Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Bioactive Sesquiterpene Quinols and Quinones from the Marine Sponge *Dysidea avara*

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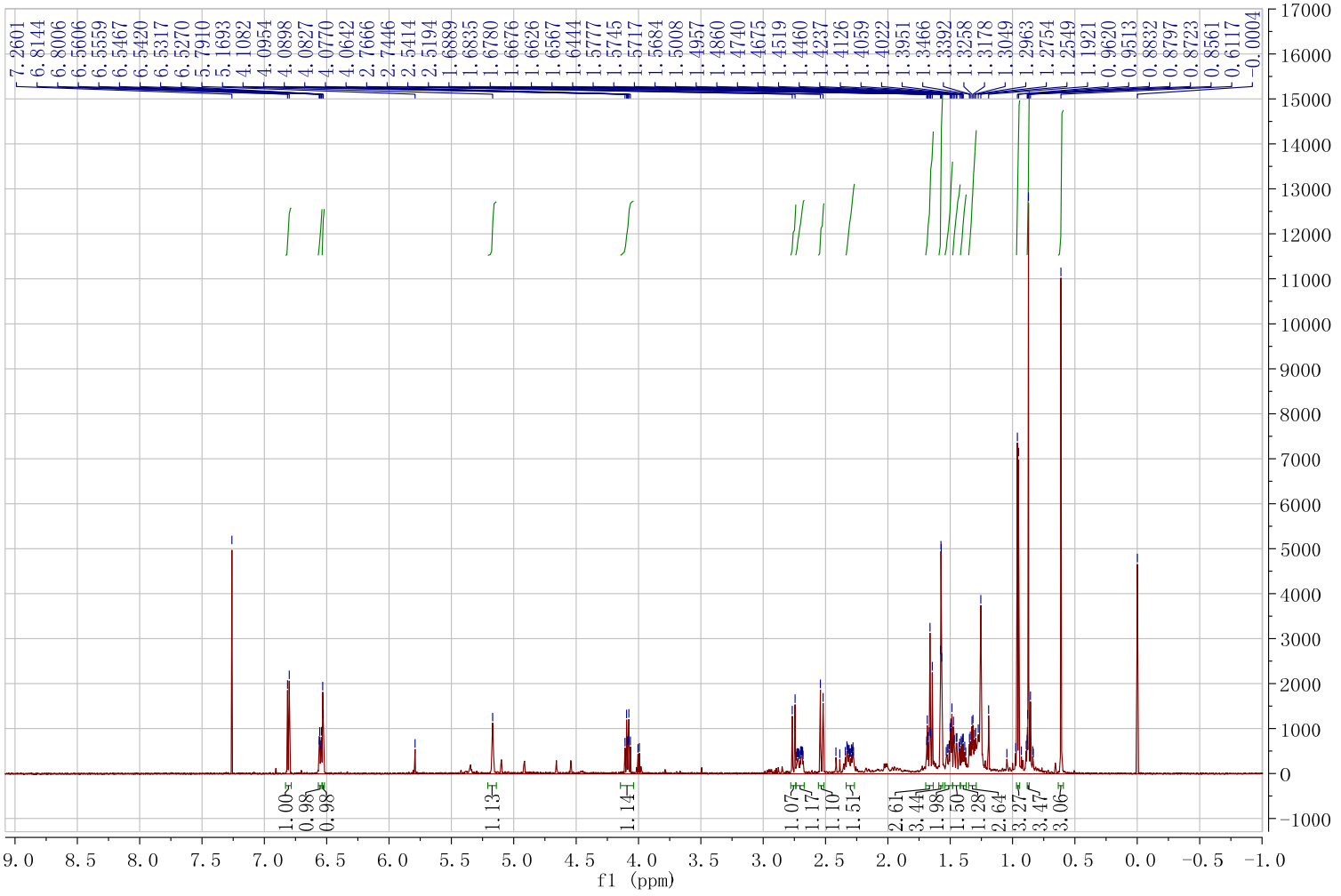
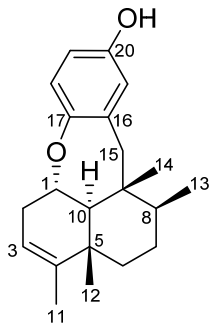
Figure S88. IR Spectrum of (5*R*,8*R*,9*S*,10*R*)-19-ethoxylavarone (**8**).





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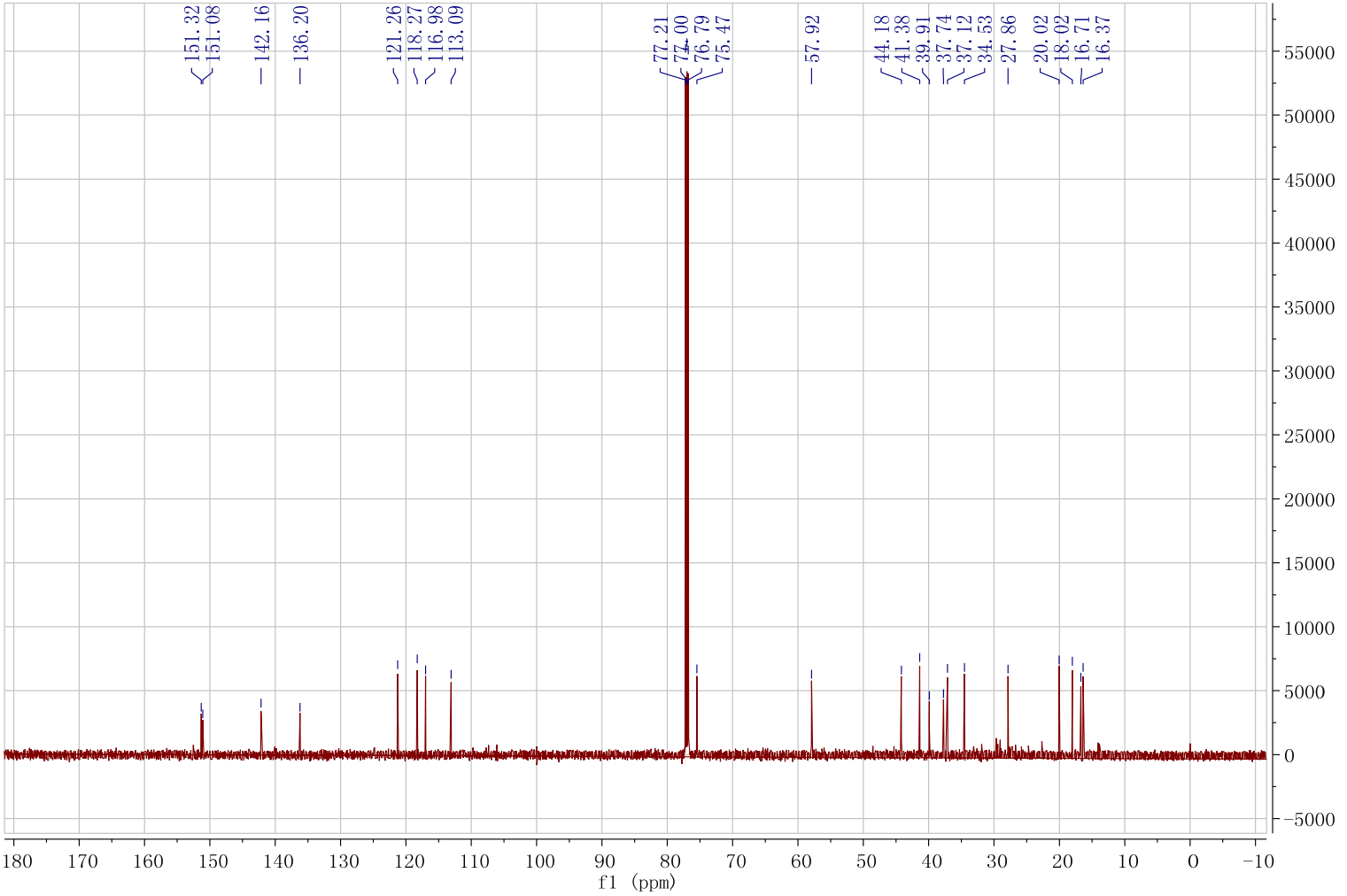

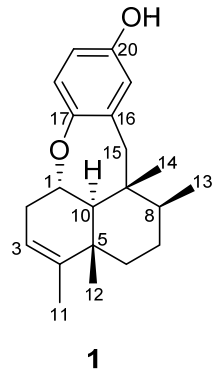

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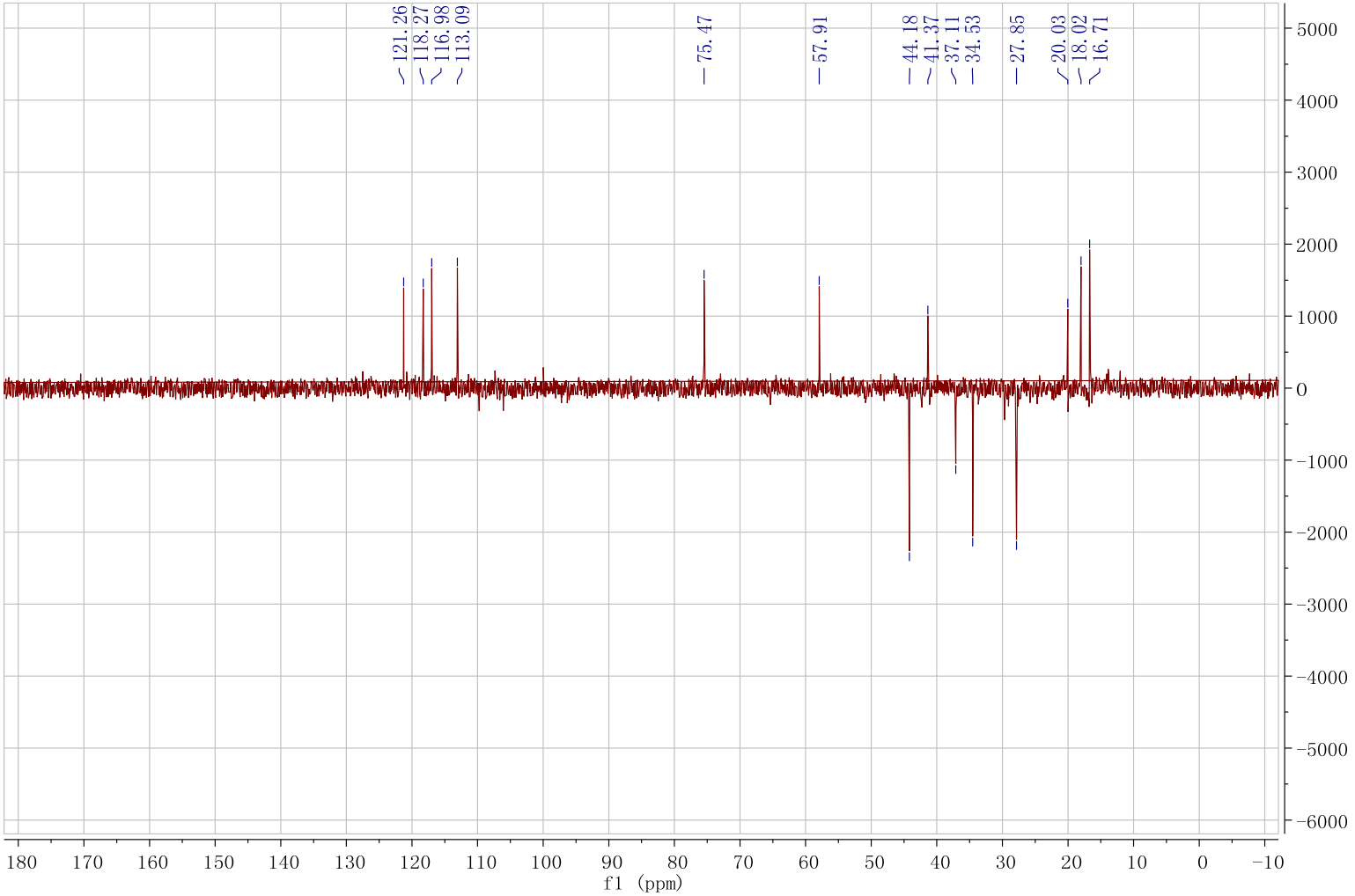
Figure S2. ^{13}C NMR Spectrum of Dysiquinol A (**1**) in $CDCl_3$.



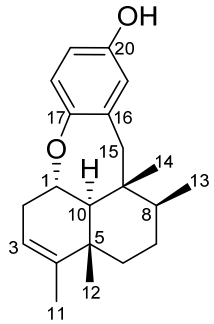


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Figure S3. DEPT135 Spectrum of Dysiquinol A (**1**) in $CDCl_3$.

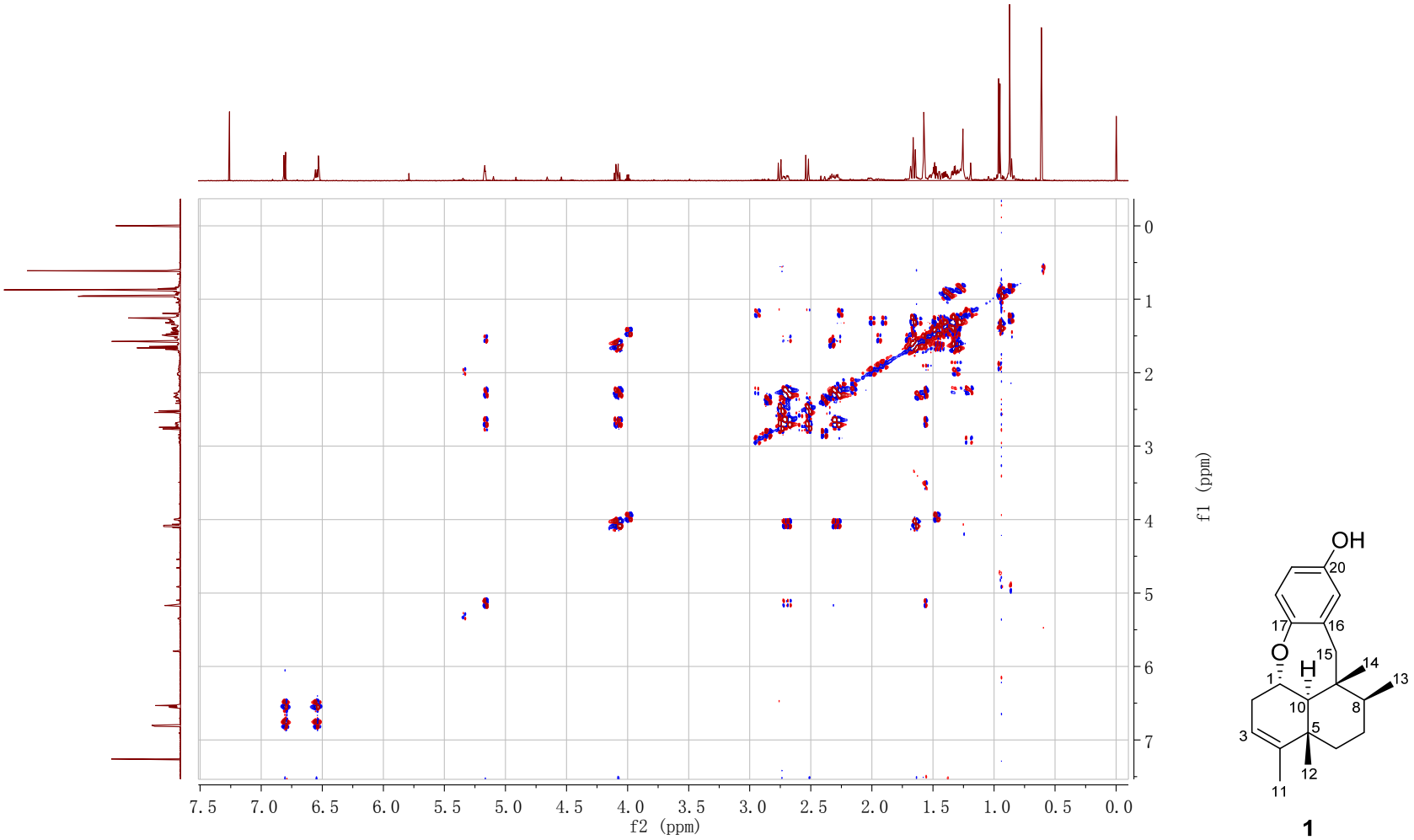

Figure S4. ^{1}H-^{1}H COSY Spectrum of Dysiquinol A (**1**) in $CDCl_3$.

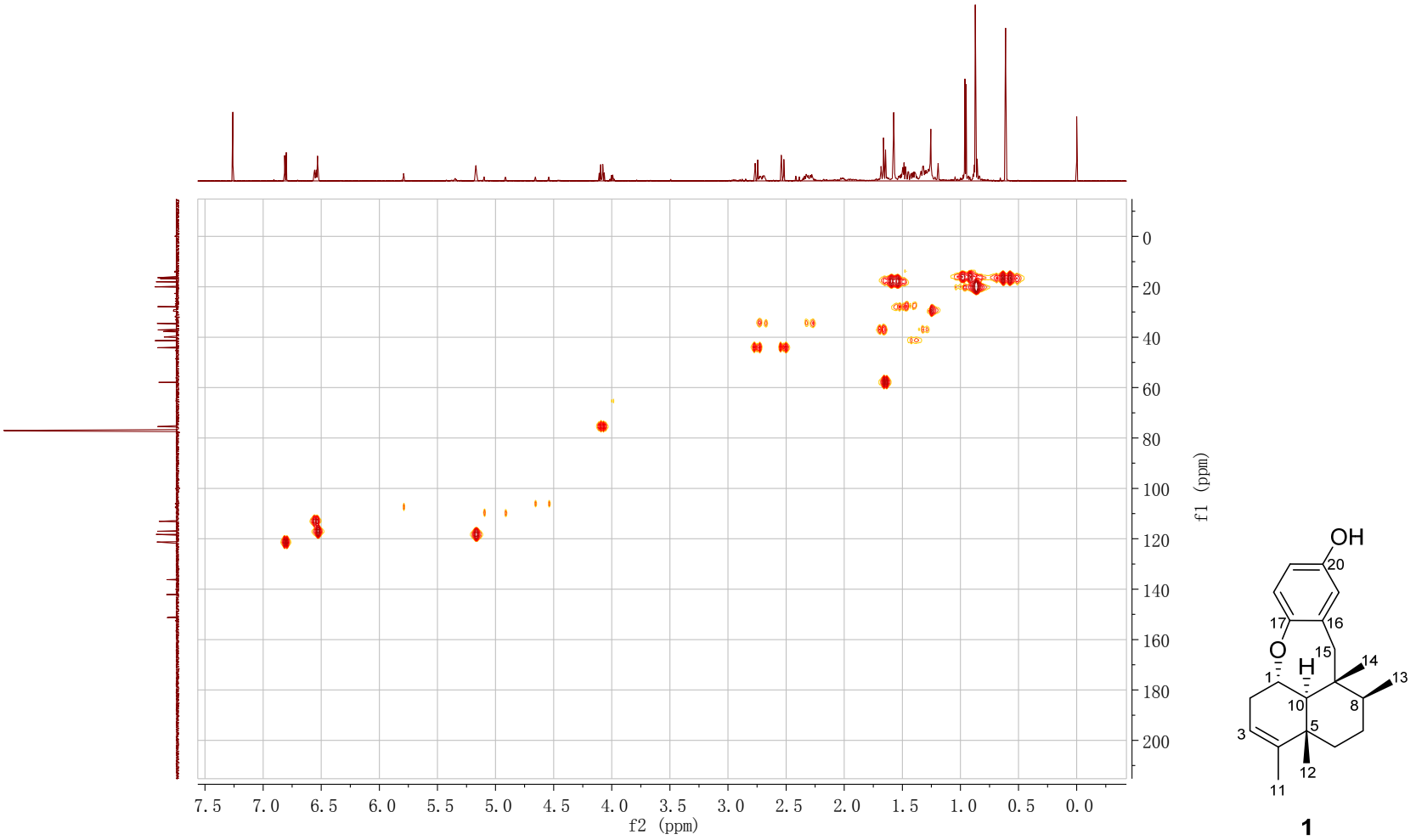

Figure S5. HSQC Spectrum of Dysiquinol A (**1**) in $CDCl_3$.

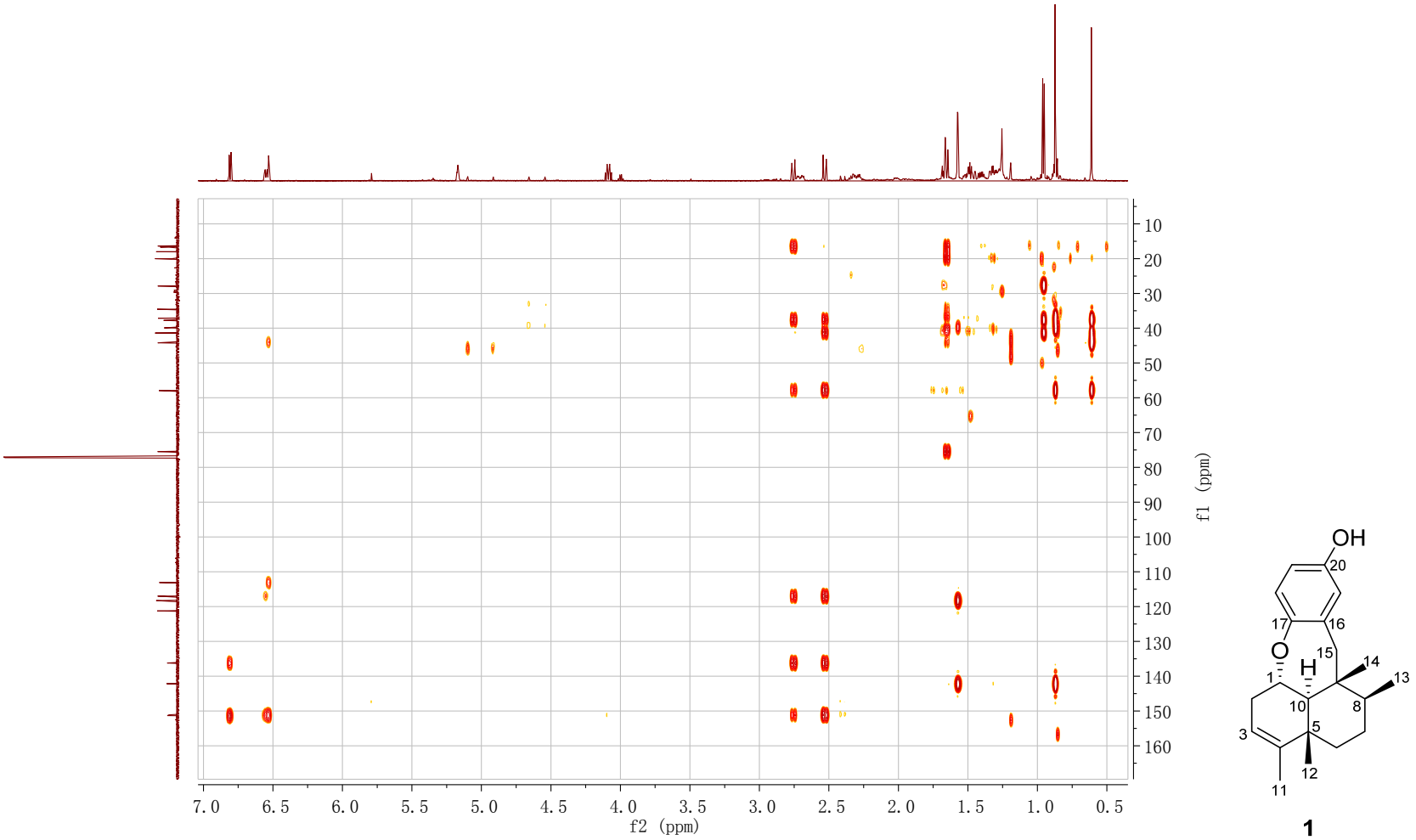

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Figure S6. HMBC Spectrum of Dysiquinol A (**1**) in $CDCl_3$.

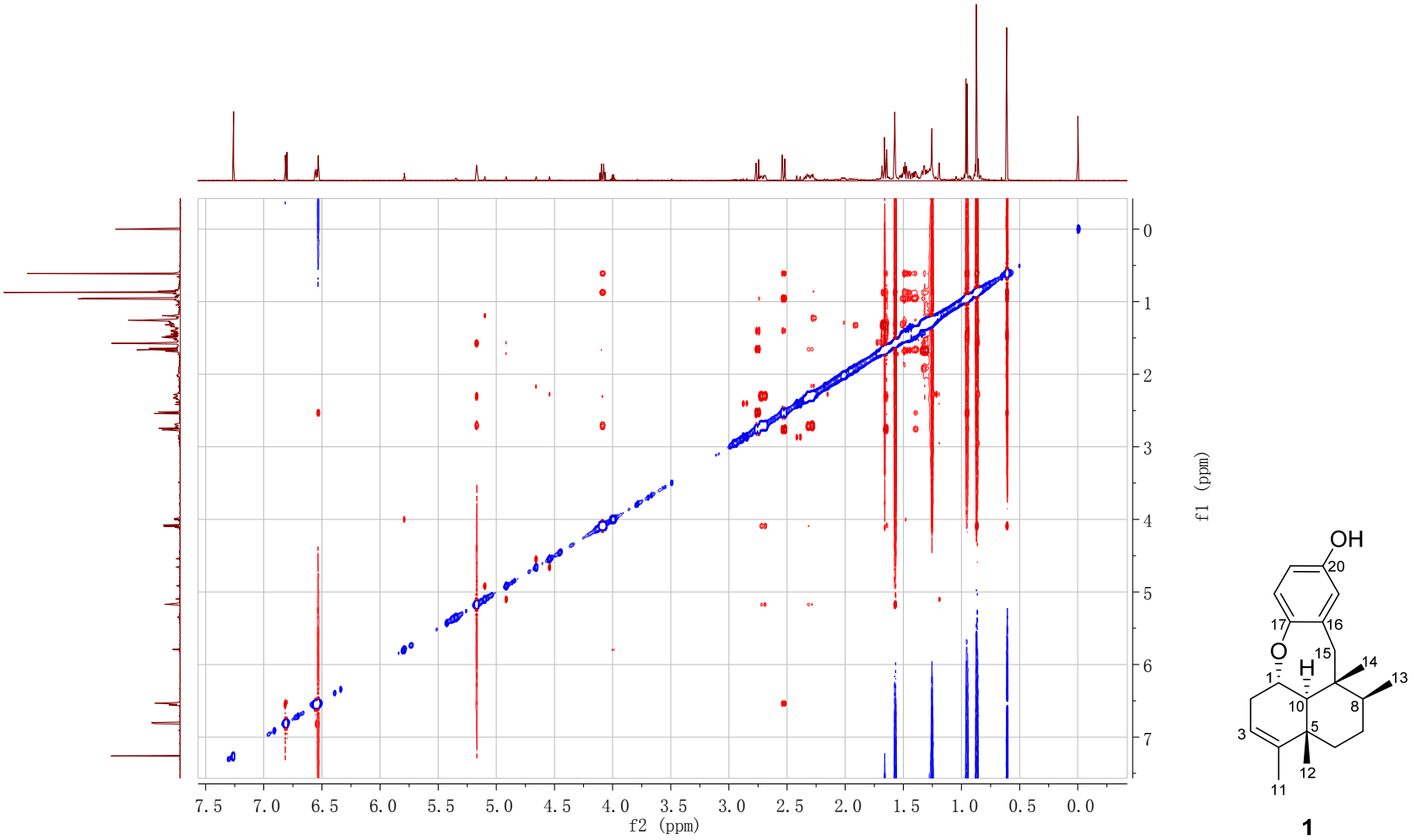

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Figure S7. NOESY Spectrum of Dysiquinol A (**1**) in $CDCl_3$.

Elemental Composition Report G2H4E3 **Page 1**

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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)
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Q-Tof micro
YA019

13-Jul-2012,10:58:39

TOF MS ES+
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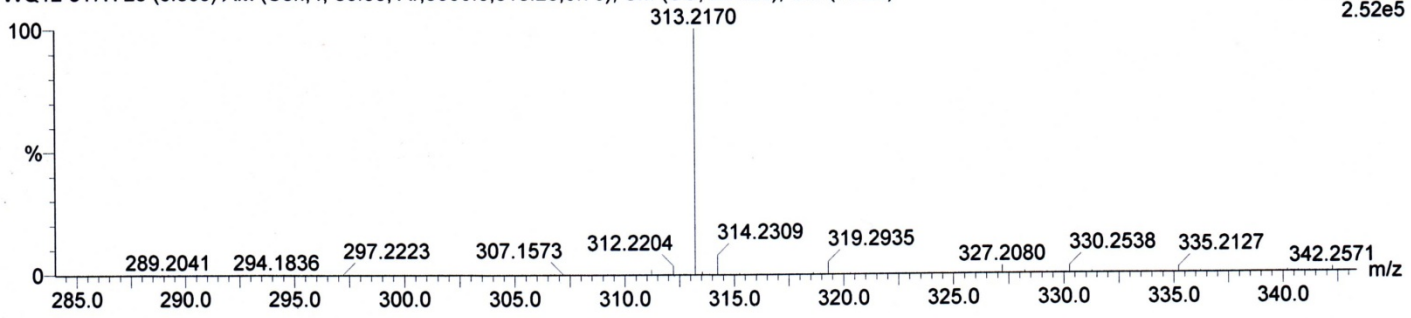

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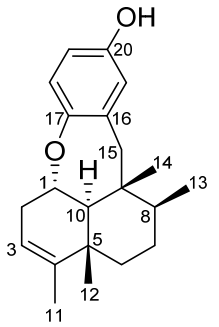

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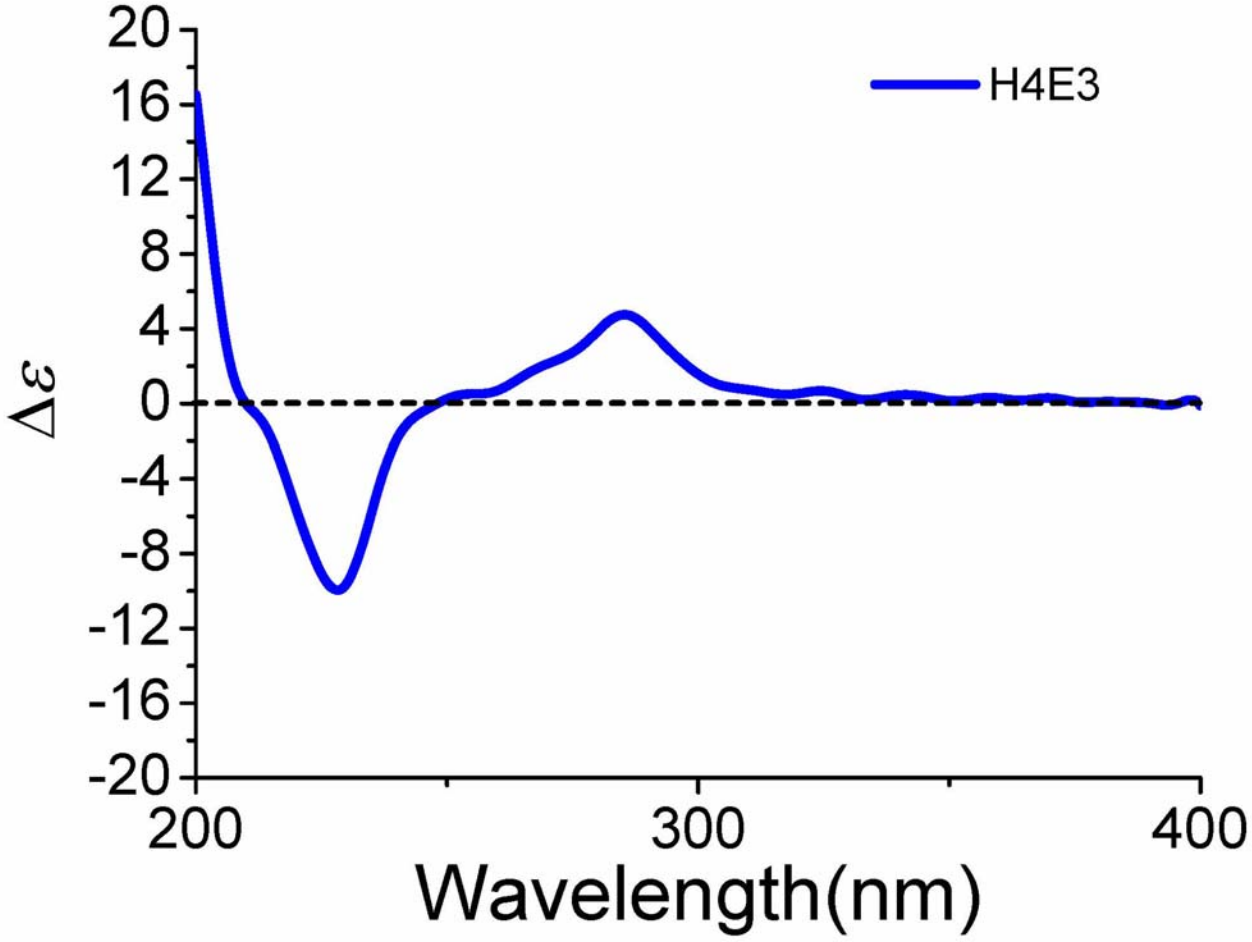
Figure S8. HRESIMS of Dysiquinol A (**1**).



