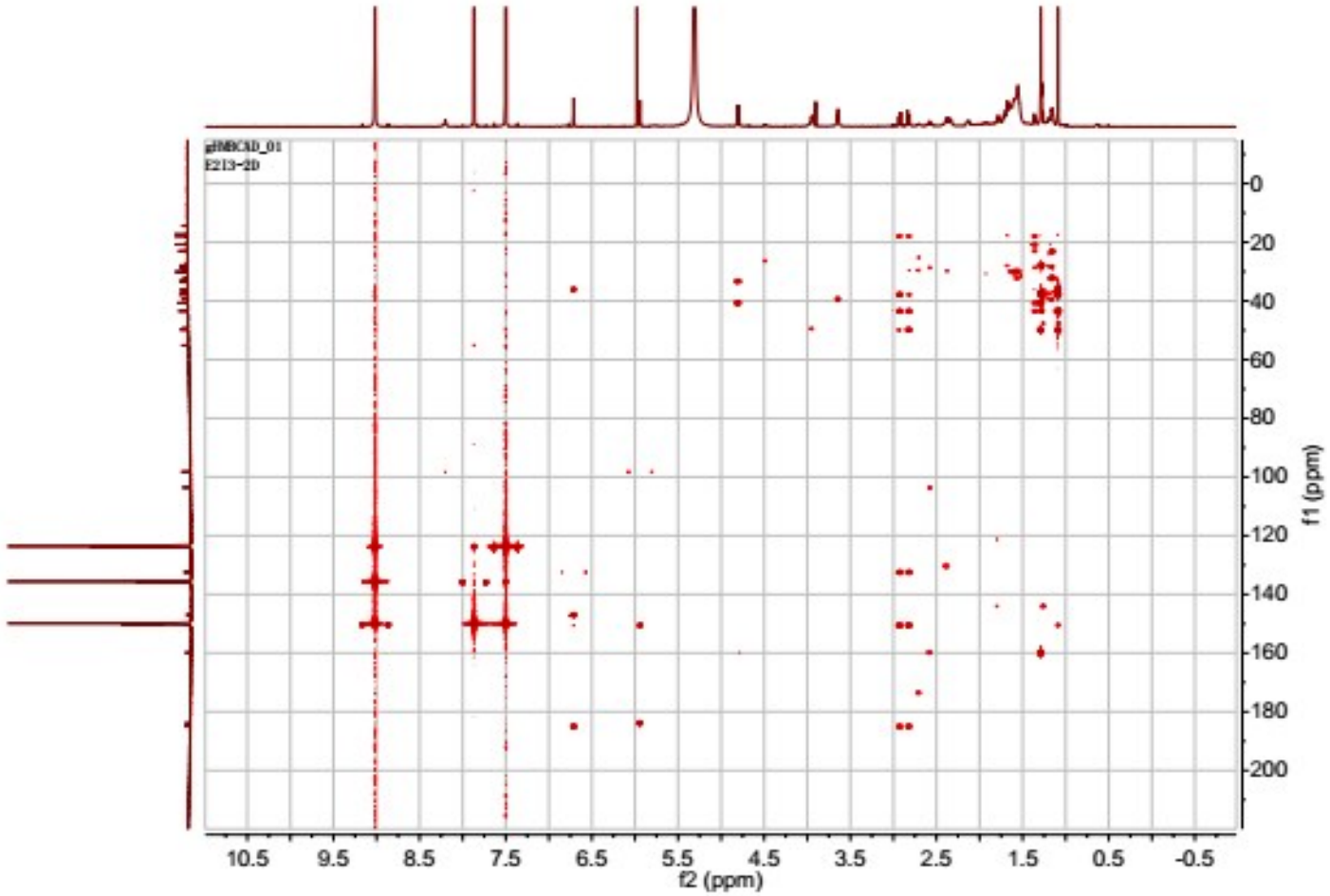
Figure S70. ^{1}H-^{1}H COSY spectrum of Compound **6** in Pyr-d_5.

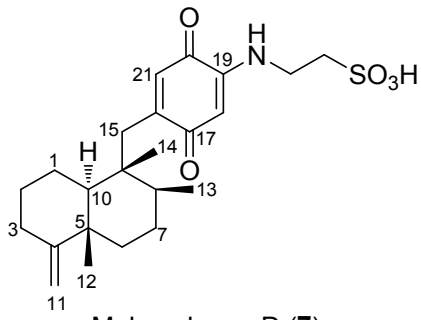




Melemeleone D (**7**)

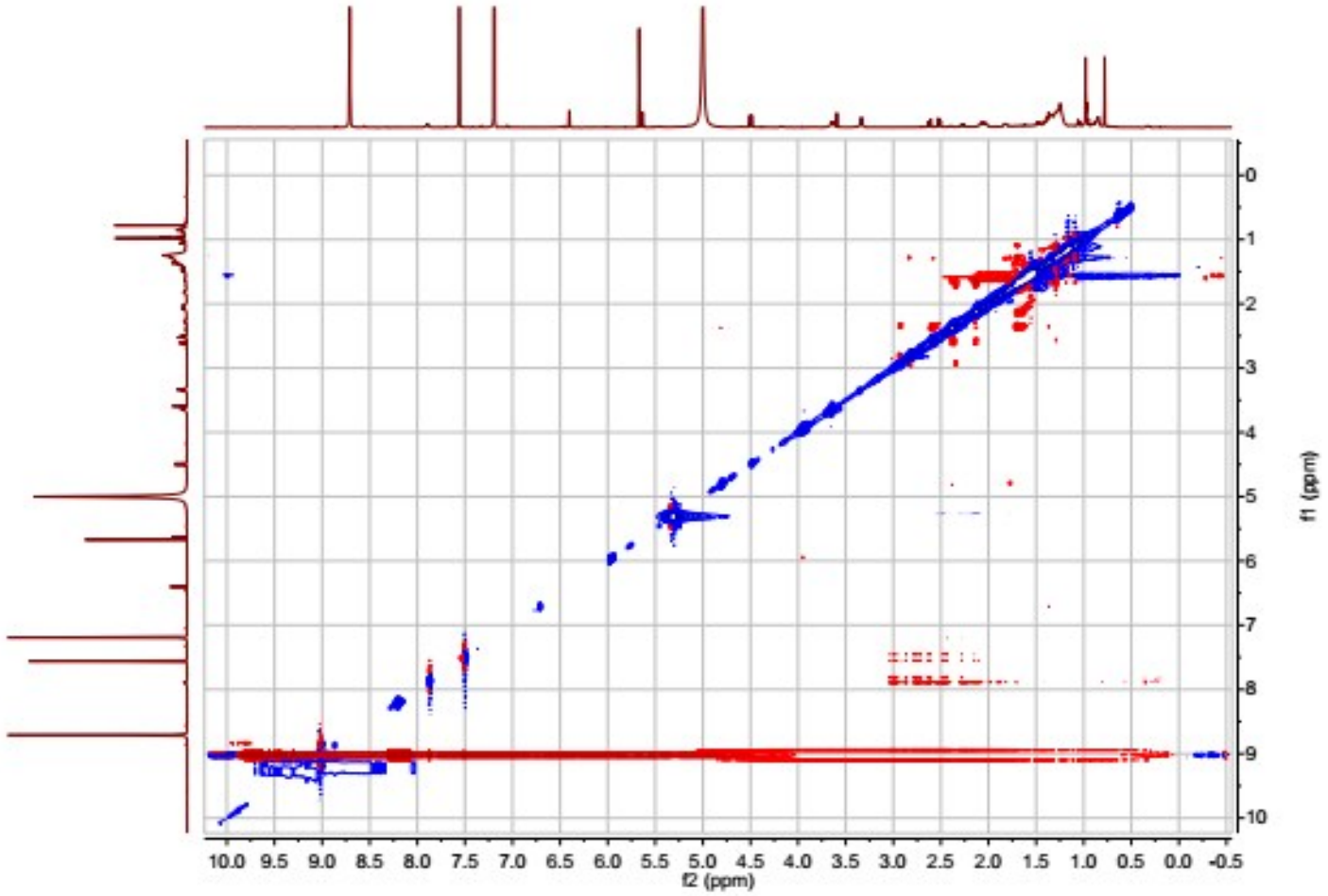
Figure S71. HSQC spectrum of Compound **7** in Pyr-d_5.

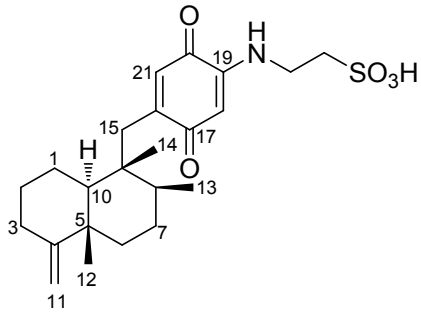




Melemeleone D (**7**)

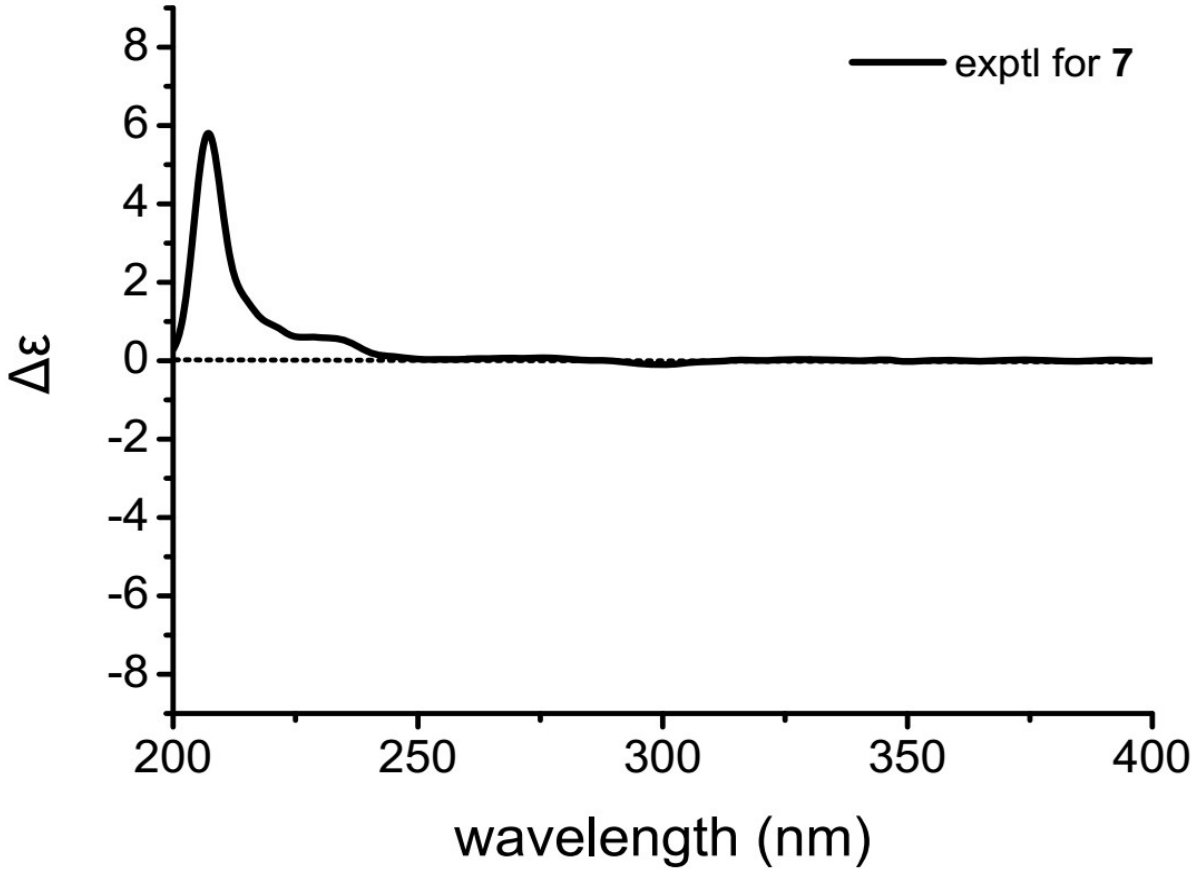
Figure S72. HMBC spectrum of Compound **7** in Pyr-d_5.

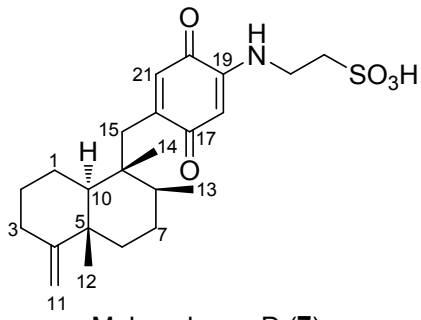




Melemeleone D (**7**)

Figure S73. NOESY spectrum of Compound **7** in Pyr-d_5.





Melemeleone D (**7**)

Figure S74. CD spectrum of Compound **7** in MeOH.

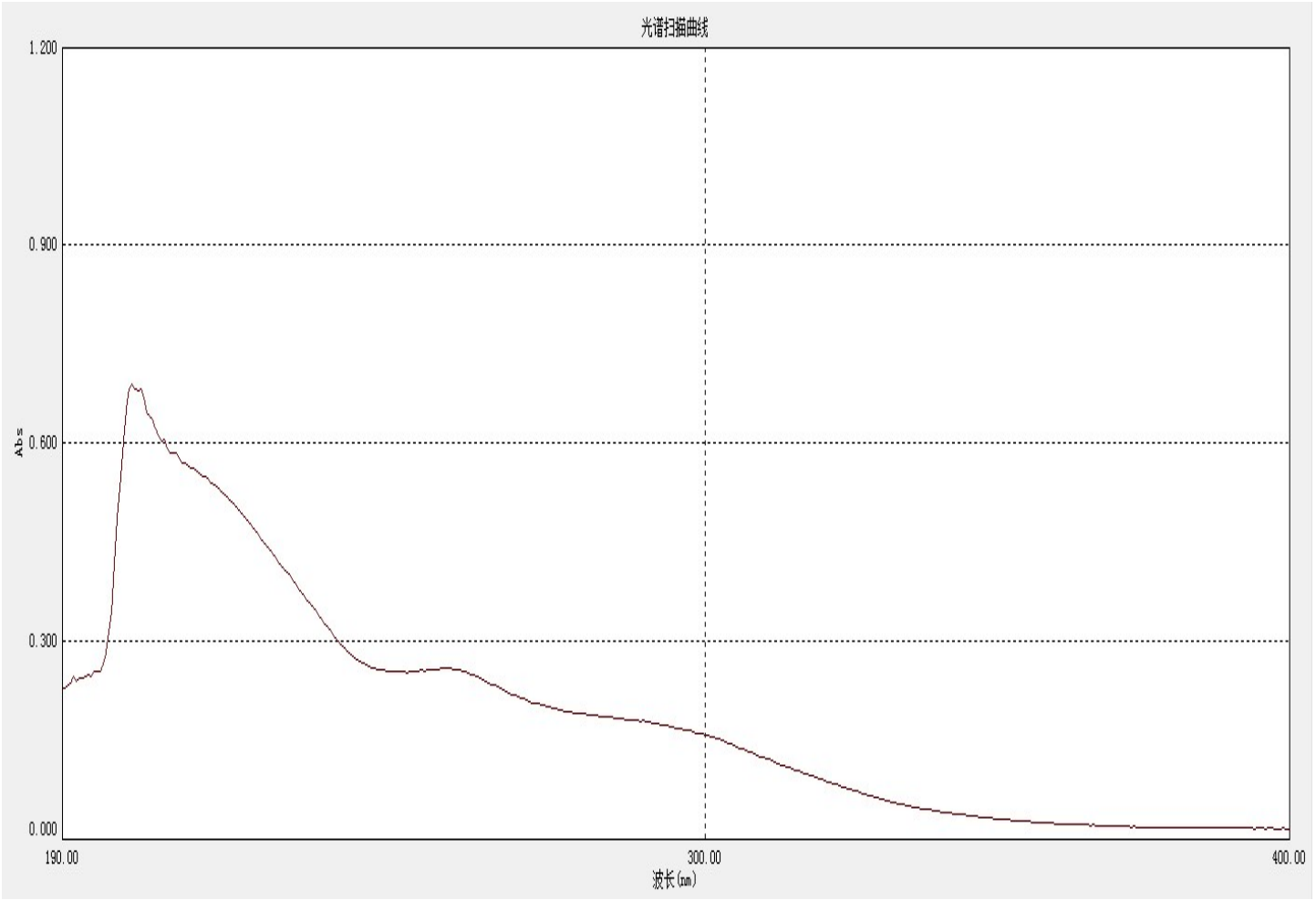
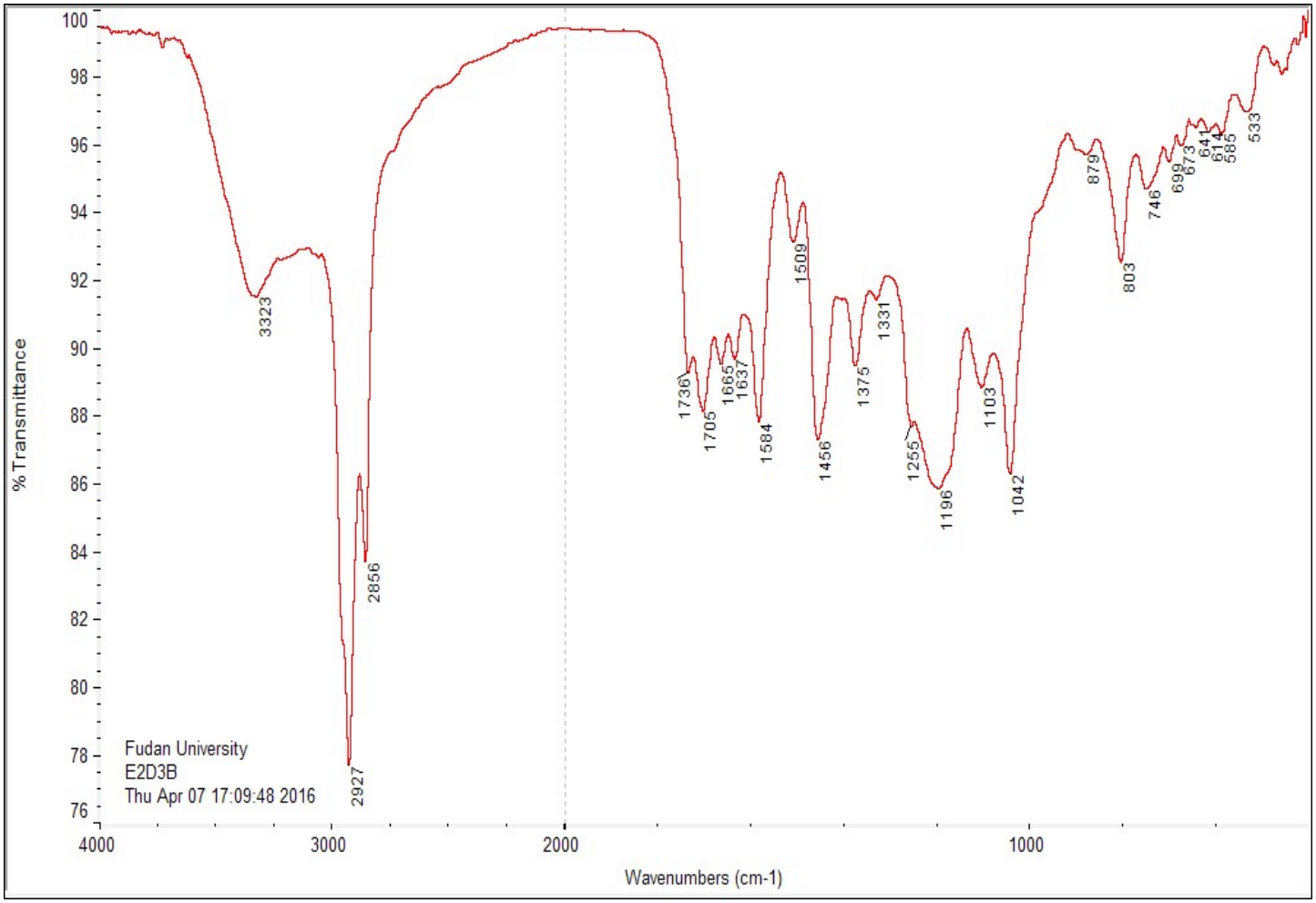


Figure S75. UV spectrum of Compound **8** in MeOH.



