

Electronic Supplementary Information

Dysidaminones A–M, Cytotoxic and NF- κ B Inhibitory Sesquiterpene

Aminoquinones from the South China Sea Sponge *Dysidea fragilis*

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Yang, Bing-Nan Han, and Hou-Wen Lin*

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Figure S101. HSQC Spectrum of Dysidaminone K (**11**) in CDCl_3 .

Figure S102. HMBC Spectrum of Dysidaminone K (**11**) in CDCl_3 .

Figure S103. NOESY Spectrum of Dysidaminone K (**11**) in CDCl_3 .

Figure S104. HRESIMS of Dysidaminone K (**11**).

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Figure S115. HRESIMS of Dysidaminone L (**12**).

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Figure S118. ^{13}C NMR Spectrum of Dysidaminone M (**13**) in CDCl_3 .

Figure S119. DEPT135 Spectrum of Dysidaminone M (**13**) in CDCl_3 .

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Figure S121. HSQC Spectrum of Dysidaminone M (**13**) in CDCl_3 .

Figure S122. HMBC Spectrum of Dysidaminone M (**13**) in CDCl_3 .

Figure S123. NOESY Spectrum of Dysidaminone M (**13**) in CDCl_3 .

Figure S124. CD Spectrum of Dysidaminone M (**13**) in MeOH.

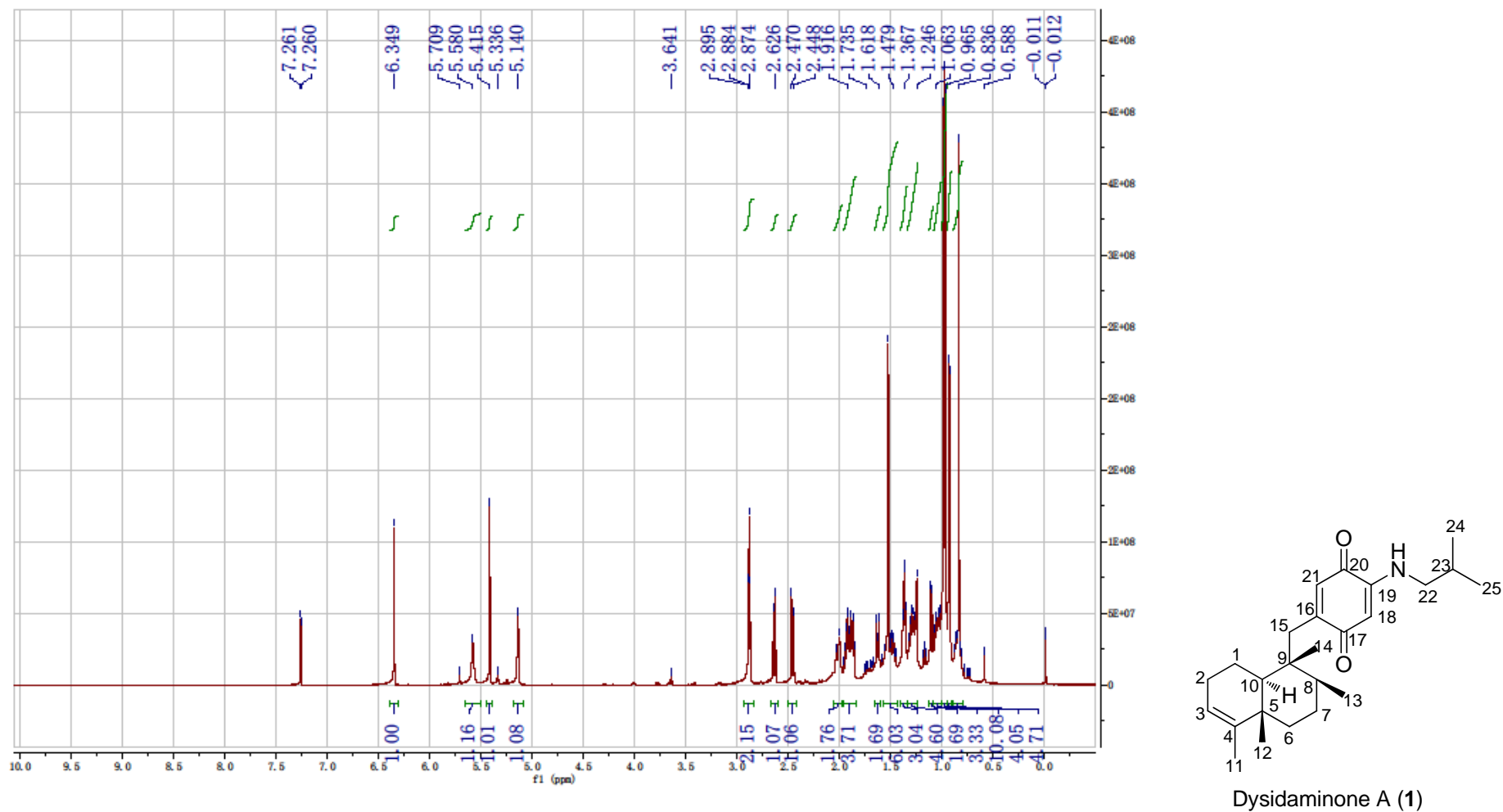


Figure S1. ^1H NMR Spectrum of Dysidaminone A (1) in CDCl_3 .

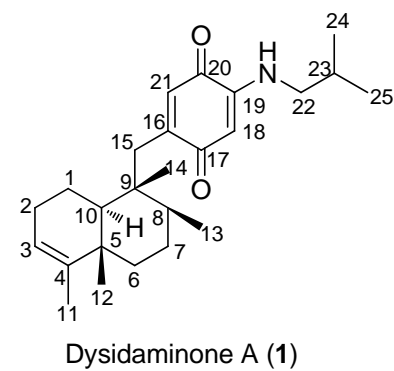
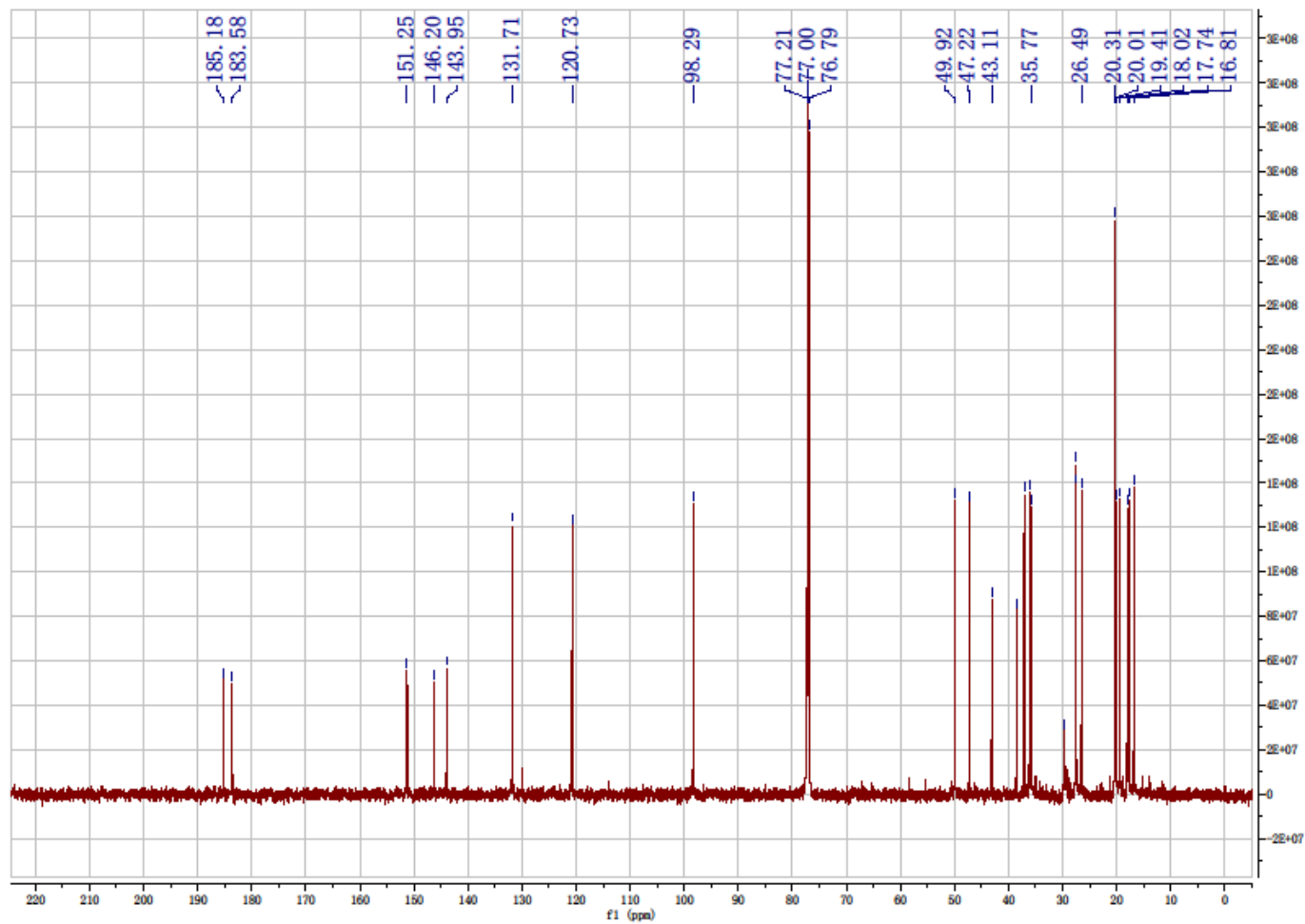


Figure S2. ^{13}C NMR Spectrum of Dysidaminone A (1) in CDCl_3 .

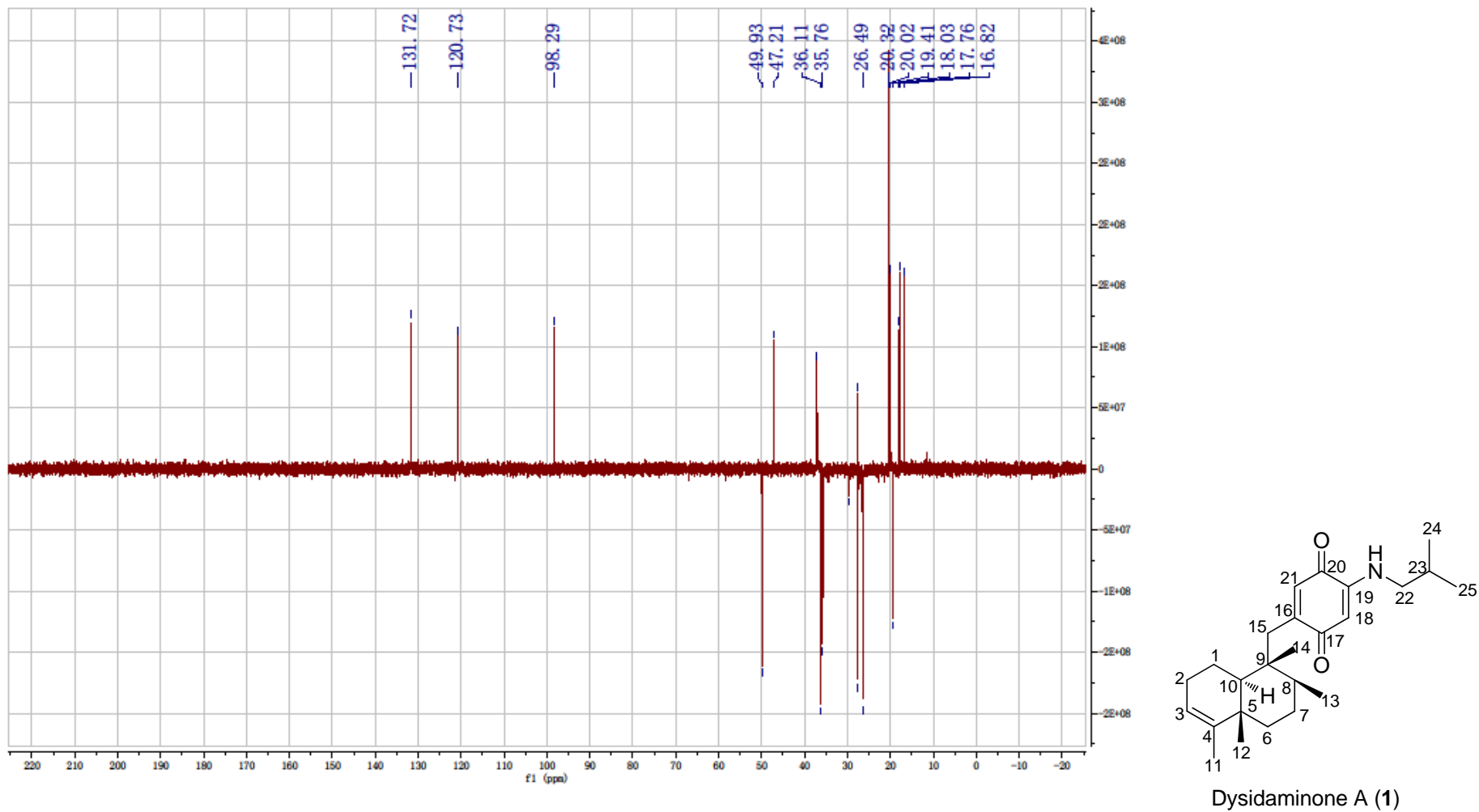


Figure S3. DEPT135 Spectrum of Dysidaminone A (1) in CDCl₃.

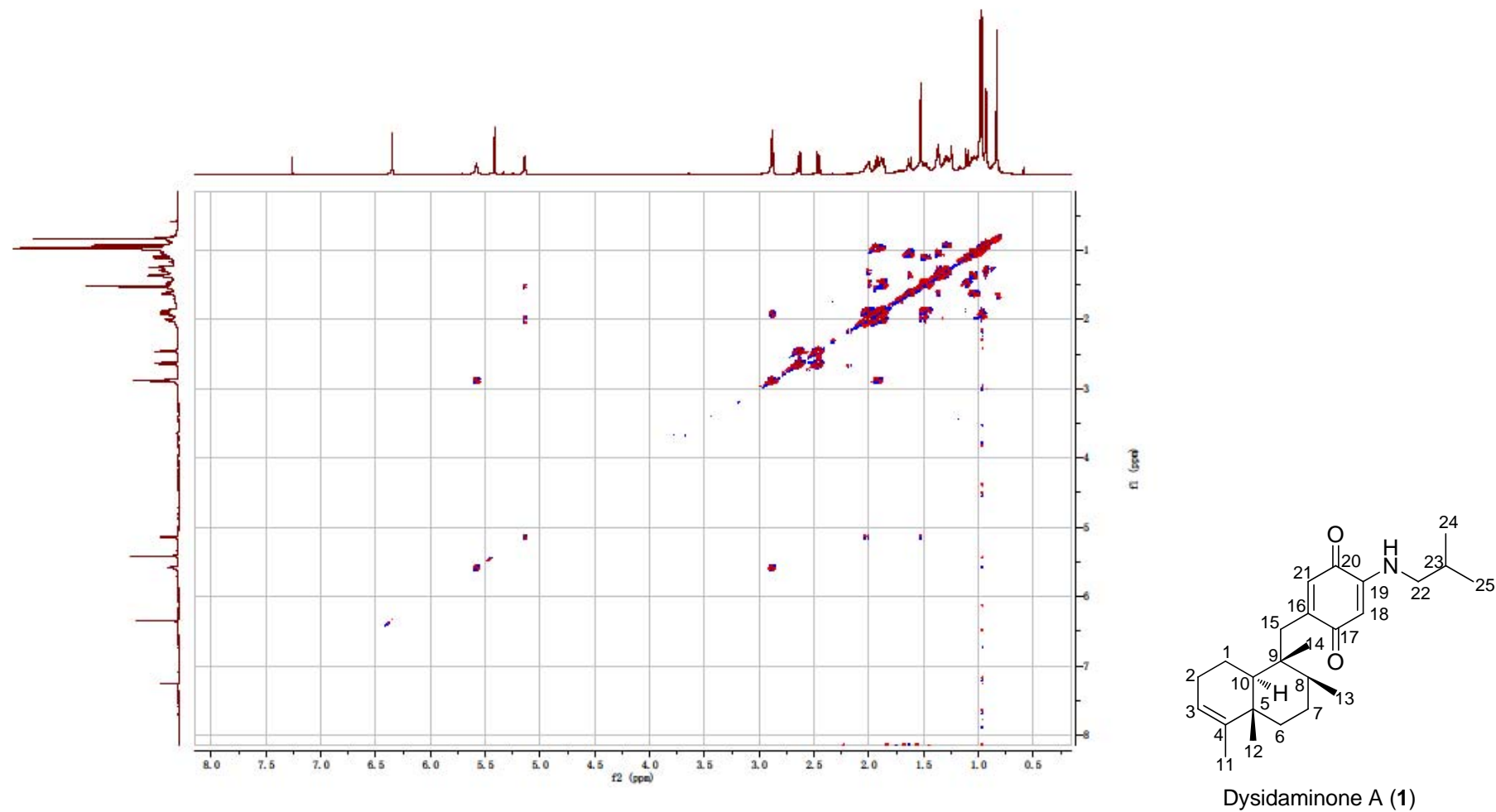


Figure S4. ^1H - ^1H COSY Spectrum of Dysidaminone A (1) in CDCl_3 .

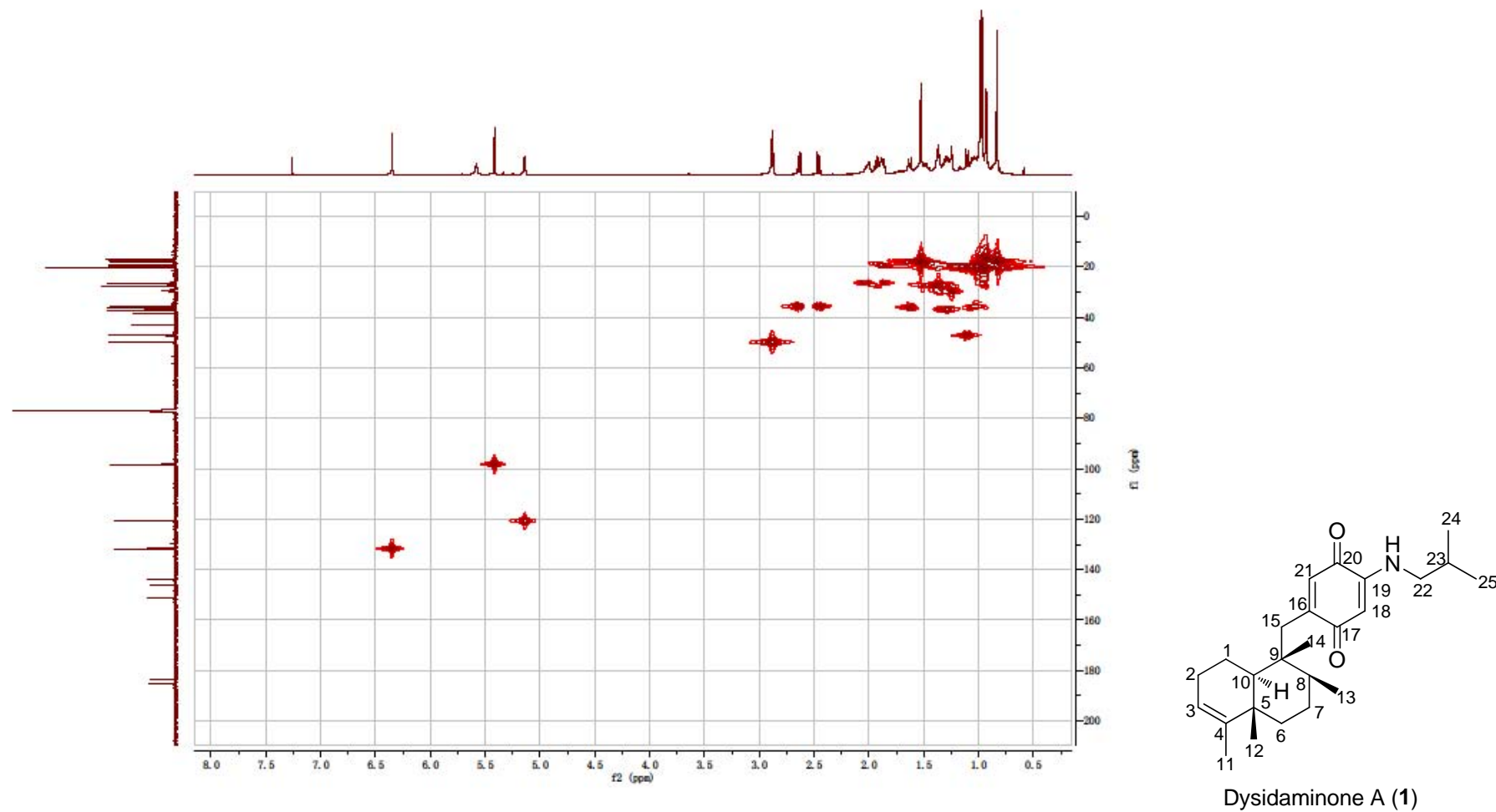


Figure S5. HSQC Spectrum of Dysidaminone A (1) in CDCl₃.

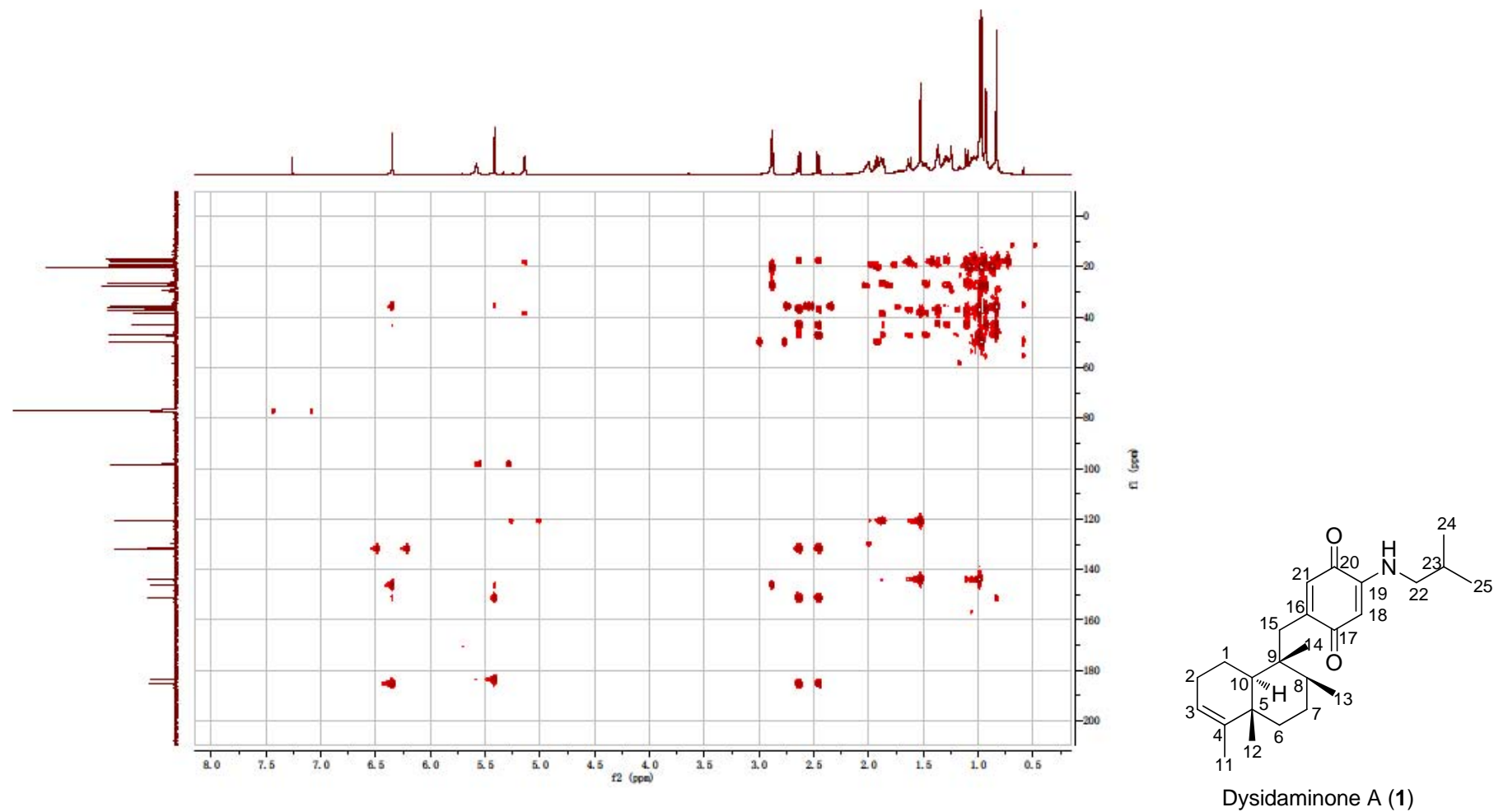


Figure S6. HMBC Spectrum of Dysidaminone A (1) in CDCl₃.

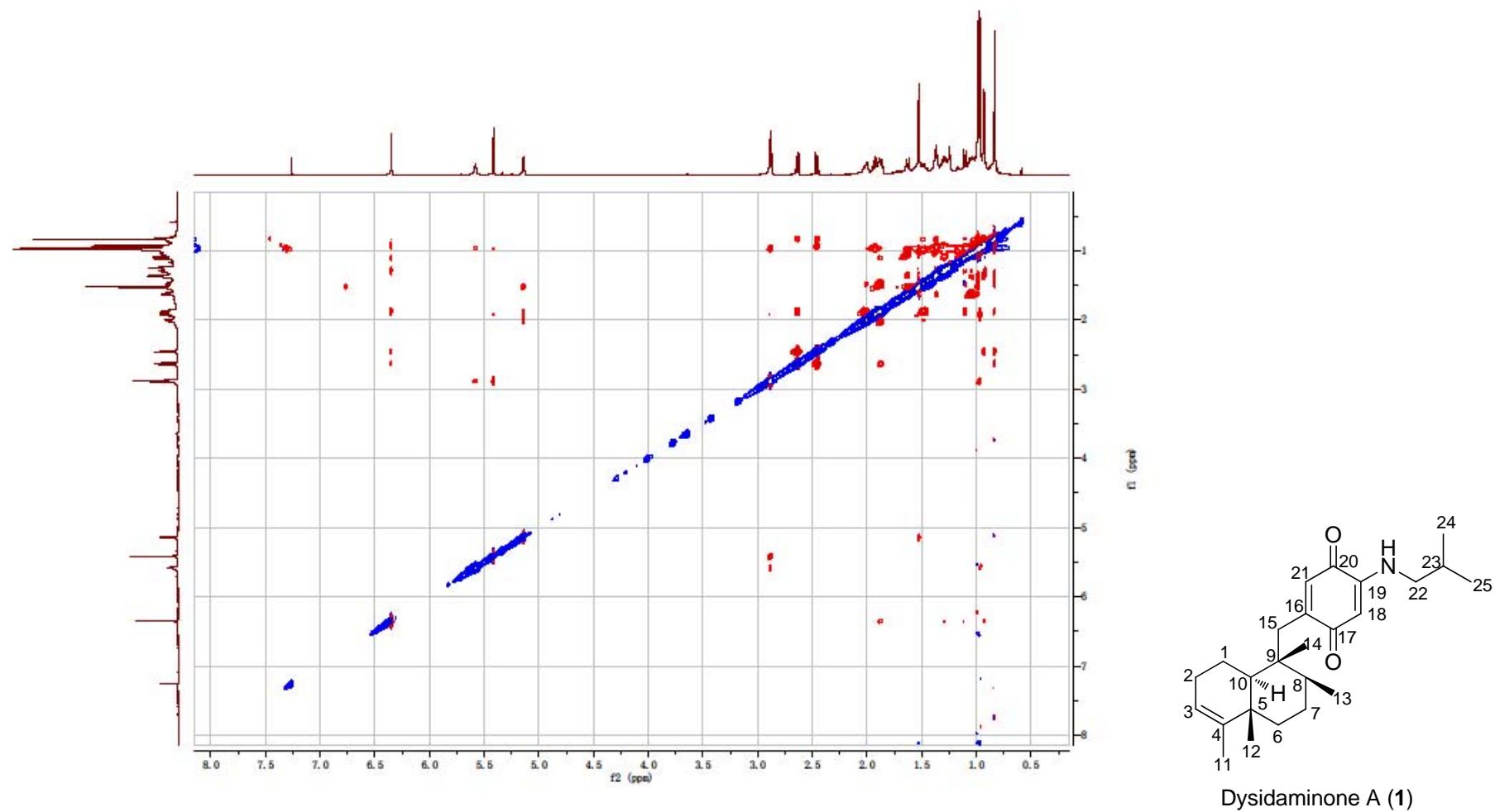


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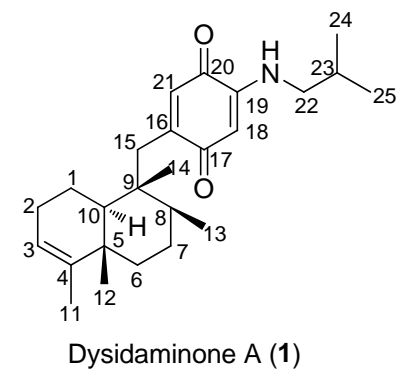
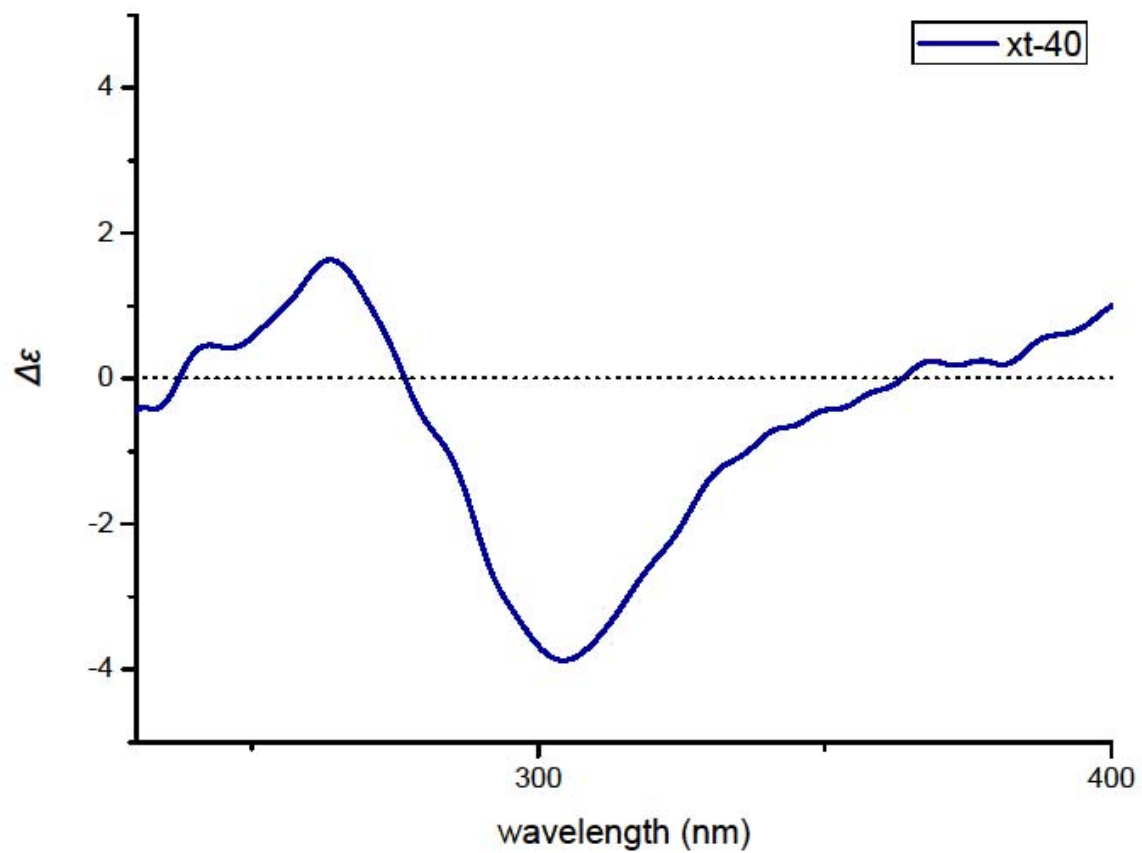


Figure S9. CD Spectrum of Dysidaminone A (1) in MeOH.

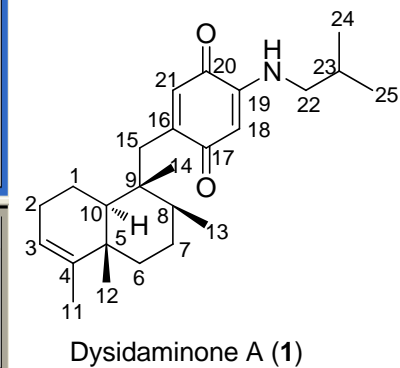
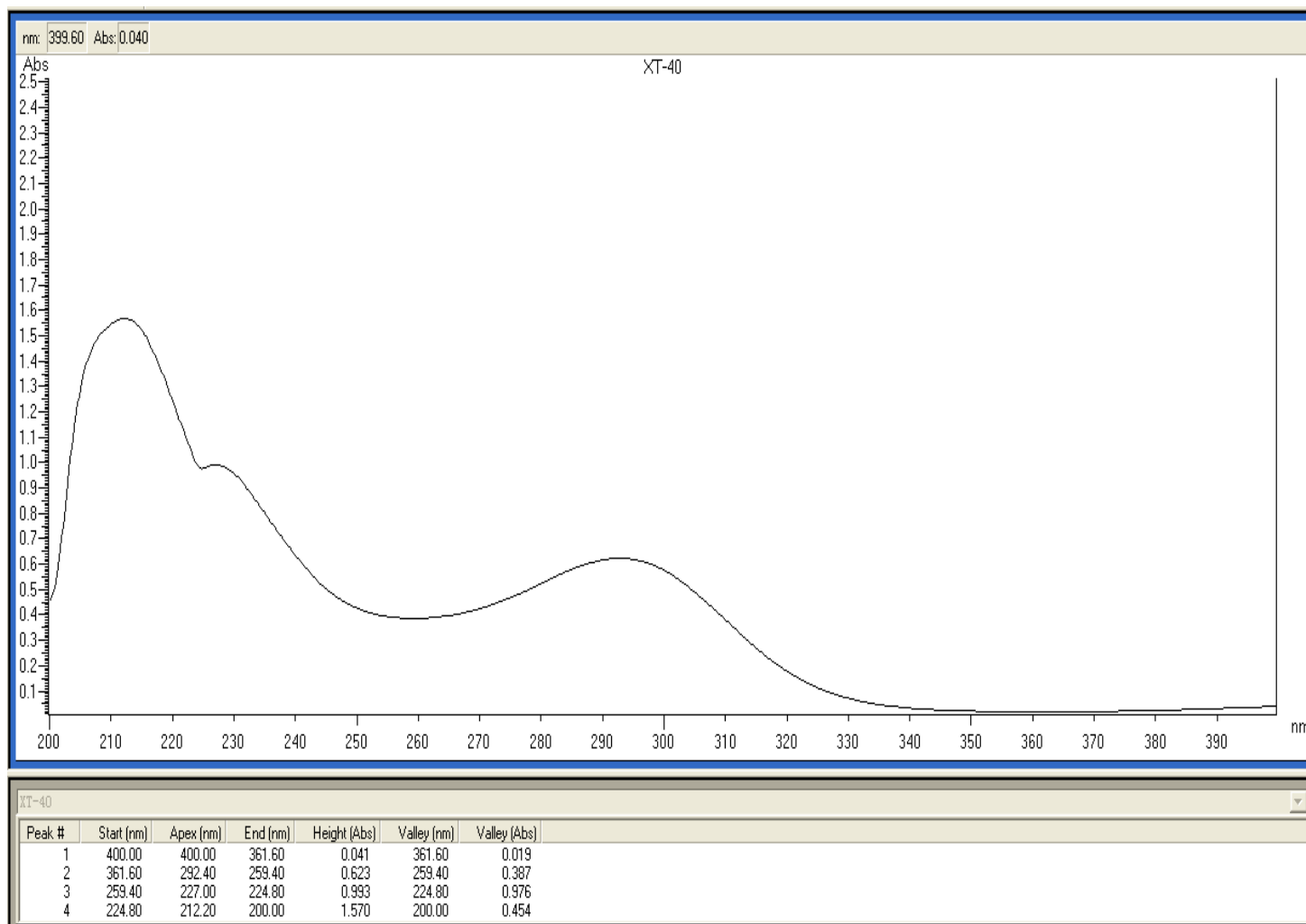


Figure S10. UV Spectrum of Dysidaminone A (1) in MeOH.

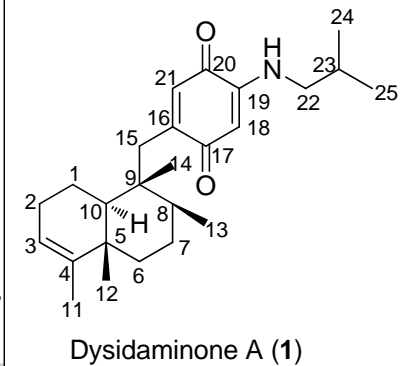
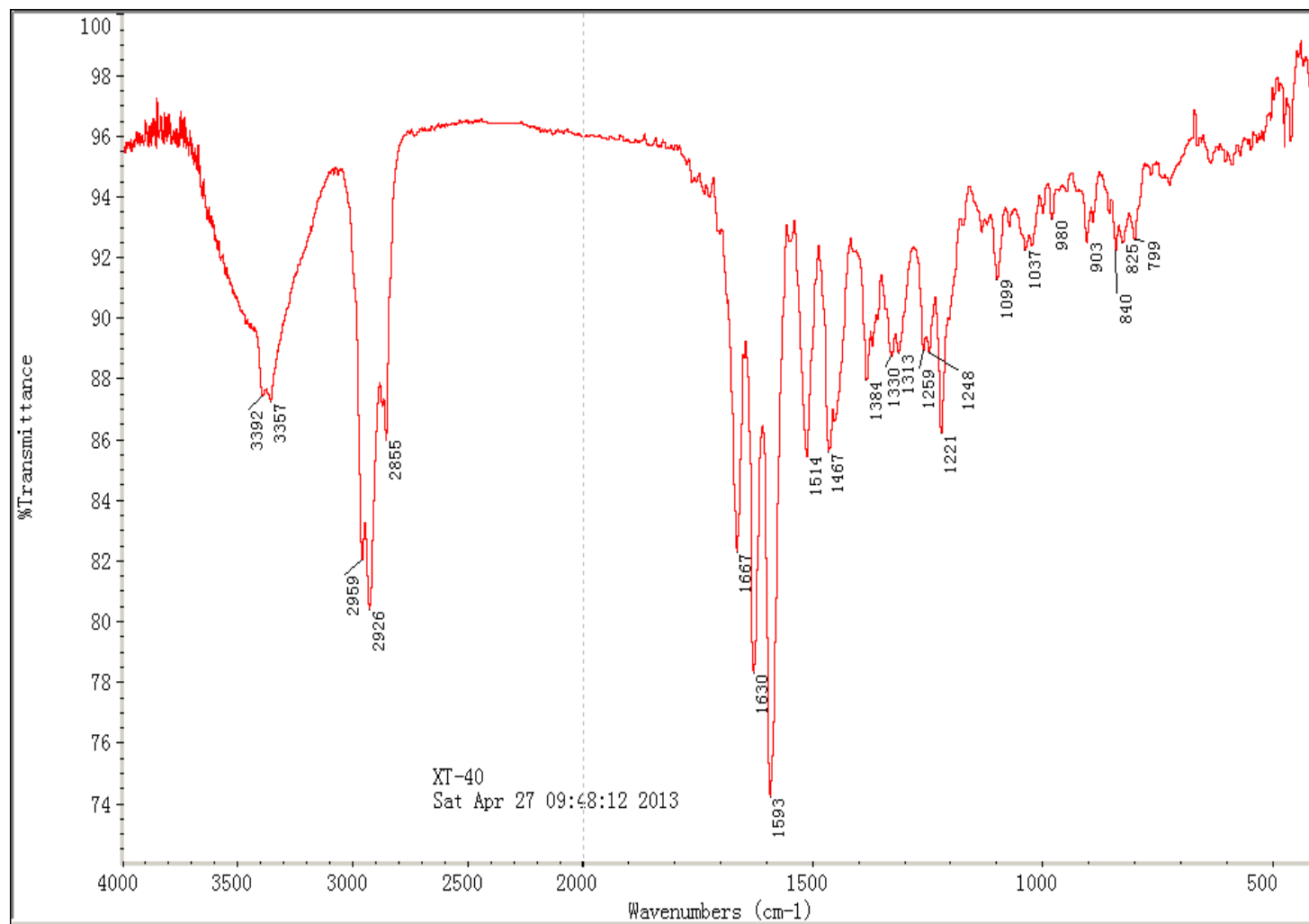


Figure S11. IR Spectrum of Dysidaminone A (1).

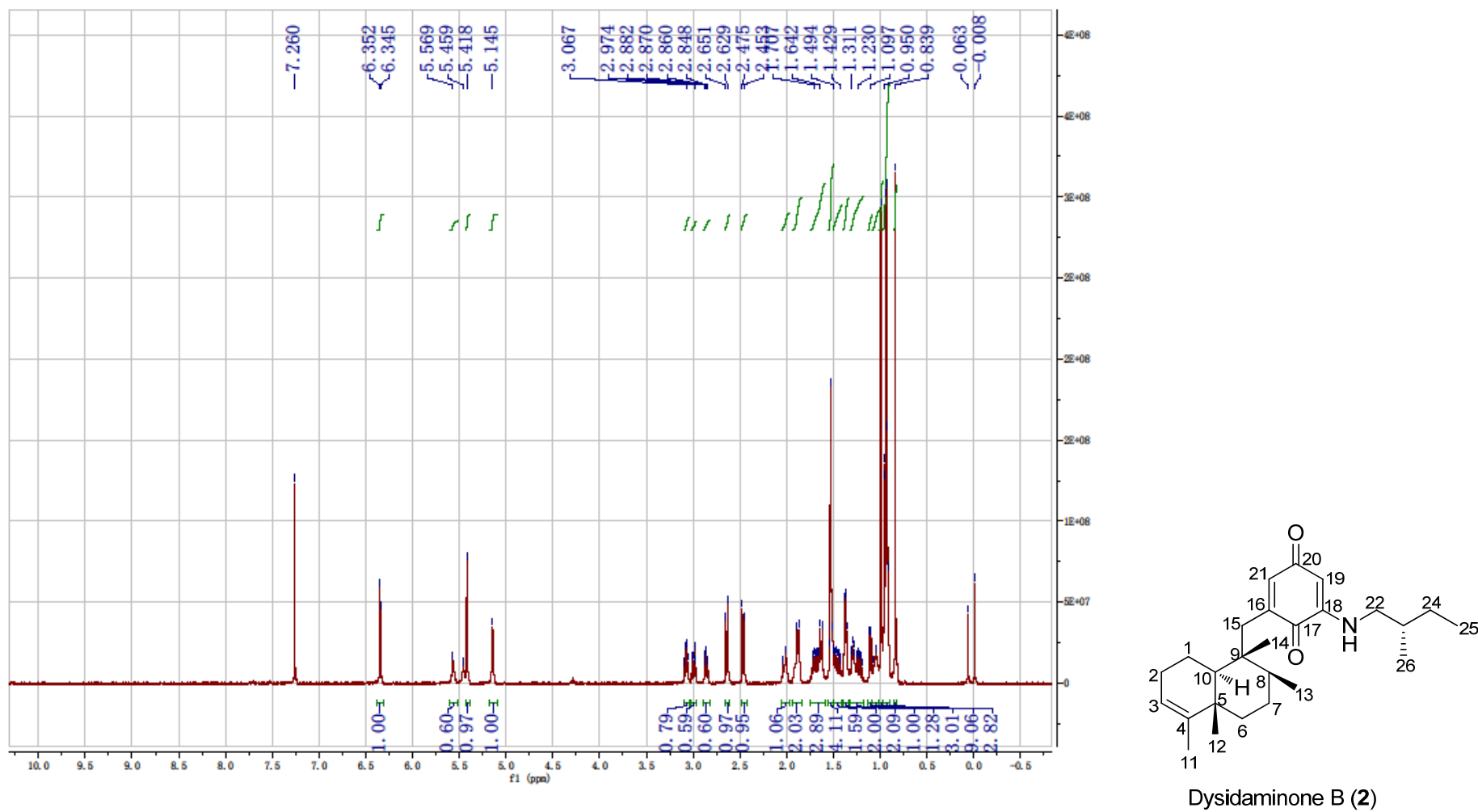
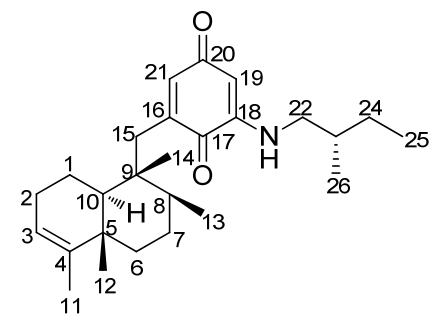
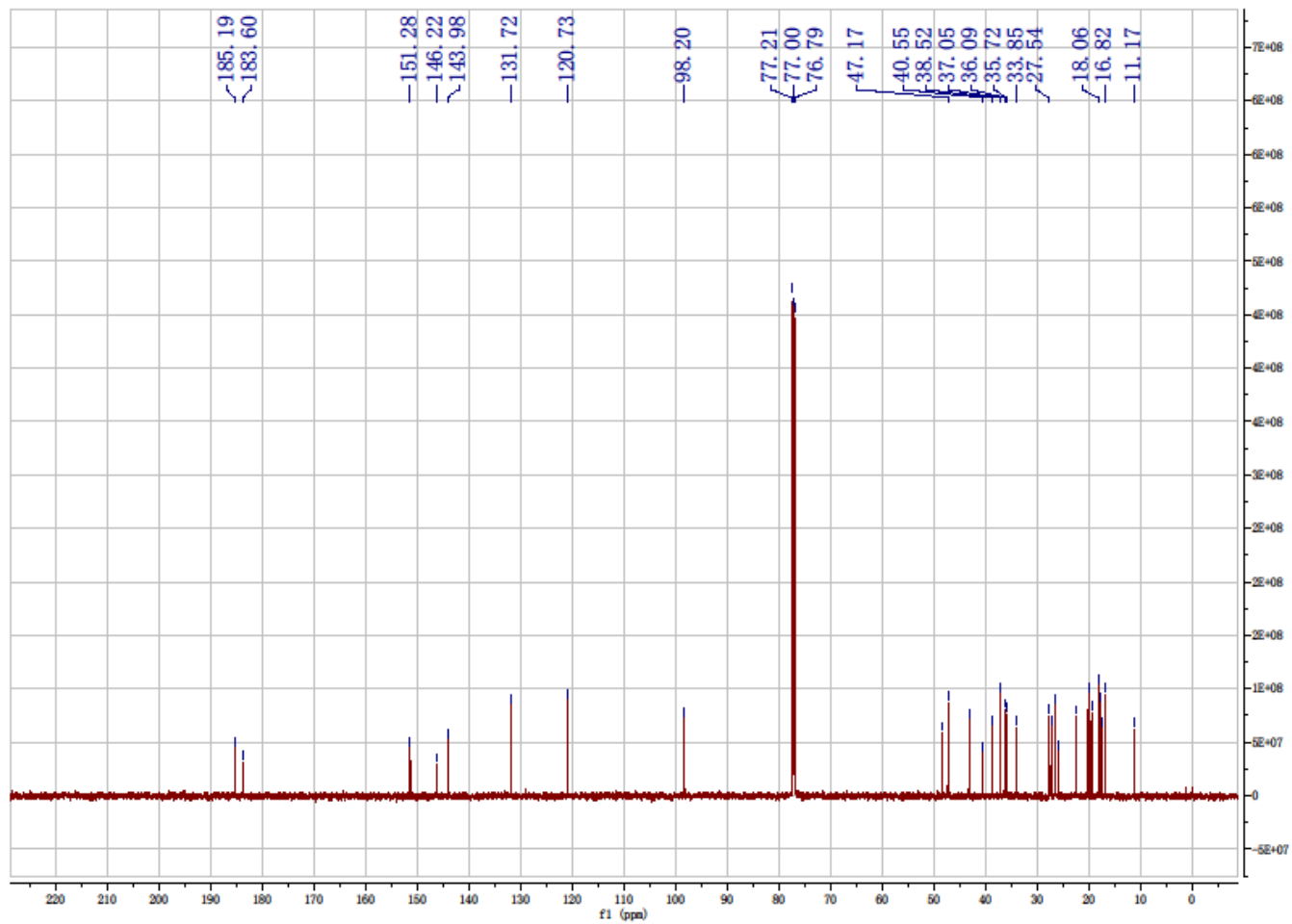


Figure S12. ¹H NMR Spectrum of Dysidaminone B (2) in CDCl₃.



Dysidaminone B (2)

Figure S13. ^{13}C NMR Spectrum of Dysidaminone B (2) in CDCl_3 .

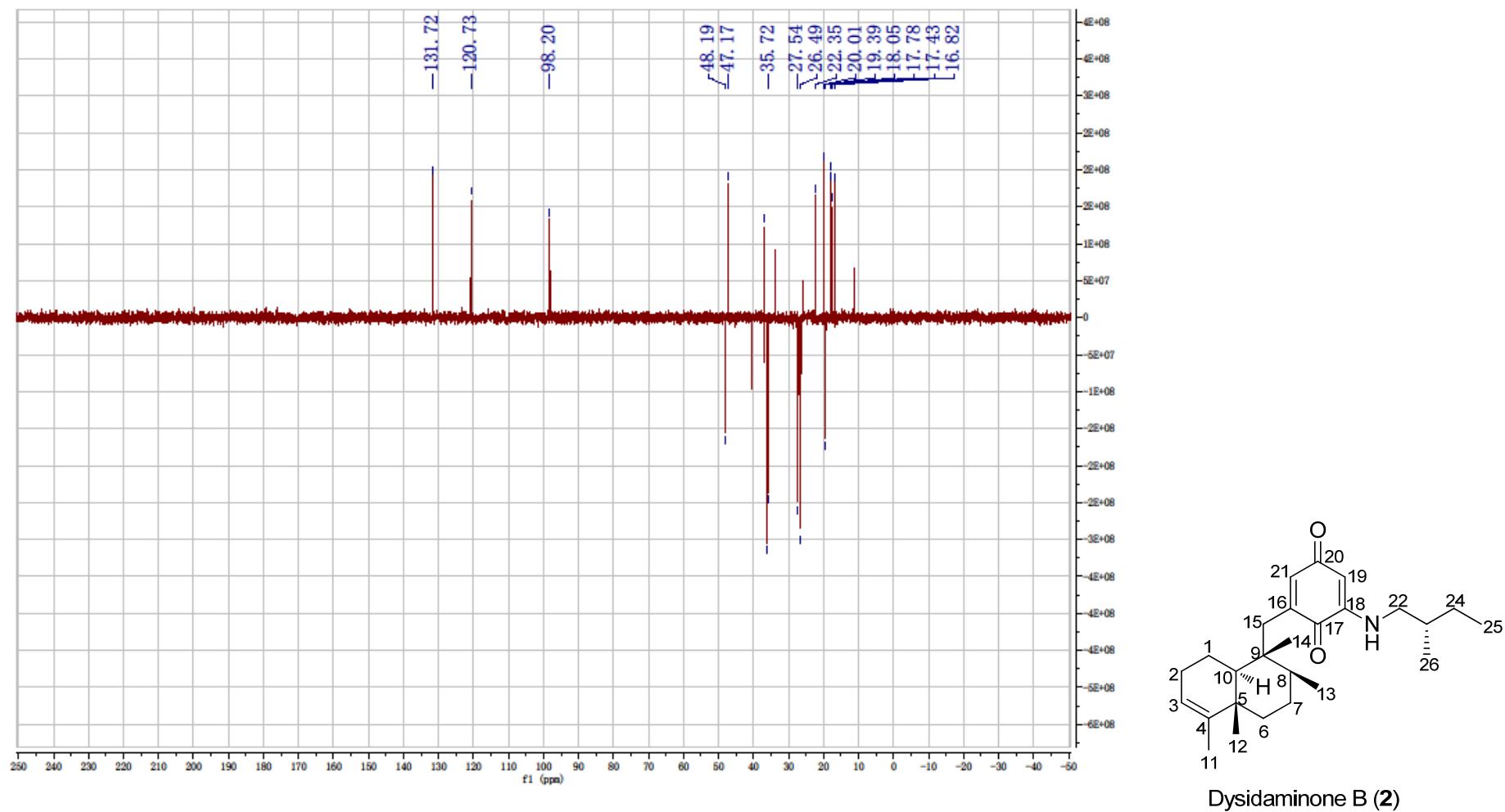


Figure S14. DEPT135 Spectrum of Dysidaminone B (2) in CDCl₃.

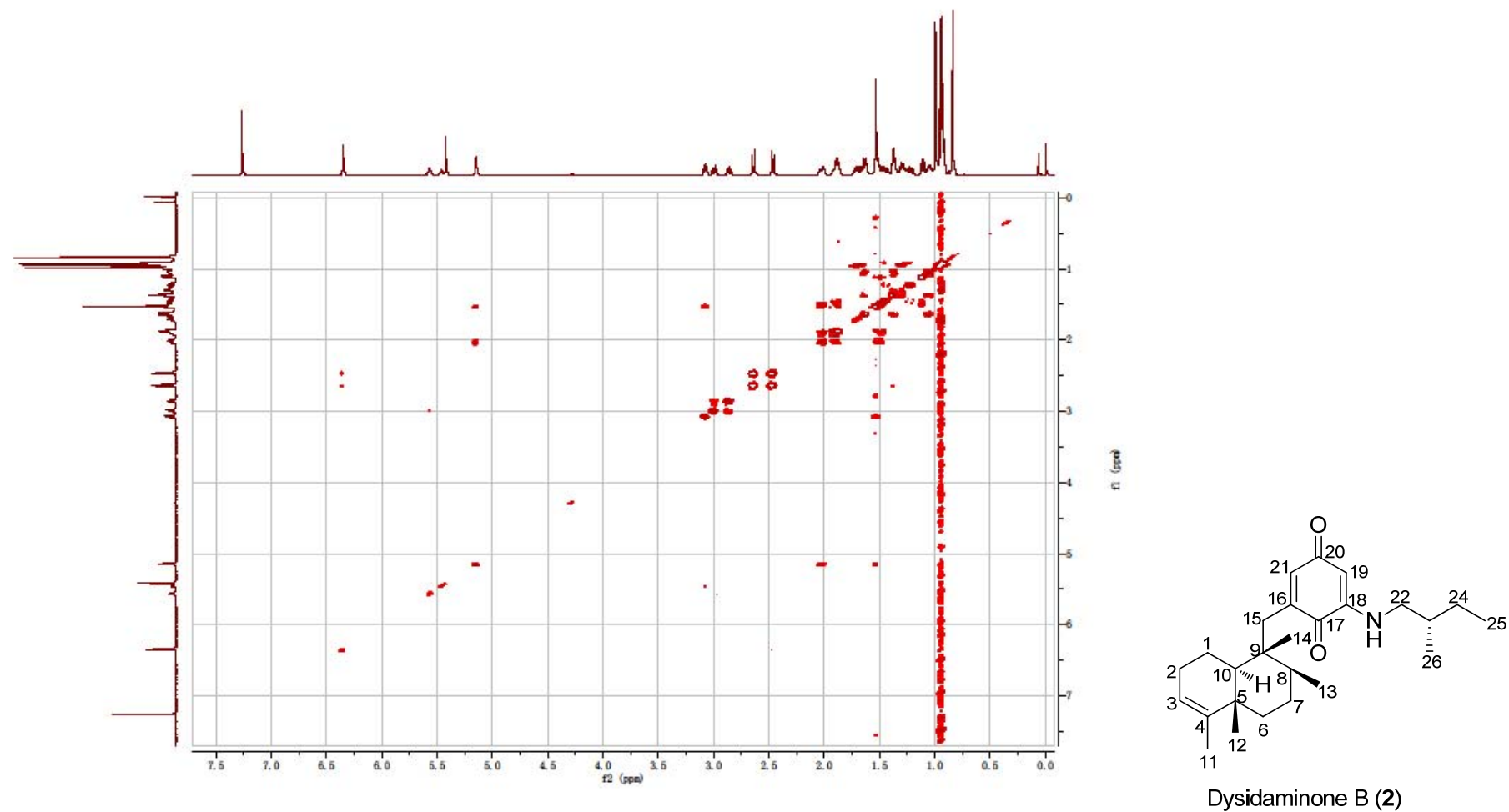


Figure S15. ^1H - ^1H COSY Spectrum of Dysidaminone B (2) in CDCl_3 .

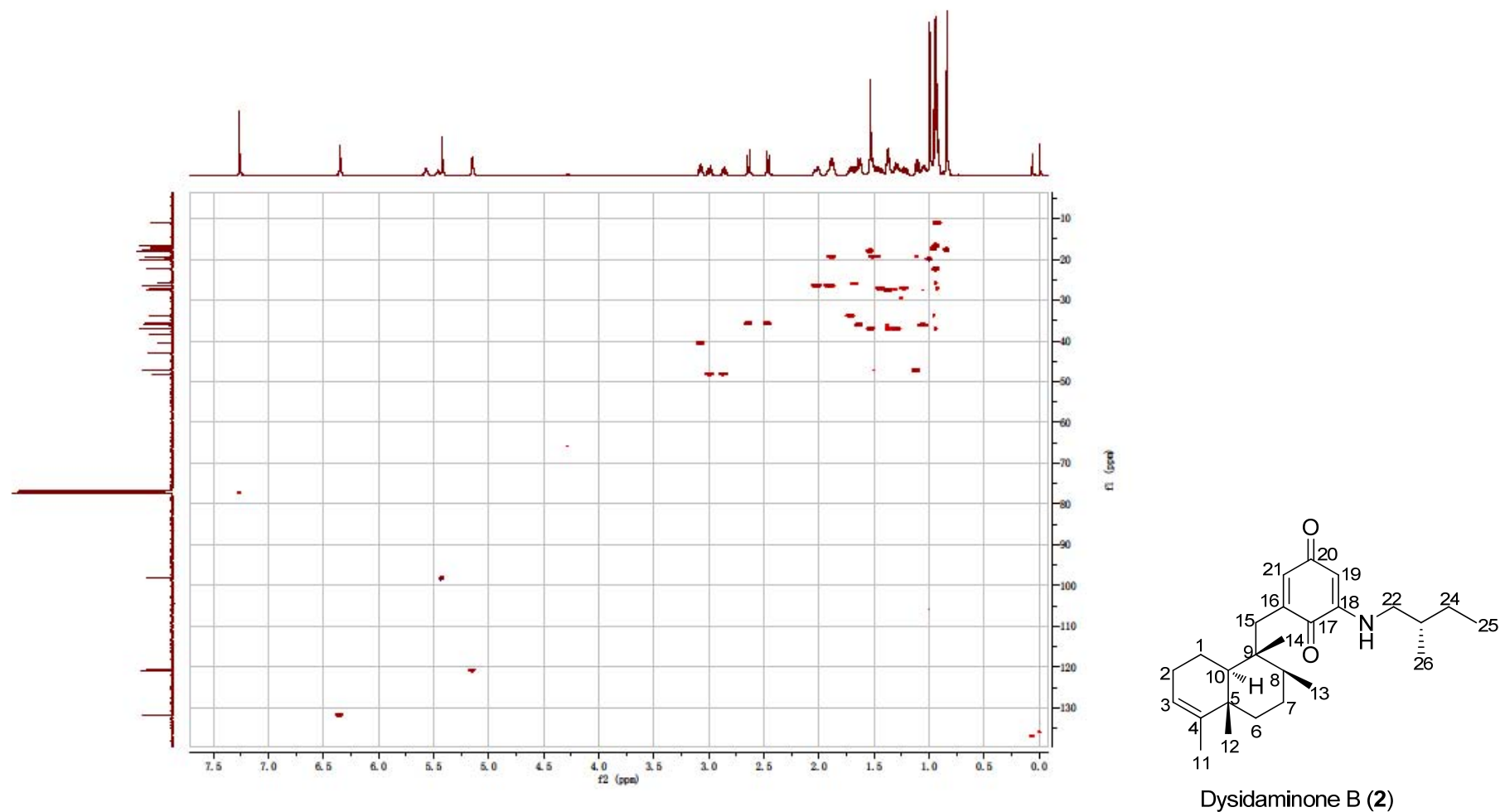


Figure S16. HSQC Spectrum of Dysidaminone B (2) in CDCl₃.