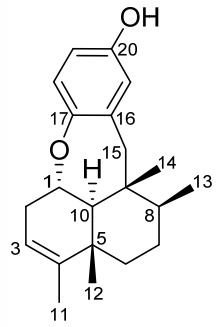


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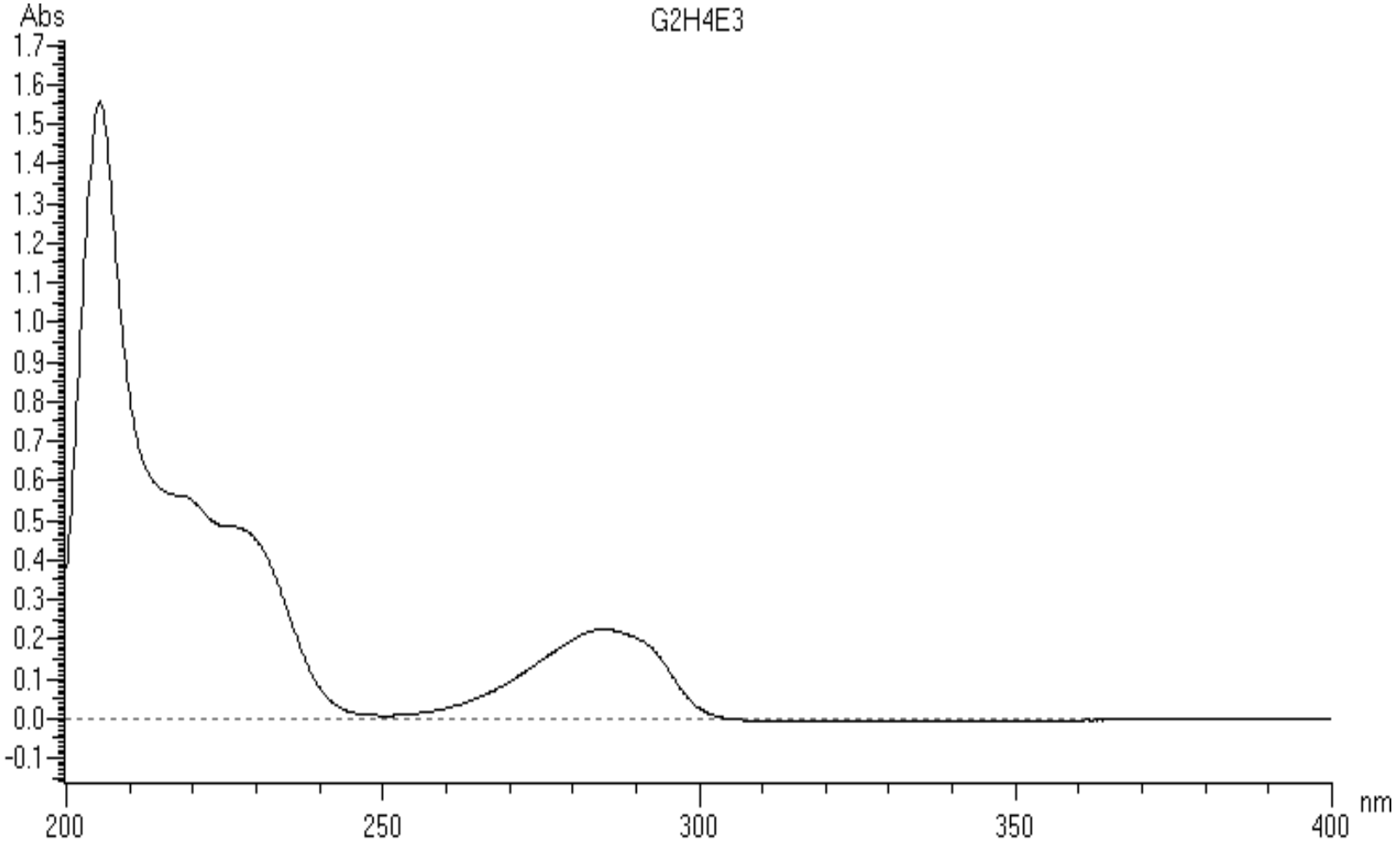
Figure S9. CD Spectrum of Dysiquinol A (**1**) in MeOH.



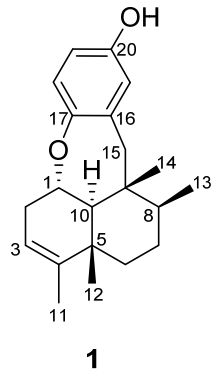


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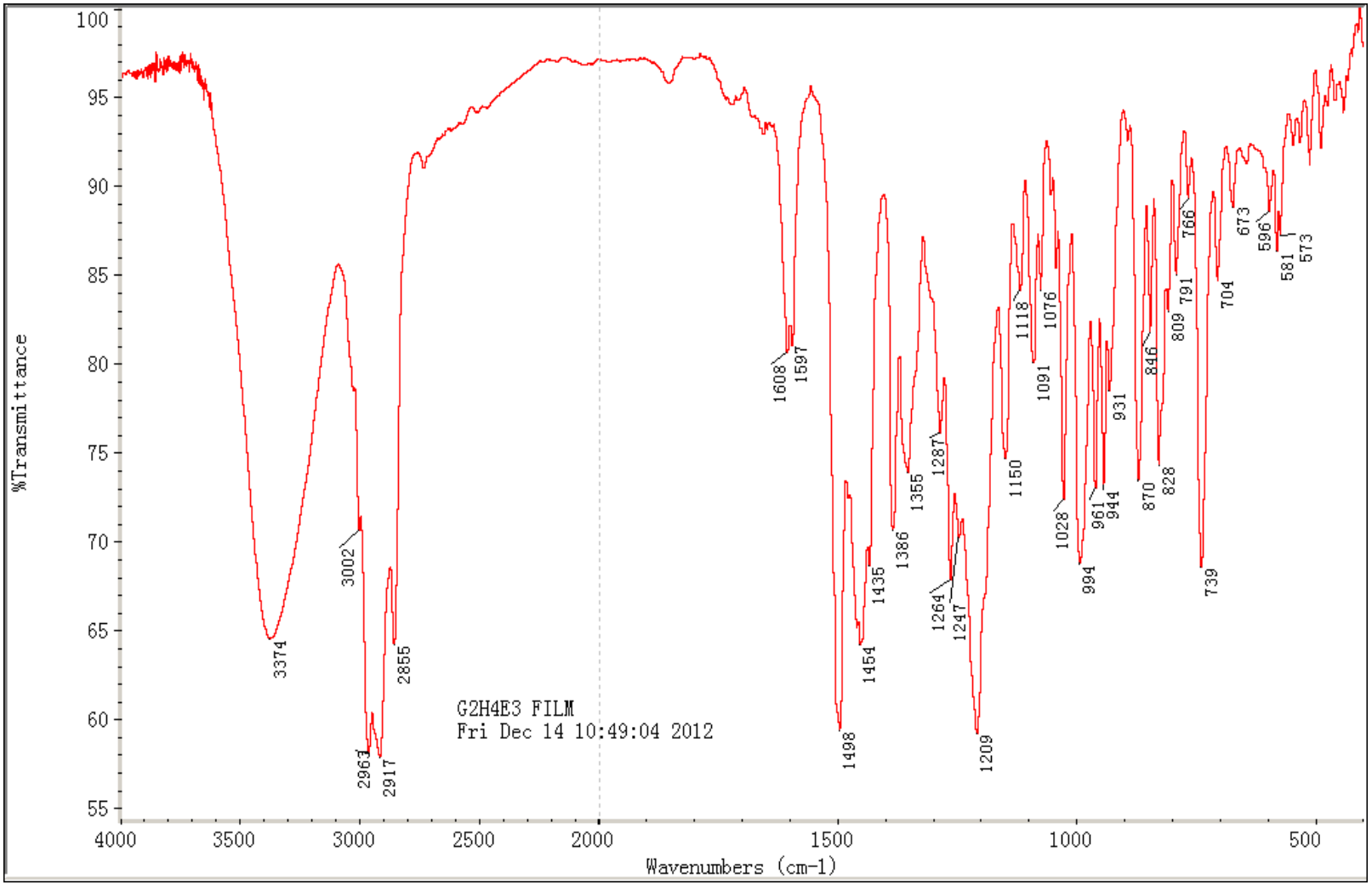
Figure S10. UV Spectrum of Dysiquinol A (**1**).



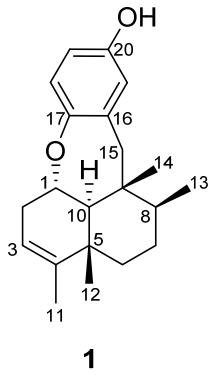


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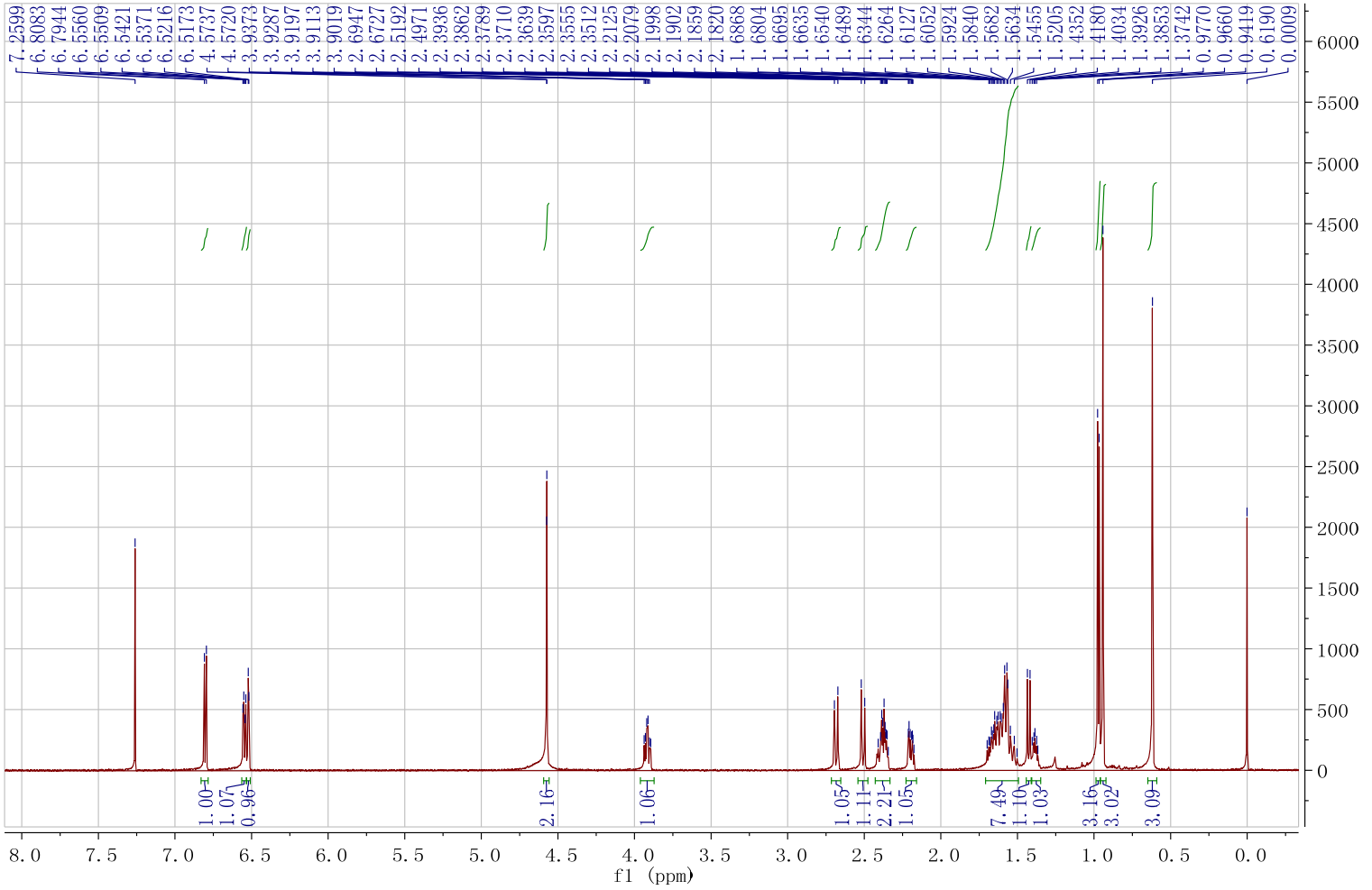
Figure S11. IR Spectrum of Dysiquinol A (**1**).



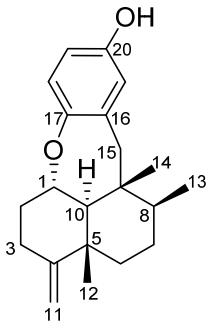


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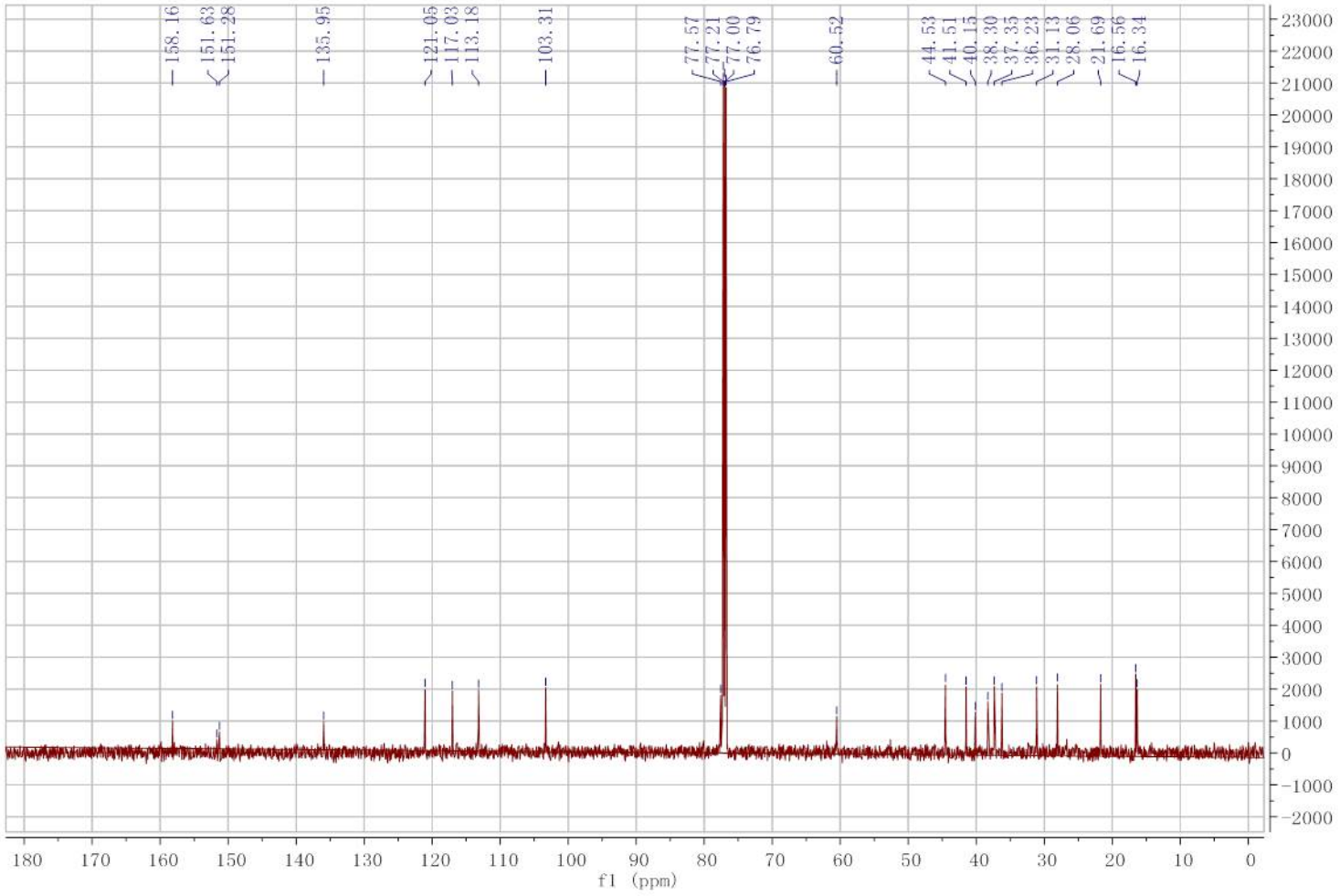
Figure S12. ^{1}H NMR Spectrum of Dysiquinol B (**2**).



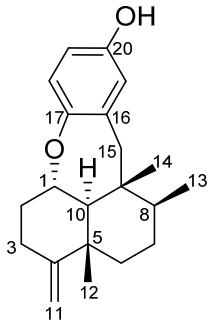


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Figure S13. ^{13}C NMR Spectrum of Dysiquinol B (**2**).

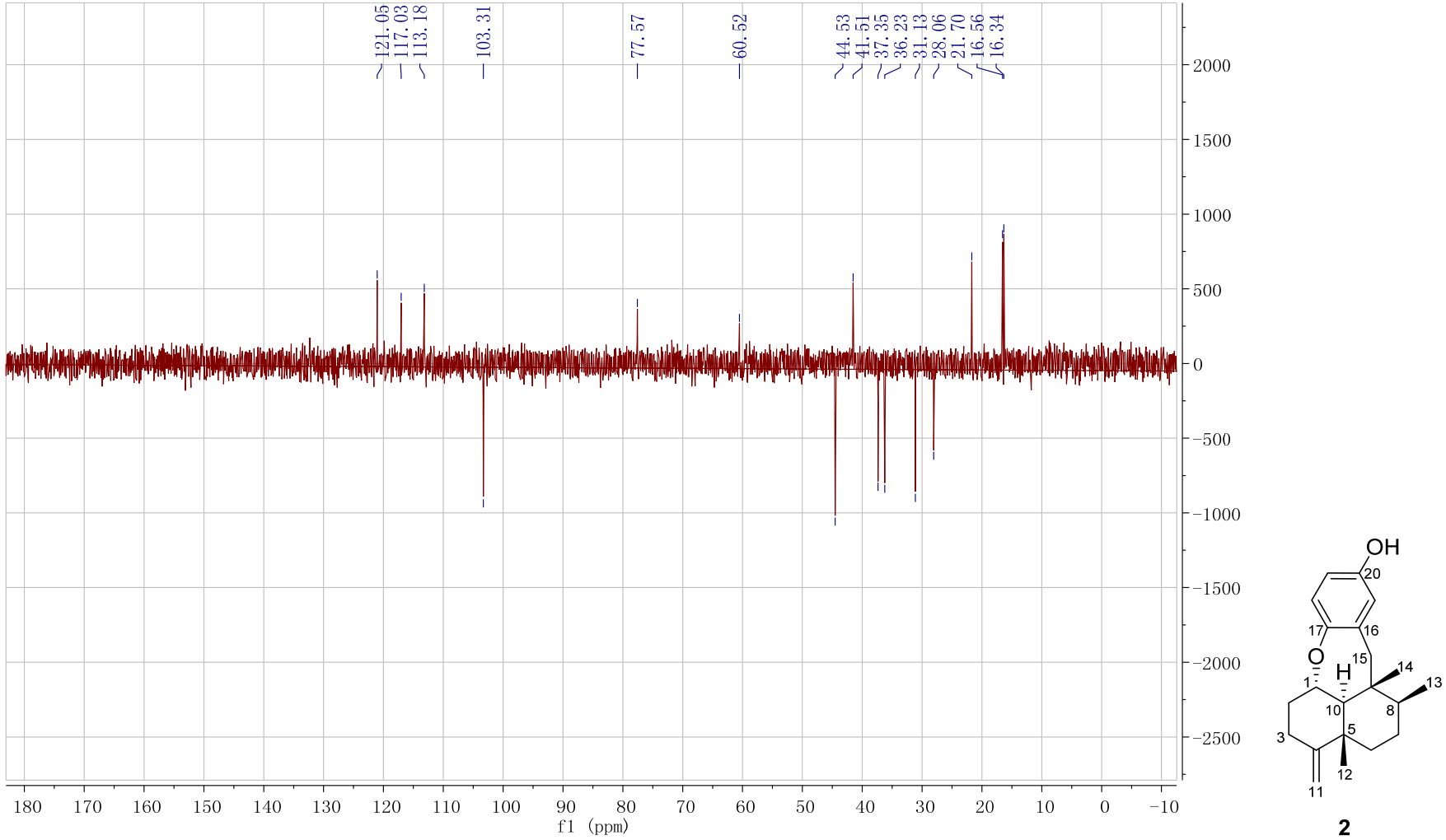

Figure S14. DEPT135 Spectrum of Dysiquinol B (**2**).

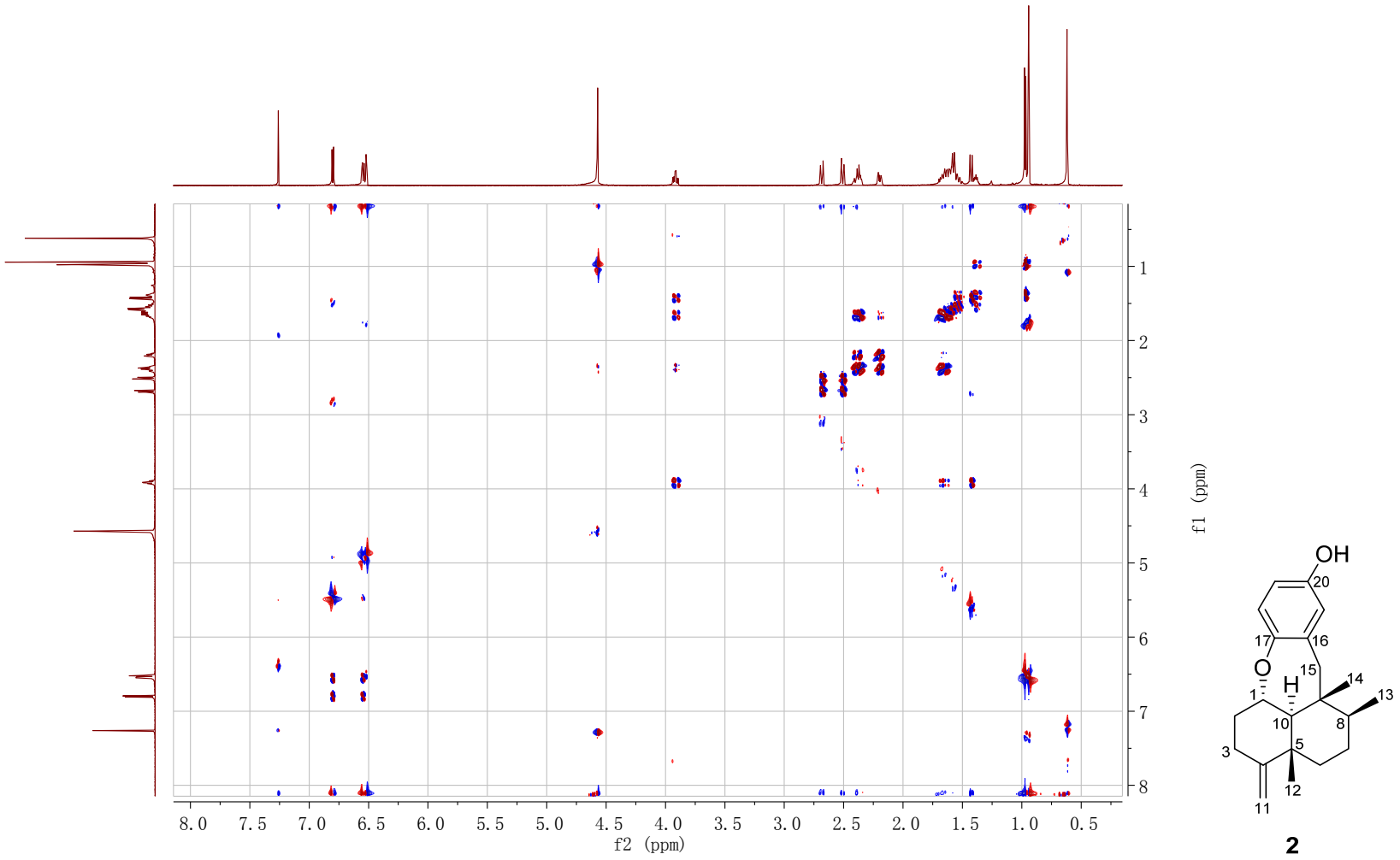

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Figure S15. ^{1}H-^{1}H COSY Spectrum of Dysiquinol B (**2**).

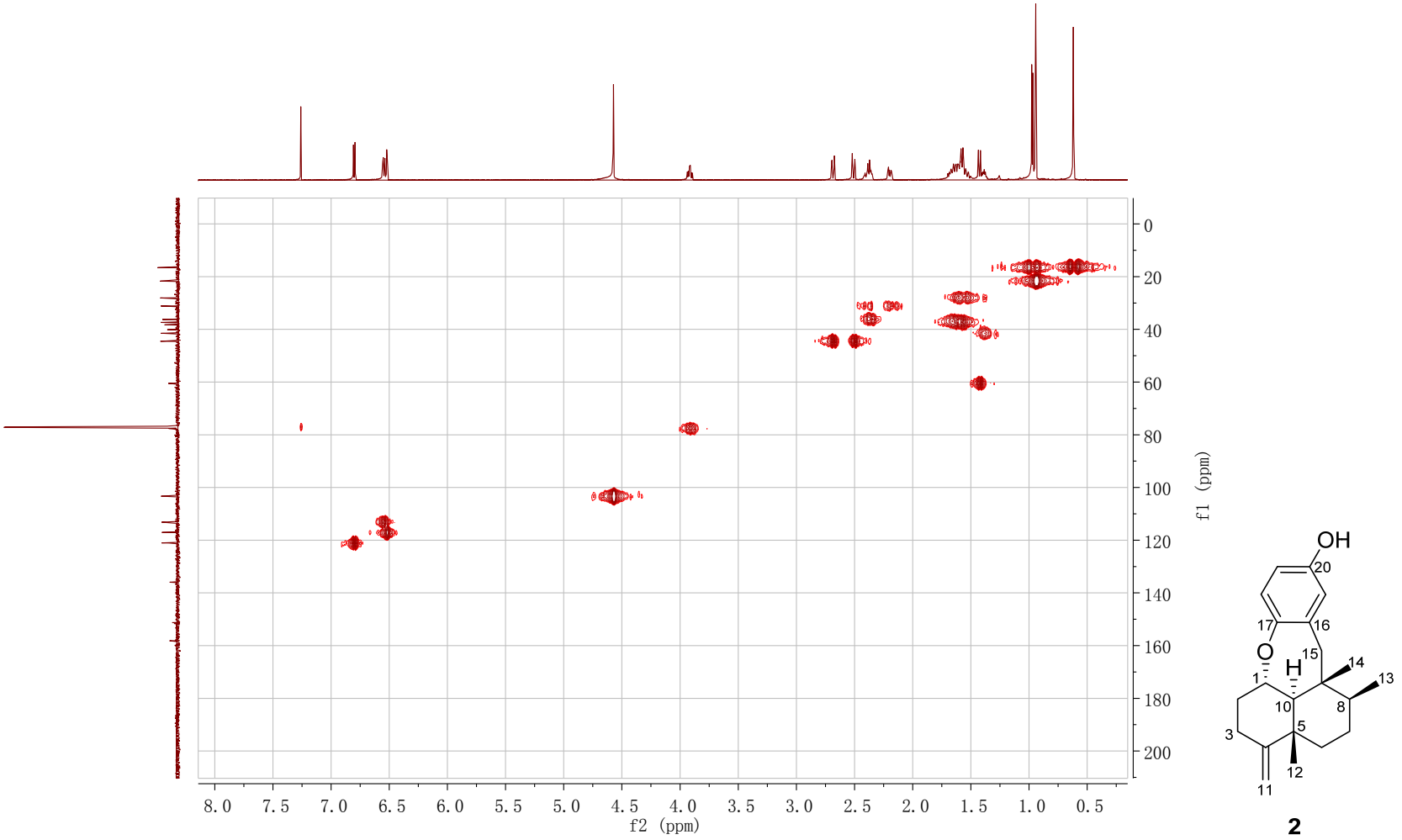

Figure S16. HSQC Spectrum of Dysiquinol B (**2**).

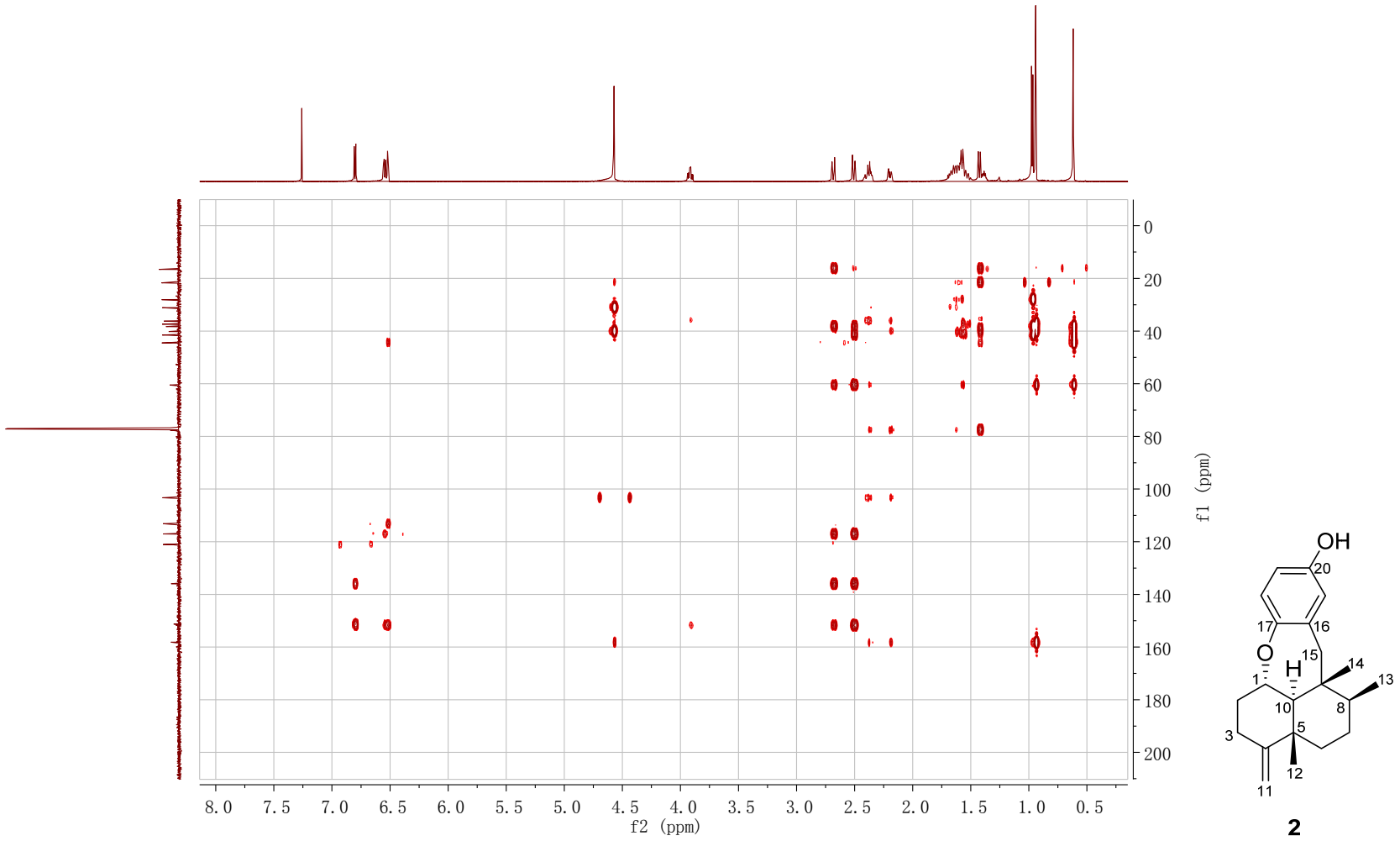

Figure S17. HMBC Spectrum of Dysiquinol B (**2**).