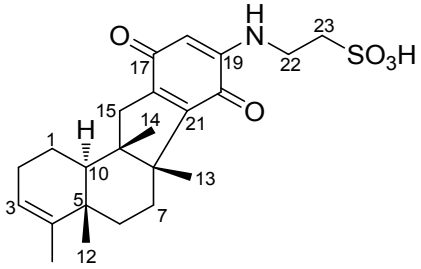
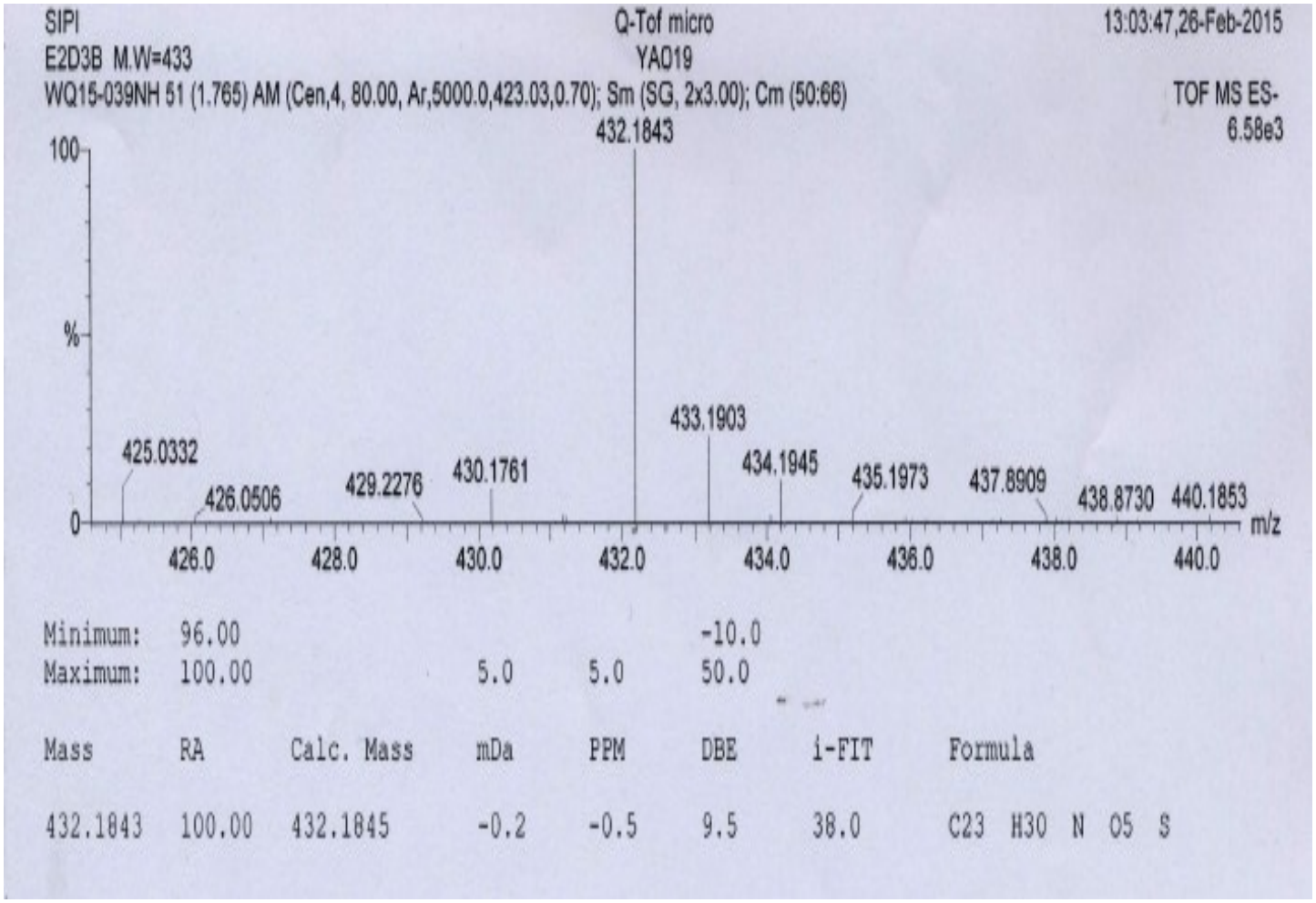
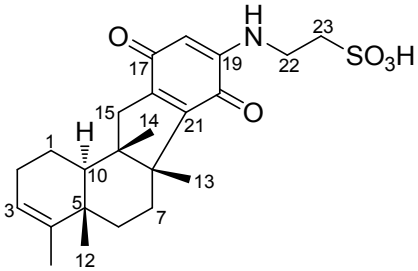


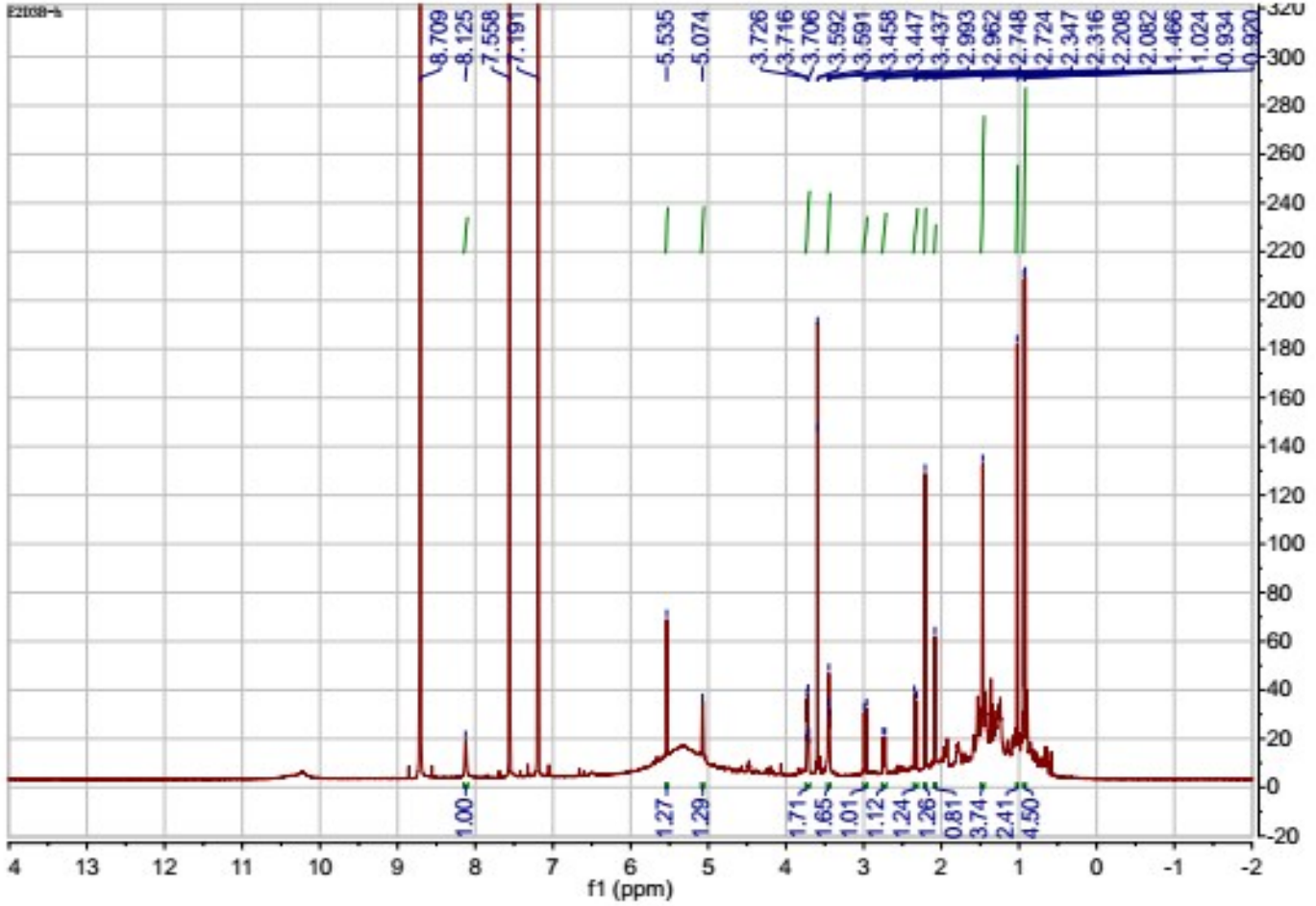
Figure S76. IR spectrum of Compound **8**.

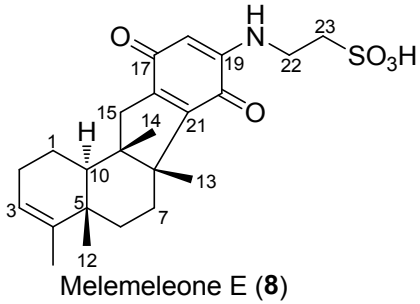




Melemeleone E (**8**)

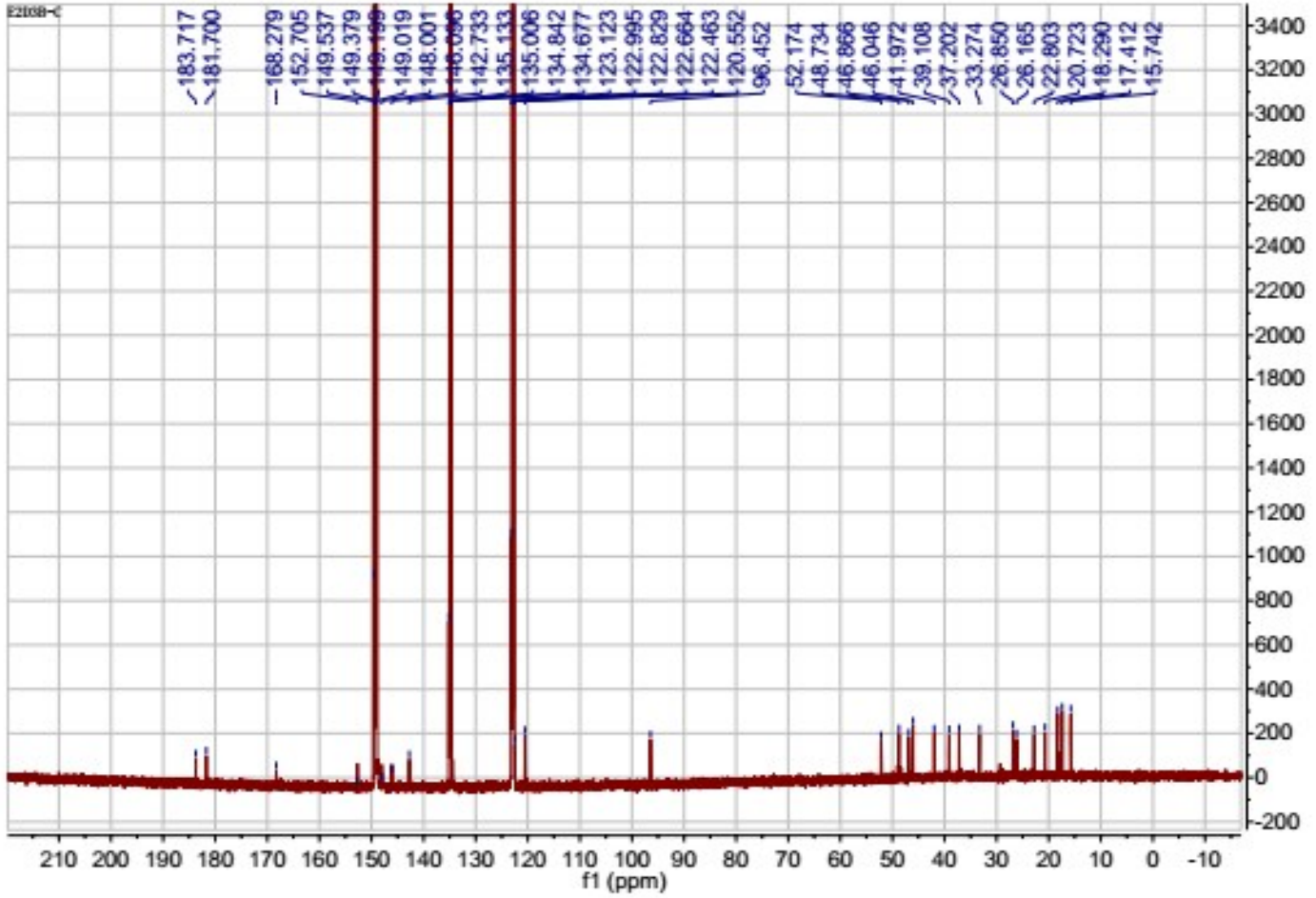
Figure S77. HRESIMS spectrum of Compound **8.**

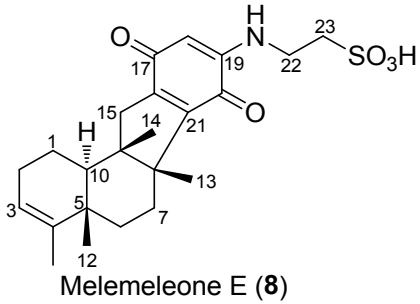




Melemeleone E (**8**)

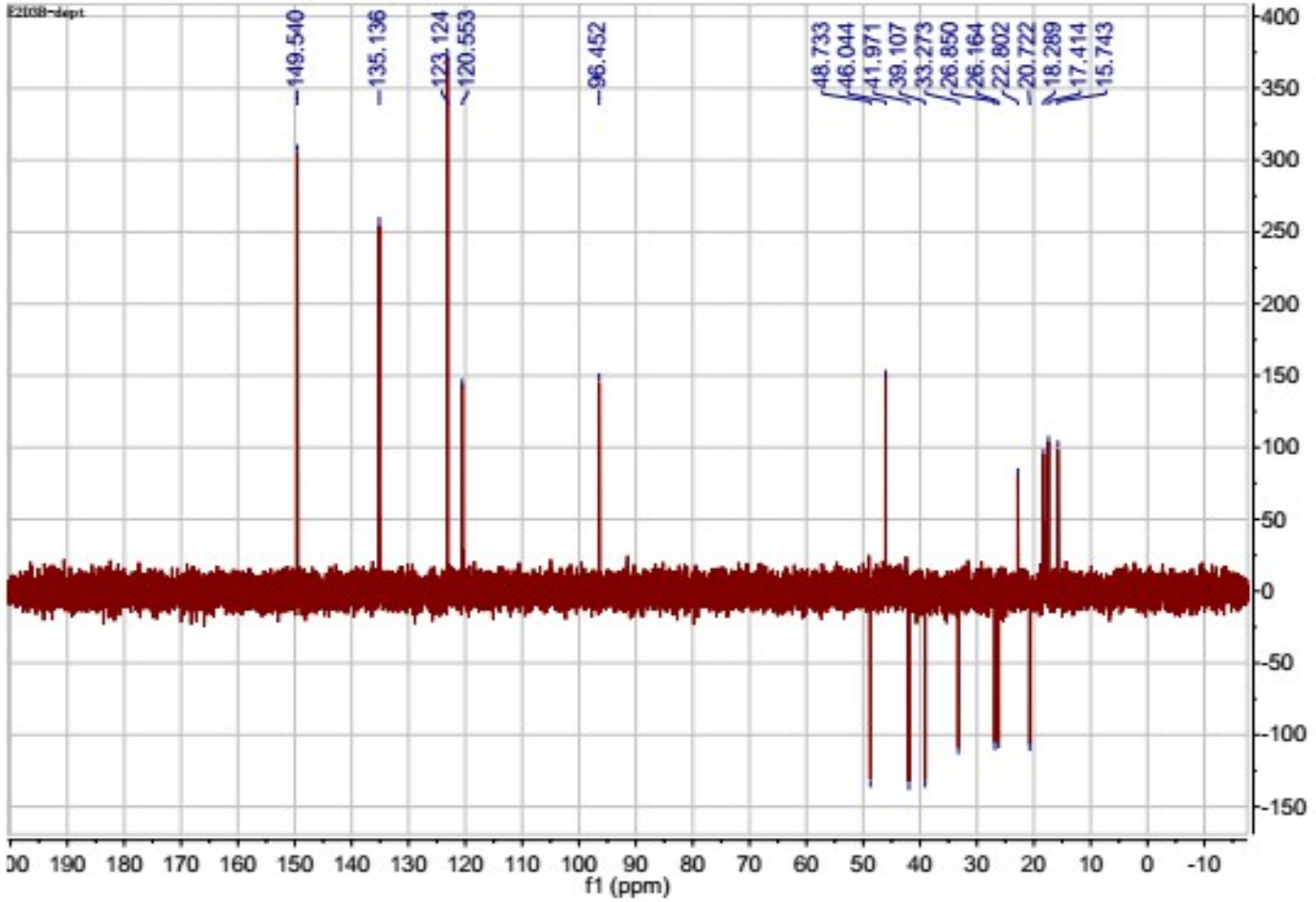
Figure S78. ^{1}H NMR spectrum of Compound **8** in Pyr-d_5.