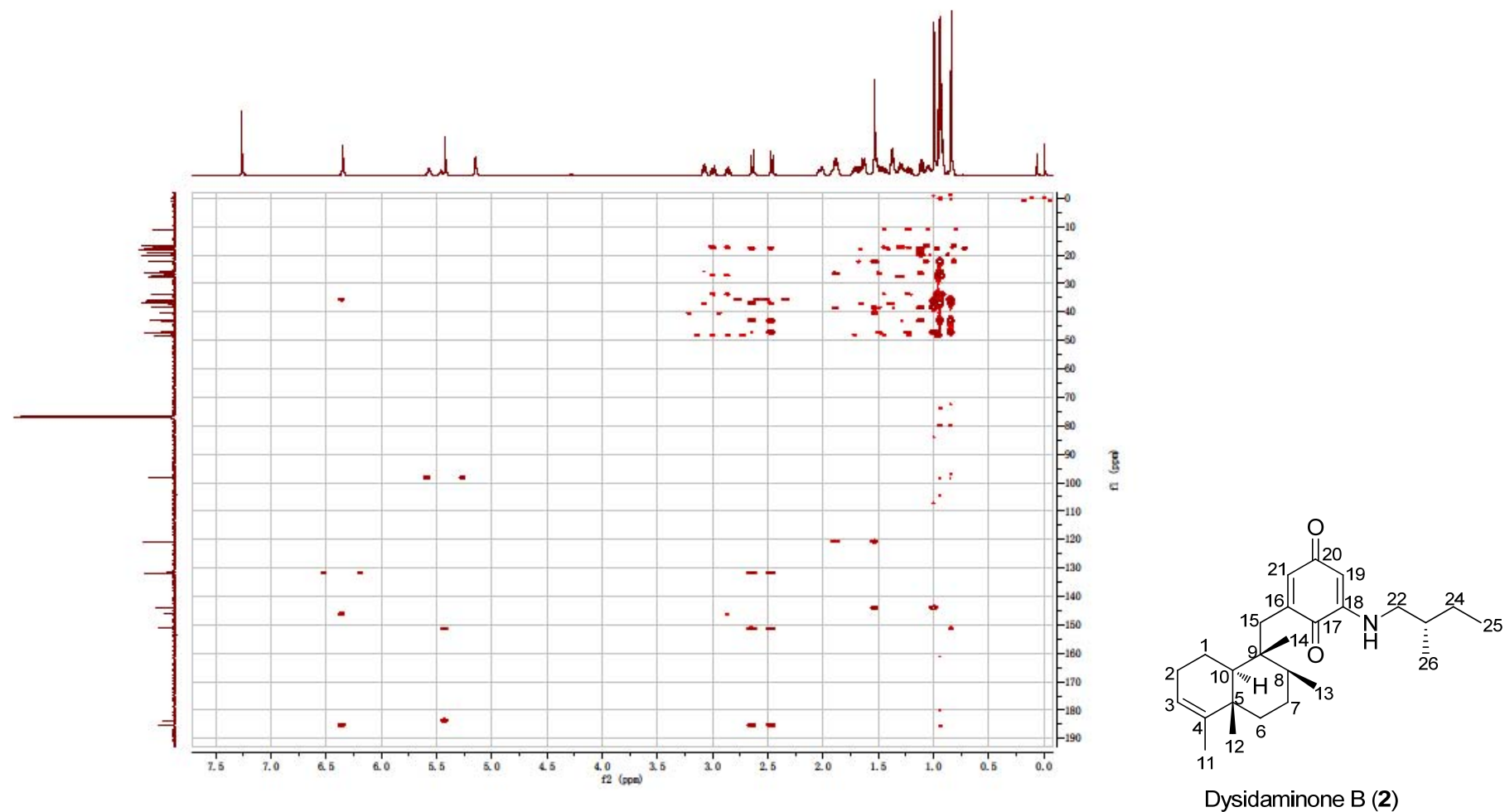


Figure S17. HMBC Spectrum of Dysidaminone B (2) in CDCl₃.

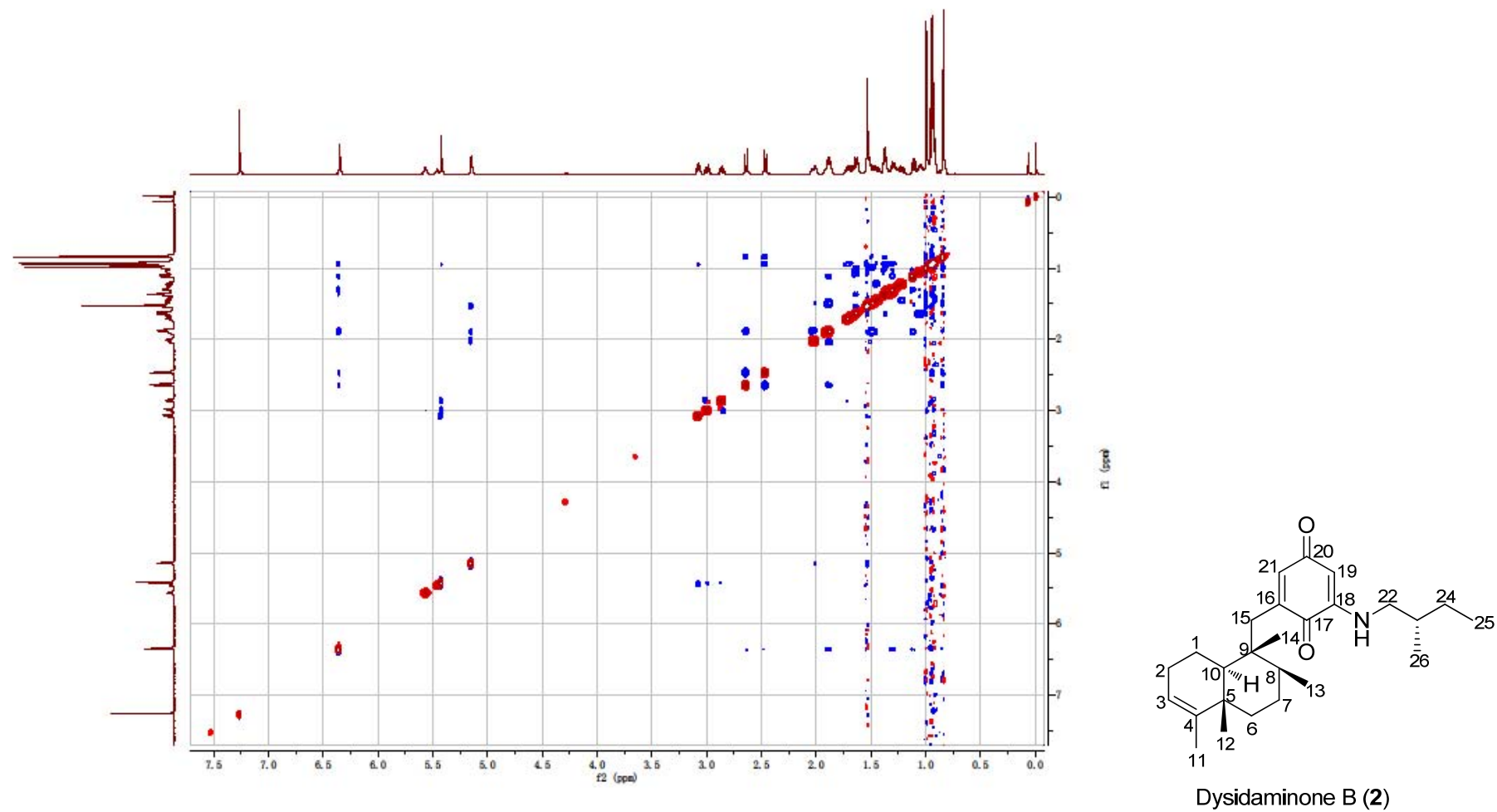


Figure S18. NOESY Spectrum of Dysidaminone B (**2**) in CDCl₃.

Elemental Composition Report

Page 1

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

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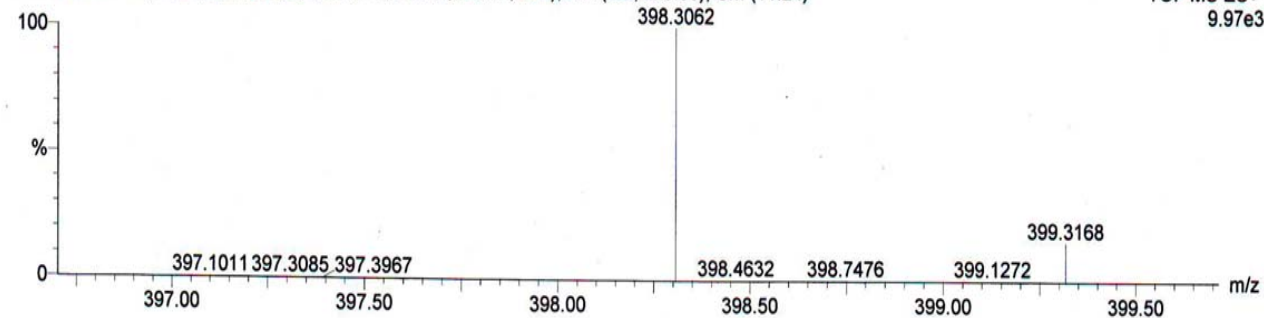
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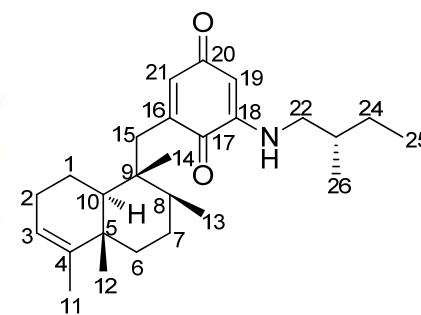
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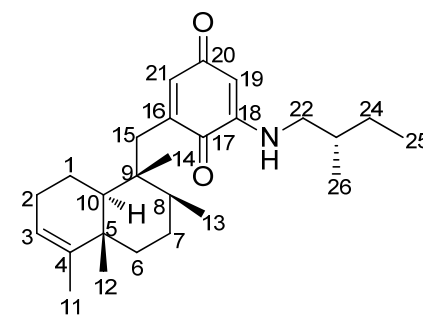
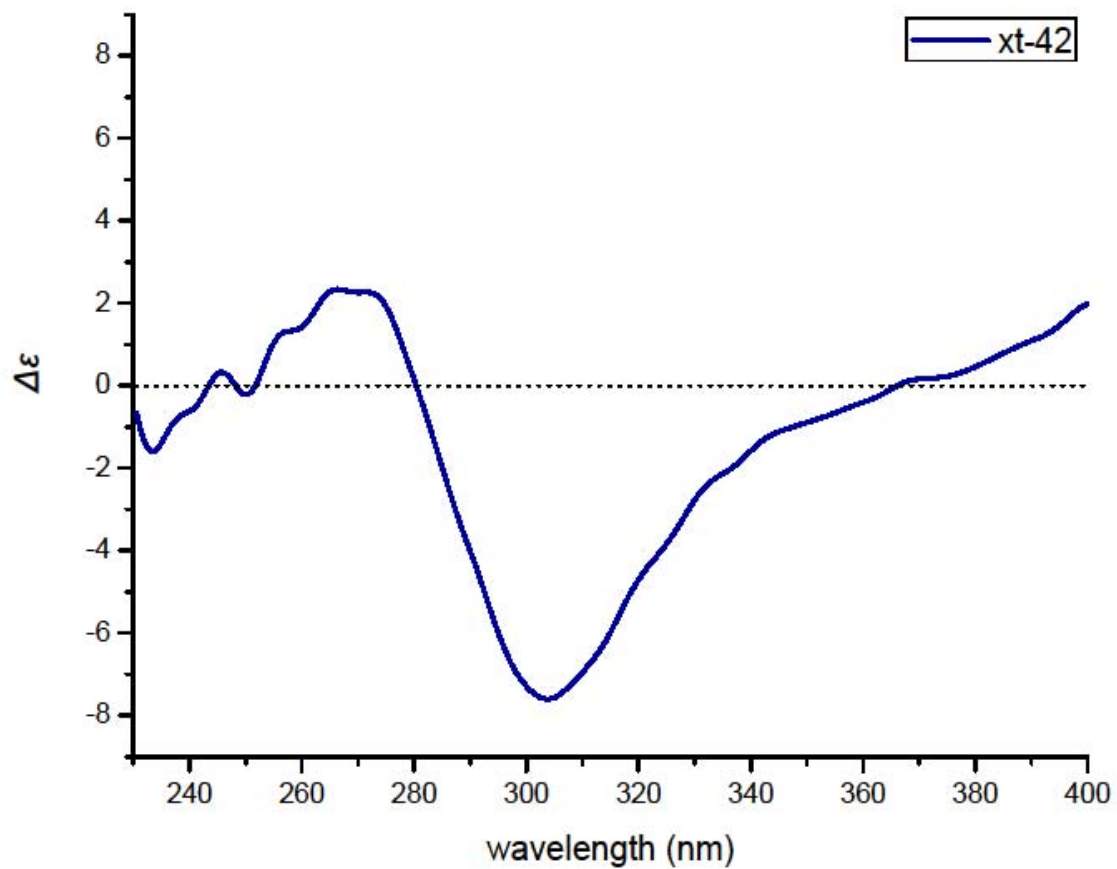
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Dysidaminone B (2)

Figure S19. HRESIMS of Dysidaminone B (2).



Dysidaminone B (2)

Figure S20. CD Spectrum of Dysidaminone B (2) in MeOH.

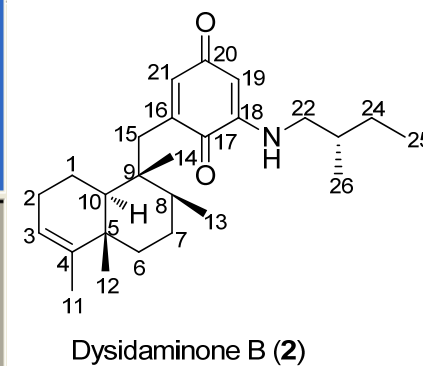
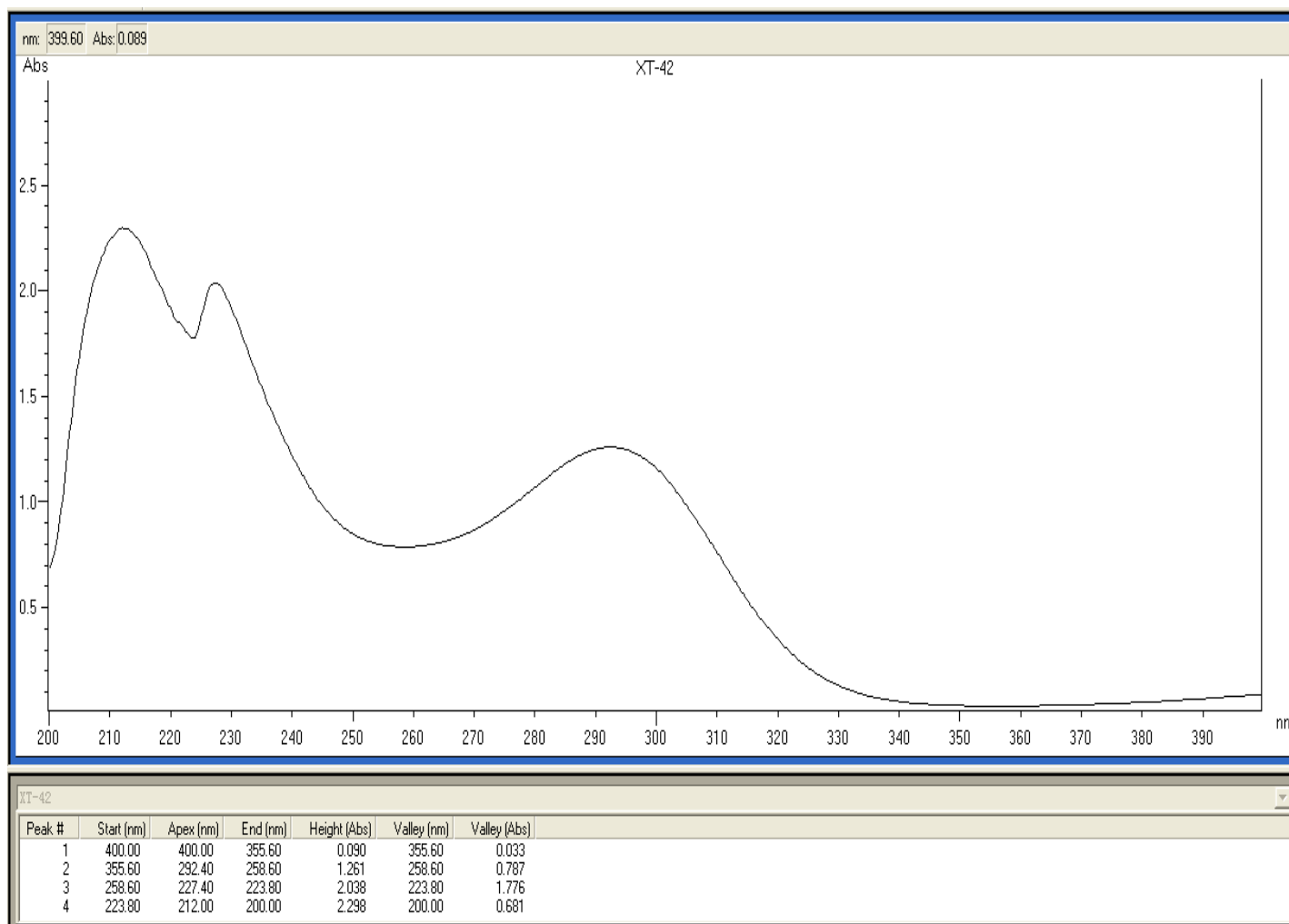


Figure S21. UV Spectrum of Dysidaminone B (2) in MeOH.

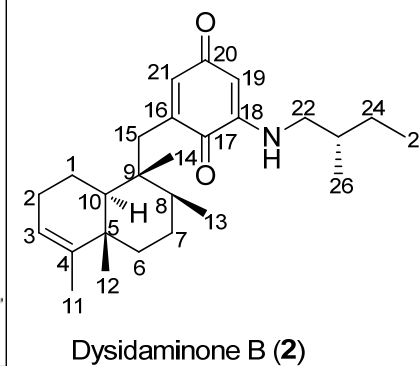
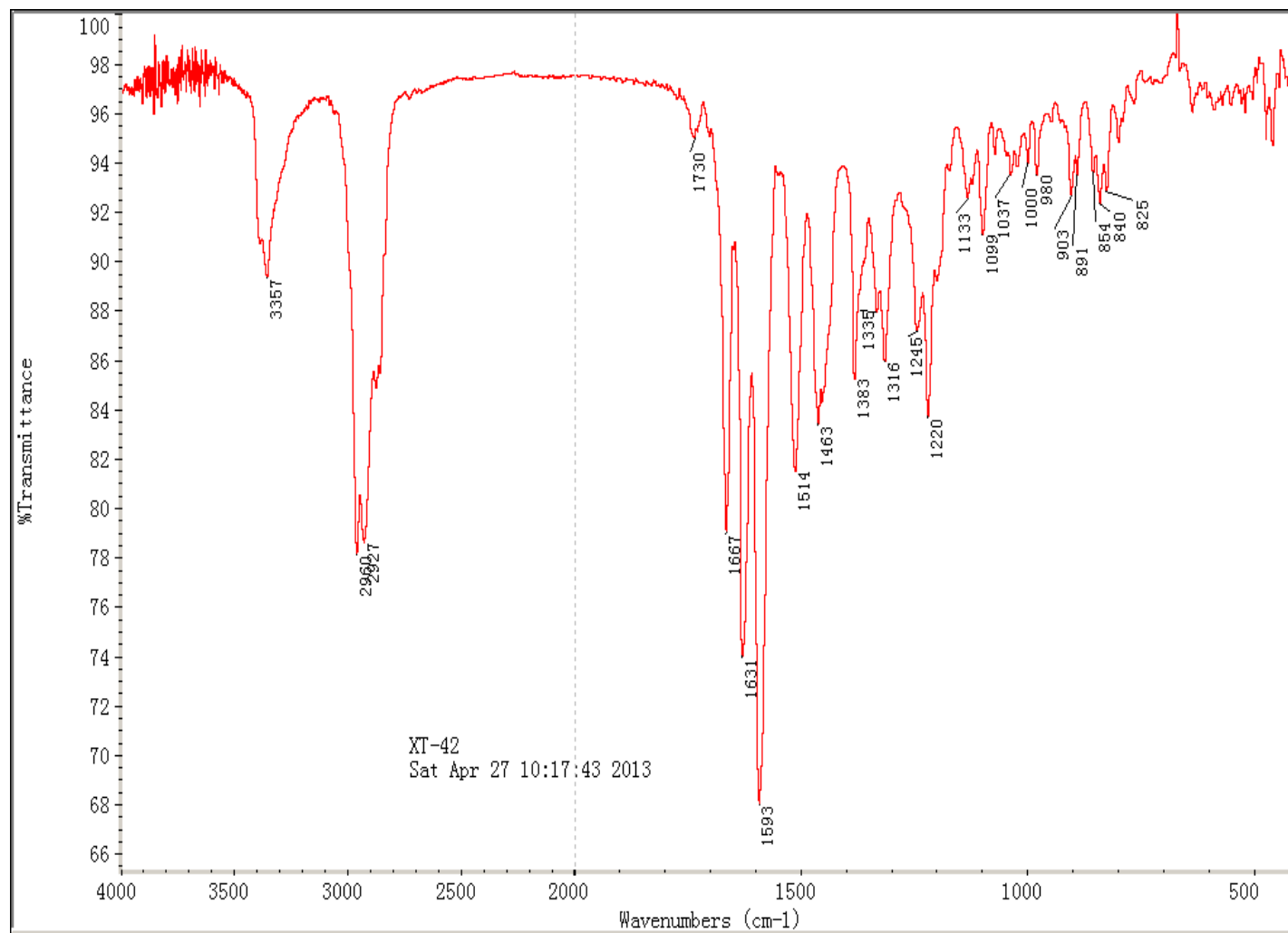
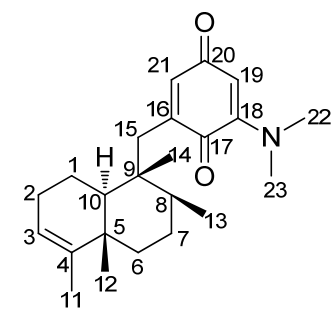
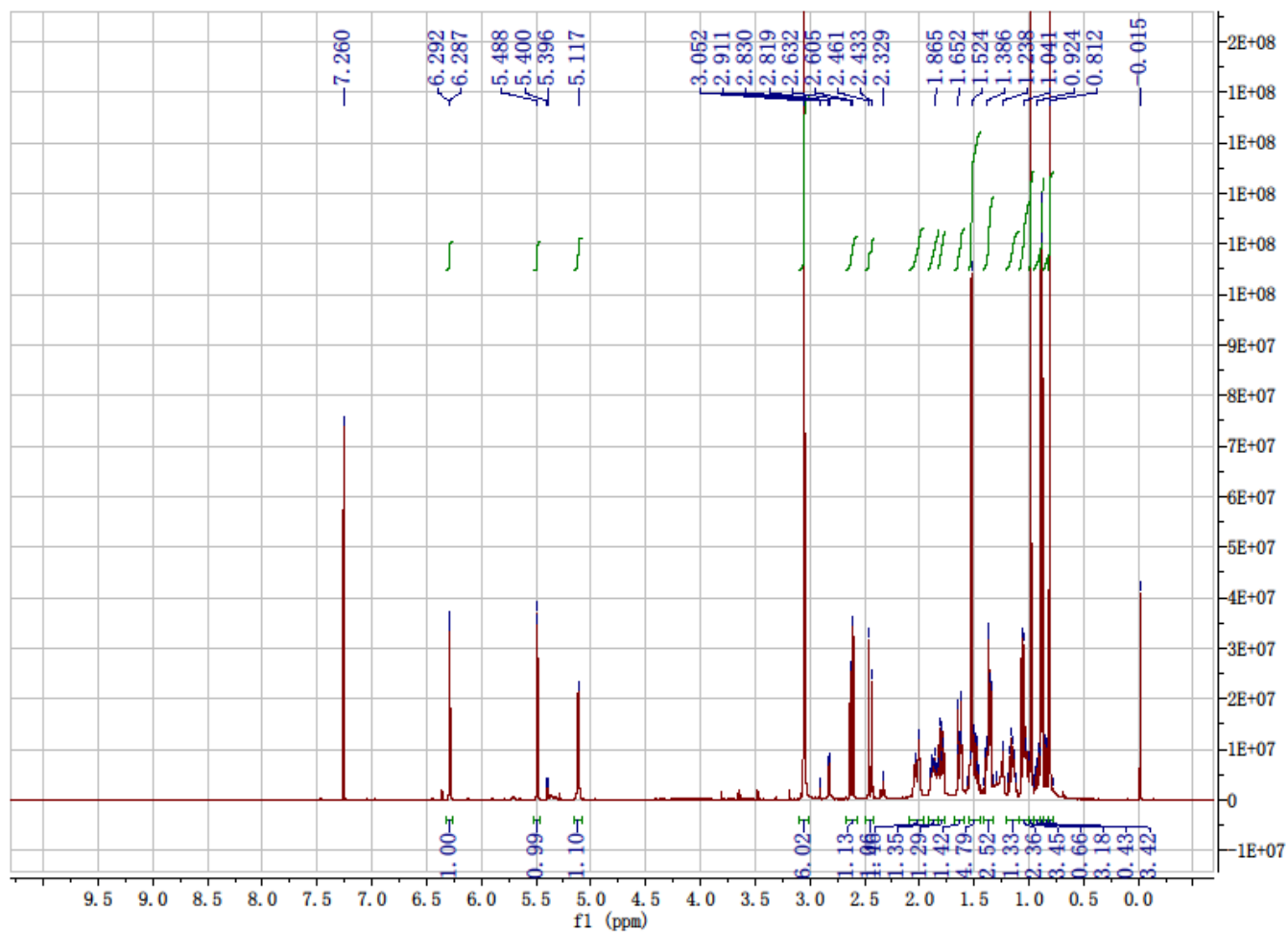
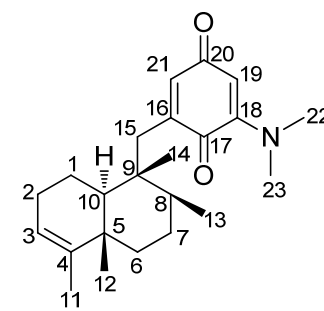
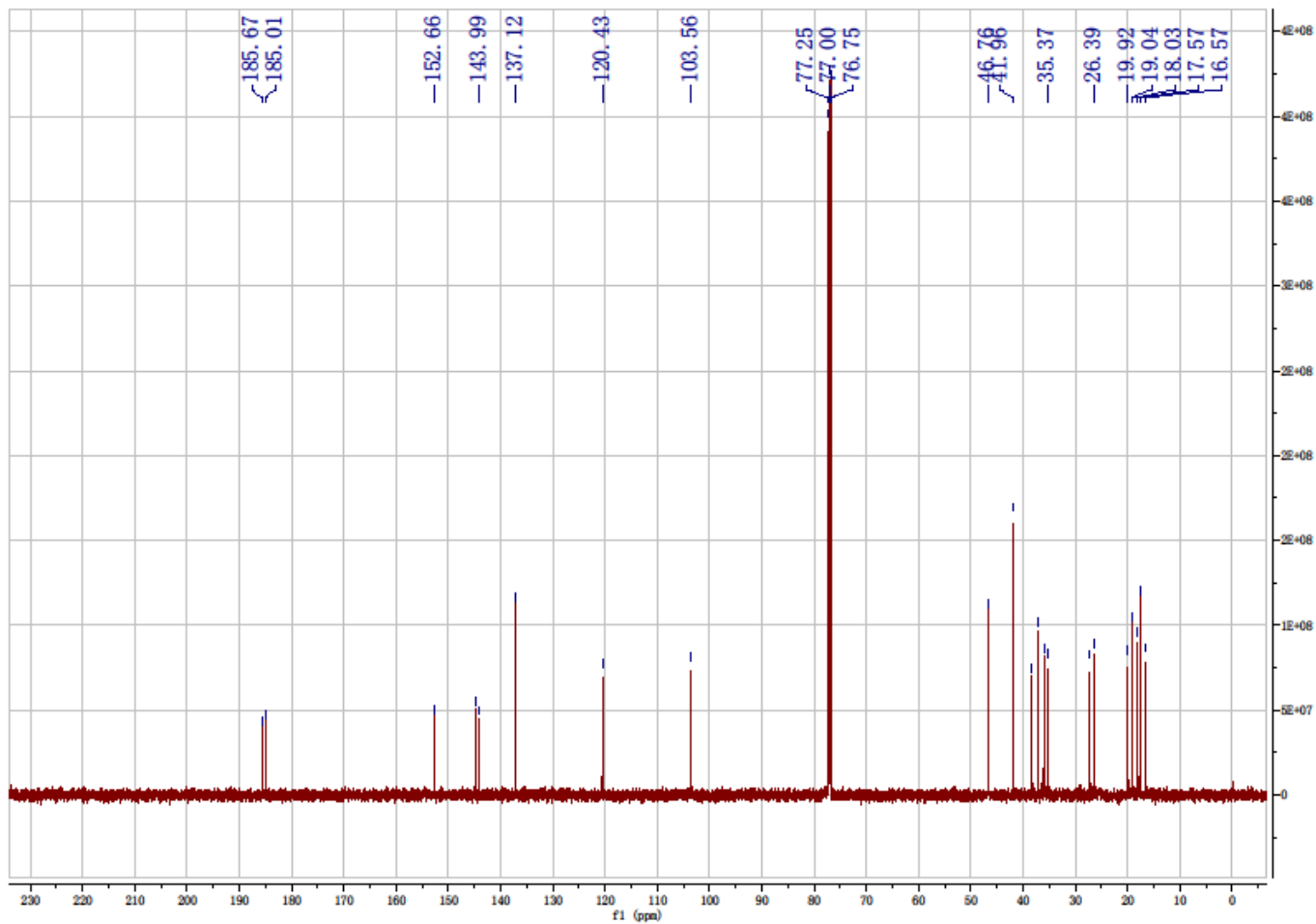


Figure S22. IR Spectrum of Dysidaminone B (2).



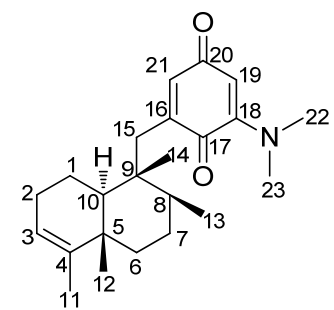
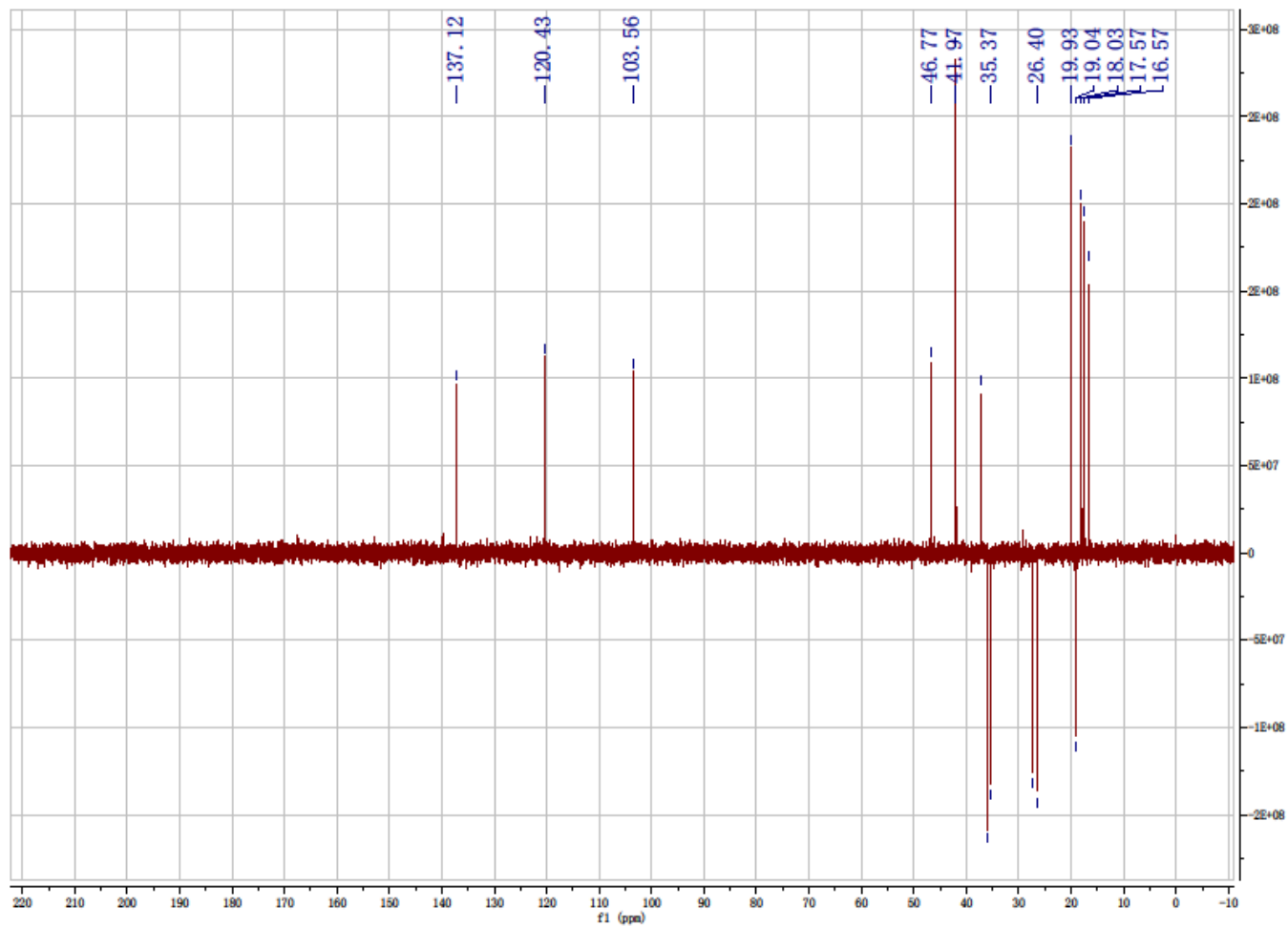
Dysidaminone C (**3**)

Figure S23. ^1H NMR Spectrum of Dysidaminone C (**3**) in CDCl_3 .



Dysidaminone C (3)

Figure S24. ^{13}C NMR Spectrum of Dysidaminone C (3) in CDCl_3 .



Dysidaminone C (**3**)

Figure S25. DEPT135 Spectrum of Dysidaminone C (**3**) in CDCl₃.

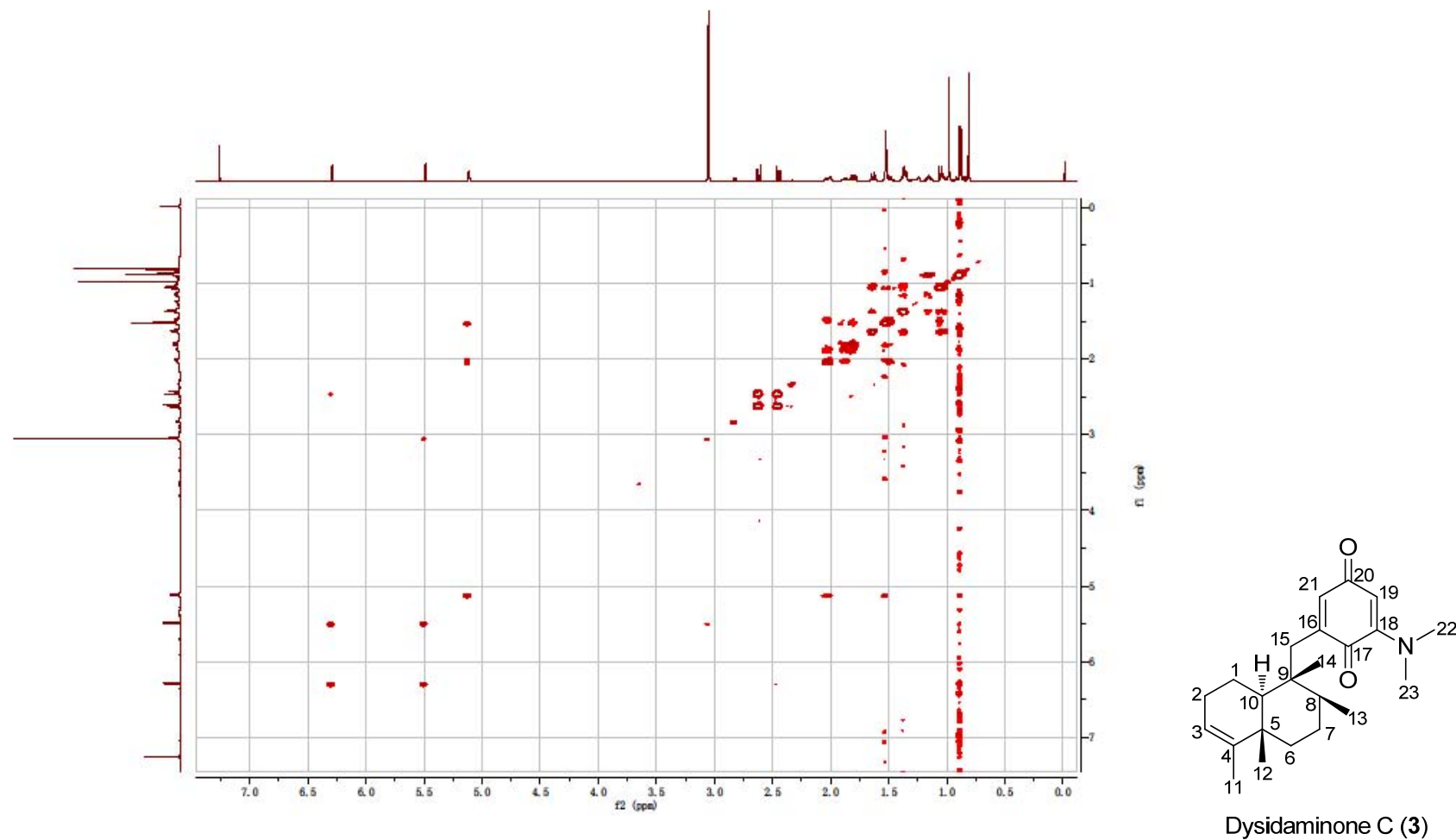


Figure S26. ^1H - ^1H COSY Spectrum of Dysidaminone C (**3**) in CDCl_3 .

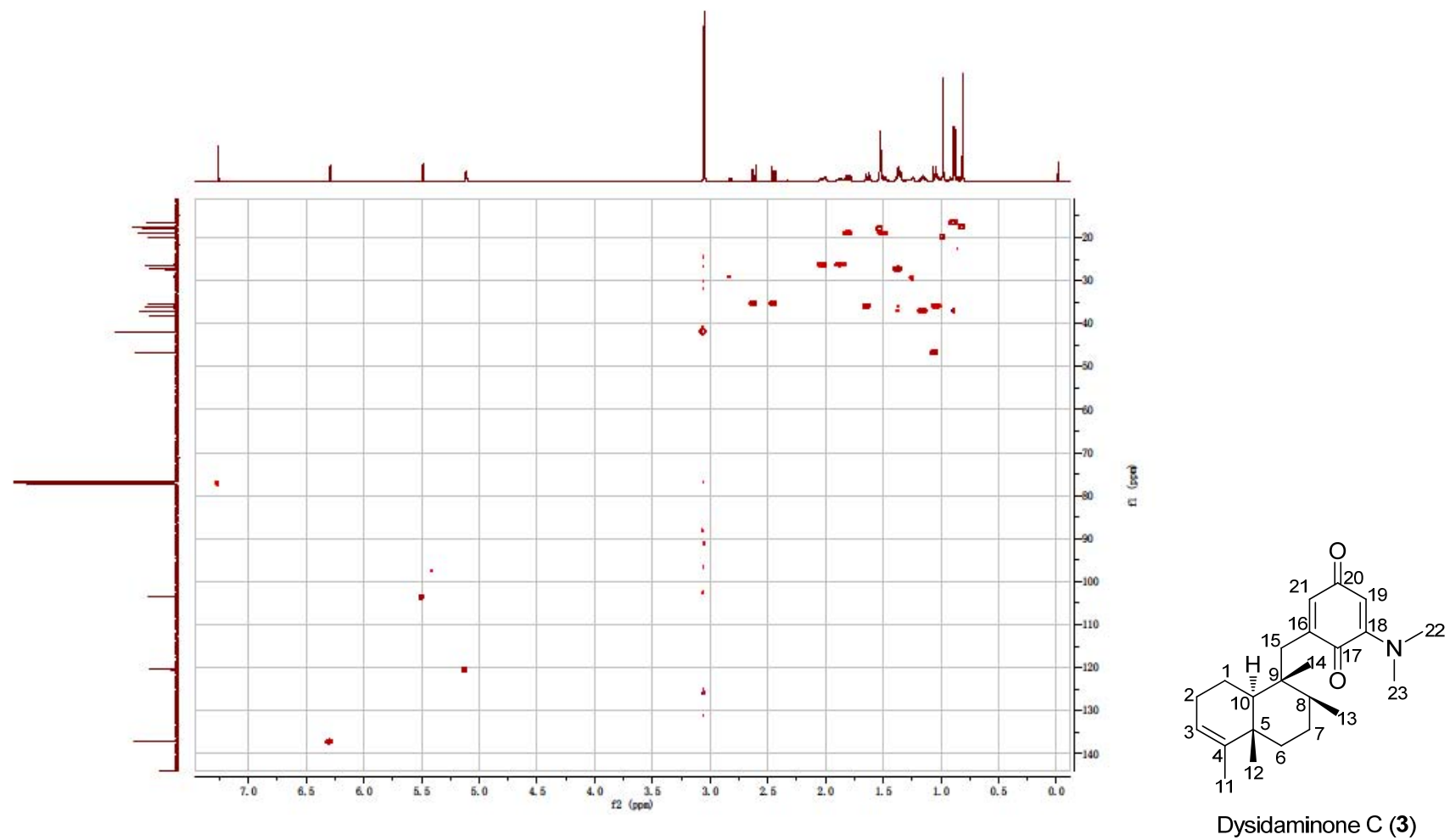


Figure S27. HSQC Spectrum of Dysidaminone C (**3**) in CDCl₃.

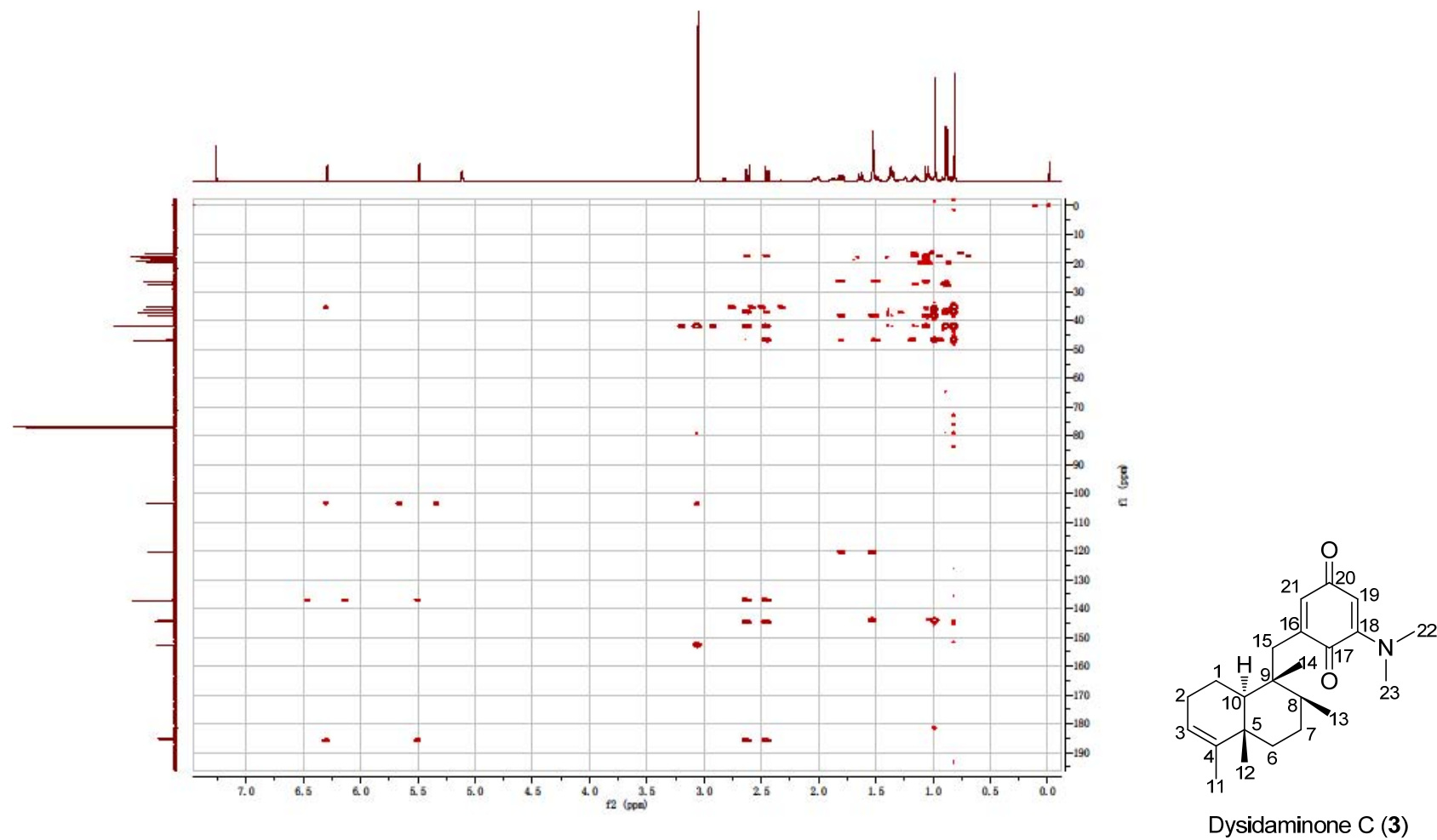


Figure S28. HMBC Spectrum of Dysidaminone C (**3**) in CDCl₃.

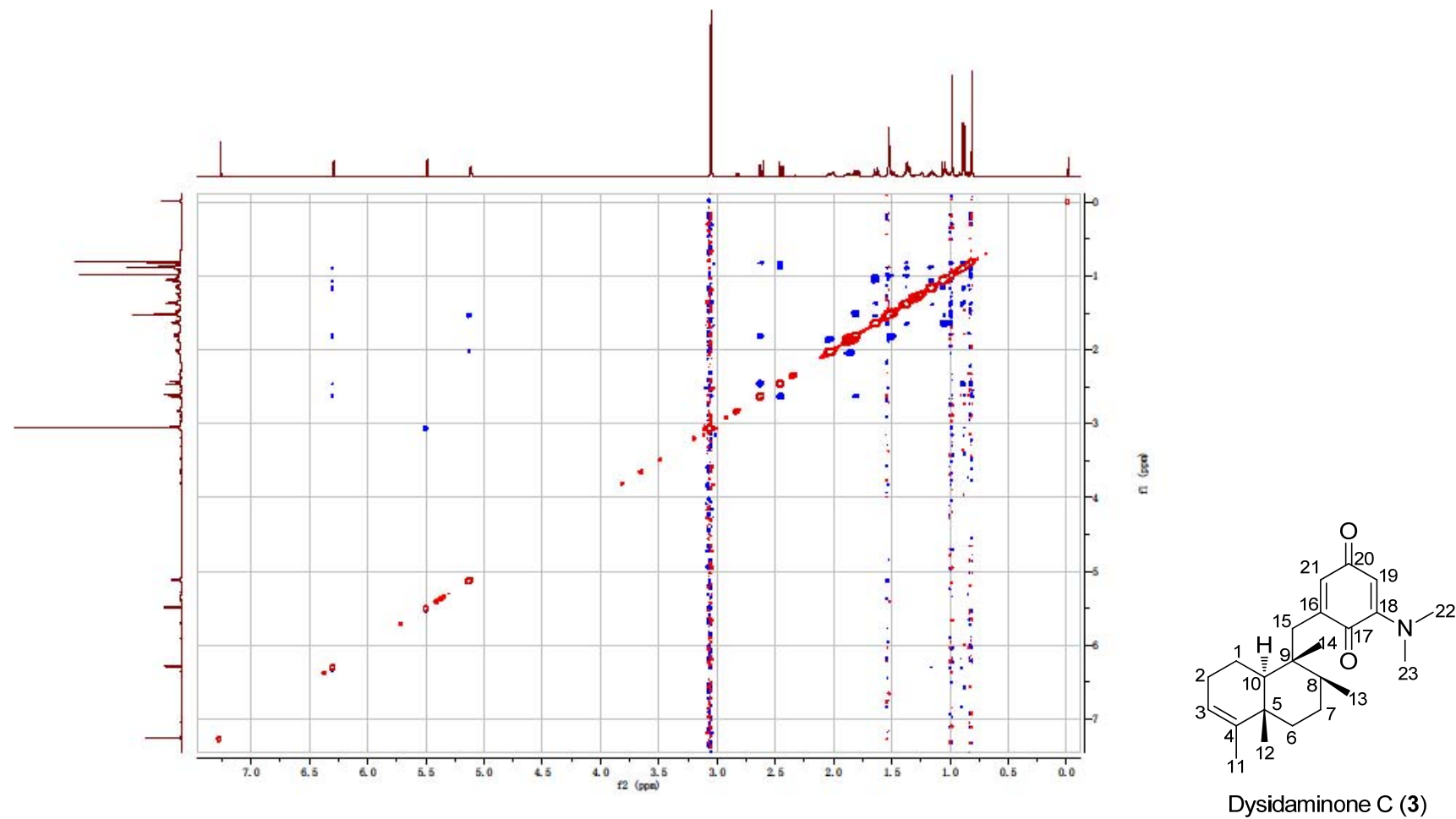


Figure S29. NOESY Spectrum of Dysidaminone C (3) in CDCl₃.

Elemental Composition Report

Page 1

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

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SIPI

XT-38 M.W.=355

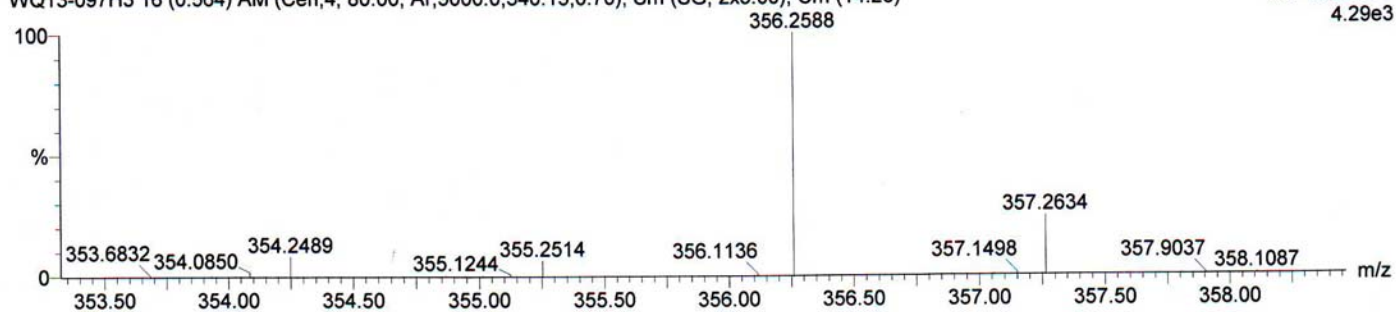
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Q-Tof micro

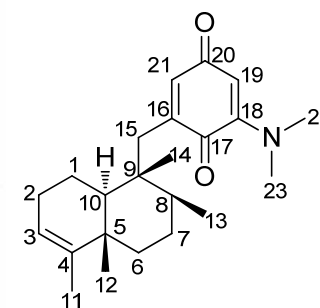
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29-Apr-2013, 15:12:33

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4.29e3

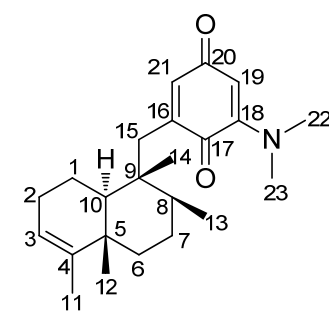
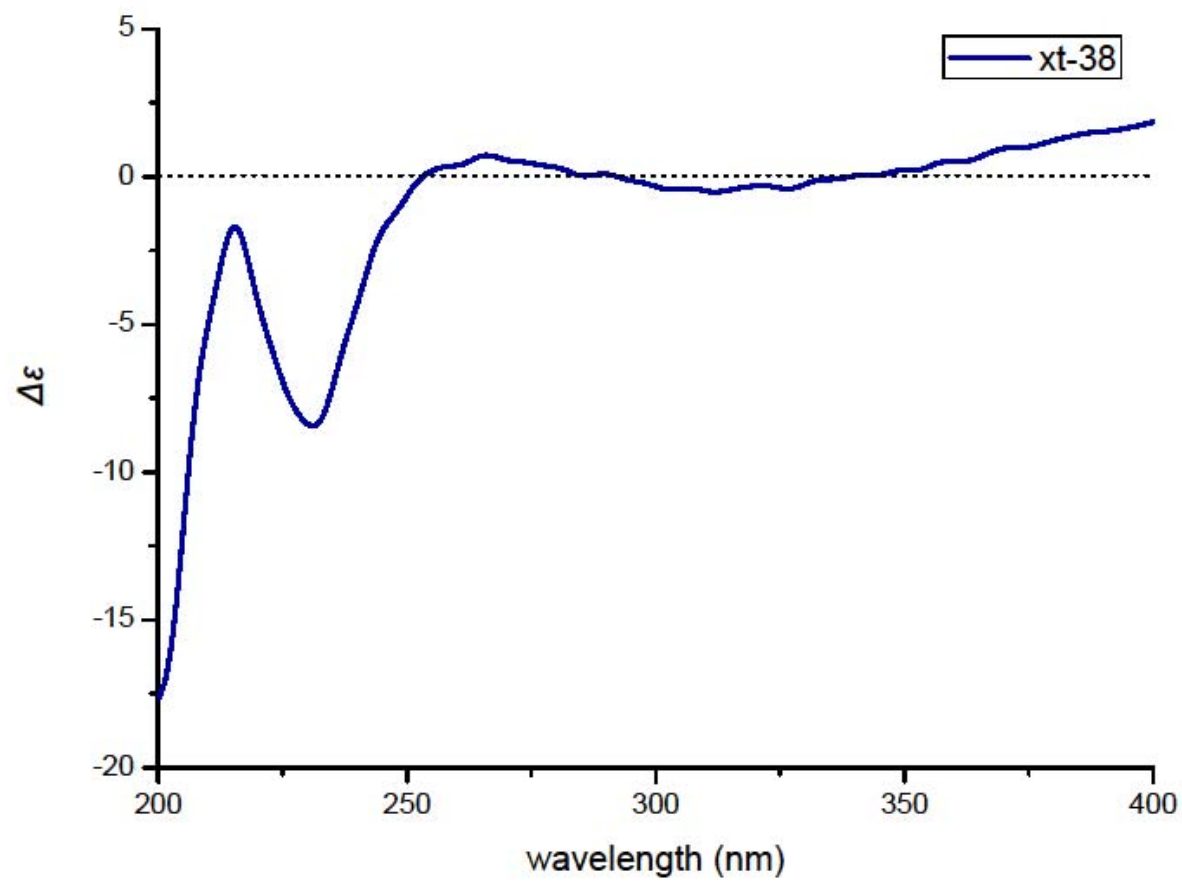


Minimum:	40.00				-1.5		
Maximum:	100.00		5.0	5.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
356.2588	100.00	356.2590	-0.2	-0.6	7.5	2775182.8	C23 H34 N O2



Dysidaminone C (3)

Figure S30. HRESIMS of Dysidaminone C (3).



Dysidaminone C (**3**)

Figure S31. CD Spectrum of Dysidaminone C (**3**) in MeOH.

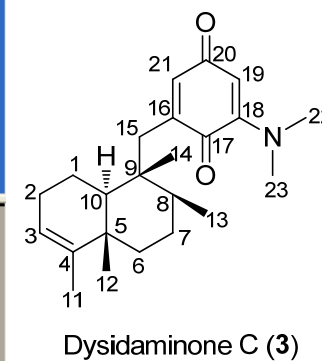
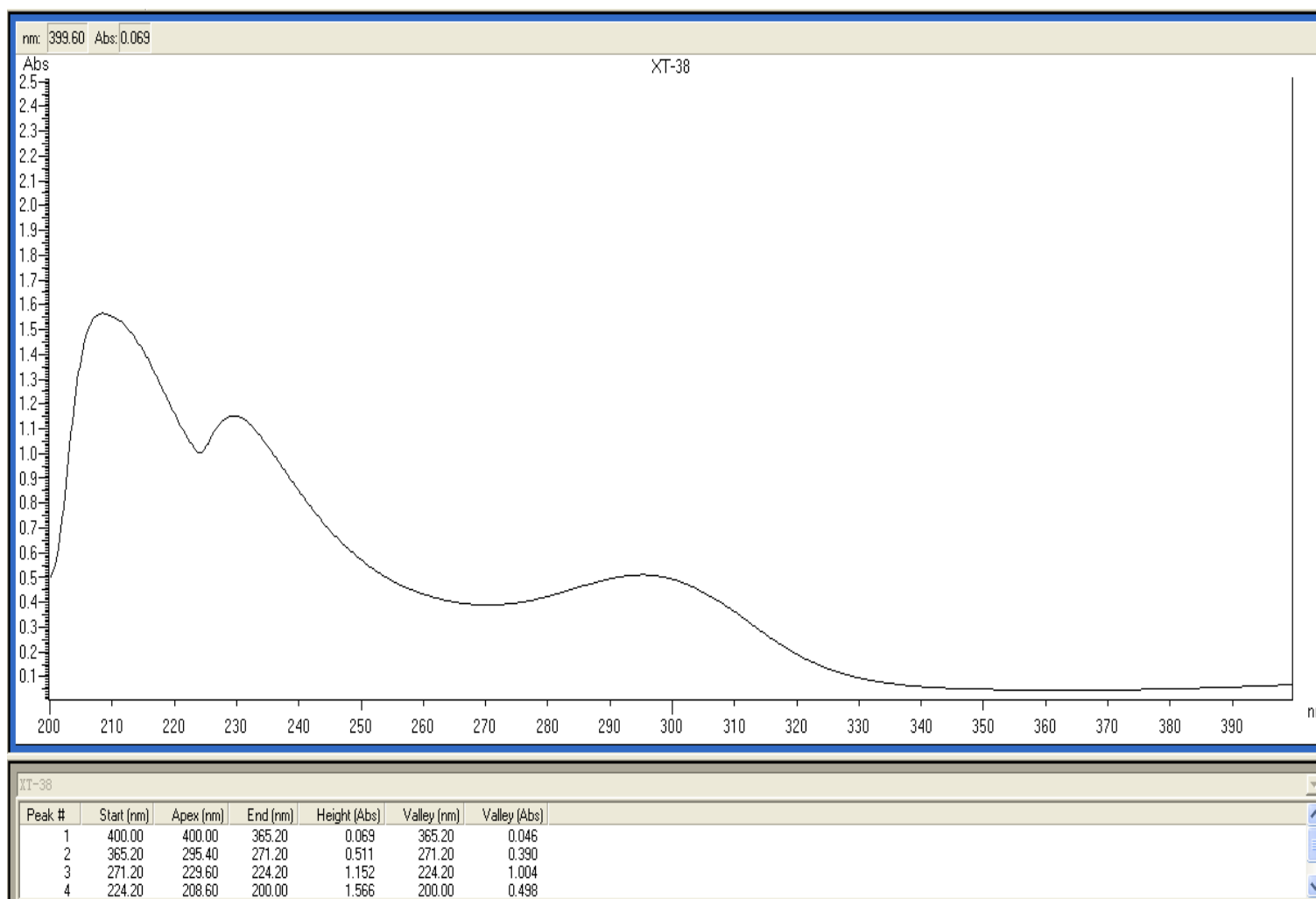


Figure S32. UV Spectrum of Dysidaminone C (3) in MeOH.