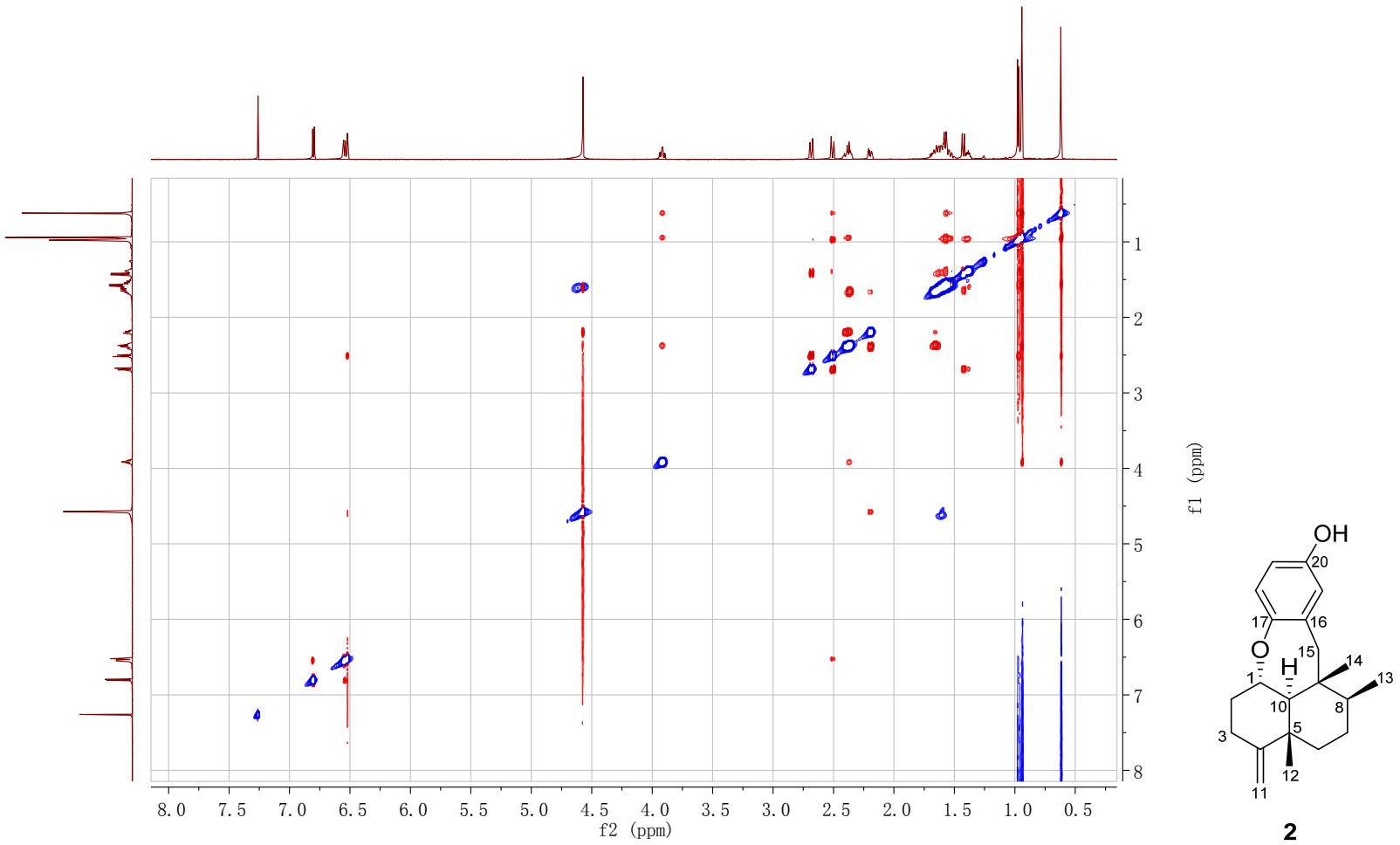

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Figure S18. NOESY Spectrum of Dysiquinol B (**2**).

Elemental Composition Report G4E2 **Page 1**

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Selected filters: None

Monoisotopic Mass, Even Electron Ions
14 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 10-25 H: 10-40 O: 1-6

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G4E2 M.W=312
WQ12-329H 56 (1.972) AM (Cen,4, 80.00, Ar,5000.0,308.05,0.70); Sm (SG, 2x1.00); Cm (55:64)

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YA019

17-Jul-2012,14:21:03
TOF MS ES+
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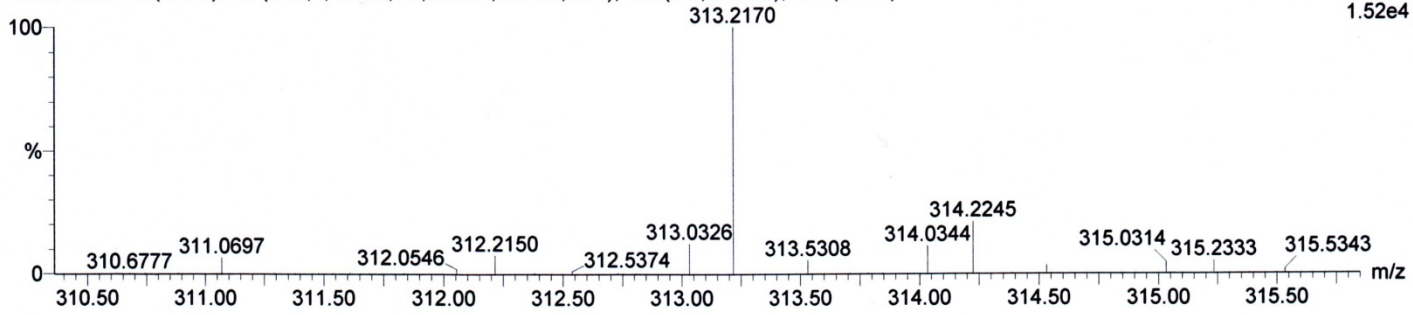

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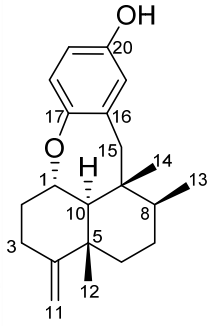

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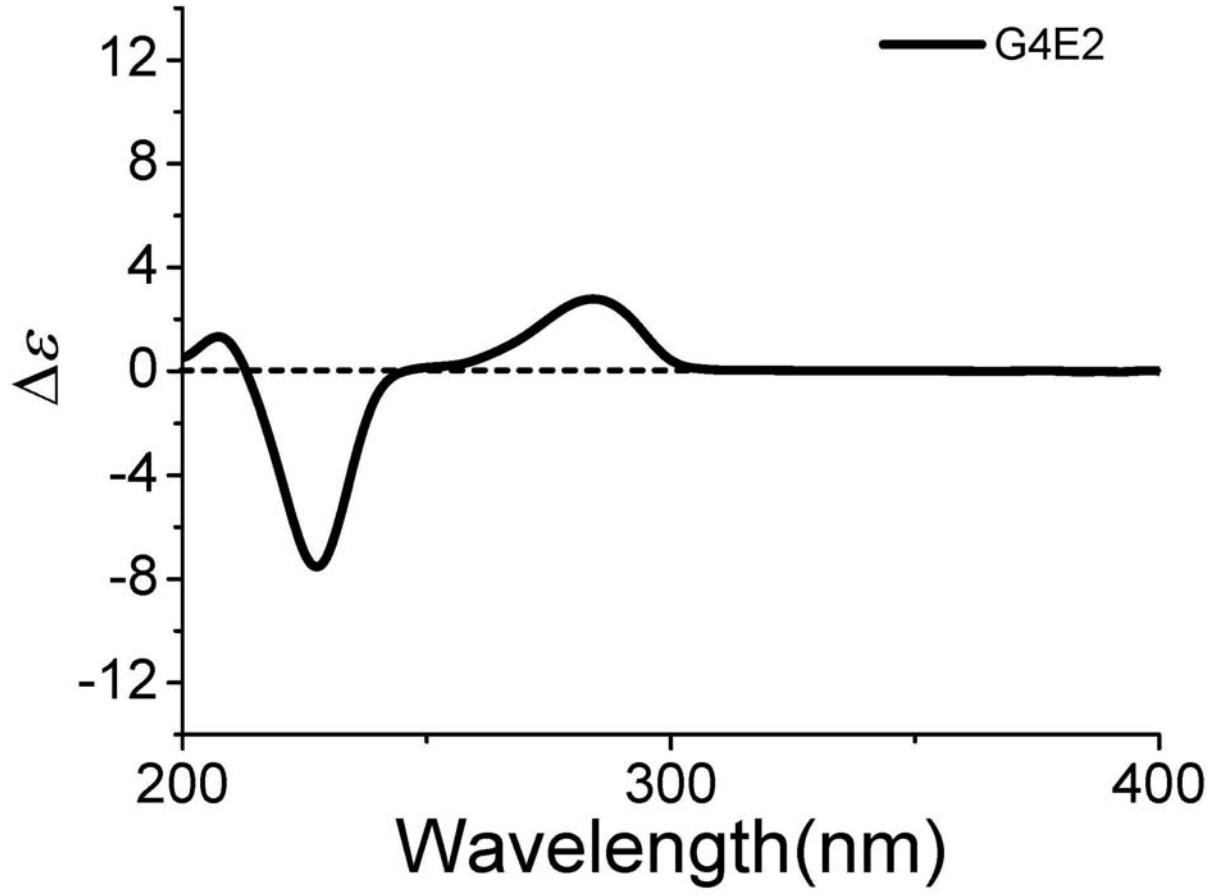
Figure S19. HRESIMS of Dysiquinol B (**2**).



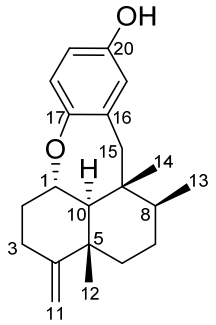


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Figure S20. CD Spectrum of Dysiquinol B (**2**) in MeOH.

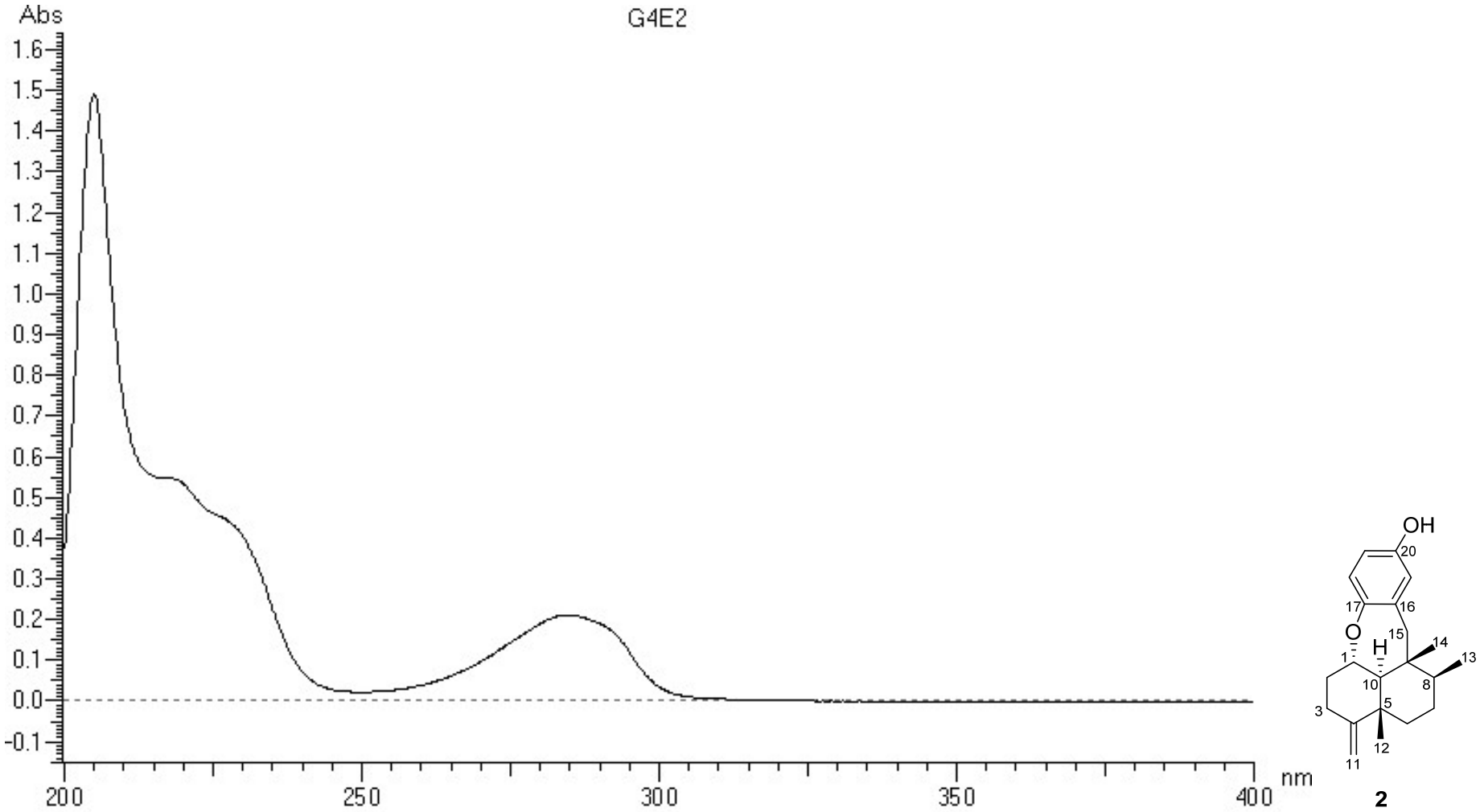


Figure S21. UV Spectrum of Dysiquinol B (**2**).

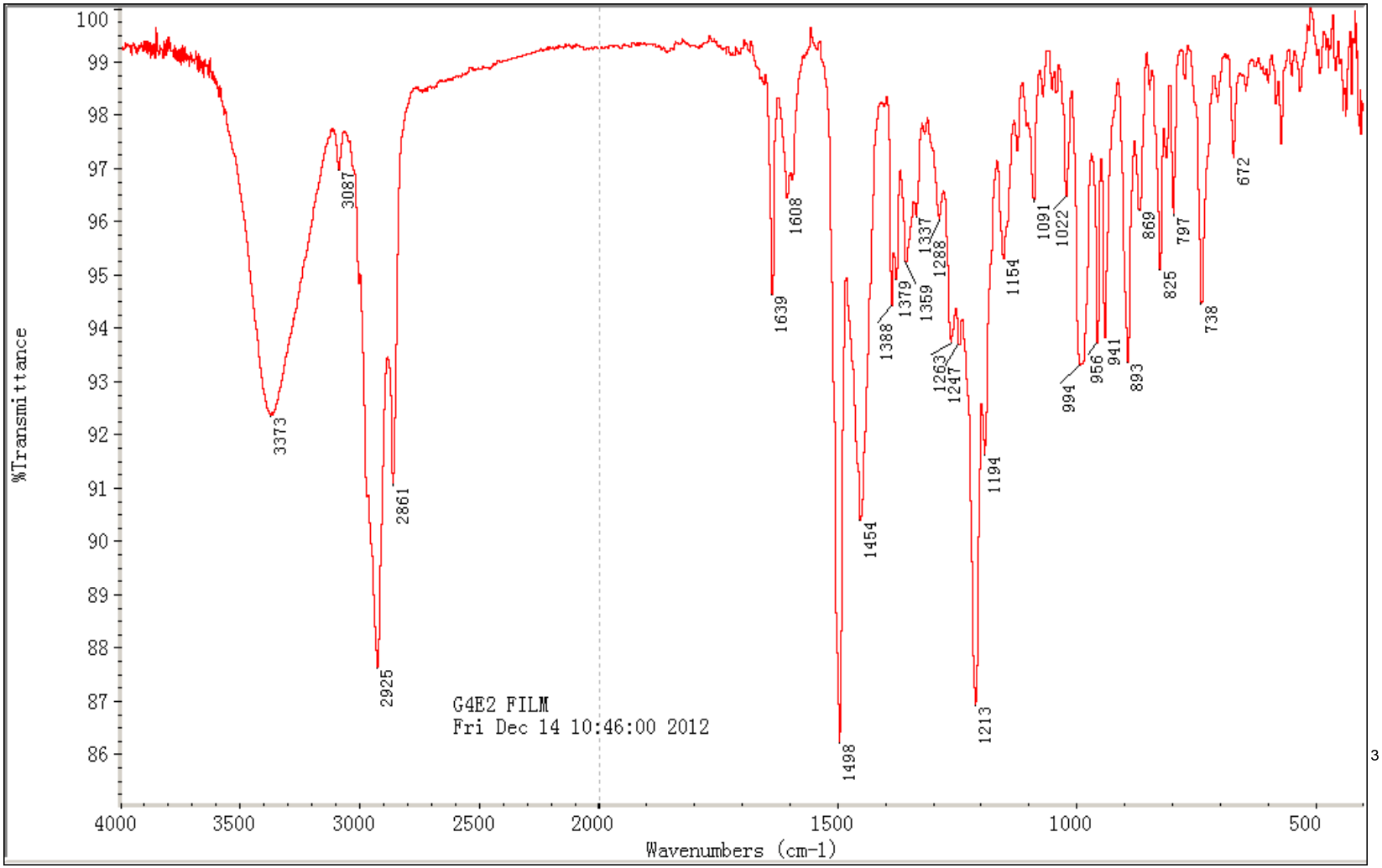
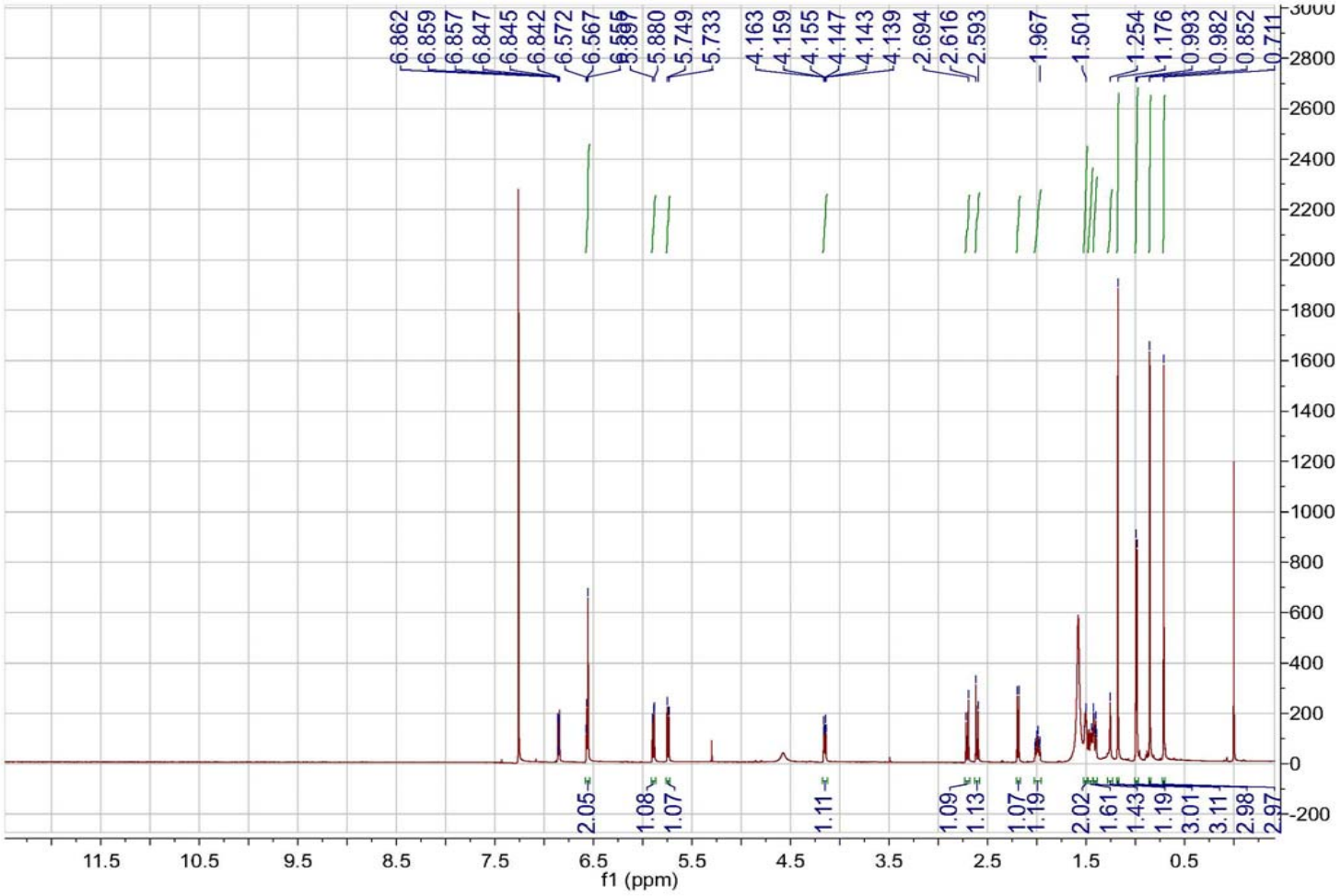
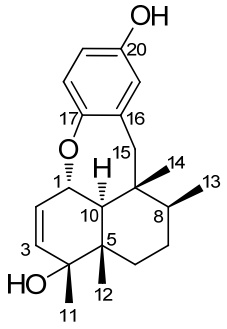


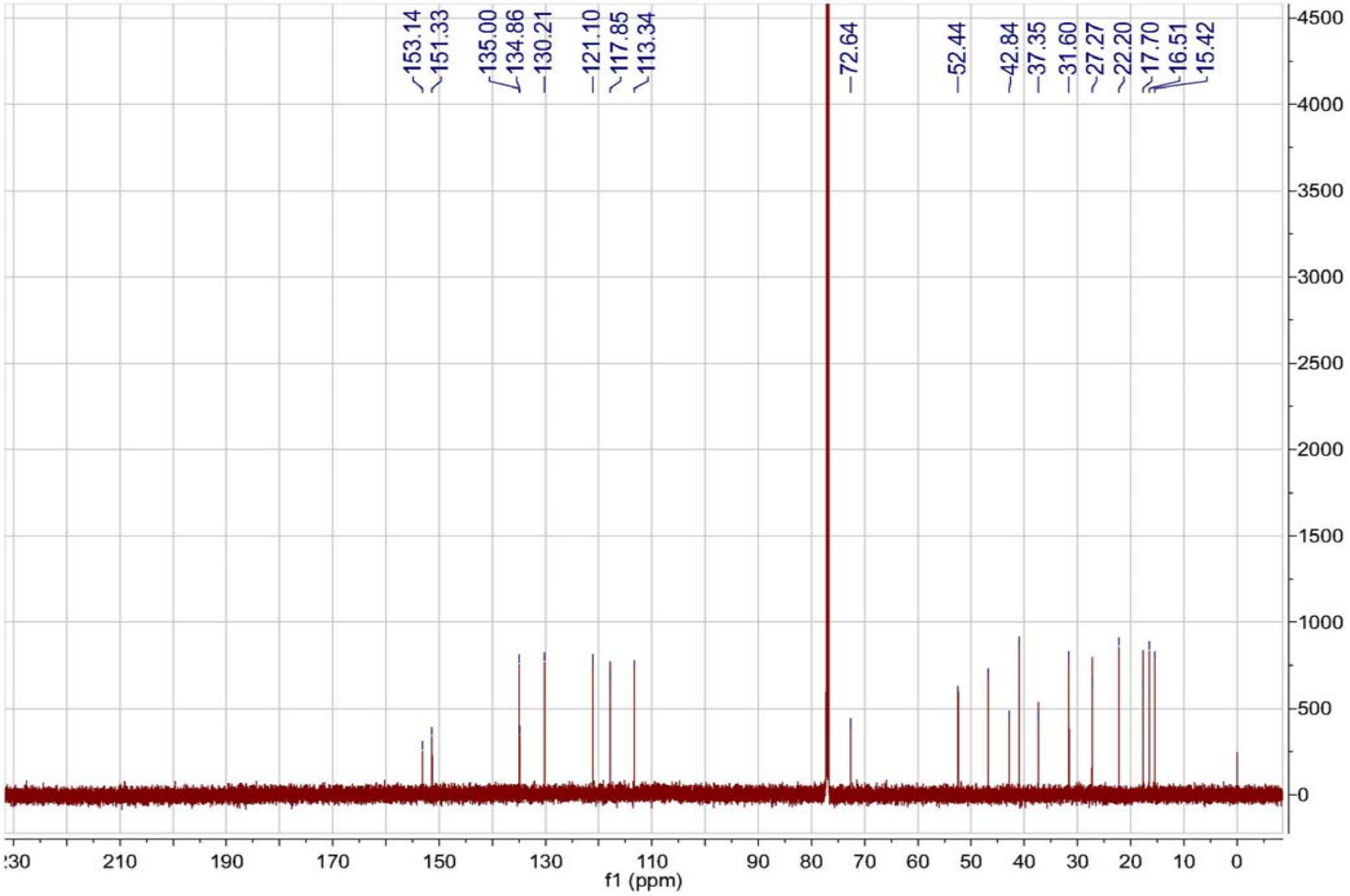
Figure S22. IR Spectrum of Dysiquinol B (**2**).

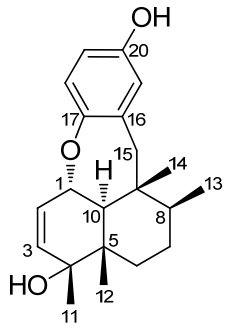




3

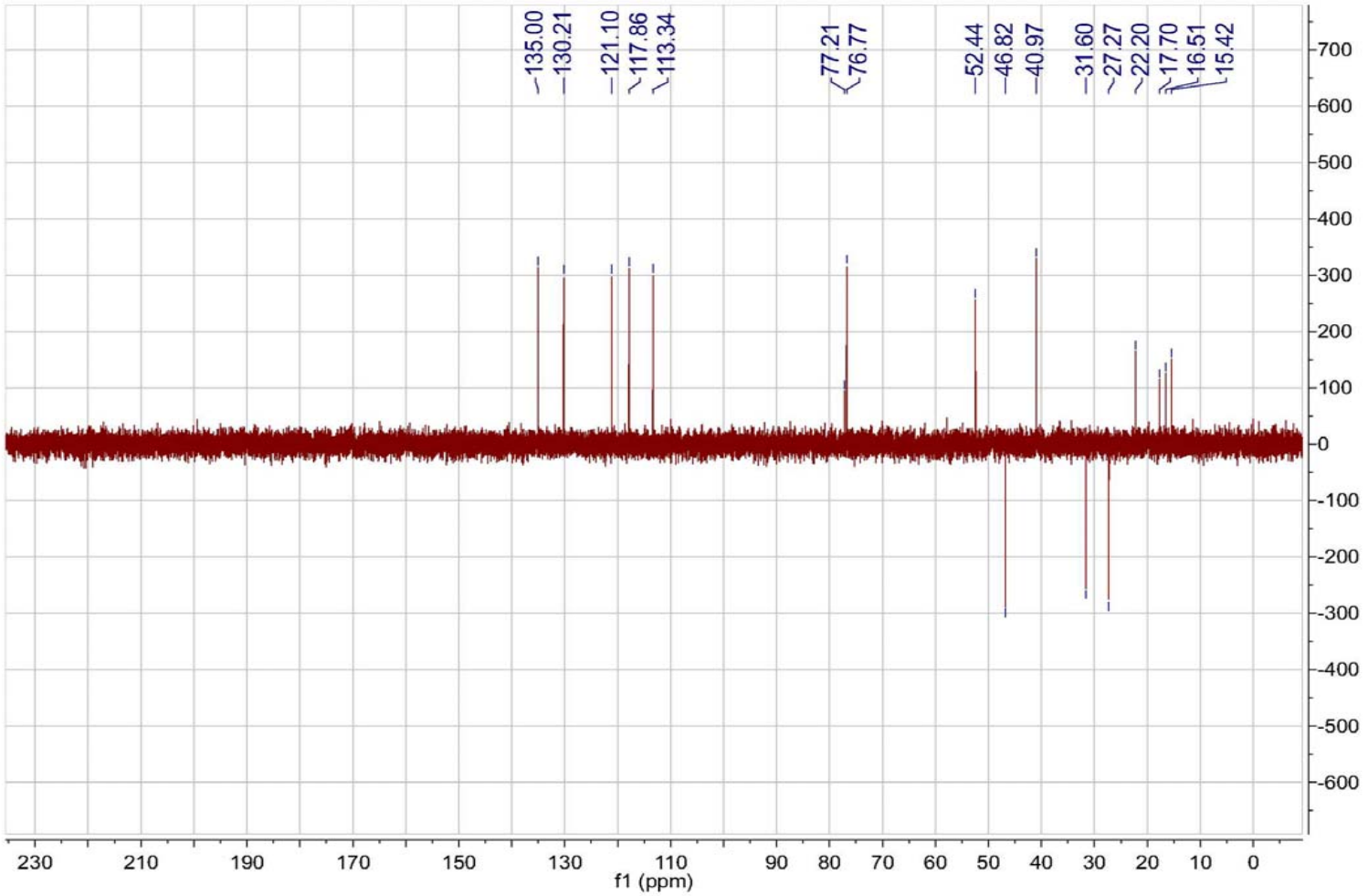
Figure S23. ^{1}H NMR Spectrum of Dysiquinol C (**3**) in $CDCl_3$.

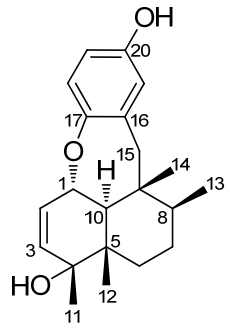




3

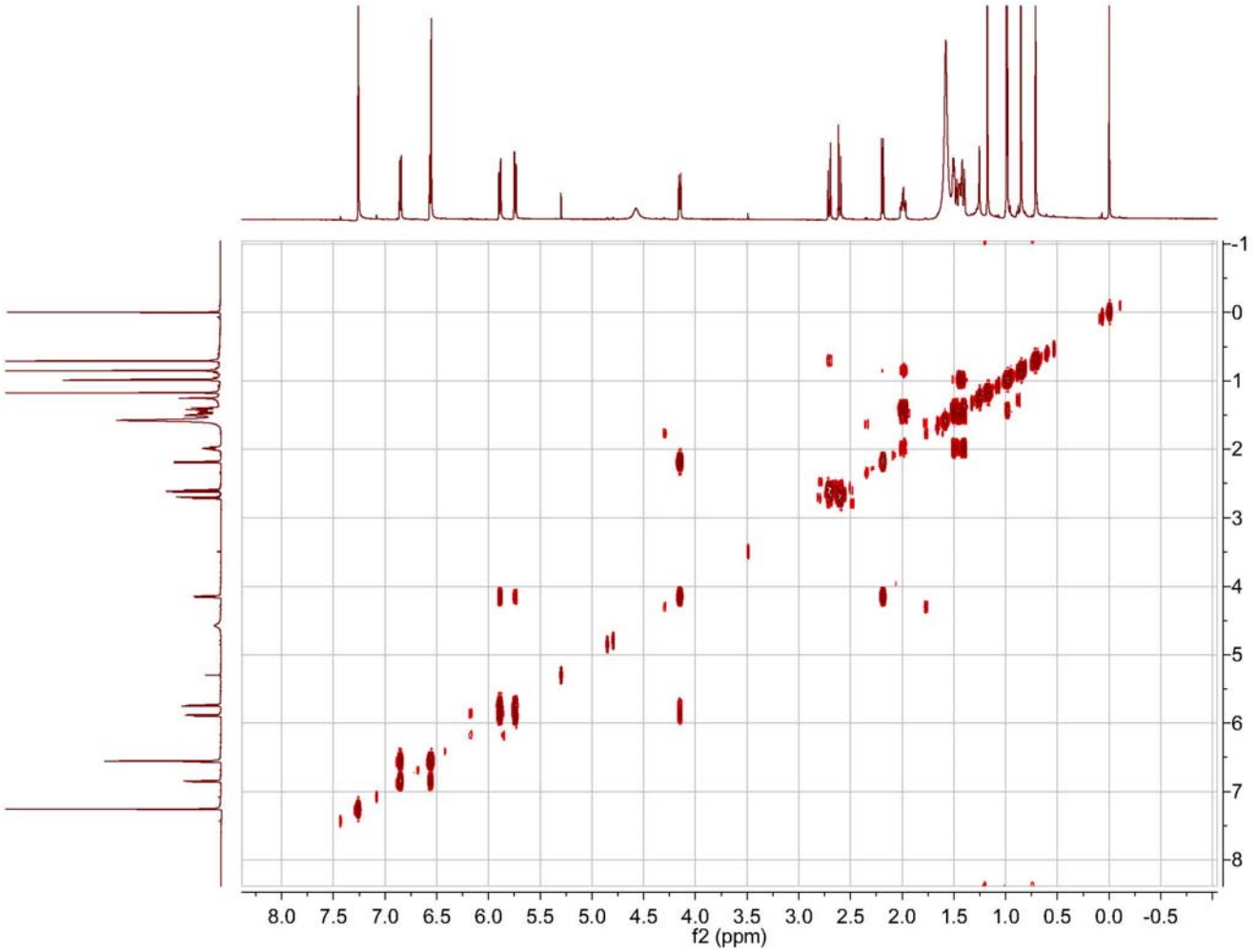
Figure S24. ^{13}C NMR Spectrum of Dysiquinol C (**3**) in $CDCl_3$.