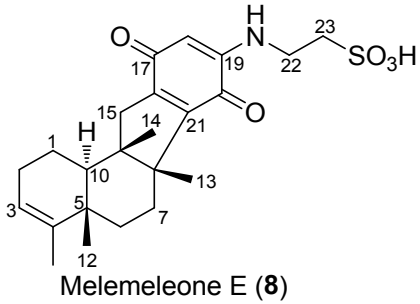




Melemeleone E (**8**)

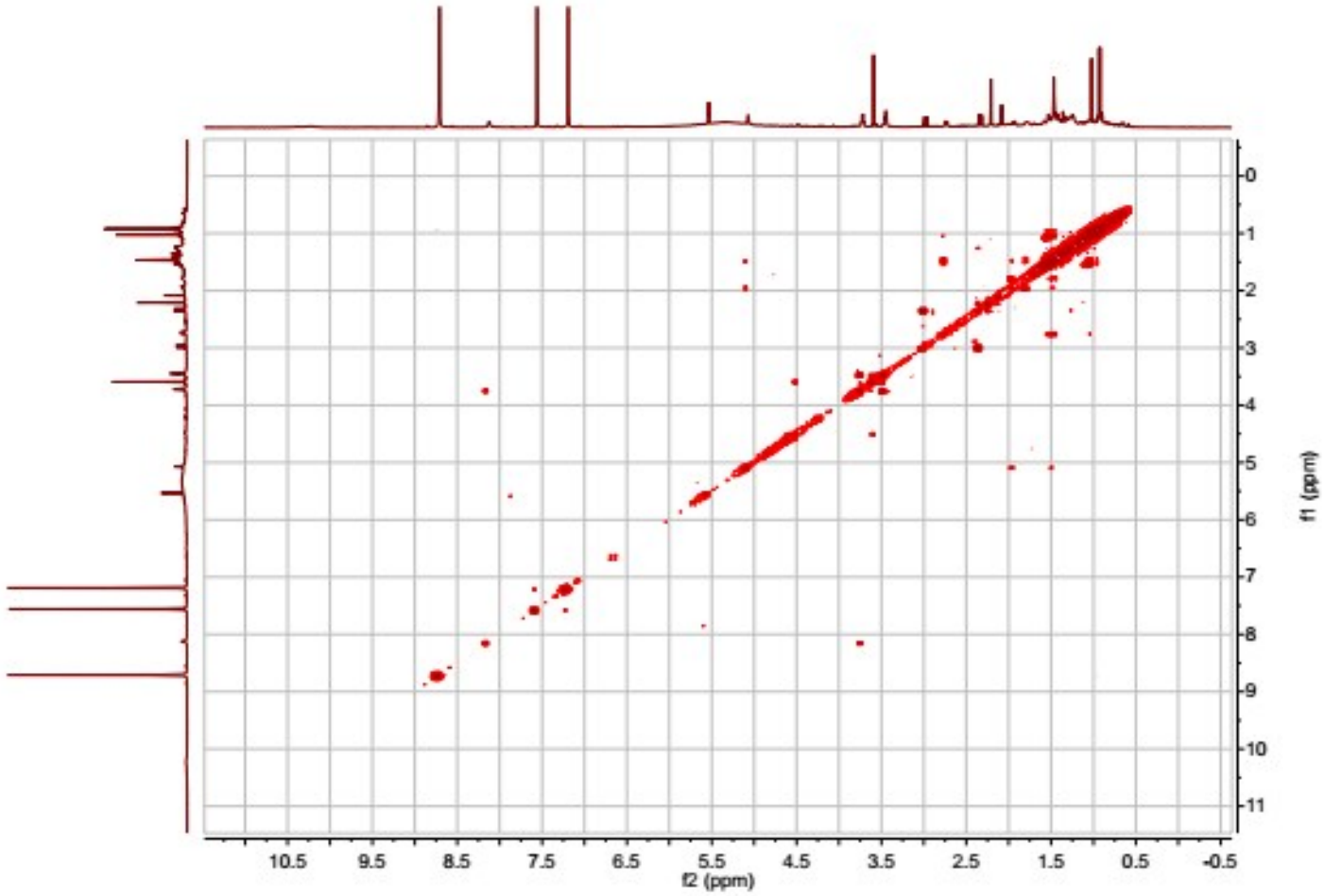
Figure S79. ^{13}C NMR spectrum of Compound **8** in Pyr-d_5.

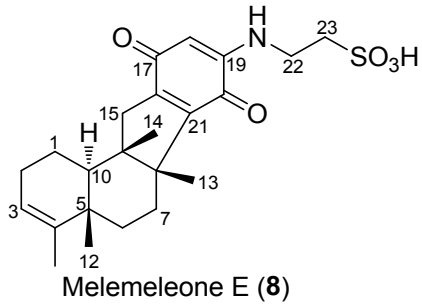




Melemeleone E (**8**)

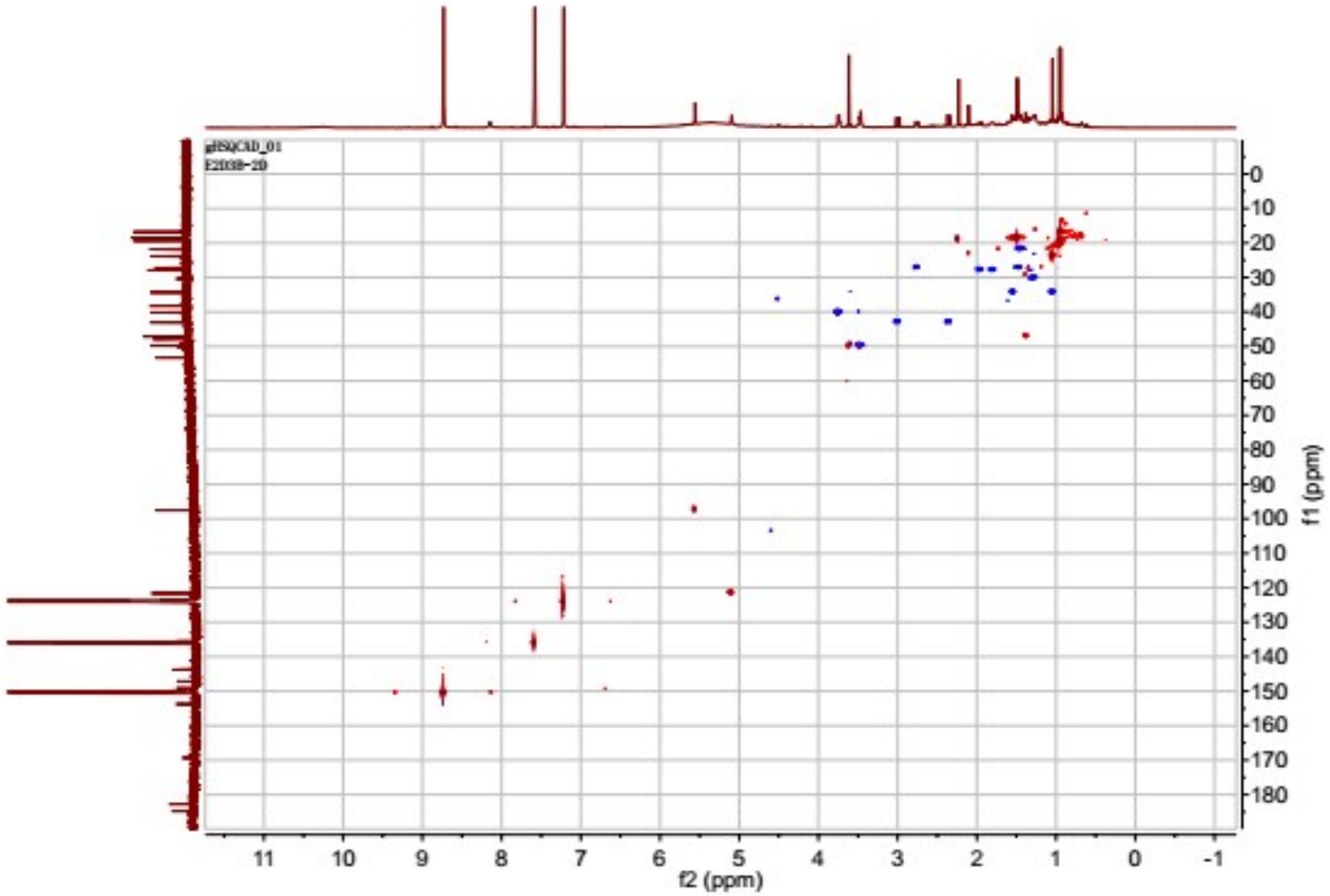
Figure S80. DEPT135 spectrum of Compound **8** in Pyr-d_5.





Melemeleone E (**8**)

Figure S81. ^{1}H-^{1}H COSY spectrum of Compound **8** in Pyr-d_5.



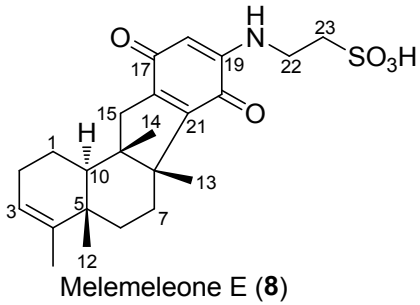
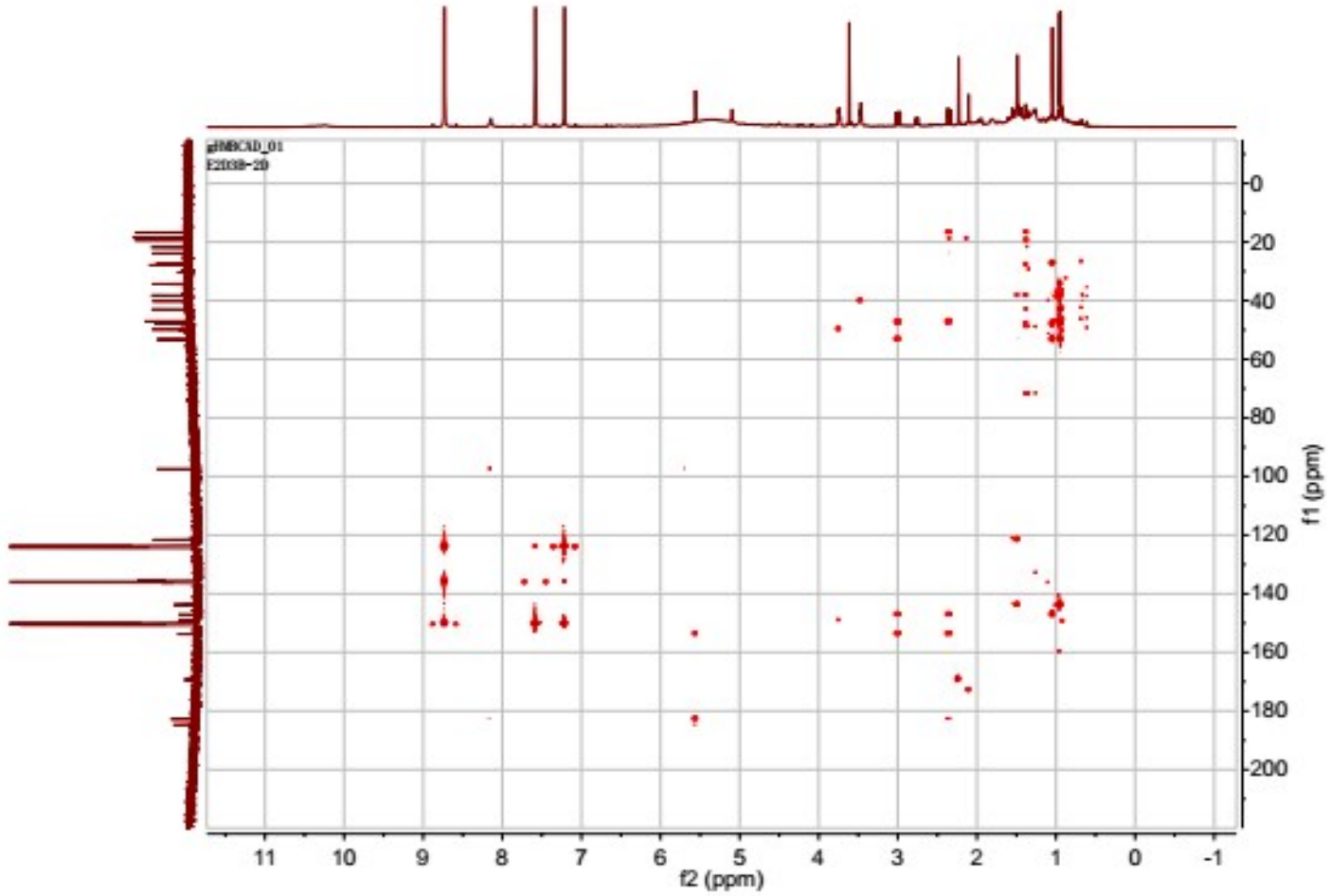


Figure S82. HSQC spectrum of Compound **8** in Pyr-d_5.



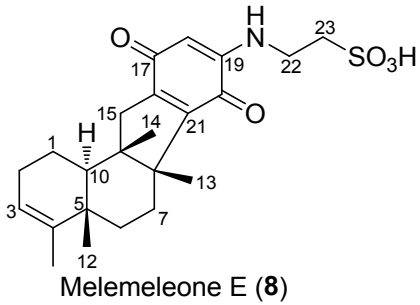
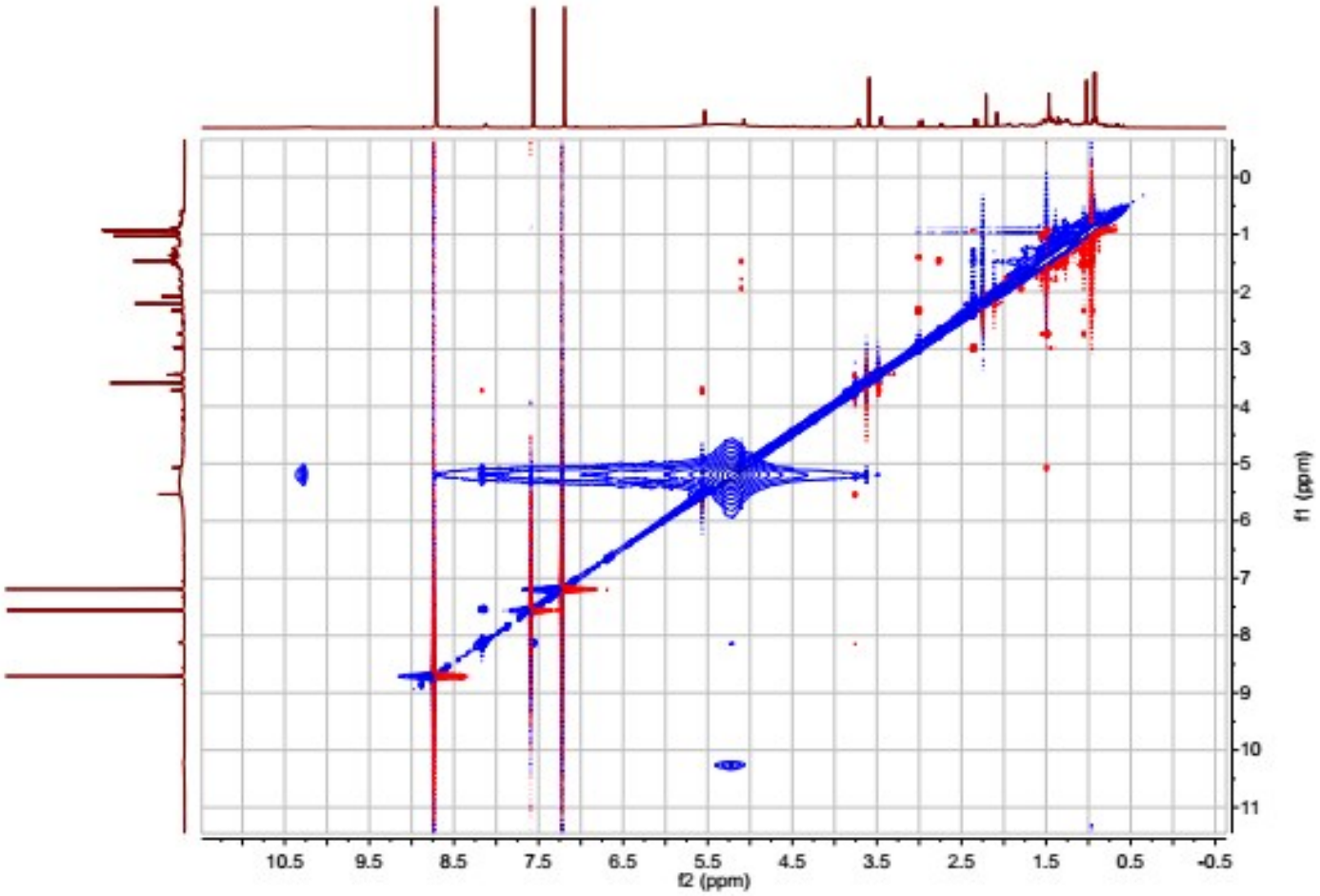
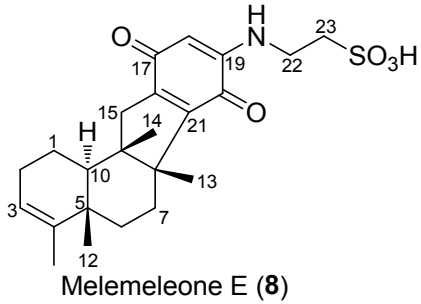


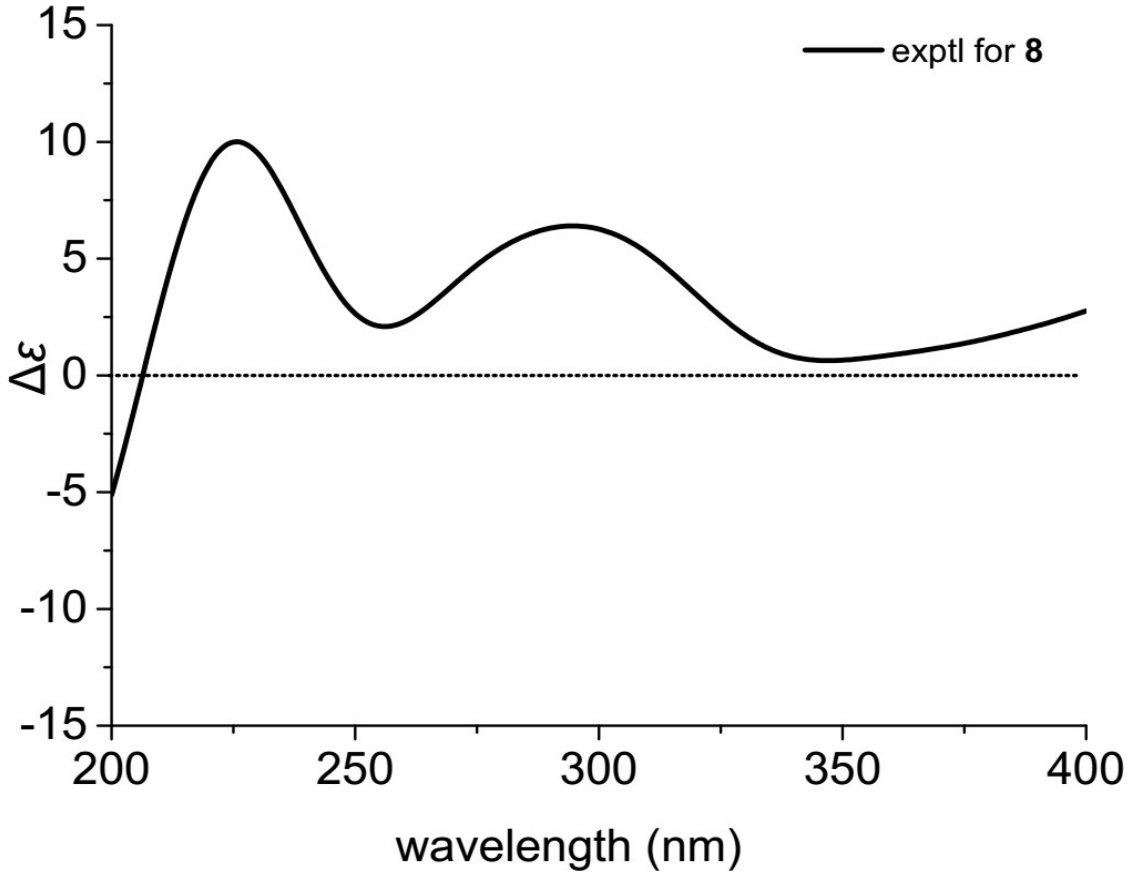
Figure S83. HMBC spectrum of Compound **8** in Pyr-d_5.