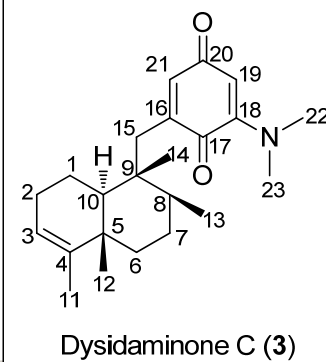
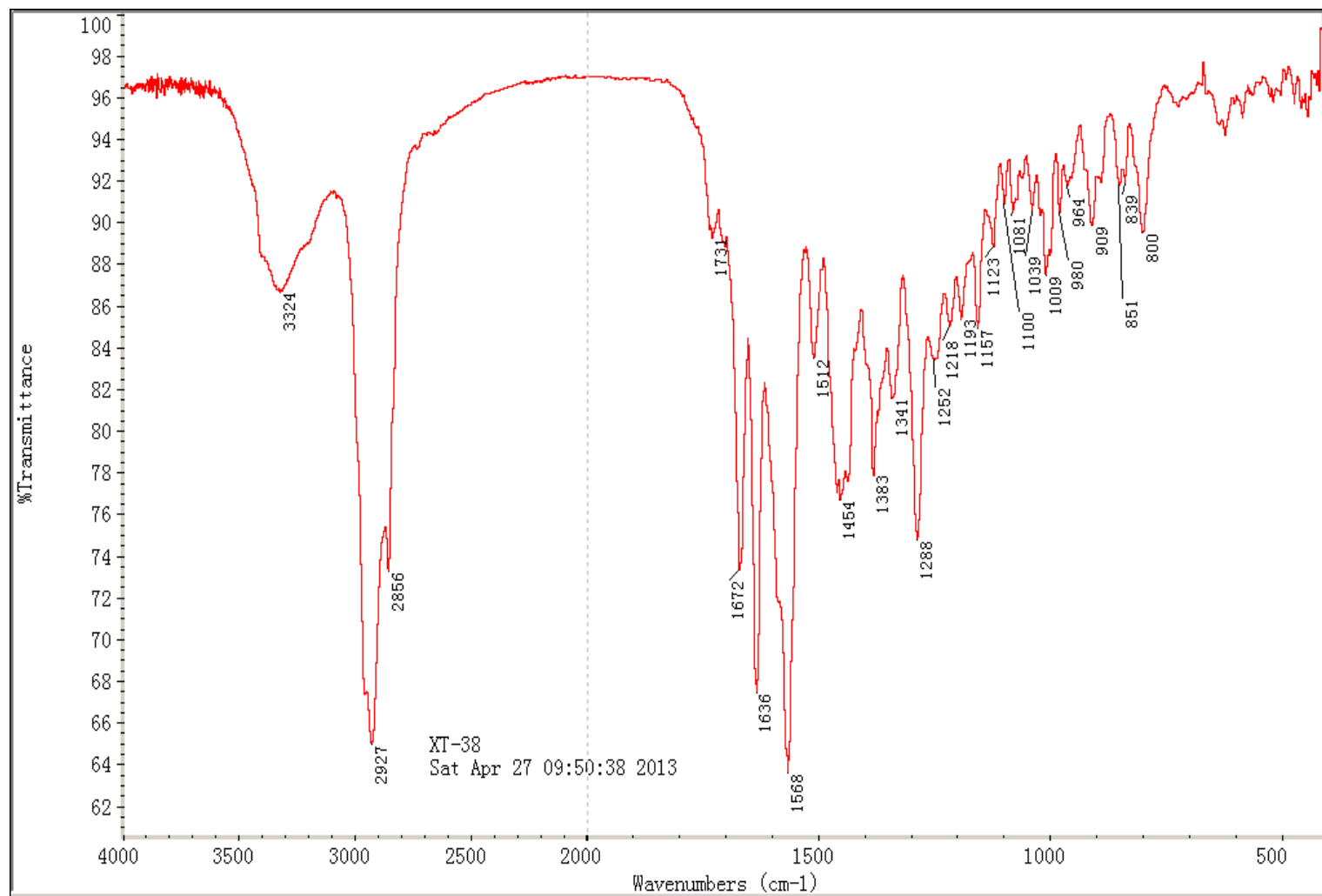
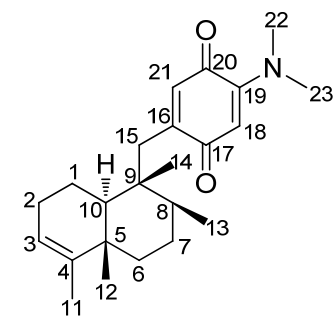
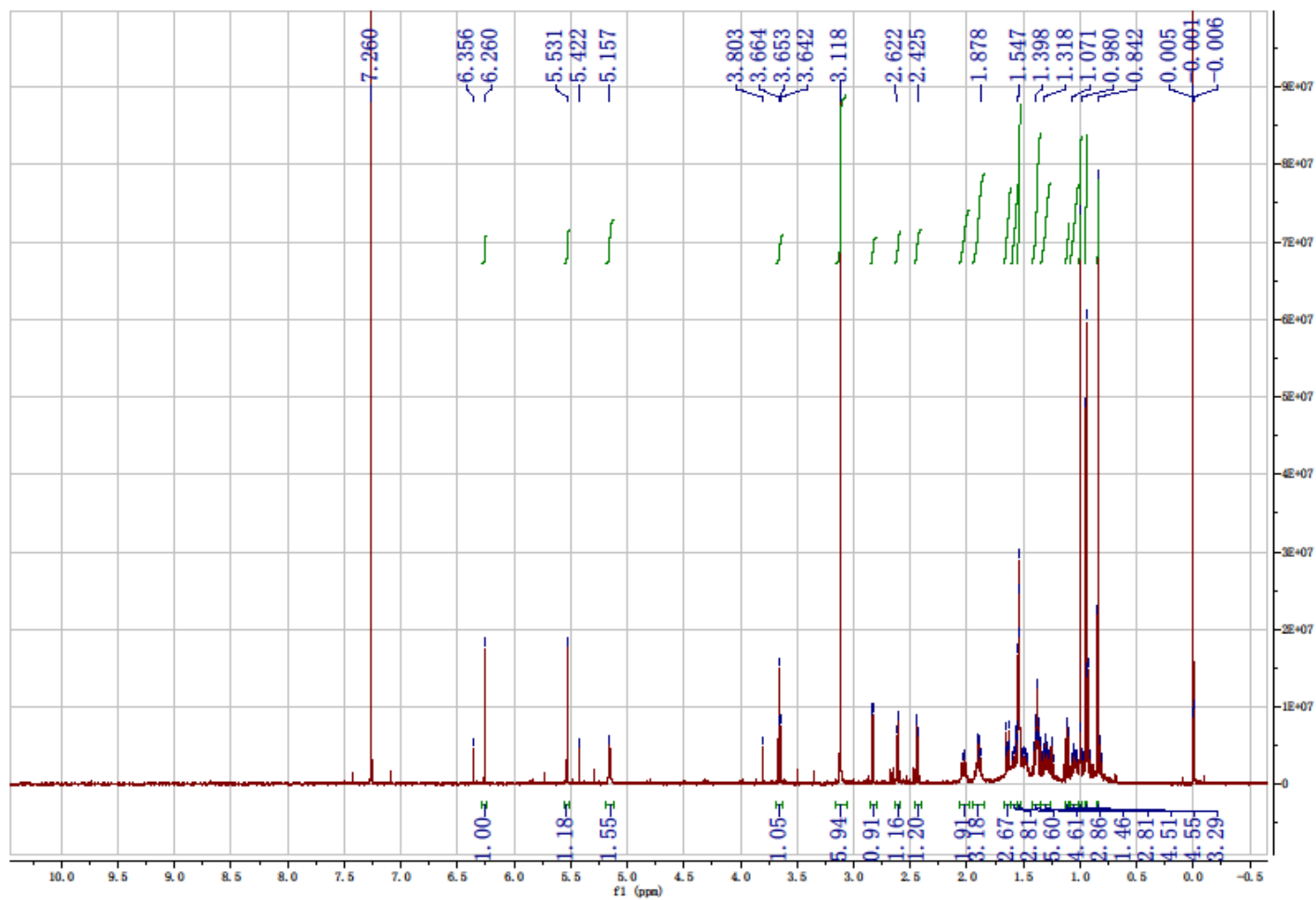


Figure S33. IR Spectrum of Dysidaminone C (3).



Dysidaminone D (4)

Figure S34. ^1H NMR Spectrum of Dysidaminone D (4) in CDCl_3 .

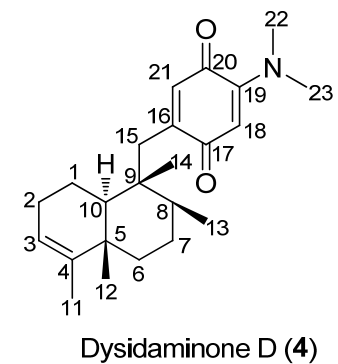
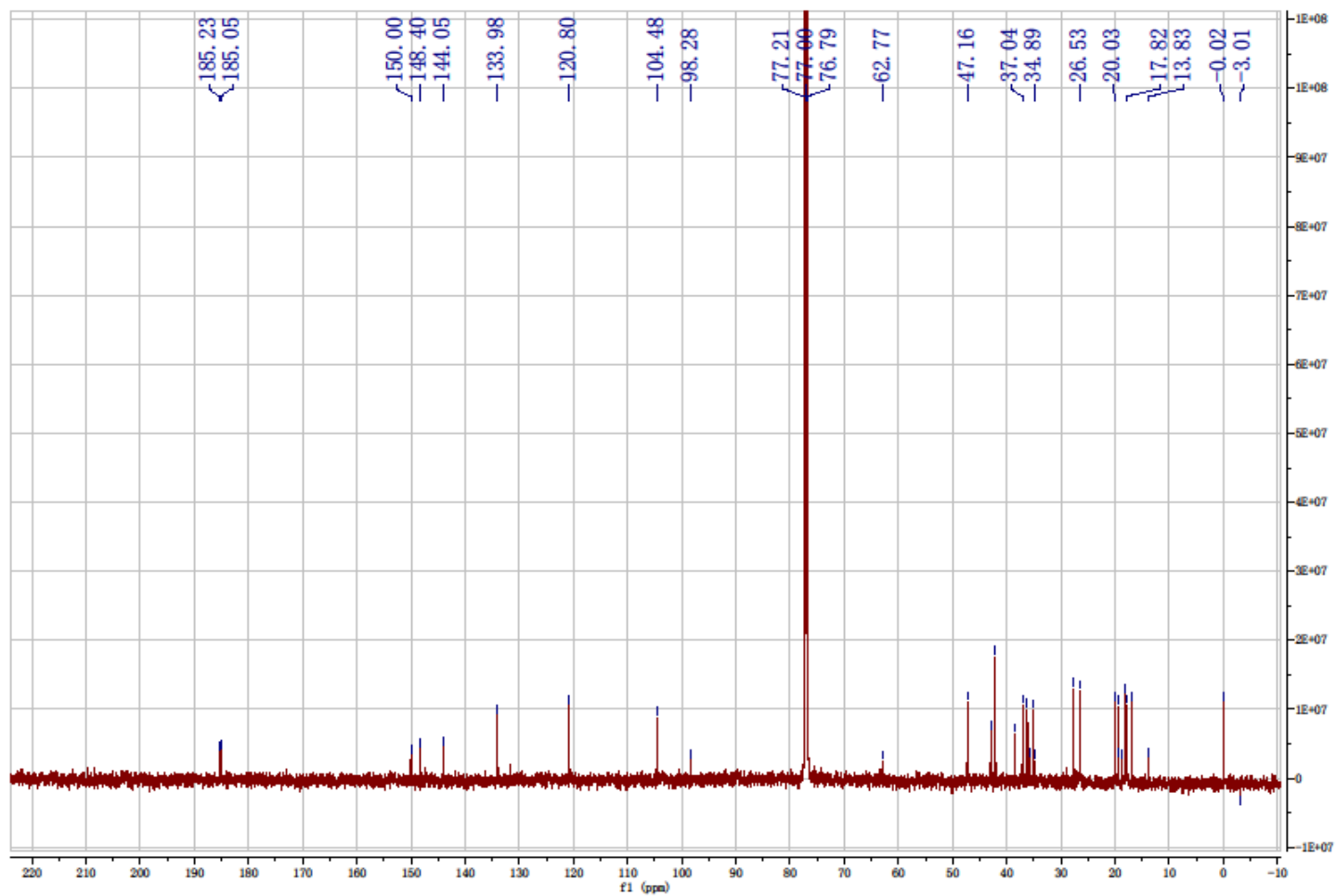


Figure S35. ^{13}C NMR Spectrum of Dysidaminone D (4) in CDCl_3 .

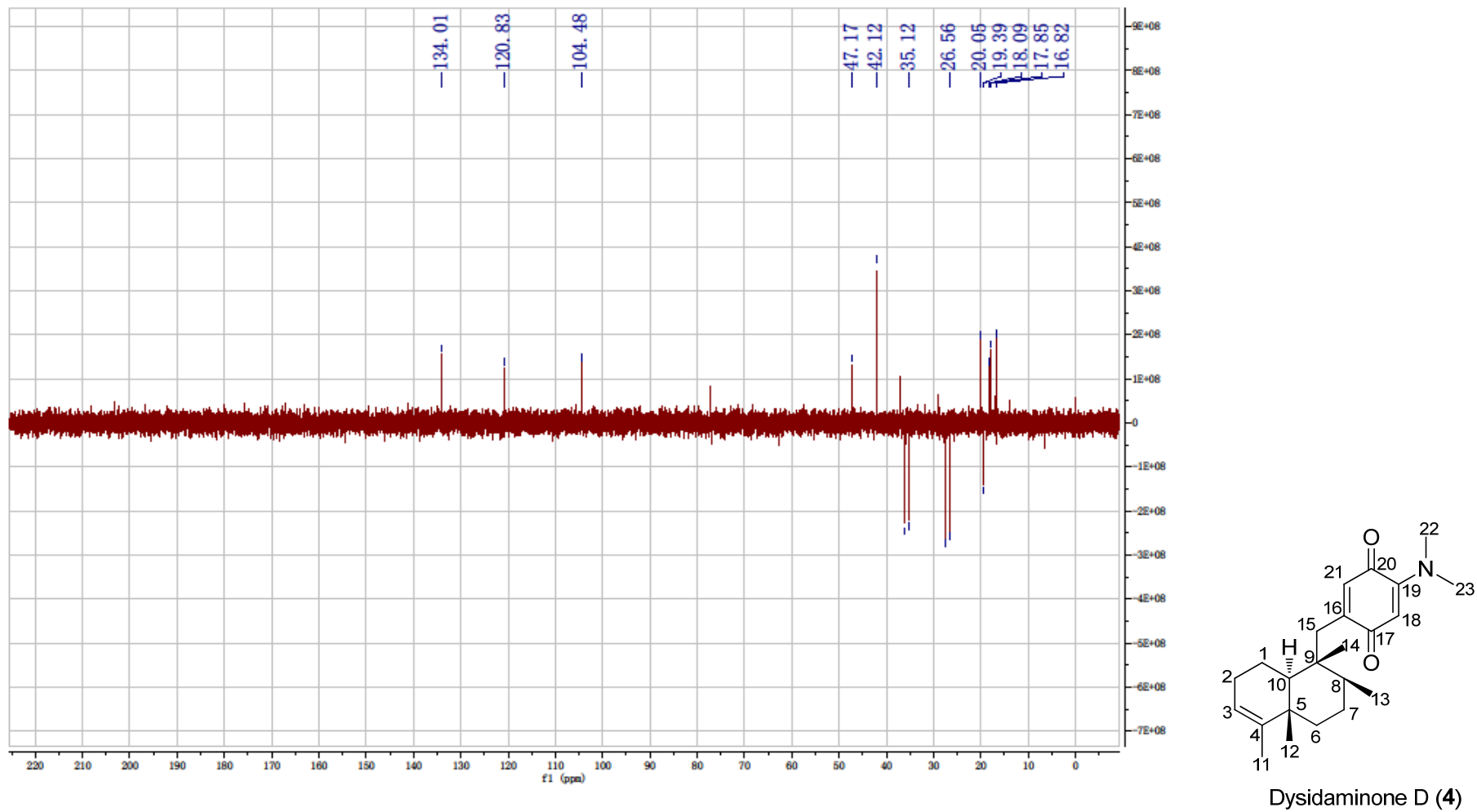


Figure S36. DEPT135 Spectrum of Dysidaminone D (4) in CDCl₃.

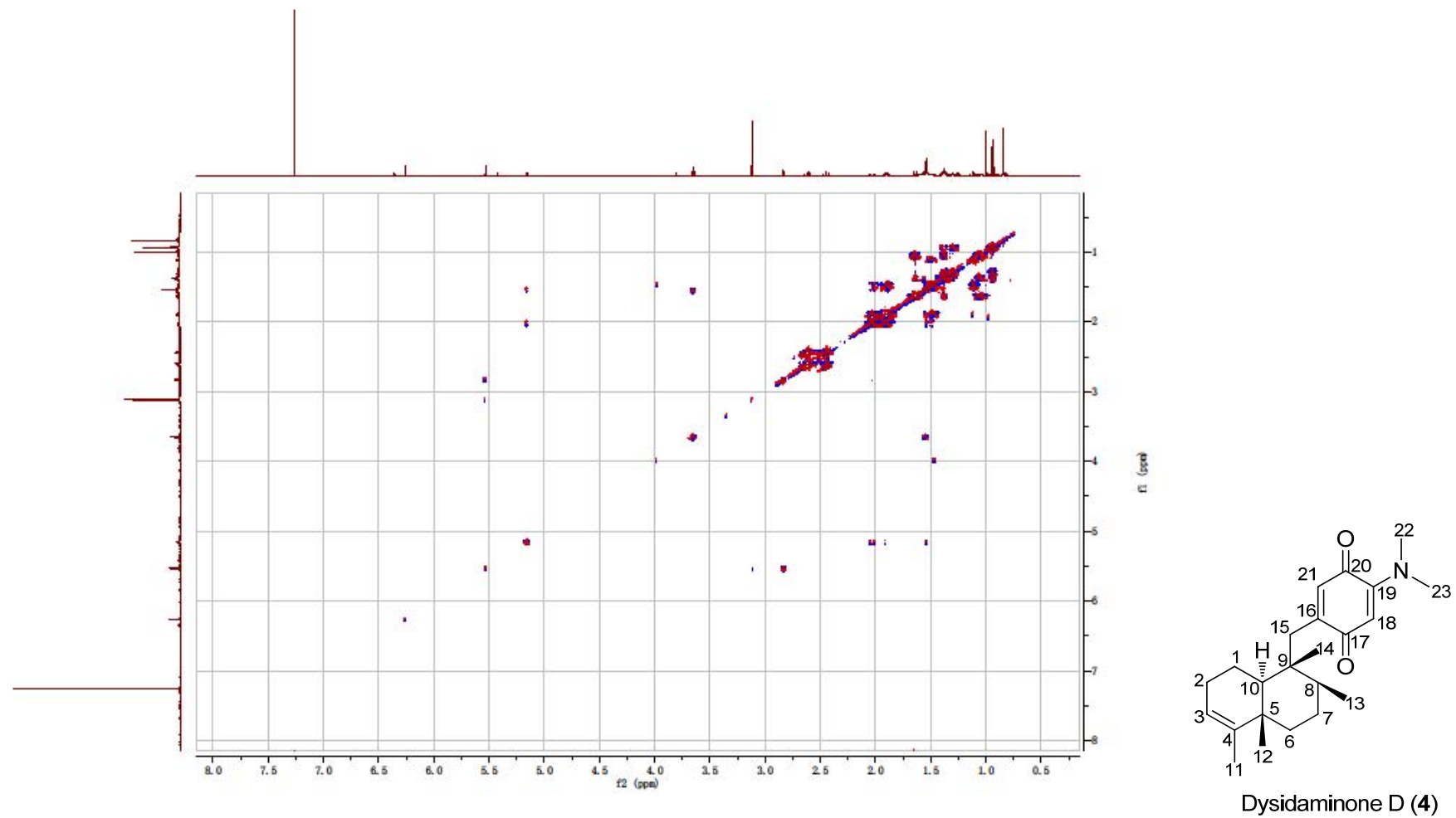


Figure S37. ^1H - ^1H COSY Spectrum of Dysidaminone D (4) in CDCl_3 .

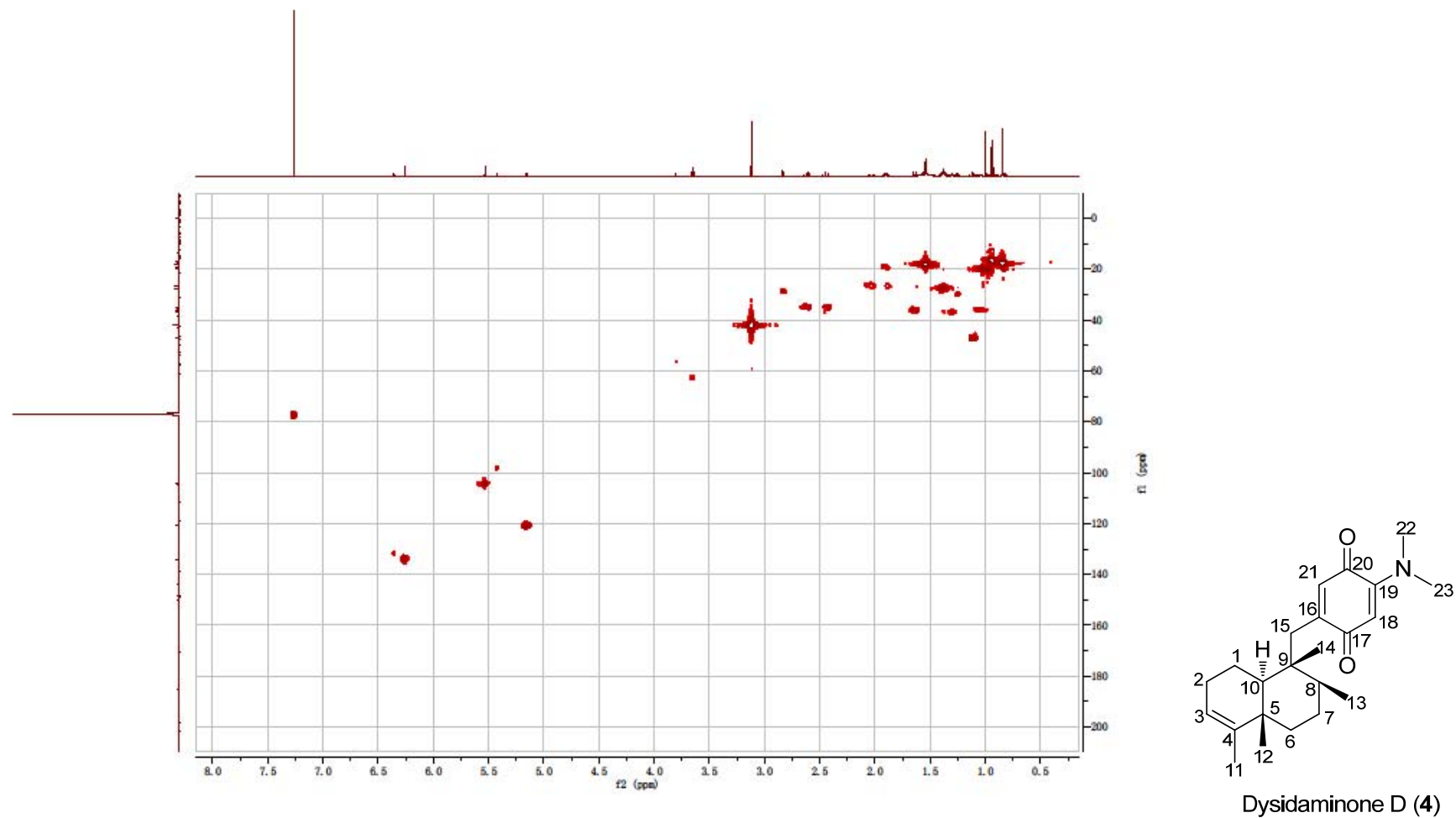


Figure S38. HSQC Spectrum of Dysidaminone D (**4**) in CDCl₃.

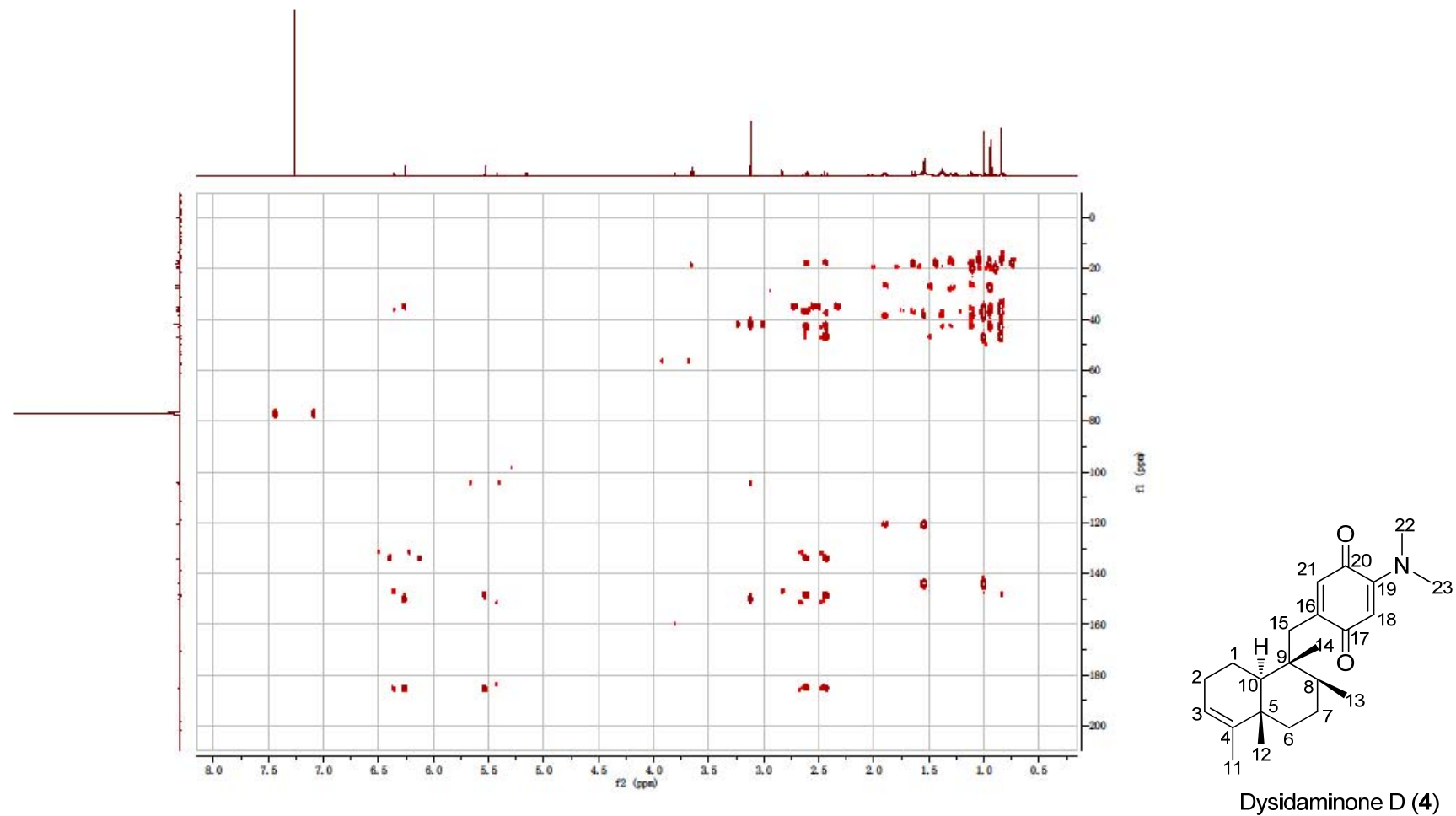


Figure S39. HMBC Spectrum of Dysidaminone D (4) in CDCl₃.

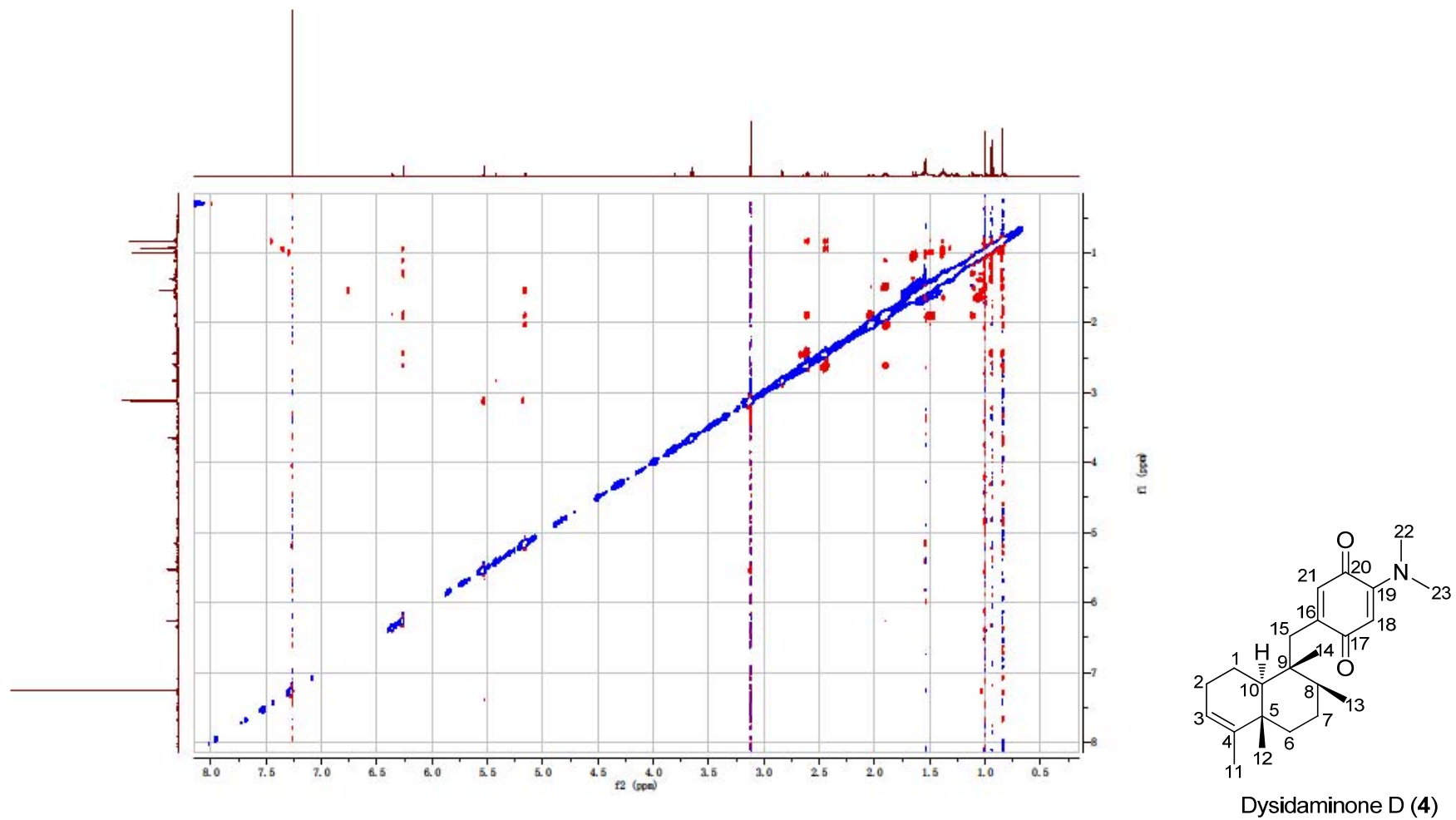


Figure S40. NOESY Spectrum of Dysidaminone D (4) in CDCl₃.

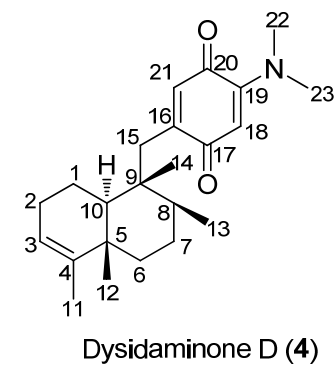
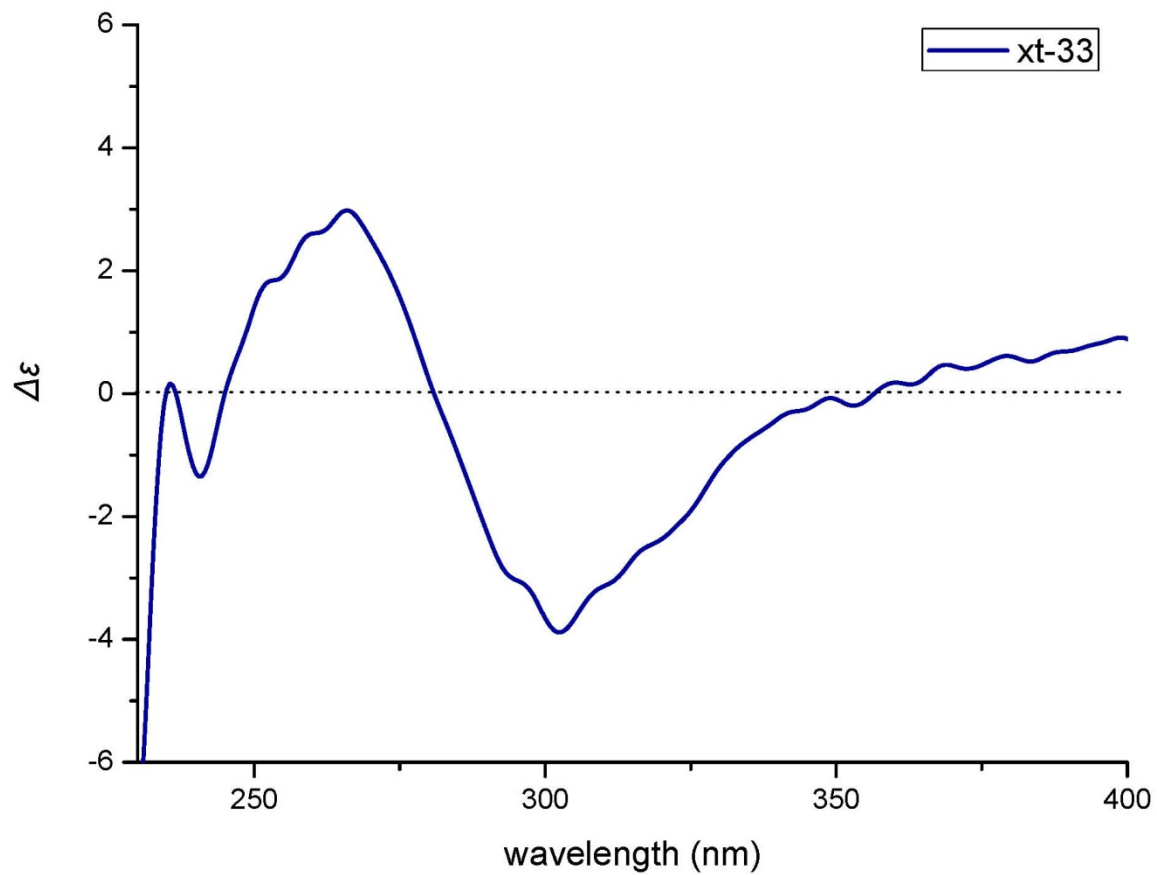


Figure S41. CD Spectrum of Dysidaminone D (4) in MeOH.

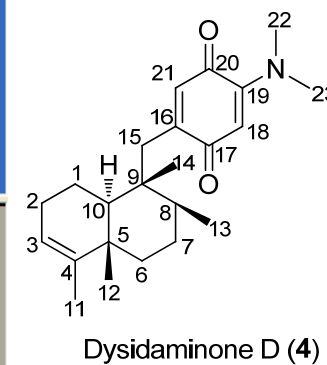
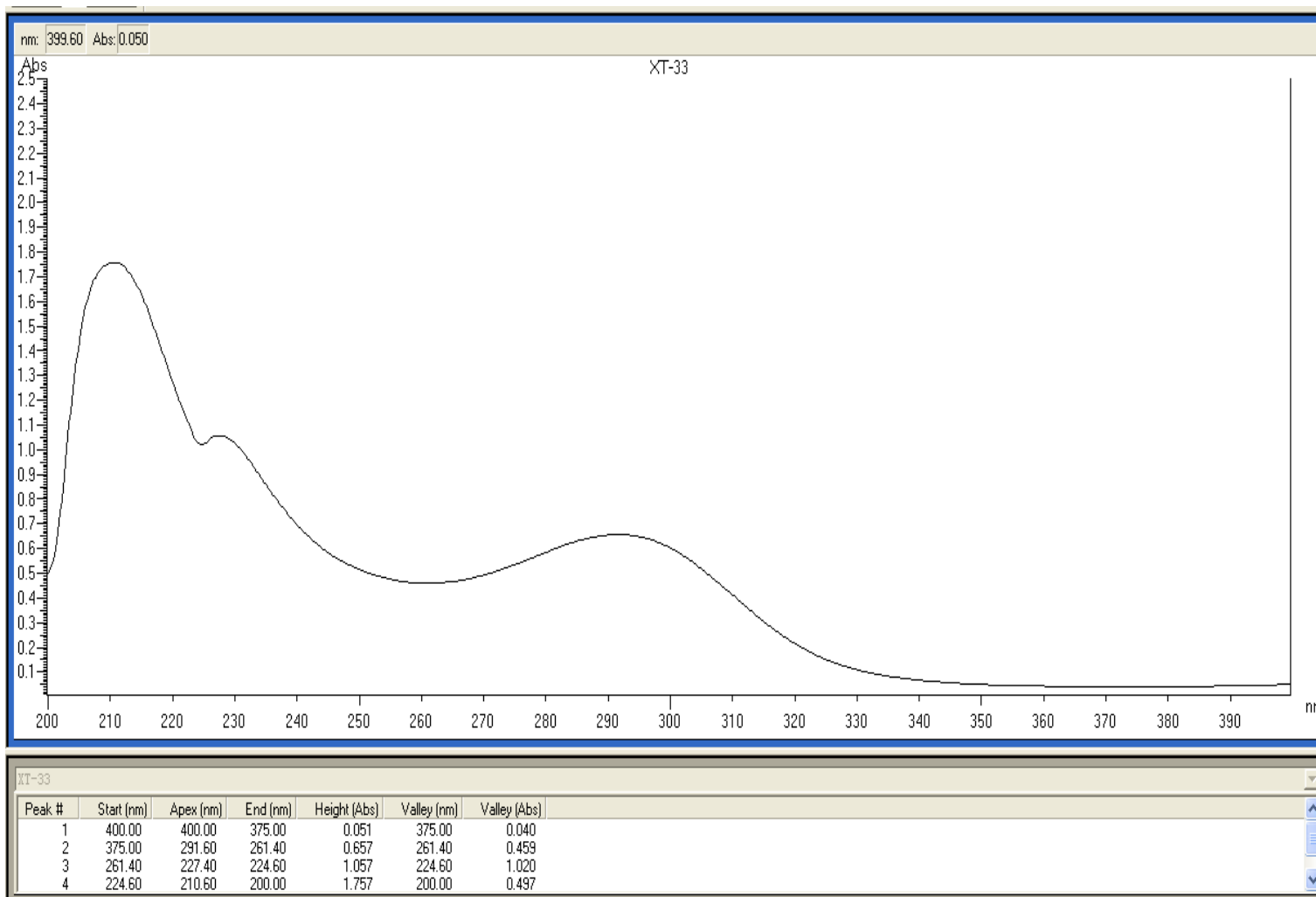


Figure S42. UV Spectrum of Dysidaminone D (4) in MeOH.

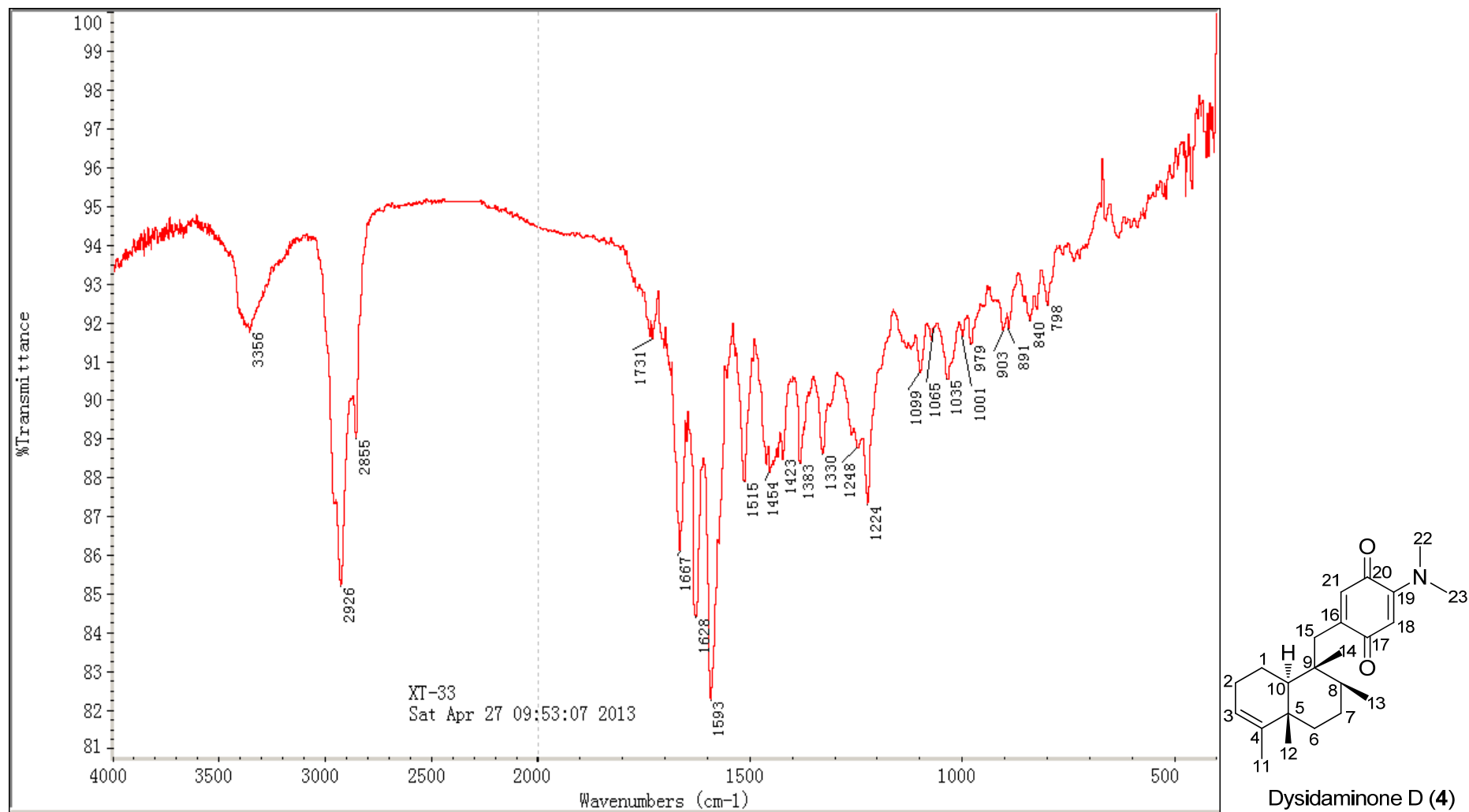
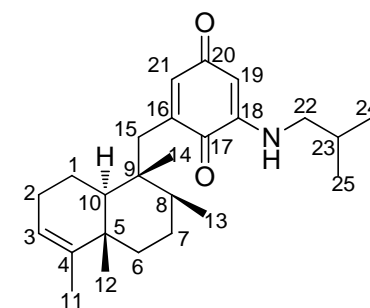
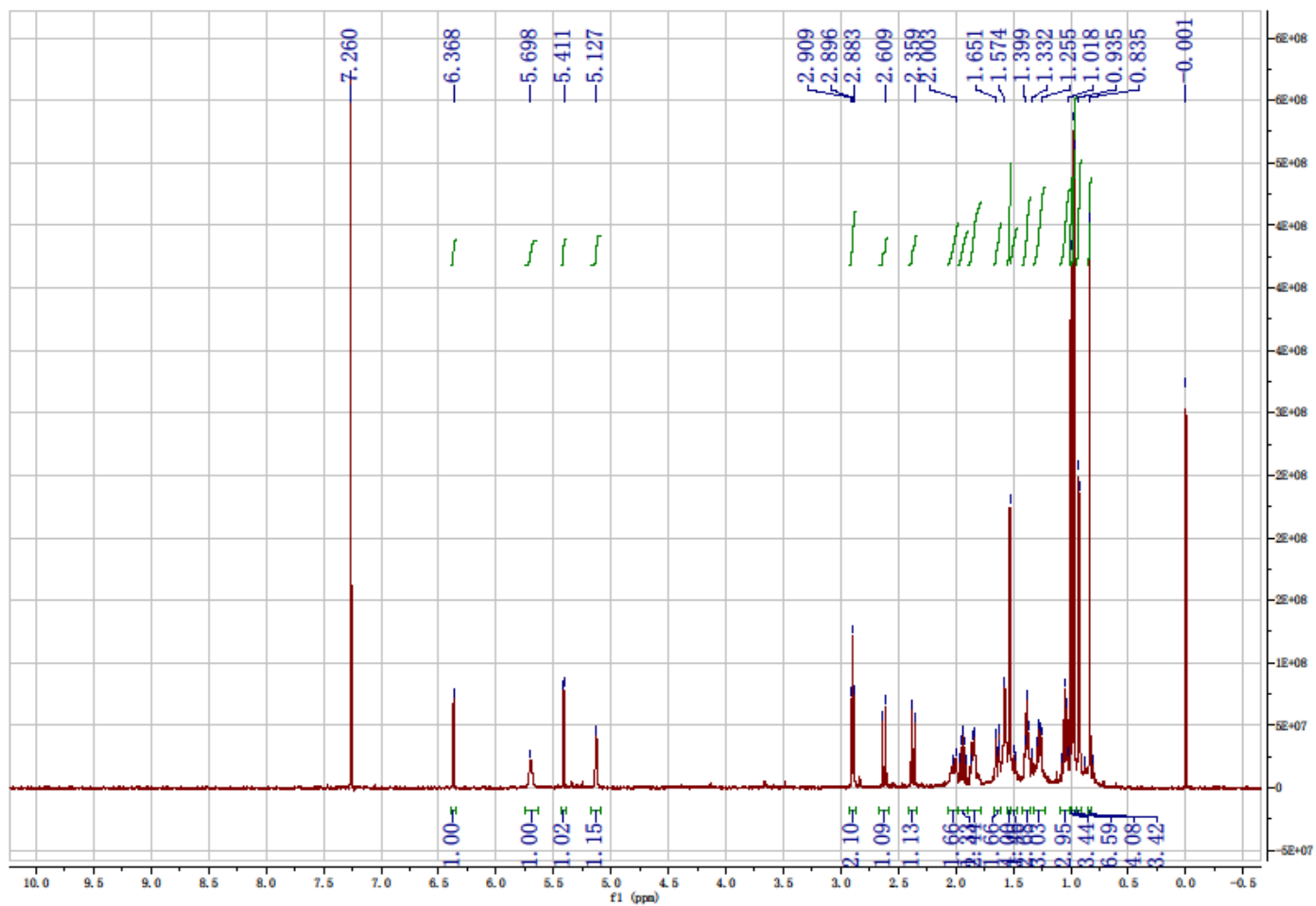
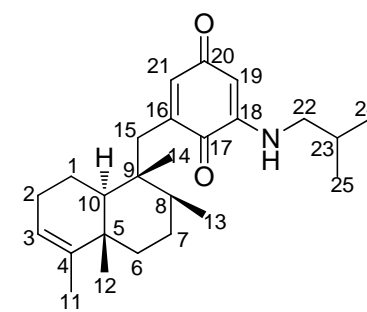
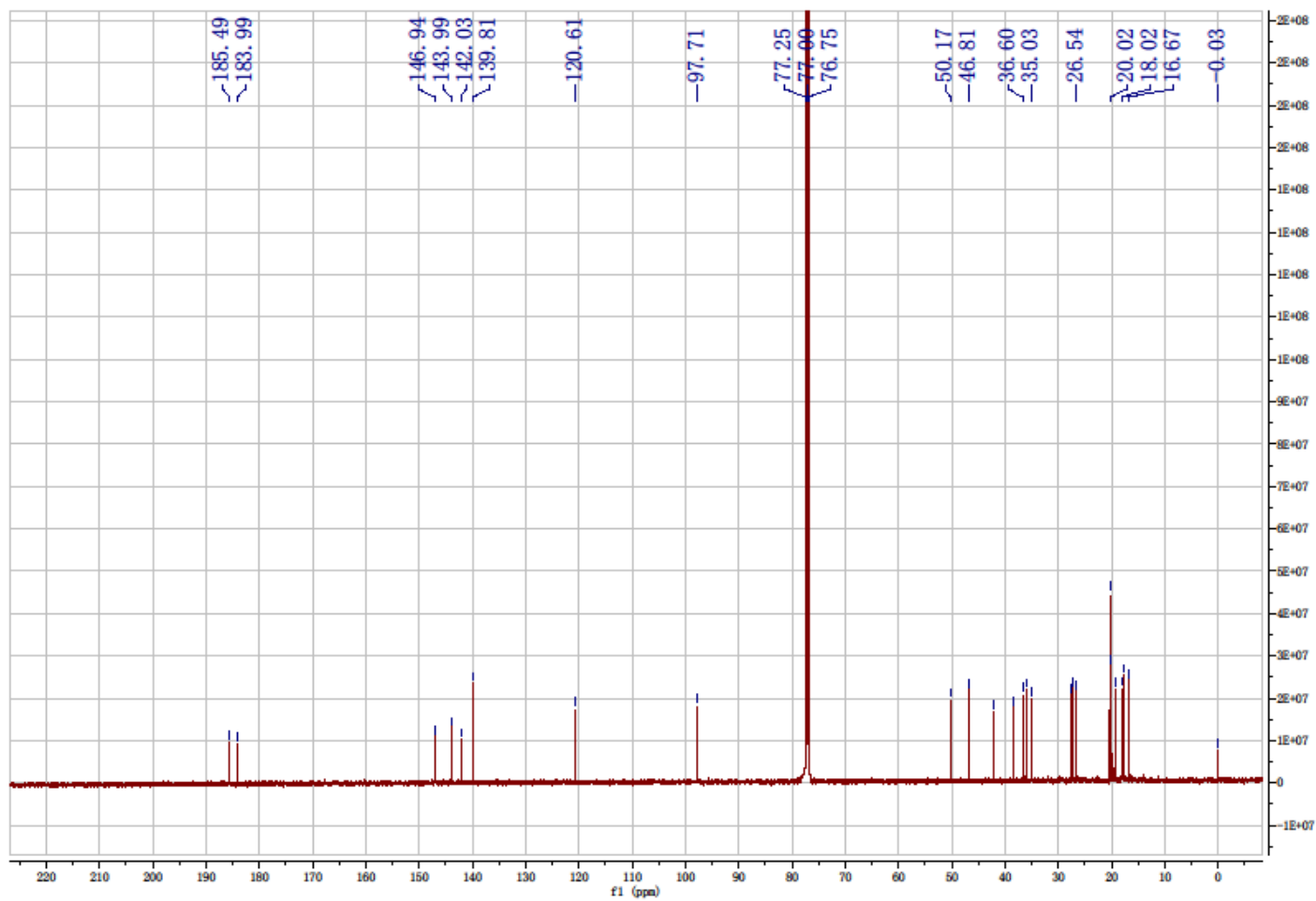


Figure S43. IR Spectrum of Dysidaminone D (4).



Dysidaminone E (5)

Figure S44. ^1H NMR Spectrum of Dysidaminone E (5) in CDCl_3 .



Dysidaminone E (5)

Figure S45. ^{13}C NMR Spectrum of Dysidaminone E (5) in CDCl_3 .

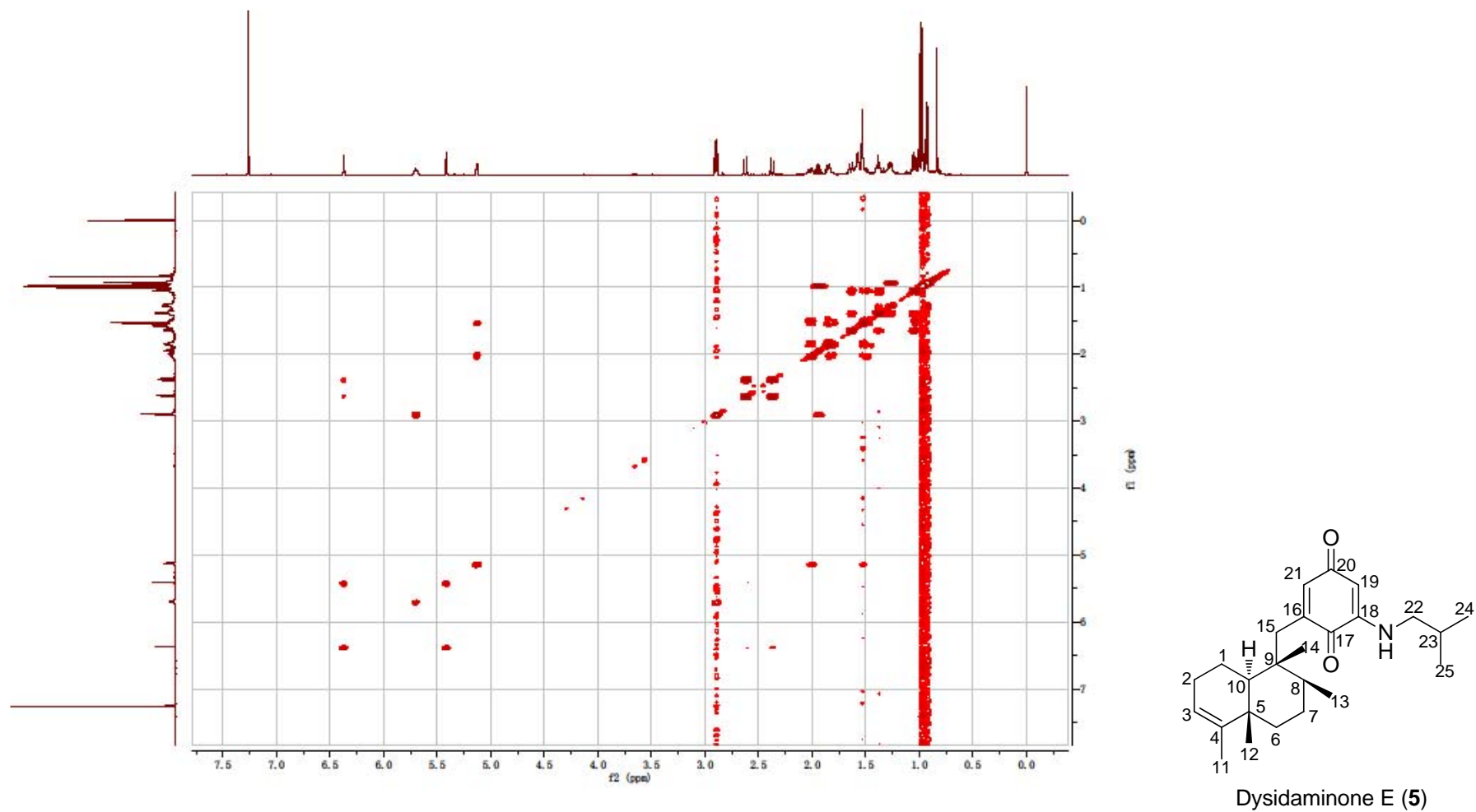


Figure S46. ^1H - ^1H COSY Spectrum of Dysidaminone E (5) in CDCl_3 .

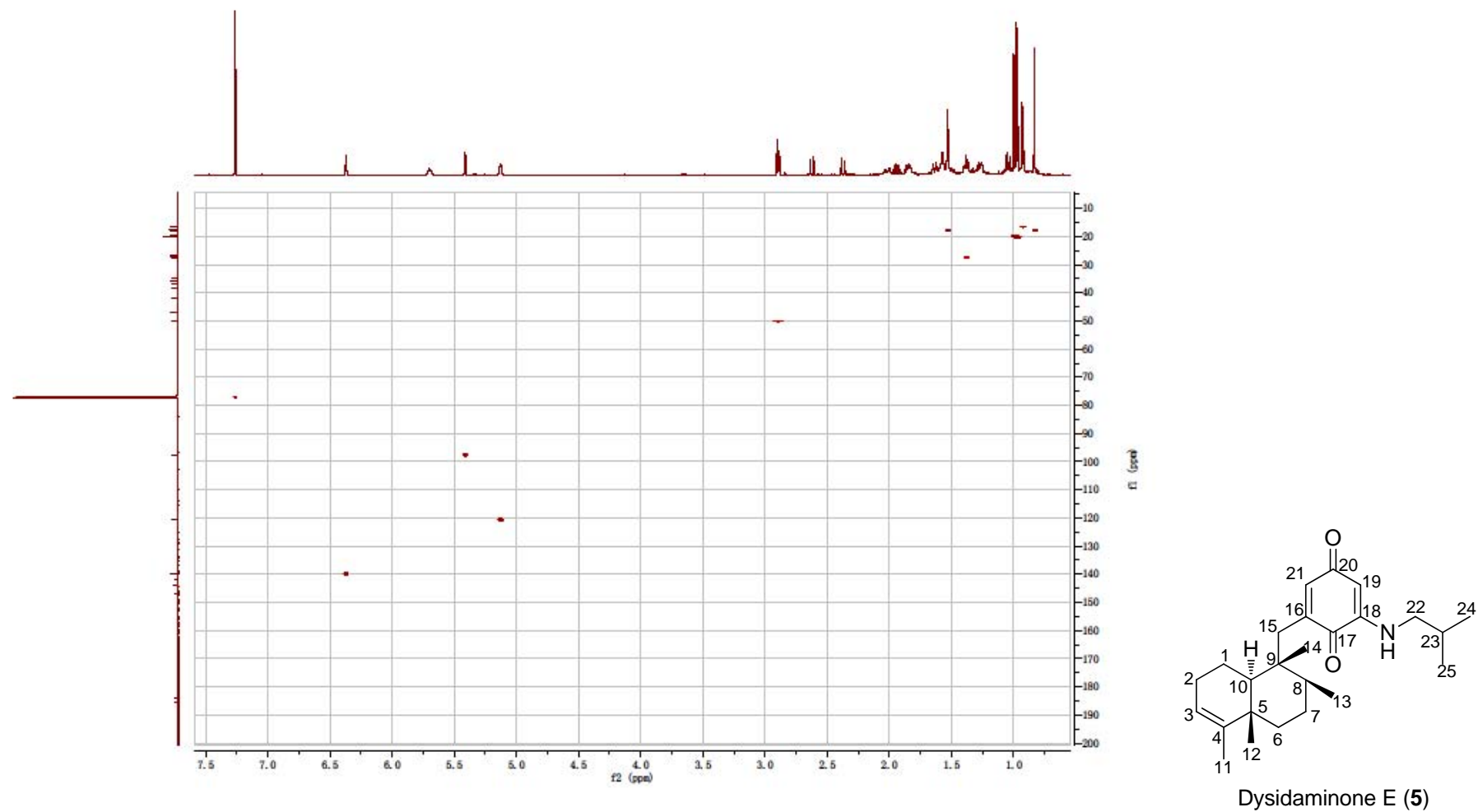


Figure S47. HSQC Spectrum of Dysidaminone E (5) in CDCl₃.