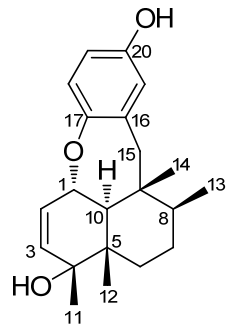




3

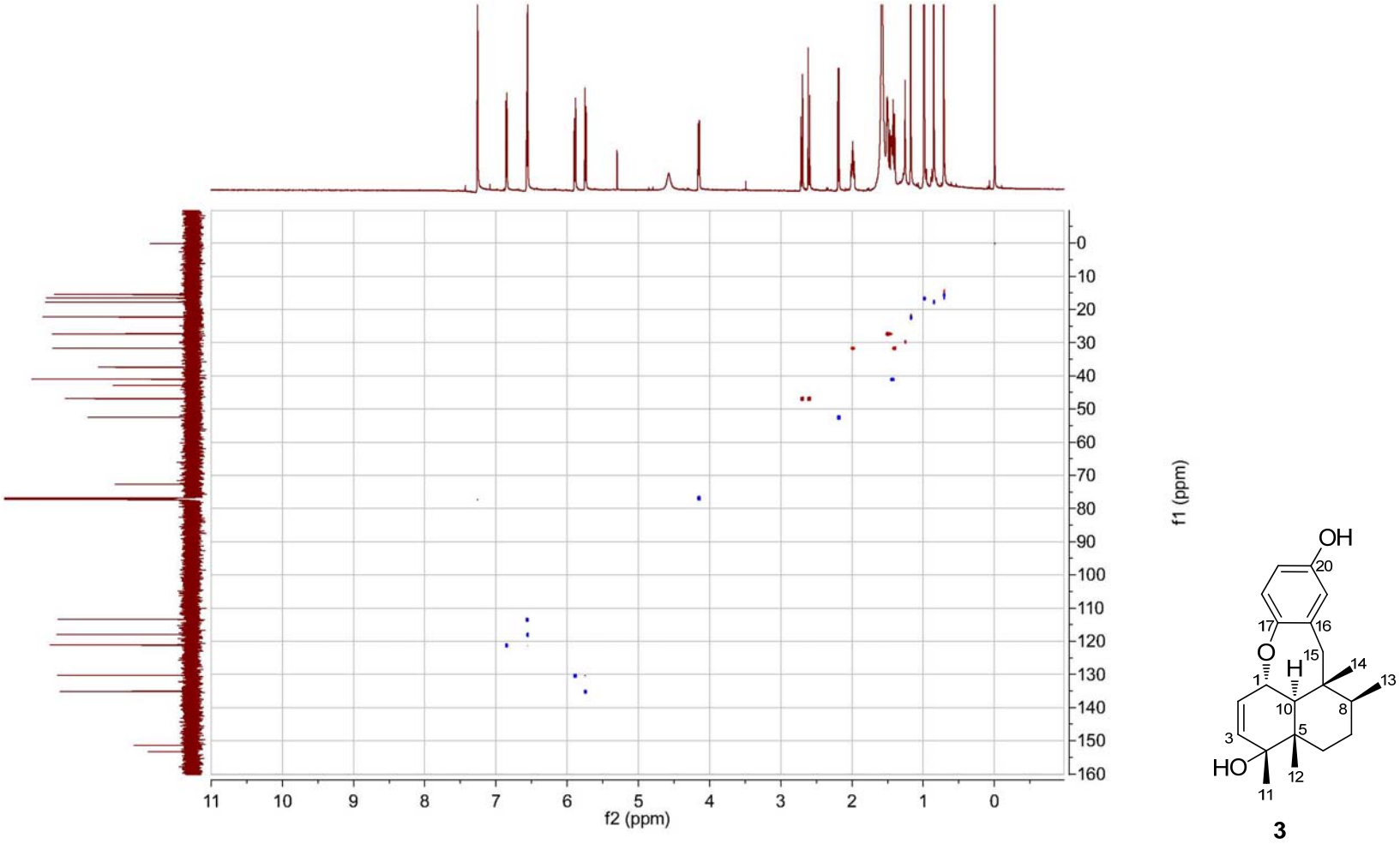
Figure S25. DEPT135 Spectrum of Dysiquinol C (**3**) in $CDCl_3$.





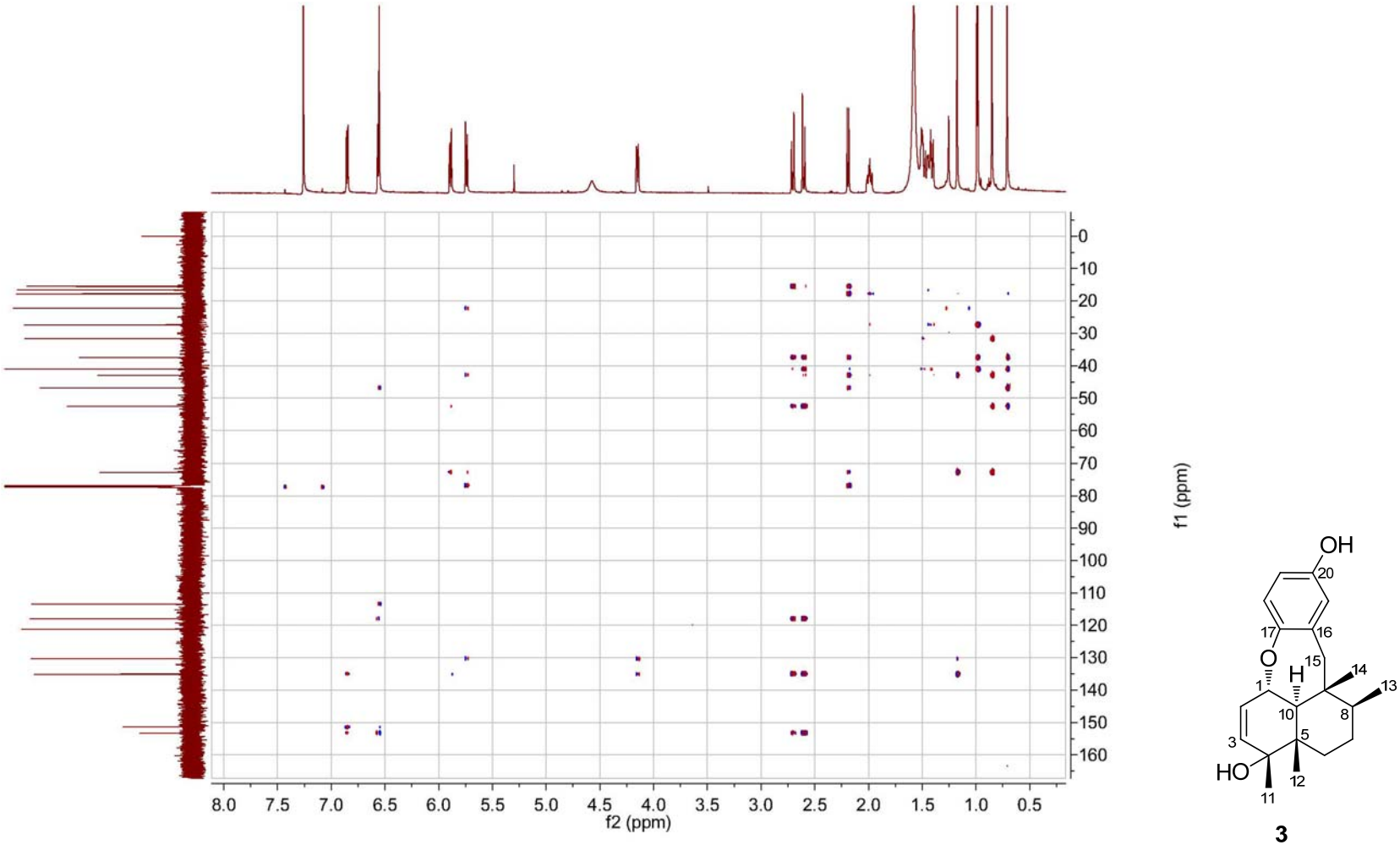
3

Figure S26. ^{1}H-^{1}H COSY Spectrum of Dysiquinol C (**3**) in $CDCl_3$.



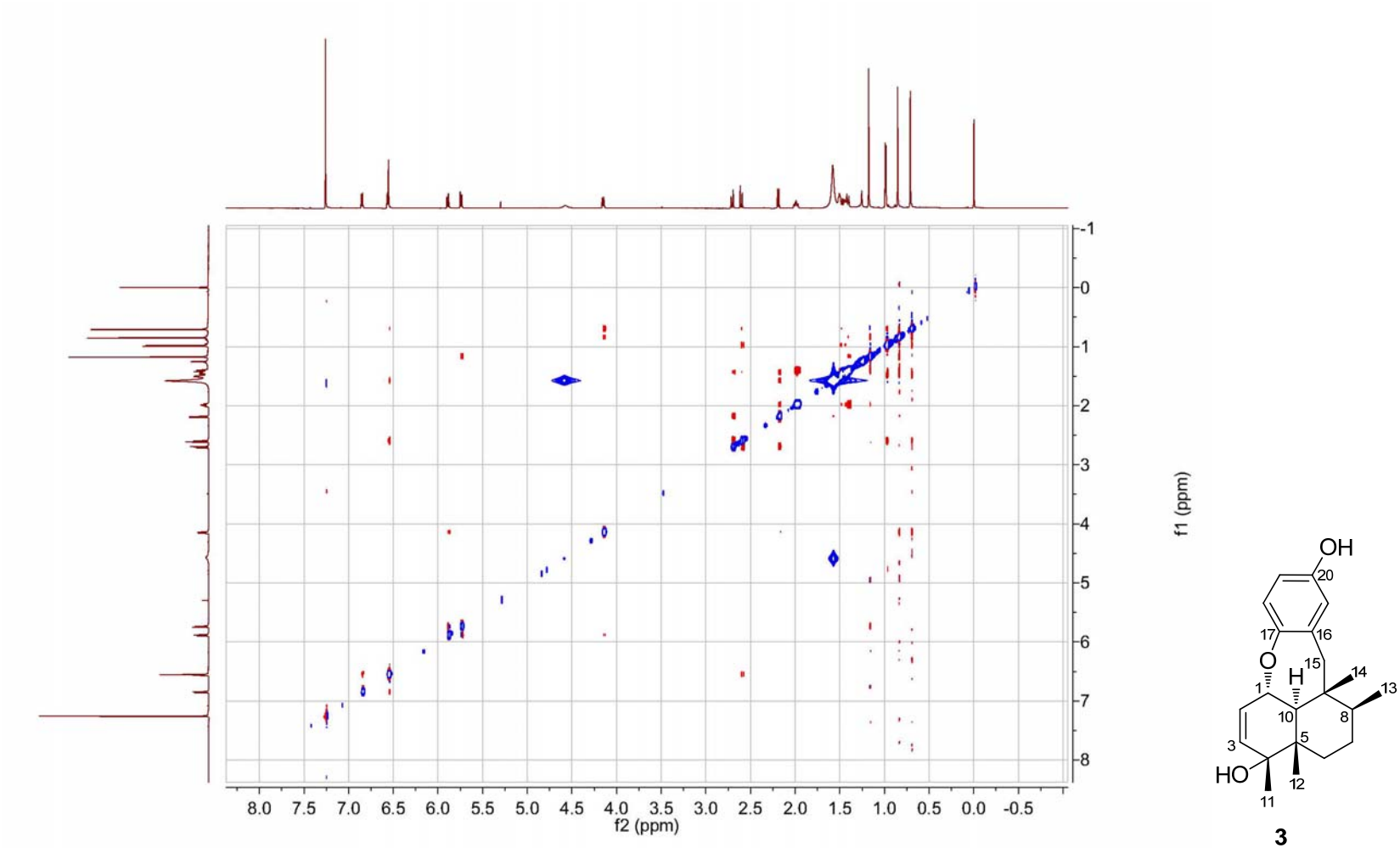
3

Figure S27. HSQC Spectrum of Dysiquinol C (**3**) in $CDCl_3$.



3

Figure S28. HMBC Spectrum of Dysiquinol C (**3**) in $CDCl_3$.



3

Figure S29. NOESY Spectrum of Dysiquinol C (**3**) in $CDCl_3$.

Elemental Composition Report Page 1

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 50.0
Selected filters: None

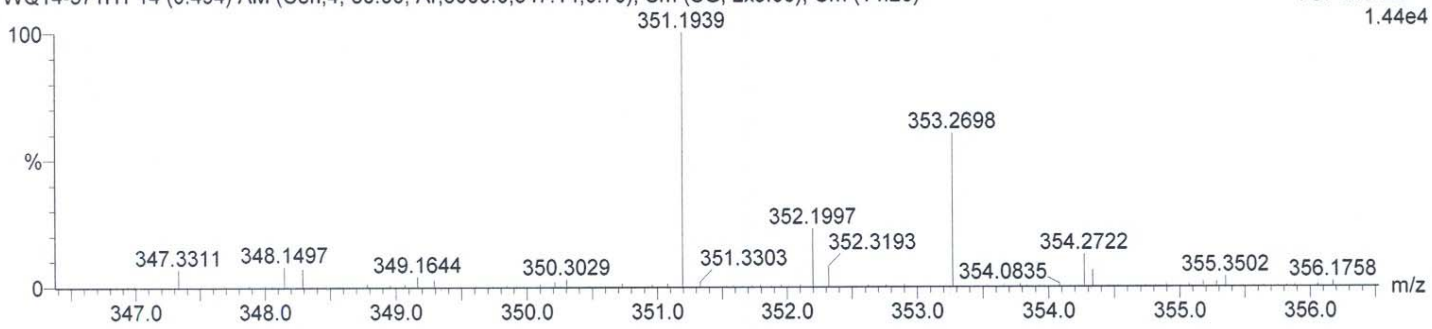
Monoisotopic Mass, Even Electron Ions
15 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-25 H: 5-40 O: 1-5 Na: 1-1

SIPI
DM-5C-1
WQ14-371H1 14 (0.494) AM (Cen,4, 80.00, Ar,5000.0,347.14,0.70); Sm (SG, 2x3.00); Cm (14:26)

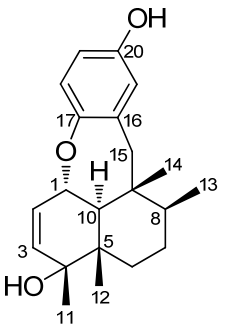
Q-Tof micro
YA019

16:41:27,15-Dec-2014

TOF MS ES+
1.44e4

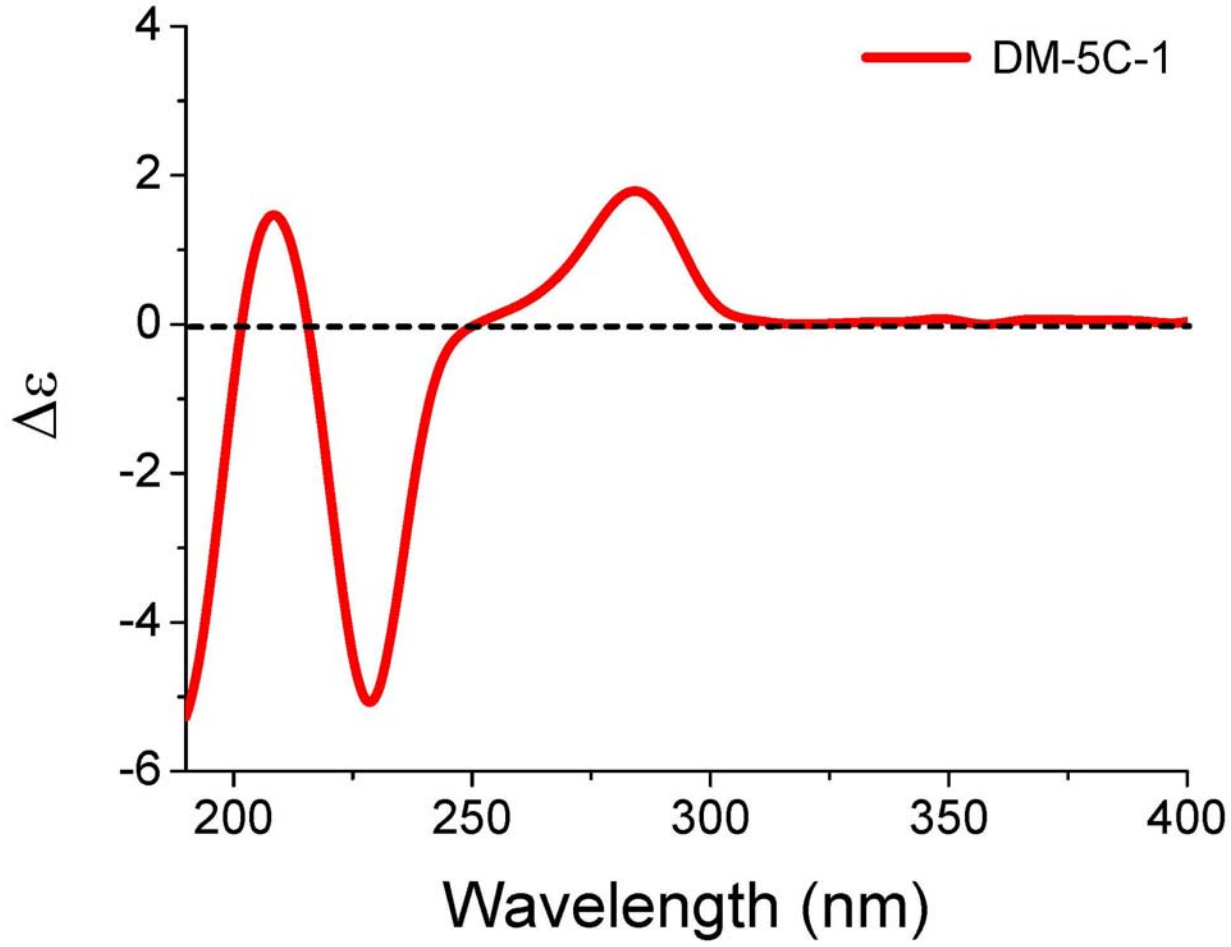


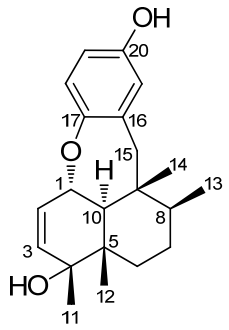
Minimum:	65.00				-10.0		
Maximum:	100.00		5.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
351.1939	100.00	351.1936	0.3	0.9	7.5	4802.6	C21 H28 O3 Na



3

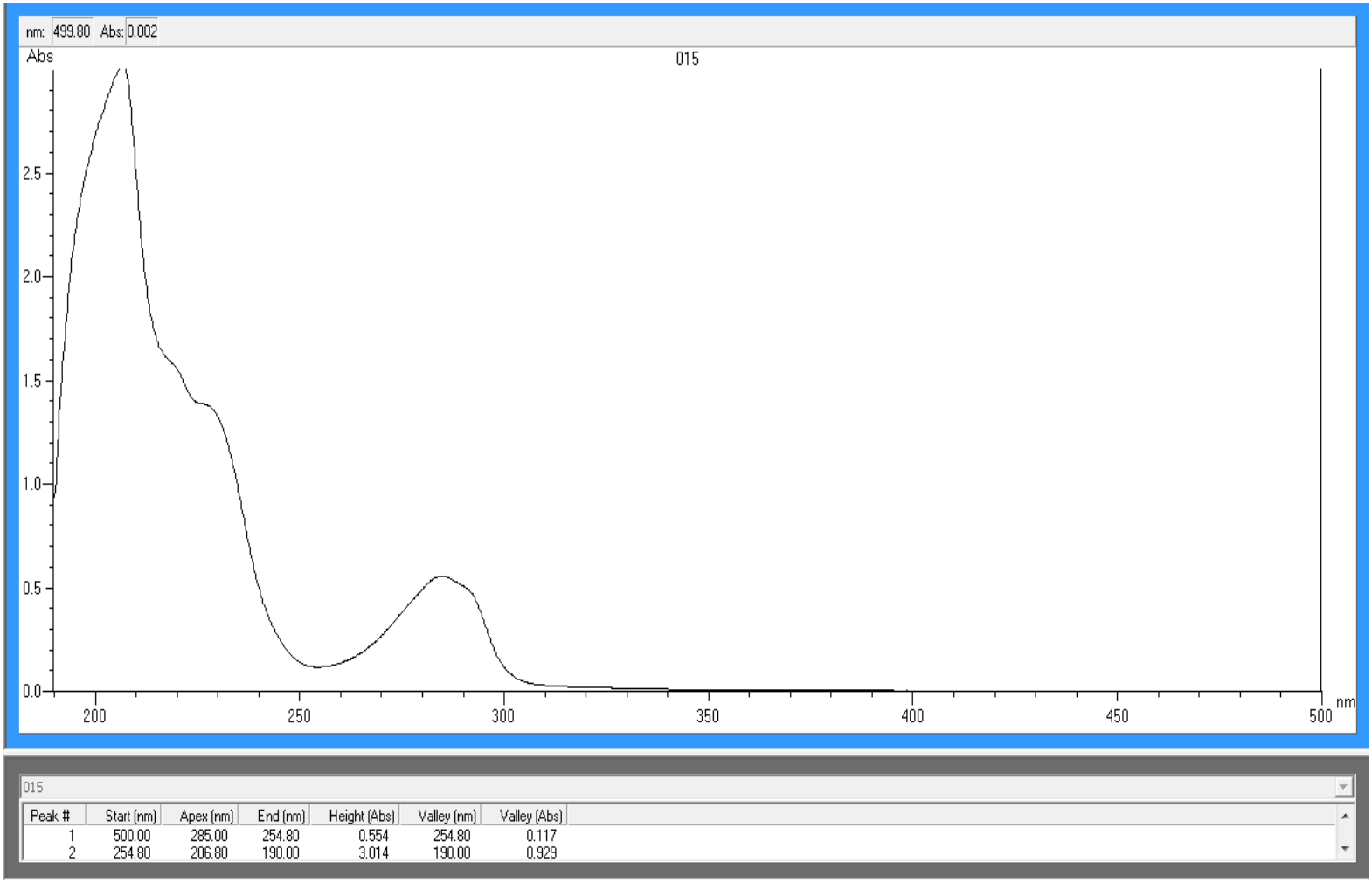
Figure S30. HRESIMS of Dysiquinol C (**3**).

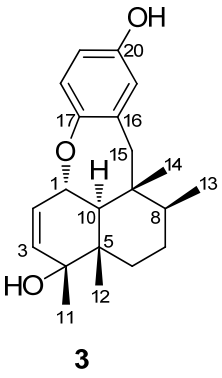




3

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





3

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

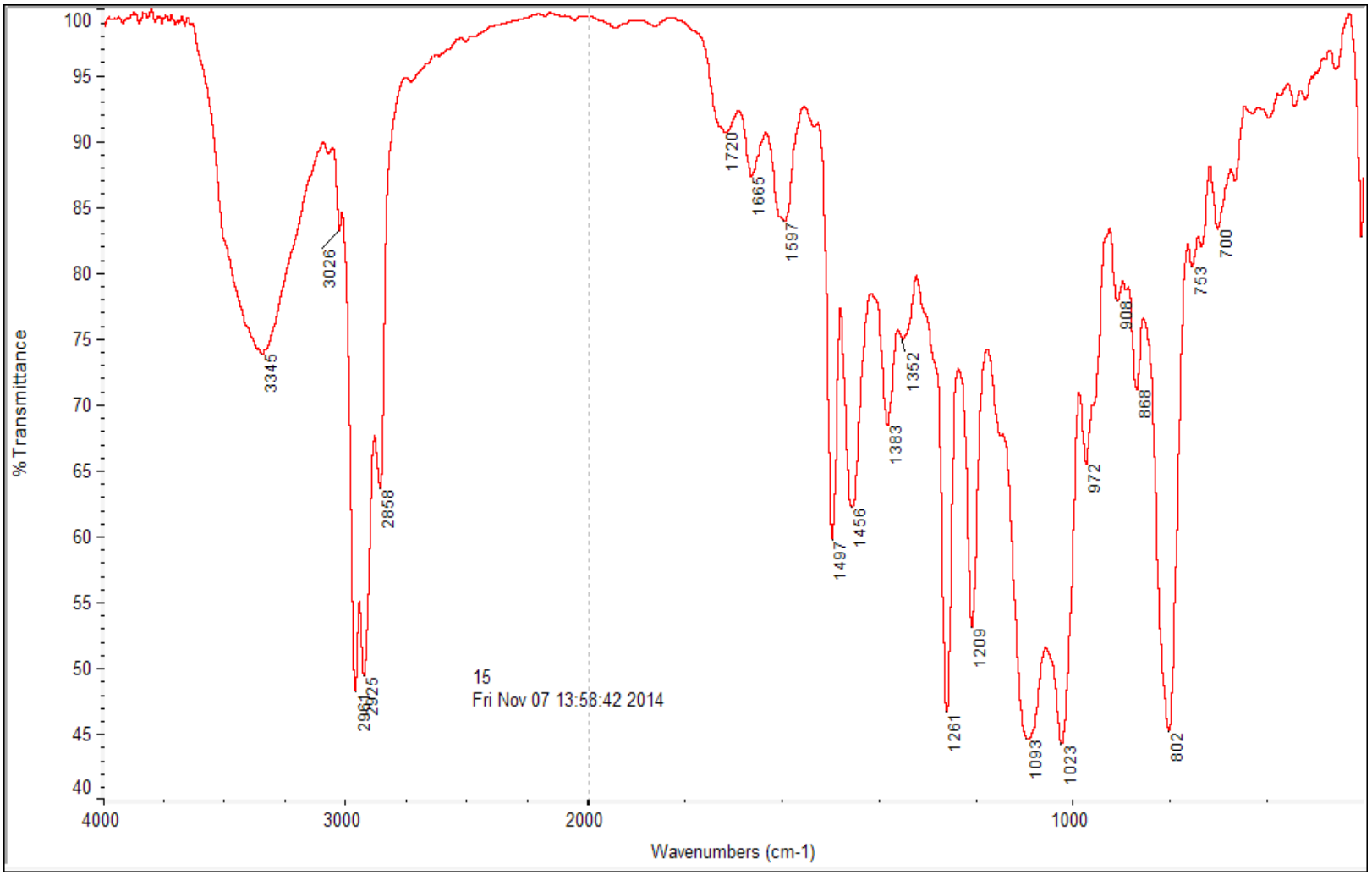
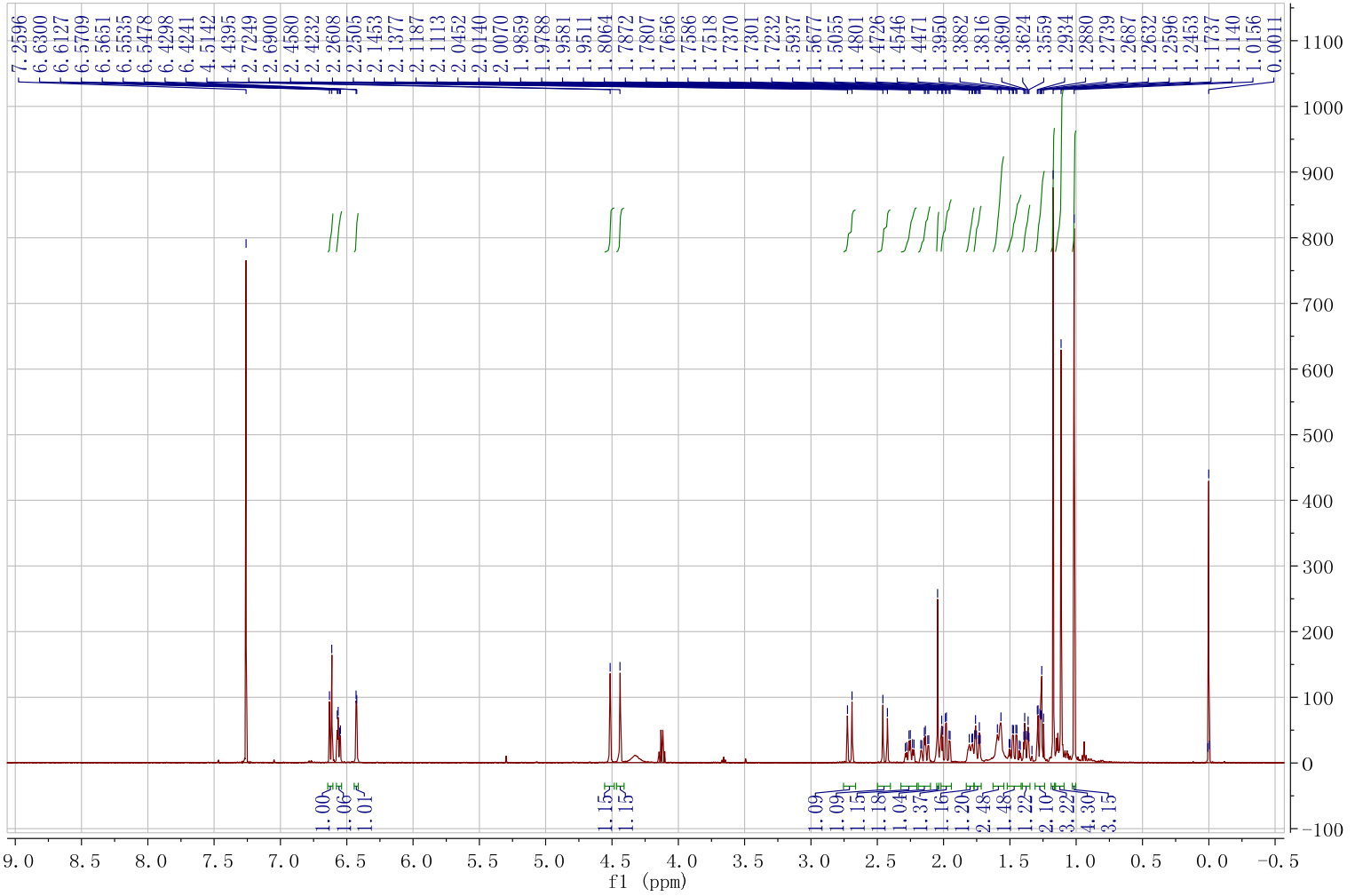
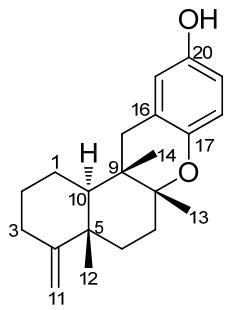


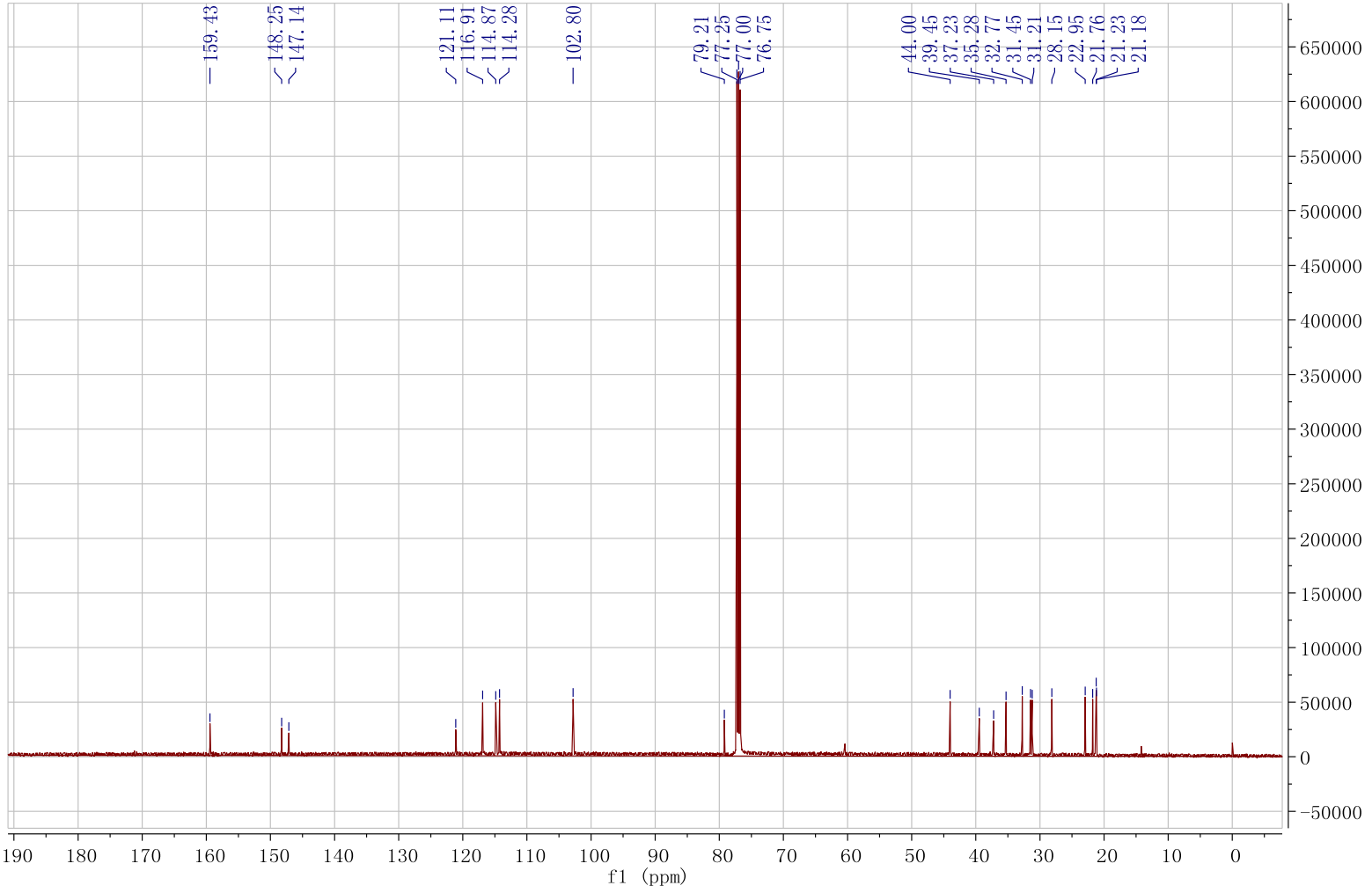
Figure S33. IR Spectrum of Dysiquinol C (**3**).