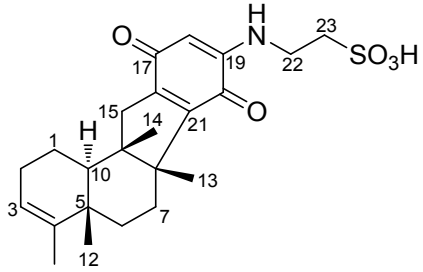




Melemeleone E (**8**)

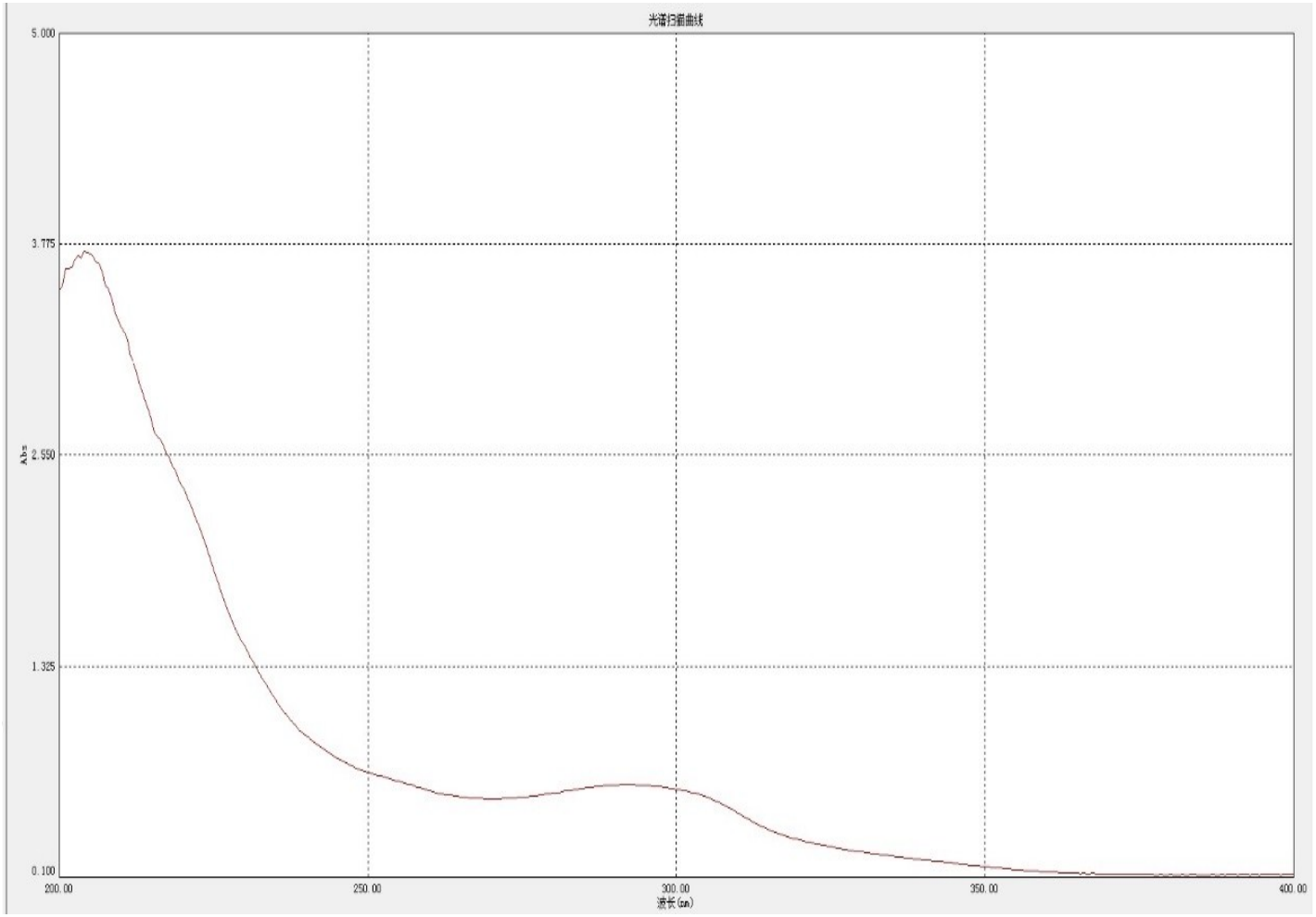
Figure S84. NOESY spectrum of Compound **8** in Pyr-d_5.

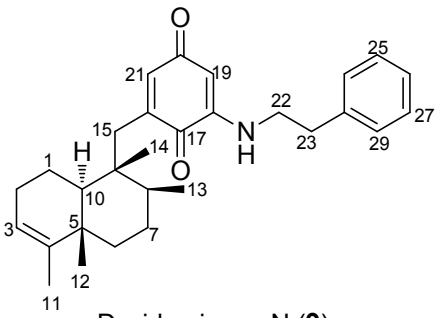




Melemeleone E (**8**)

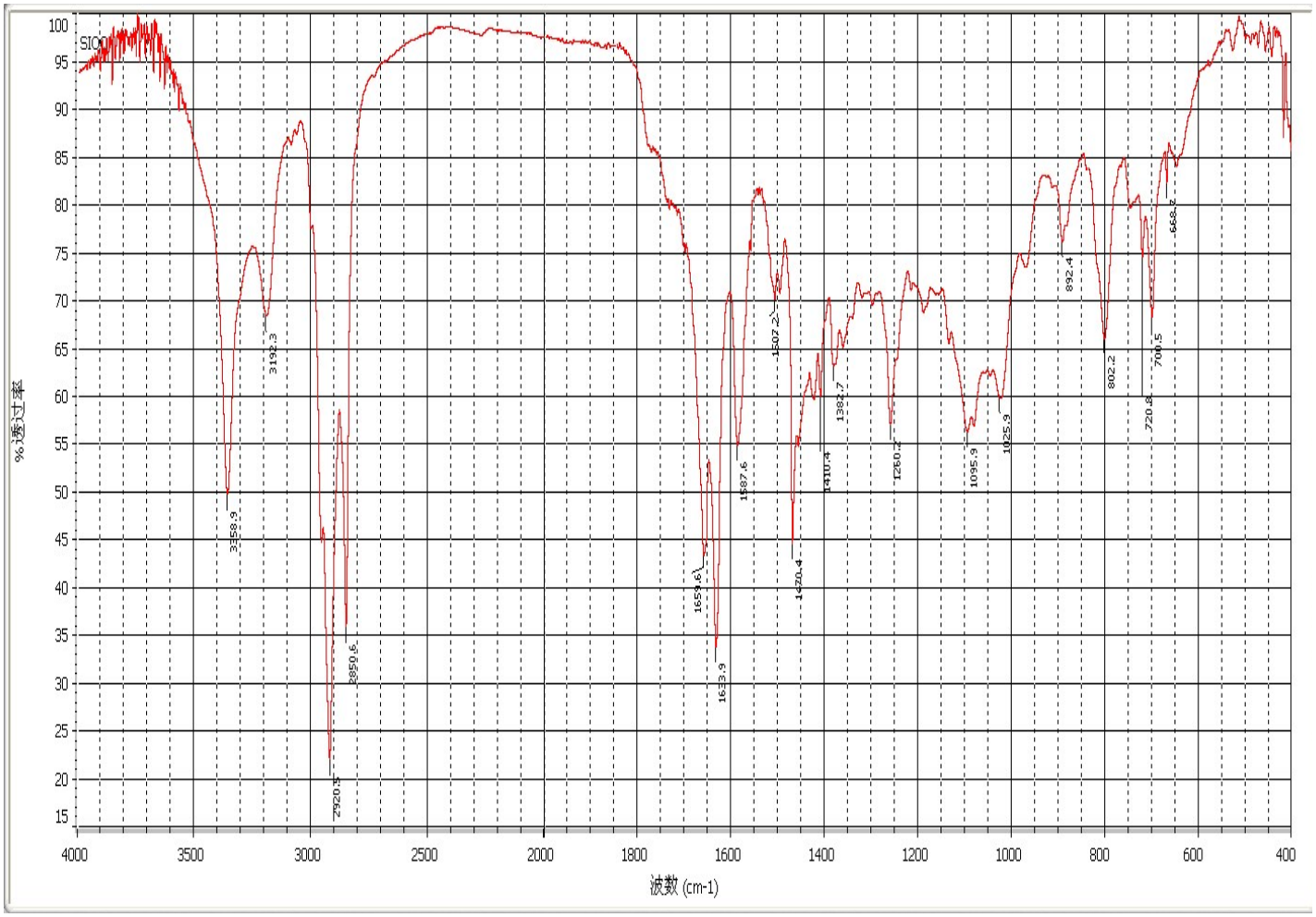
Figure S85. CD spectrum of Compound **8** in MeOH.

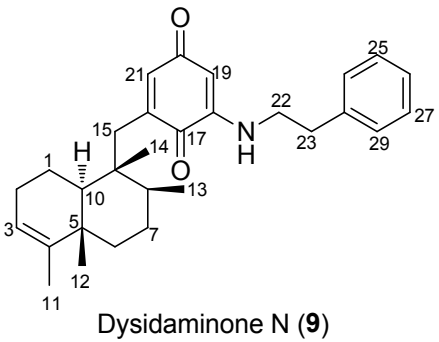




Dysidaminone N (**9**)

Figure S86. UV spectrum of Compound **9** in MeOH.



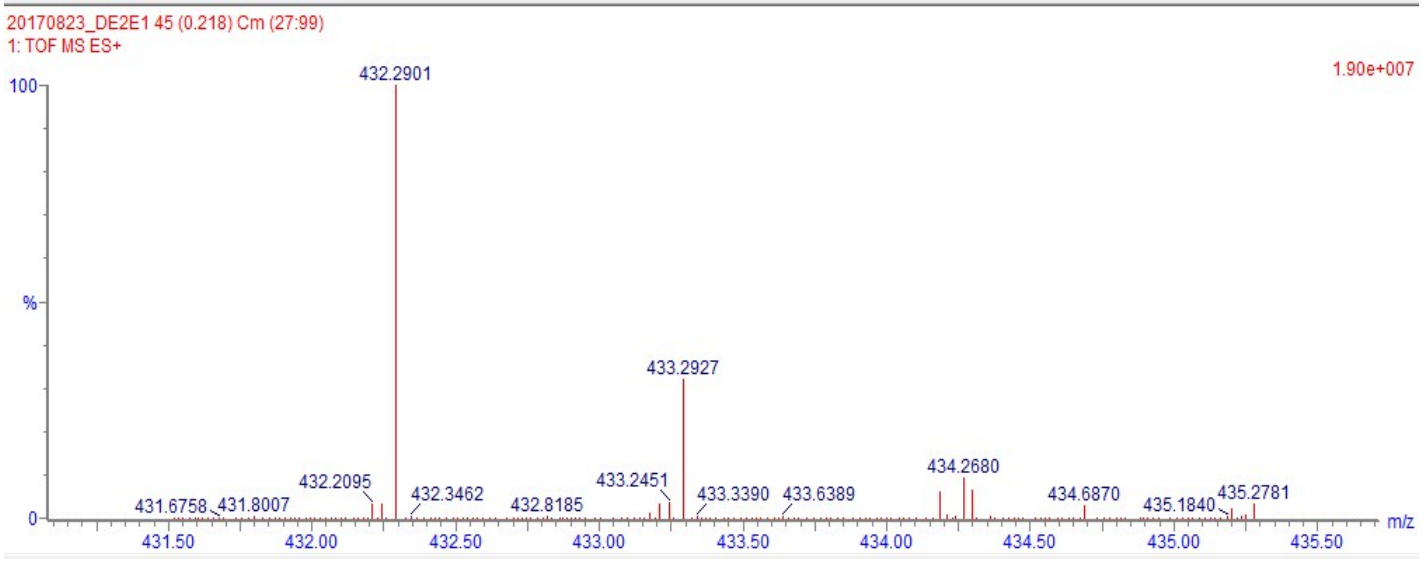


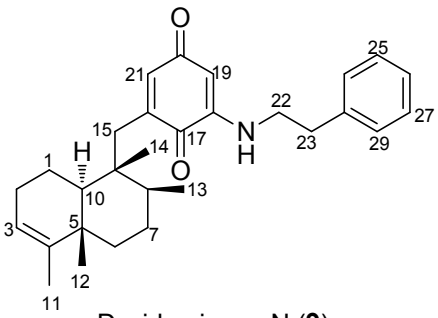
Dysidaminone N (**9**)

Figure S87. IR spectrum of Compound **9**.

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
1020 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)
Elements Used:

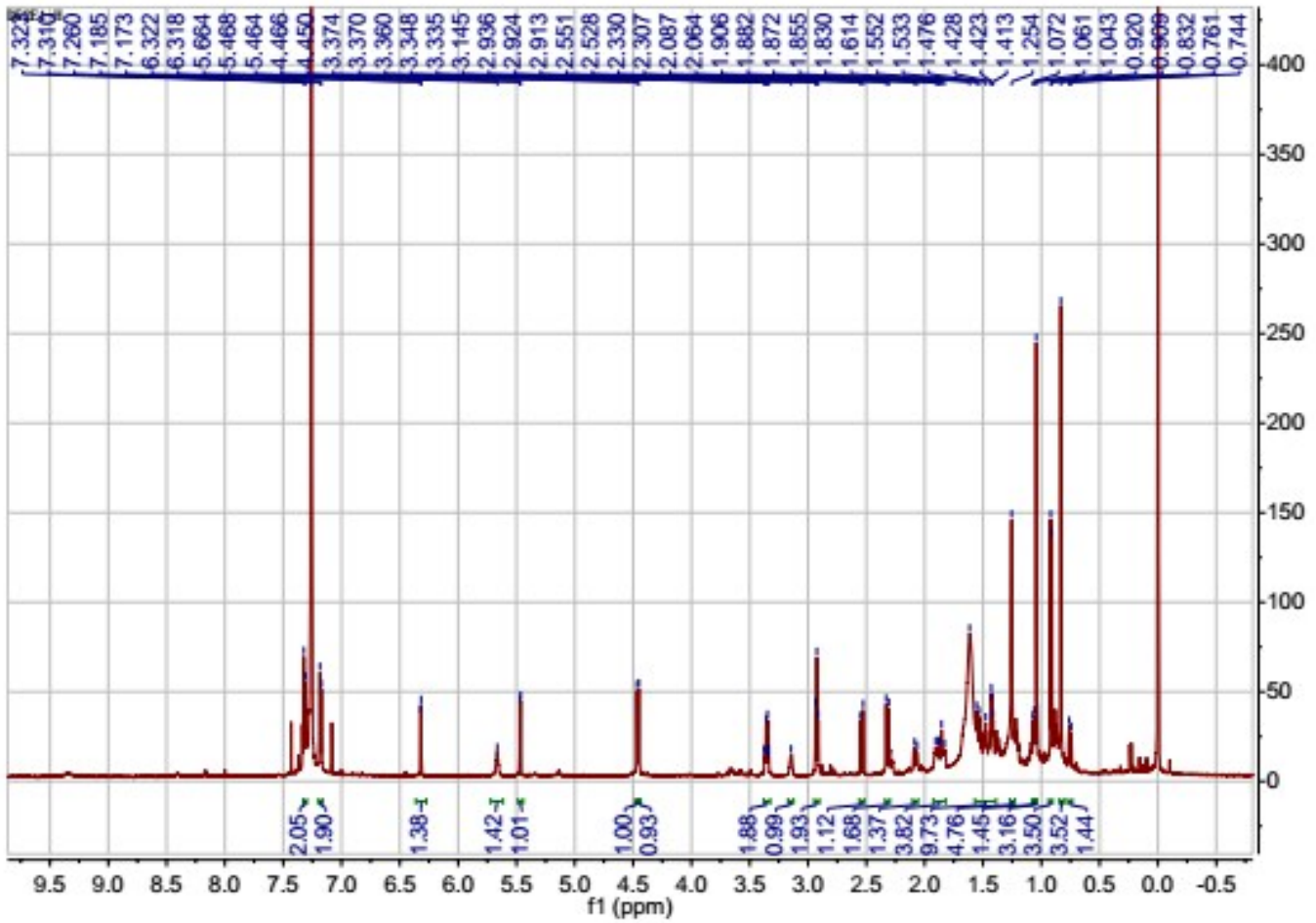
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	23Na
432.2901	432.2903	-0.2	-0.5	11.5	C29 H38 N O2	2047.5	0.046	95.53	29	38	1	2	
	432.2921	-2.0	-4.6	-1.5	C17 H42 N3 O9	2057.3	9.819	0.01	17	42	3	9	
	432.2878	2.3	5.3	8.5	C27 H39 N O2 23Na	2050.7	3.165	4.22	27	39	1	2	1
	432.2937	-3.6	-8.3	-0.5	C20 H43 N O7 23Na	2056.2	8.726	0.02	20	43	1	7	1
	432.2862	3.9	9.0	7.5	C24 H38 N3 O4	2053.6	6.071	0.23	24	38	3	4	





Dysidaminone N (**9**)

Figure S88. HRESIMS spectrum of Compound **9**.