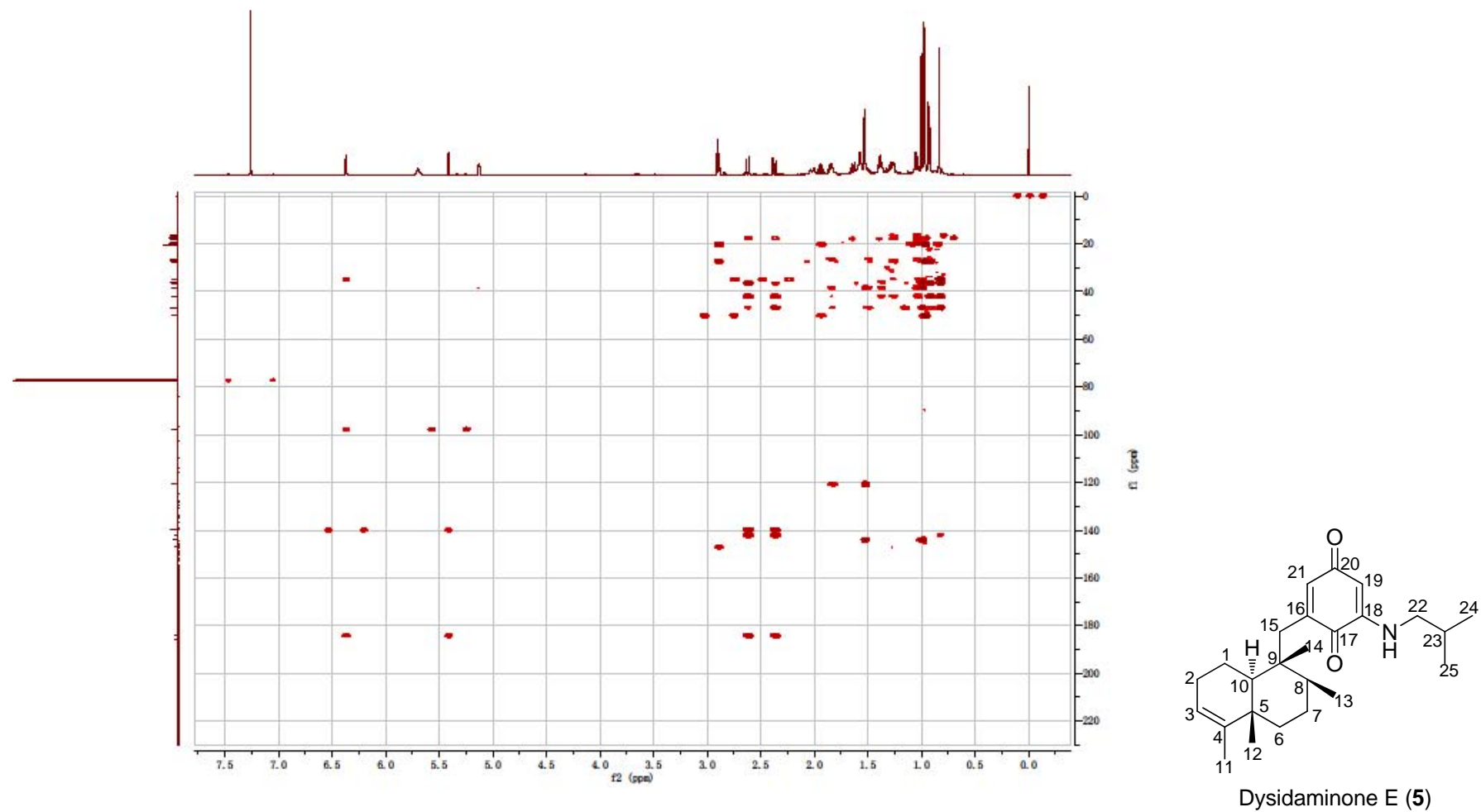
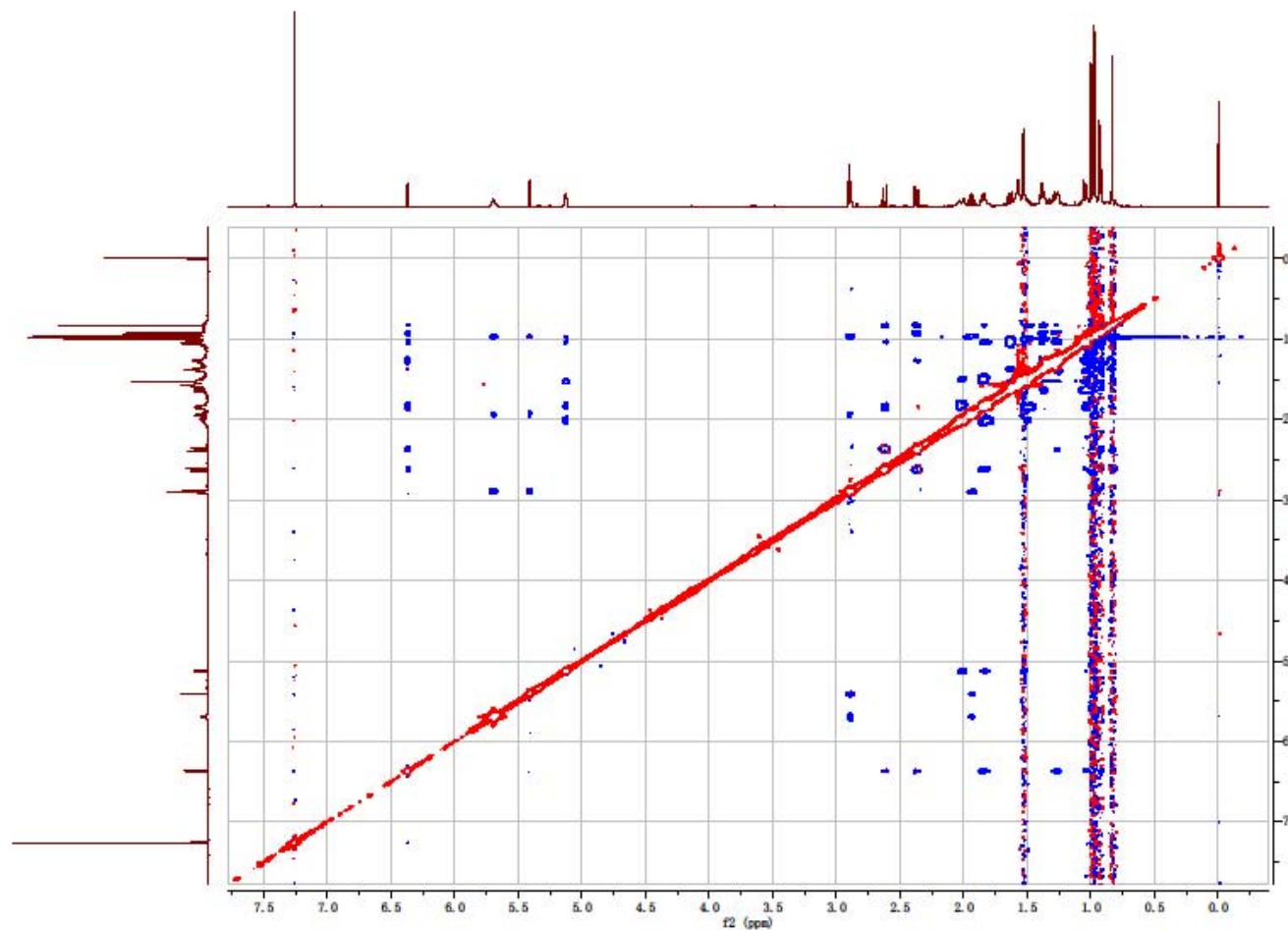
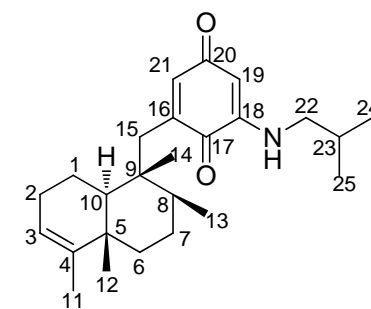


Figure S48. HMBC Spectrum of Dysidaminone E (**5**) in CDCl₃.



f1 (ppm)



Dysidaminone E (5)

Figure S49. NOESY Spectrum of Dysidaminone E (5) in CDCl₃.

Elemental Composition Report

Page 1

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 10-30 H: 10-40 N: 1-1 O: 1-4

SIPI

XT-28 M.W=383

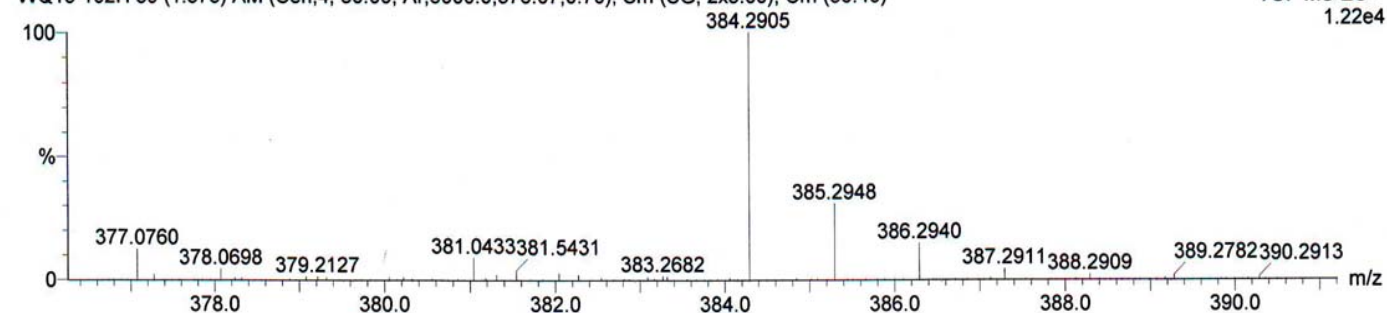
WQ13-102H 39 (1.373) AM (Cen,4, 80.00, Ar,5000.0,376.07,0.70); Sm (SG, 2x3.00); Cm (30:40)

Q-ToF micro

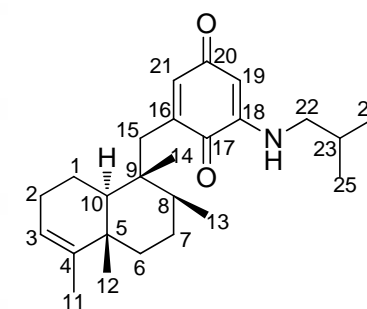
YA019

30-Apr-2013,15:05:58

TOF MS ES+
1.22e4



Minimum:	40.00								
Maximum:	100.00		5.0	5.0	-1.5				
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula		
384.2905	100.00	384.2903	0.2	0.5	7.5	439.1	C25 H38 N O2		



Dysidaminone E (5)

Figure S50. HRESIMS of Dysidaminone E (5).

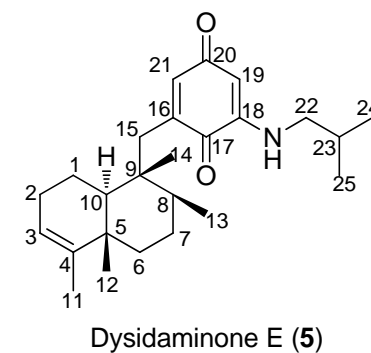
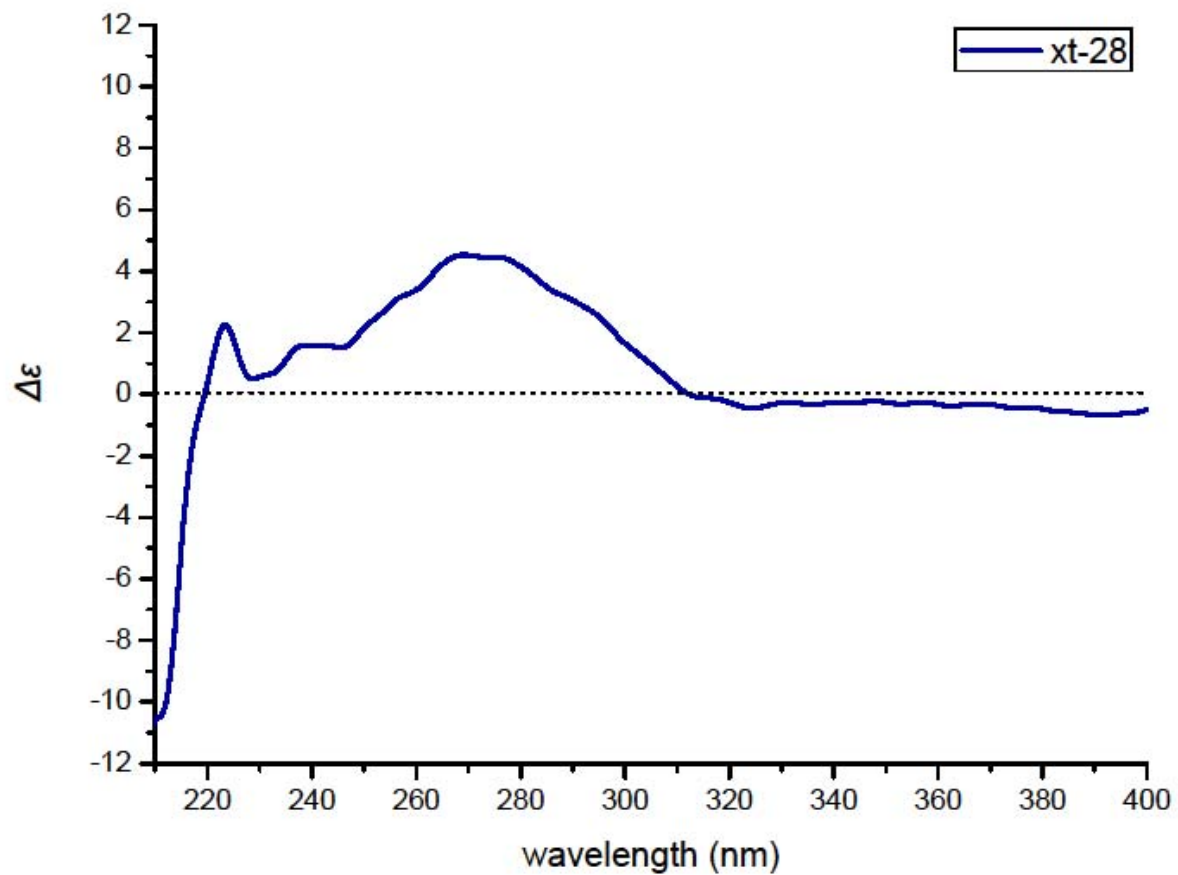


Figure S51. CD Spectrum of Dysidaminone E (**5**) in MeOH.

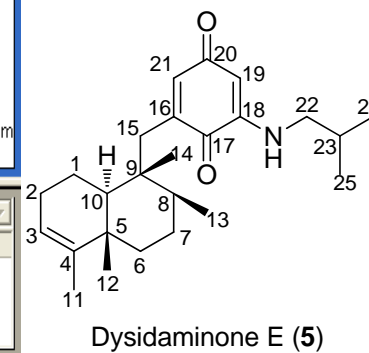
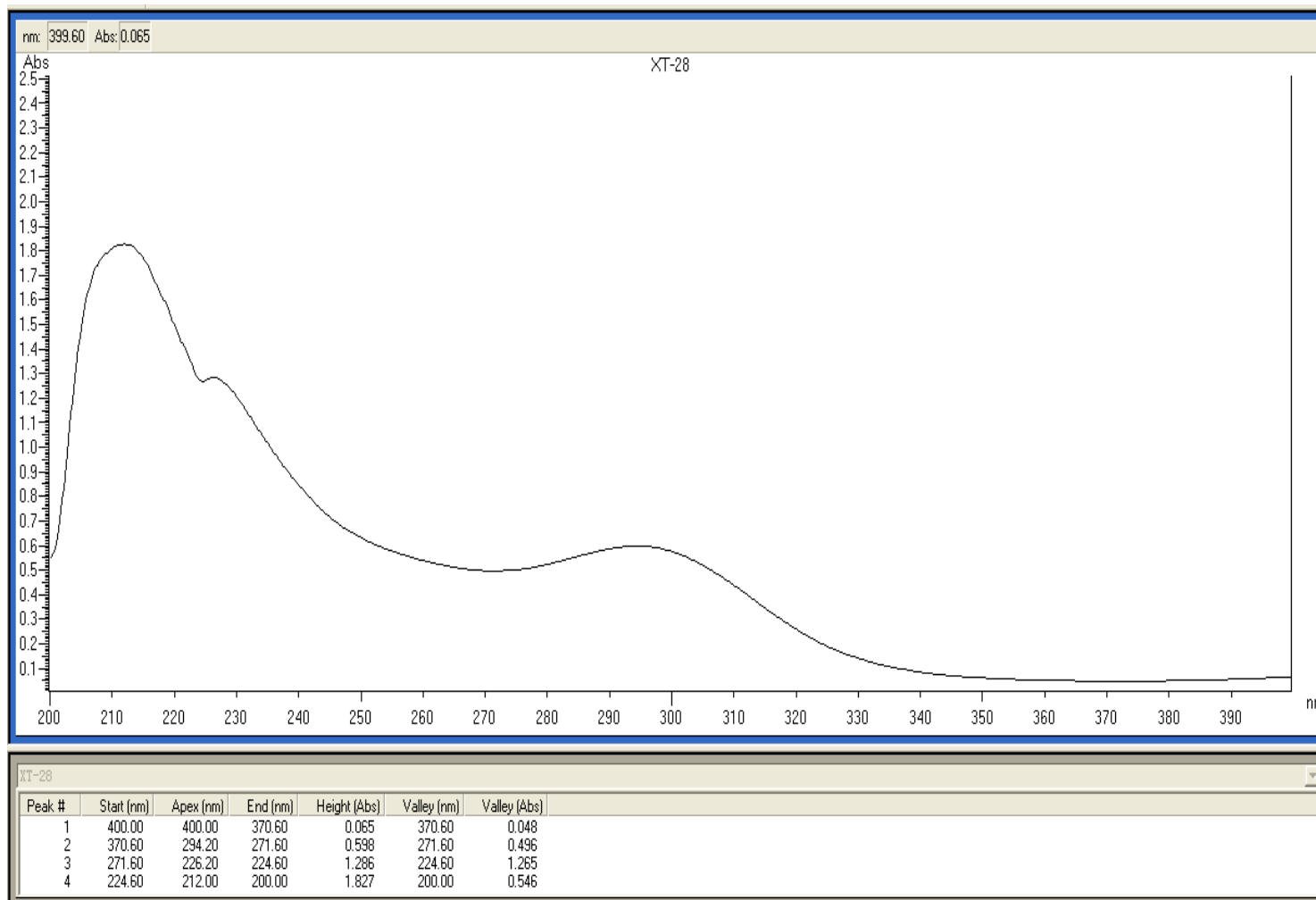


Figure S52. UV Spectrum of Dysidaminone E (5) in MeOH.

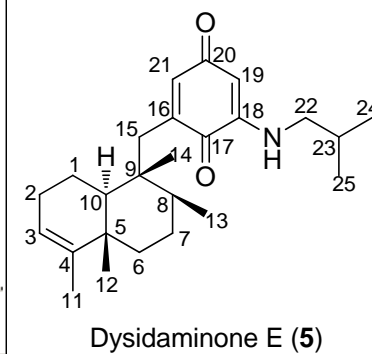
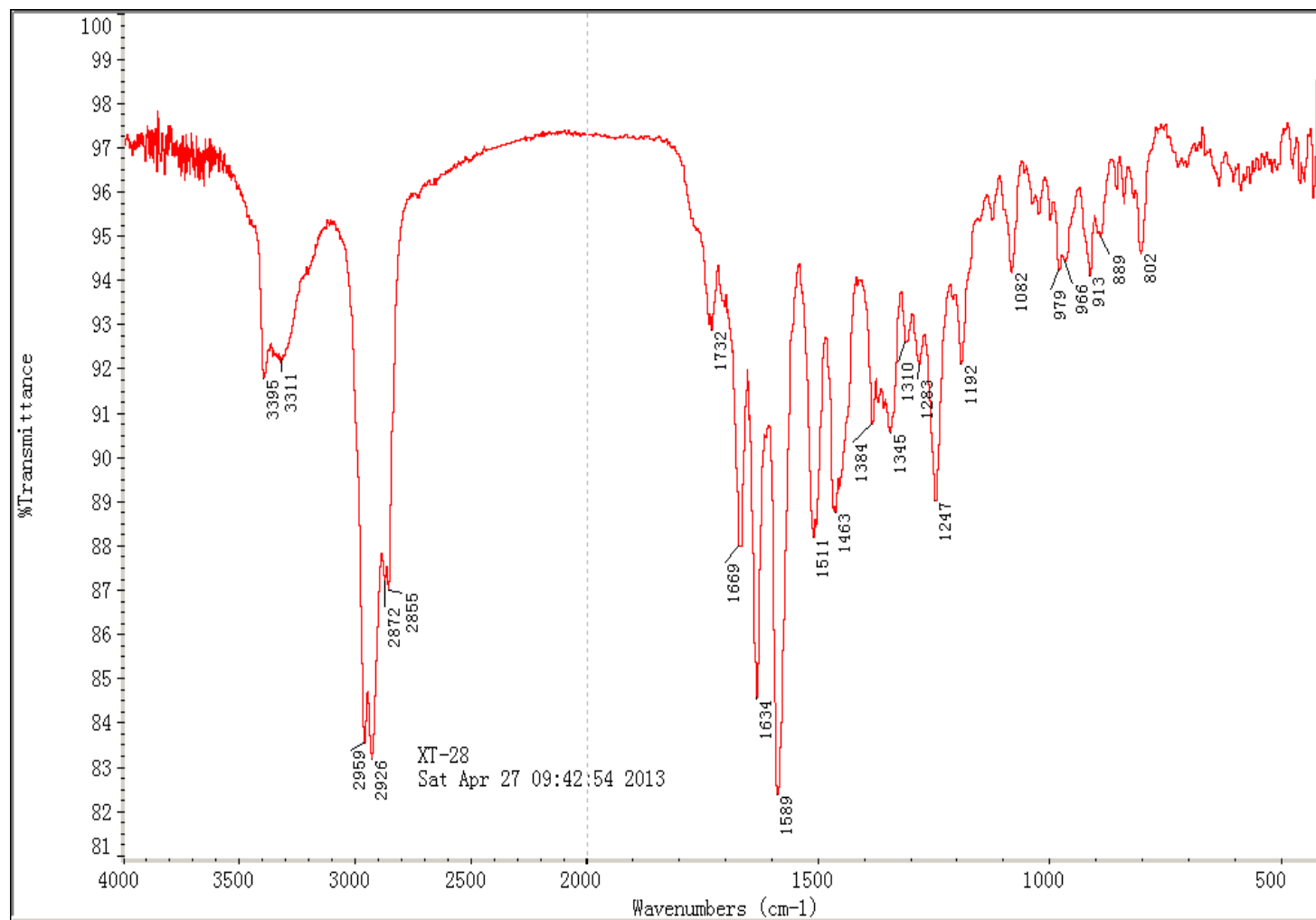
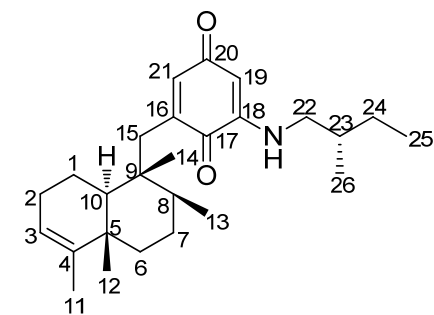
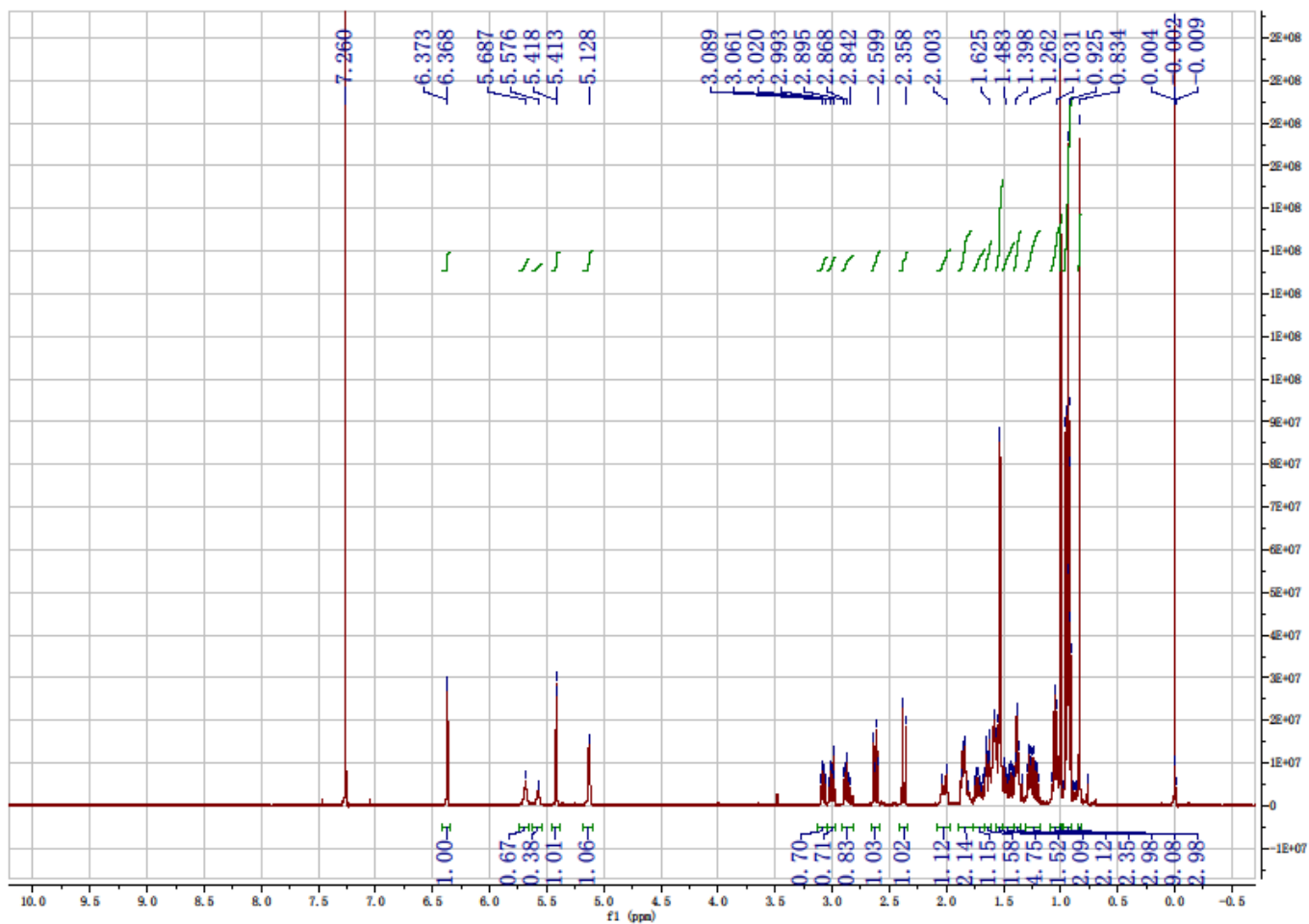


Figure S53. IR Spectrum of Dysidaminone E (5).



Dysidaminone F (6)

Figure S54. ^1H NMR Spectrum of Dysidaminone F (6) in CDCl_3 .

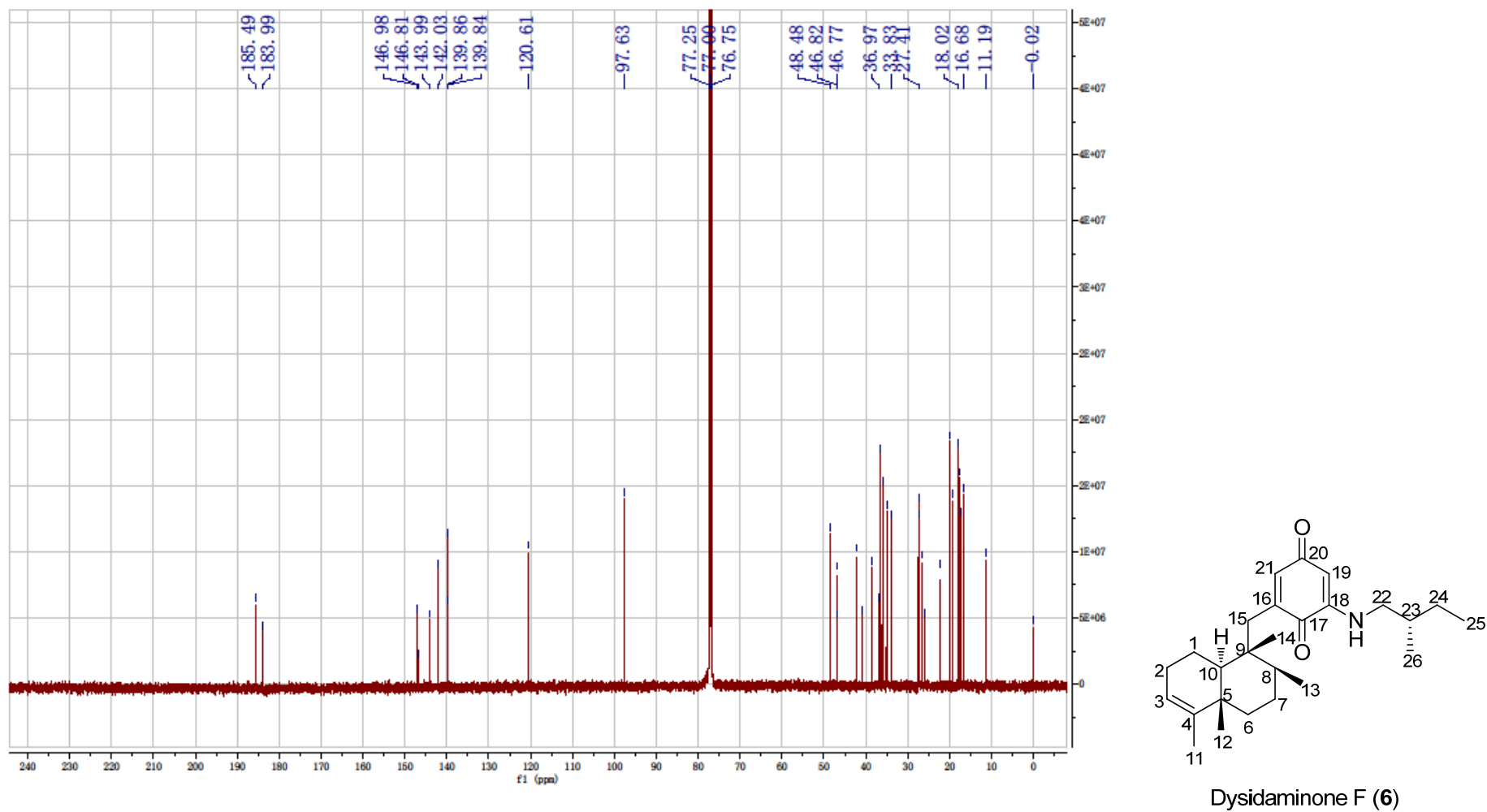


Figure S55. ^{13}C NMR Spectrum of Dysidaminone F (6) in CDCl_3 .

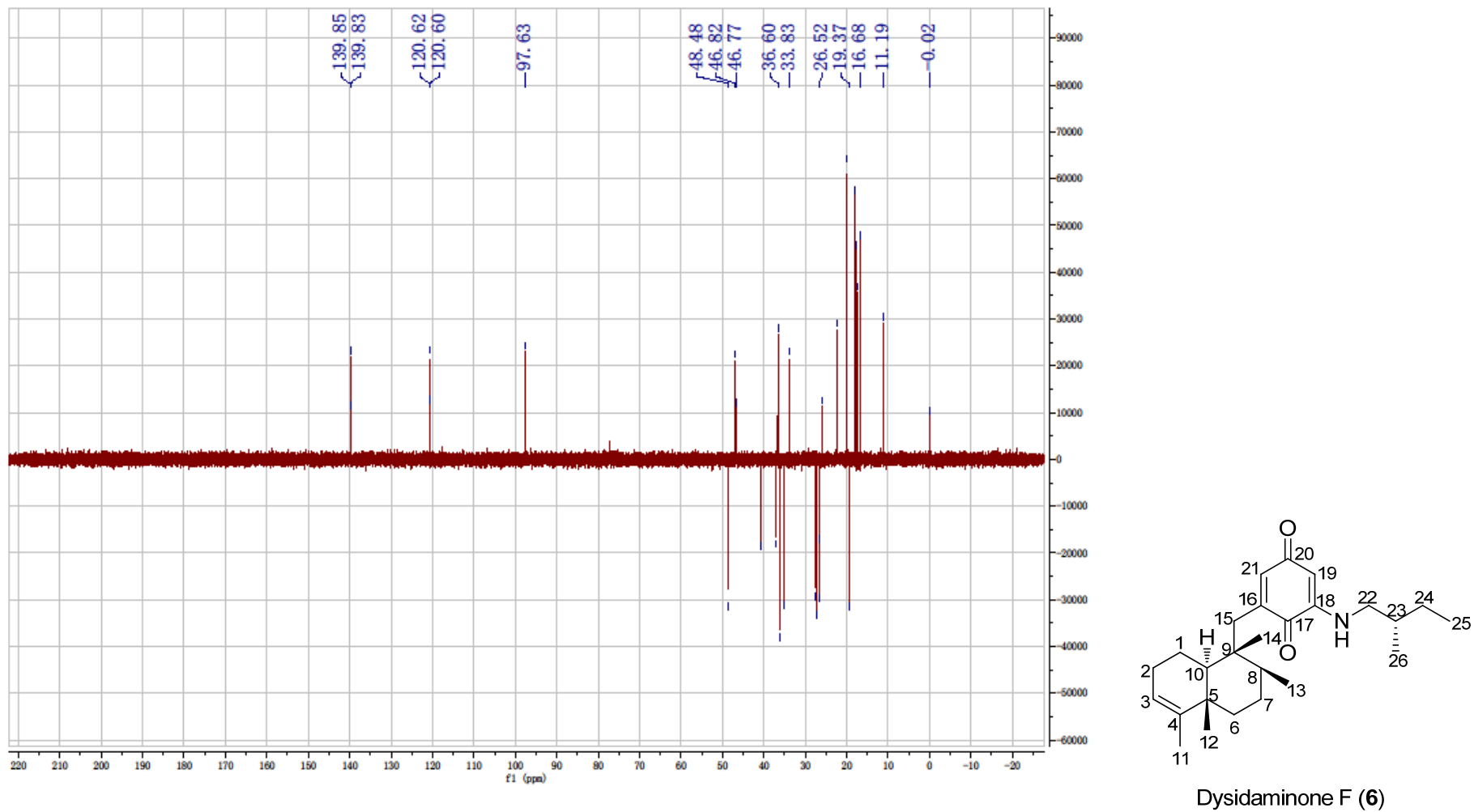


Figure S56. DEPT135 Spectrum of Dysidaminone F (6) in CDCl₃.

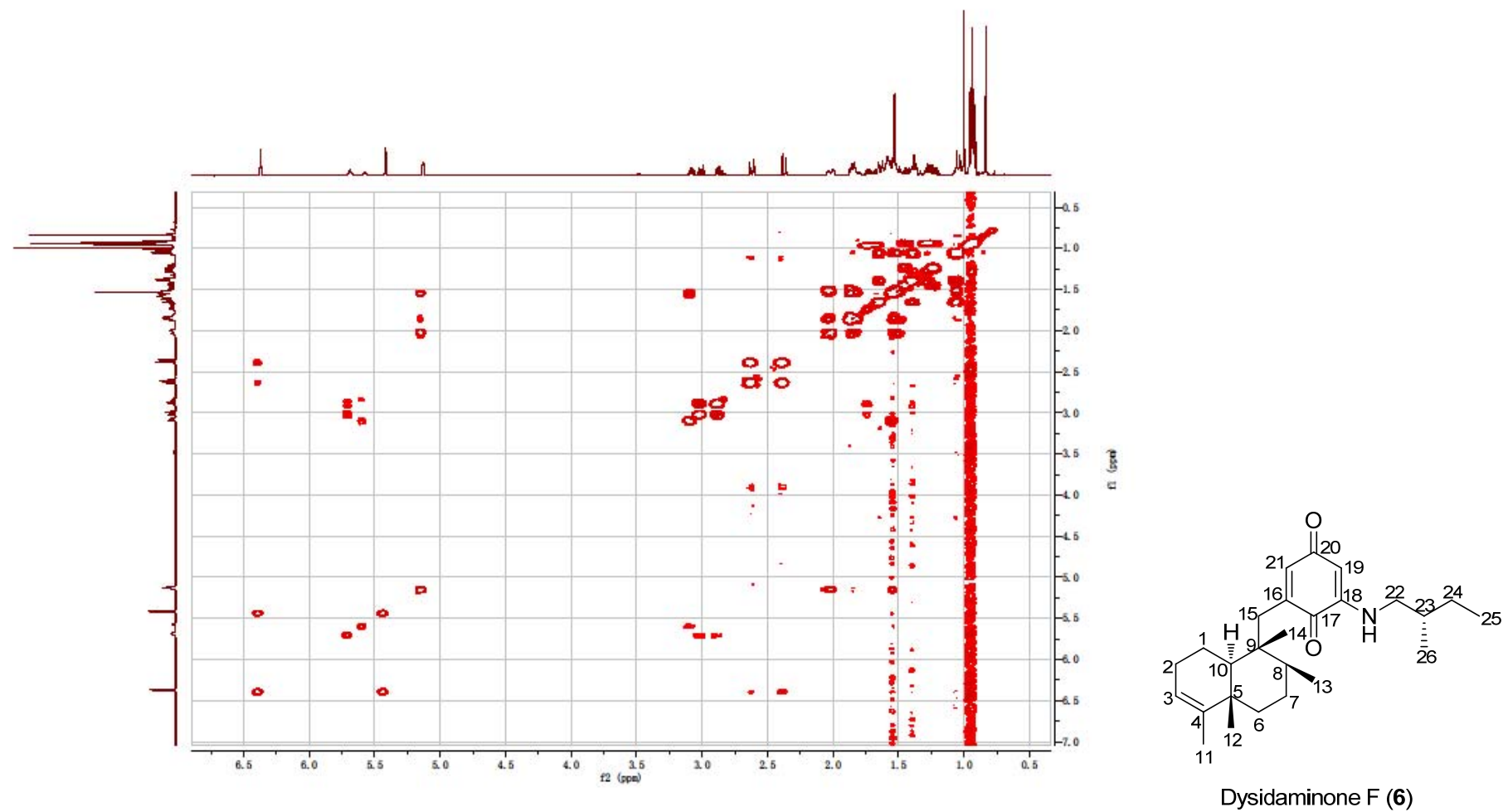


Figure S57. ¹H-¹H COSY Spectrum of Dysidaminone F (**6**) in CDCl₃.

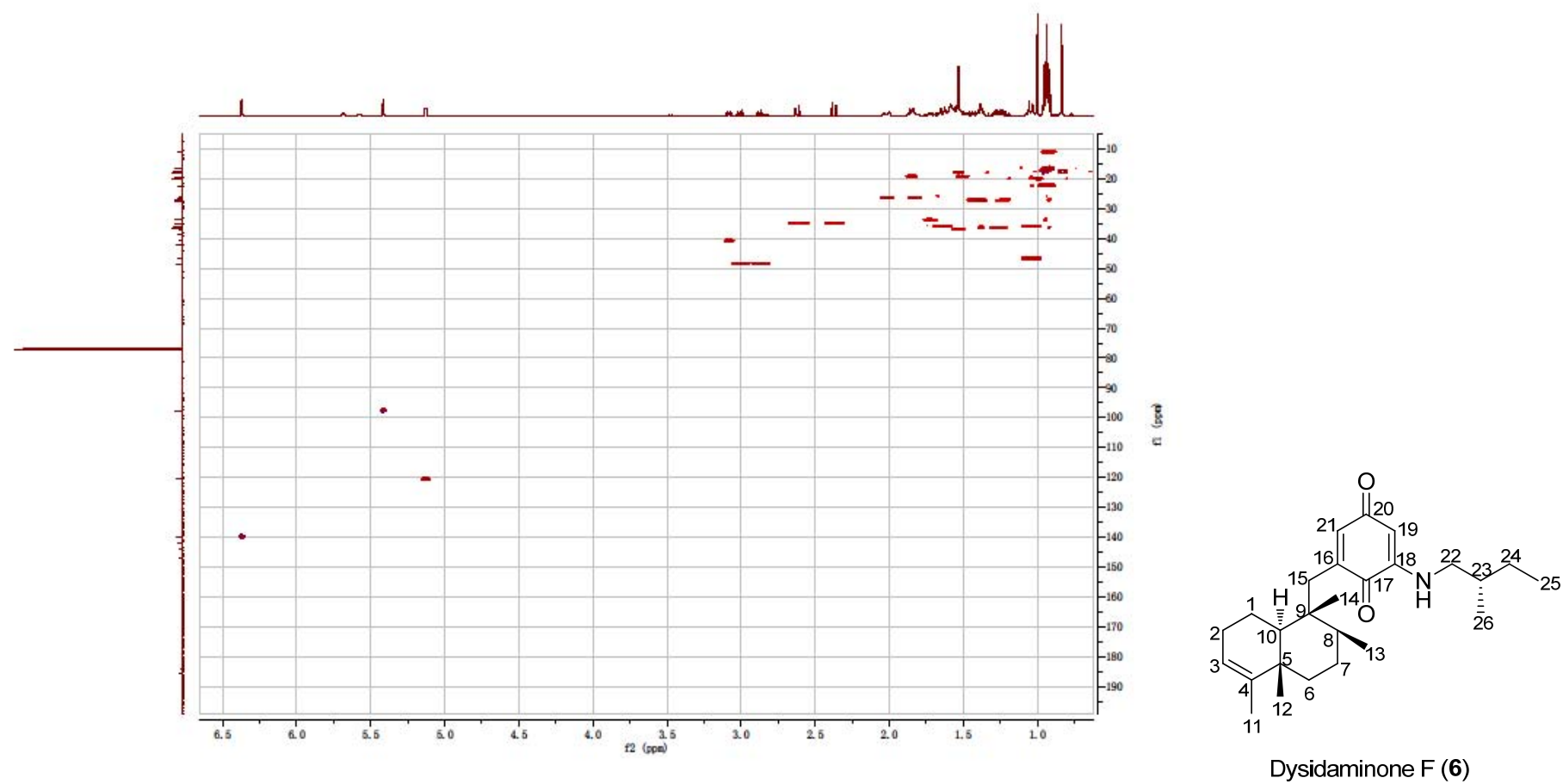


Figure S58. HSQC Spectrum of Dysidaminone F (6) in CDCl₃.

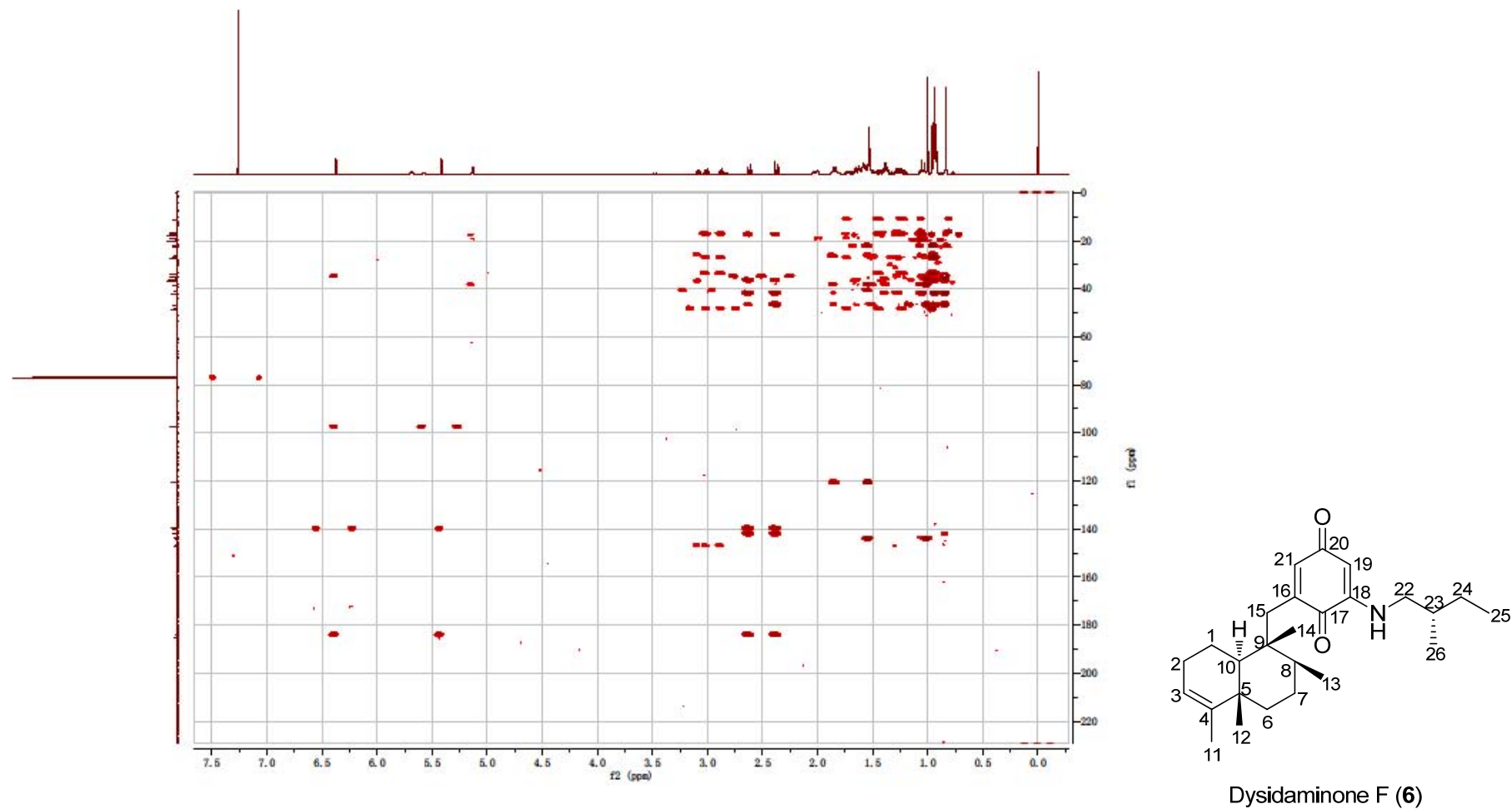


Figure S59. HMBC Spectrum of Dysidaminone F (**6**) in CDCl₃.

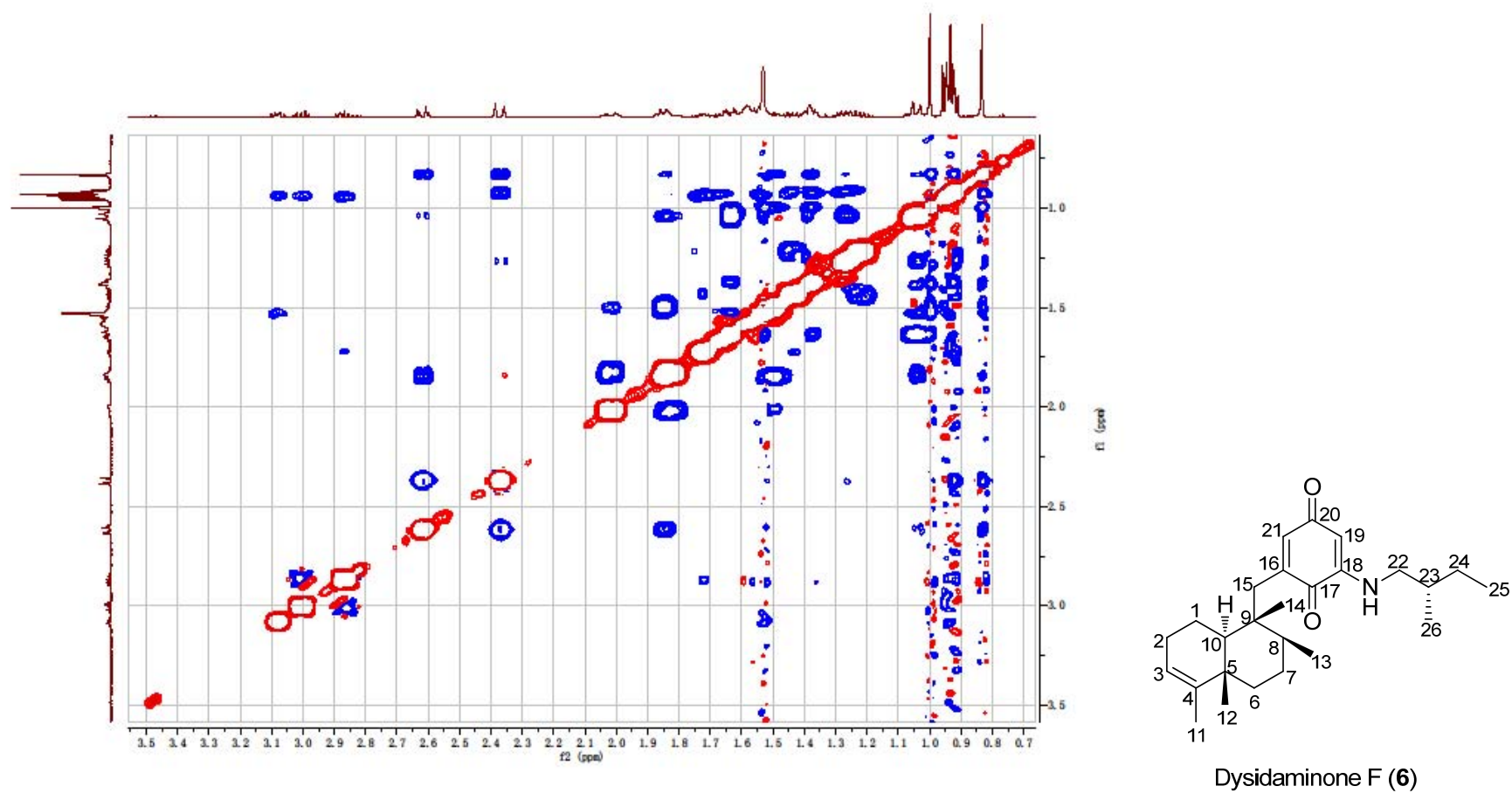


Figure S60. NOESY Spectrum of Dysidaminone F (6) in CDCl₃.

Elemental Composition Report

Page 1

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions

6 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 10-30 H: 10-50 N: 1-1 O: 1-2 Na: 1-1

SIPI

XT-31 M.W=397

WQ13-109H1 20 (0.691) AM (Cen,4, 80.00, Ar,5000.0,407.22,0.70); Sm (SG, 2x3.00); Cm (13:20)

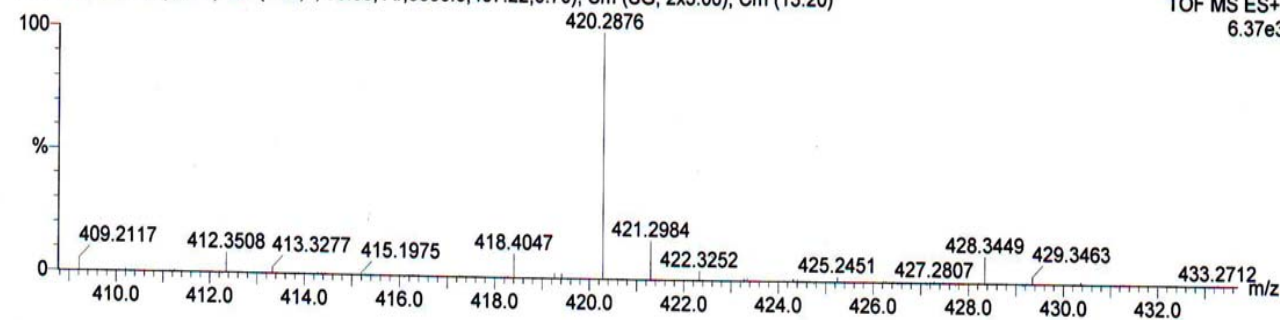
Q-ToF micro

YA019

08-May-2013,14:35:41

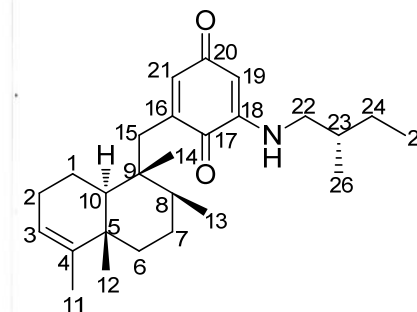
TOF MS ES+

6.37e3



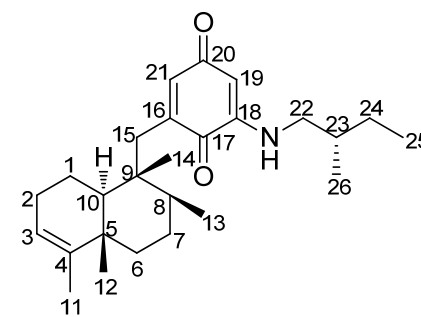
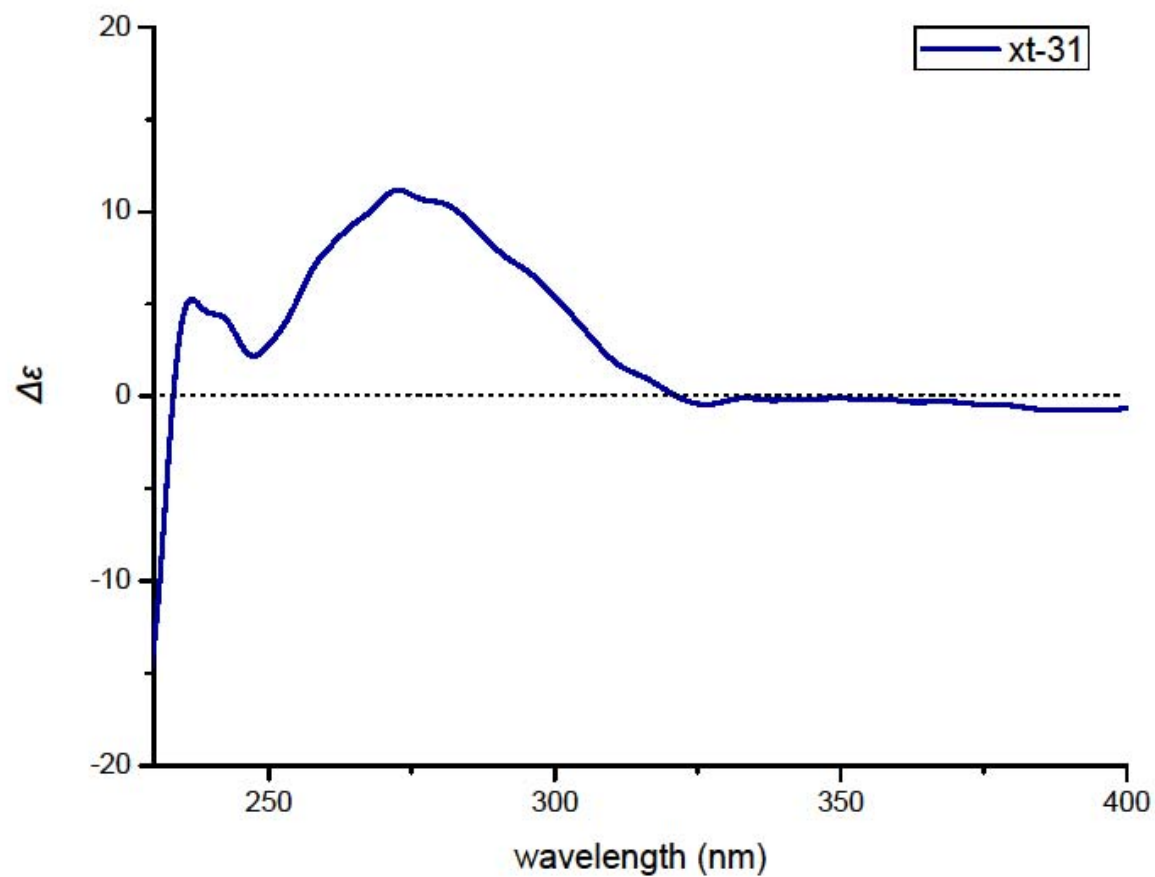
Minimum: 50.00
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
420.2876	100.00	420.2878	-0.2	-0.5	7.5	275.5	C ₂₆ H ₃₉ N O ₂ Na



Dysidaminone F (6)

Figure S61. HRESIMS of Dysidaminone F (6).



Dysidaminone F (6)

Figure S62. CD Spectrum of Dysidaminone F (6) in MeOH.

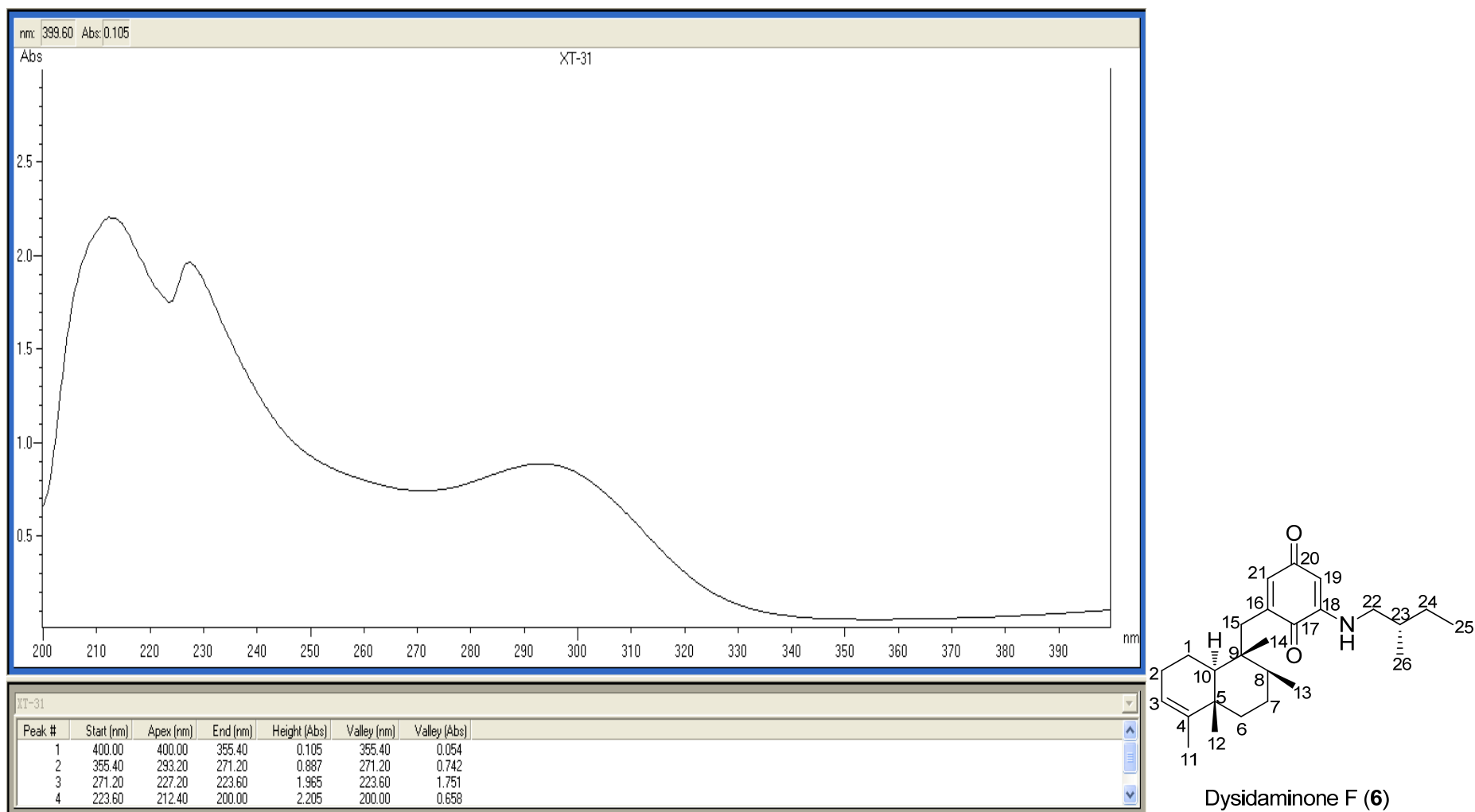


Figure S63. UV Spectrum of Dysidaminone F (6) in MeOH.