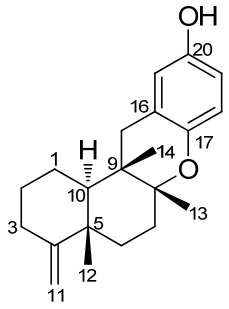




4

Figure S34. ^{1}H NMR Spectrum of Dysiquinol D (**4**).





4

Figure S35. ^{13}C NMR Spectrum of Dysiquinol D (**4**).

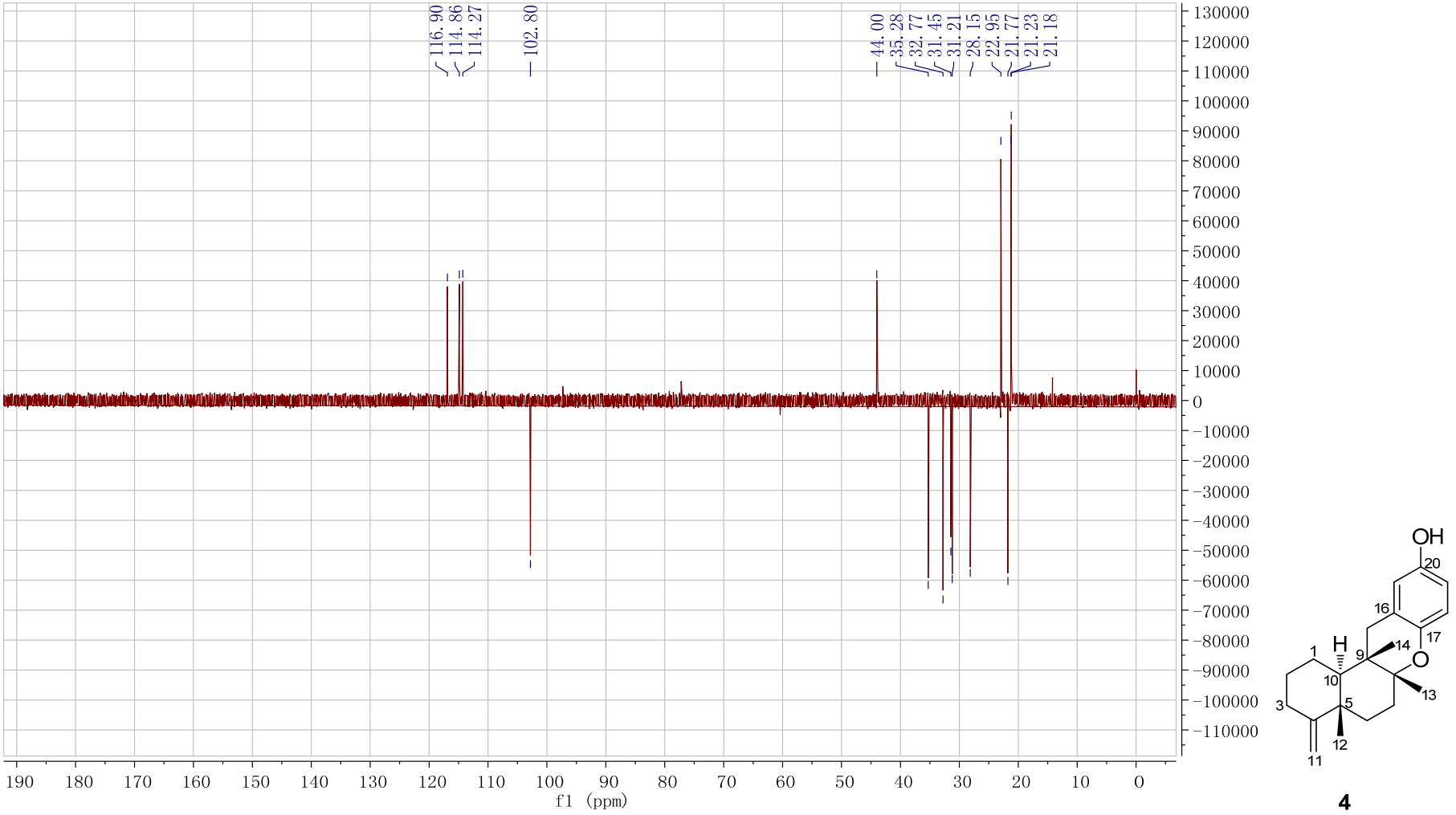
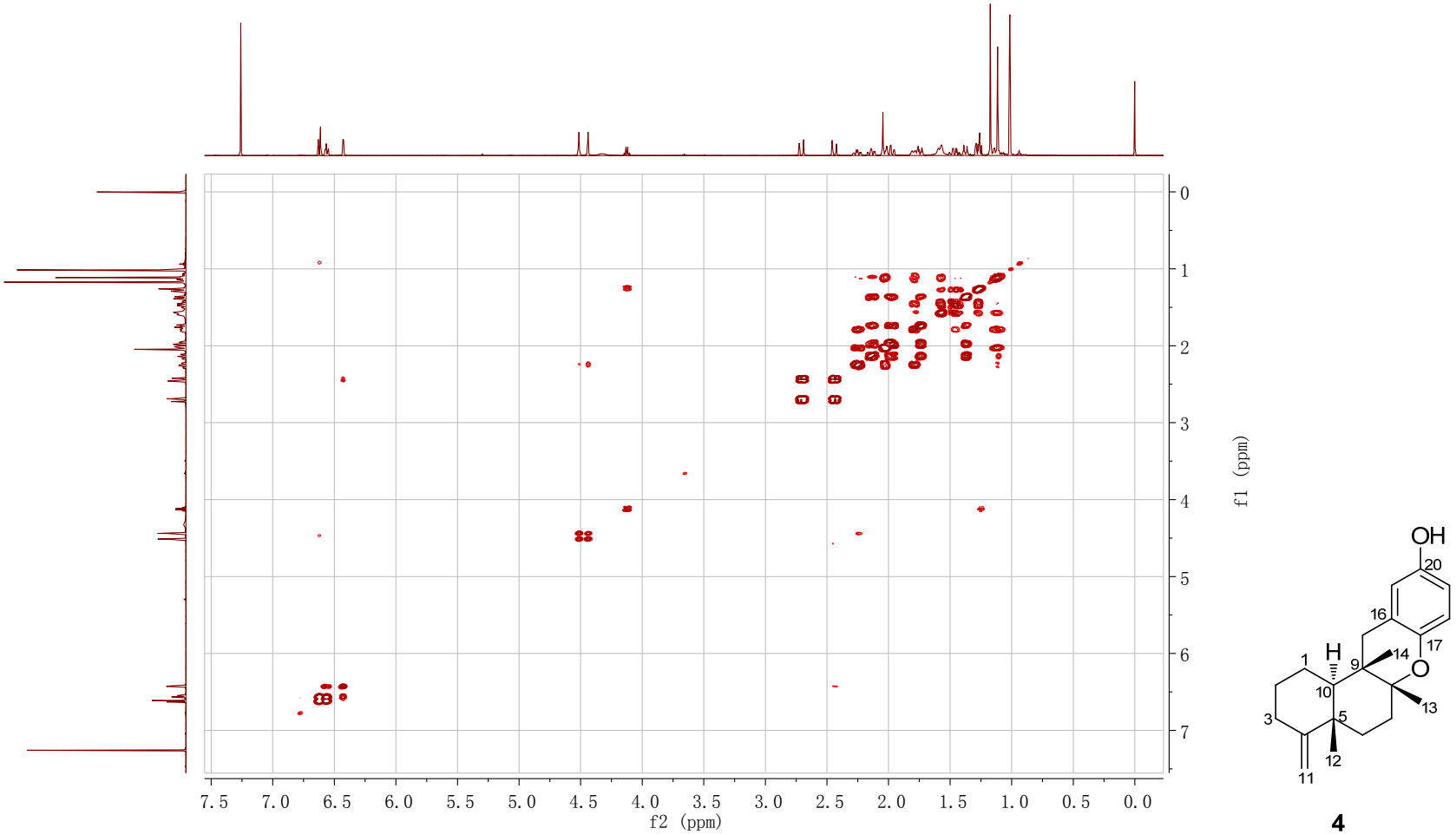


Figure S36. DEPT Spectrum of Dysiquinol D (**4**).



4

Figure S37. ^{1}H-^{1}H COSY Spectrum of Dysiquinol D (**4**).

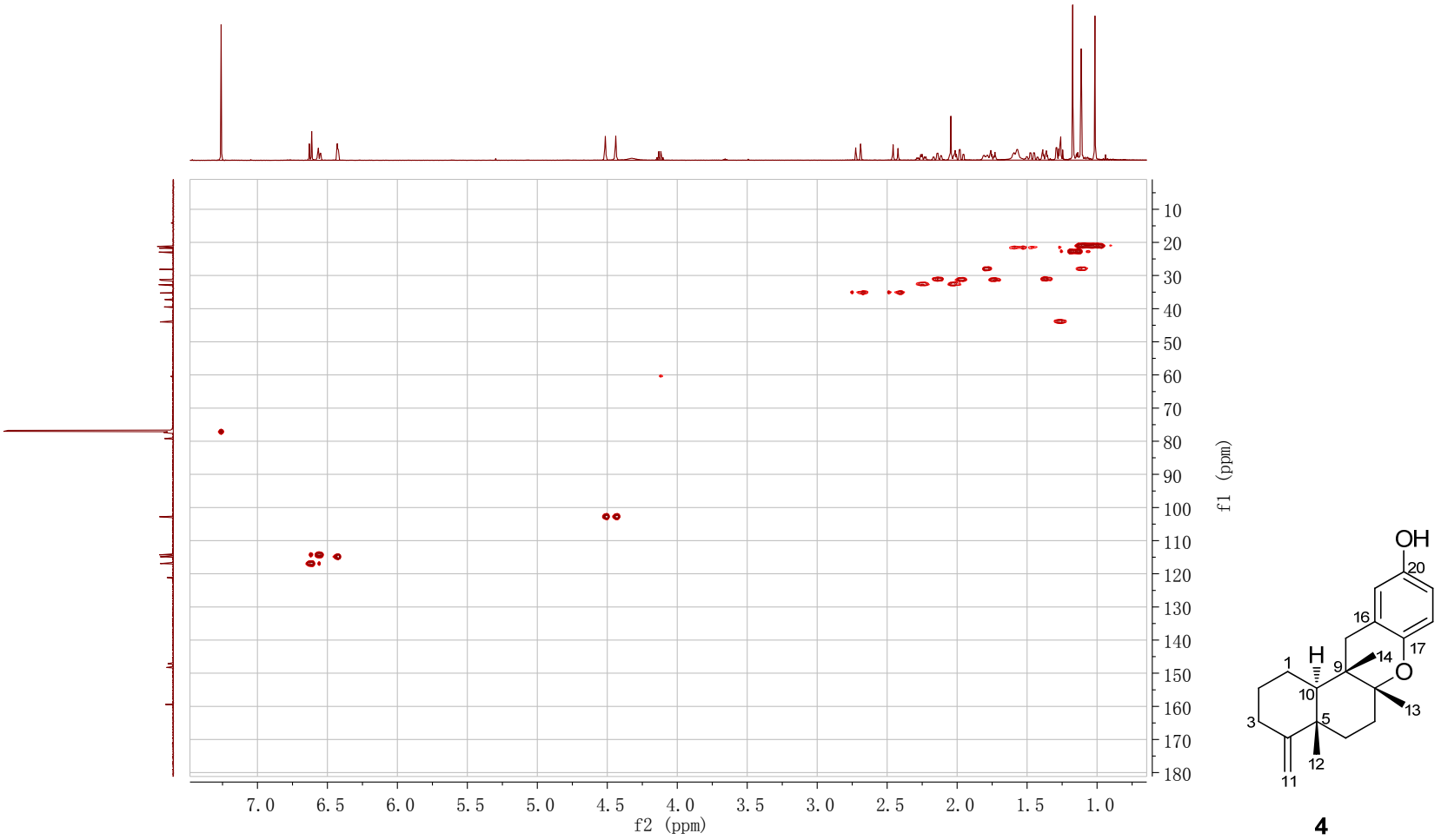
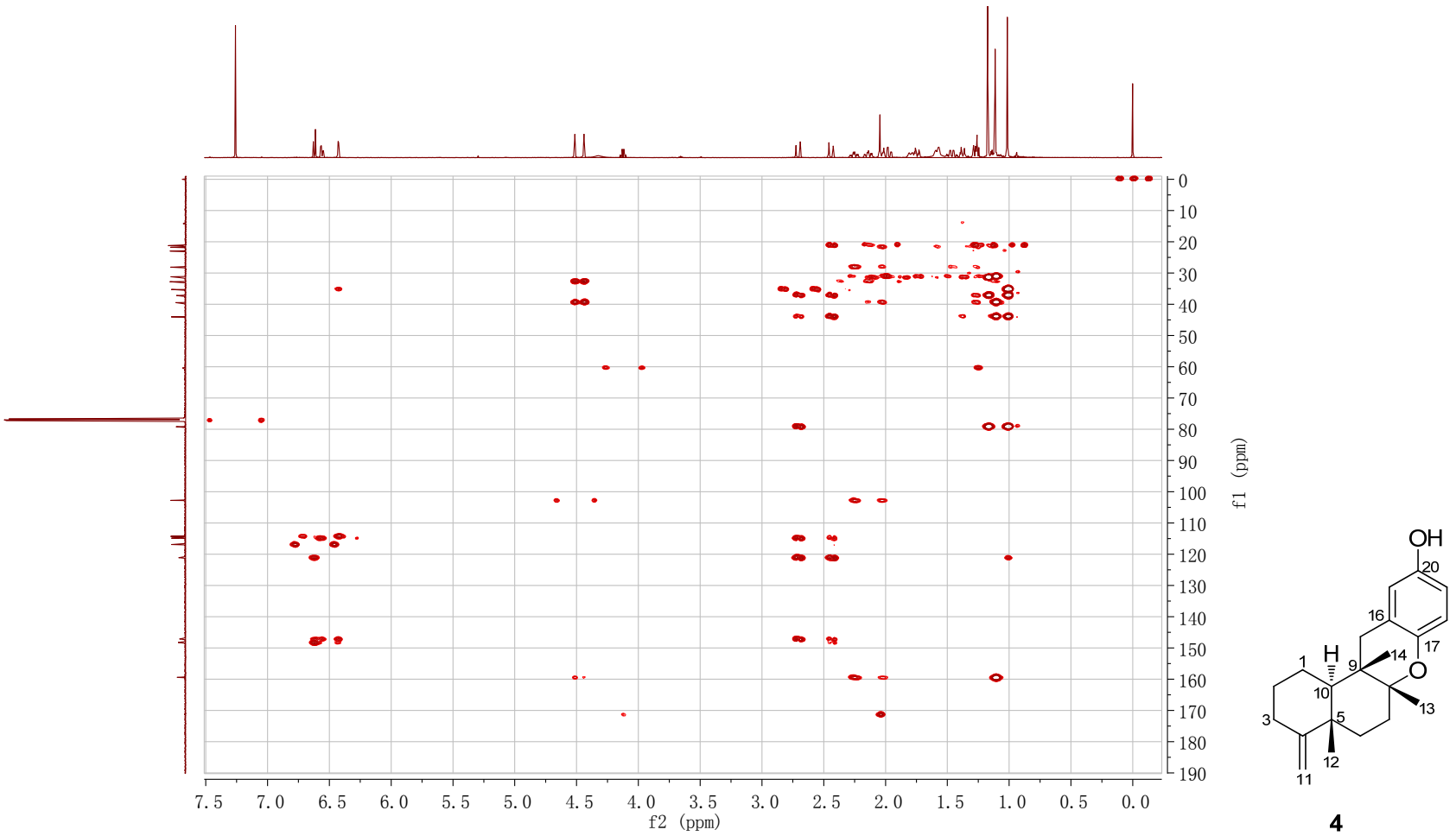
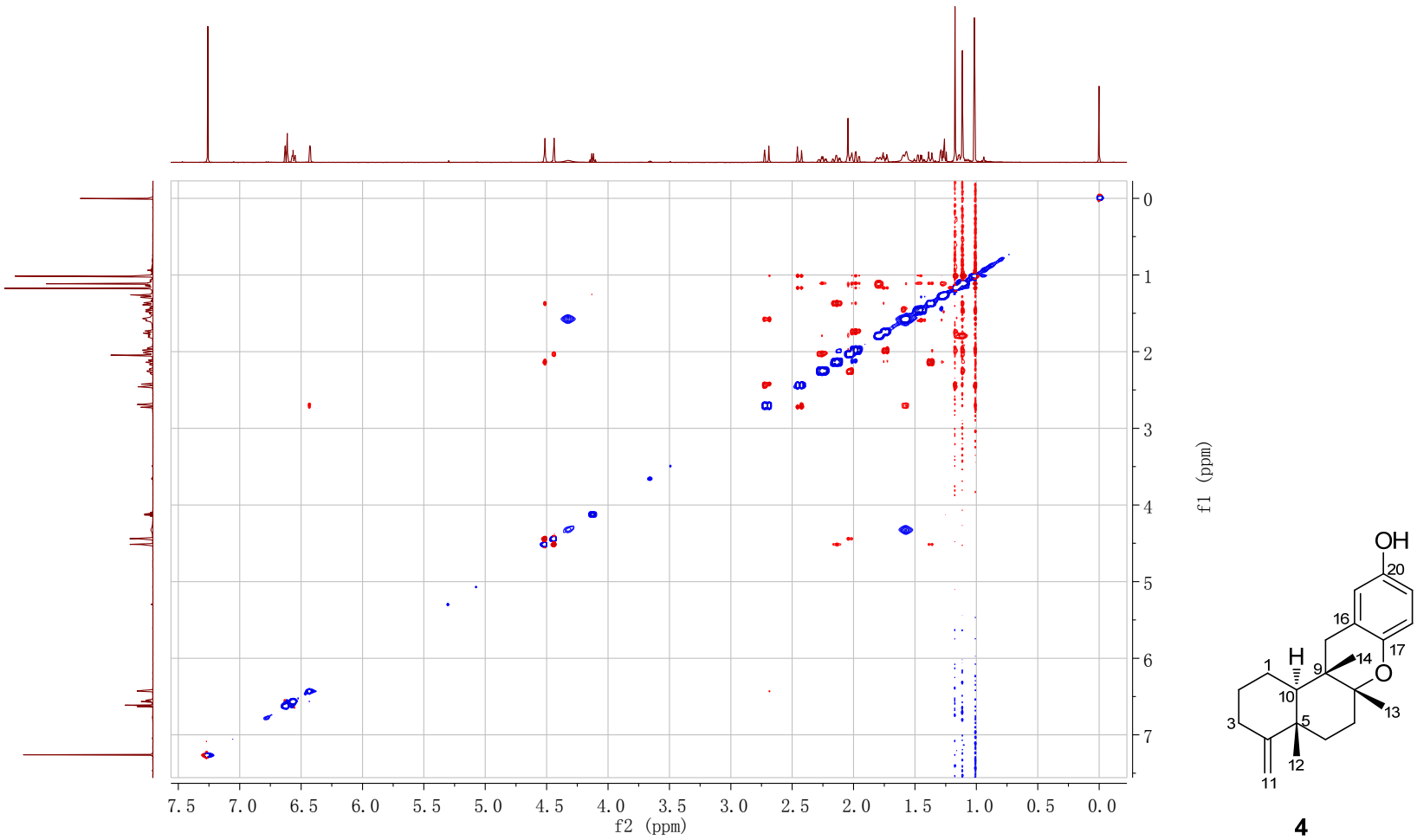


Figure S38. HSQC Spectrum of Dysiquinol D (**4**).



4

Figure S39. HMBC Spectrum of Dysiquinol D (**4**).



4

Figure S40. NOESY Spectrum of Dysiquinol D (**4**).

Elemental Composition Report XT-15 **Page 1**

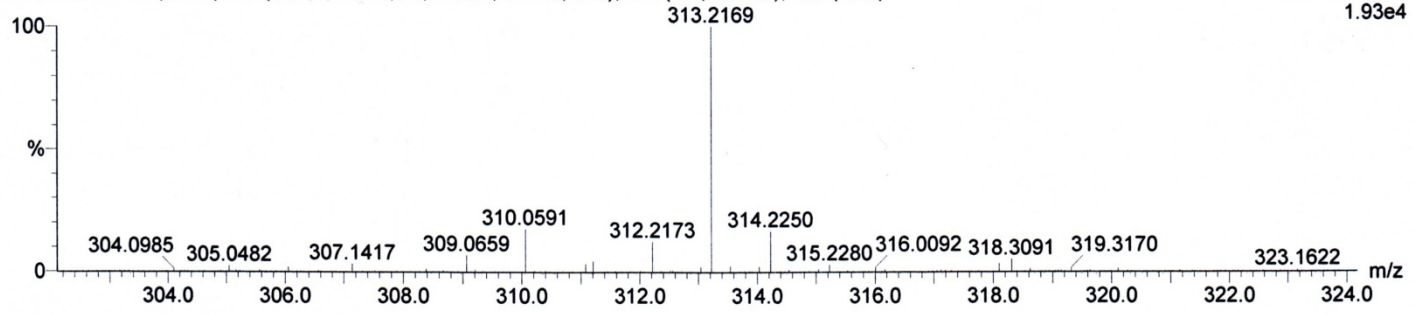
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
14 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 10-25 H: 10-40 O: 1-6

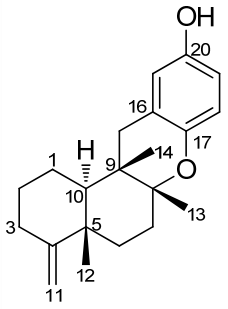
SIPI
XT-15 M.W=312
WQ12-324H 10 (0.352) AM (Cen,4, 80.00, Ar,5000.0,308.05,0.70); Sm (SG, 2x1.00); Cm (2:11)

Q-Tof micro
YA019

16-Jul-2012,15:28:35
TOF MS ES+
1.93e4

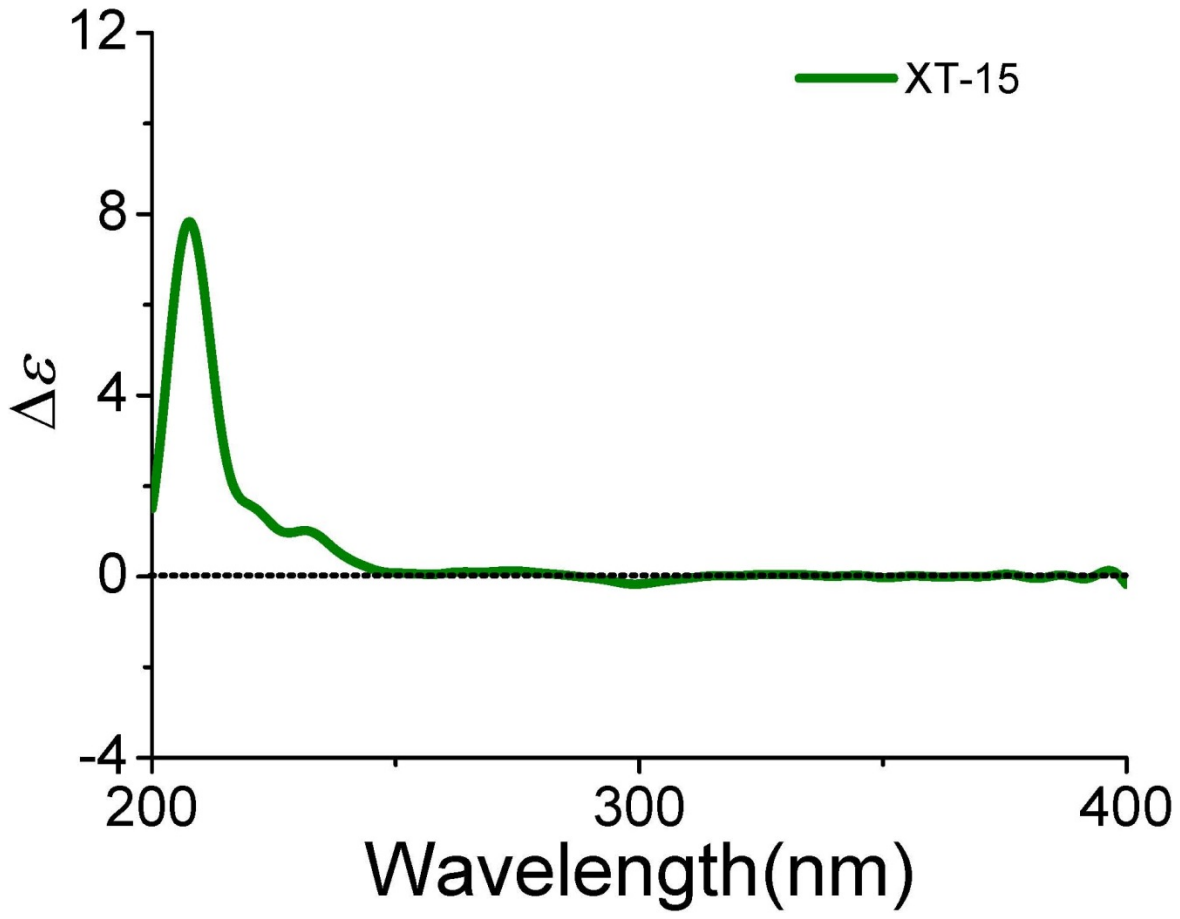


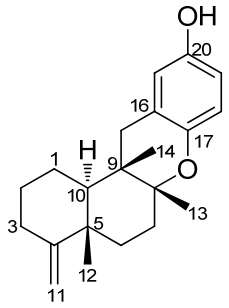
Minimum:	70.00				-1.5		
Maximum:	100.00		5.0	20.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
313.2169	100.00	313.2168	0.1	0.3	7.5	249.0	C21 H29 O2



4

Figure S41. HRESIMS of Dysiquinol D (**4**).





4

Figure S42. CD Spectrum of Dysiquinol D (**4**) in MeOH.

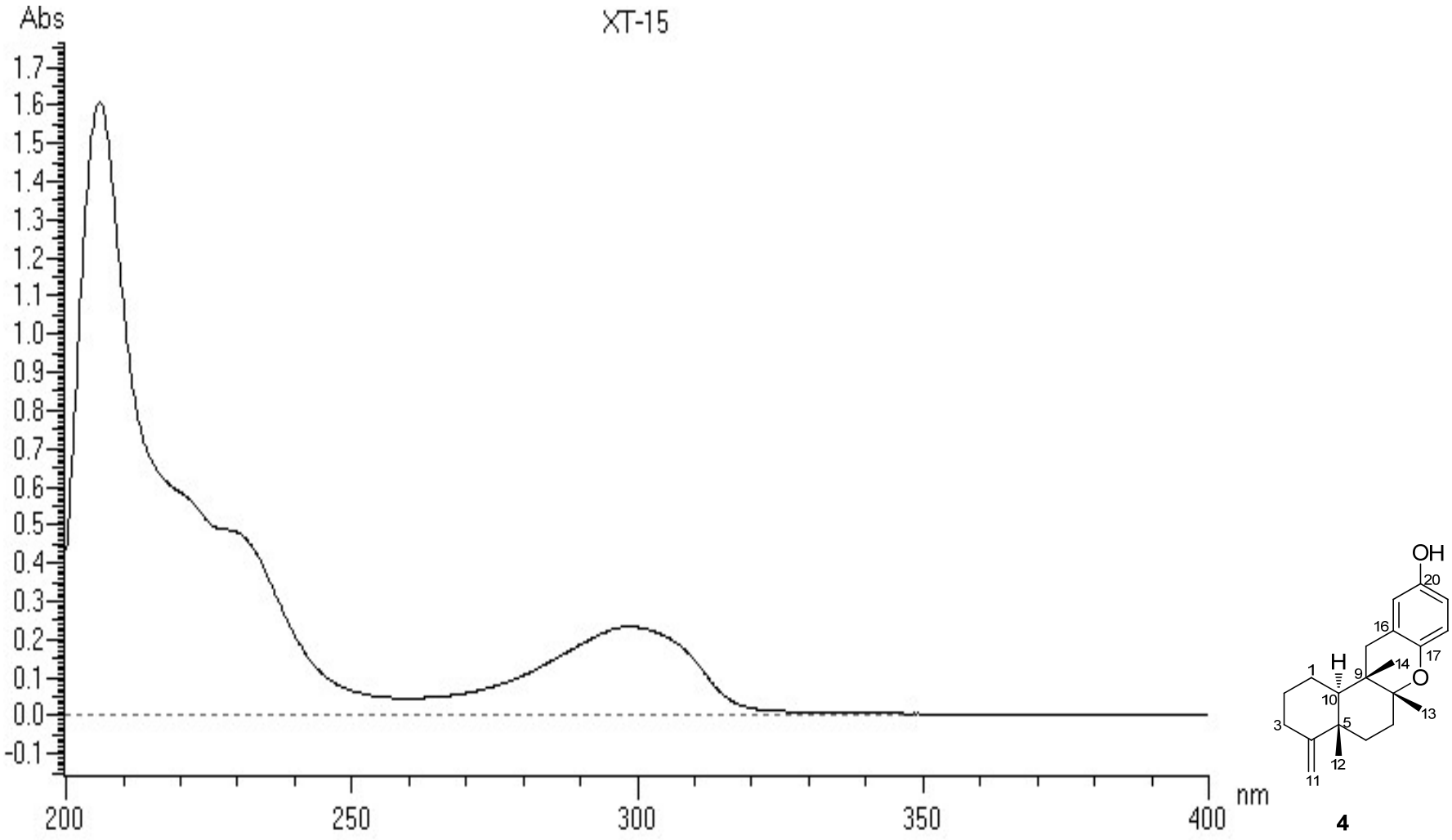
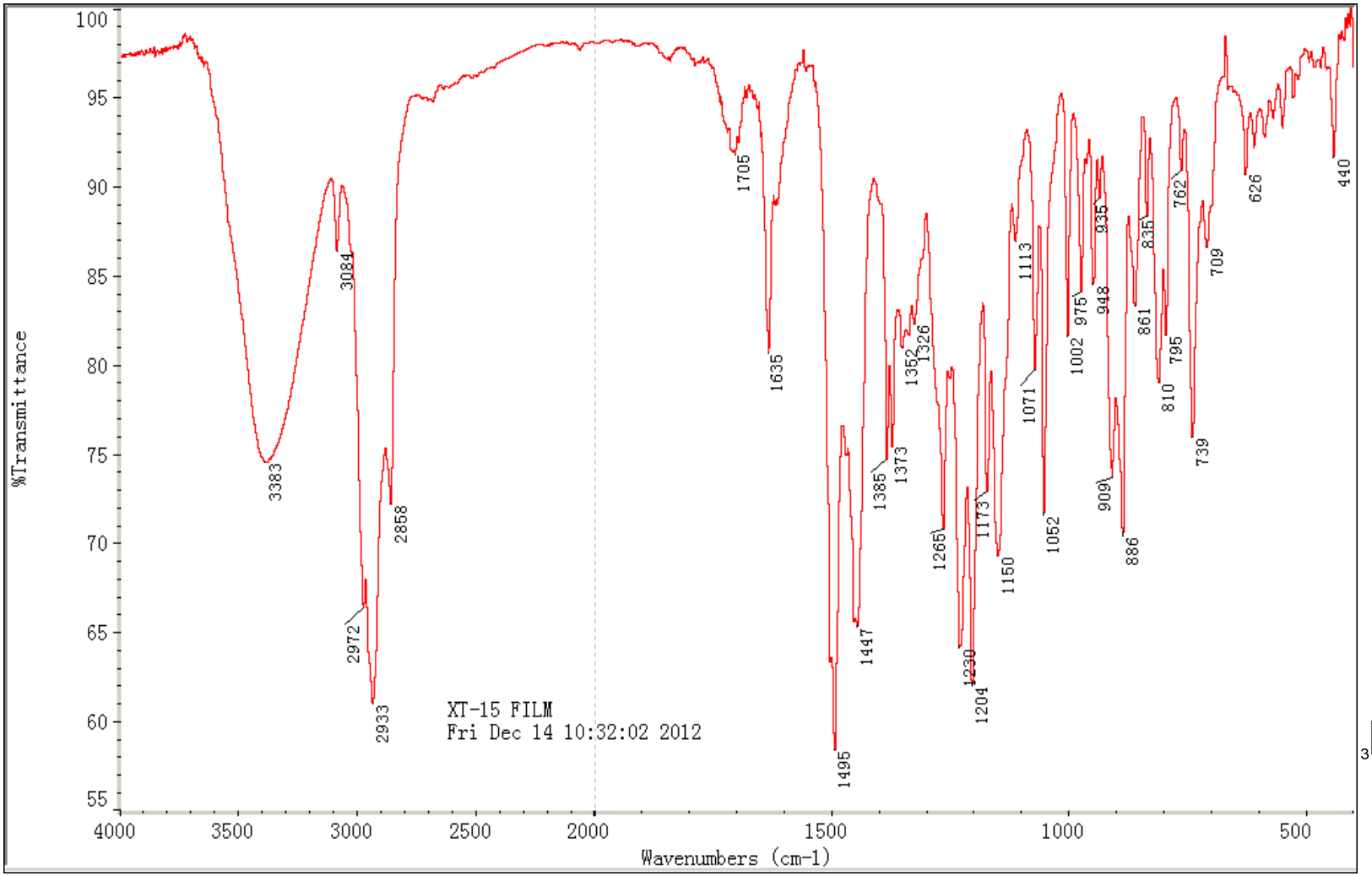
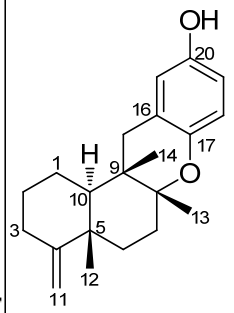