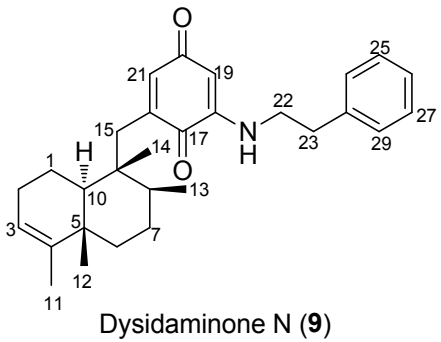
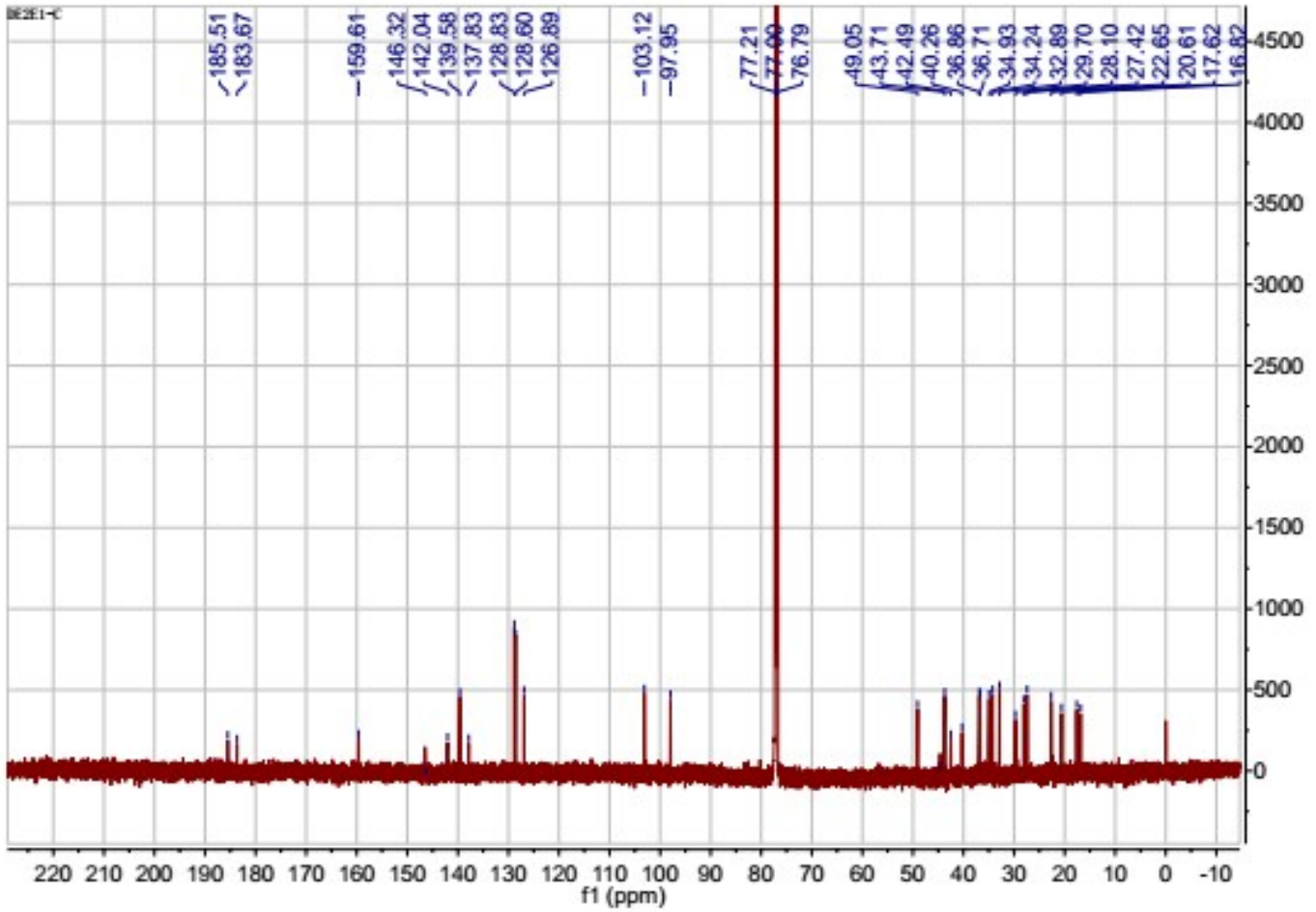
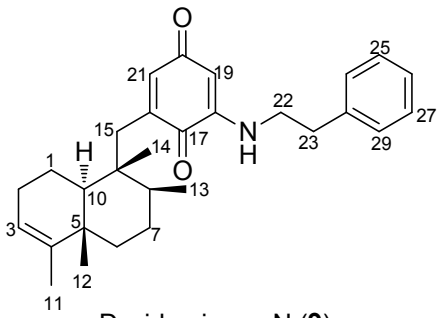


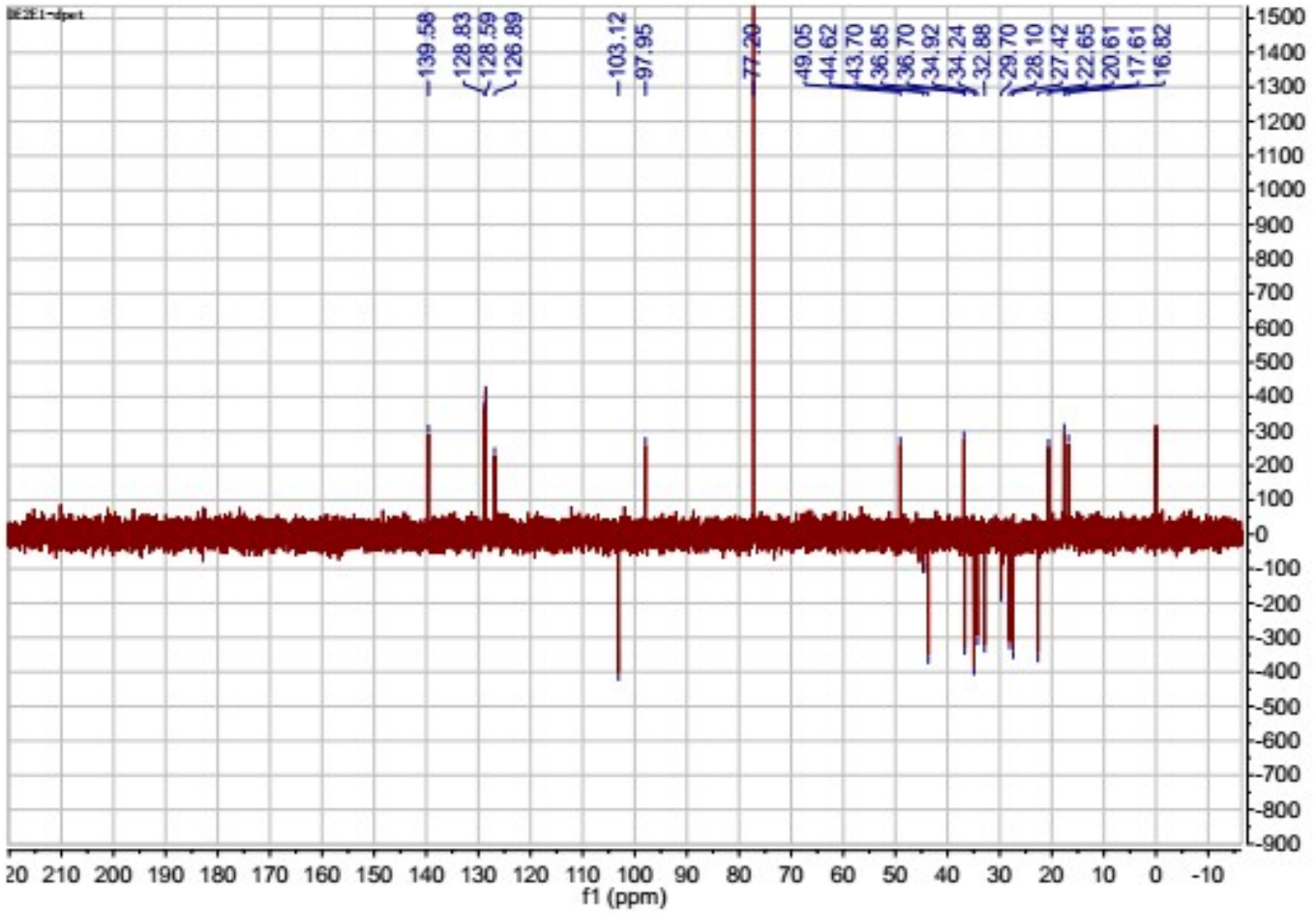
Figure S89. ^{1}H NMR spectrum of Compound **9** in $CDCl_3$.

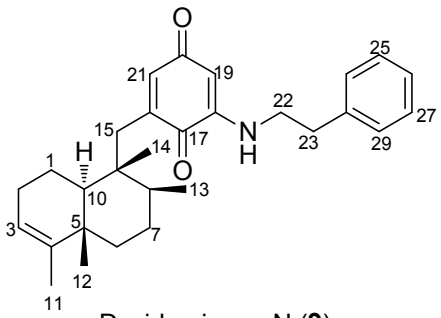




Dysidaminone N (**9**)

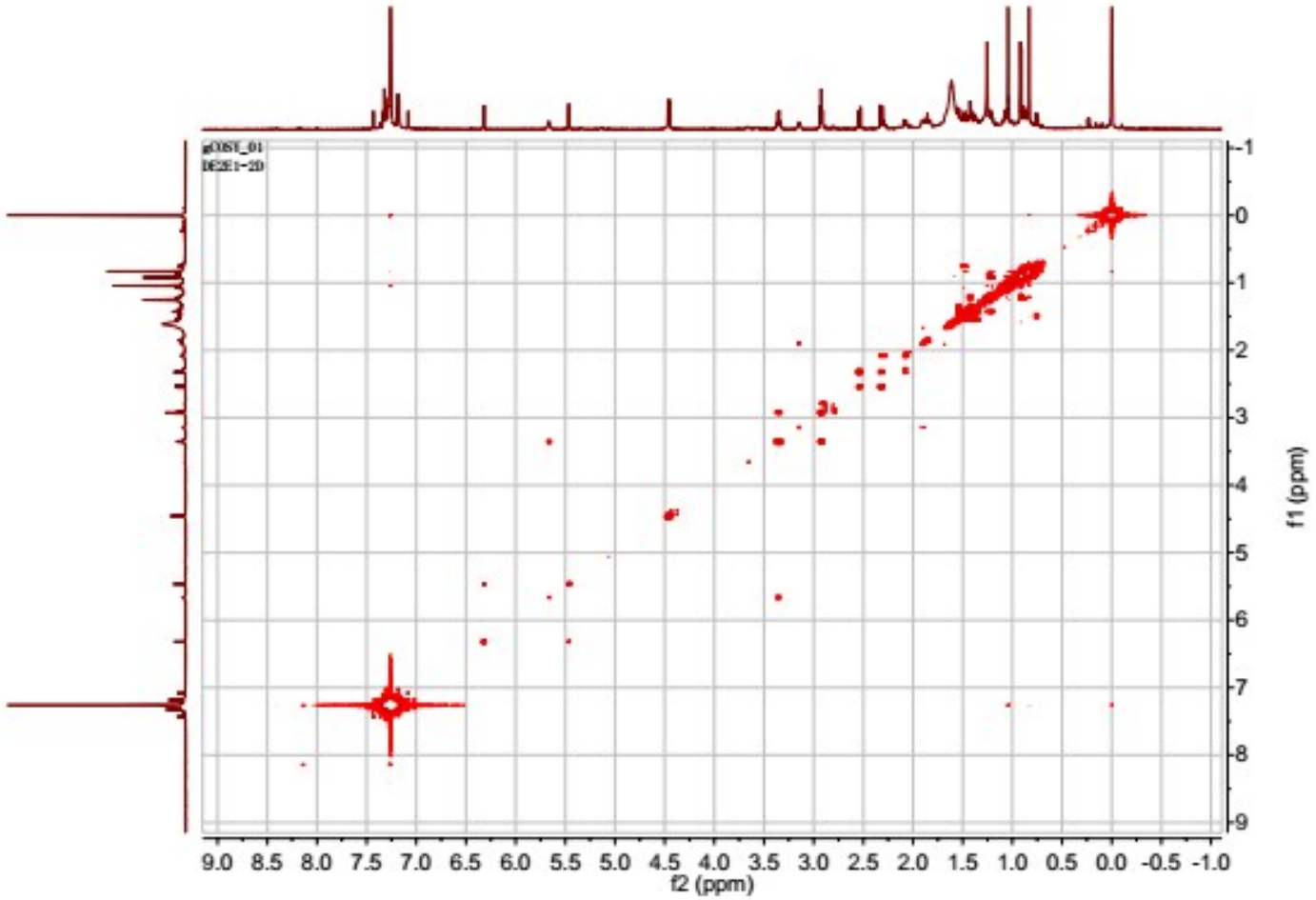
Figure S90. ^{13}C NMR spectrum of Compound **9** in $CDCl_3$.

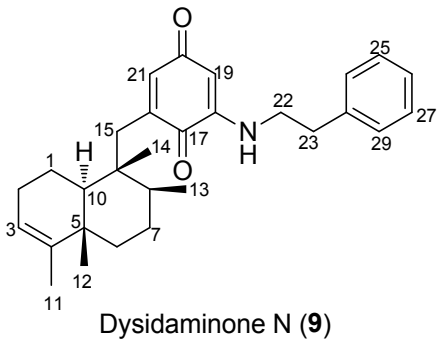




Dysidaminone N (**9**)

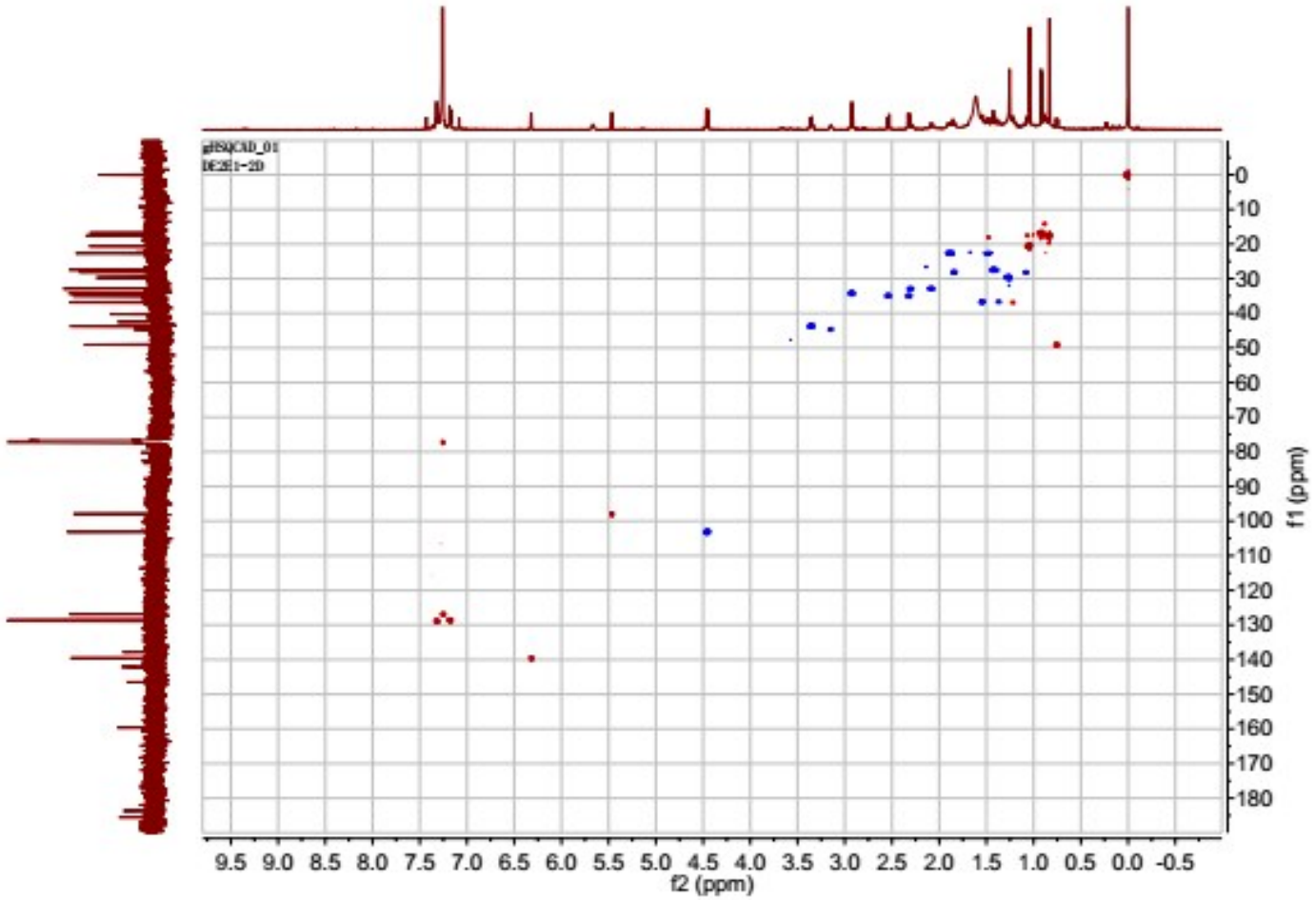
Figure S91. DEPT135 spectrum of Compound **9** in $CDCl_3$.

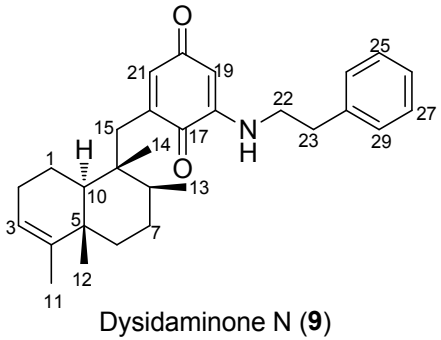




Dysidaminone N (**9**)

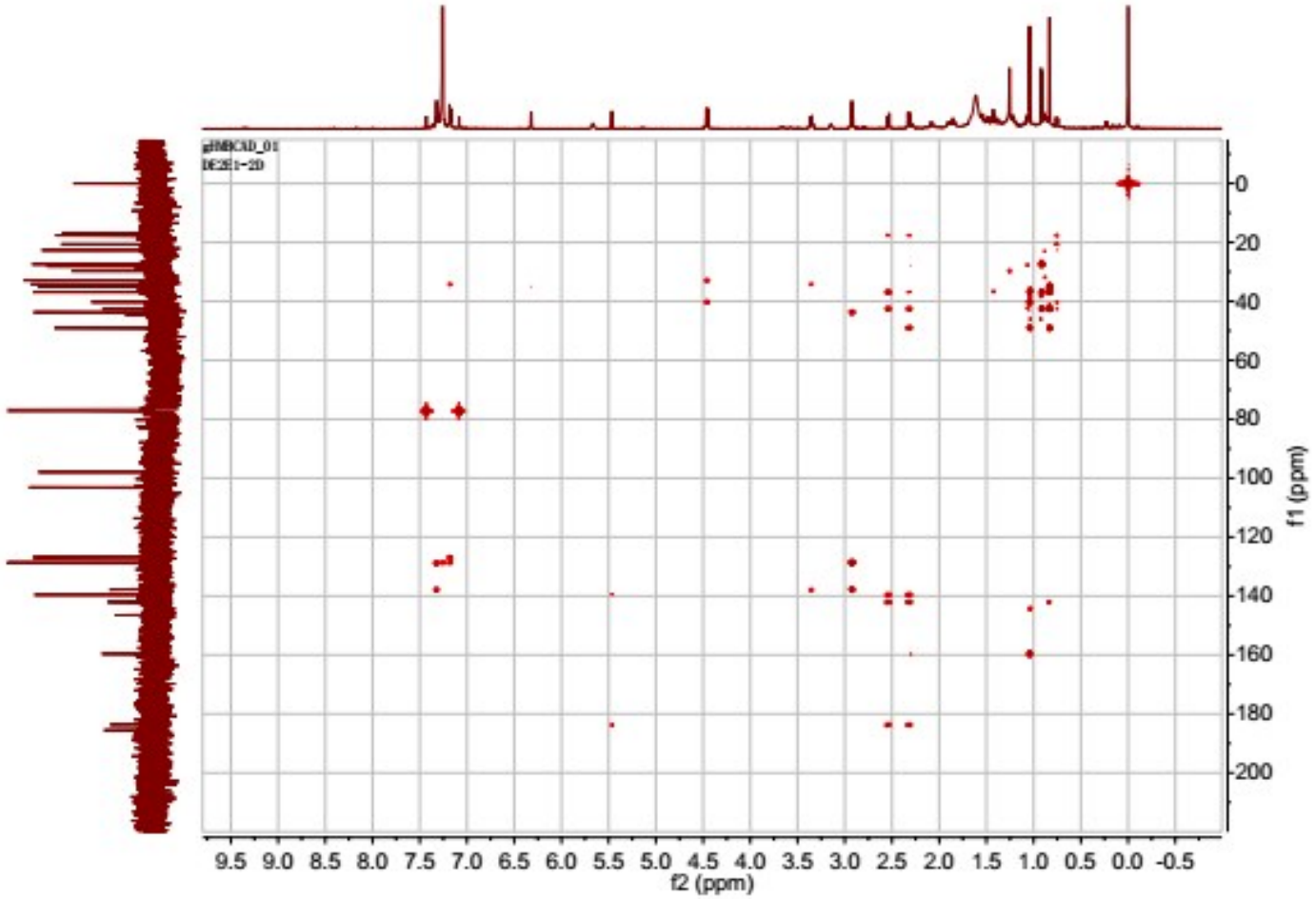
Figure S92. ^{1}H-^{1}H COSY spectrum of Compound **9** in $CDCl_3$.