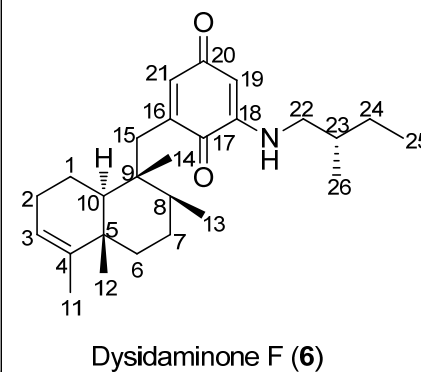
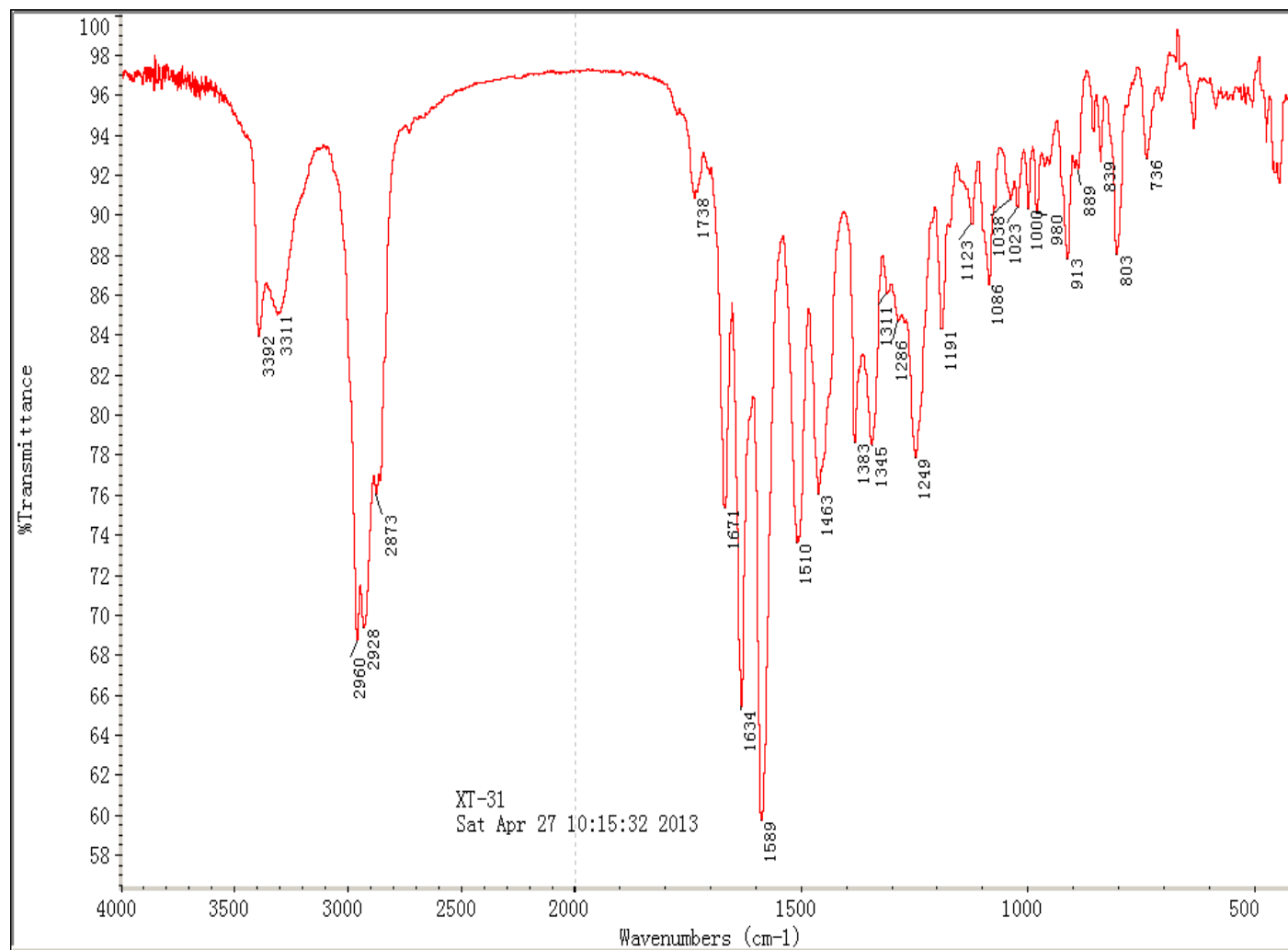
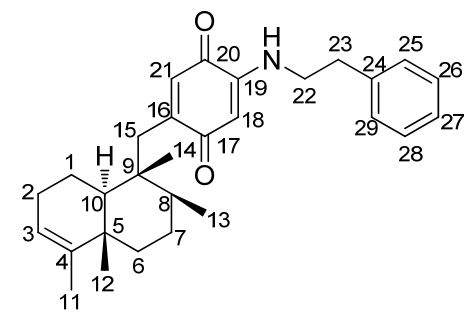
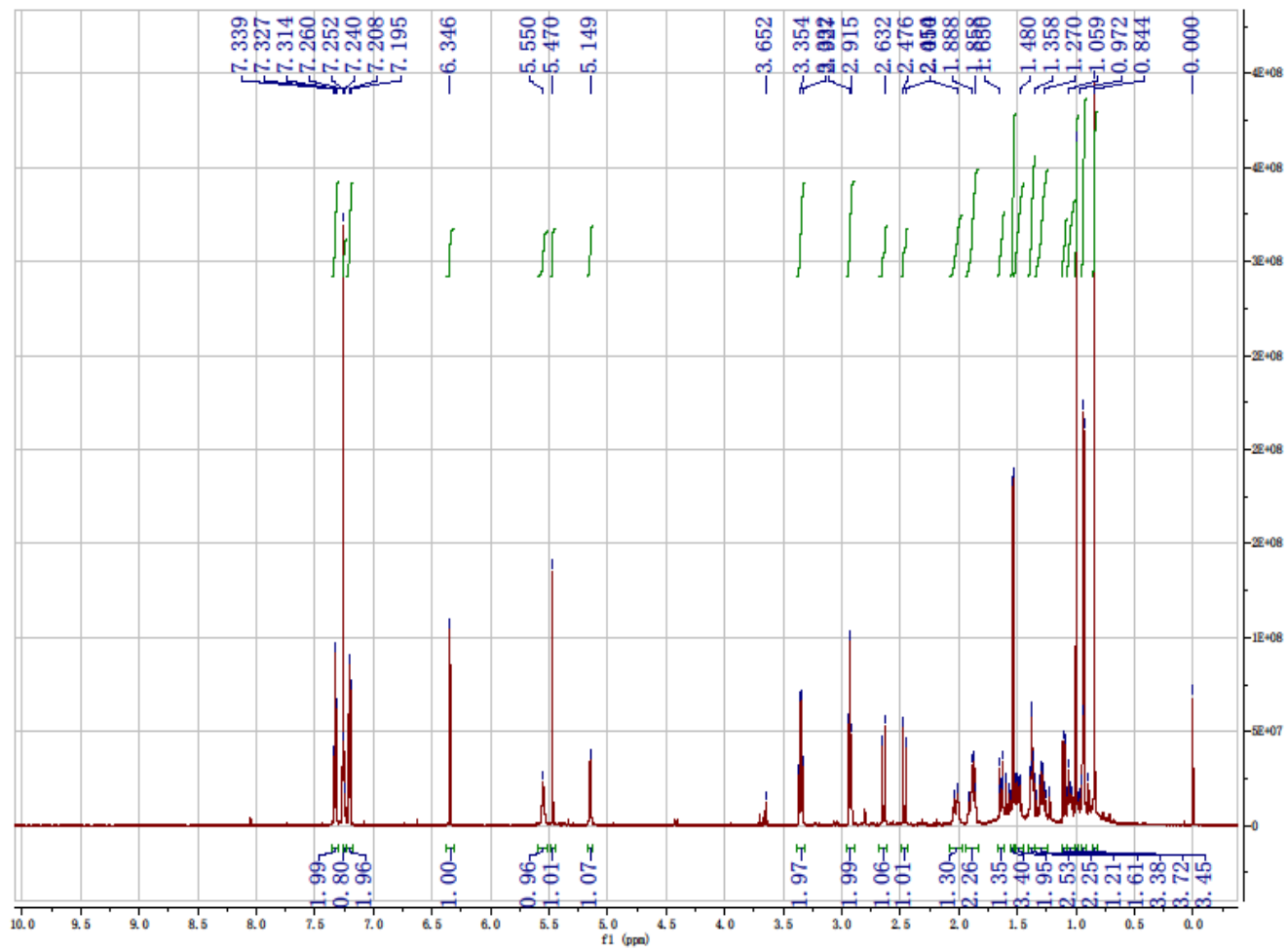
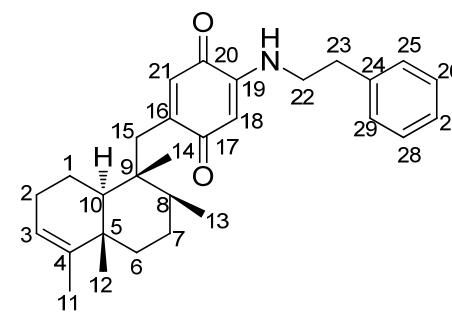
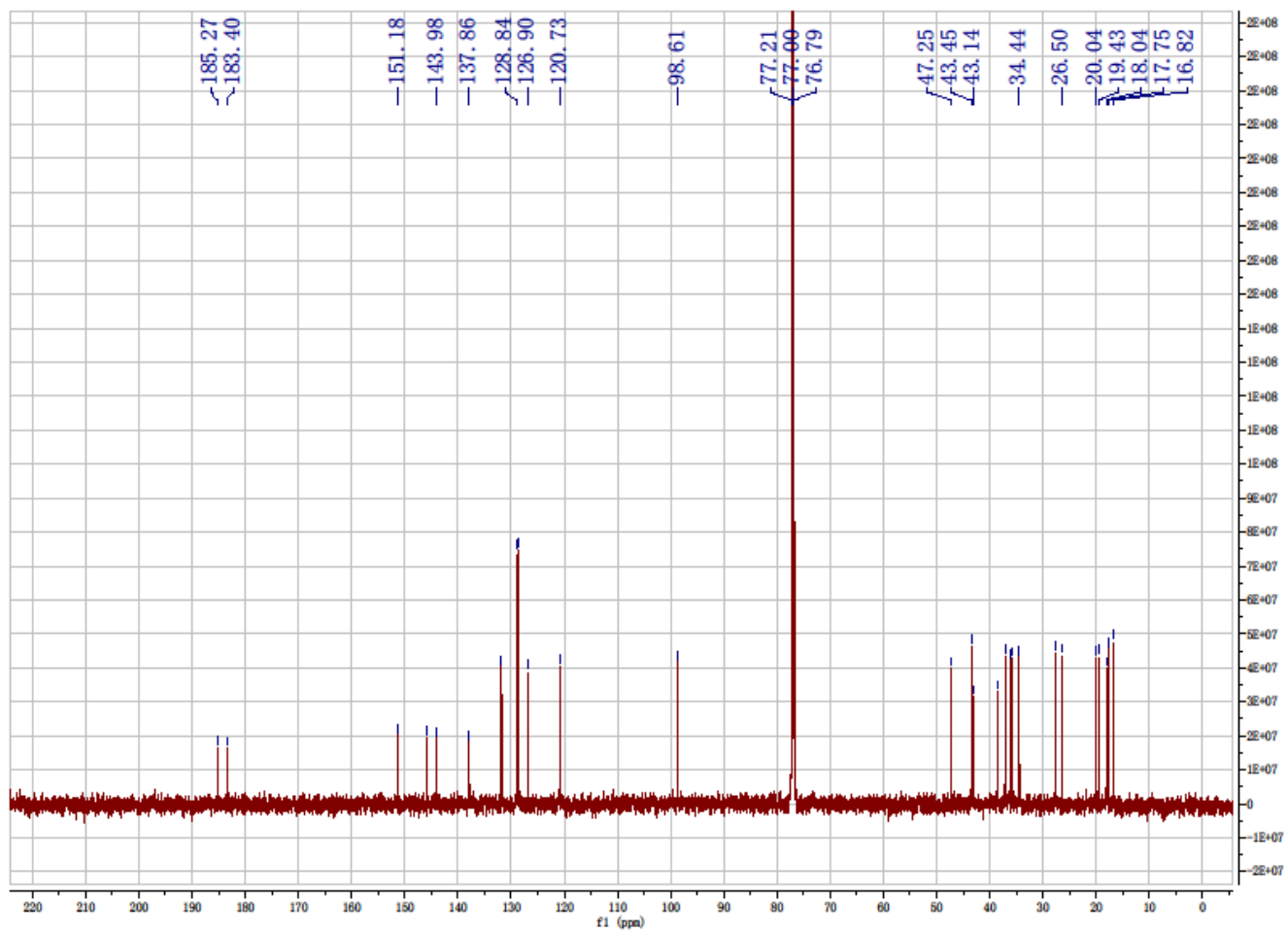


Figure S64. IR Spectrum of Dysidaminone F (6).



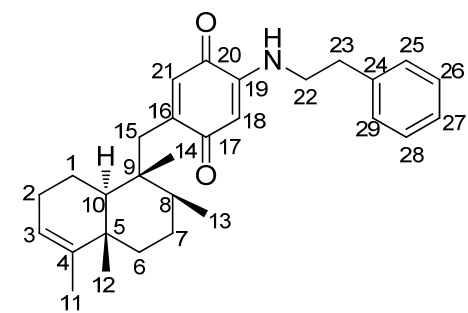
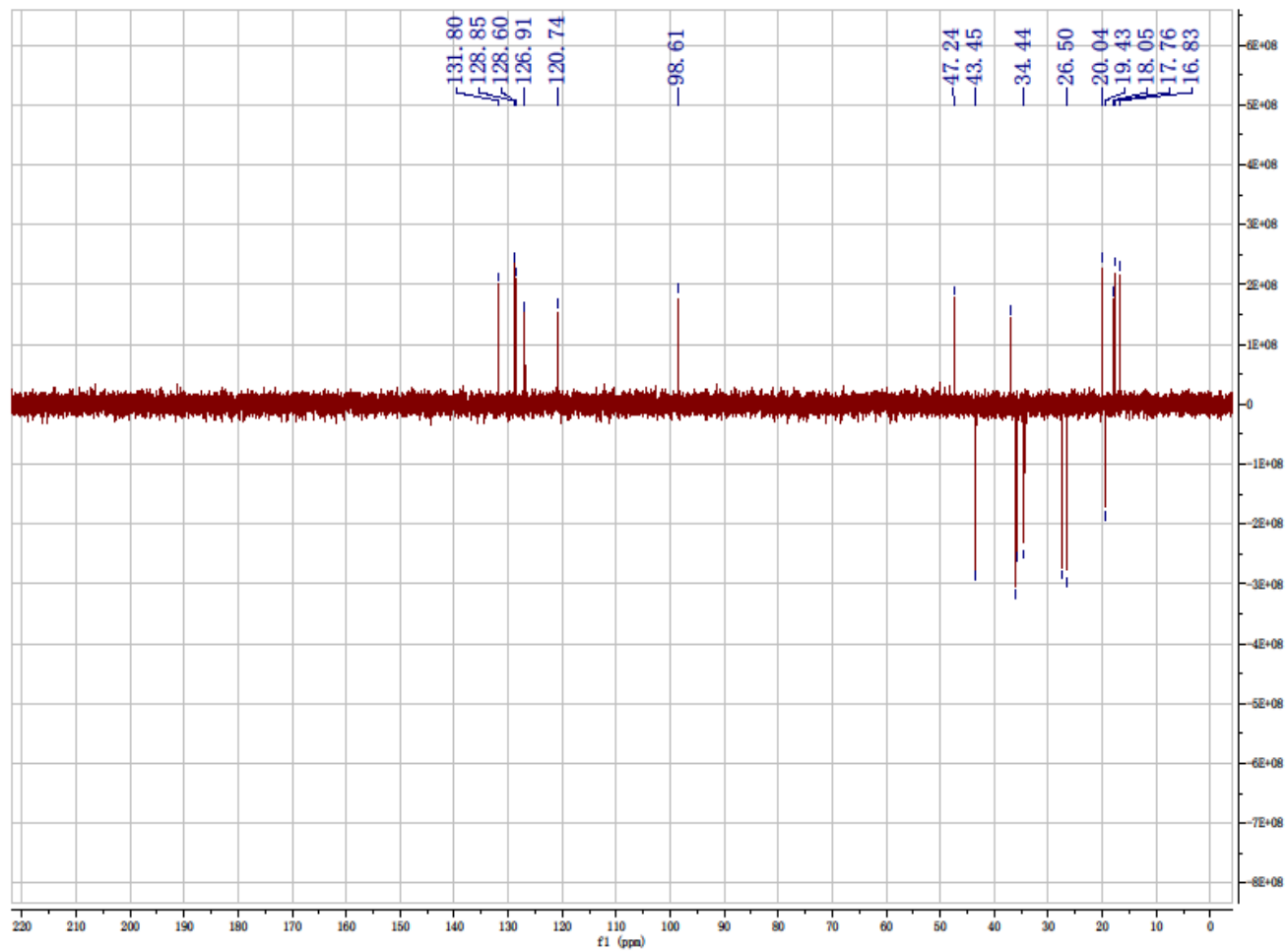
Dysidaminone G (7)

Figure S65. ^1H NMR Spectrum of Dysidaminone G (7) in CDCl_3 .



Dysidaminone G (7)

Figure S66. ^{13}C NMR Spectrum of Dysidaminone G (7) in CDCl_3 .



Dysidaminone G (7)

Figure S67. DEPT135 Spectrum of Dysidaminone G (7) in CDCl₃.

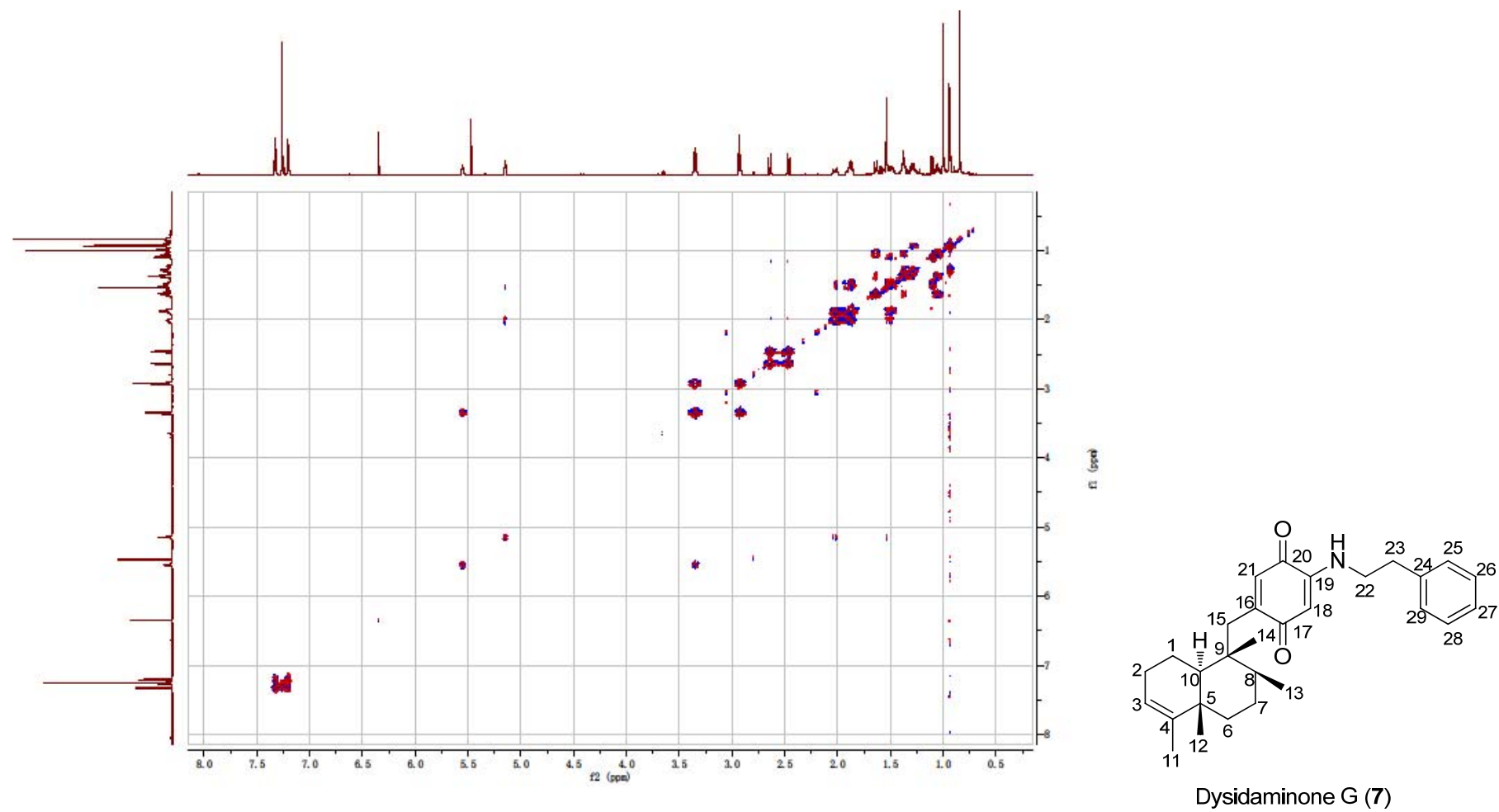


Figure S68. ^1H - ^1H COSY Spectrum of Dysidaminone G (7) in CDCl_3 .

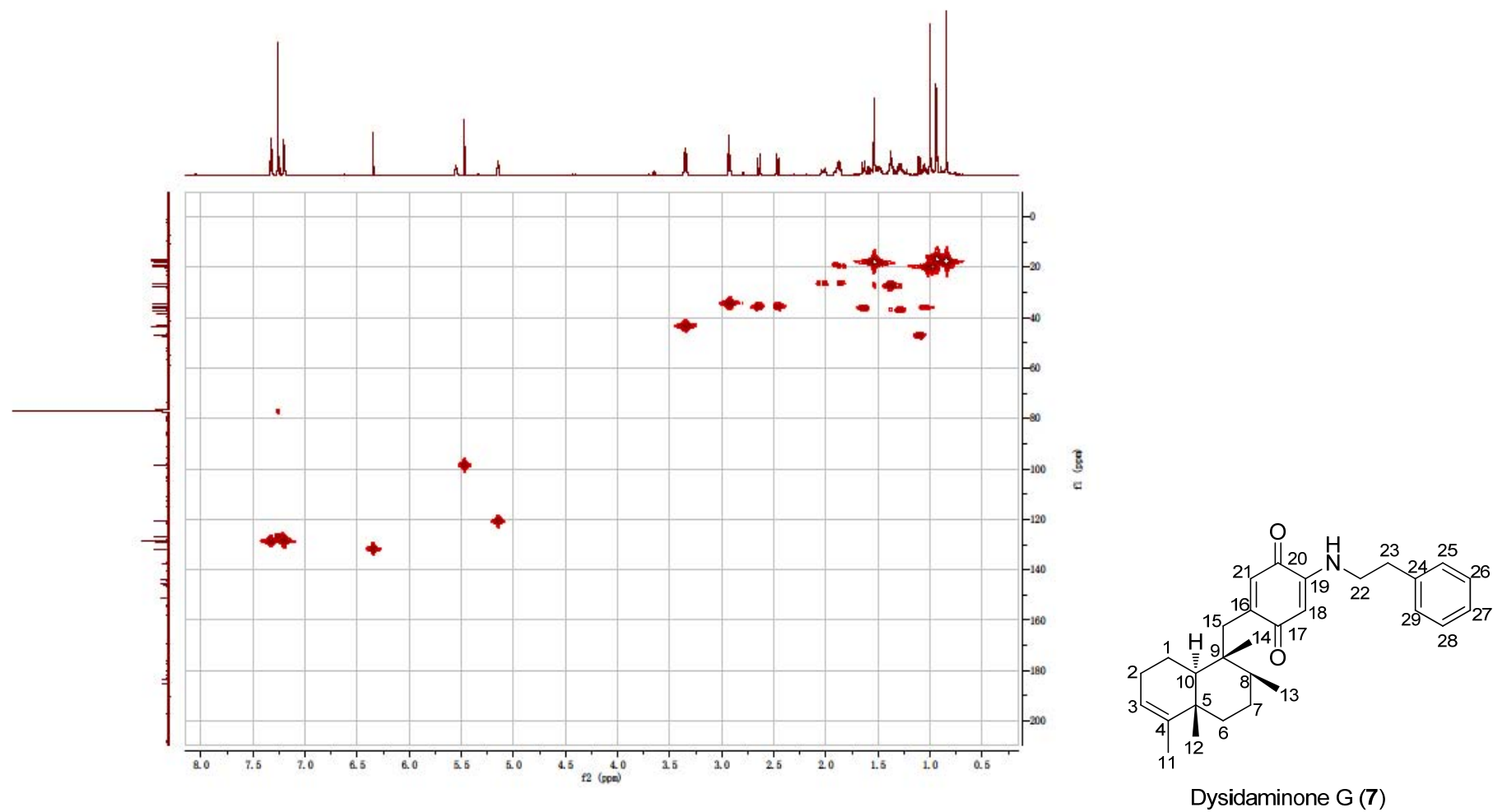


Figure S69. HSQC Spectrum of Dysidaminone G (7) in CDCl₃.

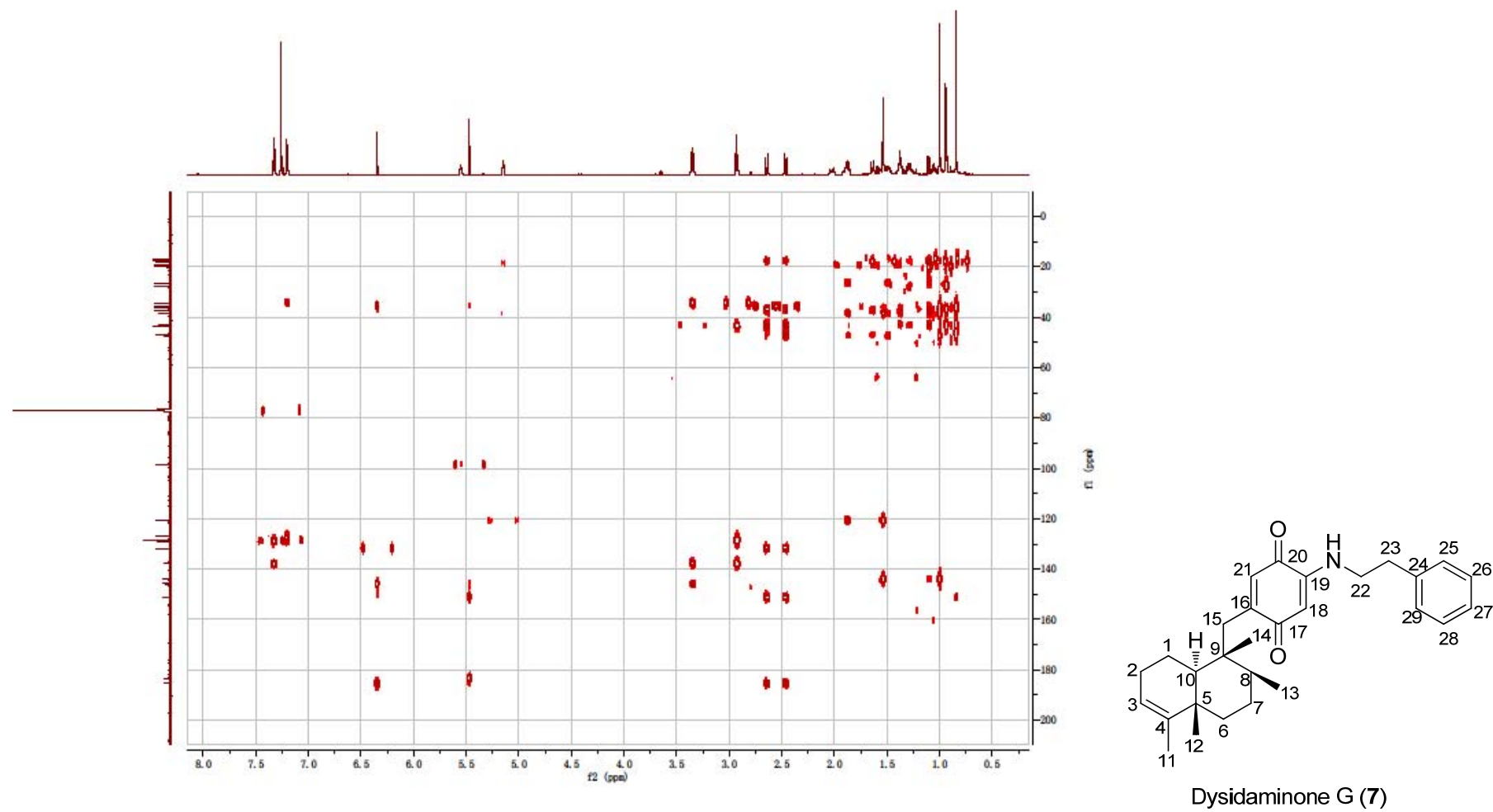


Figure S70. HMBC Spectrum of Dysidaminone G (7) in CDCl₃.

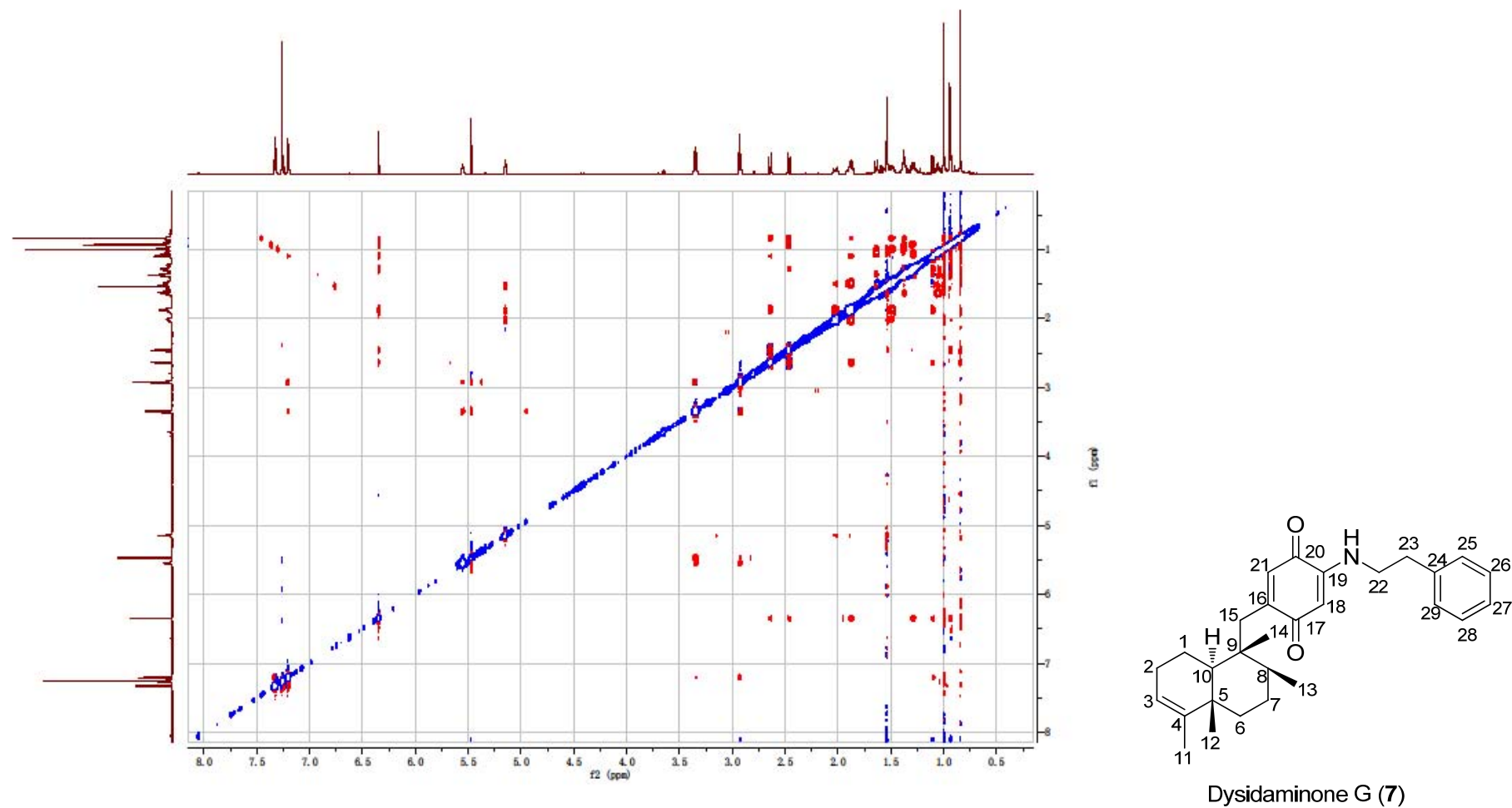


Figure S71. NOESY Spectrum of Dysidaminone G (7) in CDCl₃.

Elemental Composition Report

Page 1

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 10-30 H: 10-40 N: 1-1 O: 1-4

SIPI

XT-30 M.W=431

WQ13-099H 31 (1.070) AM (Cen,4, 80.00, Ar,5000.0,425.05,0.70); Sm (SG, 2x3.00); Cm (23:33)

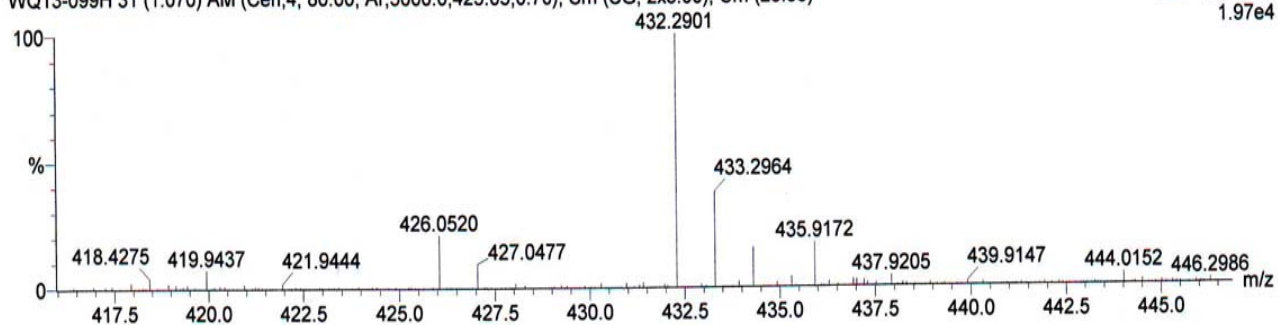
Q-ToF micro

YA019

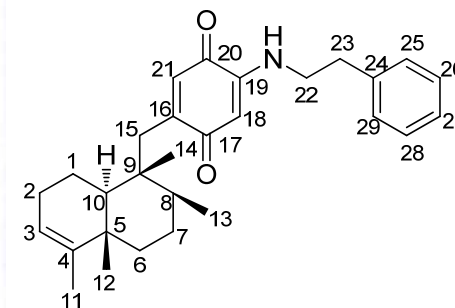
432.2901

30-Apr-2013,13:57:38

TOF MS ES+
1.97e4



Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
432.2901	100.00	432.2903	-0.2	-0.5	11.5	615.0	C ₂₉ H ₃₈ N O ₂



Dysidaminone G (7)

Figure S72. HRESIMS of Dysidaminone G (7).

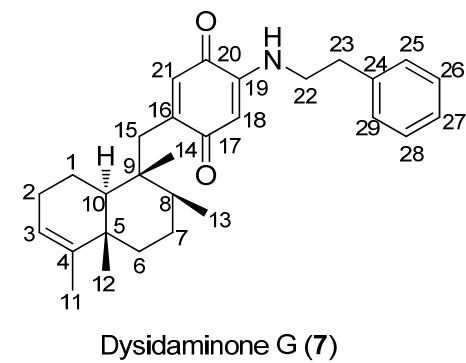
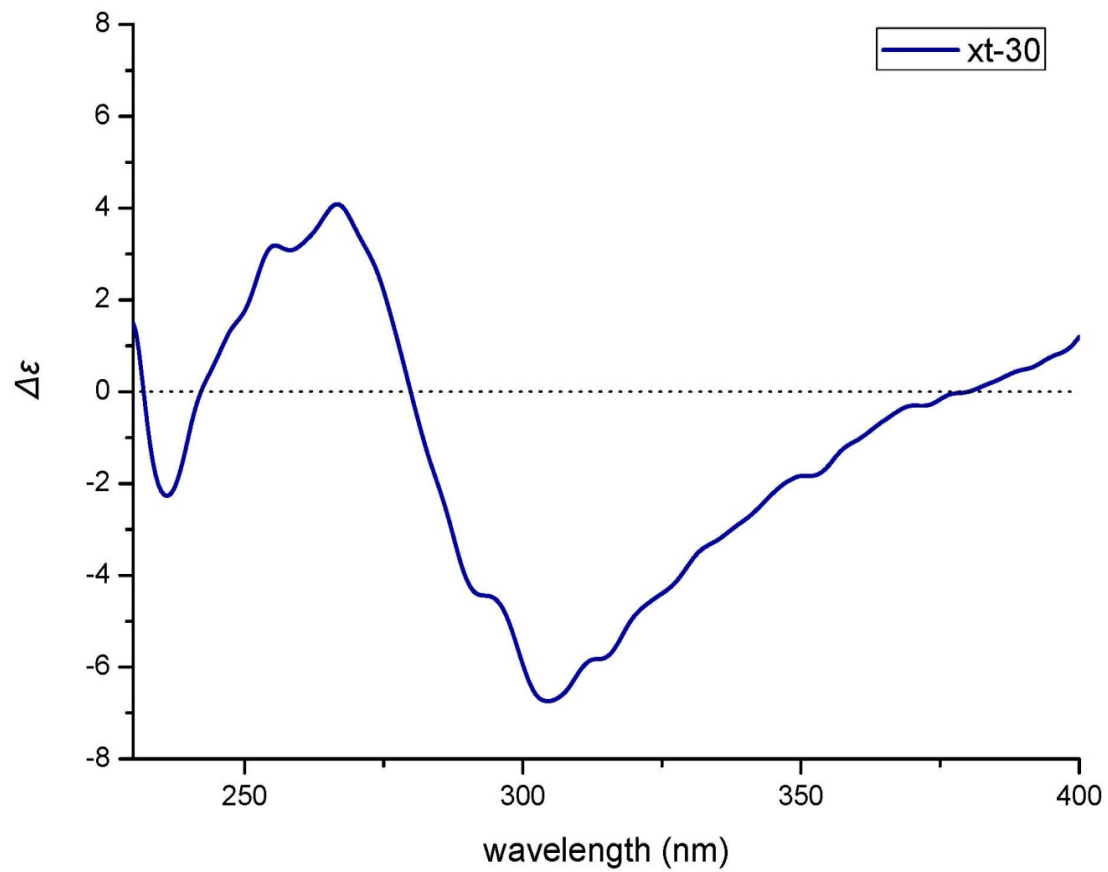


Figure S73. CD Spectrum of Dysidaminone G (7) in MeOH.

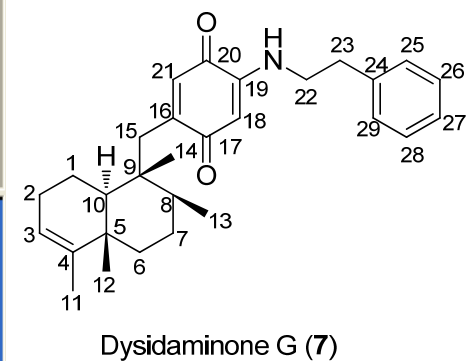
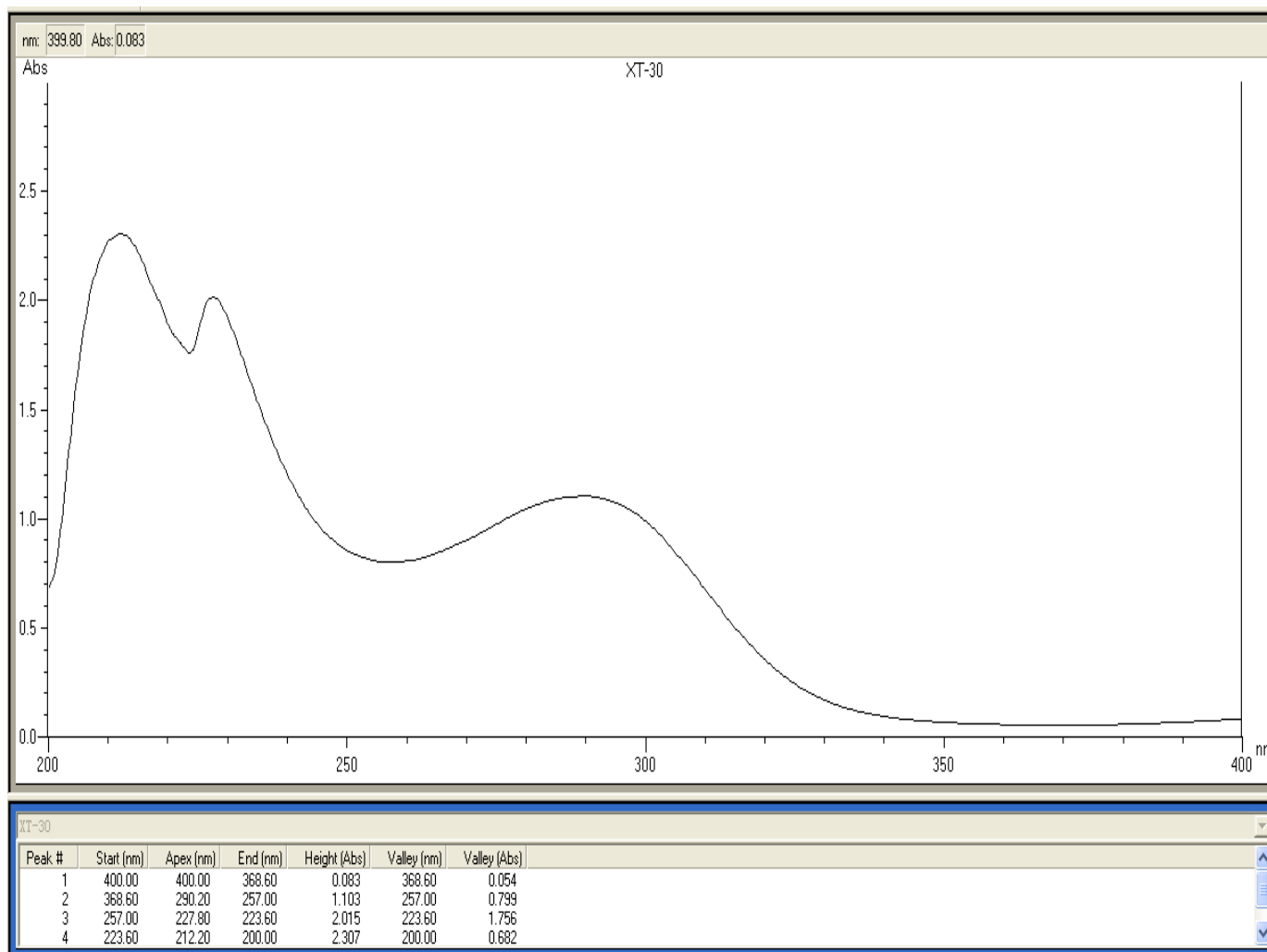


Figure S74. UV Spectrum of Dysidaminone G (7) in MeOH.

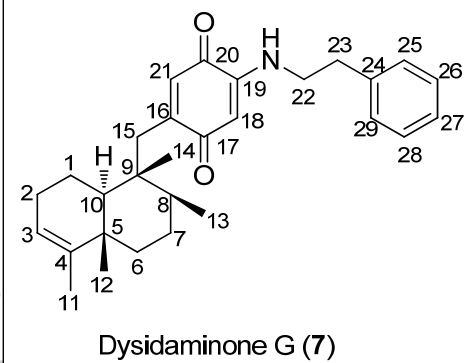
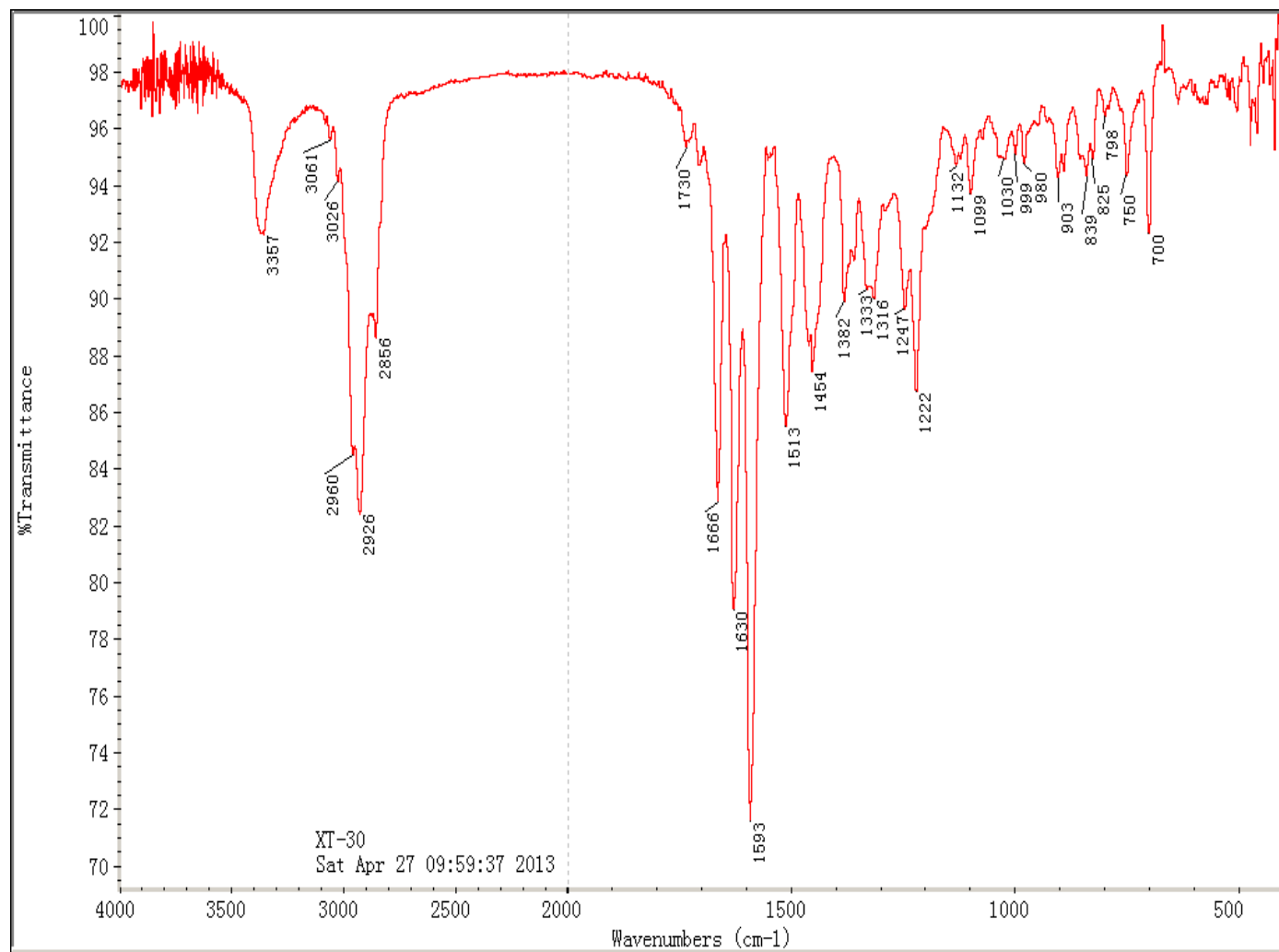


Figure S75. IR Spectrum of Dysidaminone G (7).

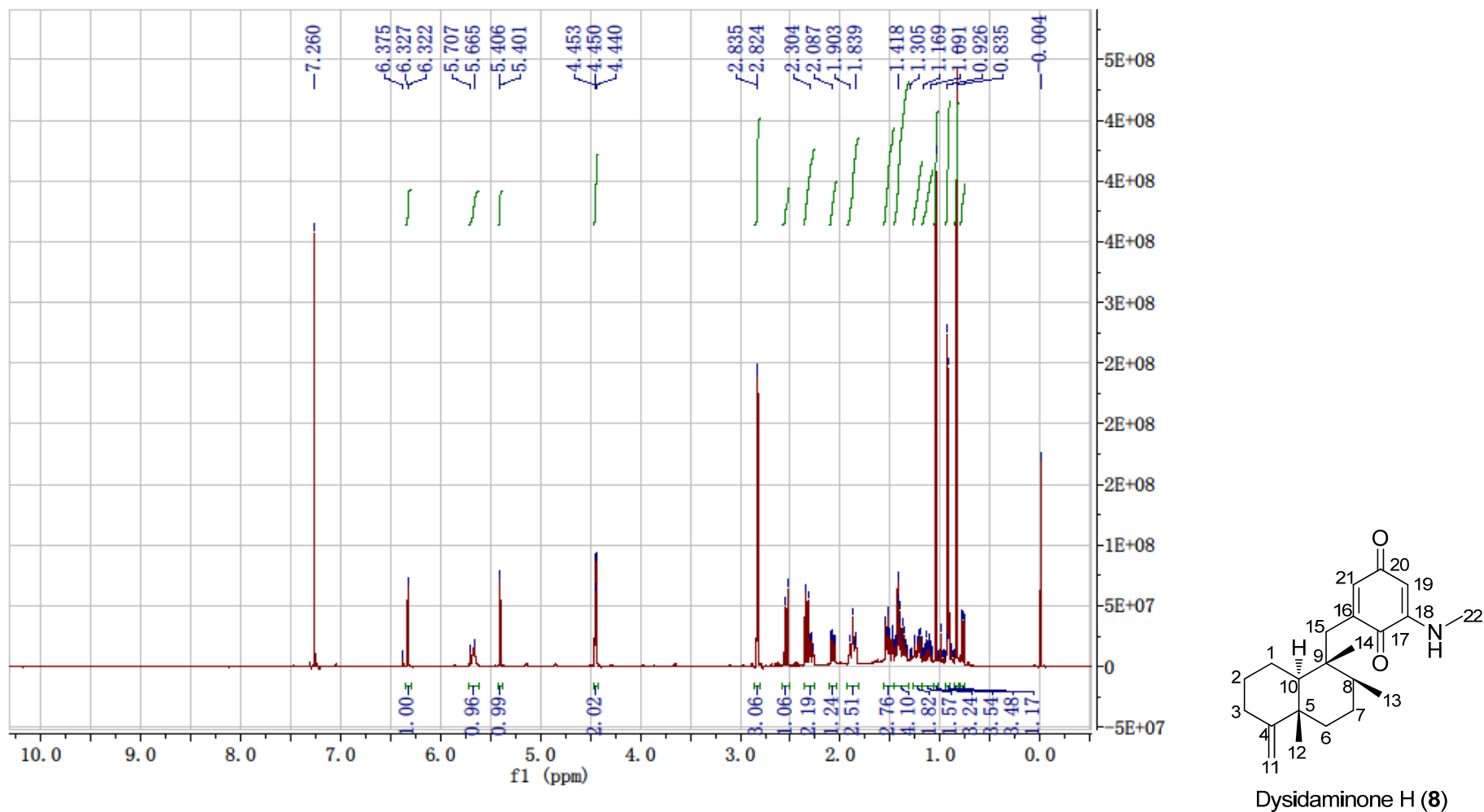


Figure S76. ¹H NMR Spectrum of Dysidaminone H (8) in CDCl₃.

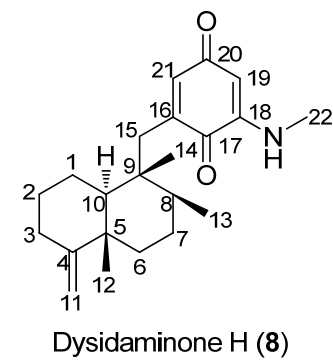
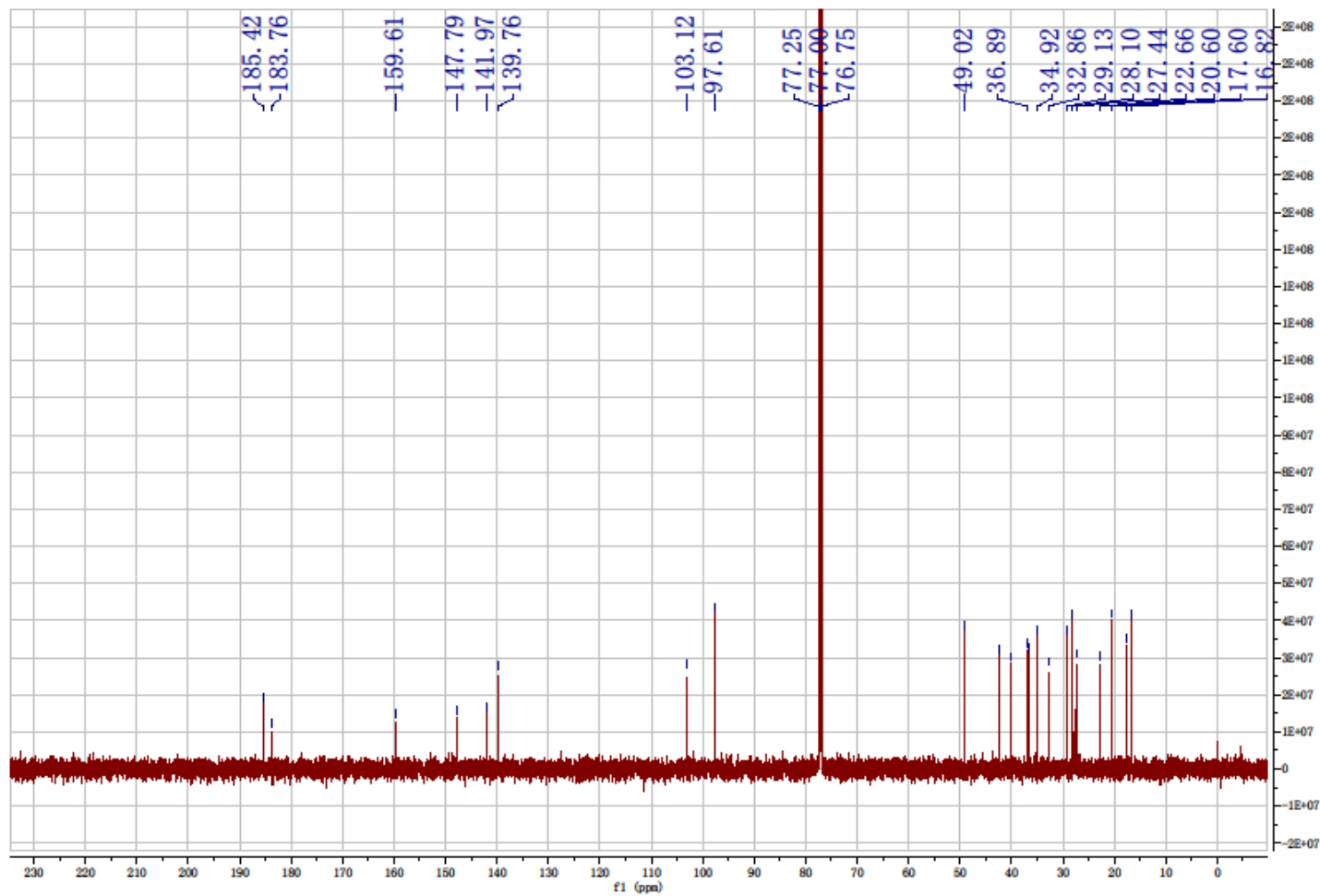


Figure S77. ^{13}C NMR Spectrum of Dysidaminone H (8) in CDCl_3 .

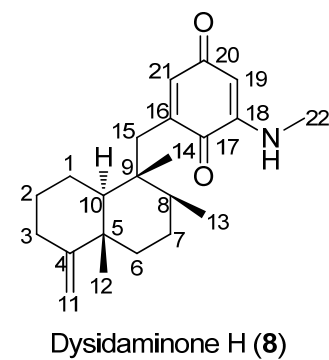
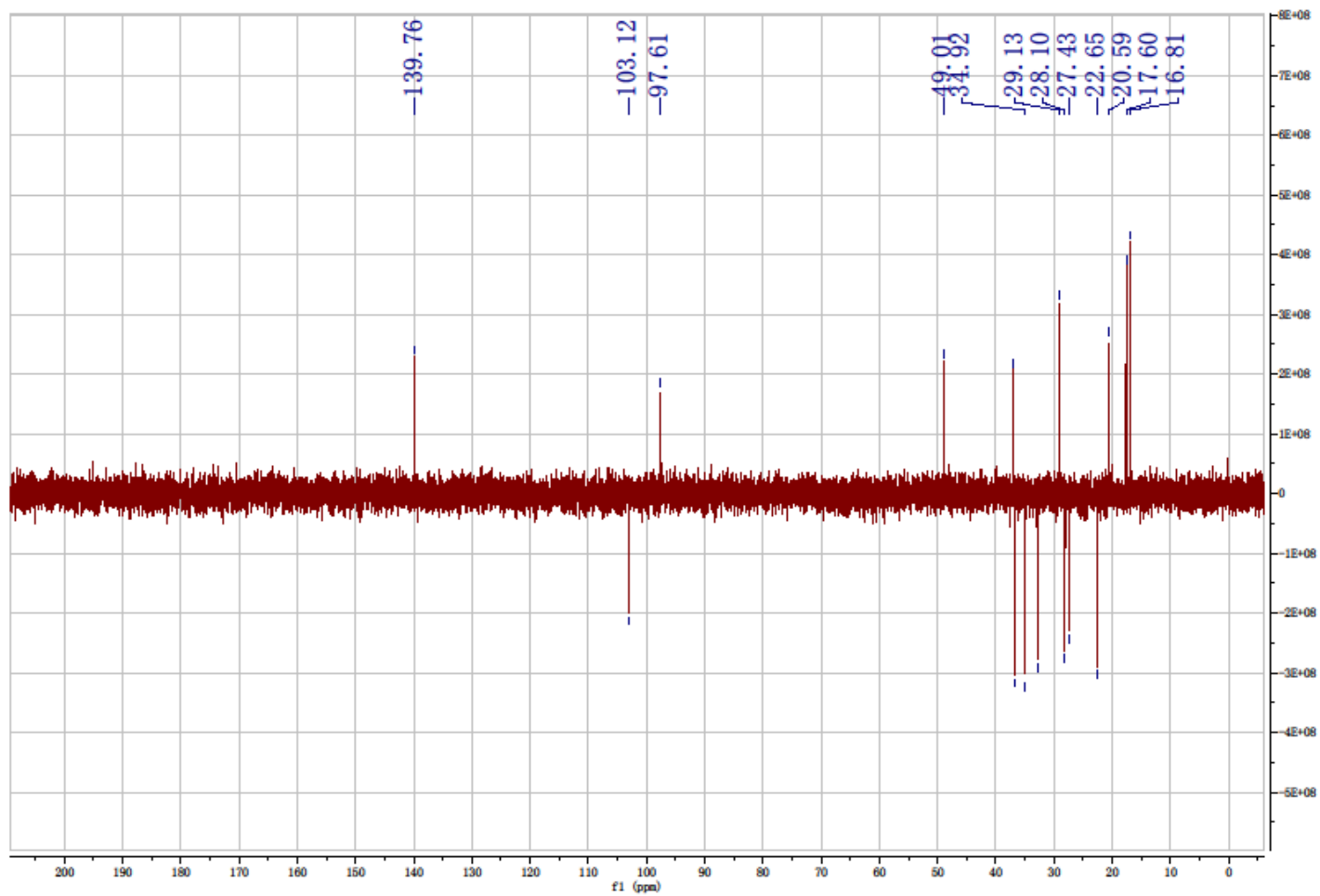


Figure S78. DEPT135 Spectrum of Dysidaminone H (8) in CDCl₃.