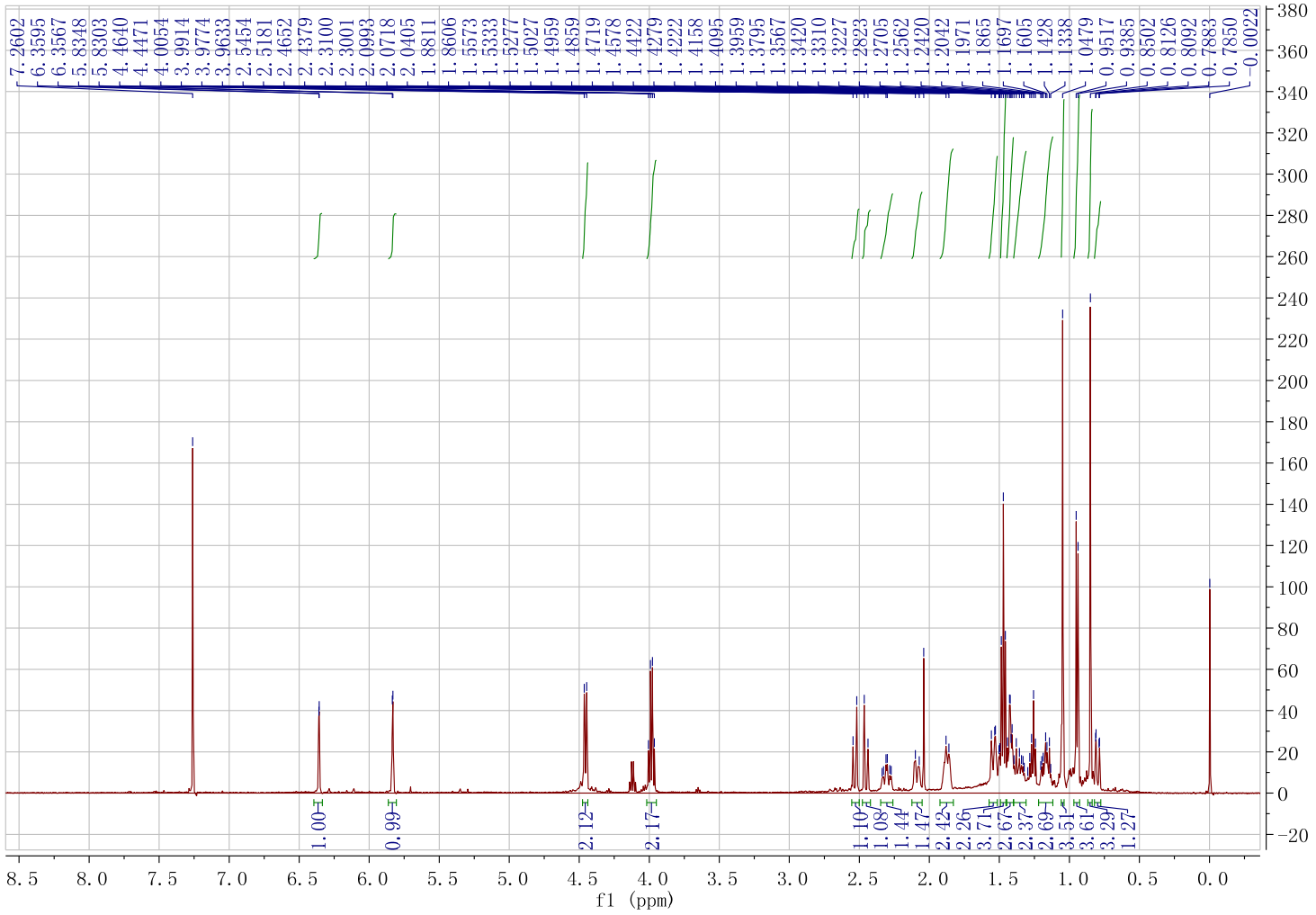
Figure S43. UV Spectrum of Dysiquinol D (**4**).

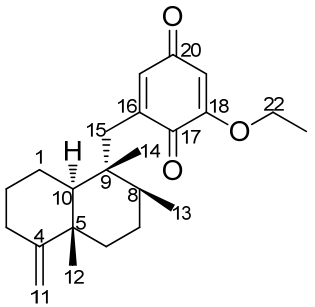




4

Figure S44. IR Spectrum of Dysiquinol D (**4**).





5

Figure S45. ^{1}H NMR Spectrum of (5*S*,8*S*,9*R*,10*S*)-18-ethoxylneoavarone (**5**).

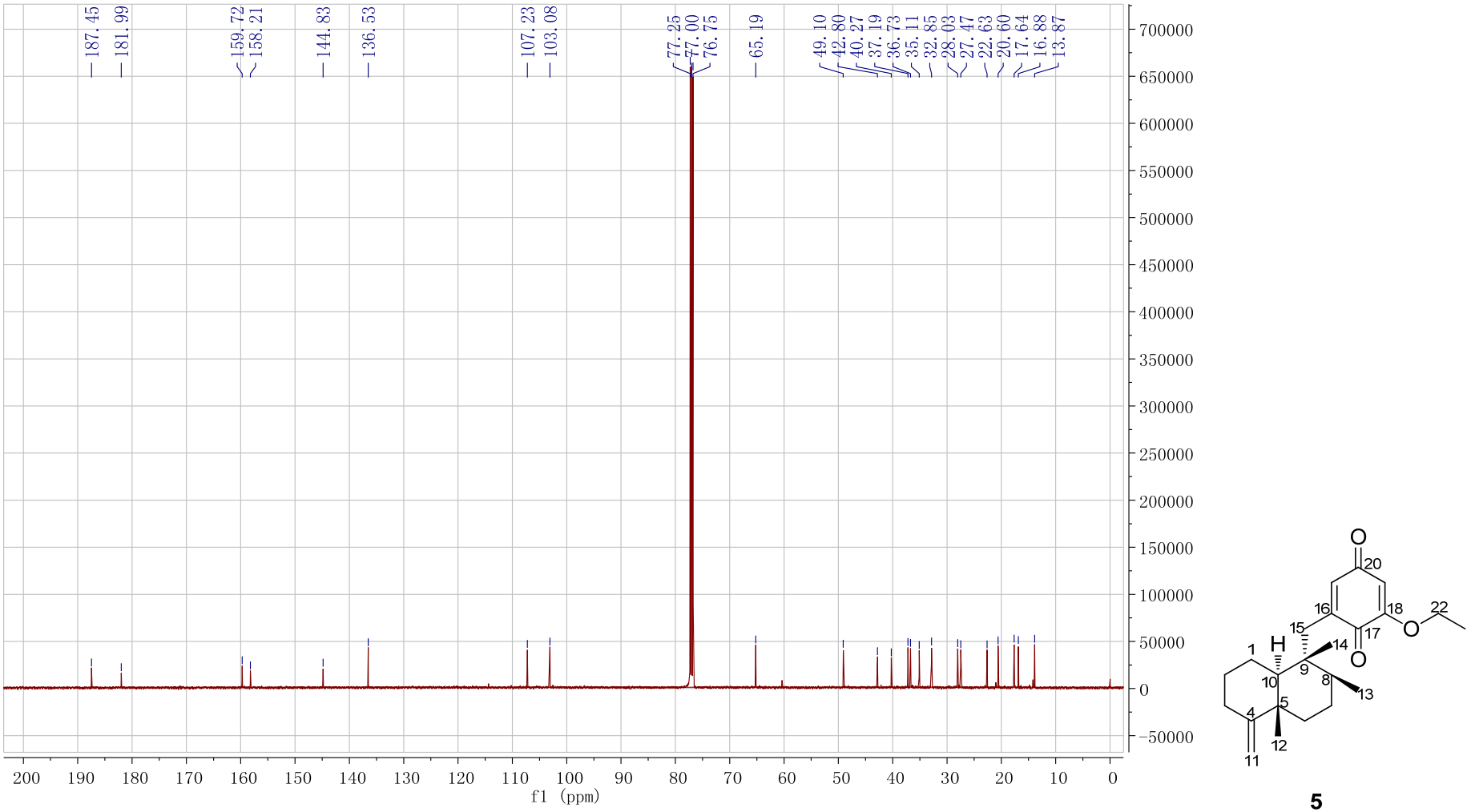
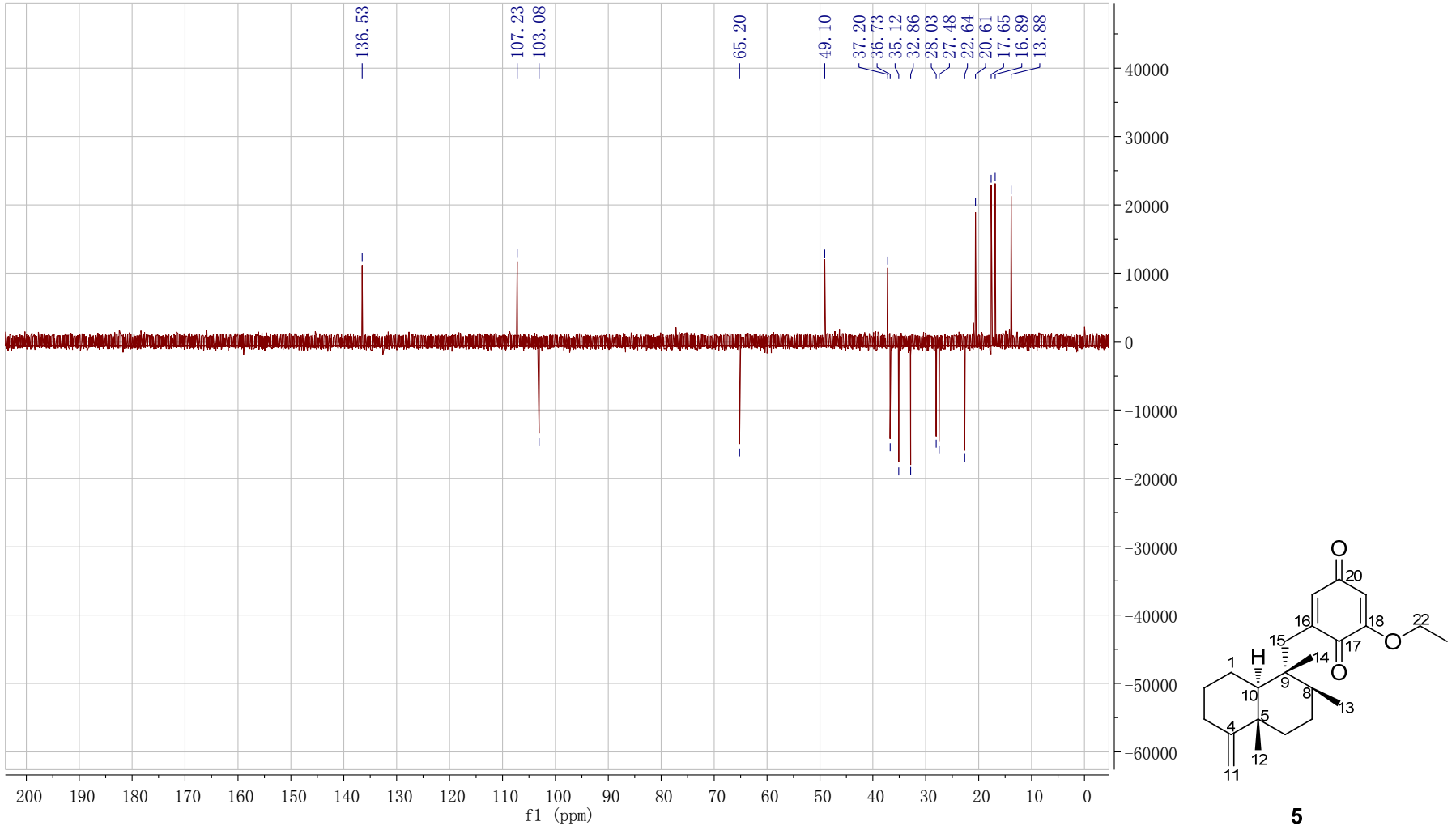
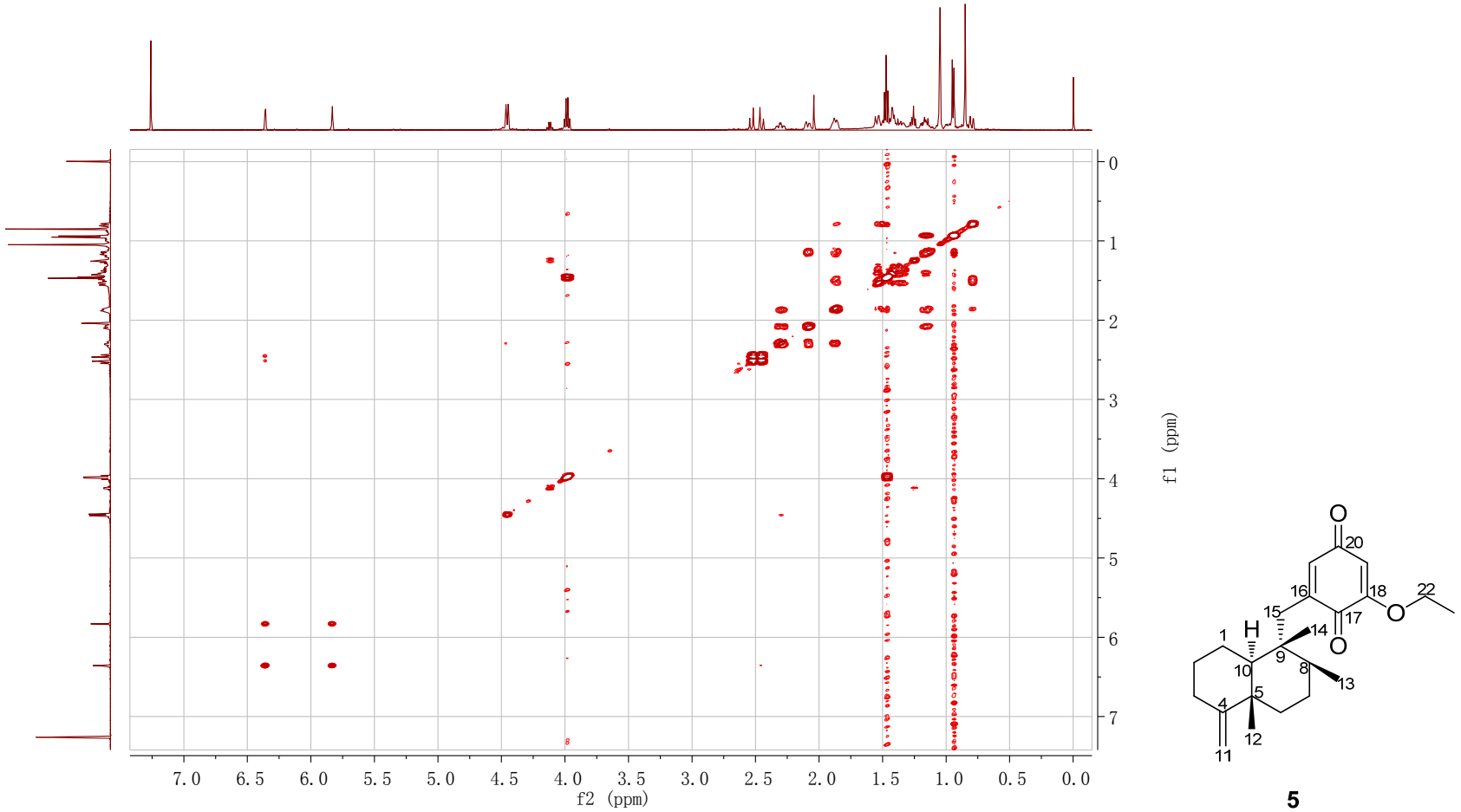


Figure S46. ^{13}C NMR Spectrum of (5*S*,8*S*,9*R*,10*S*)-18-ethoxylneoavarone (**5**).



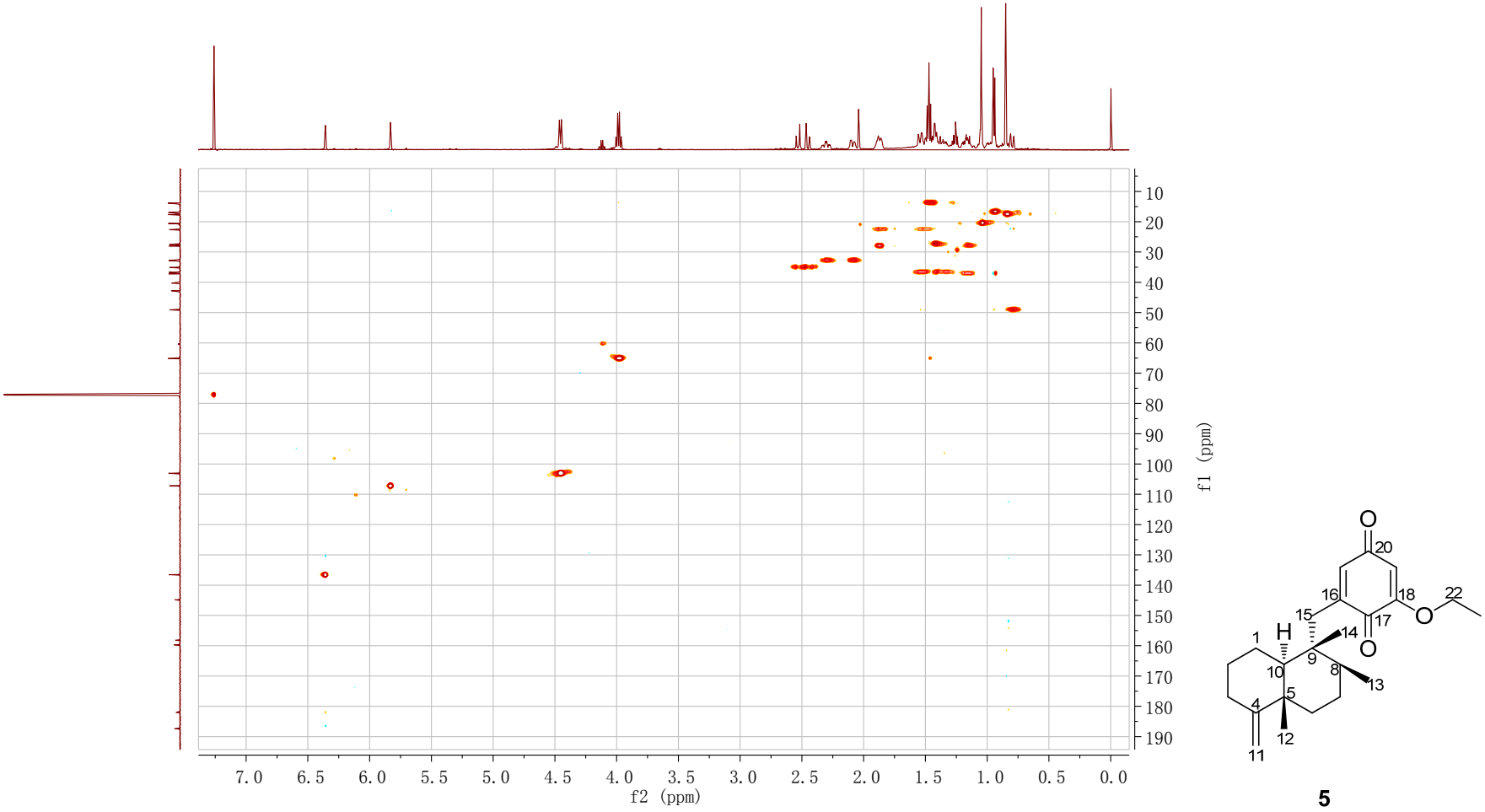
5

Figure S47. DEPT135 Spectrum of (5*S*,8*S*,9*R*,10*S*)-18-ethoxylneoavarone (**5**).



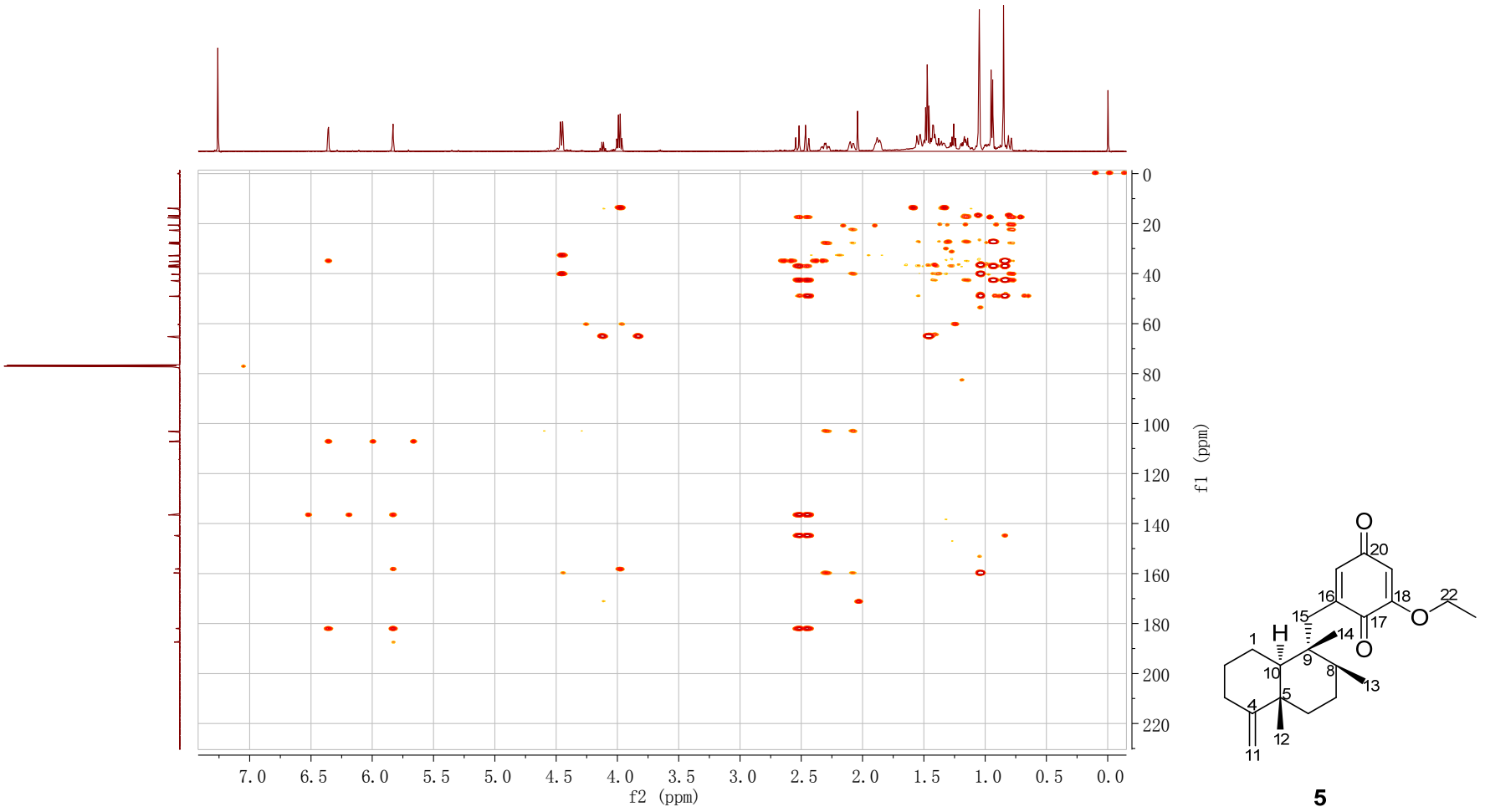
5

Figure S48. ^{1}H-^{1}H COSY Spectrum of (5*S*,8*S*,9*R*,10*S*)-18-ethoxylneoavarone (**5**).



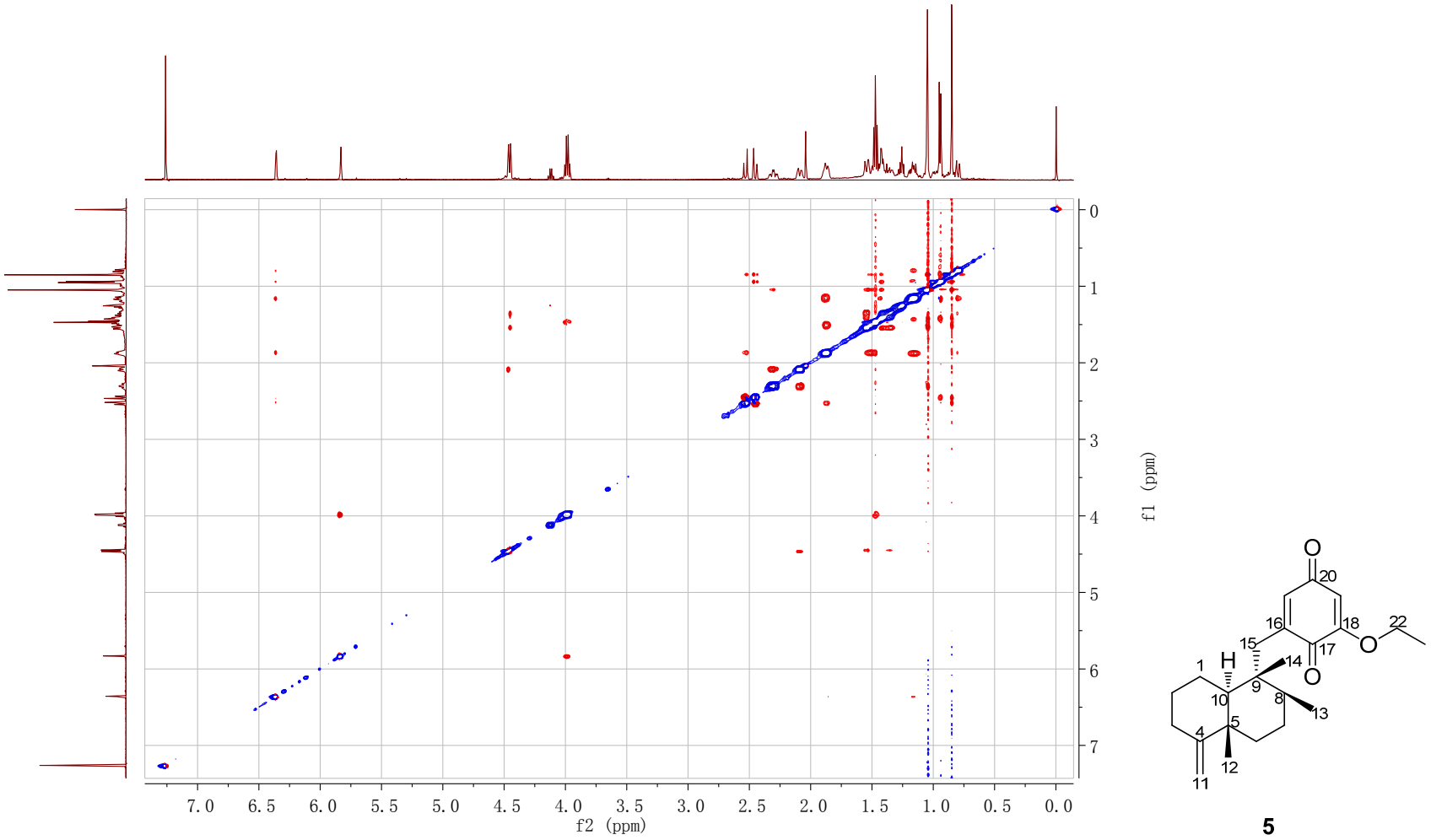
5

Figure S49. HSQC Spectrum of (5*S*,8*S*,9*R*,10*S*)-18-ethoxylneoavarone (**5**).



5

Figure S50. HMBC Spectrum of (5*S*,8*S*,9*R*,10*S*)-18-ethoxylneoavarone (**5**).



5

Figure S51. NOESY Spectrum of (5*S*,8*S*,9*R*,10*S*)-18-ethoxylneoavarone (**5**).