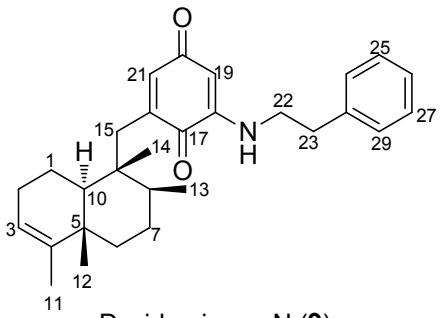




Dysidaminone N (**9**)

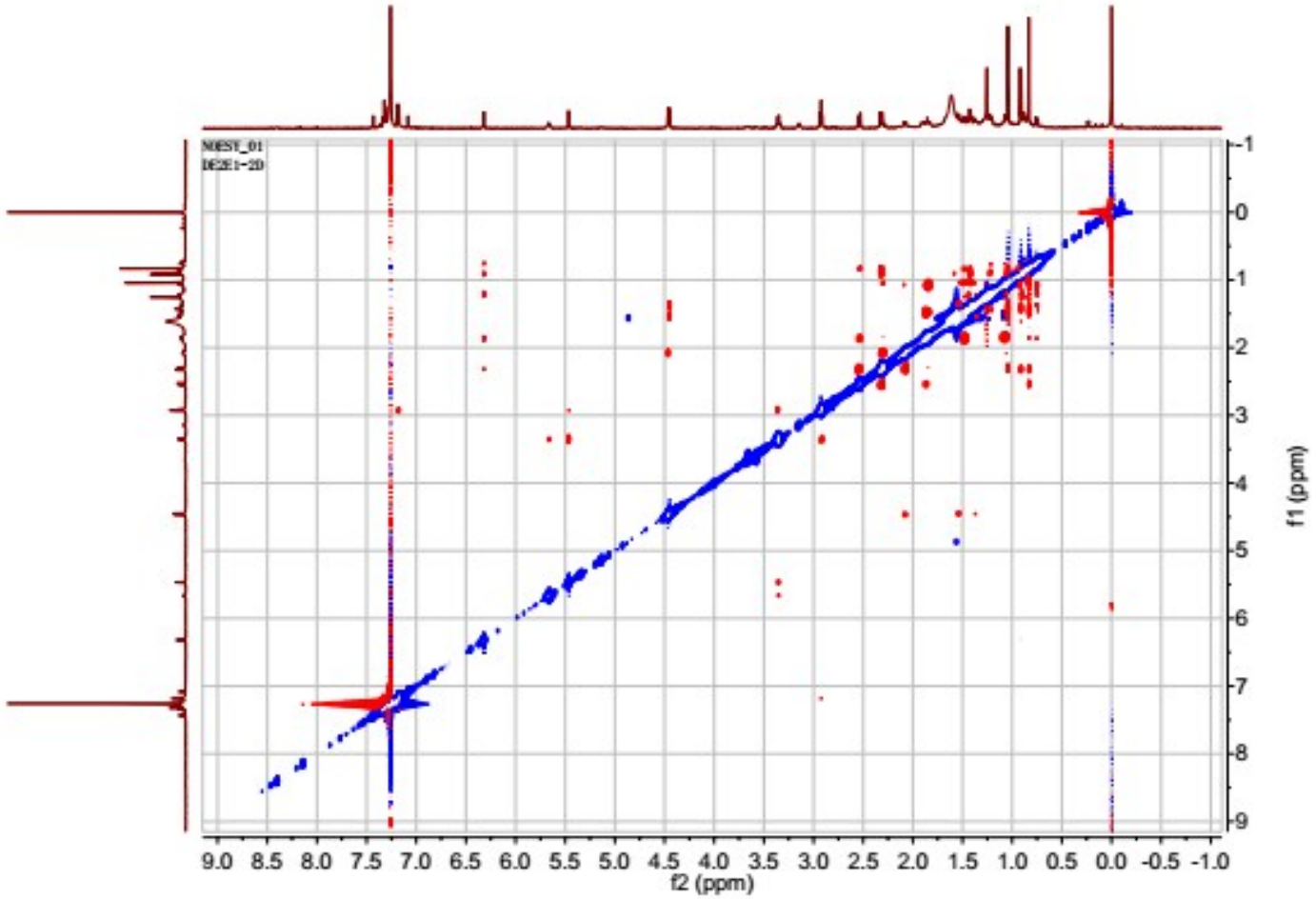
Figure S93. HSQC spectrum of Compound **9** in $CDCl_3$.

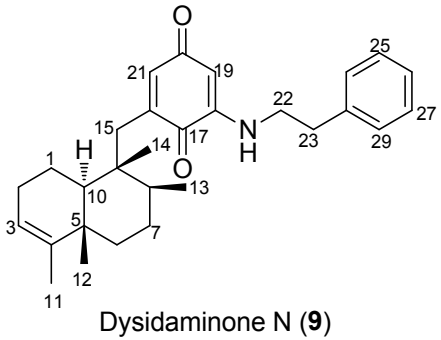




Dysidaminone N (**9**)

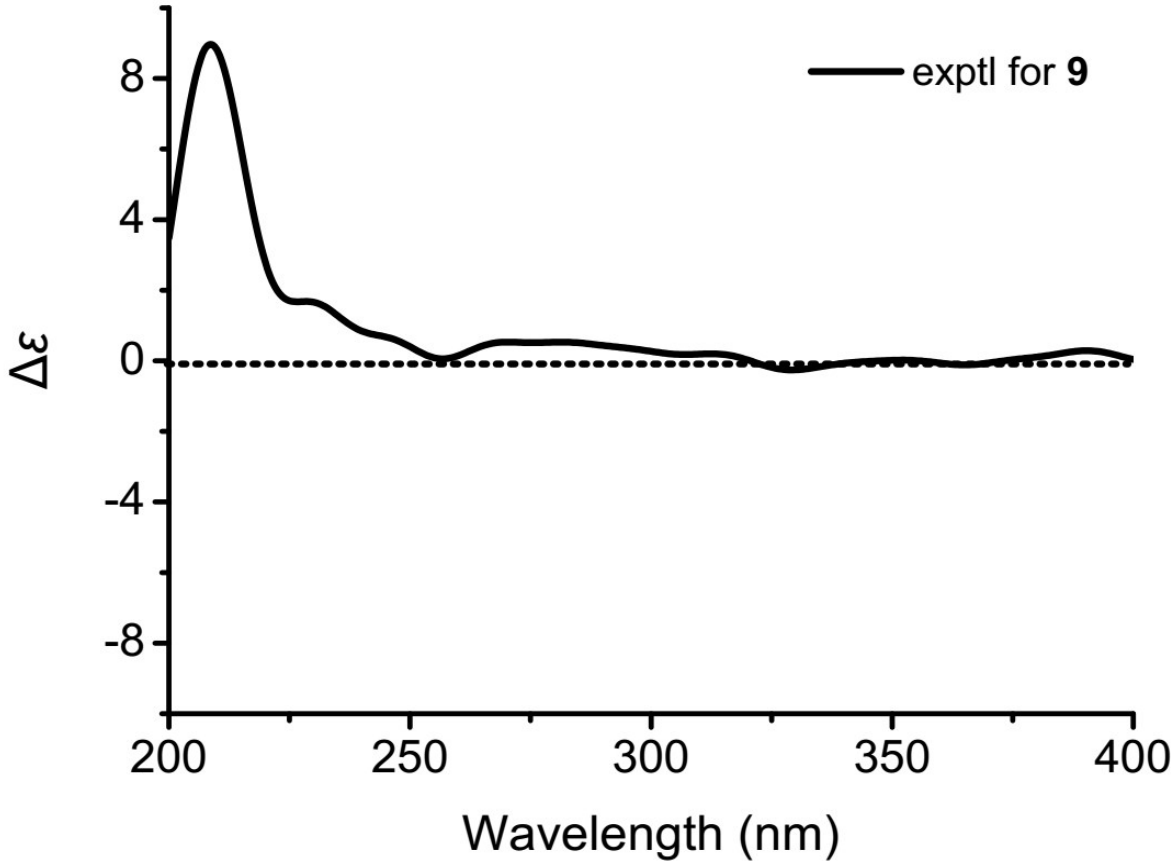
Figure S94. HMBC spectrum of Compound **9** in $CDCl_3$.

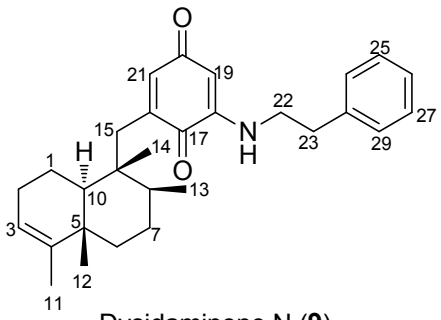




Dysidaminone N (**9**)

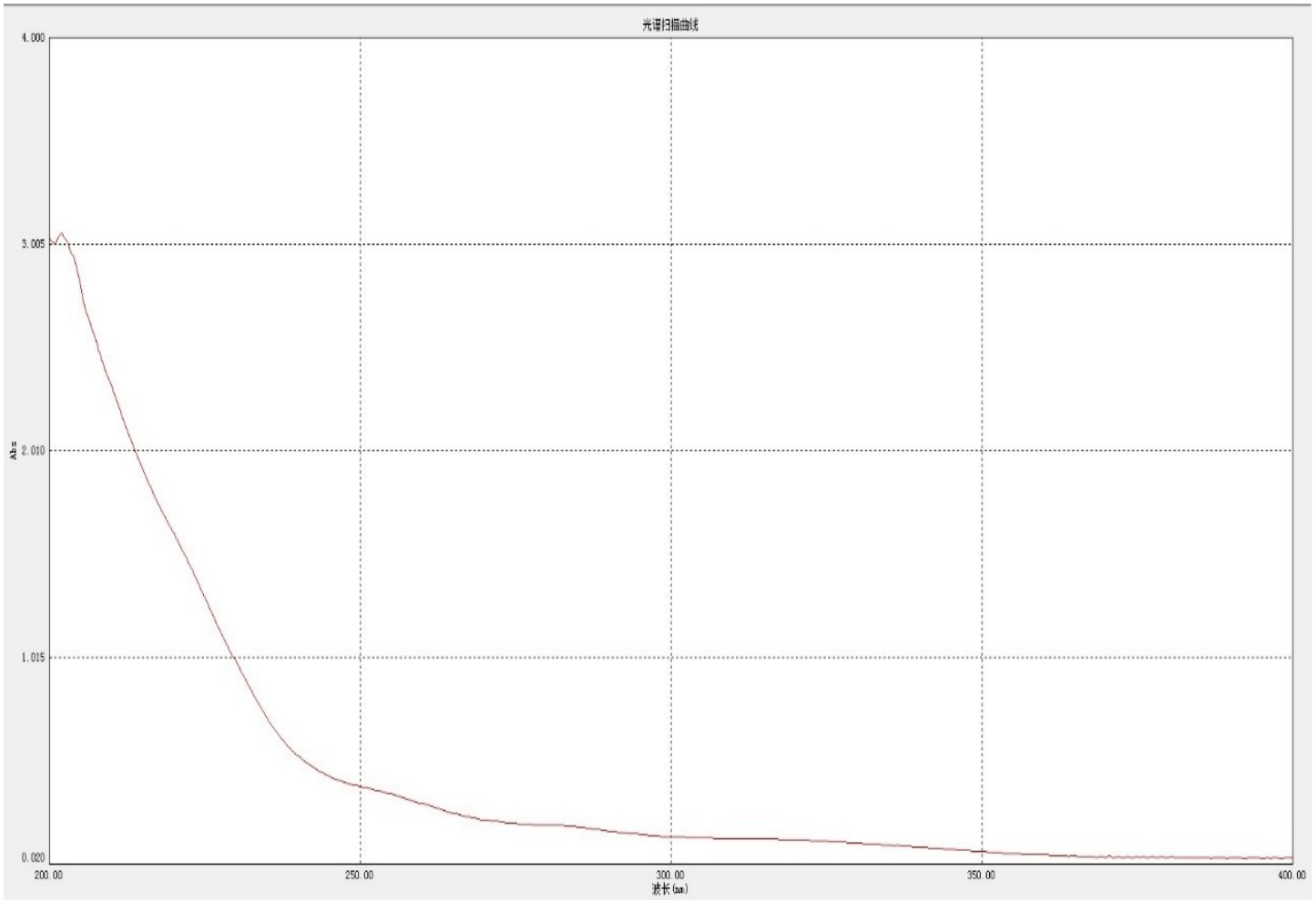
Figure S95. NOESY spectrum of Compound **9** in $CDCl_3$.

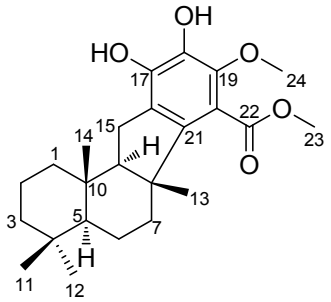




Dysidaminone N (**9**)

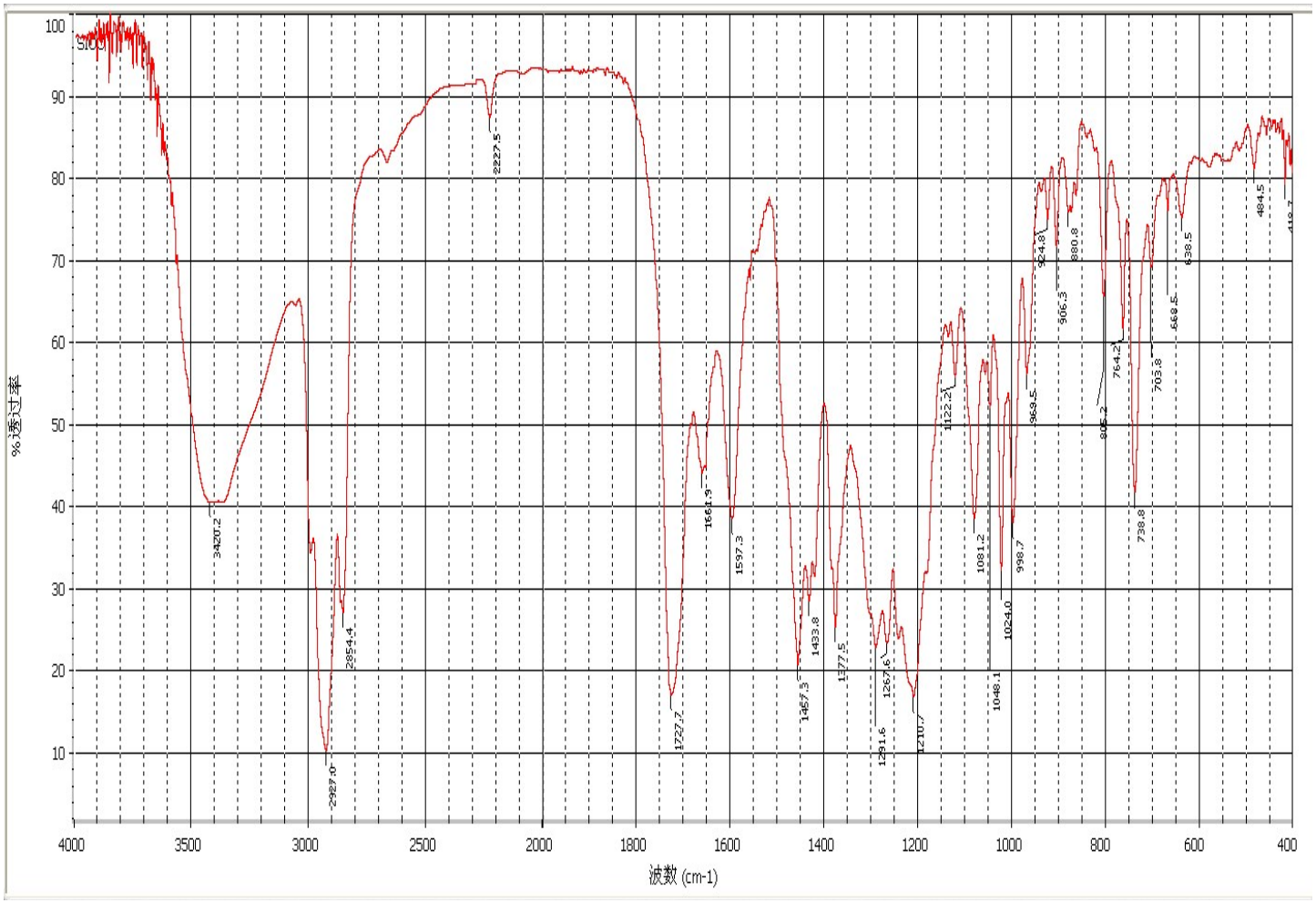
Figure S96. CD spectrum of Compound **9** in $CDCl_3$.