Elemental Composition Report

Page 1

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

22 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 10-24 H: 10-40 N: 1-3 O: 1-3 Na: 1-1

SIPI

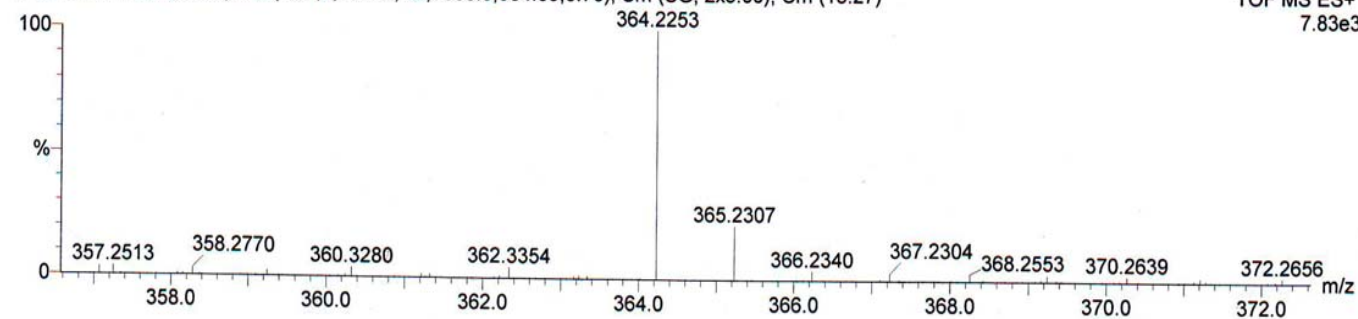
XT-35 M.W=341

WQ13-089H1 24 (0.830) AM (Cen,4, 80.00, Ar,5000.0,354.09,0.70); Sm (SG, 2x3.00); Cm (15:27)

Q-ToF micro
YA019

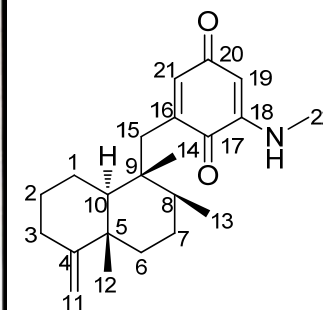
22-Apr-2013,13:29:40

TOF MS ES+
7.83e3



Minimum: 60.00
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
364.2253	100.00	364.2252	0.1	0.3	7.5	20.7	C22 H31 N O2 Na



Dysidaminone H (8)

Figure S79. HRESIMS of Dysidaminone H (8).

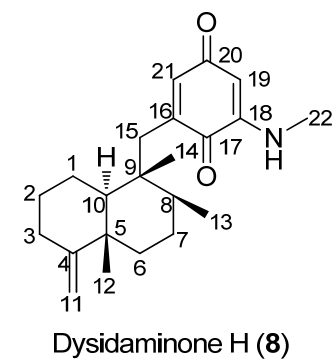
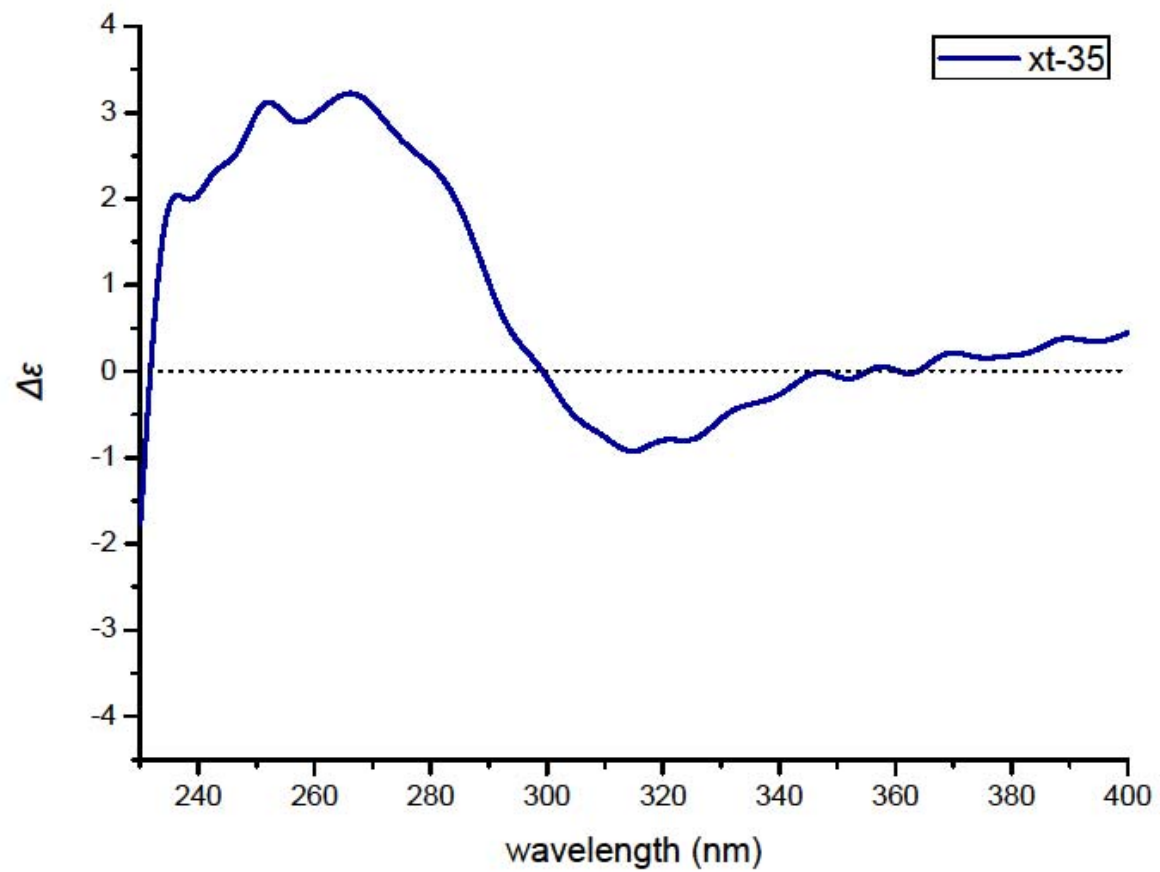


Figure S80. CD Spectrum of Dysidaminone H (8) in MeOH.

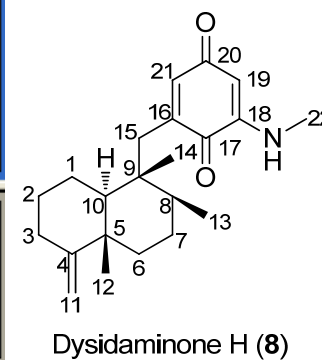
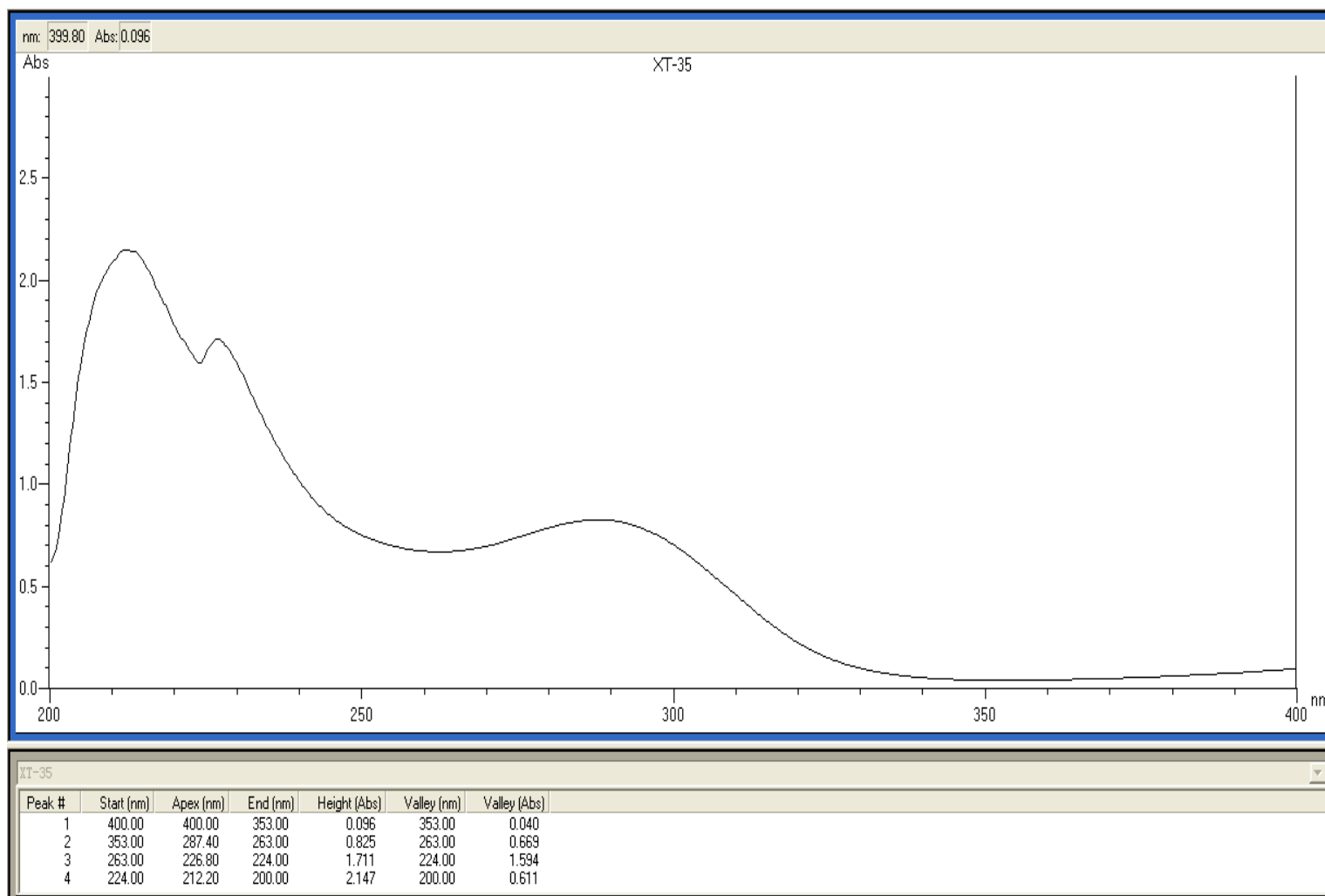


Figure S81. UV Spectrum of Dysidaminone H (**8**) in MeOH.

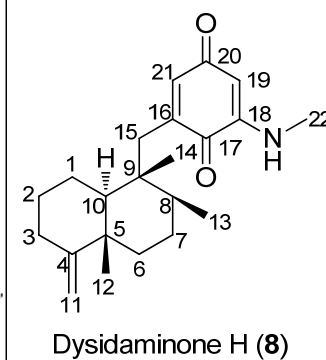
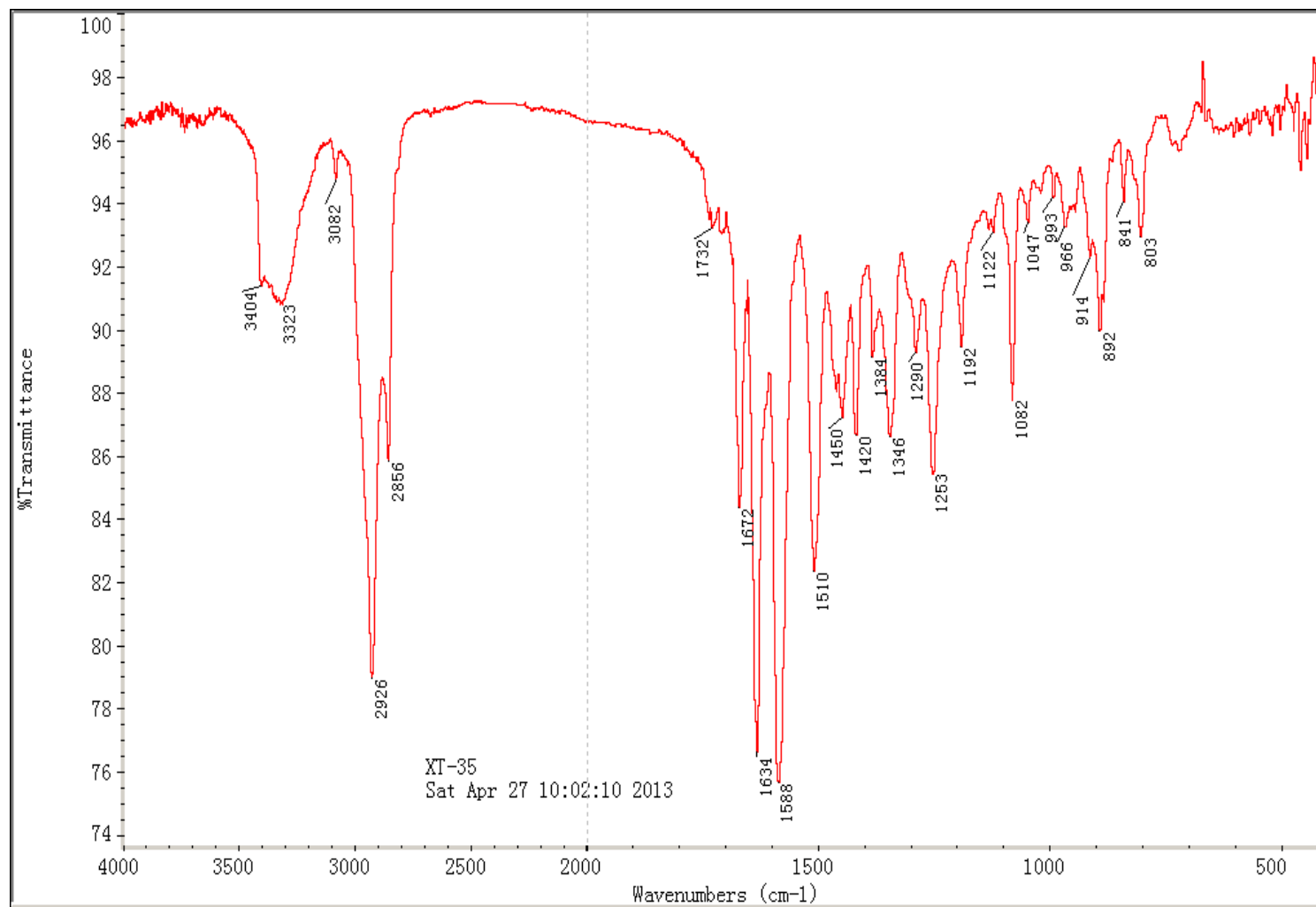
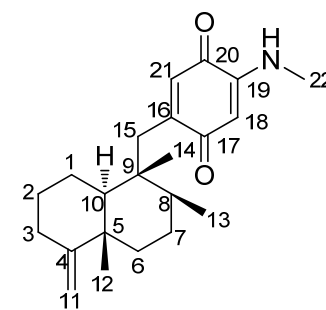
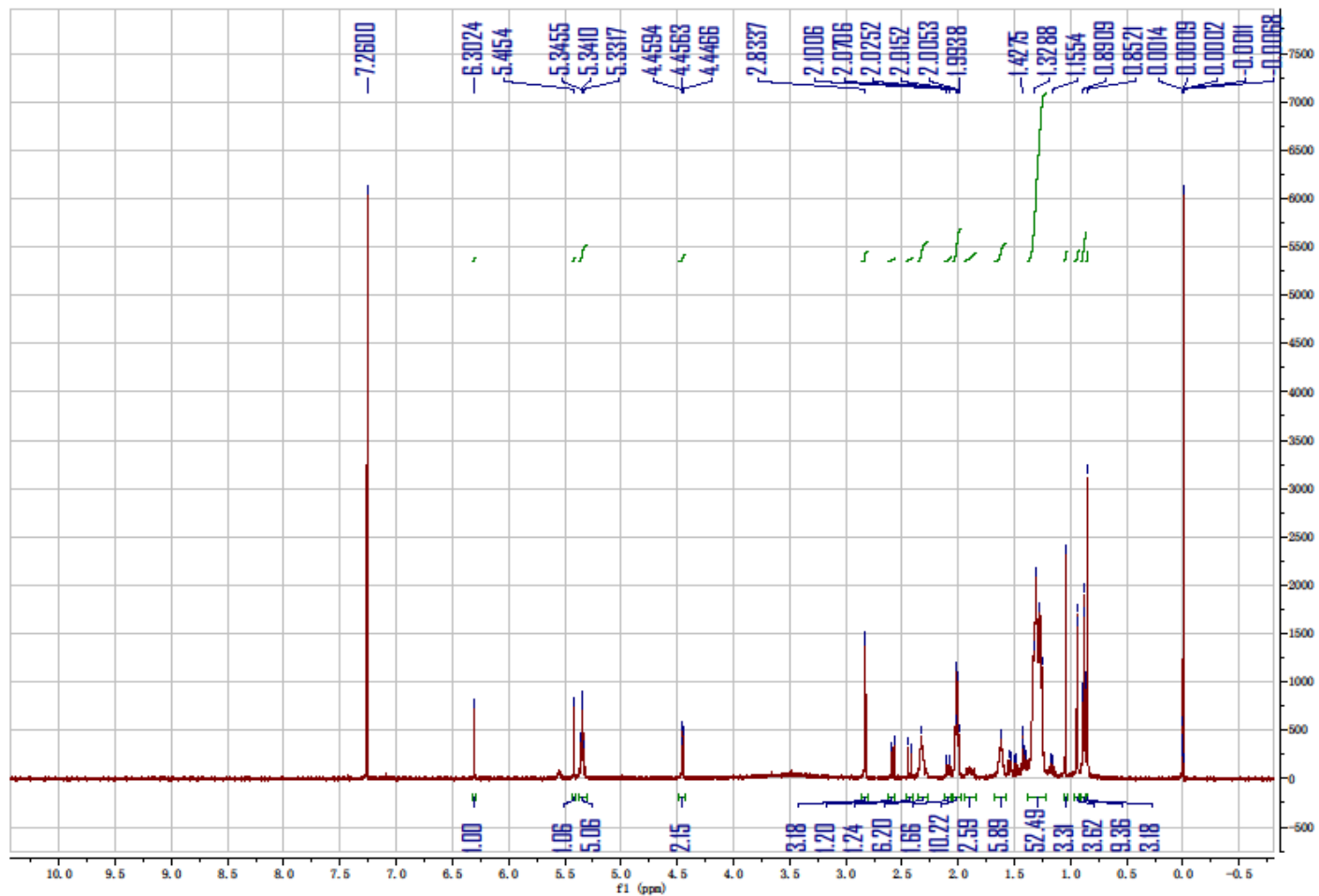


Figure S82. IR Spectrum of Dysidaminone H (8).



Dysidaminone I (9)

Figure S83. ^1H NMR Spectrum of Dysidaminone I (9) in CDCl_3 .

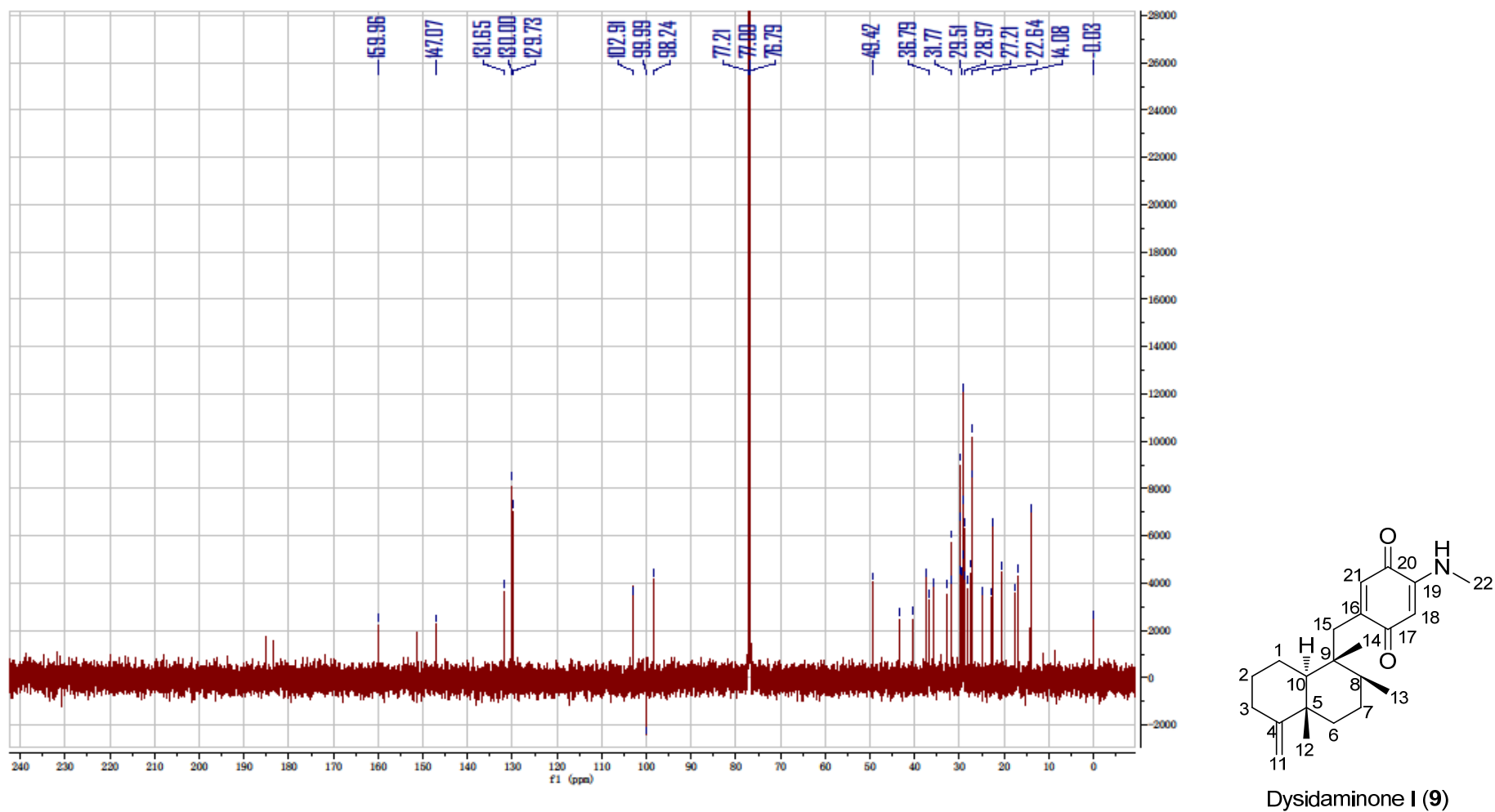


Figure S84. ¹³C NMR Spectrum of Dysidaminone I (9) in CDCl₃.

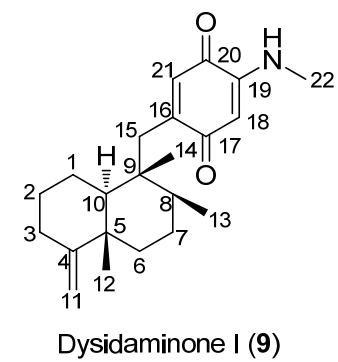
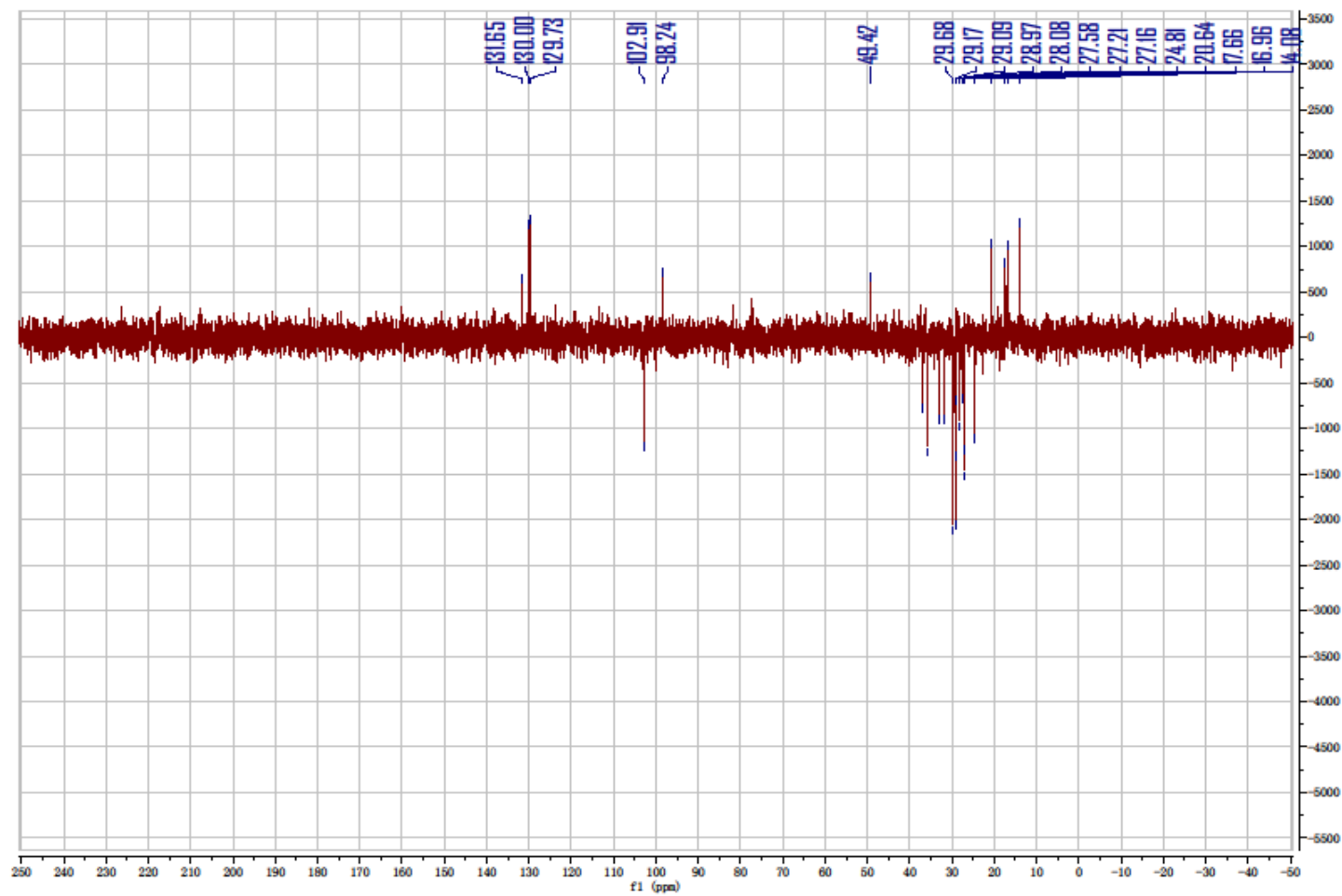


Figure S85. DEPT135 Spectrum of Dysidaminone I (9) in CDCl₃.

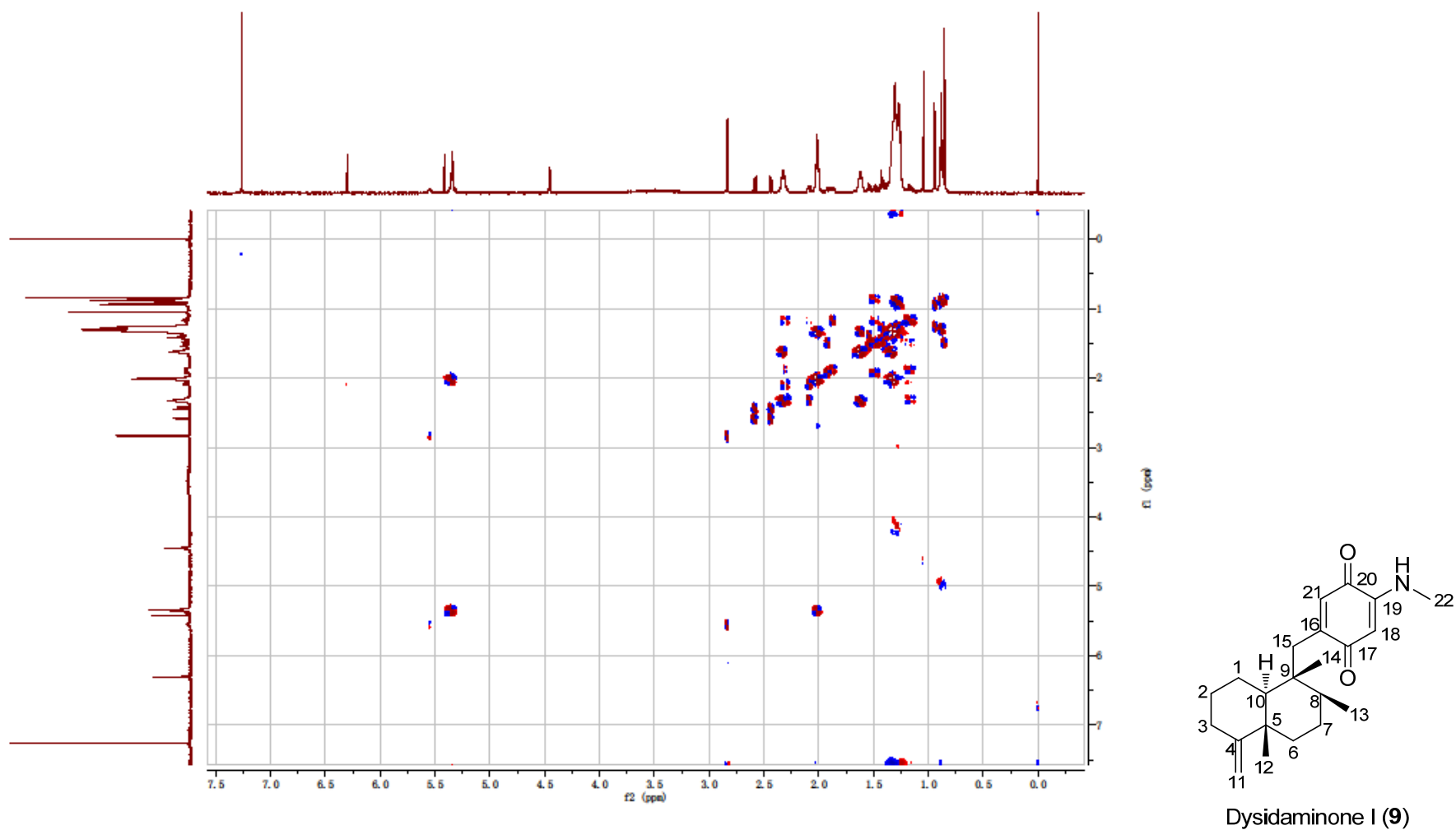


Figure S86. ^1H - ^1H COSY Spectrum of Dysidaminone I (9) in CDCl_3 .

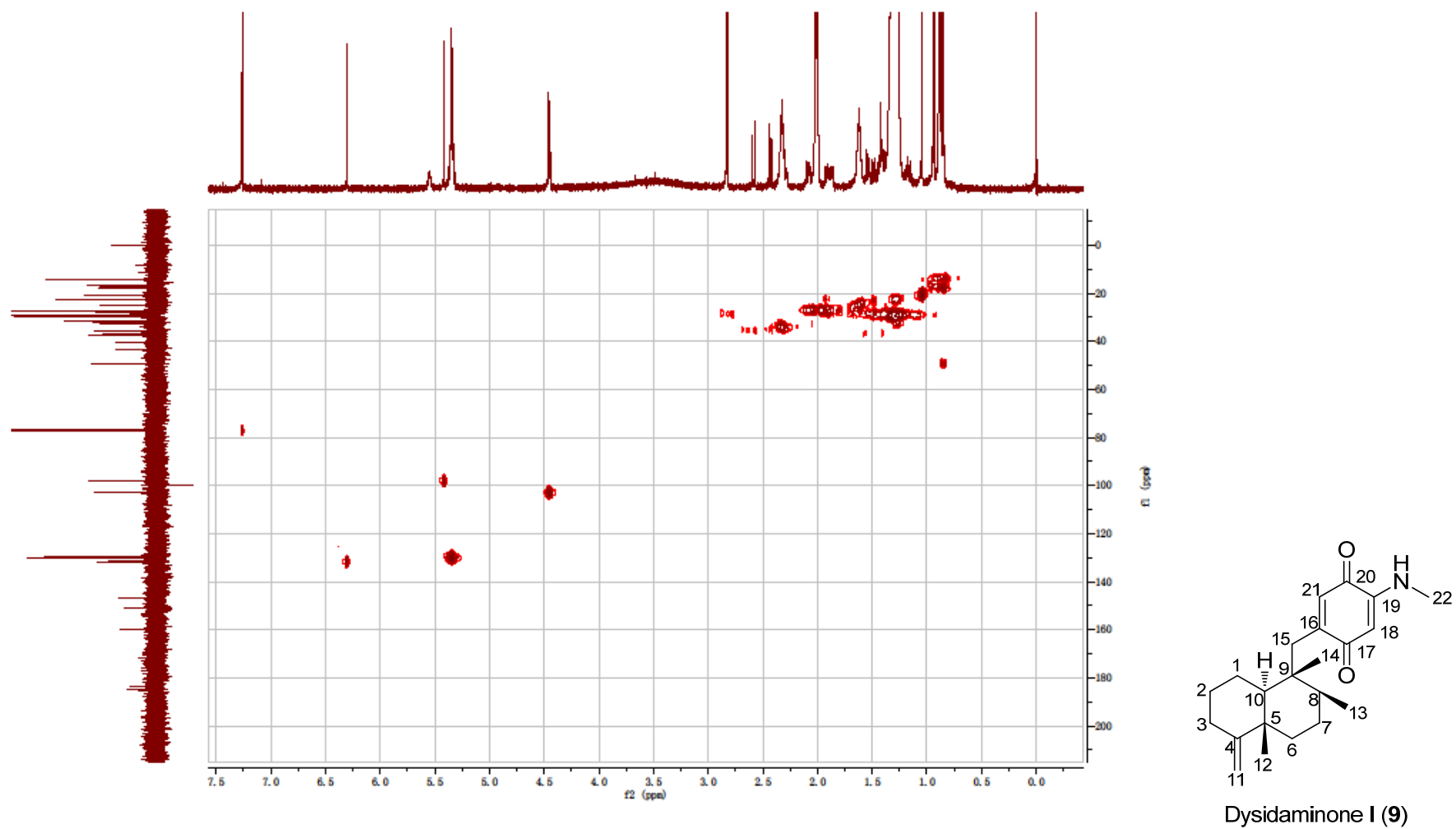


Figure S87. HSQC Spectrum of Dysidaminone I (**9**) in CDCl₃.

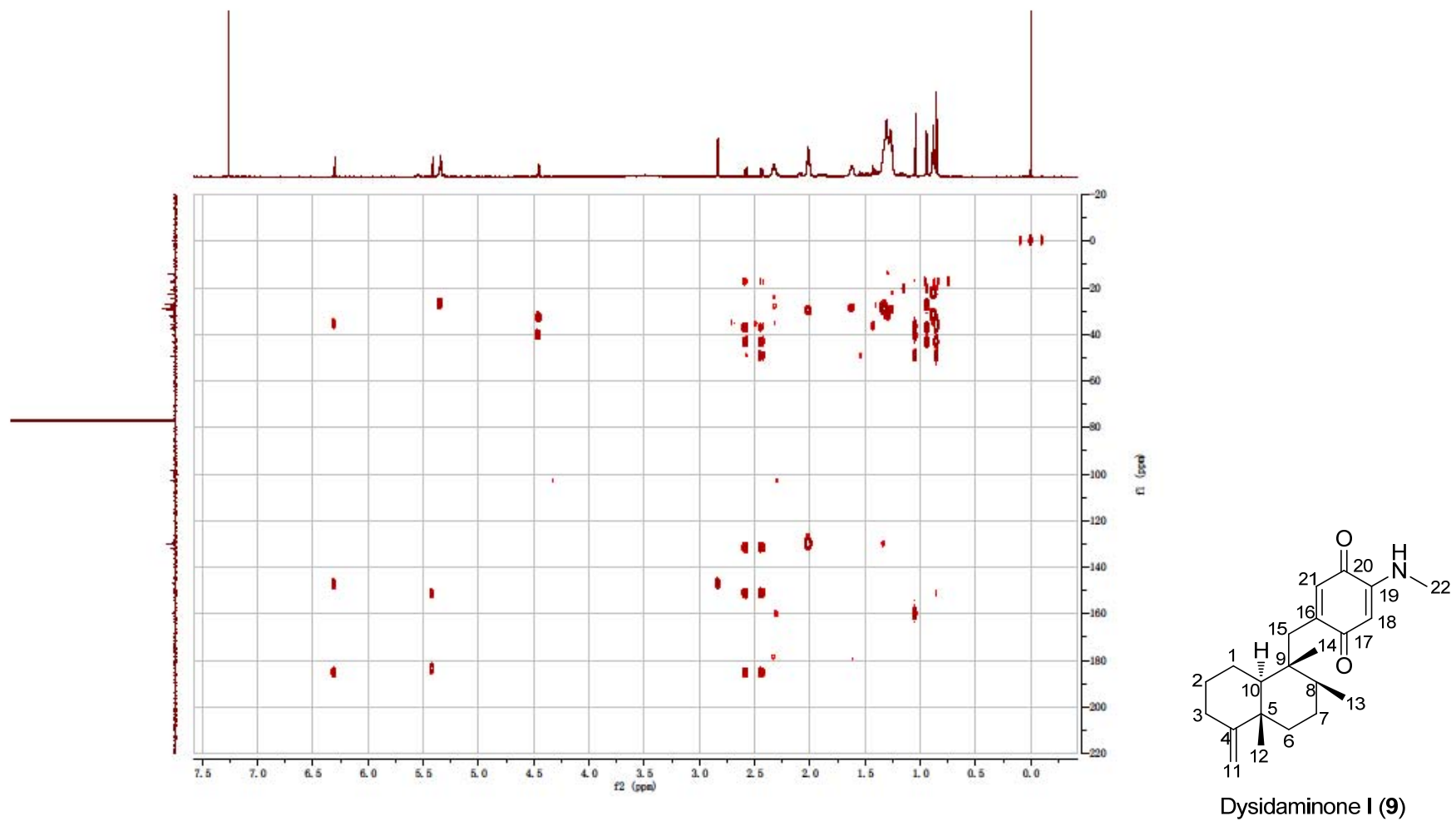


Figure S88. HMBC Spectrum of Dysidaminone I (**9**) in CDCl₃.

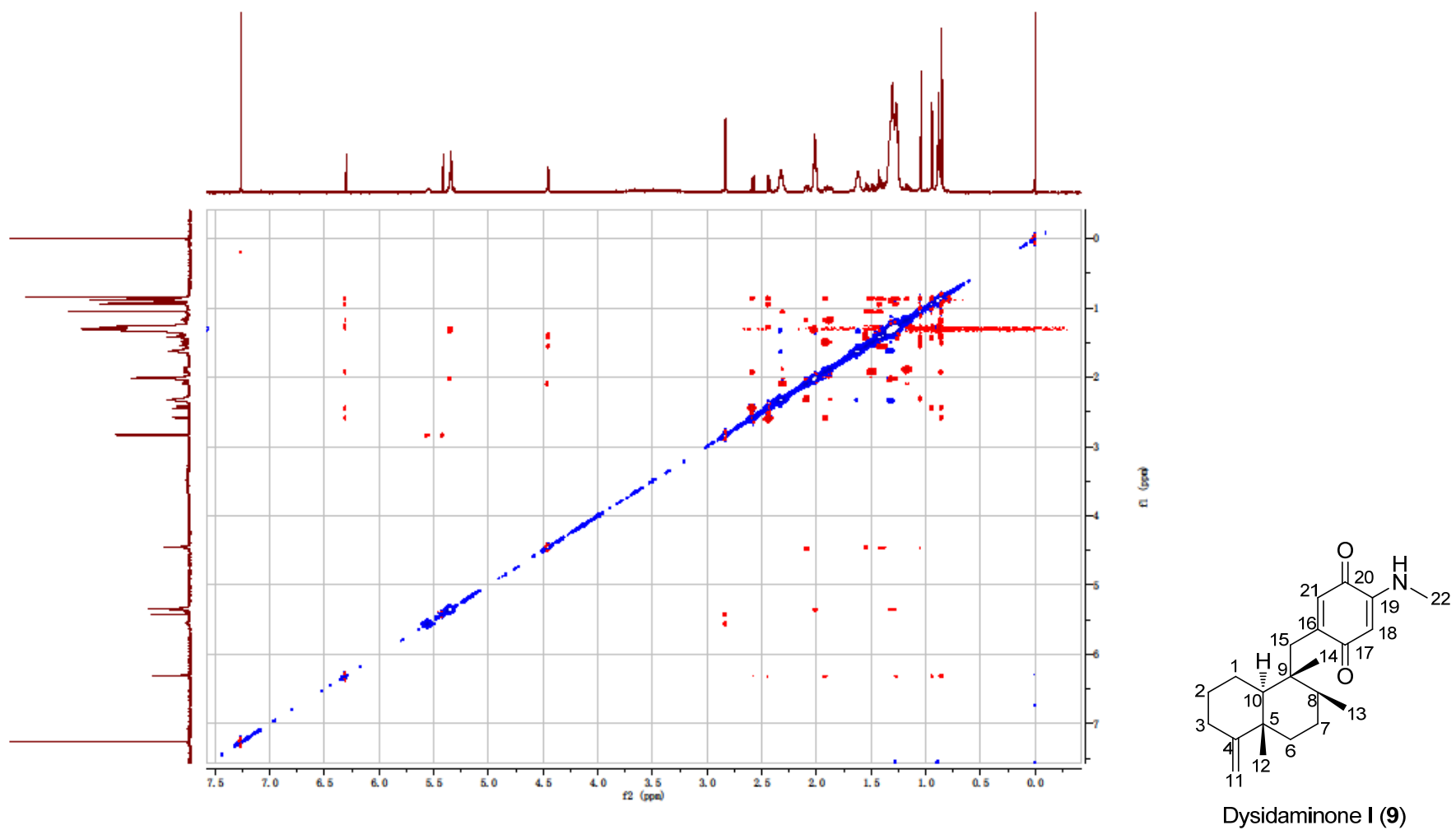
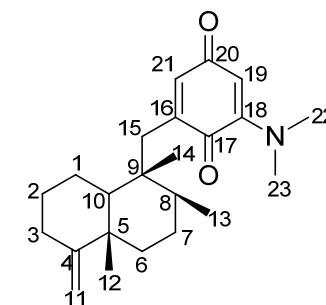
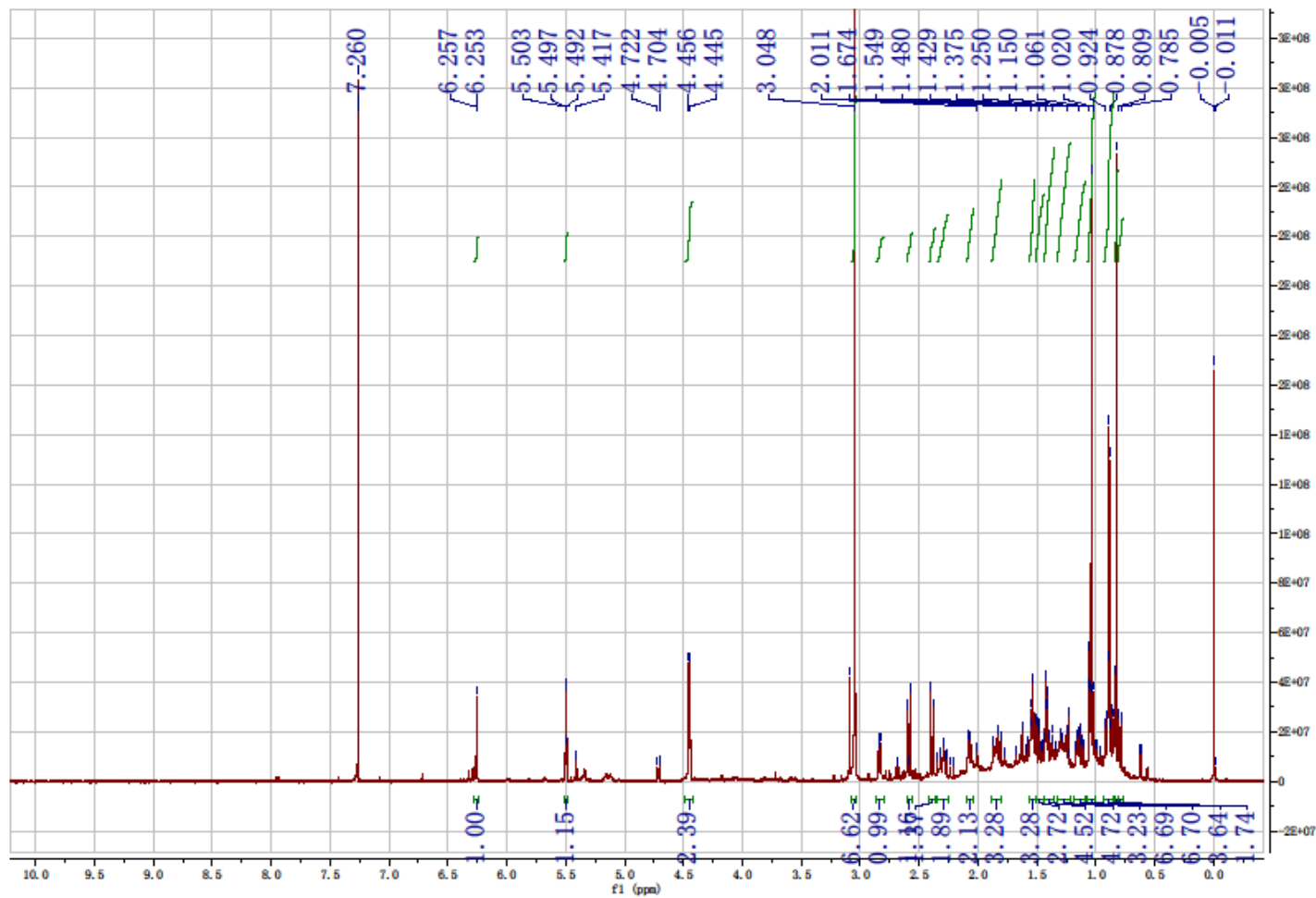
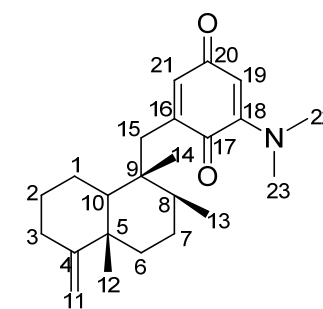
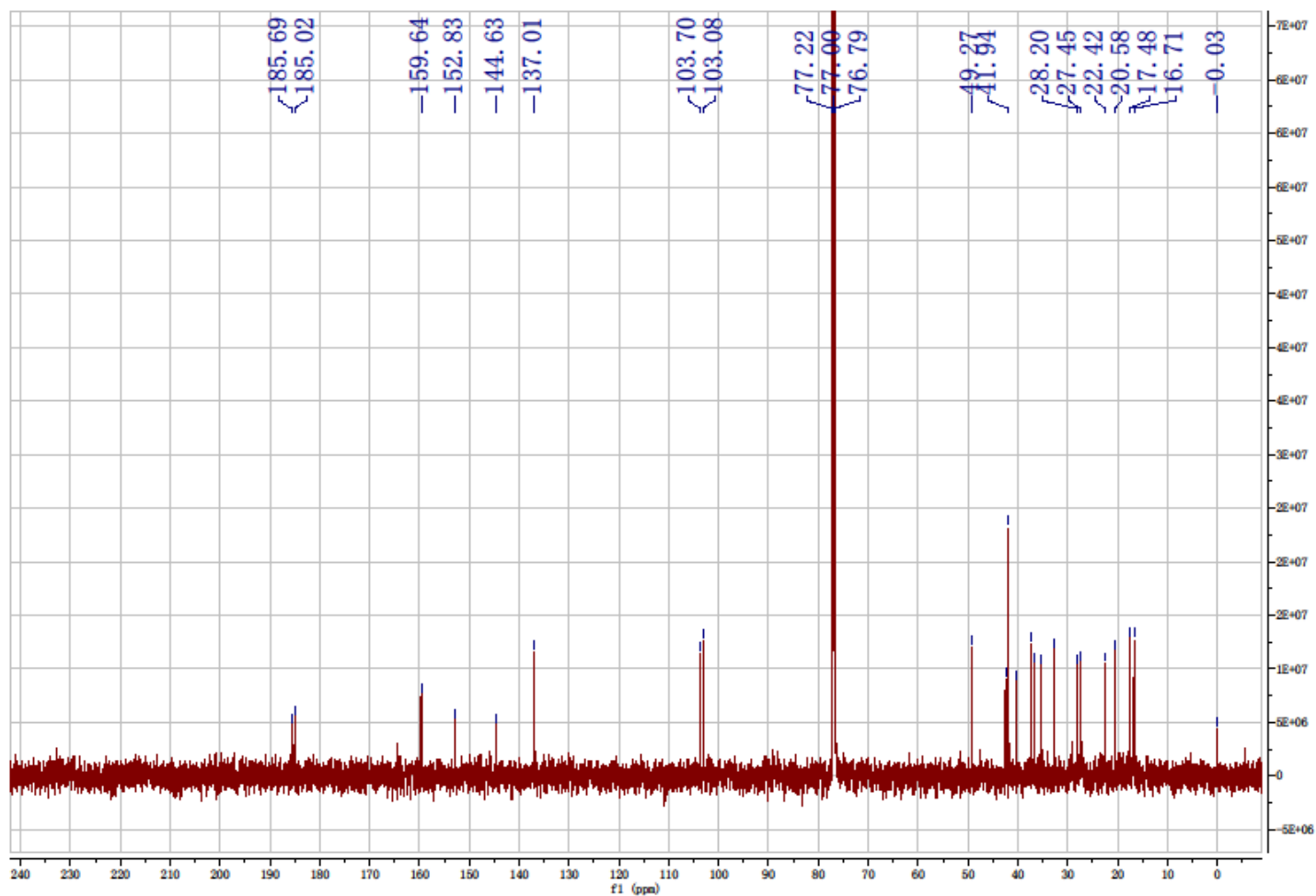


Figure S89. NOESY Spectrum of Dysidaminone I (9) in CDCl₃.



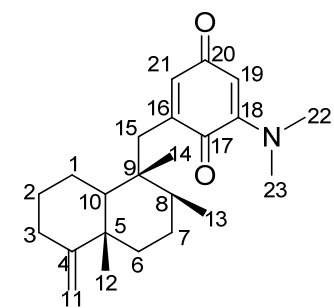
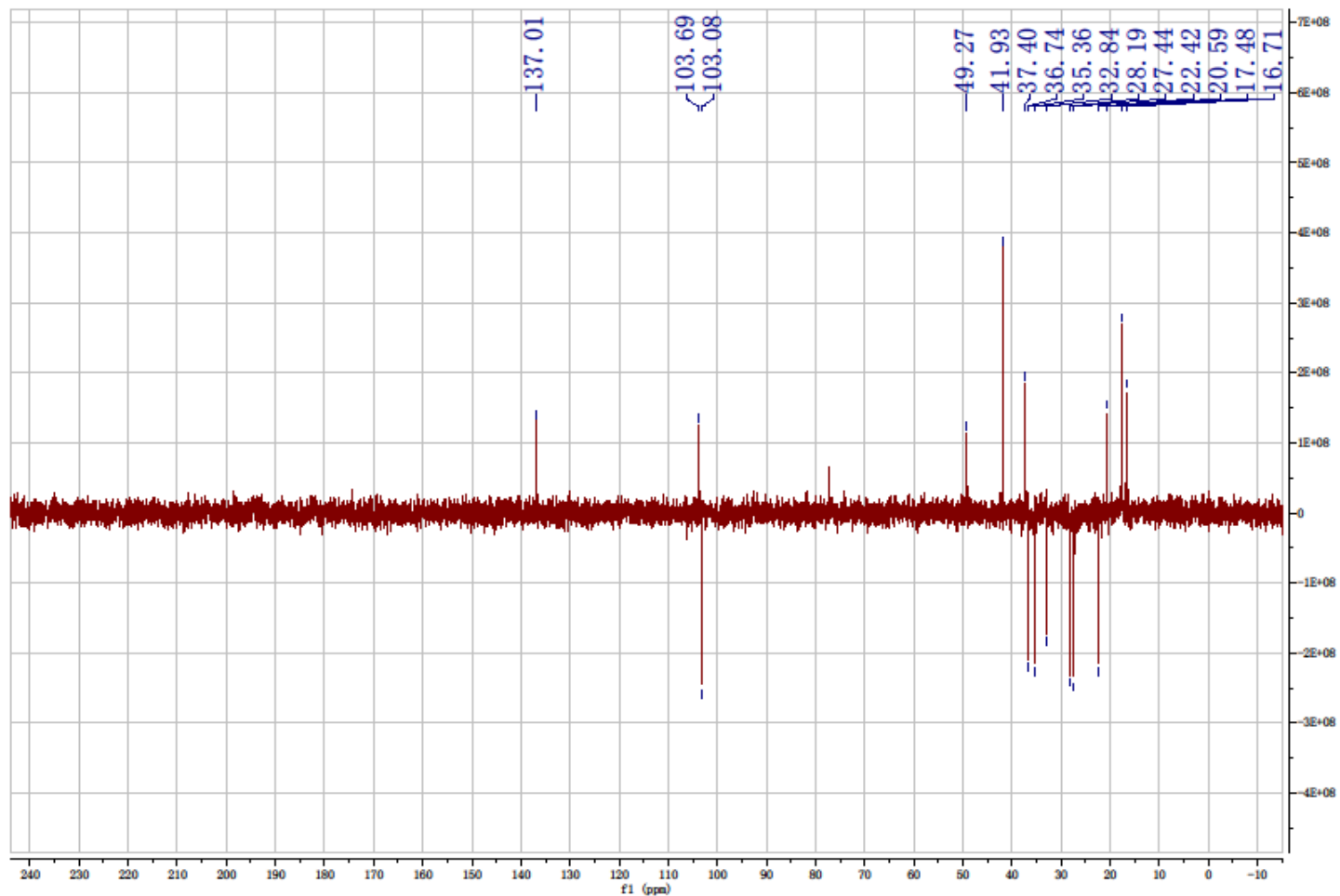
Dysidaminone J (**10**)

Figure S90. ^1H NMR Spectrum of Dysidaminone J (**10**) in CDCl_3 .



Dysidaminone J (**10**)

Figure S91. ^{13}C NMR Spectrum of Dysidaminone J (**10**) in CDCl_3 .



Dysidaminone J (**10**)

Figure S92. ^1H - ^1H COSY Spectrum of Dysidaminone J (**10**) in CDCl_3 .

Elemental Composition Report

Page 1

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
23 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 10-24 H: 10-40 N: 1-3 O: 1-3

SIPI

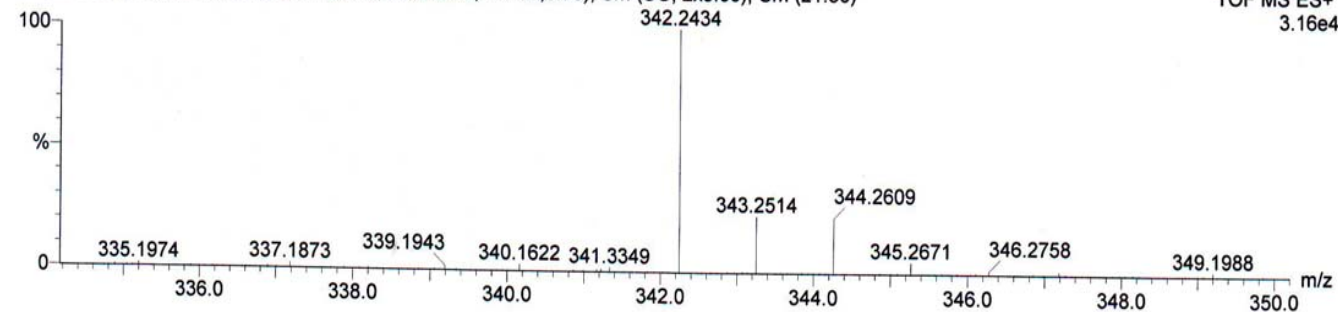
XT-37A M.W=341

WQ13-088H 30 (1.037) AM (Cen,4, 80.00, Ar,5000.0,354.09,0.70); Sm (SG, 2x3.00); Cm (21:30)

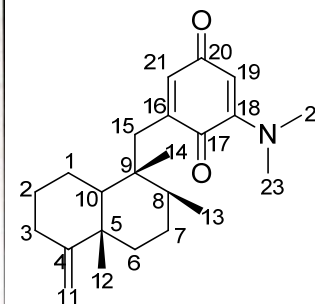
Q-ToF micro
YA019
342.2434

22-Apr-2013,13:09:19

TOF MS ES+
3.16e4



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Maximum:	100.00		5.0	10.0	-1.5				
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula		
342.2434	100.00	342.2433	0.1	0.3	7.5	2575.7	C22 H32 N O2		



Dysidaminone J (10)

Figure S93. HRESIMS of Dysidaminone J (10).

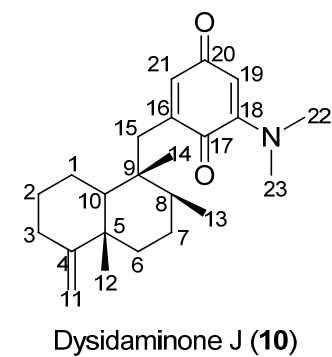
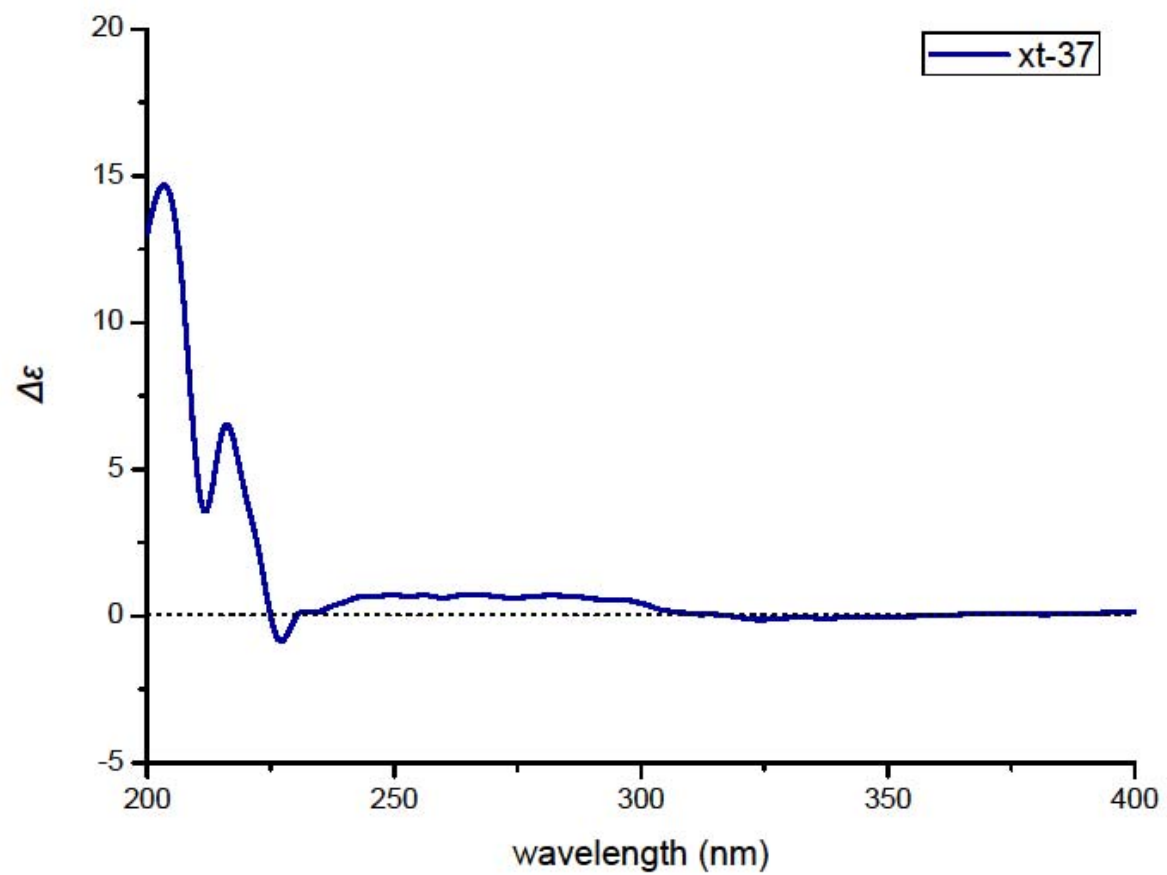


Figure S94. CD Spectrum of Dysidaminone J (**10**) in MeOH.