Elemental Composition Report XT-7

Page 1

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

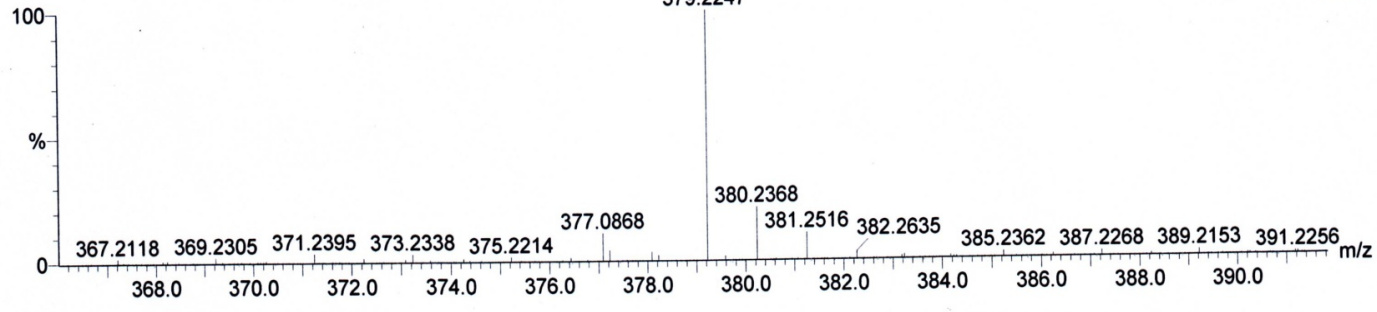
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 10-25 H: 10-40 O: 1-6 Na: 1-1

SIPI
XT-7 M.W=356
WQ12-323H 51 (1.797) AM (Cen,4, 80.00, Ar,5000.0,376.07,0.70); Sm (SG, 2x1.00); Cm (38:56)

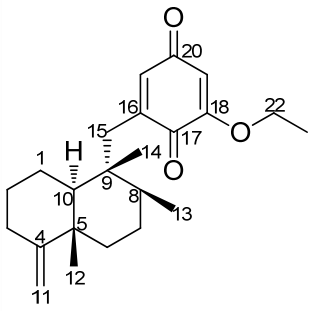
Q-Tof micro
YA019

16-Jul-2012,15:05:05

TOF MS ES+
4.68e4

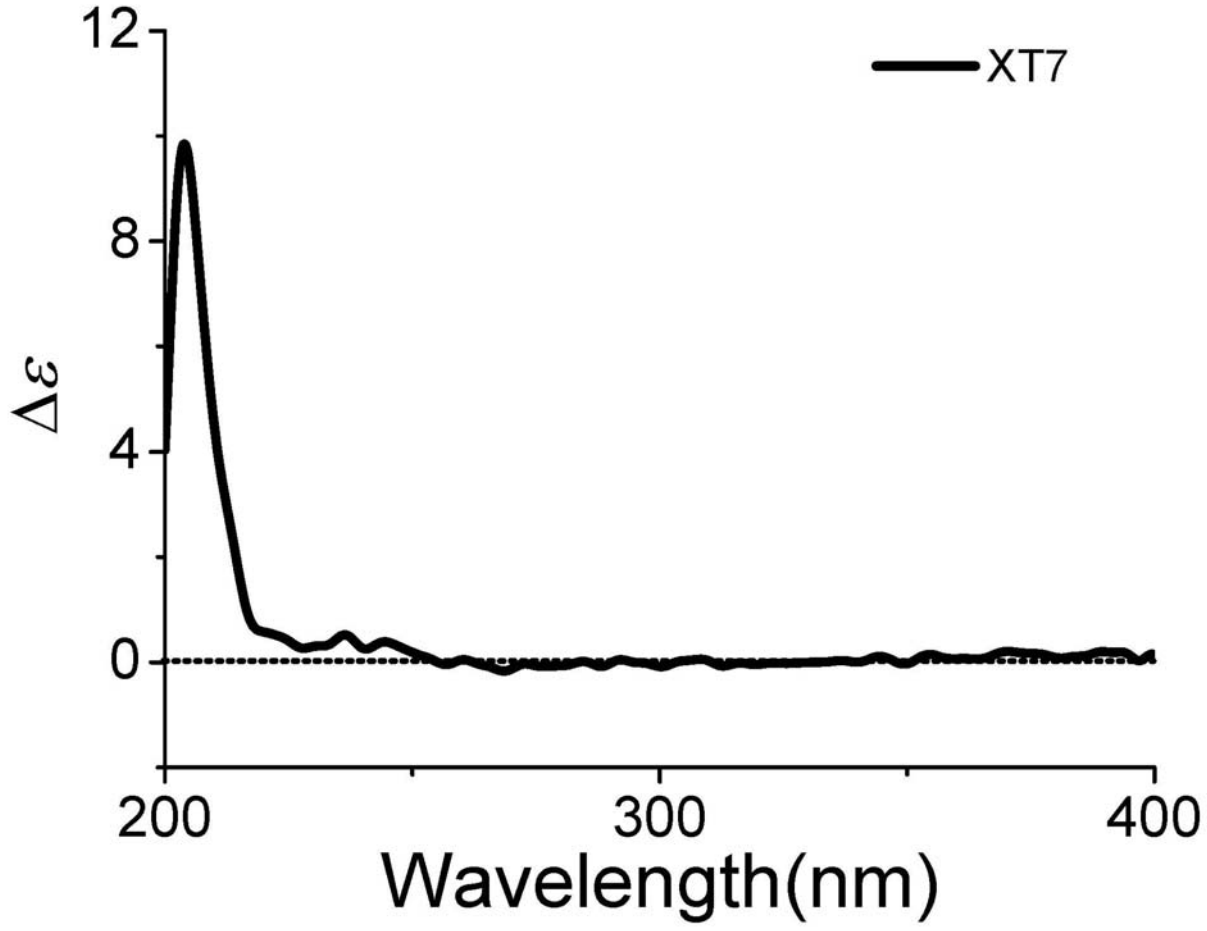


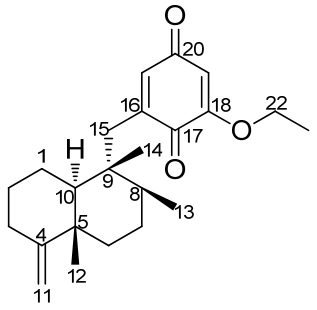
Minimum:	70.00				-1.5		
Maximum:	100.00		5.0	20.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
379.2247	100.00	379.2249	-0.2	-0.5	7.5	1299.5	C23 H32 O3 Na



5

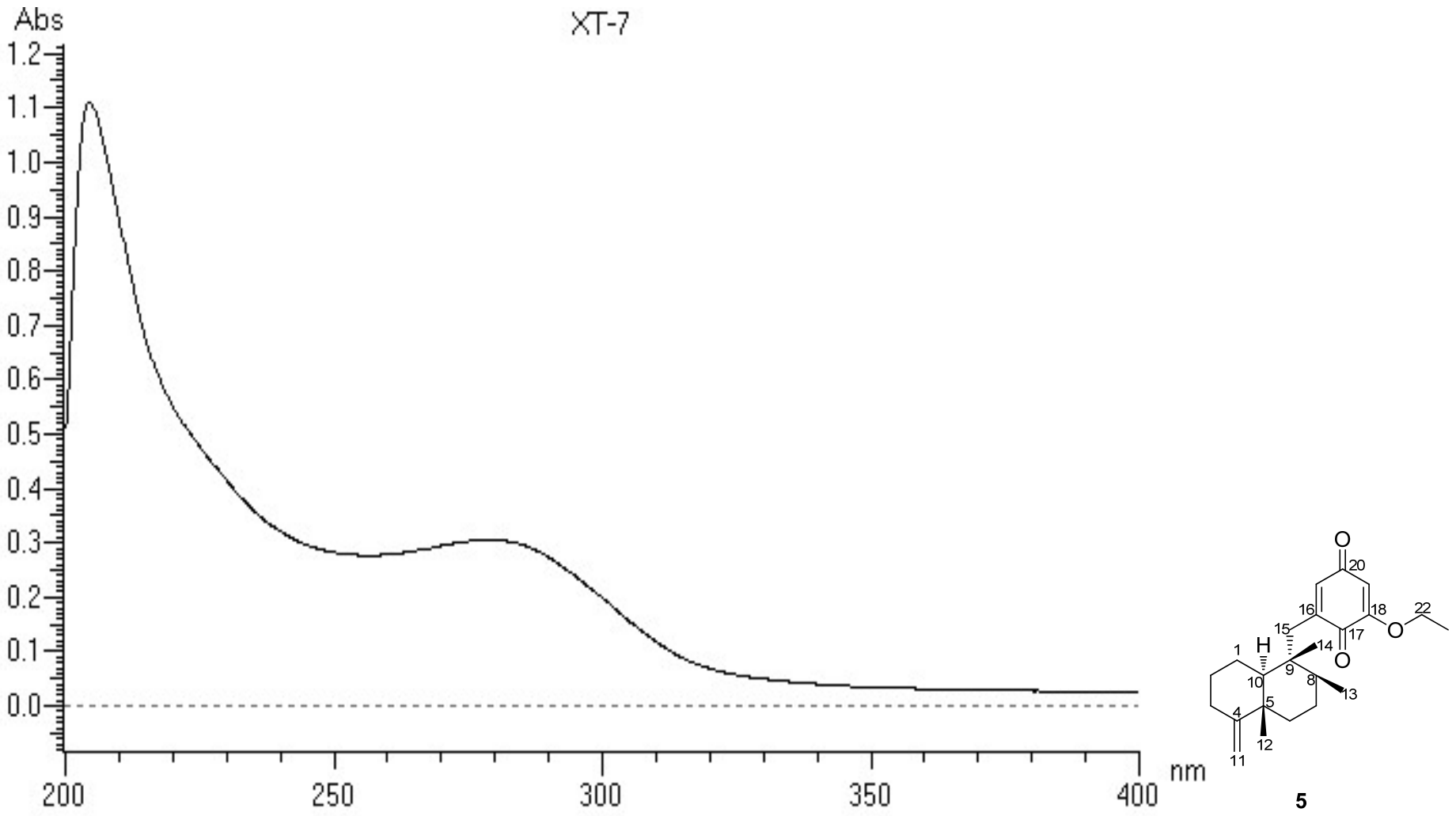
Figure S52. HRESIMS of (5*S*,8*S*,9*R*,10*S*)-18-ethoxylneoavarone (**5**).





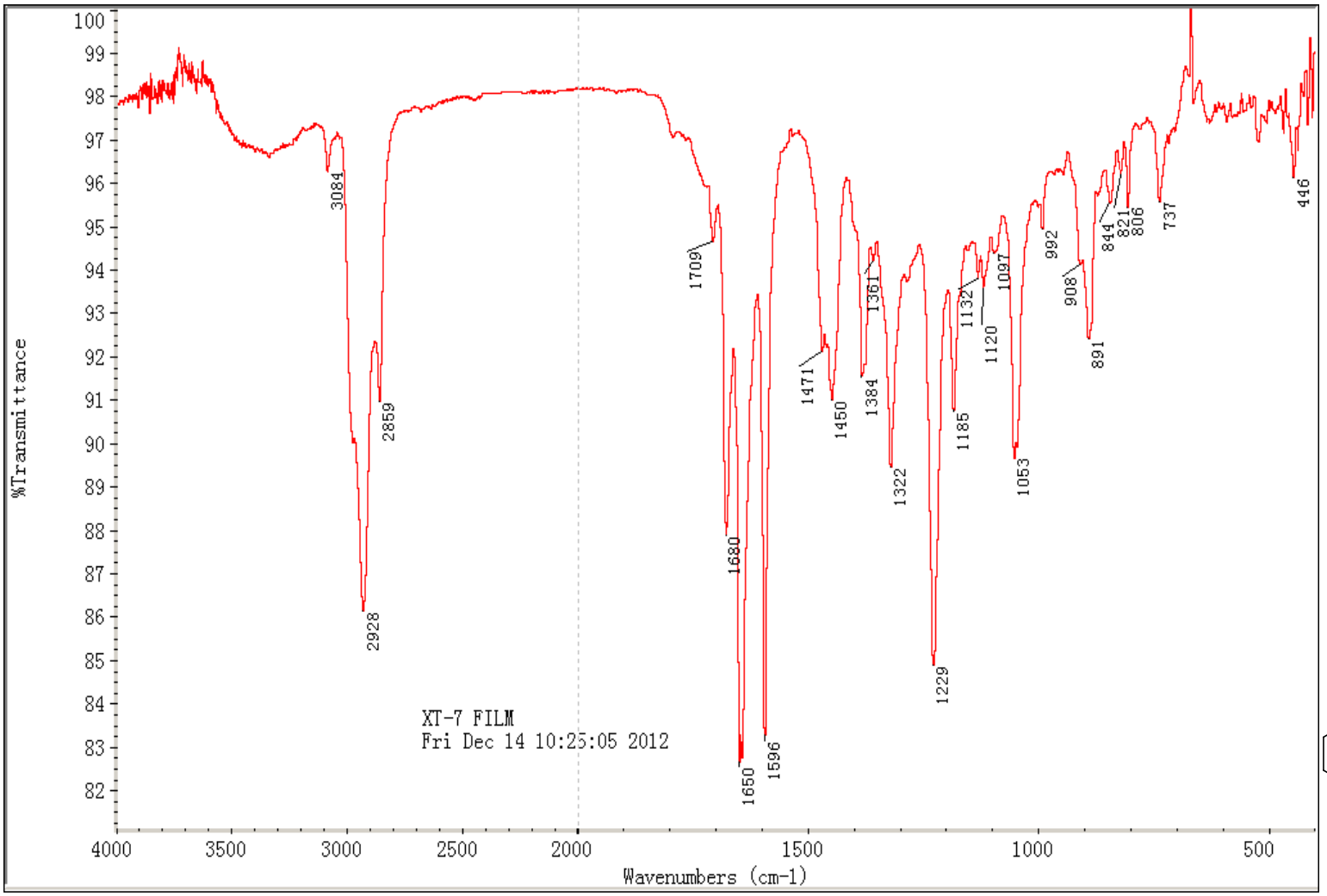
5

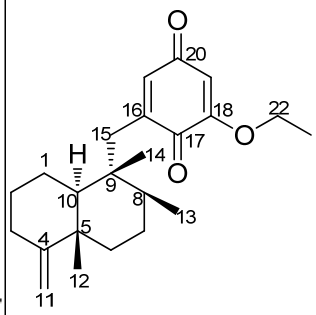
Figure S53. CD Spectrum of (5*S*,8*S*,9*R*,10*S*)-18-ethoxylneoavarone (**5**) in MeOH.



5

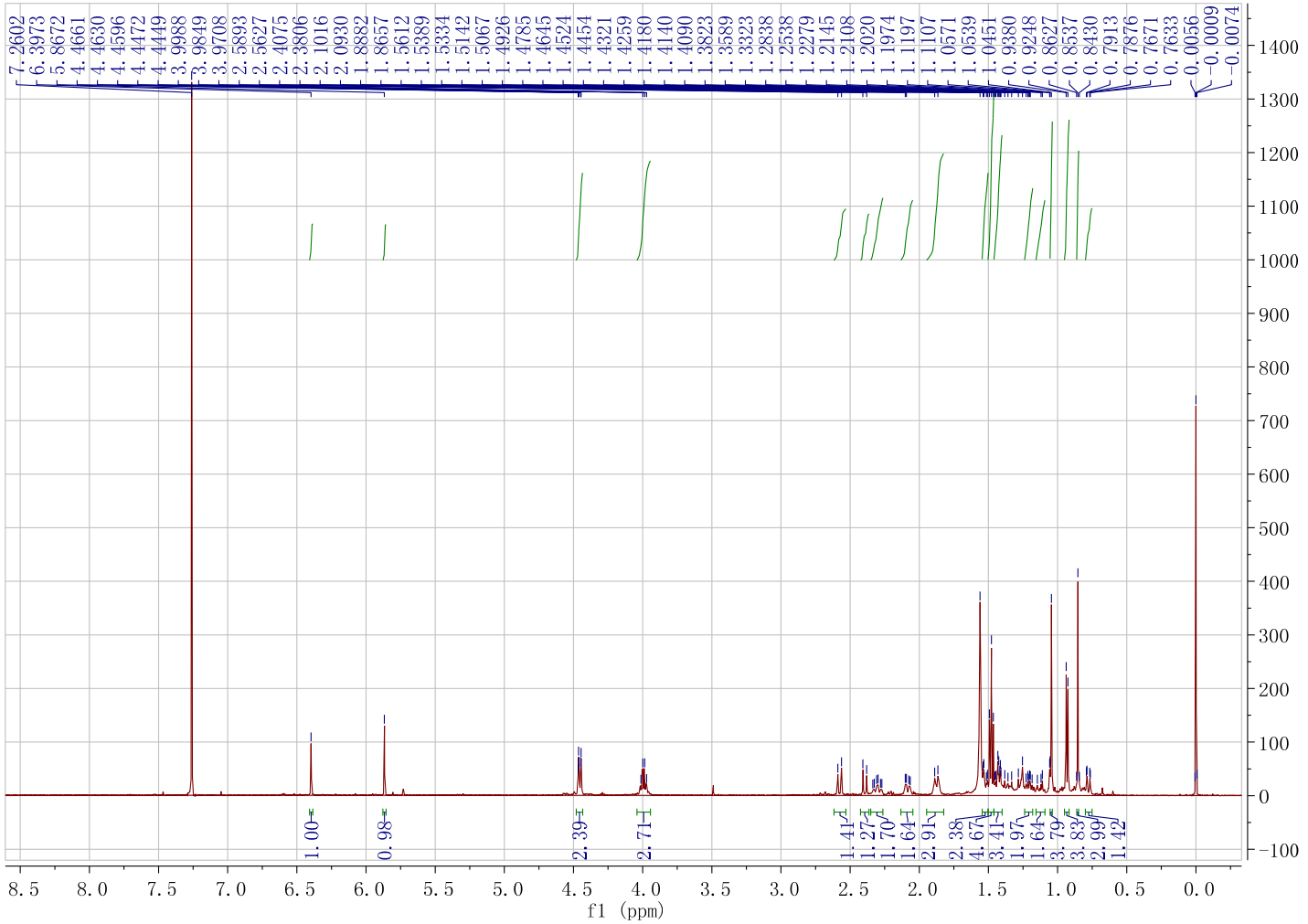
Figure S54. UV Spectrum of (5*S*,8*S*,9*R*,10*S*)-18-ethoxylneoavarone (**5**).

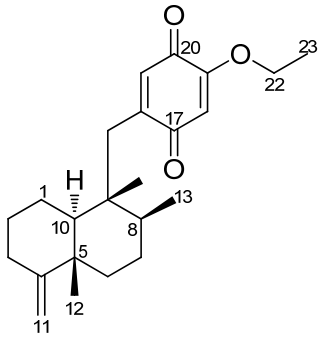




5

Figure S55. IR Spectrum of (5*S*,8*S*,9*R*,10*S*)-18-ethoxylneoavarone (**5**).





6

Figure S56. ^{1}H NMR Spectrum of (5*S*,8*S*,9*R*,10*S*)-19-ethoxylneoavarone (**6**).

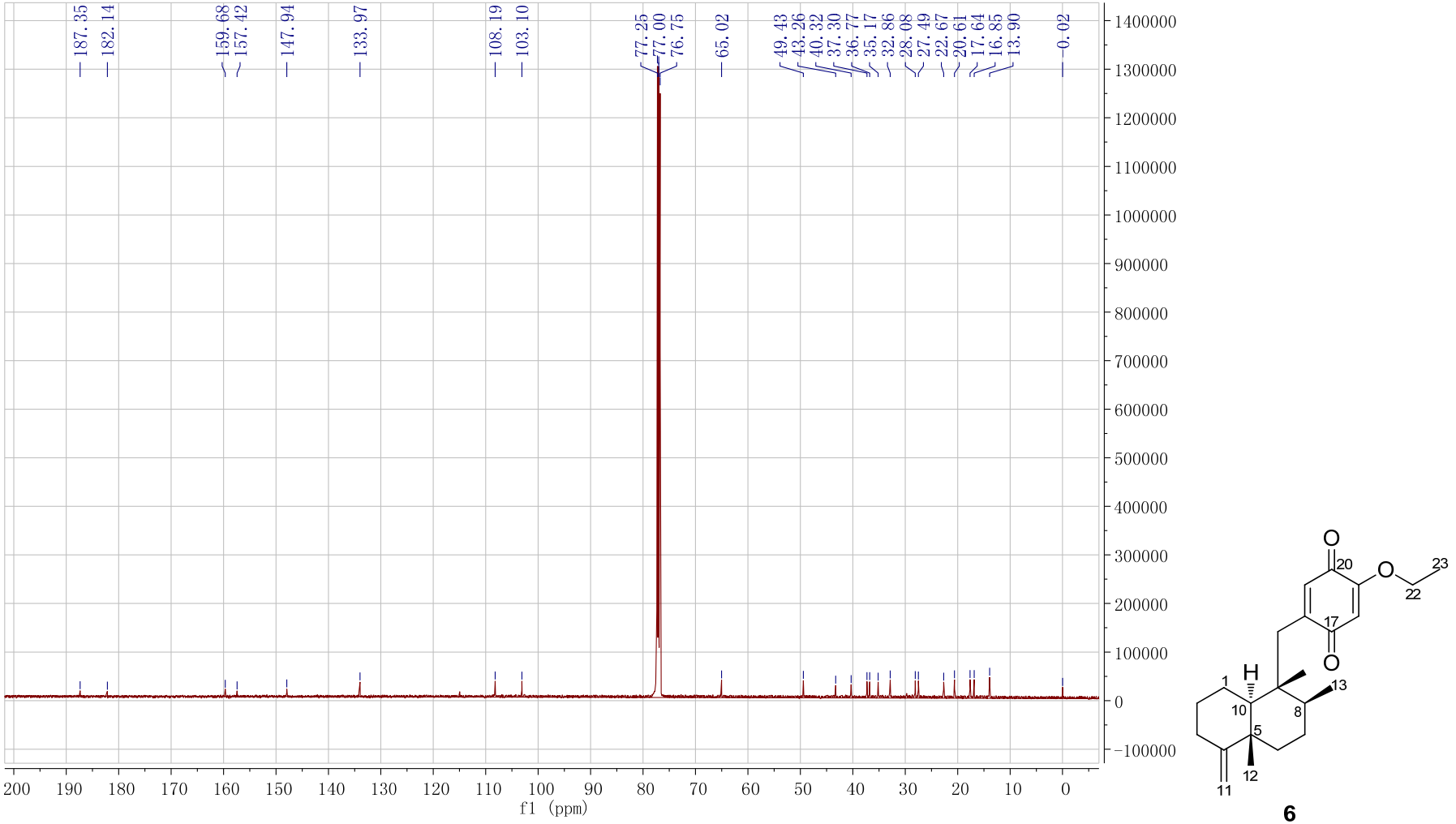


Figure S57. ^{13}C NMR Spectrum of (5*S*,8*S*,9*R*,10*S*)-19-ethoxylneoavarone (**6**).

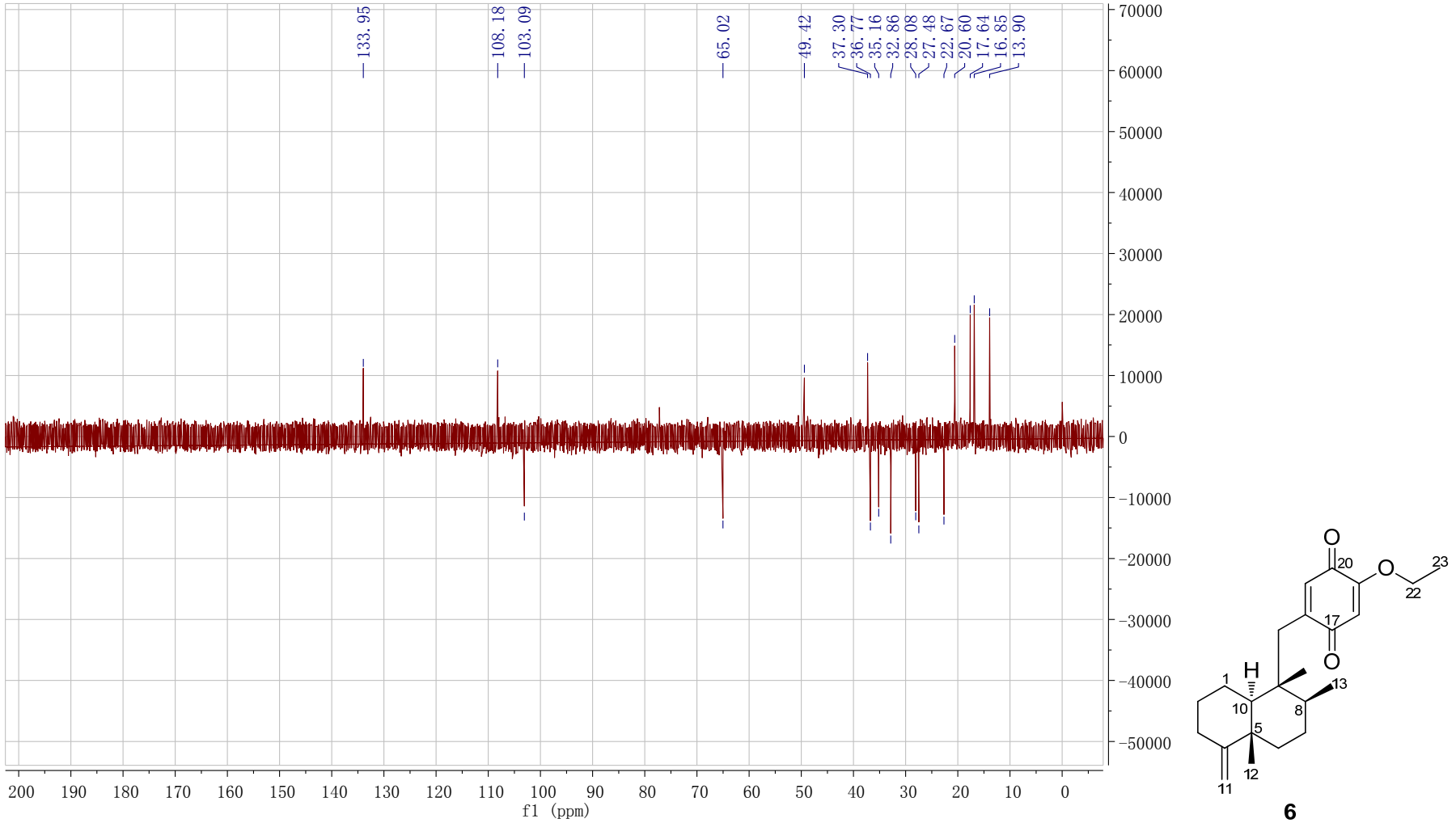
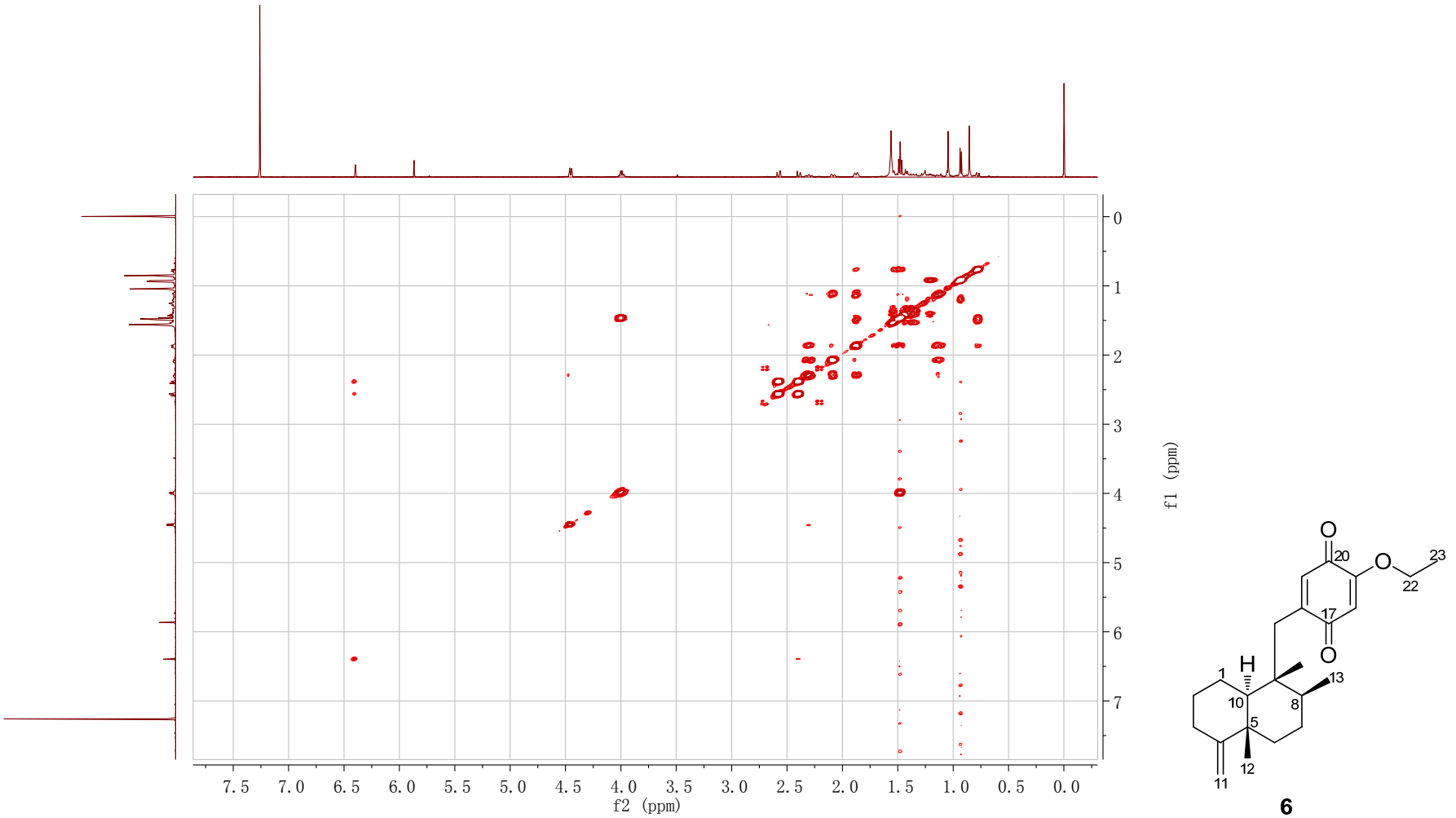


Figure S58. DEPT135 Spectrum of (5*S*,8*S*,9*R*,10*S*)-19-ethoxylneoavarone (**6**).



6

Figure S59. ^{1}H-^{1}H COSY Spectrum of (5*S*,8*S*,9*R*,10*S*)-19-ethoxylneoavarone (**6**).

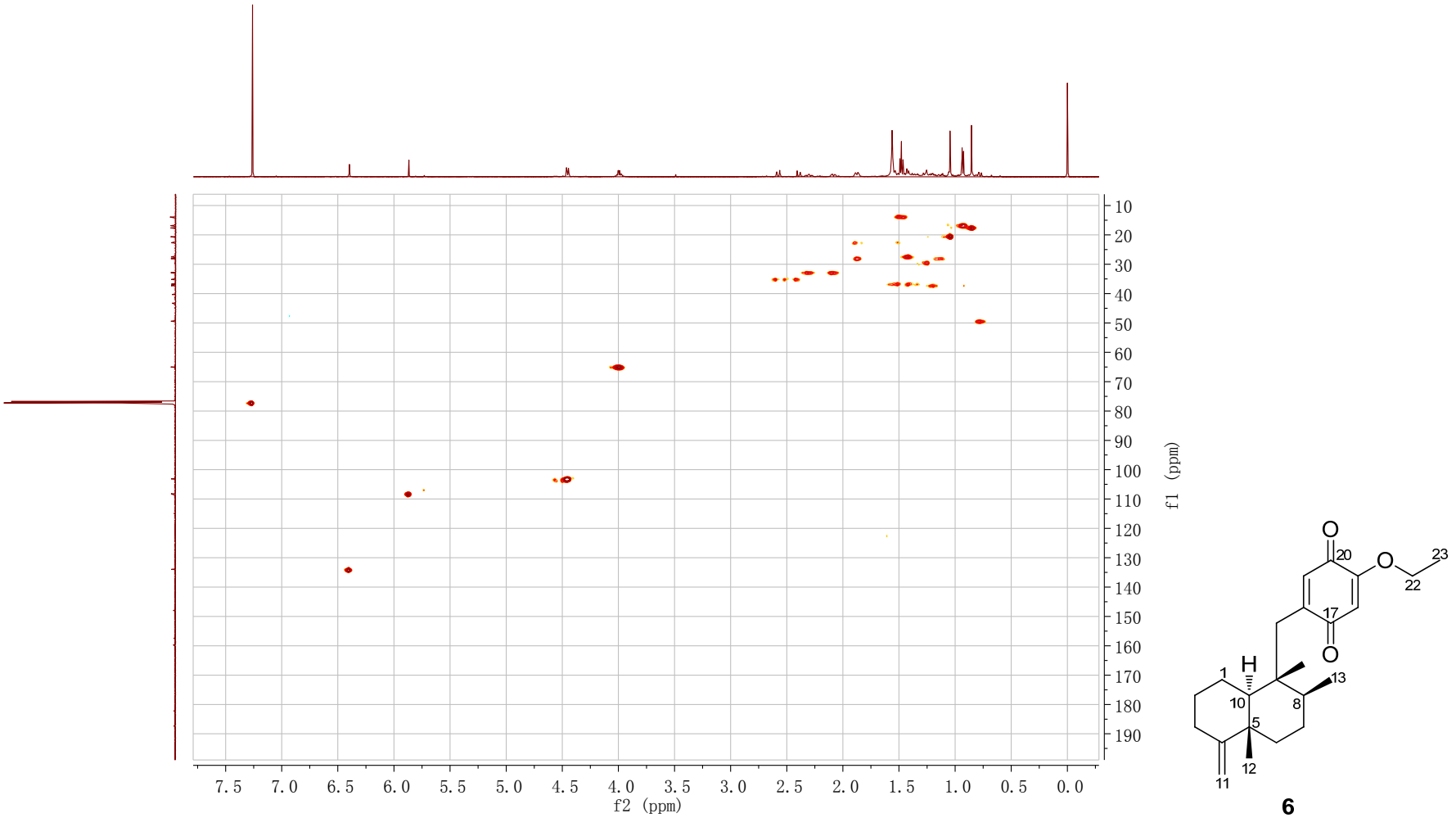


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Figure S60. HSQC Spectrum of (5*S*,8*S*,9*R*,10*S*)-19-ethoxylneoavarone (**6**).