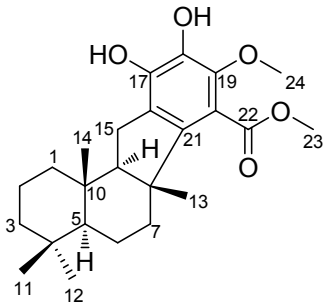




19-*O*-methylpelorol (**10**)

Figure S97. UV spectrum of Compound **10** in MeOH.



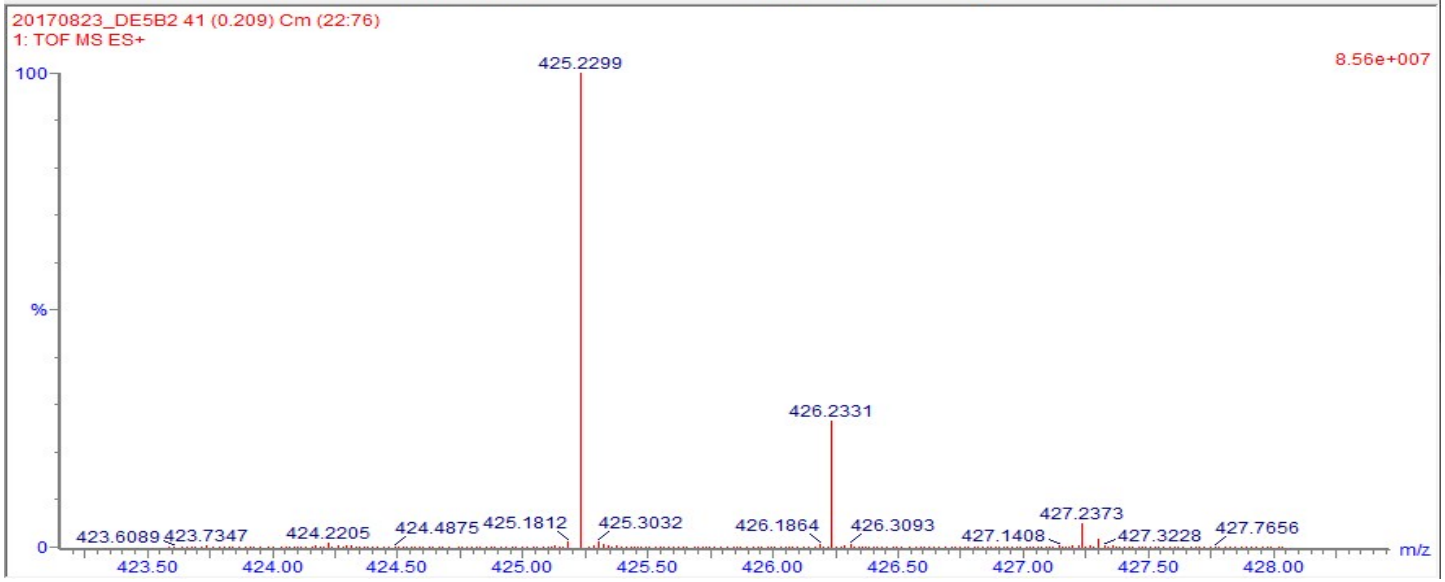


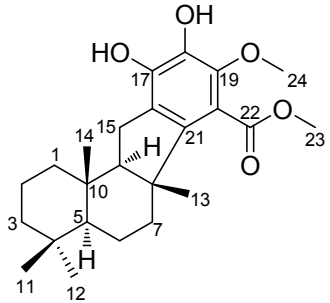
19-*O*-methylpelorol (**10**)

Figure S98. IR spectrum of Compound **10**.

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
1637 formula(e) evaluated with 12 results within limits (up to 50 closest results for each mass)
Elements Used:

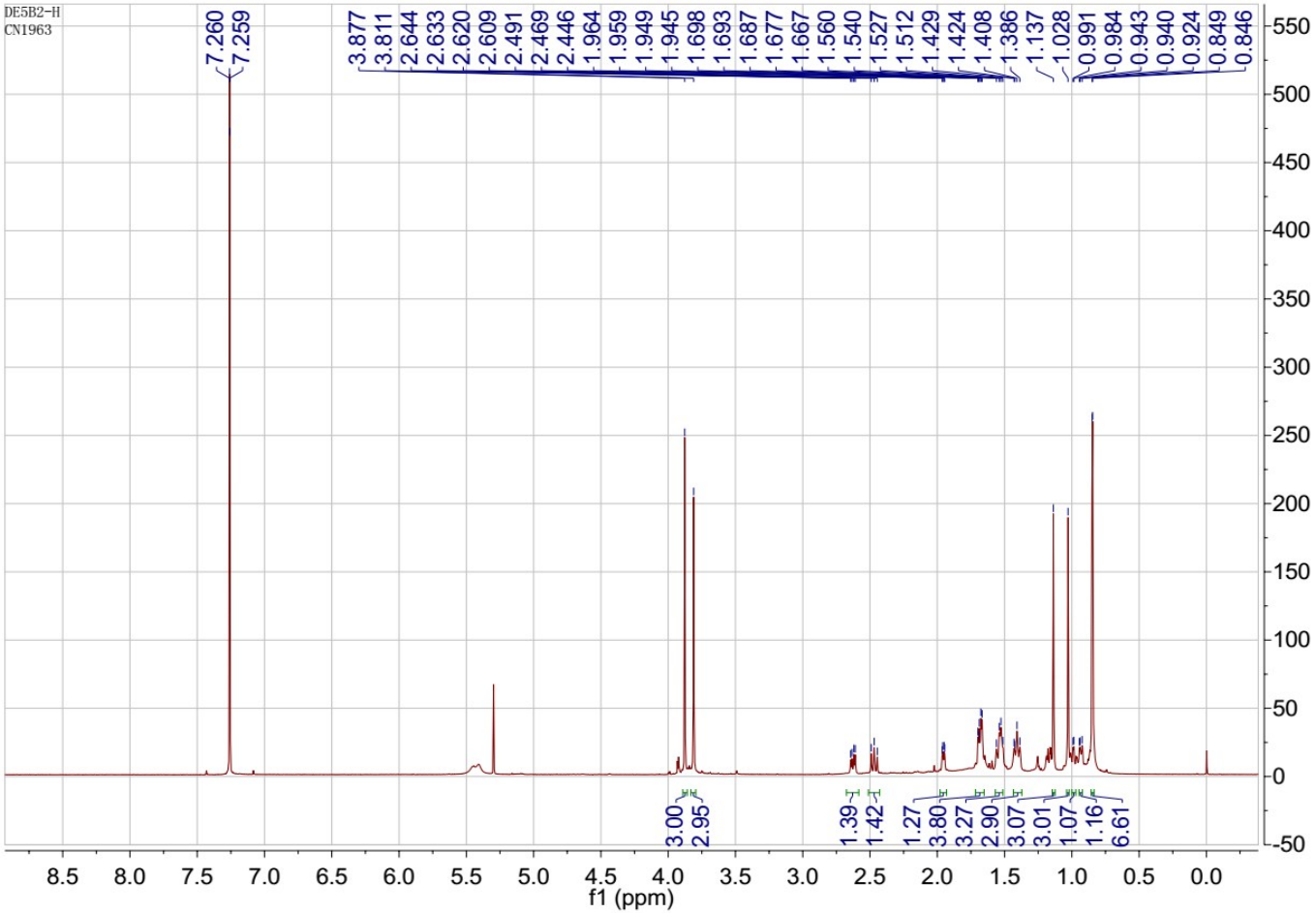
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	23Na
425.2299	425.2304	-0.5	-1.2	7.5	C24 H34 O5 23Na	2525.6	0.098	90.69	24	34		5	1
	425.2328	-2.9	-6.8	10.5	C26 H33 O5	2528.6	3.058	4.70	26	33		5	
	425.2301	-0.2	-0.5	11.5	C22 H29 N6 O3	2529.5	3.981	1.87	22	29	6	3	
	425.2317	-1.8	-4.2	12.5	C25 H30 N4 O 23Na	2529.6	4.044	1.75	25	30	4	1	1
	425.2288	1.1	2.6	6.5	C21 H33 N2 O7	2530.5	4.964	0.70	21	33	2	7	
	425.2341	-4.2	-9.9	15.5	C27 H29 N4 O	2532.0	6.504	0.15	27	29	4	1	
	425.2277	2.2	5.2	8.5	C20 H30 N6 O3 23Na	2532.6	7.057	0.09	20	30	6	3	1
	425.2269	3.0	7.1	19.5	C33 H29	2533.6	8.037	0.03	33	29			

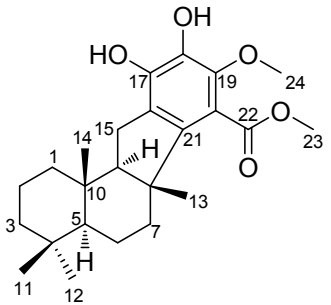




19-*O*-methylpelorol (**10**)

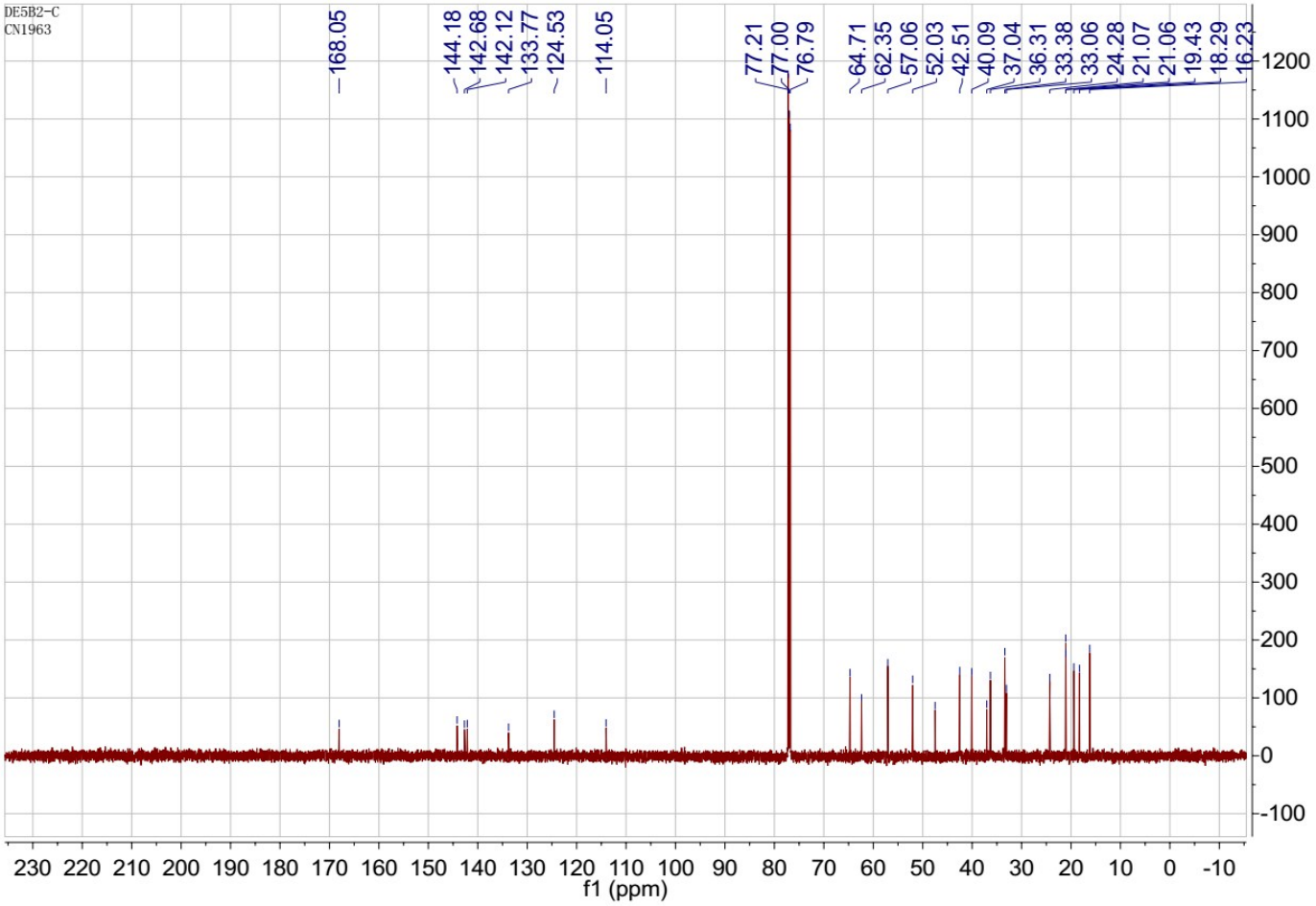
Figure S99. HRESIMS spectrum of Compound **10**.

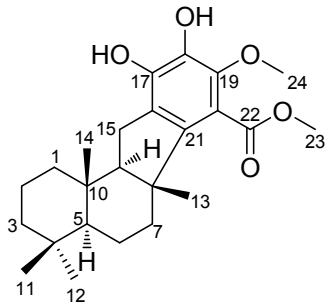




19-*O*-methylpelorol (**10**)

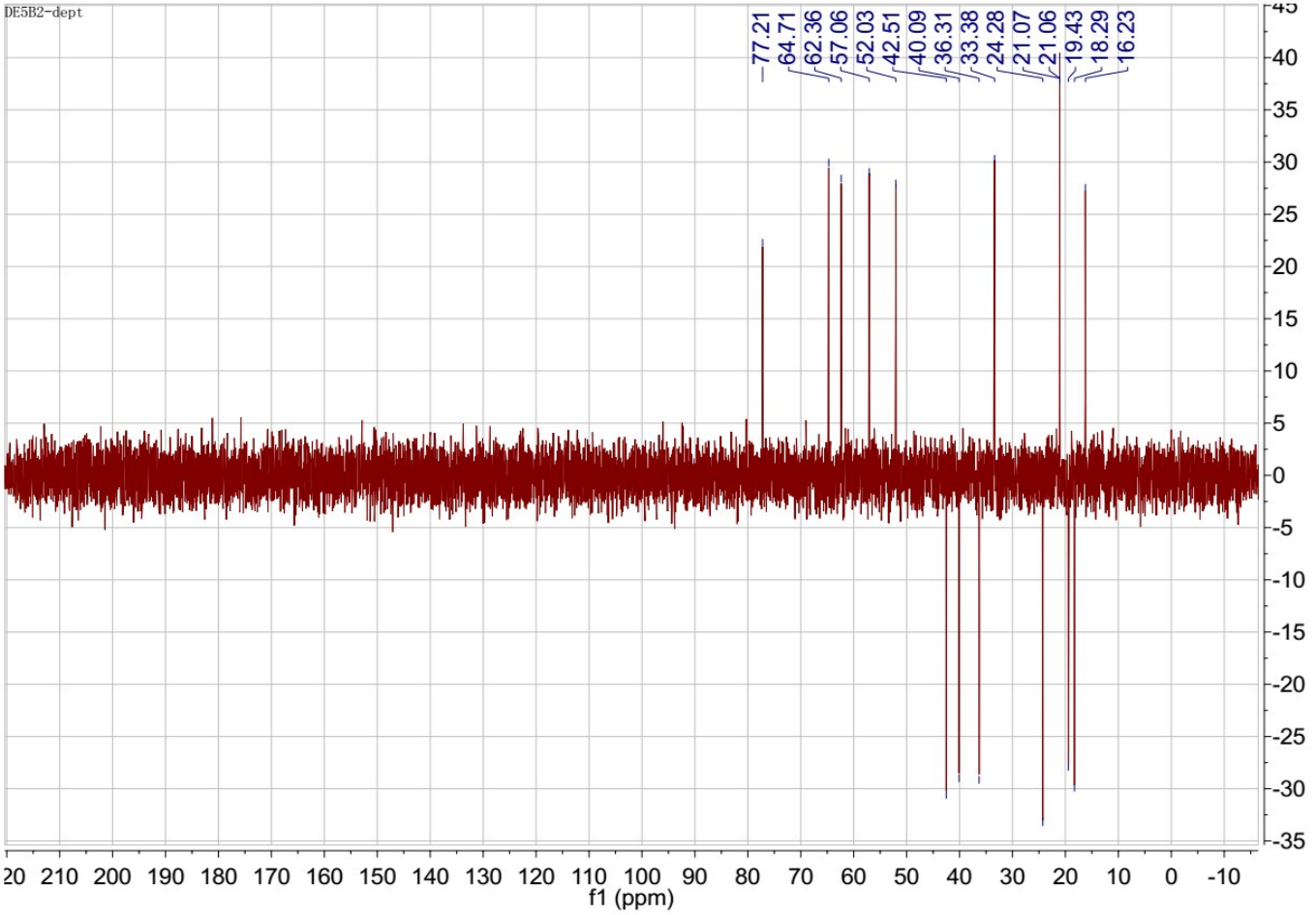
Figure S100. ^{1}H NMR spectrum of Compound **10** in $CDCl_3$.

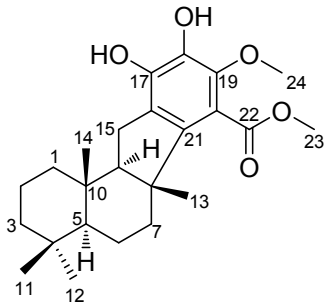




19-*O*-methylpelorol (**10**)

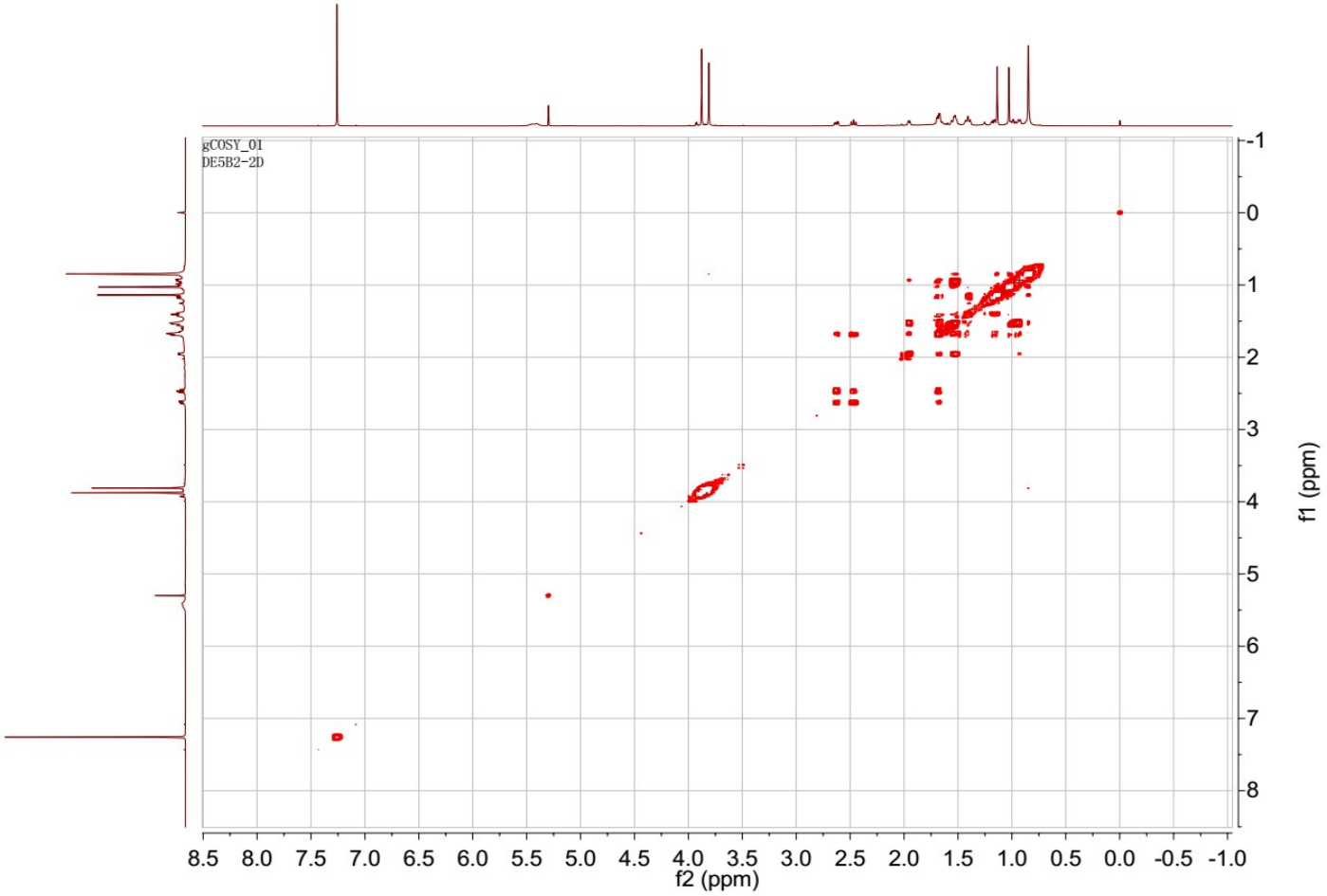
Figure S101. ^{13}C NMR spectrum of Compound **10** in $CDCl_3$.