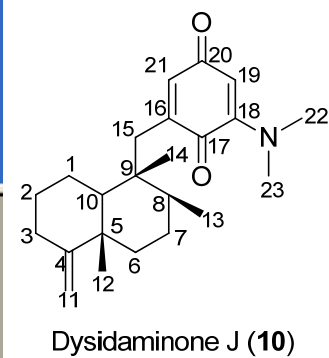
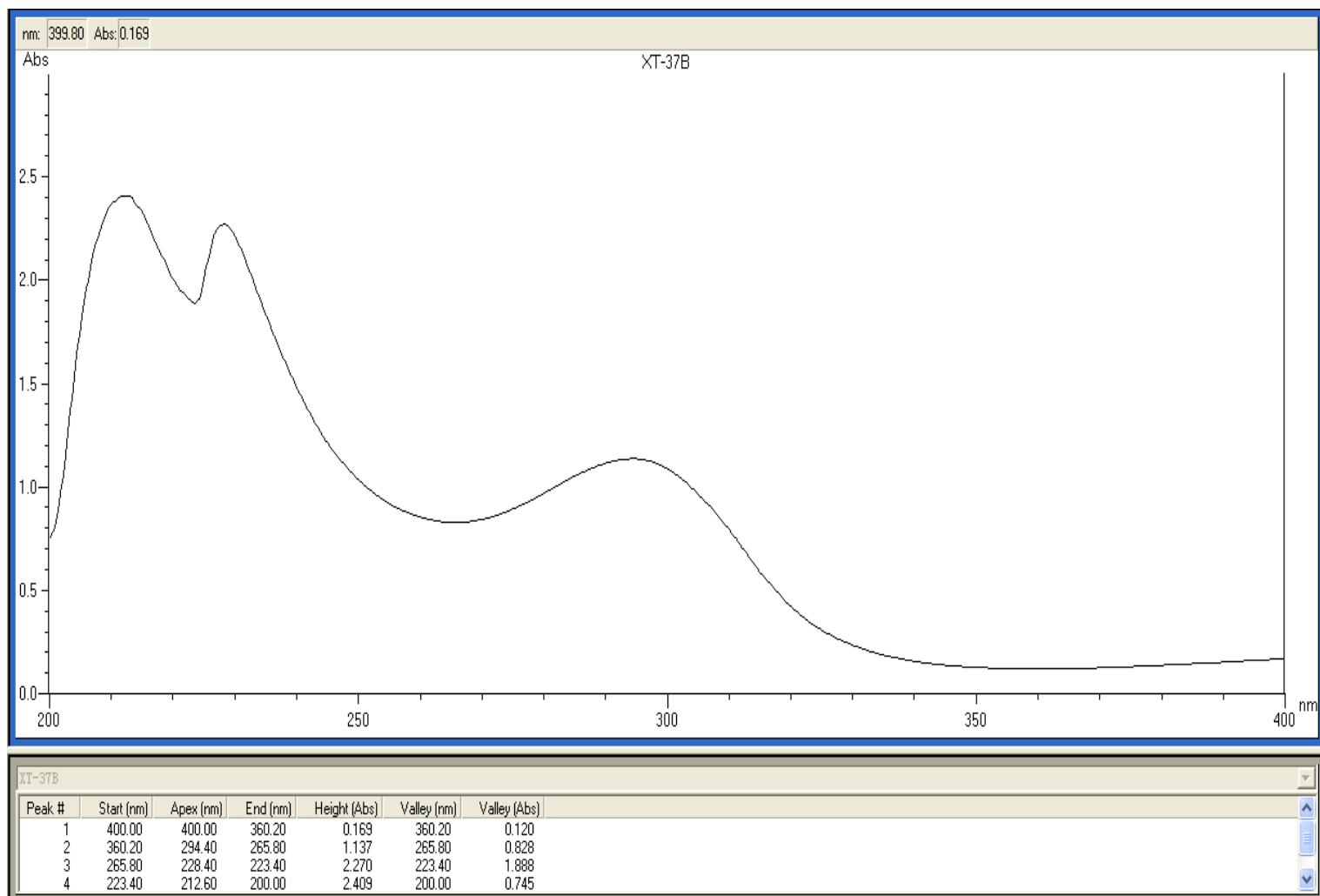


Figure S95. UV Spectrum of Dysidaminone J (**10**) in MeOH.

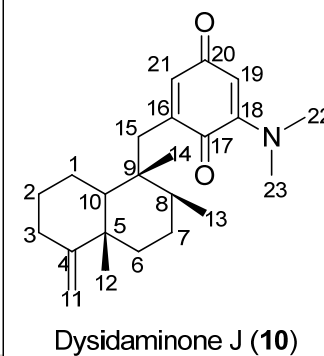
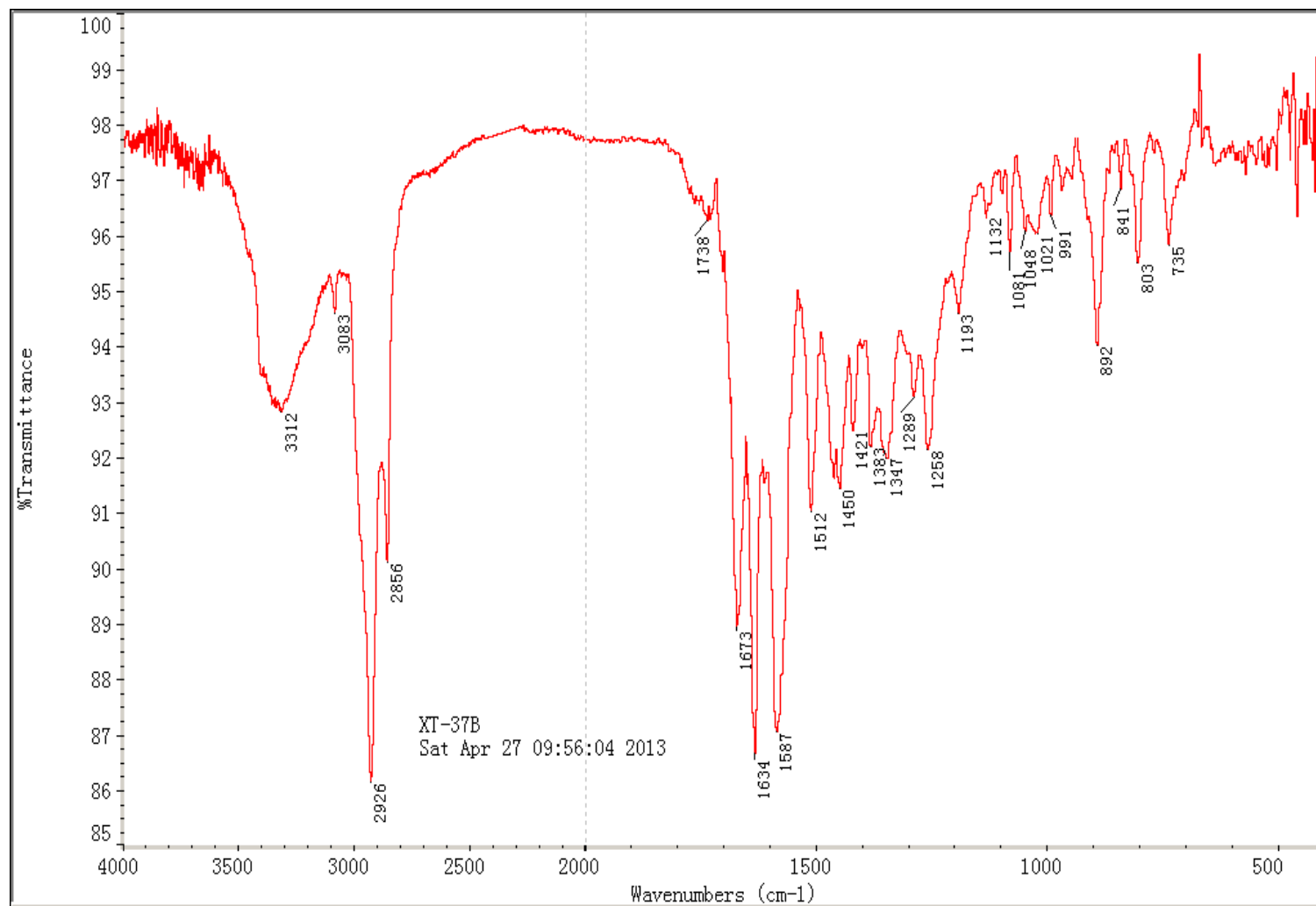


Figure S96. IR Spectrum of Dysidaminone J (**10**).

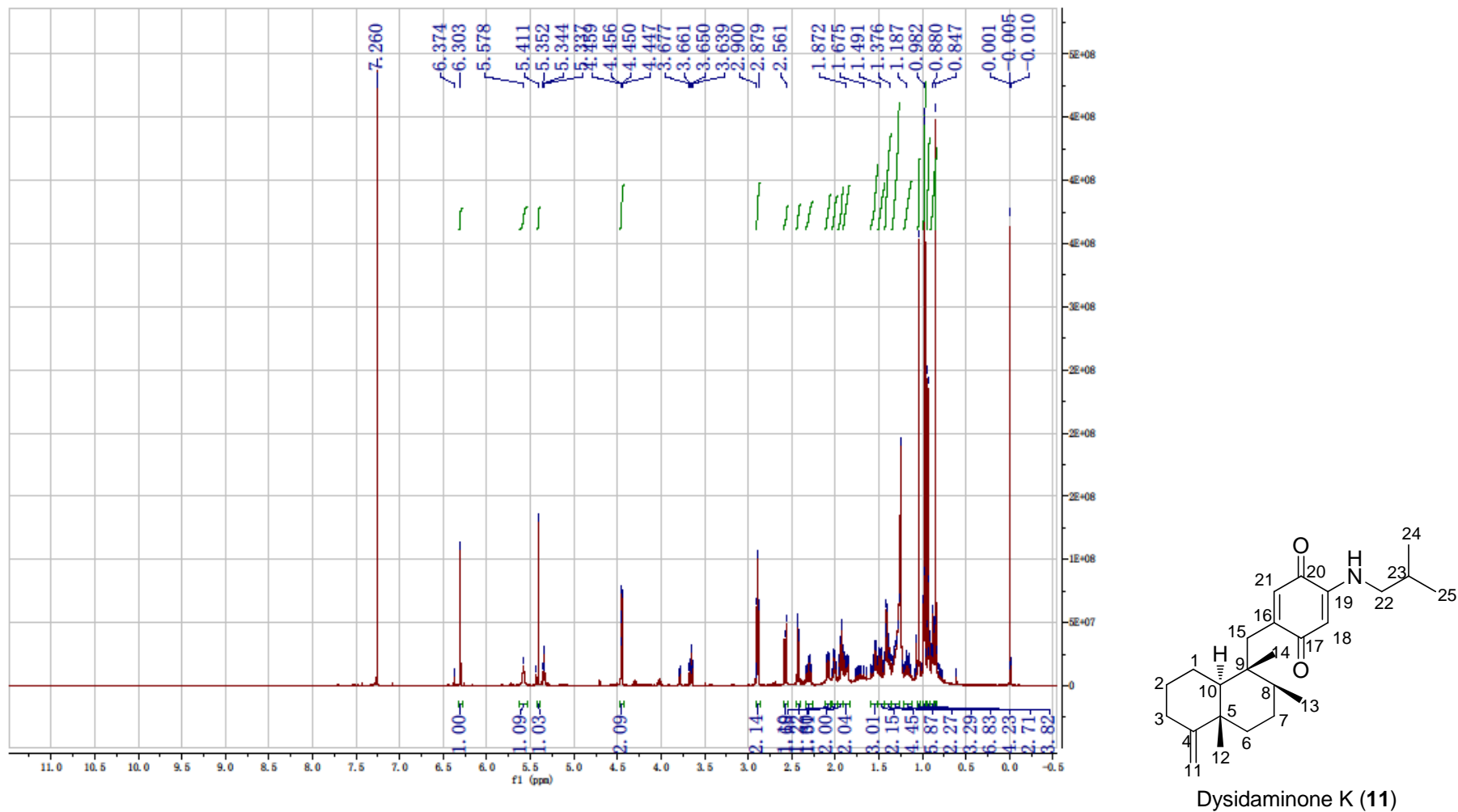


Figure S97. ¹H NMR Spectrum of Dysidaminone K (**11**) in CDCl₃.

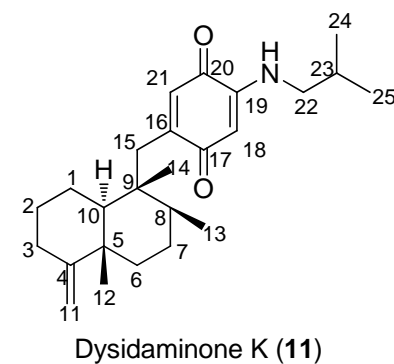
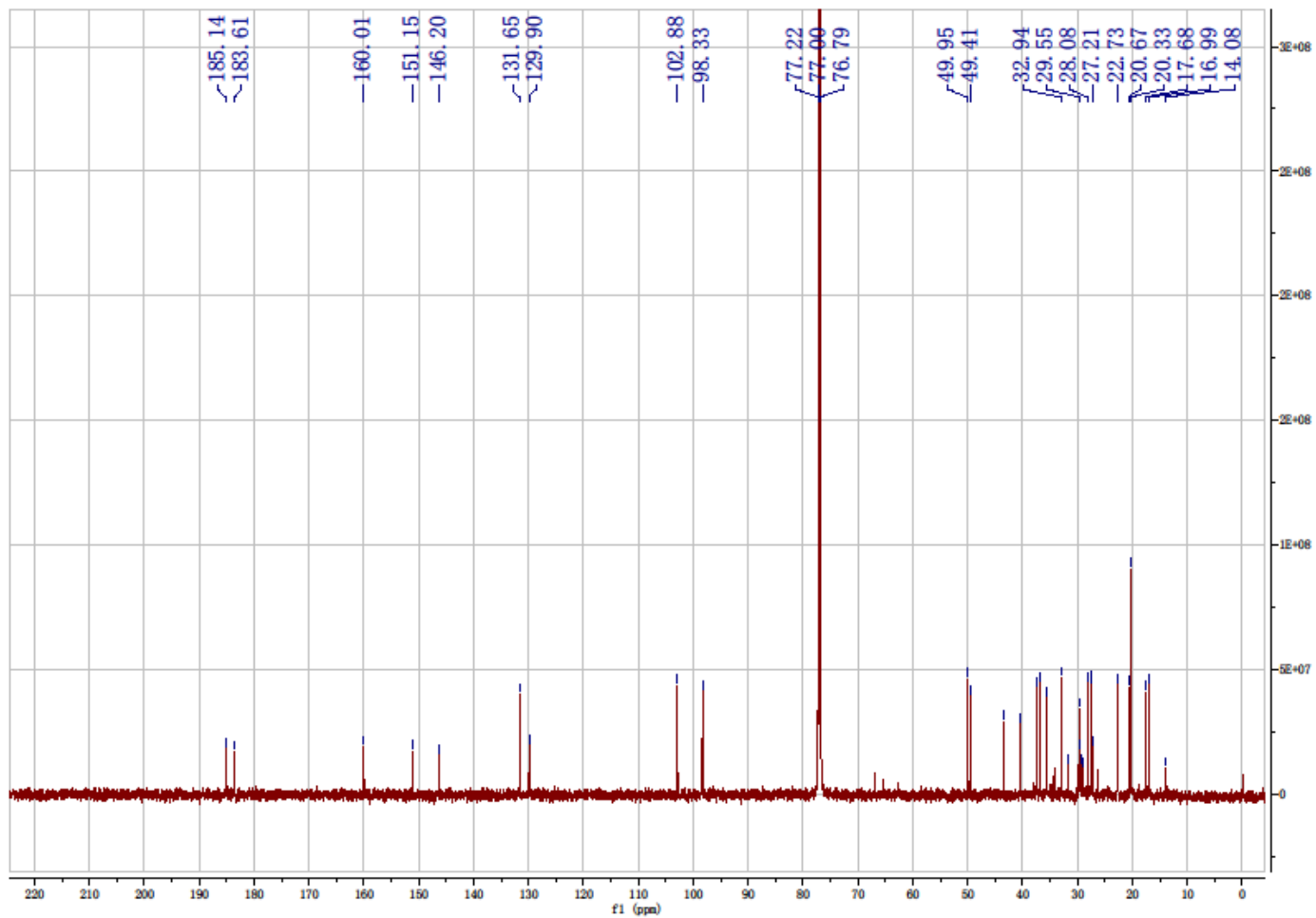


Figure S98. ^{13}C NMR Spectrum of Dysidaminone K (11) in CDCl_3 .

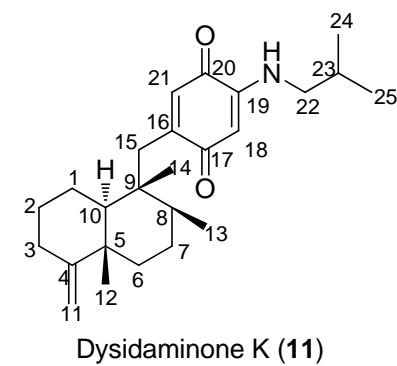
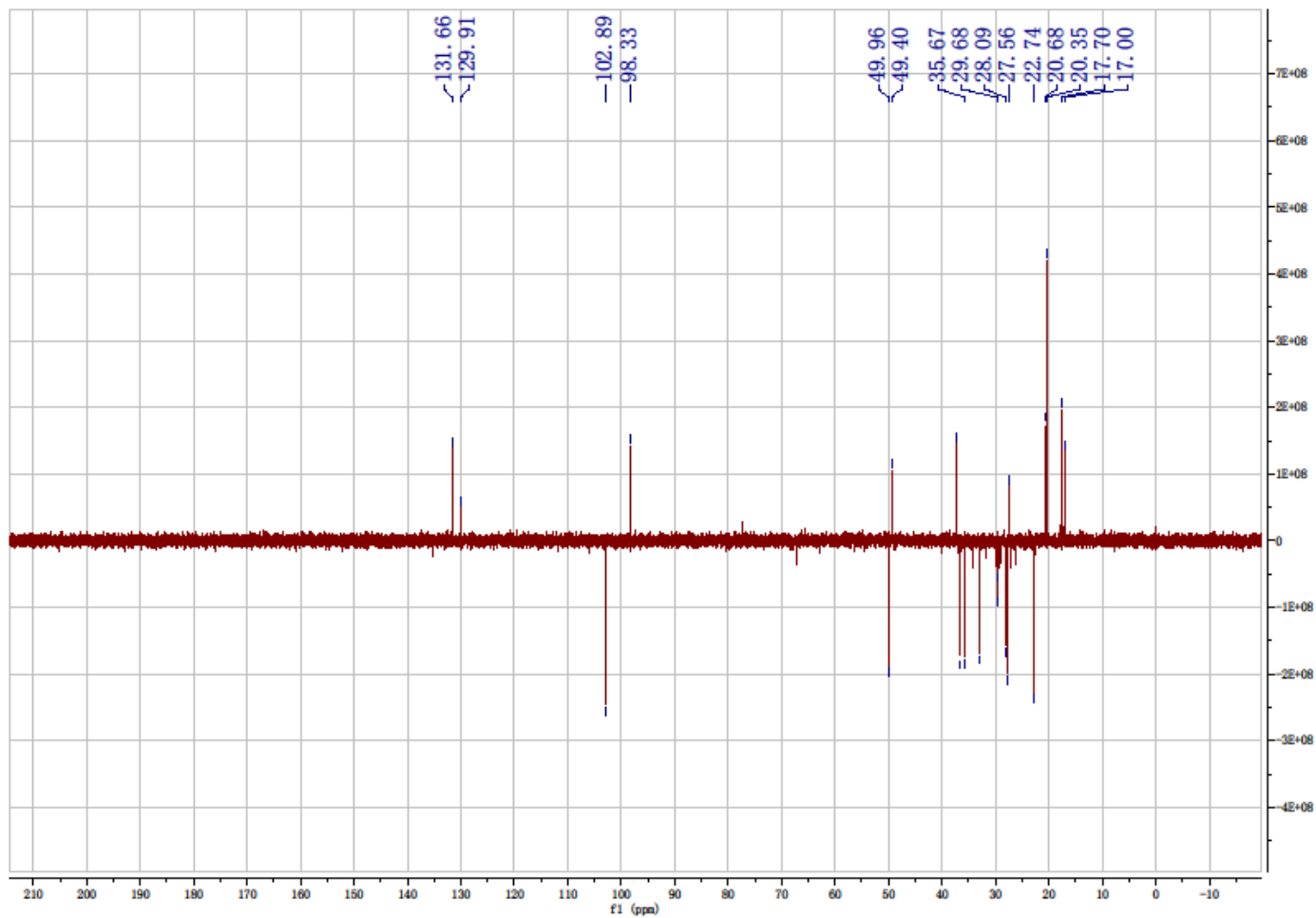


Figure S99. DEPT135 Spectrum of Dysidaminone K (**11**) in CDCl₃.

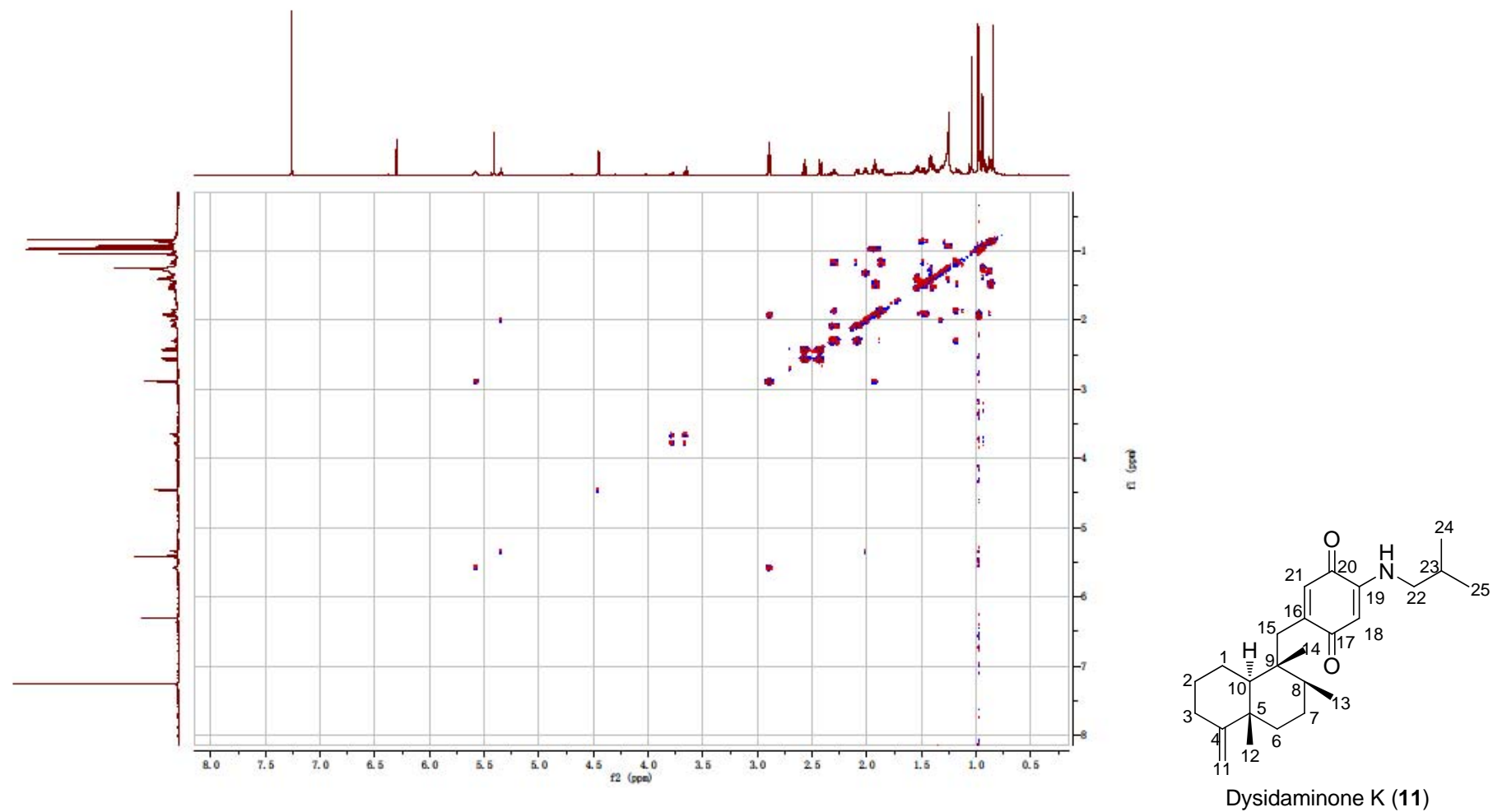


Figure S100. ^1H - ^1H COSY Spectrum of Dysidaminone K (11) in CDCl_3 .

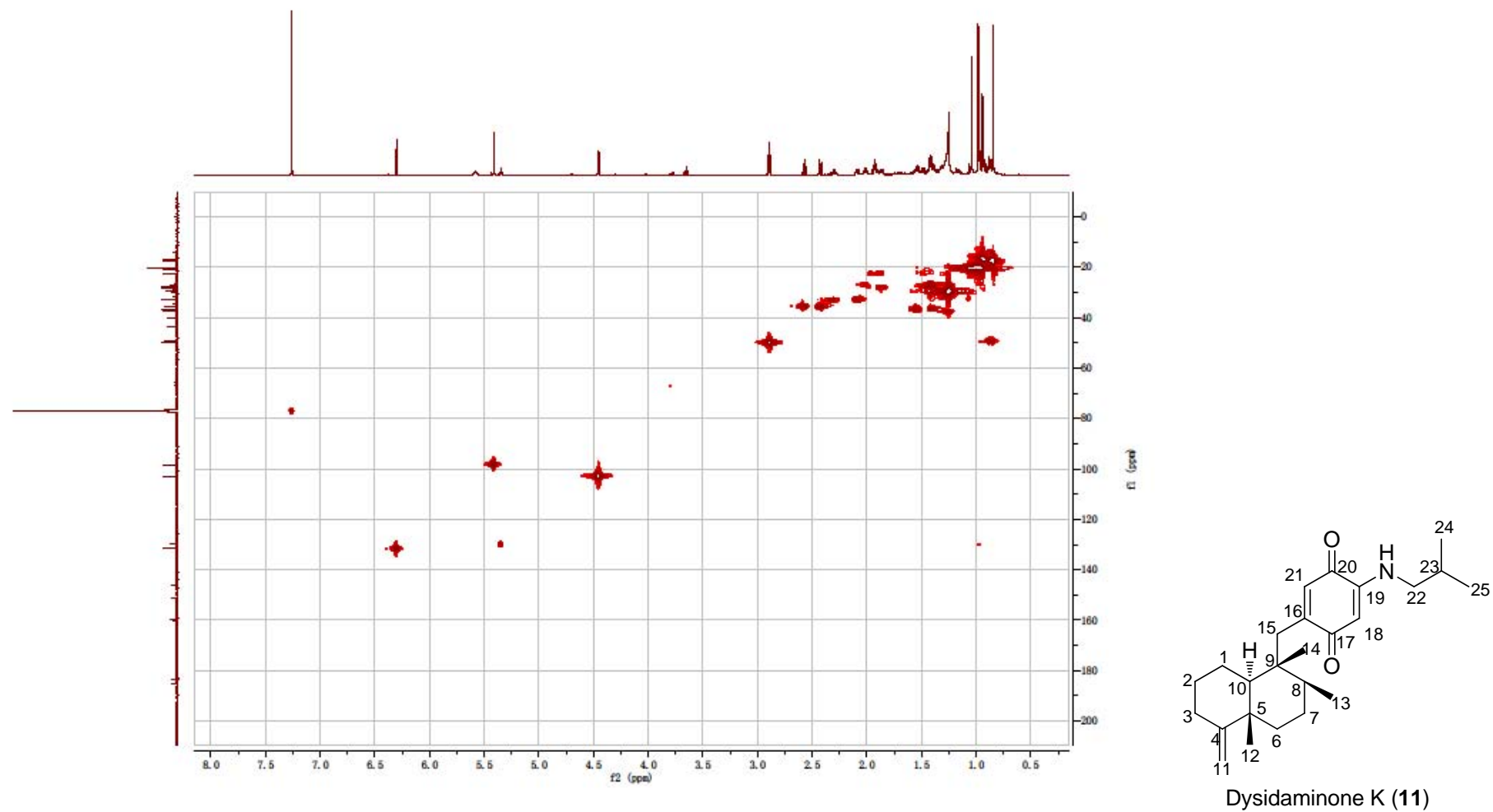


Figure S101. HSQC Spectrum of Dysidaminone K (**11**) in CDCl₃.

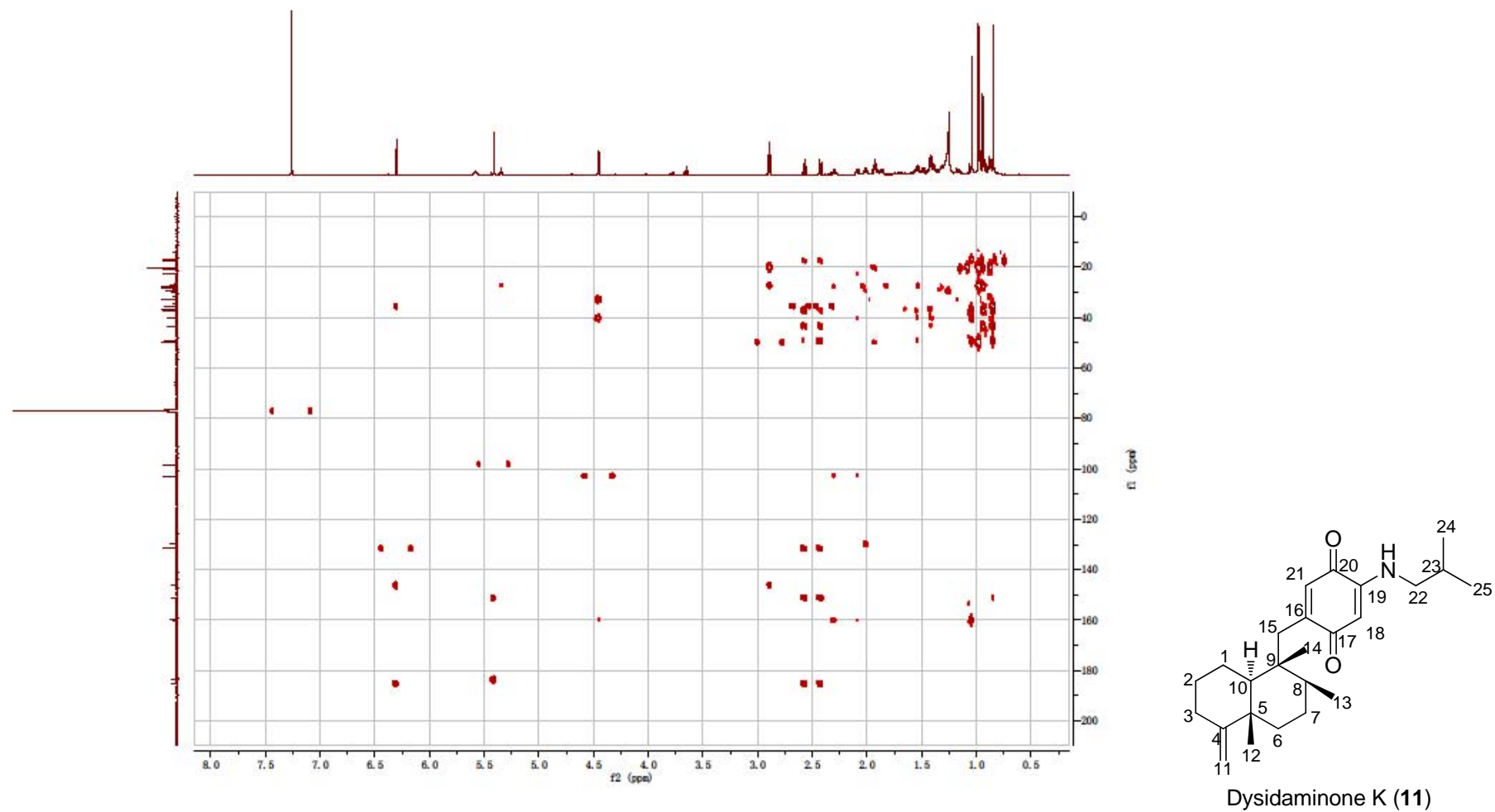


Figure S102. HMBC Spectrum of Dysidaminone K (**11**) in CDCl₃.

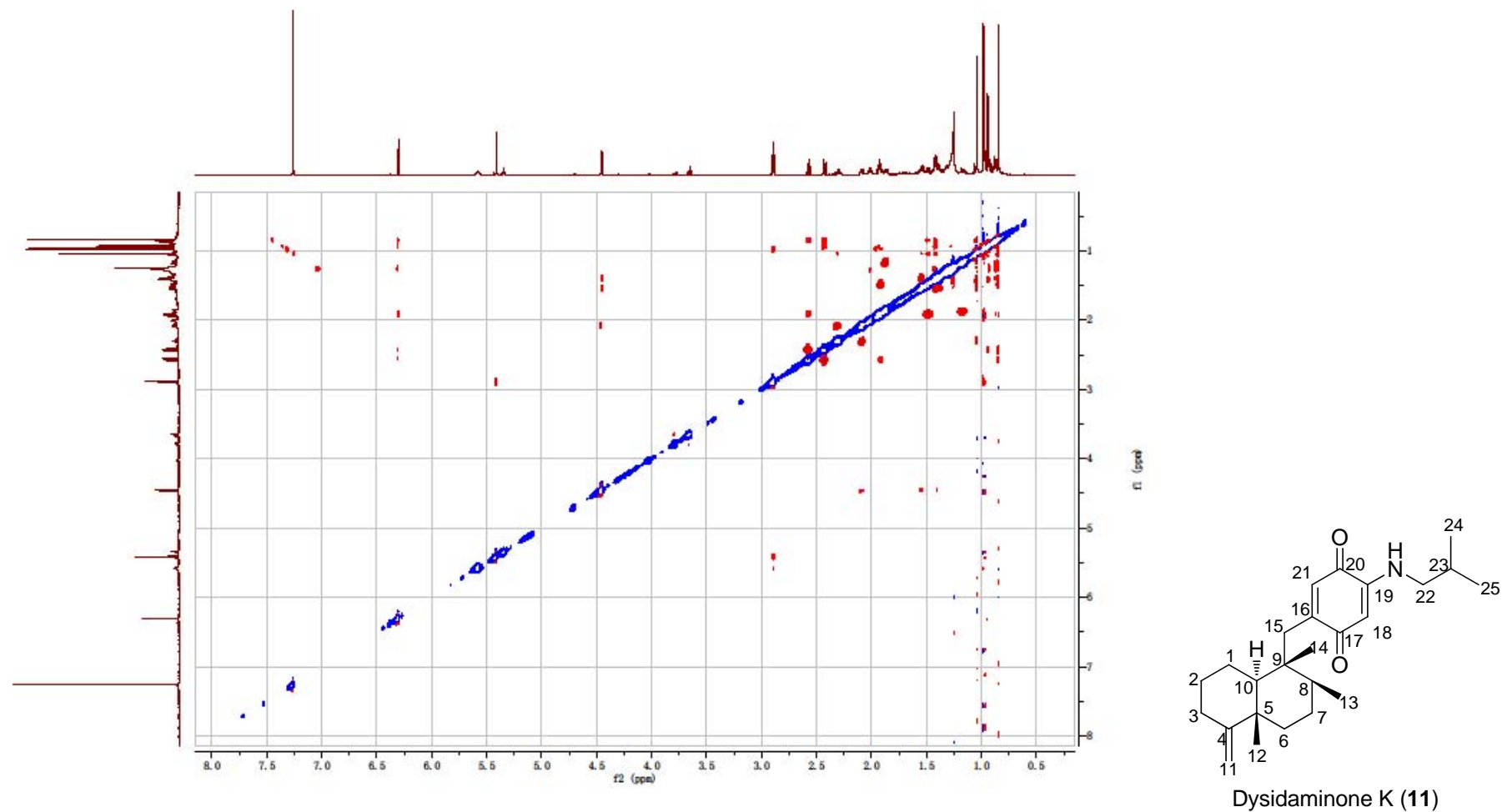


Figure S103. NOESY Spectrum of Dysidaminone K (**11**) in CDCl₃.

Elemental Composition Report

Page 1

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 10-27 H: 10-40 N: 1-1 O: 1-4

SIPI

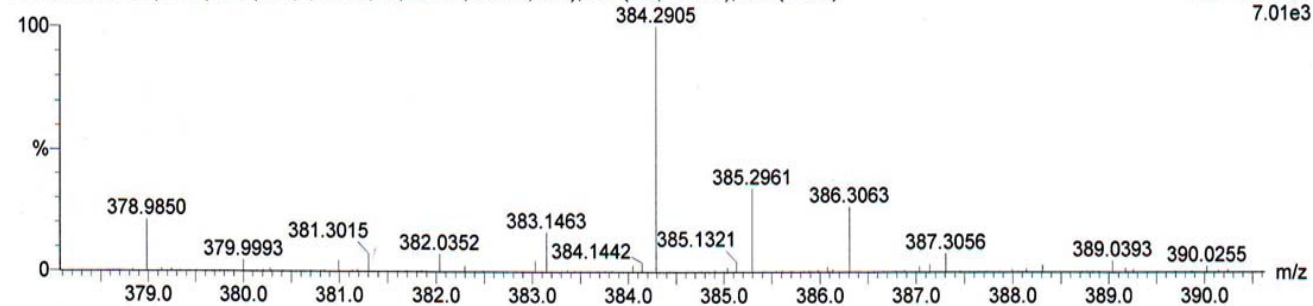
XT-39 M.W=383

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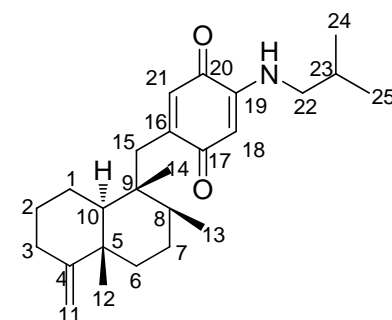
Q-ToF micro
YA019

29-Apr-2013, 14:34:49

TOF MS ES+
7.01e3

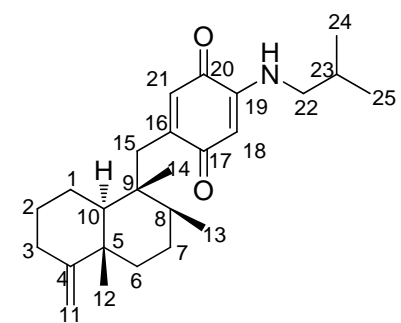
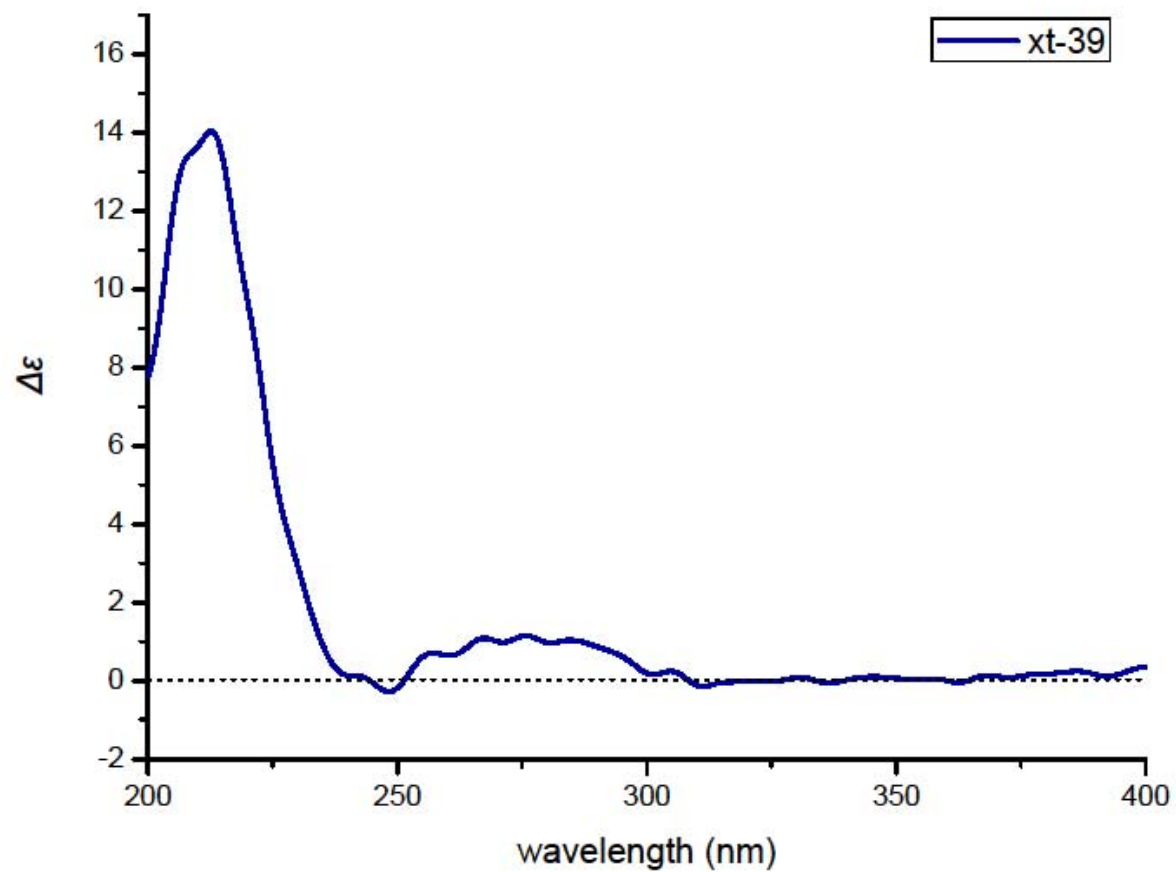


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Maximum:	100.00		5.0	10.0	50.0			
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
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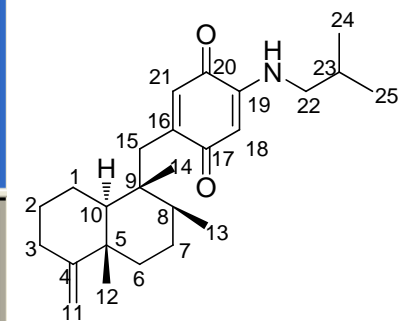
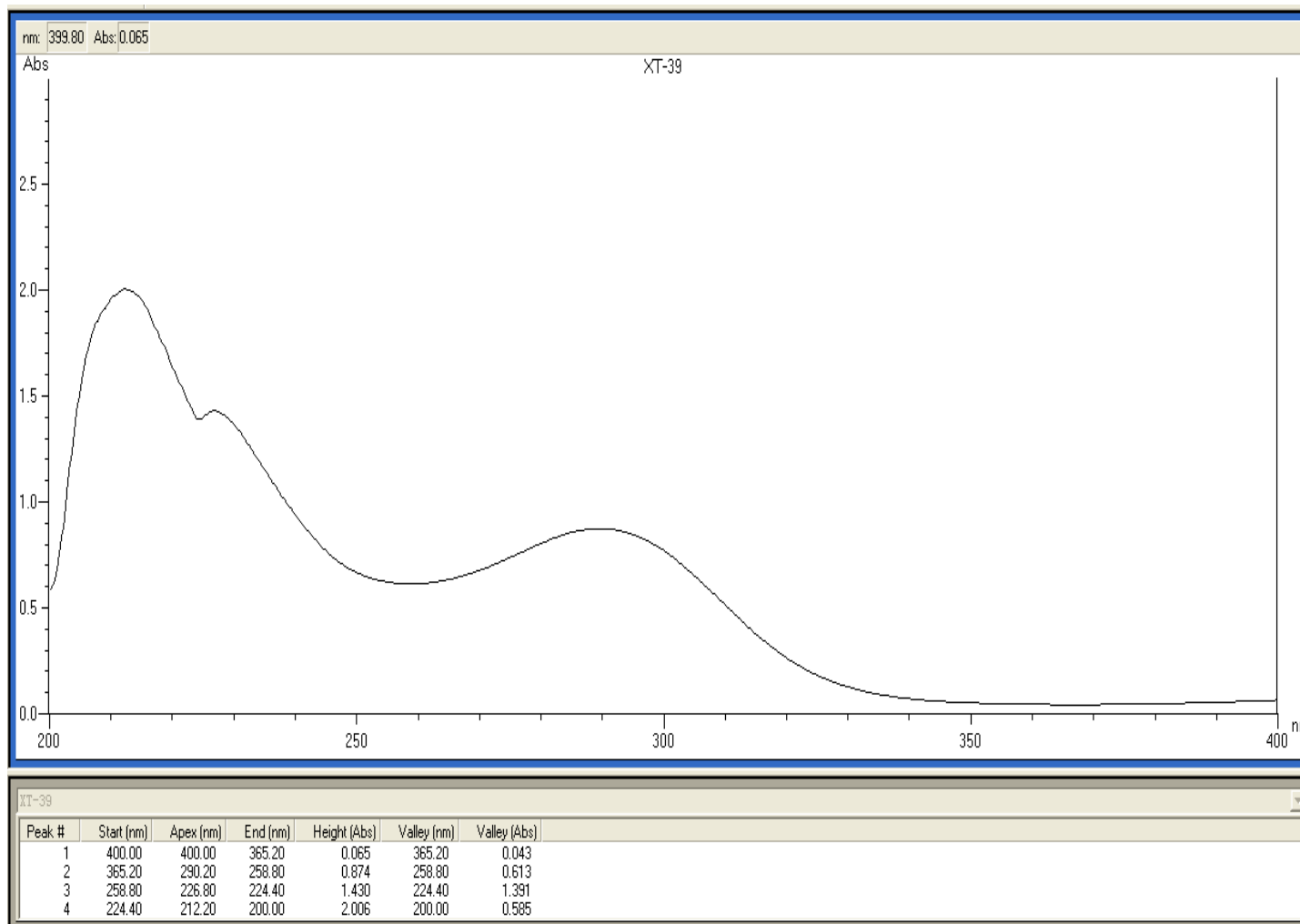
Dysidaminone K (11)

Figure S104. HRESIMS of Dysidaminone K (11).



Dysidaminone K (11)

Figure S105. CD Spectrum of Dysidaminone K (11) in MeOH.



Dysidaminone K (11)

Figure S106. UV Spectrum of Dysidaminone K (11) in MeOH.

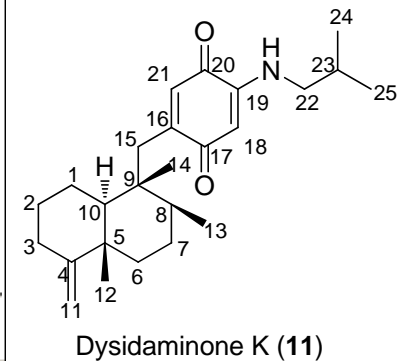
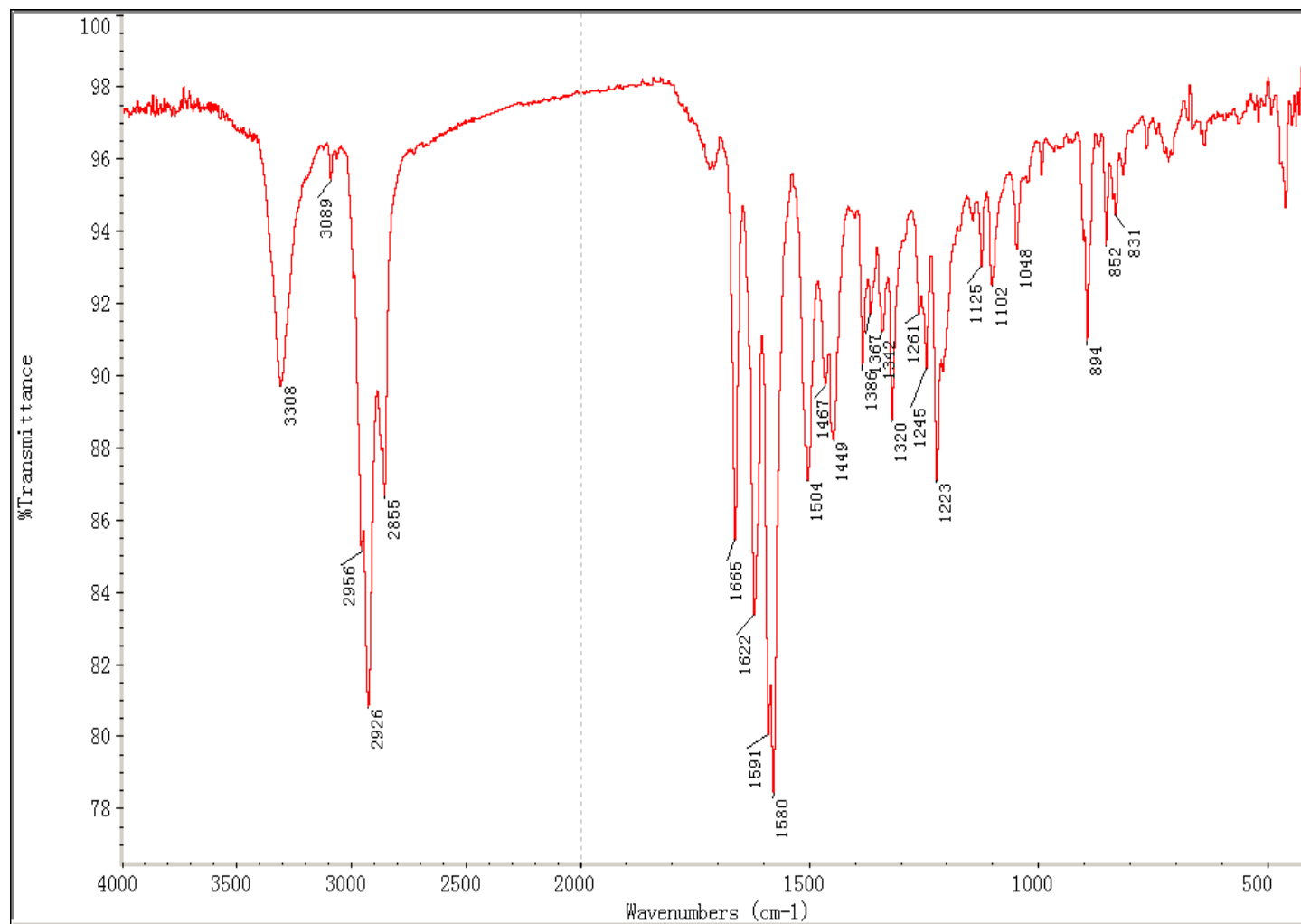
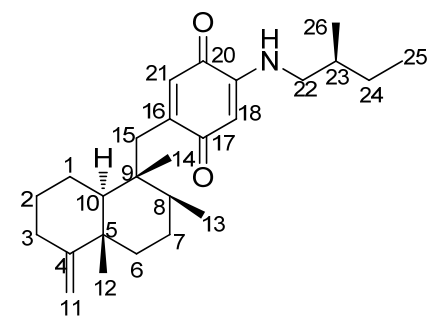
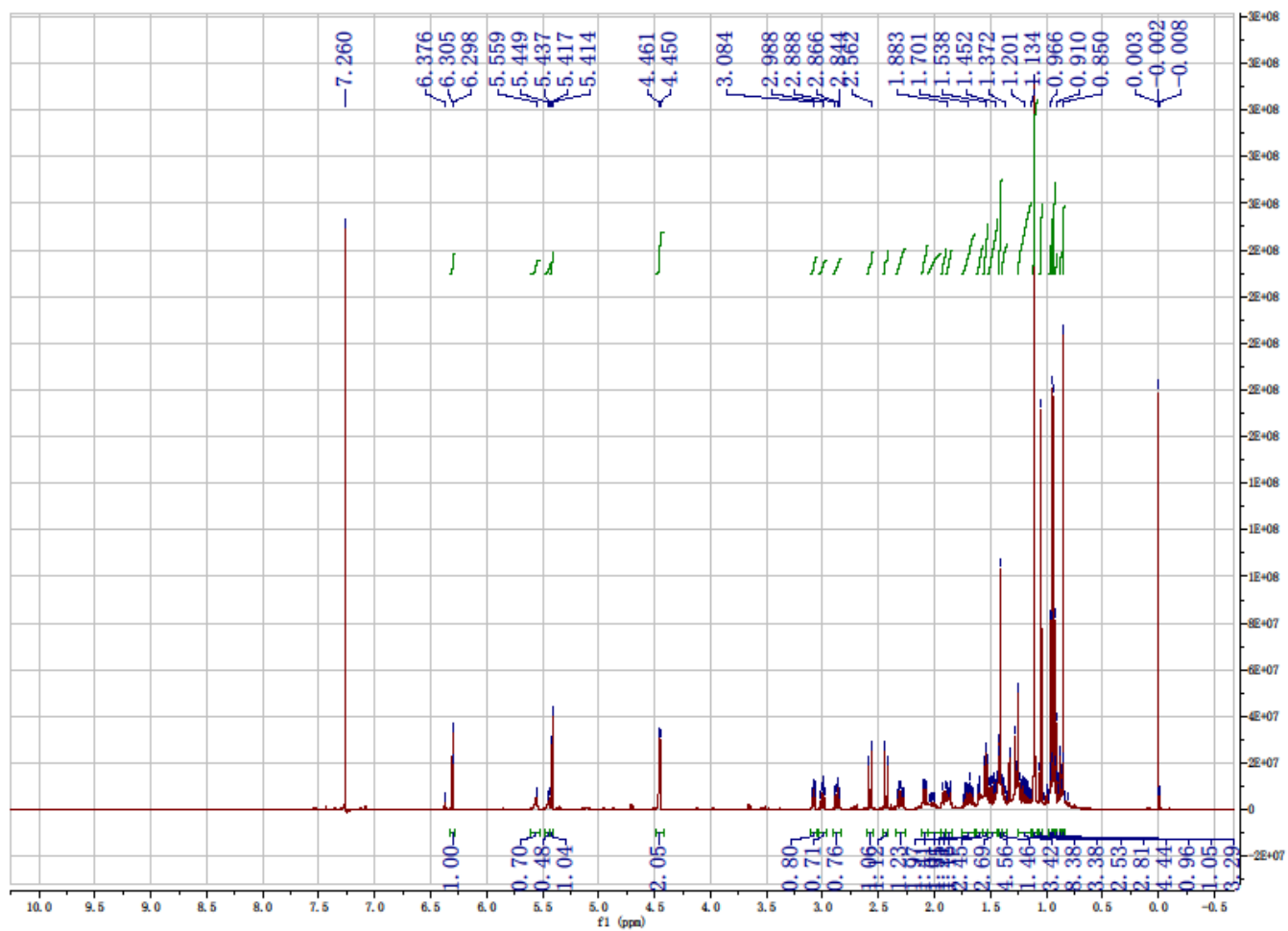
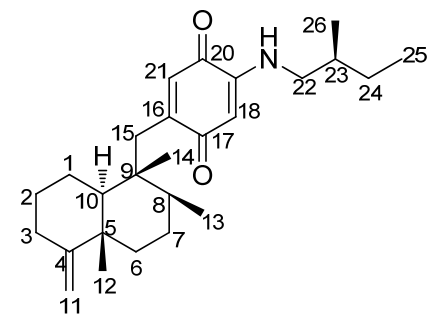
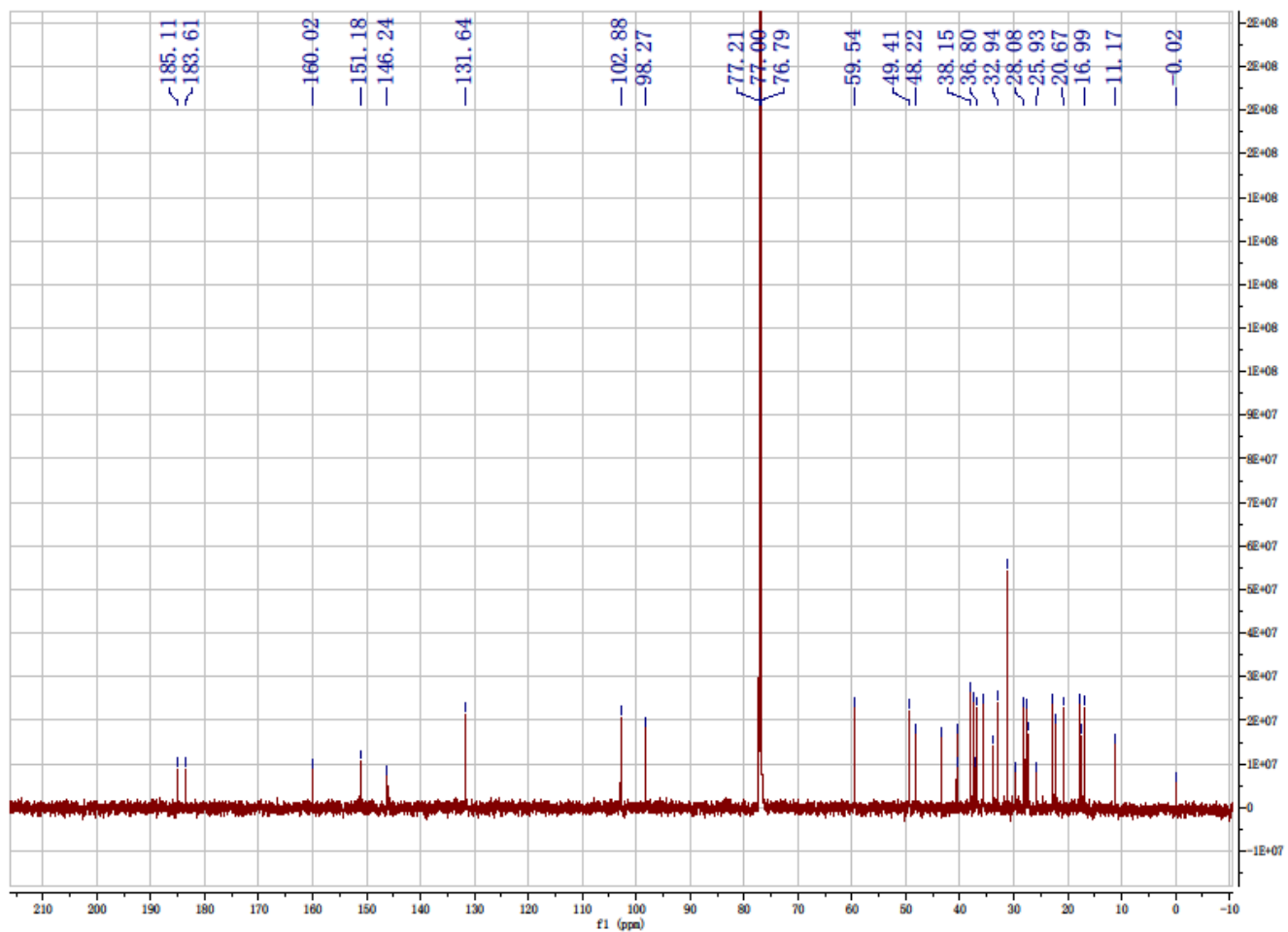


Figure S107. IR Spectrum of Dysidaminone K (11).



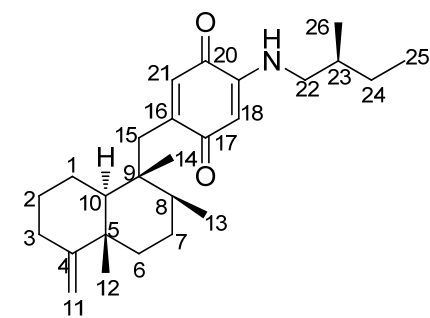
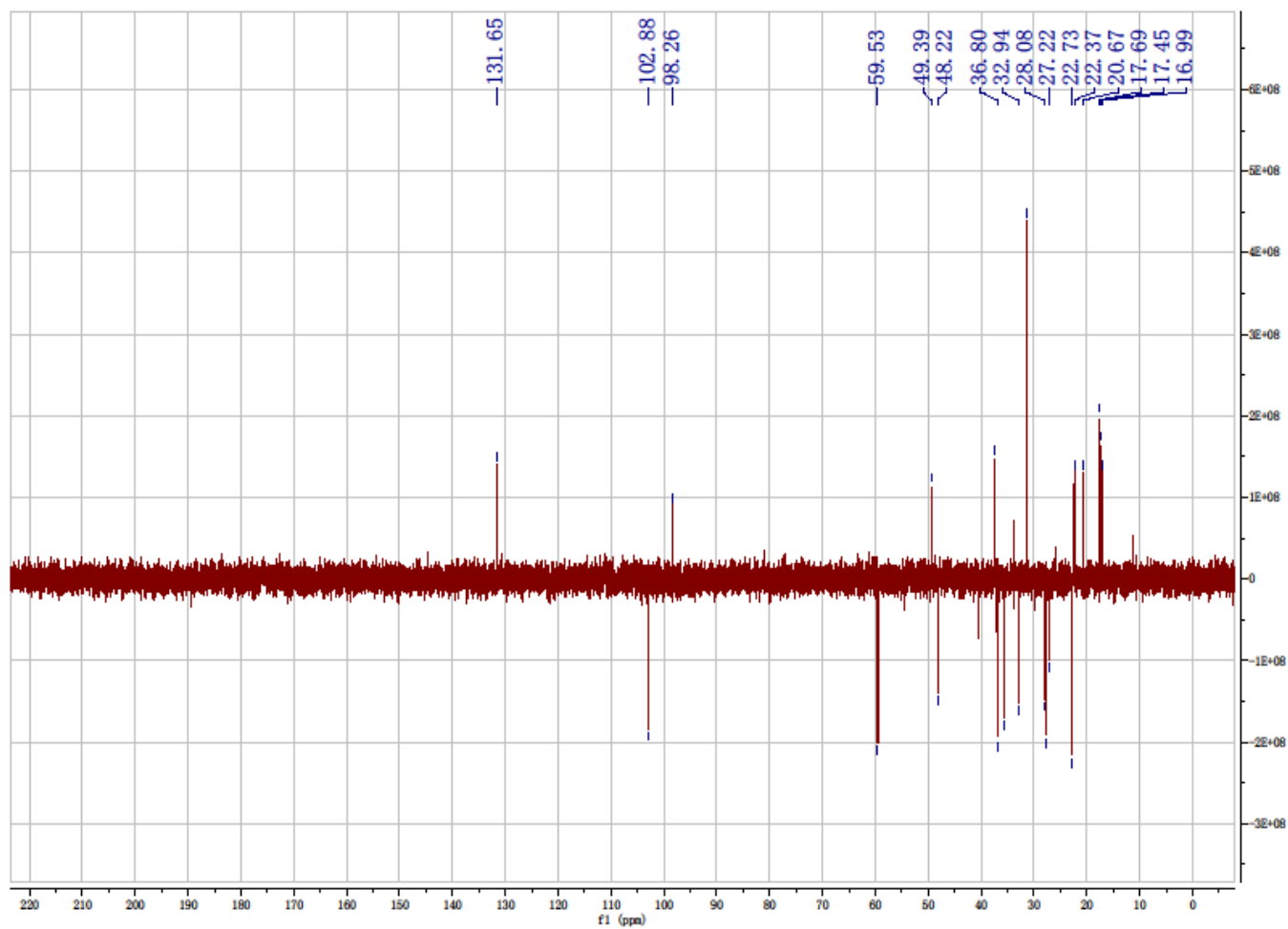
Dysidaminone L (12)

Figure S108. ^1H NMR Spectrum of Dysidaminone L (12) in CDCl_3 .



Dysidaminone L (**12**)

Figure S109. ^{13}C NMR Spectrum of Dysidaminone L (**12**) in CDCl_3 .



Dysidaminone L (12)

Figure S110. DEPT135 Spectrum of Dysidaminone L (12) in CDCl_3 .

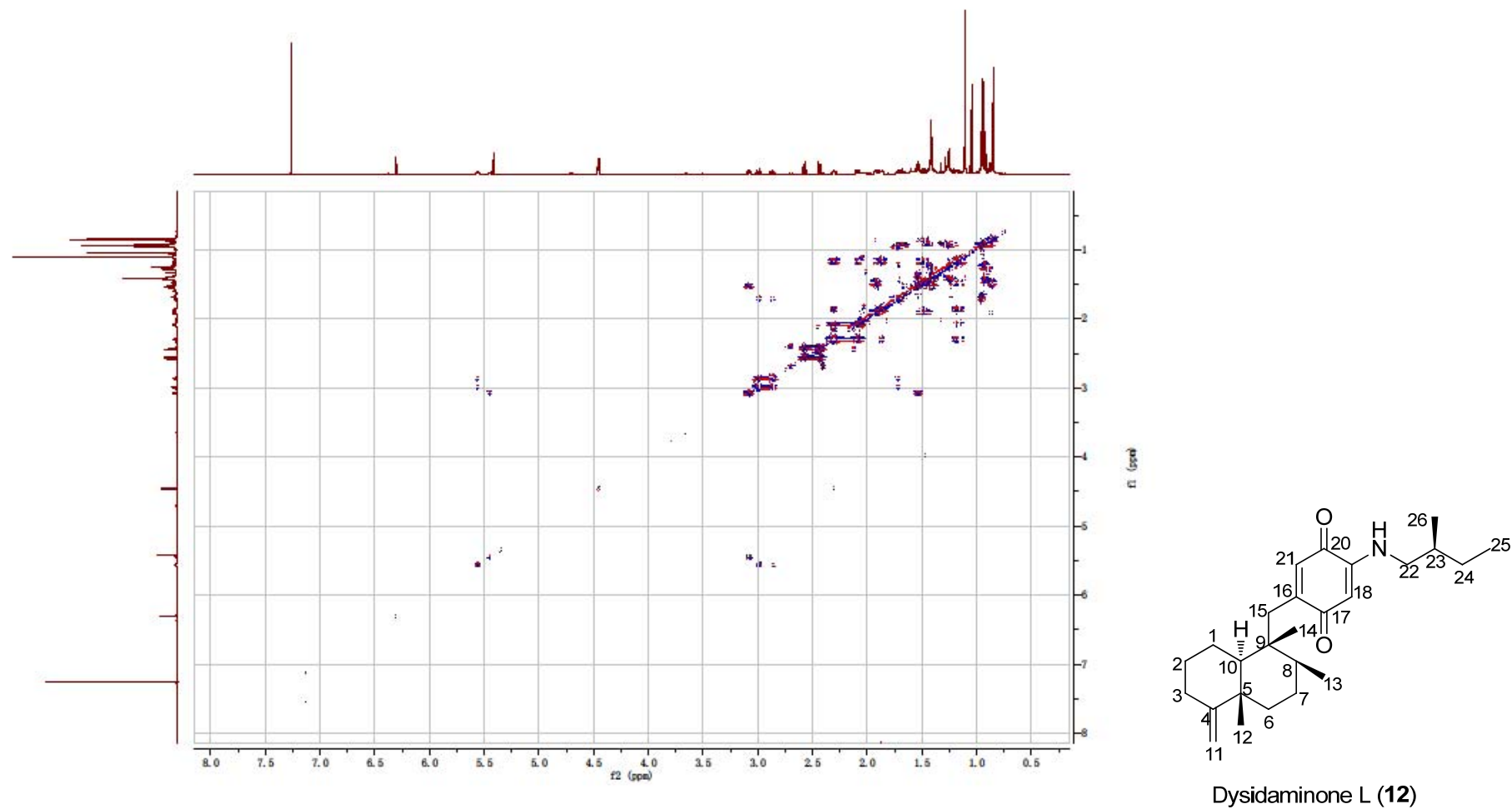


Figure S111. ^1H - ^1H COSY Spectrum of Dysidaminone L (12) in CDCl_3 .

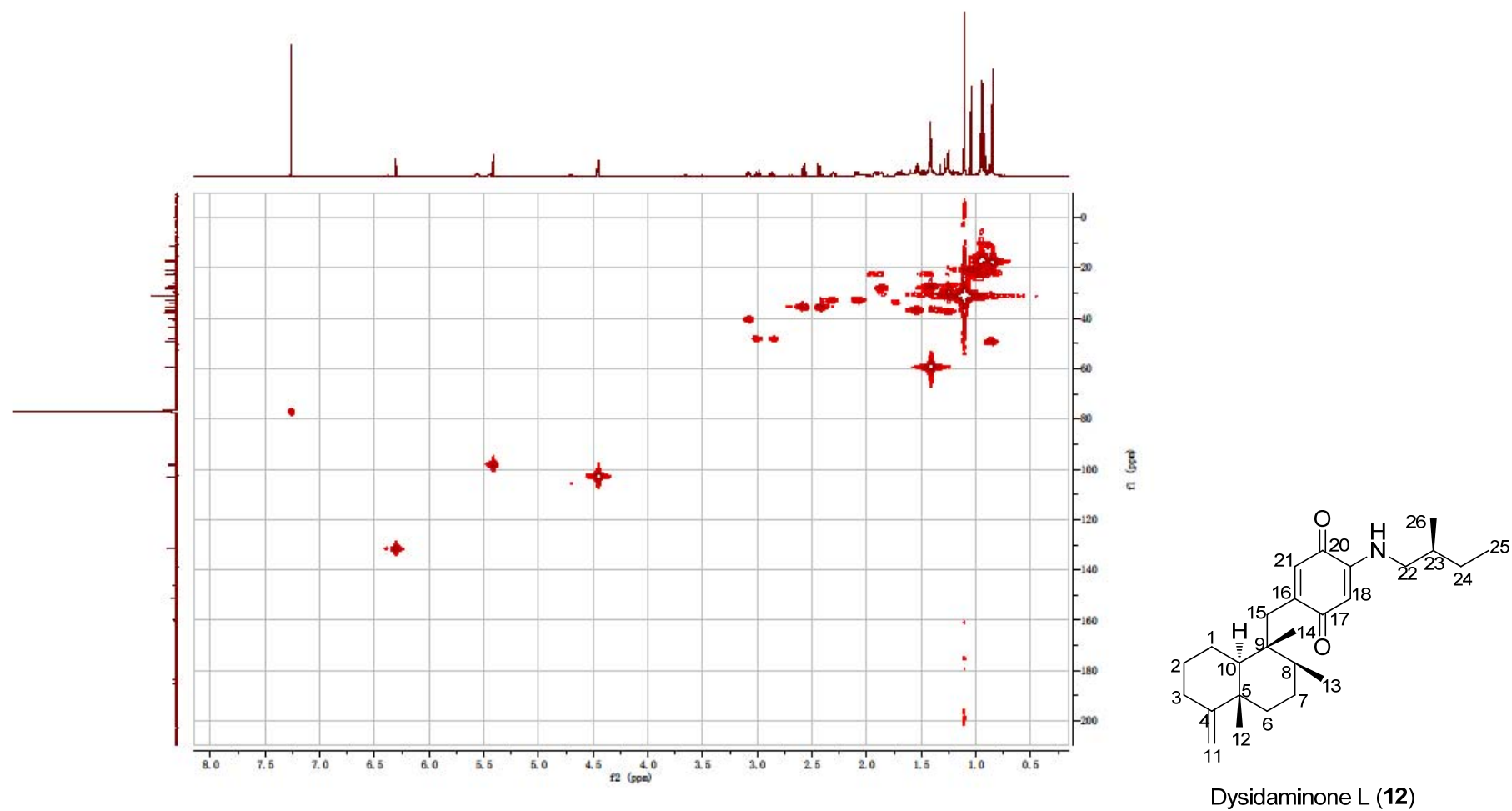


Figure S112. HSQC Spectrum of Dysidaminone L (**12**) in CDCl₃.

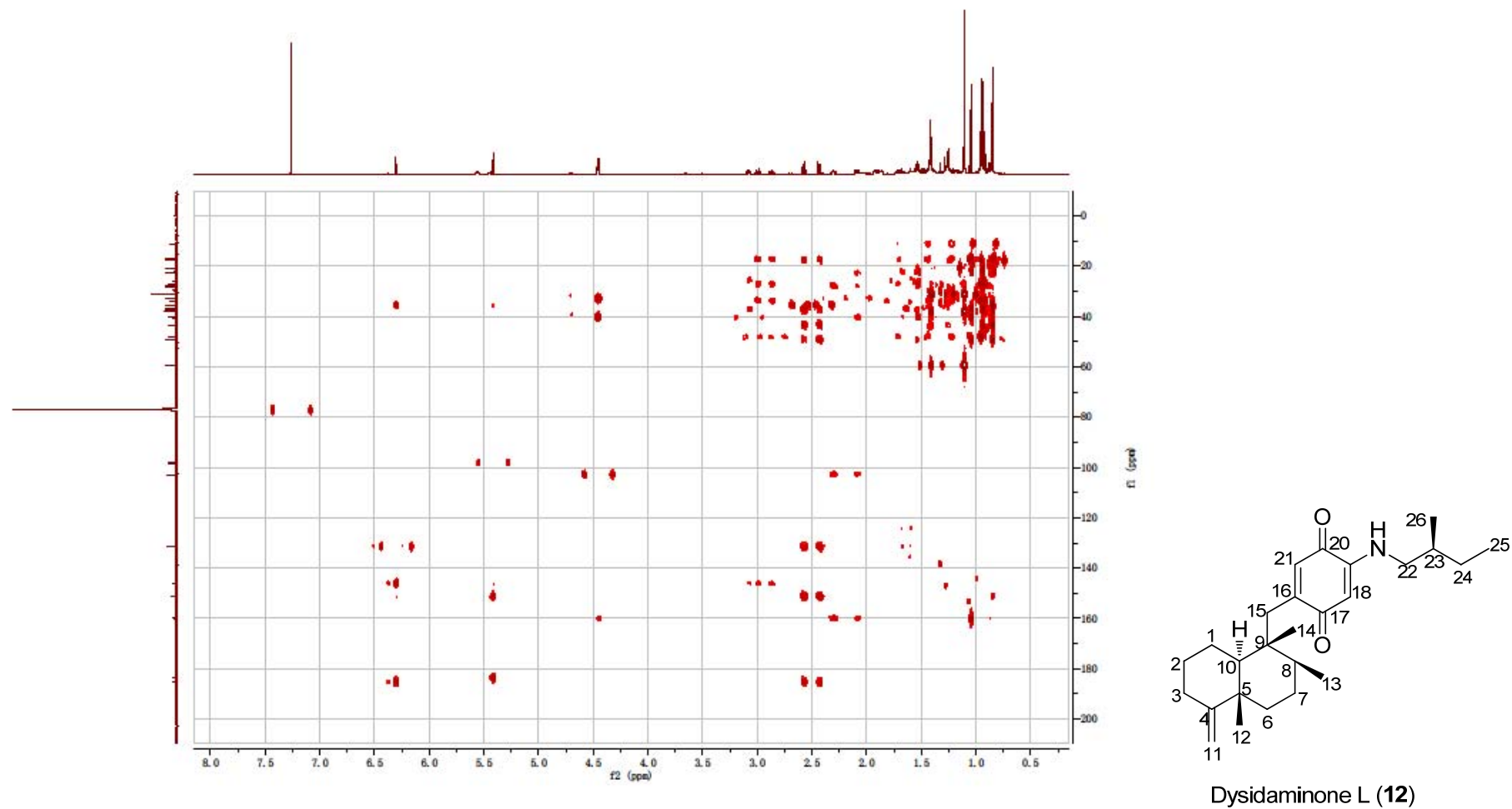


Figure S113. HMBC Spectrum of Dysidaminone L (**12**) in CDCl₃.

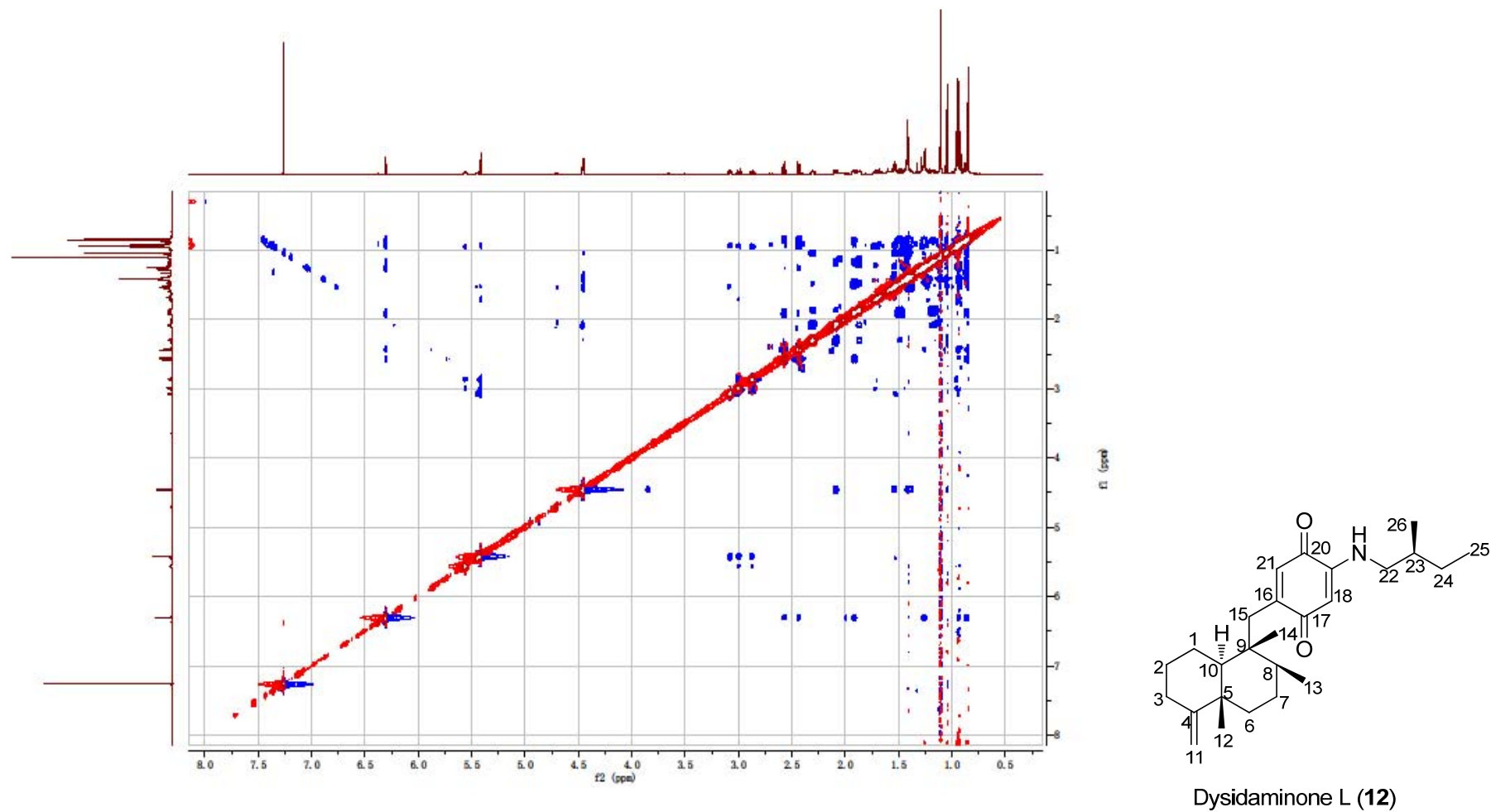


Figure S114. NOESY Spectrum of Dysidaminone L (**12**) in CDCl₃.

Elemental Composition Report

Page 1

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

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SIP1

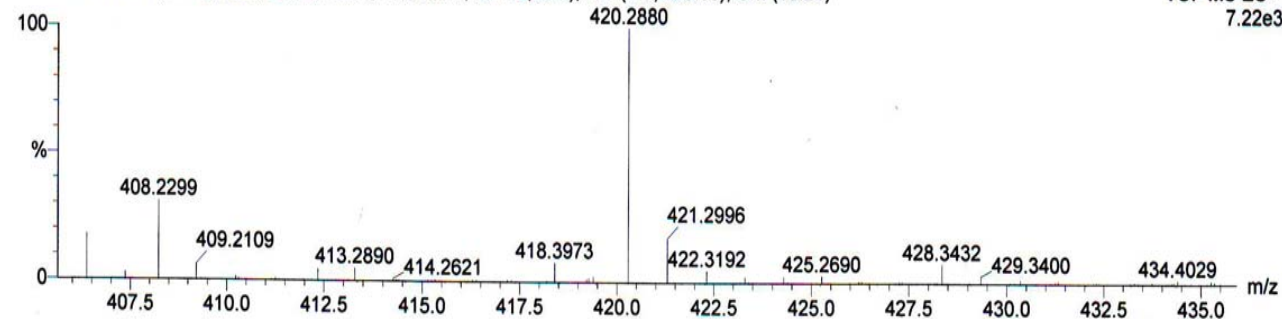
XT-41 M.W=397

WQ13-110H1 13 (0.449) AM (Cen,4, 80.00, Ar,5000.0,407.22,0.70); Sm (SG, 2x3.00); Cm (13:21)

Q-Tof micro
YA019
420.2880

08-May-2013,15:04:03

TOF MS ES+
7.22e3

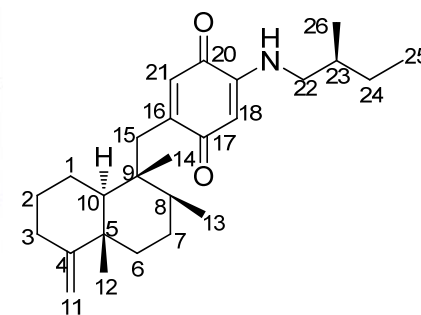


Minimum: 50.00

Maximum: 100.00

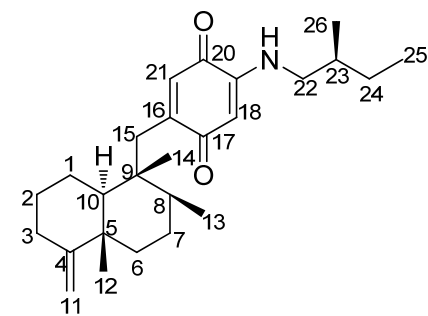
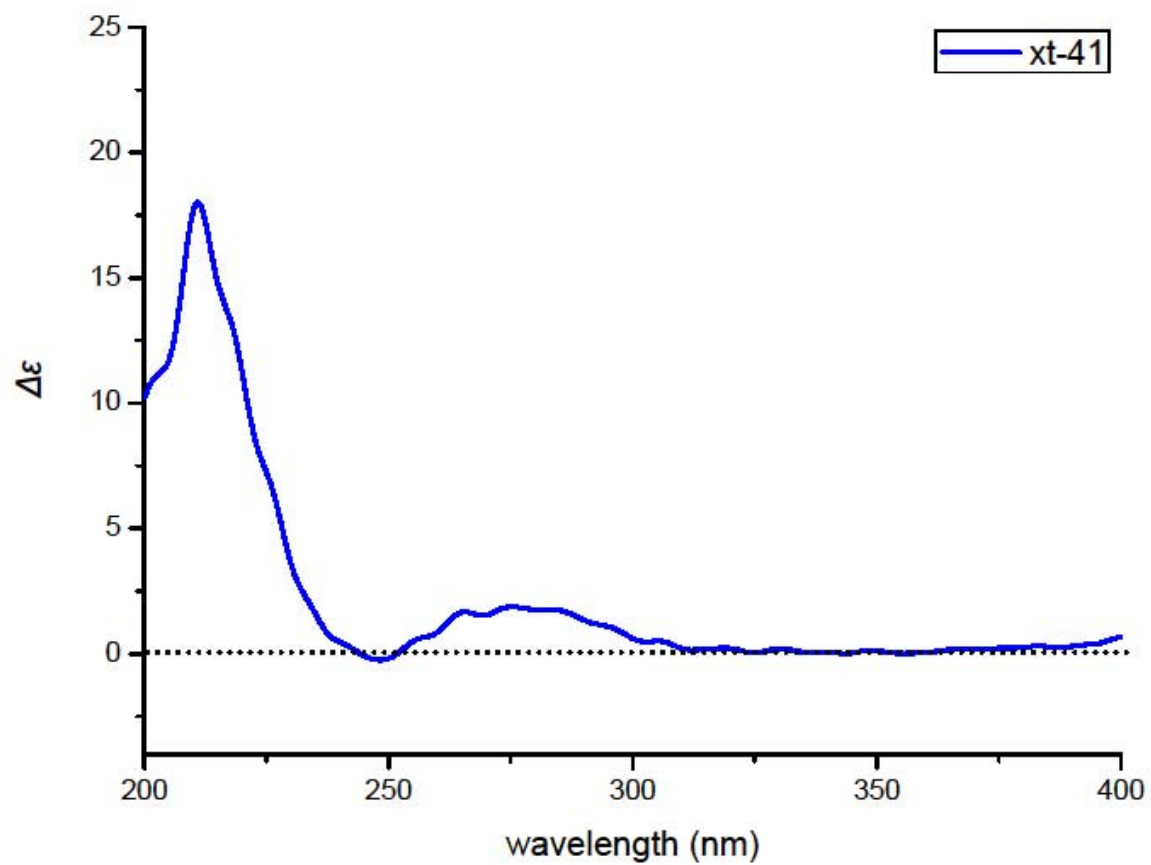
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
------	----	------------	-----	-----	-----	-------	---------

420.2880	100.00	420.2878	0.2	0.5	7.5	232.0	C26 H39 N O2 Na
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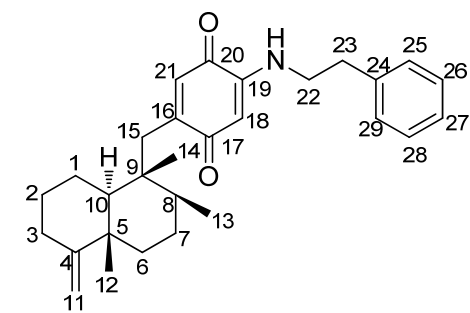
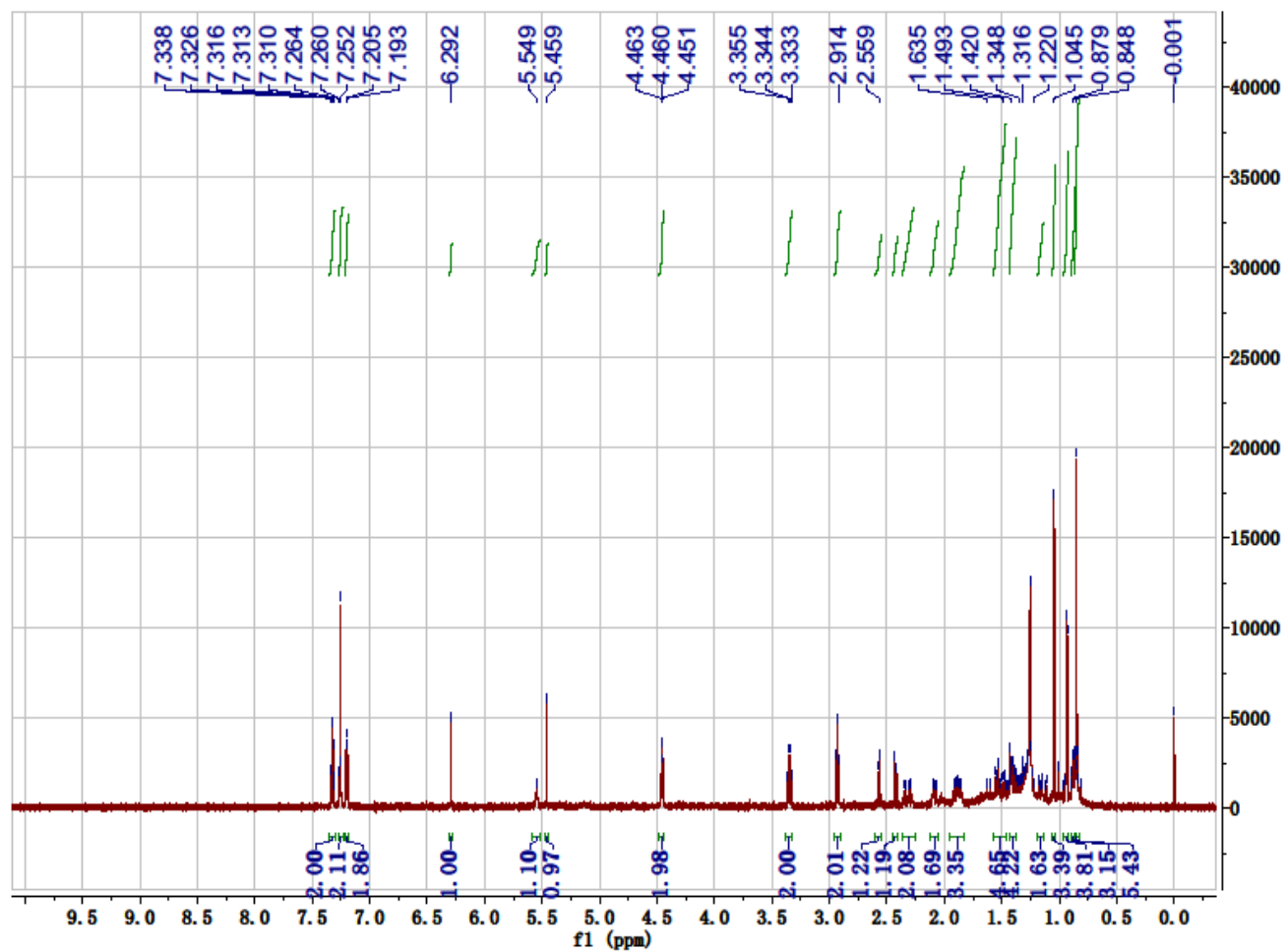
Dysidaminone L (**12**)

Figure S115. HRESIMS of Dysidaminone L (**12**).



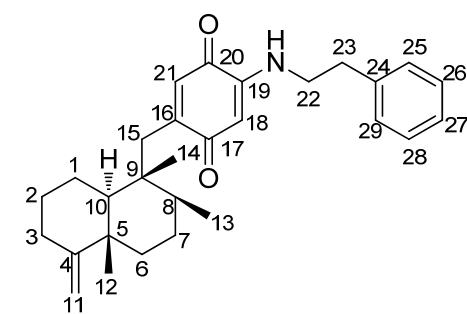
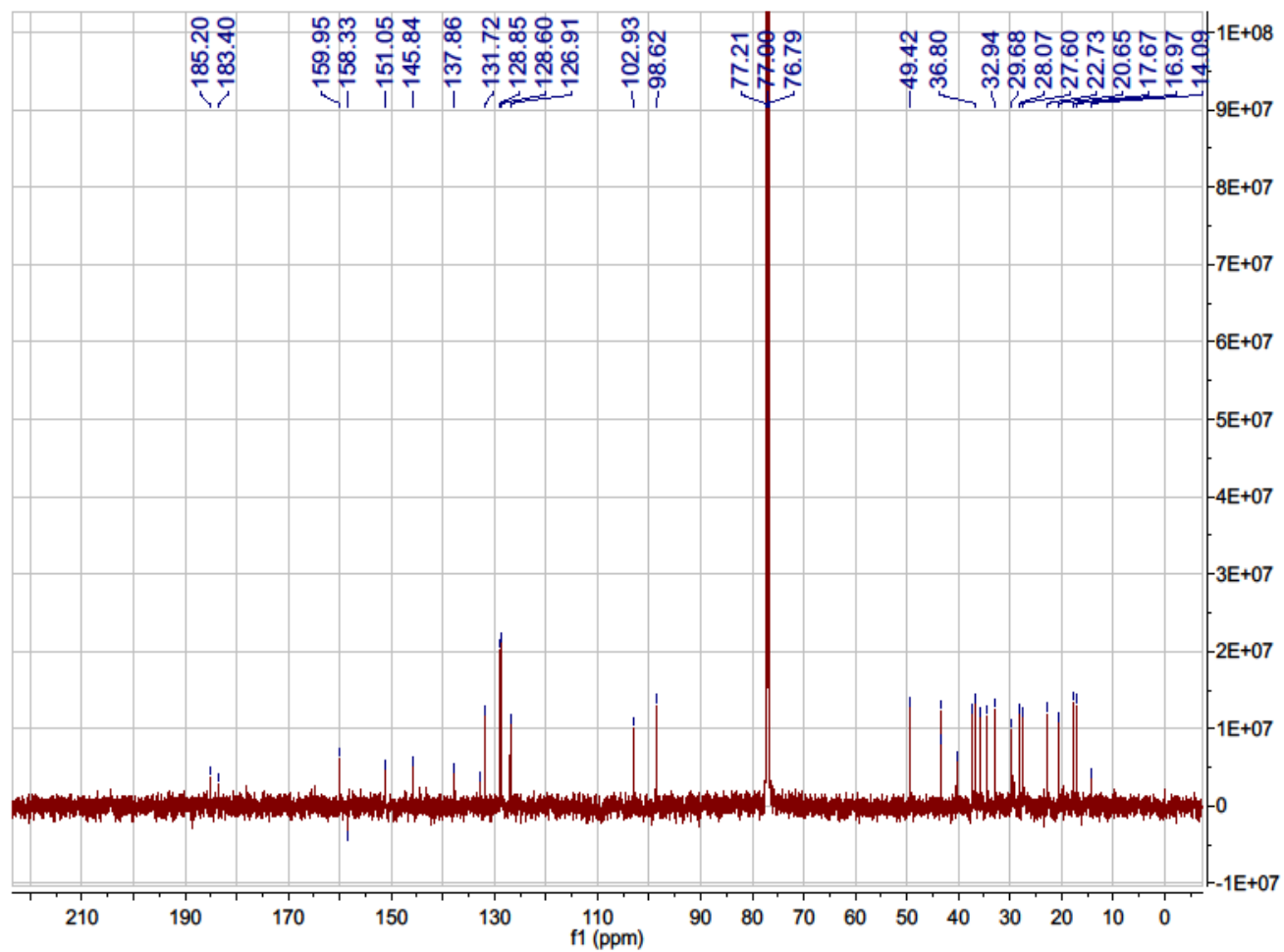
Dysidaminone L (**12**)

Figure S116. CD Spectrum of Dysidaminone L (**12**) in MeOH.



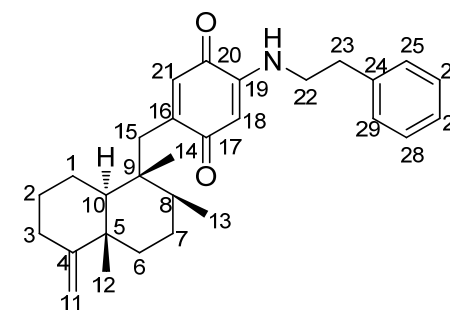
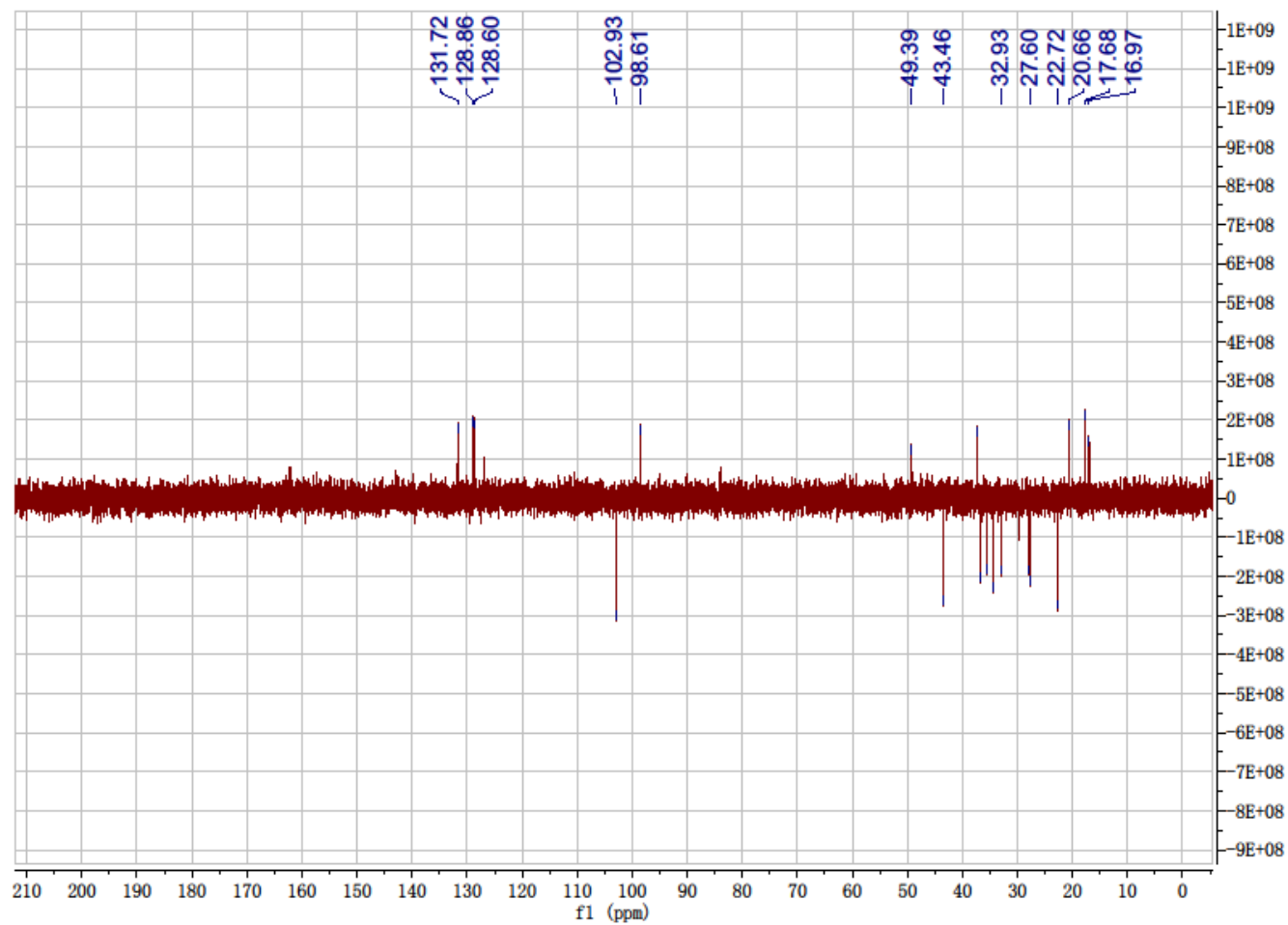
Dysidaminone M (**13**)

Figure S117. ^1H NMR Spectrum of Dysidaminone M (**13**) in CDCl_3 .



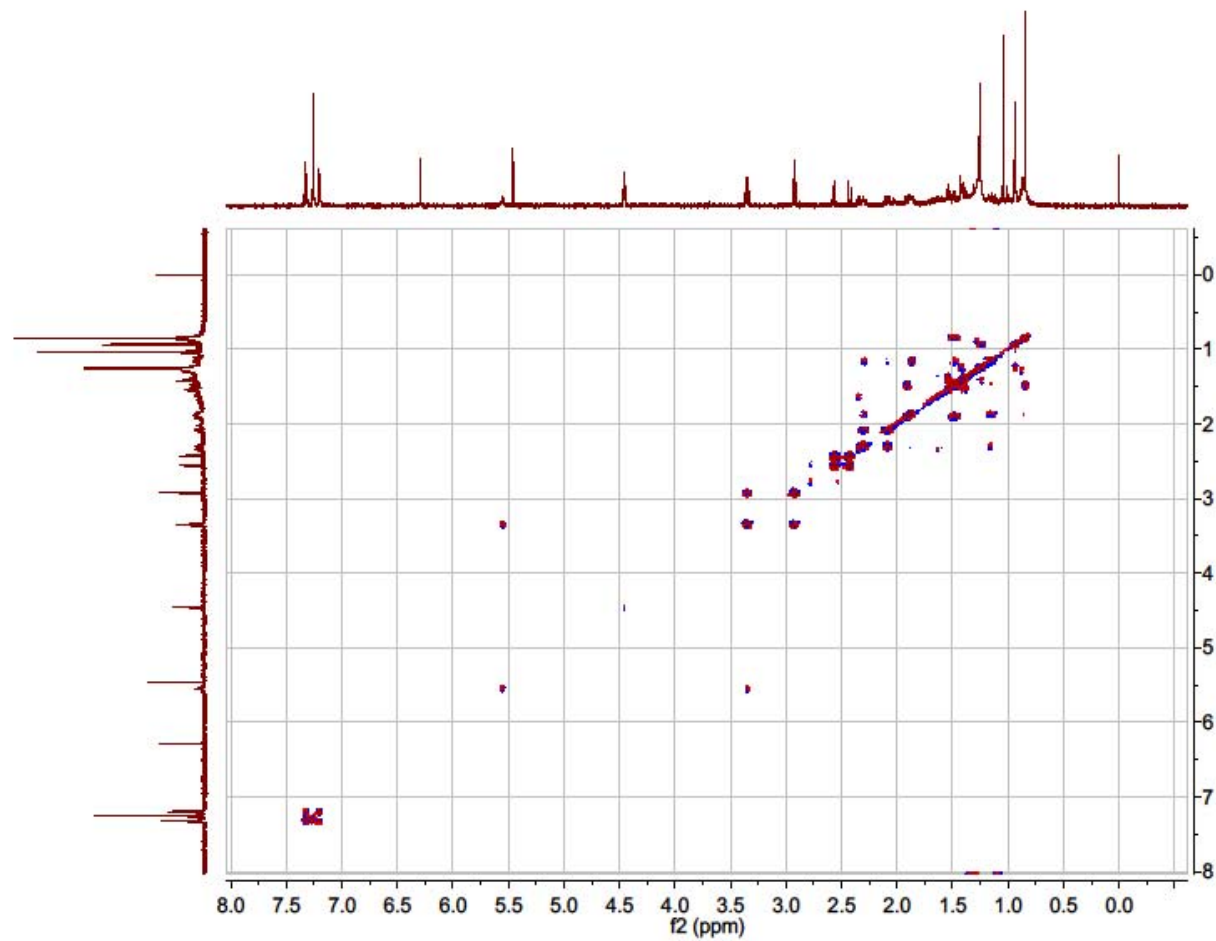
Dysidaminone M (13)

Figure S118. ^{13}C NMR Spectrum of Dysidaminone M (13) in CDCl_3 .

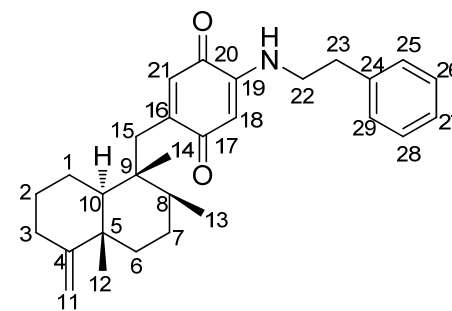


Dysidaminone M (**13**)

Figure S119. DEPT135 Spectrum of Dysidaminone M (**13**) in CDCl_3 .



f1 (ppm)



Dysidaminone M (**13**)

Figure S120. ^1H - ^1H COSY Spectrum of Dysidaminone M (**13**) in CDCl_3 .

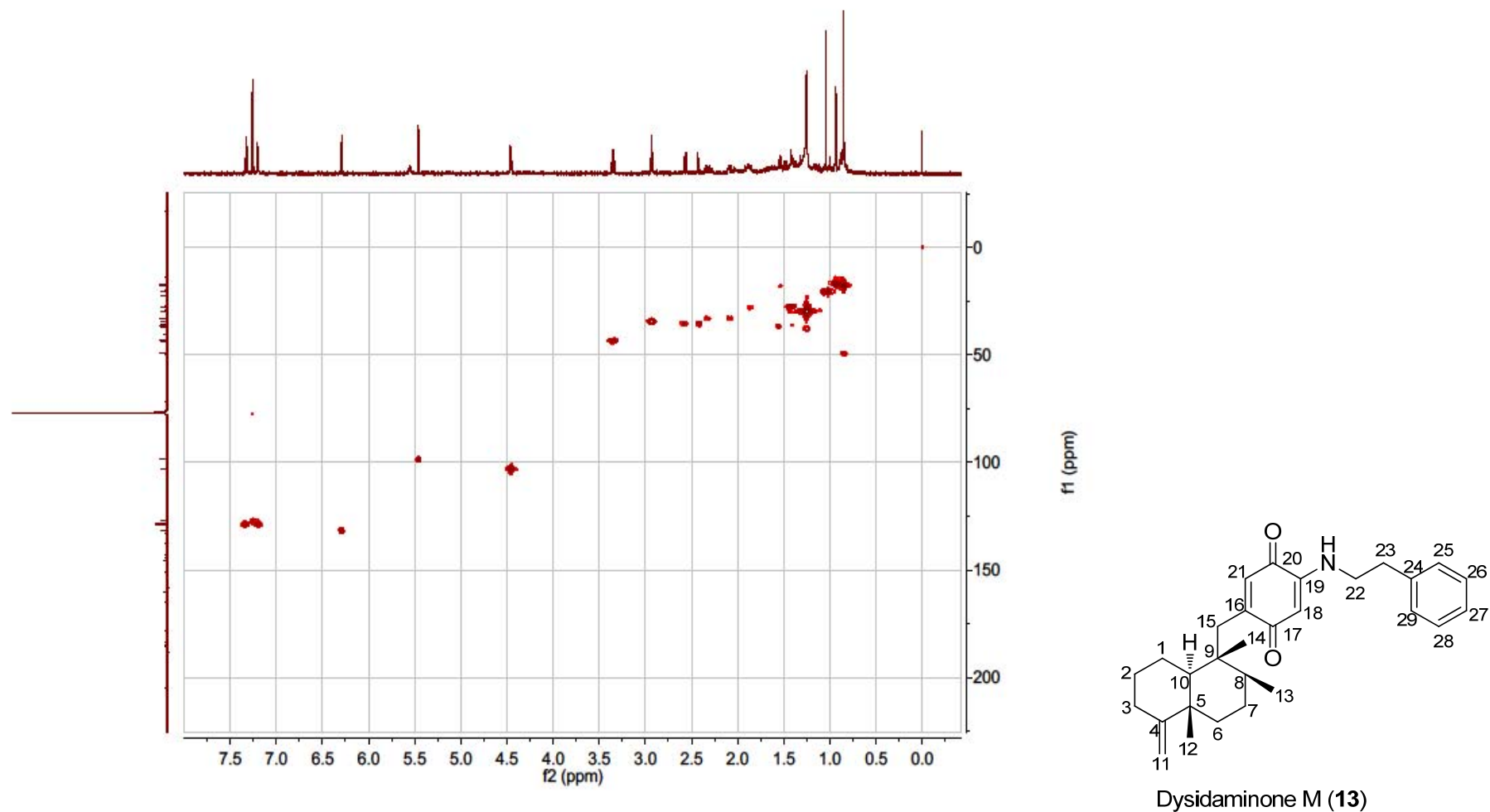
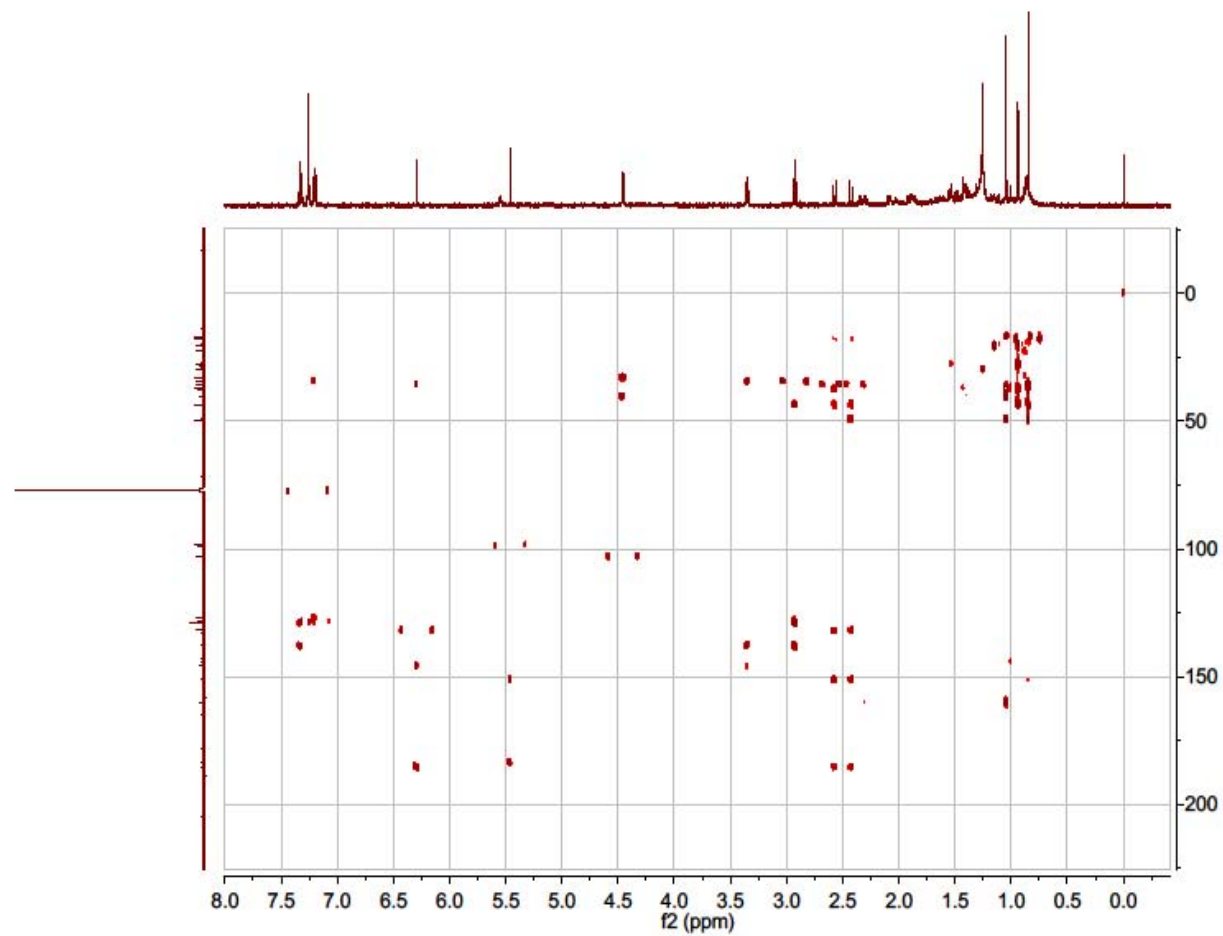
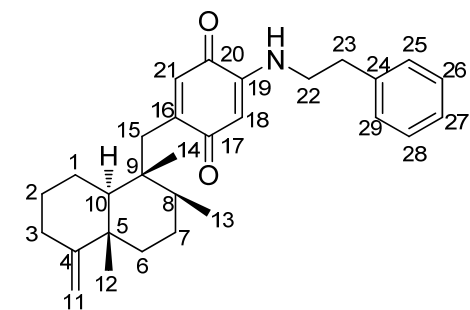


Figure S121. HSQC Spectrum of Dysidaminone M (13) in CDCl₃.



f1 (ppm)



Dysidaminone M (**13**)

Figure S122. HMBC Spectrum of Dysidaminone M (**13**) in CDCl₃.

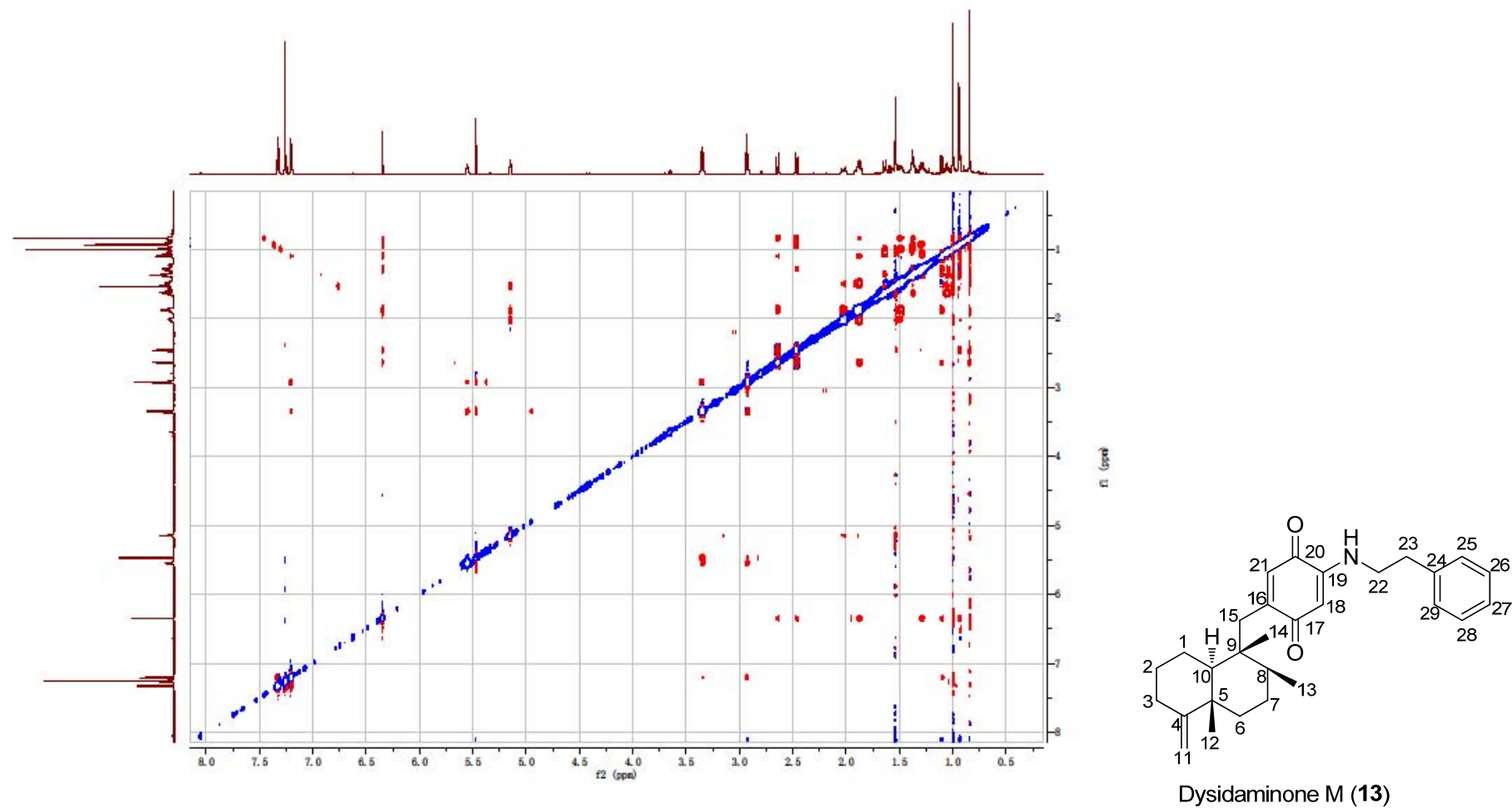
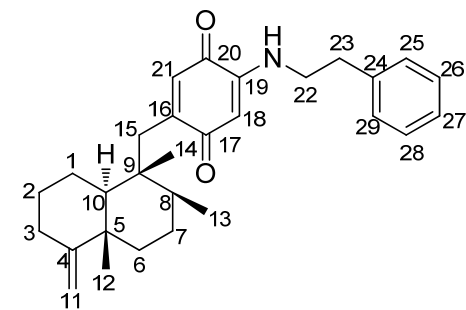
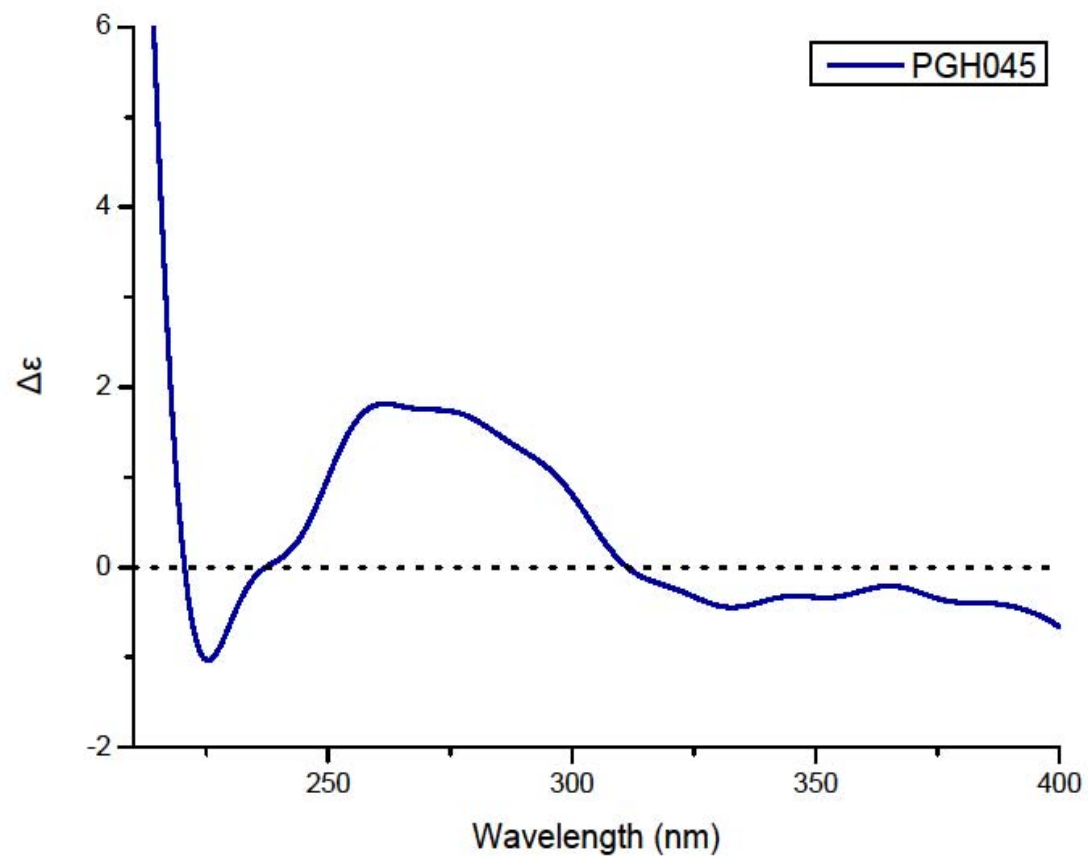


Figure S123. NOESY Spectrum of Dysidaminone M (13) in CDCl₃.



Dysidaminone M (**13**)

Figure S124. CD Spectrum of Dysidaminone M (**13**) in MeOH.