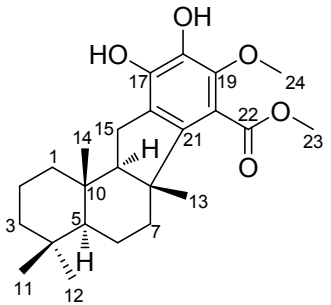




19-*O*-methylpelorol (**10**)

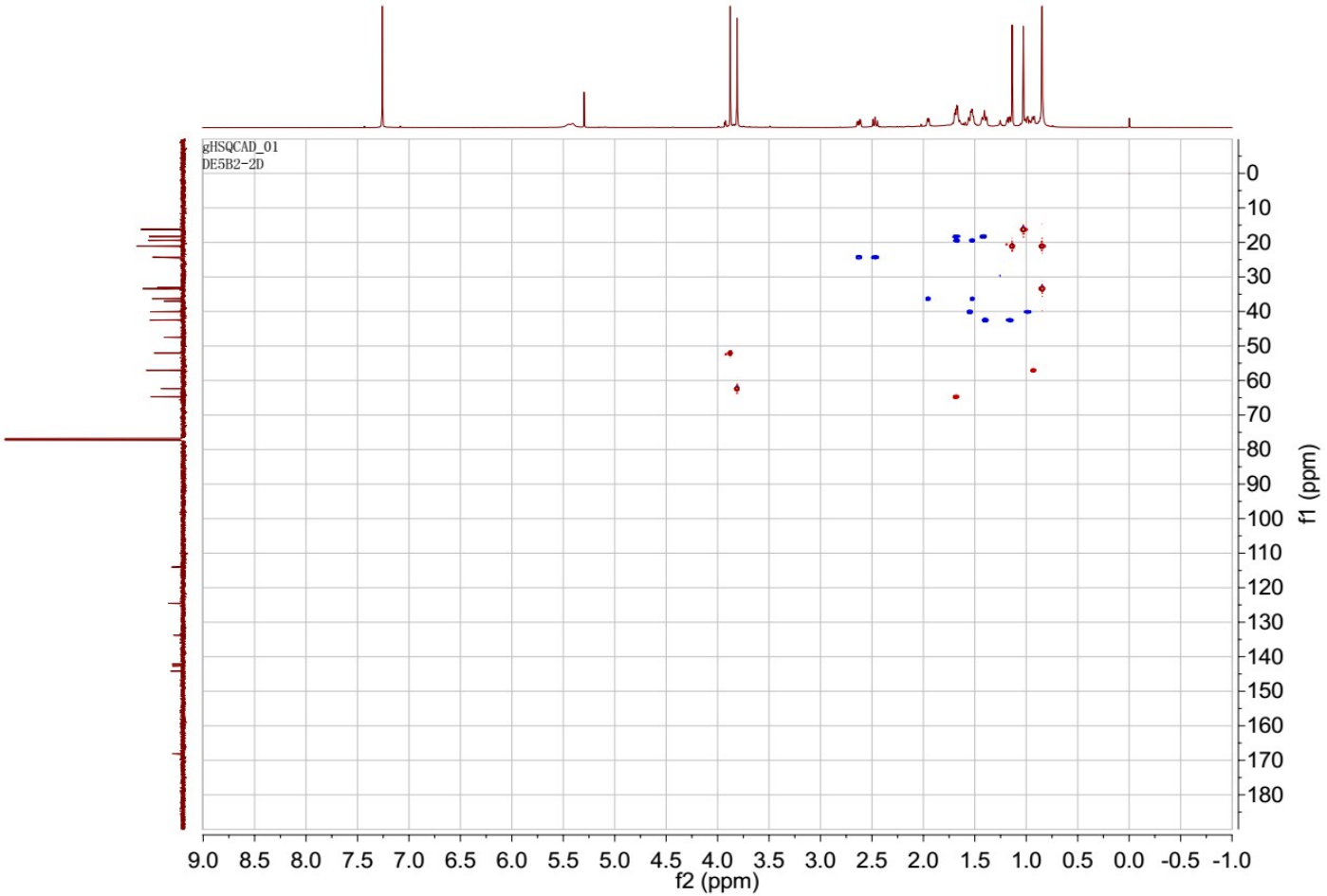
Figure S102. DEPT135 spectrum of Compound **10** in $CDCl_3$.

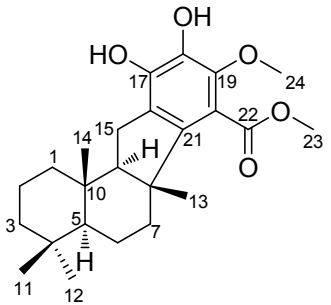




19-*O*-methylpelorol (**10**)

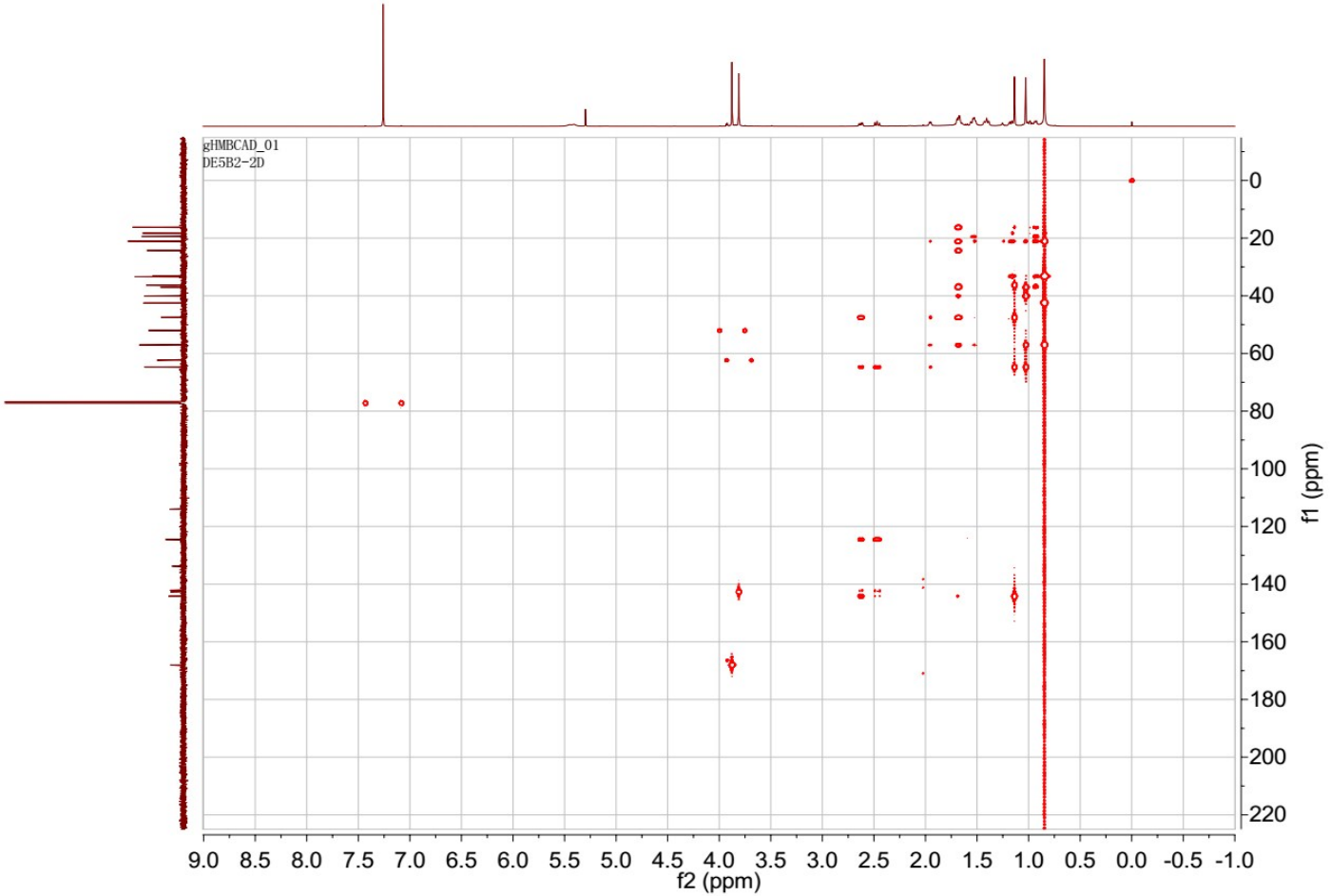
Figure S103. ^{1}H-^{1}H COSY spectrum of Compound **10** in $CDCl_3$.

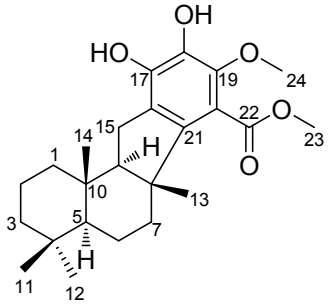




19-*O*-methylpelorol (**10**)

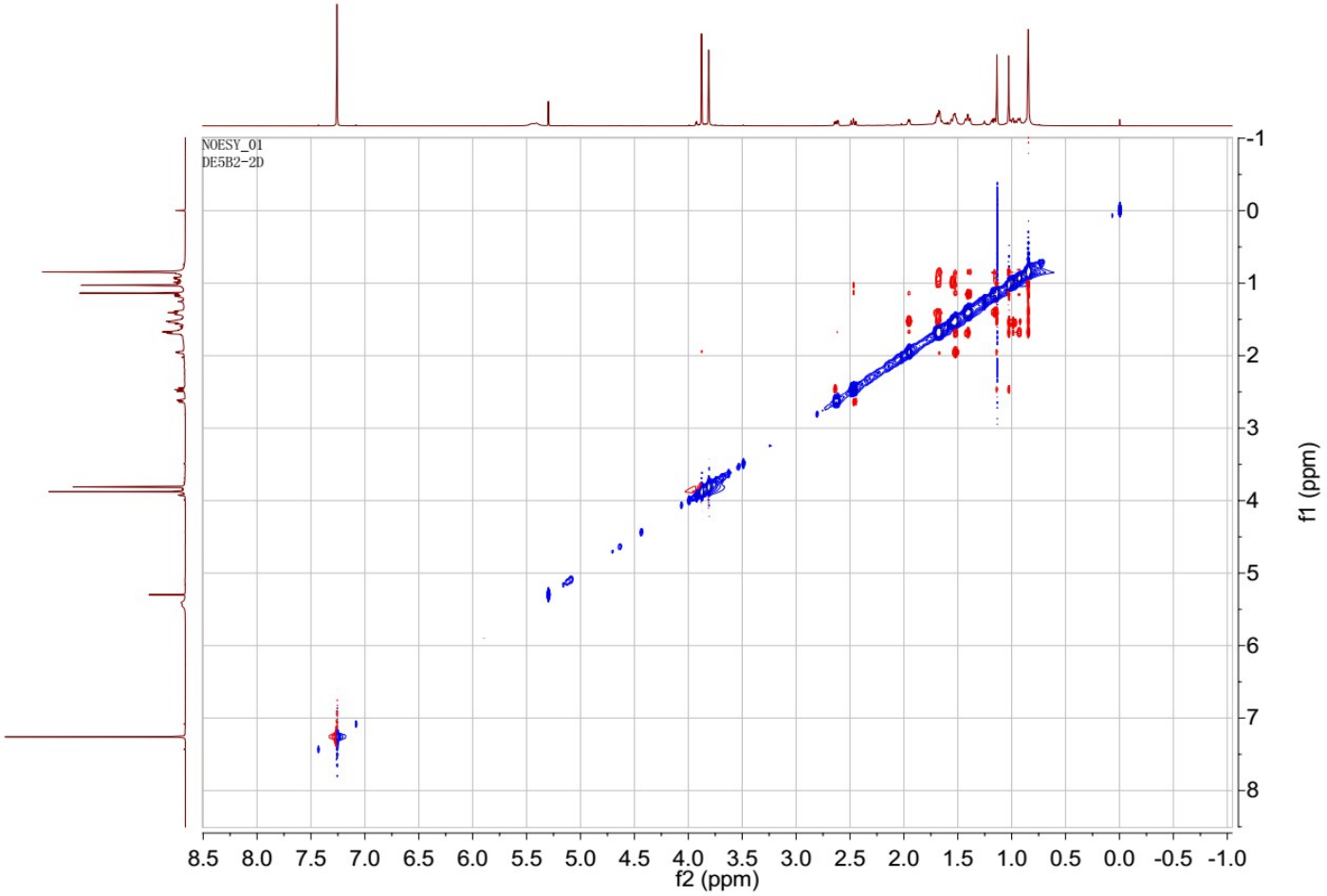
Figure S104. HSQC spectrum of Compound **10** in $CDCl_3$.

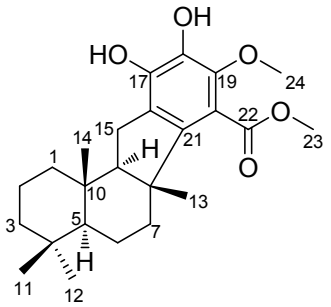




19-*O*-methylpelorol (**10**)

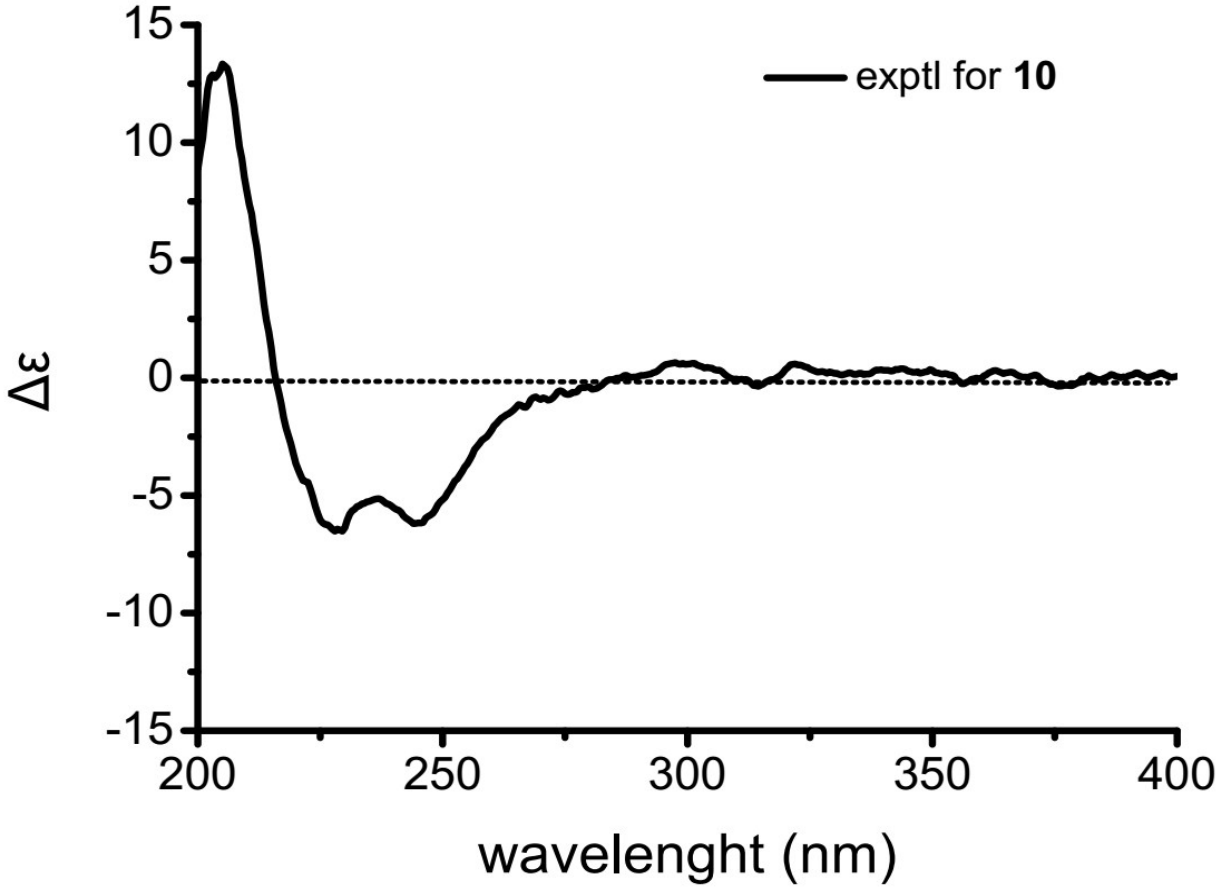
Figure S105. HSQC spectrum of Compound **10** in $CDCl_3$.

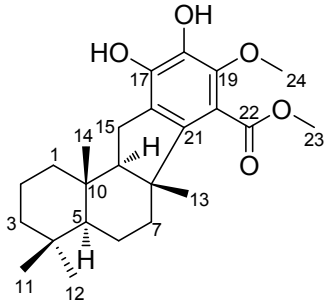




19-*O*-methylpelorol (**10**)

Figure S106. NOESY spectrum of Compound **10** in $CDCl_3$.





19-*O*-methylpelorol (**10**)

Figure S107. CD spectrum of Compound **10** in MeOH.