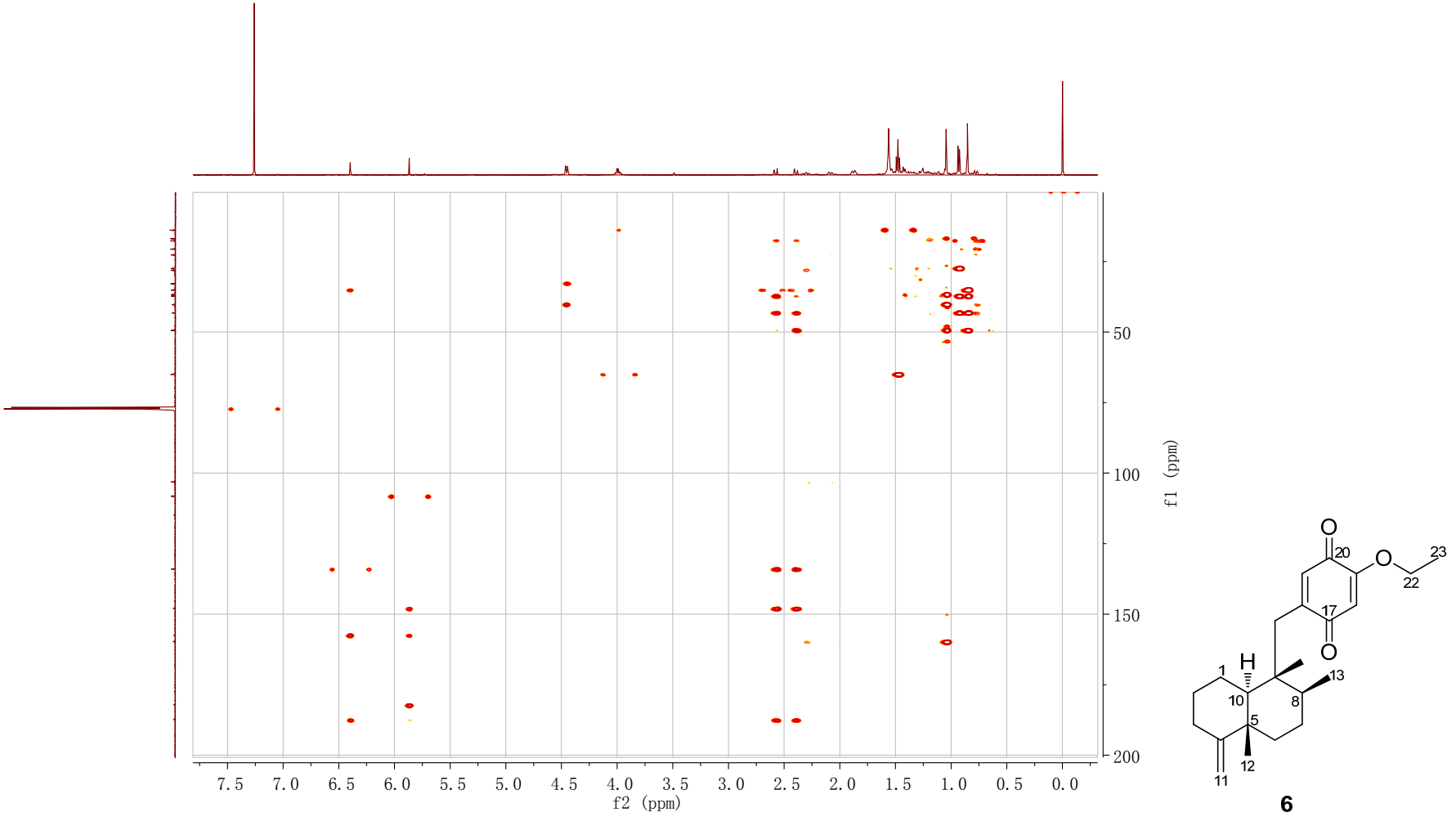
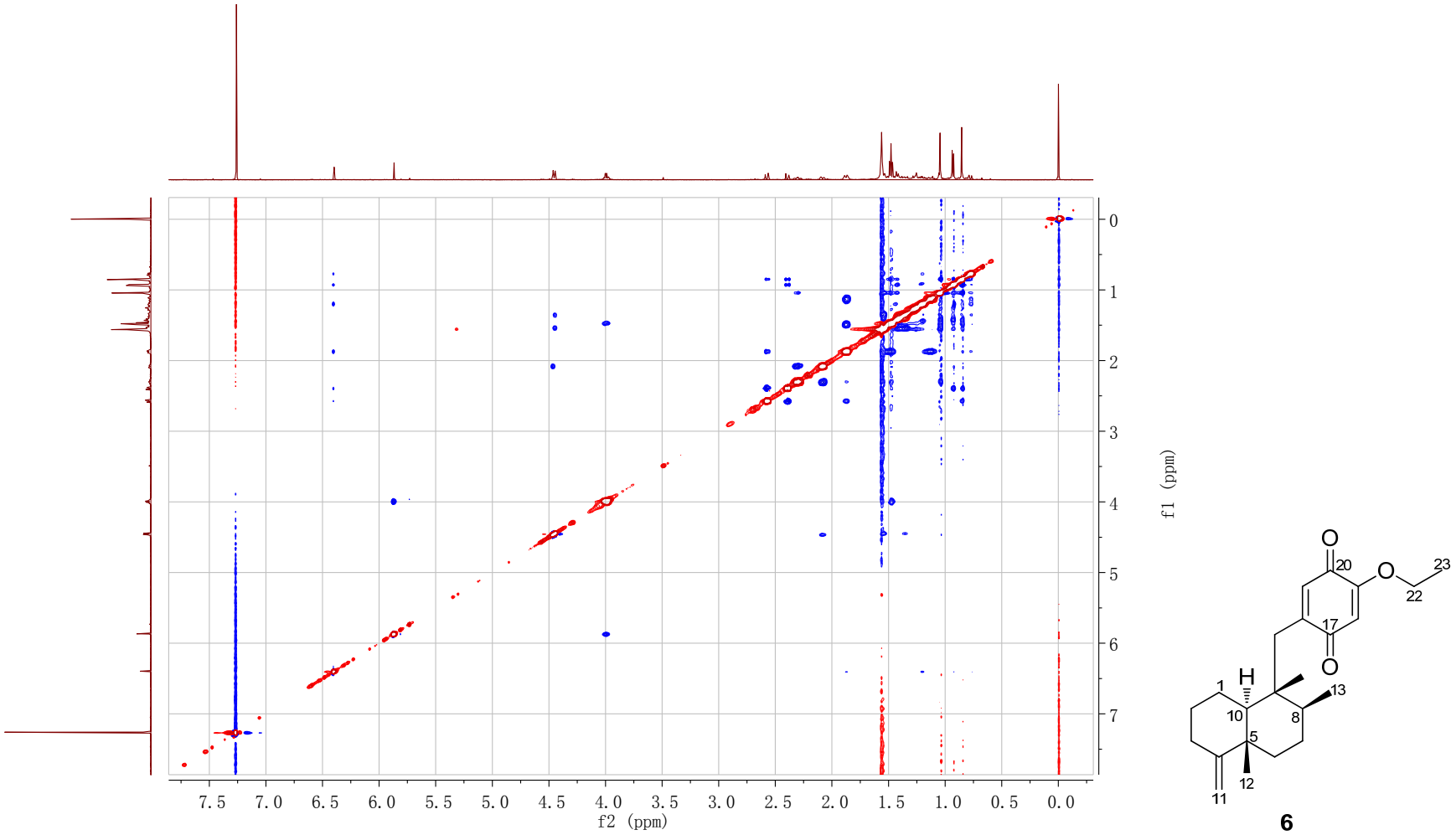


Figure S61. HMBC Spectrum of (5*S*,8*S*,9*R*,10*S*)-19-ethoxylneoavarone (**6**).



6

Figure S62. NOESY Spectrum of (5*S*,8*S*,9*R*,10*S*)-19-ethoxylneoavarone (**6**).

Elemental Composition Report XT-4

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

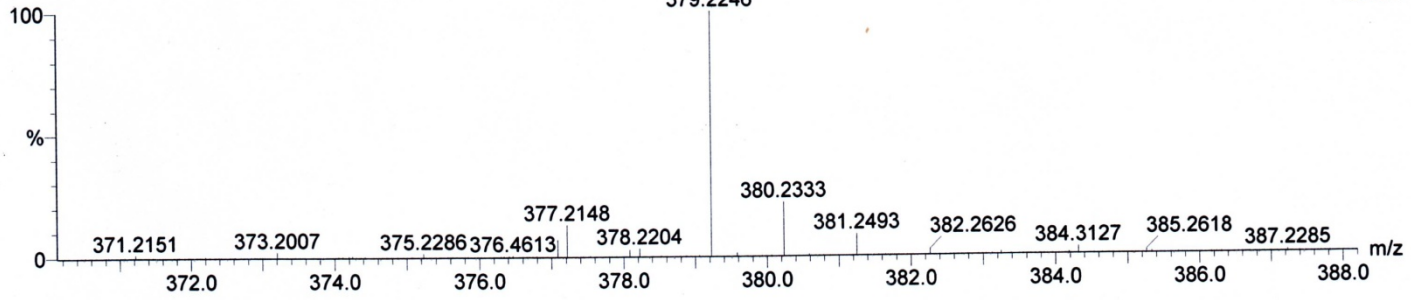
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 10-25 H: 10-40 O: 1-6 Na: 1-1

SIPI
XT-4 M.W=356
WQ12-321H 30 (1.056) AM (Cen,4, 80.00, Ar,5000.0,376.07,0.70); Sm (SG, 2x1.00); Cm (22:30)

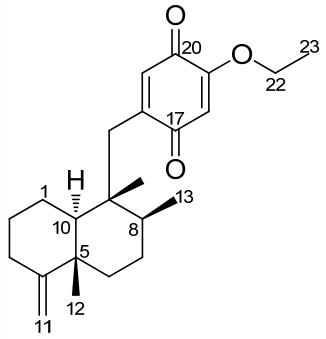
Q-Tof micro
YA019

16-Jul-2012,14:33:28

TOF MS ES+
2.56e4

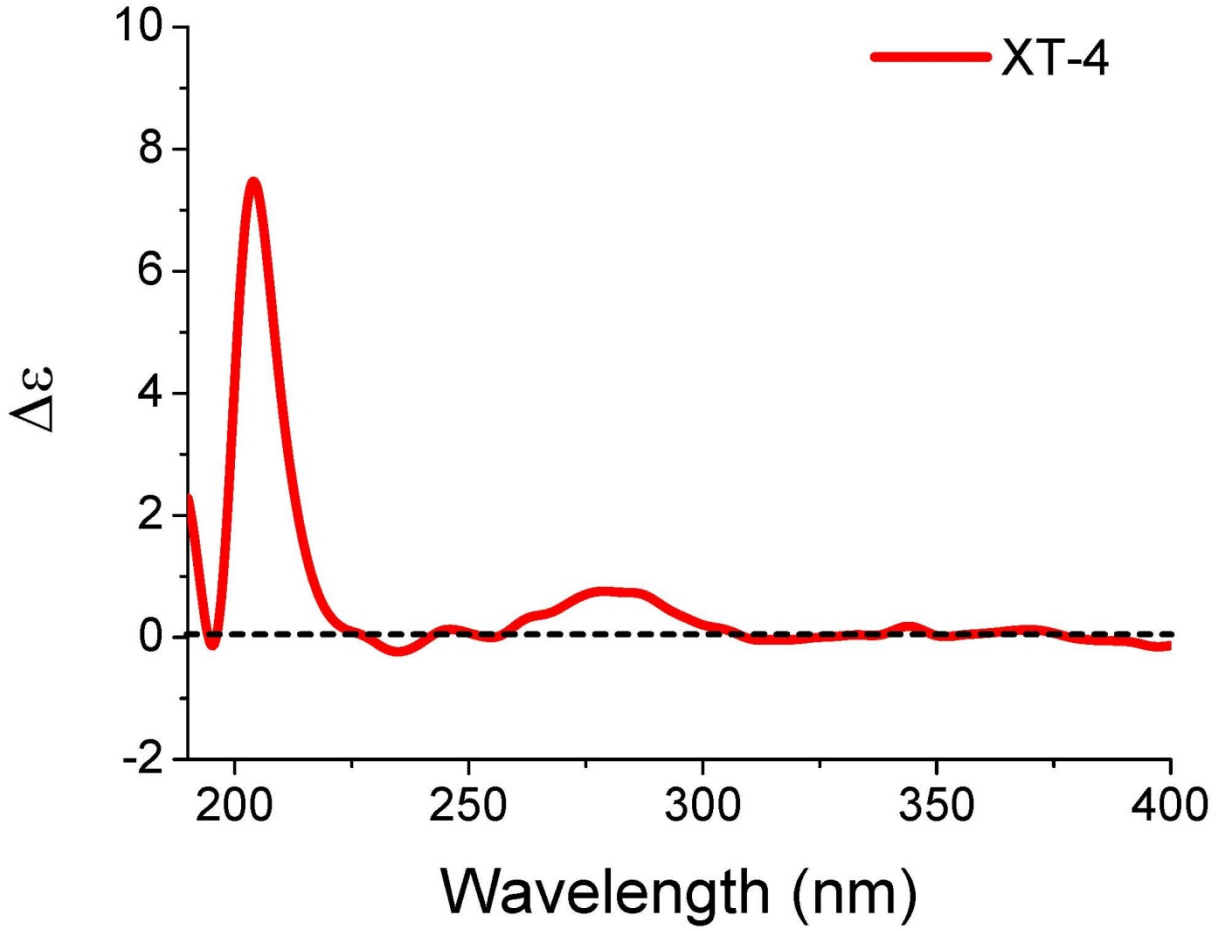


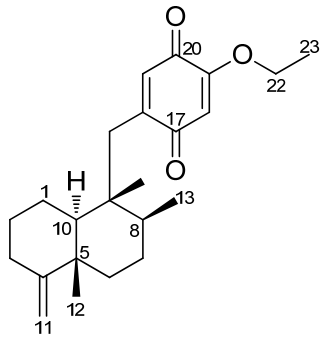
Minimum:	70.00				-1.5		
Maximum:	100.00		5.0	20.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
379.2246	100.00	379.2249	-0.3	-0.8	7.5	448.3	C23 H32 O3 Na



6

Figure S63. HRESIMS of 19-eth(5*S*,8*S*,9*R*,10*S*)-19-ethoxylneoavarone (**6**).





6

Figure S64. CD Spectrum of (5*S*,8*S*,9*R*,10*S*)-19-ethoxylneoavarone (**6**) in MeOH.

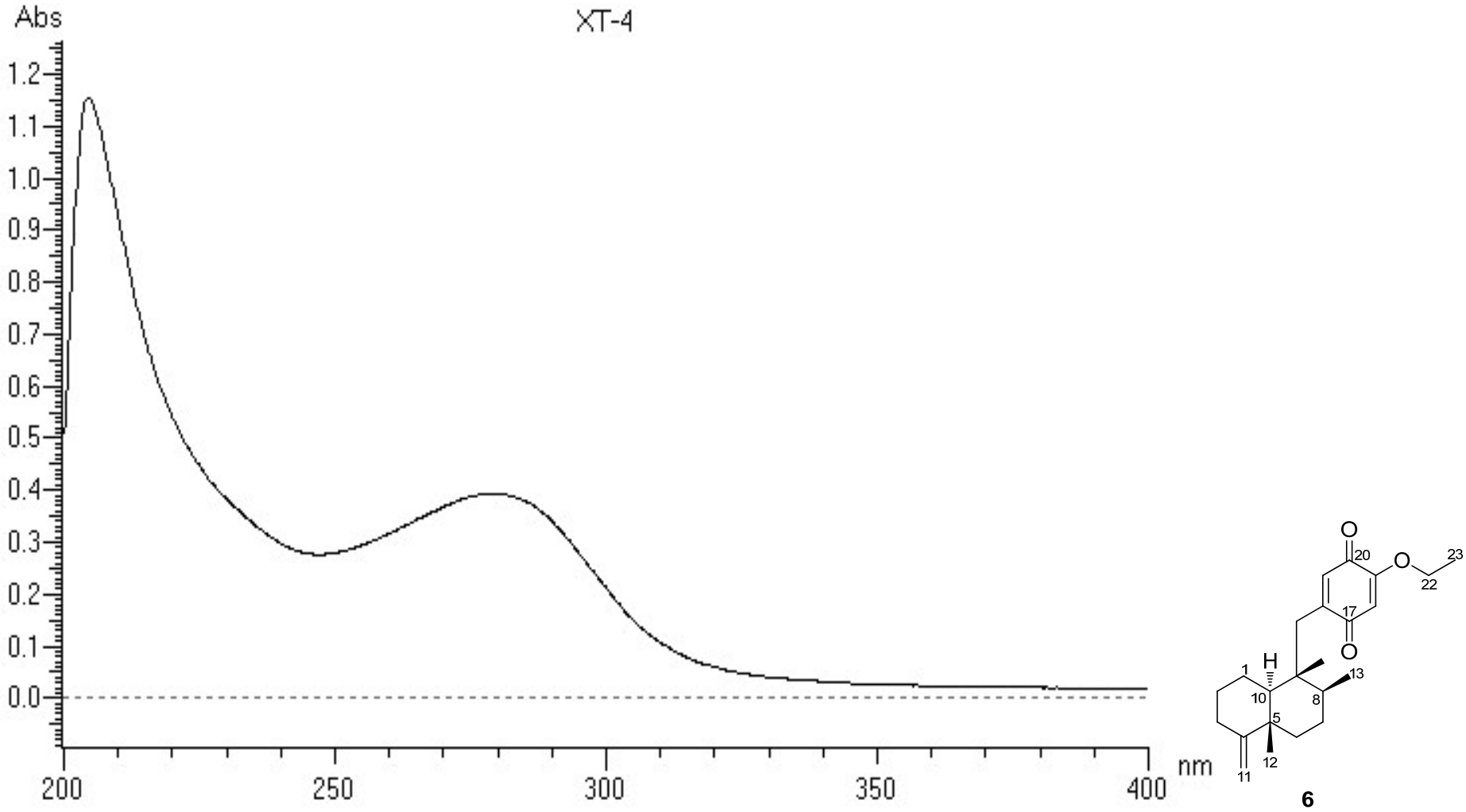
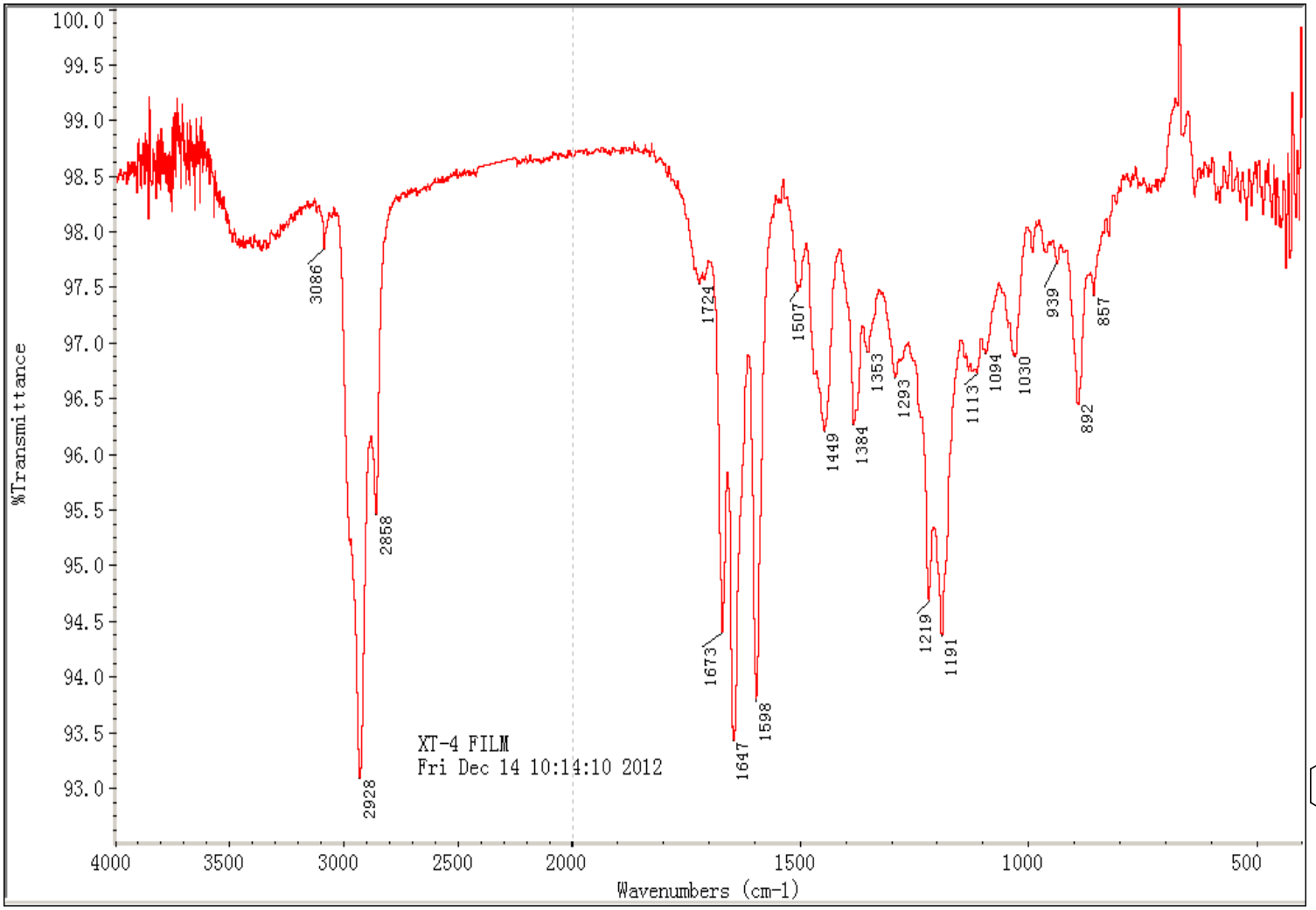
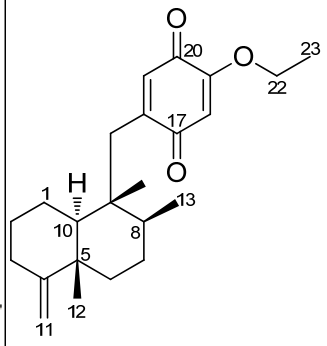


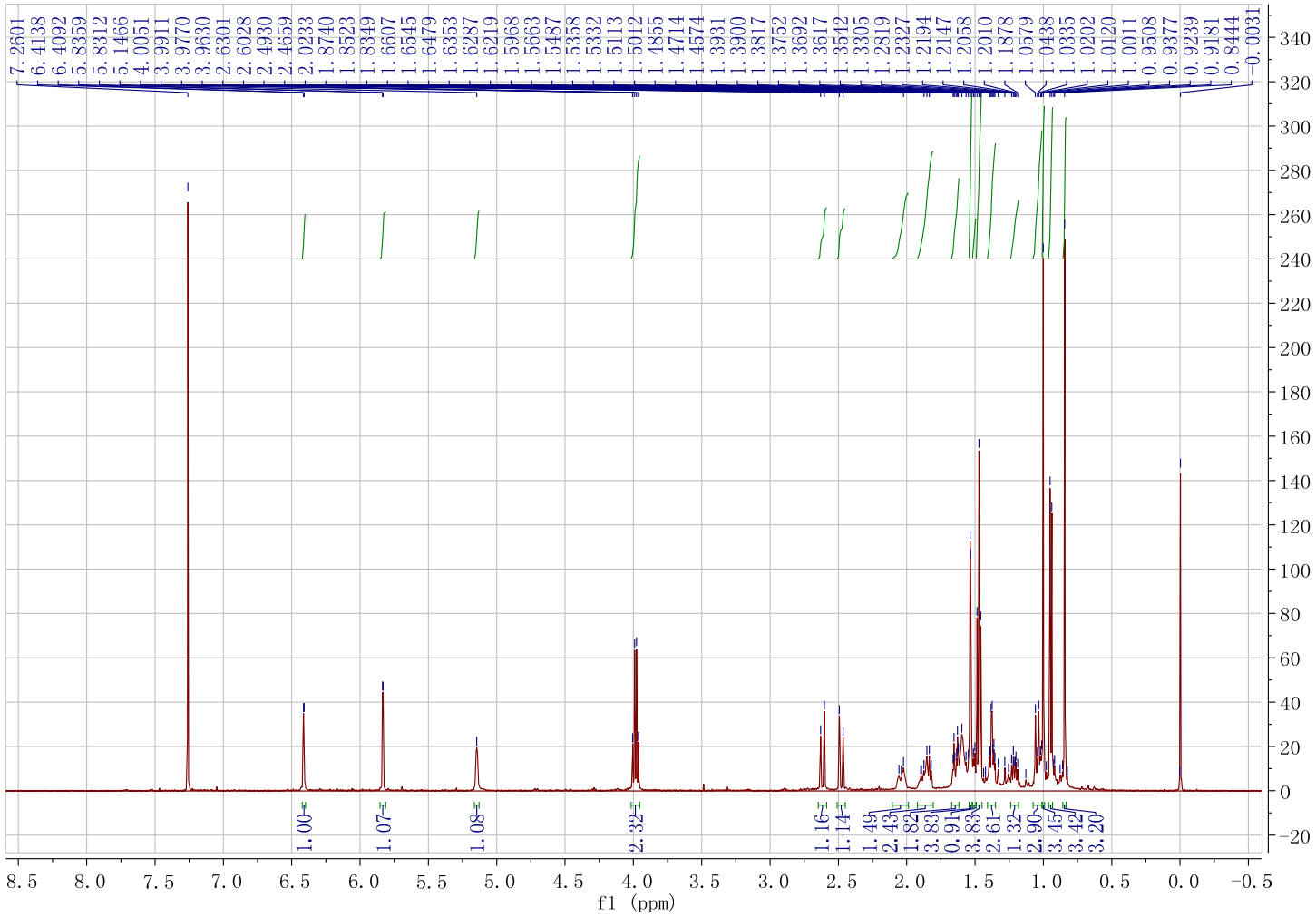
Figure S65. UV Spectrum of (5*S*,8*S*,9*R*,10*S*)-19-ethoxylneoavarone (**6**).

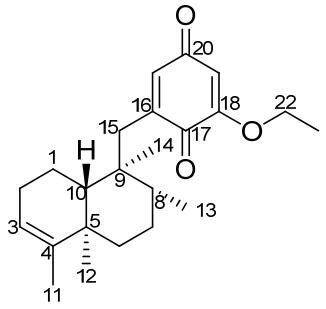




6

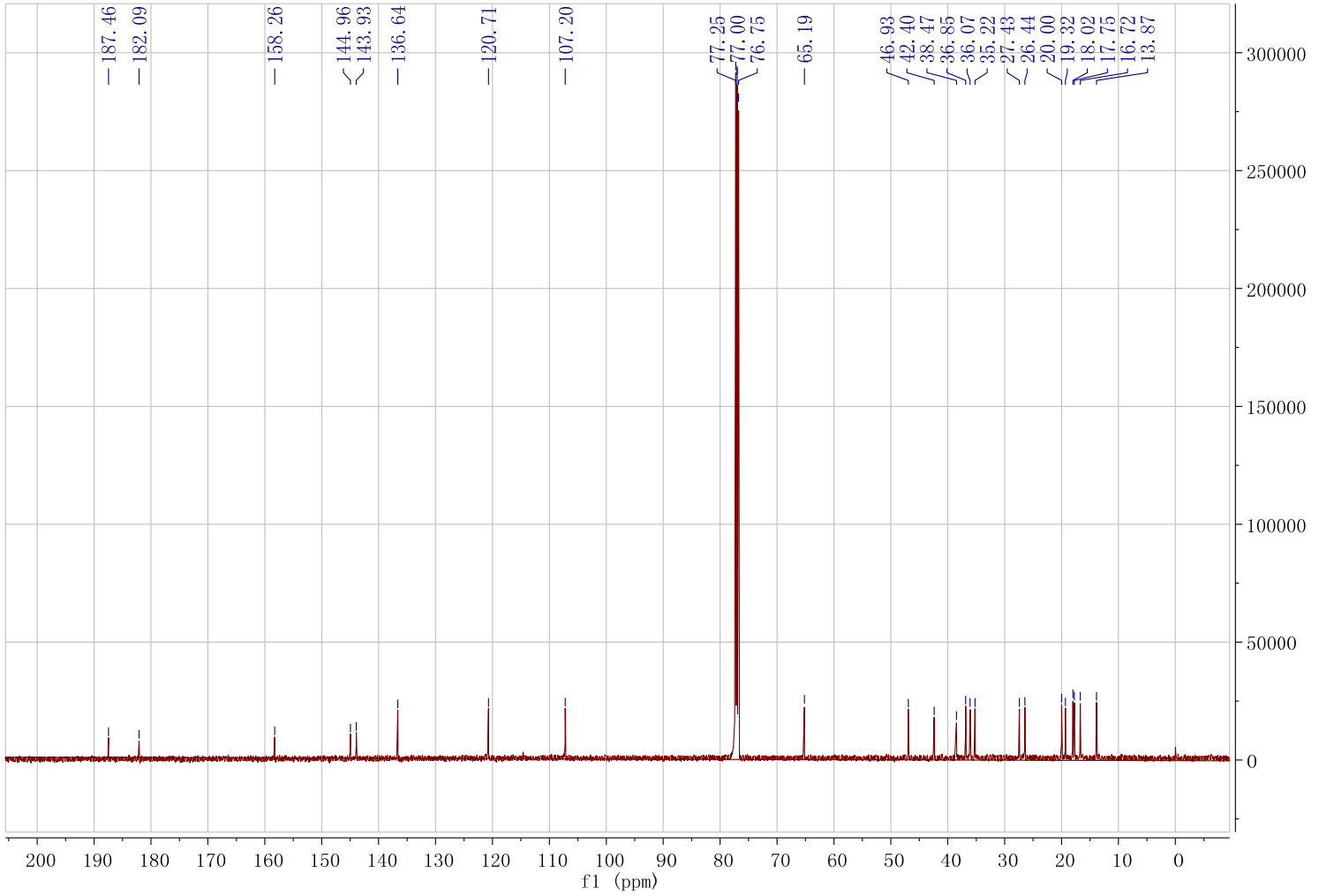
Figure S66. IR Spectrum of (5*S*,8*S*,9*R*,10*S*)-19-ethoxylneoavarone (**6**).

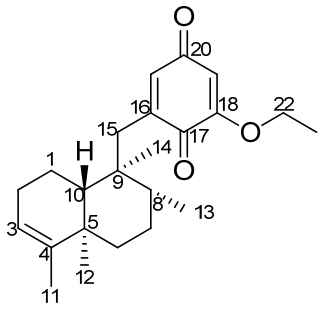




7

Figure S67. ^{1}H NMR Spectrum of (5*R*,8*R*,9*S*,10*R*)-18-ethoxylavarone (**7**).





7

Figure S68. ^{13}C NMR Spectrum of (5*R*,8*R*,9*S*,10*R*)-18-ethoxylavarone (**7**).

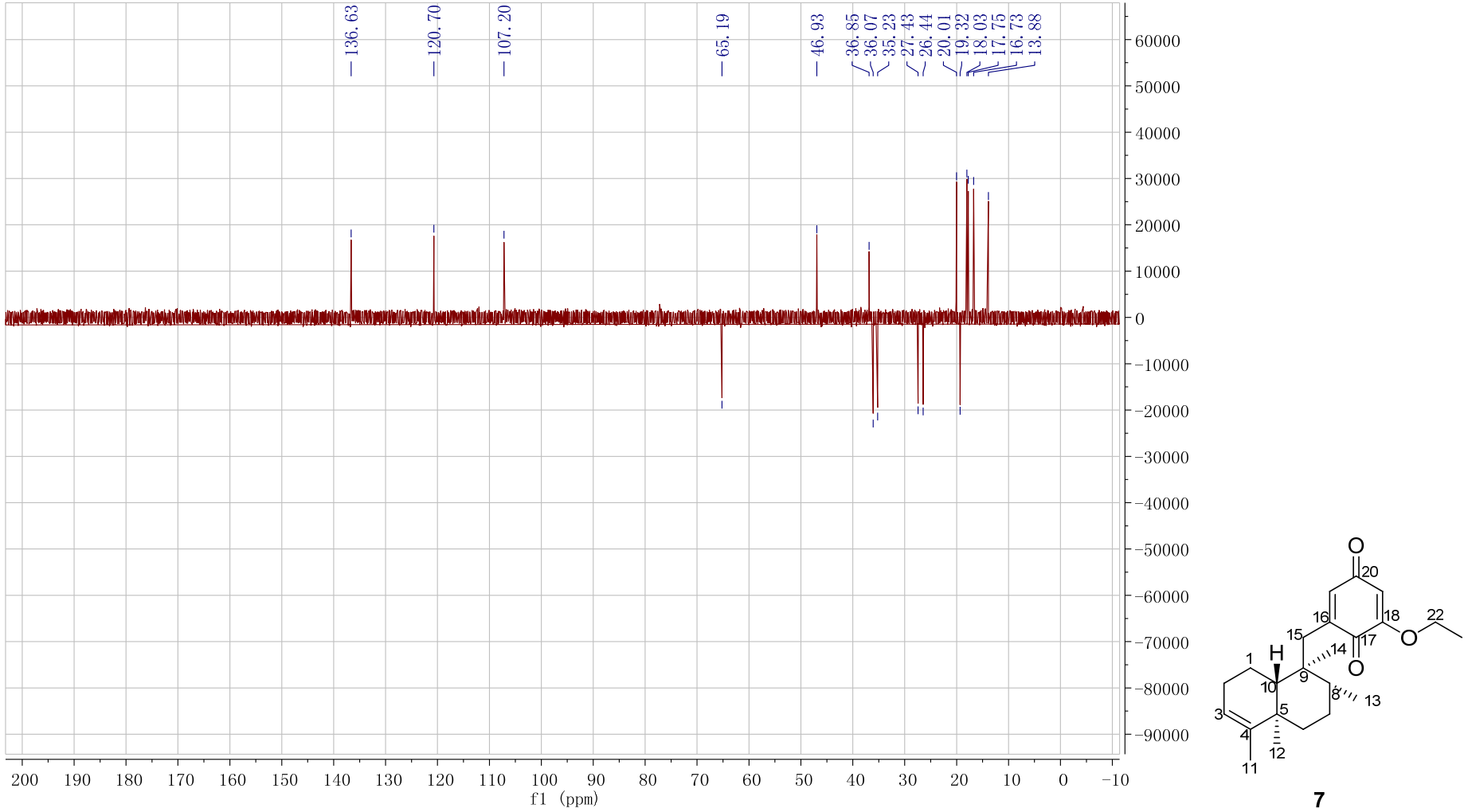
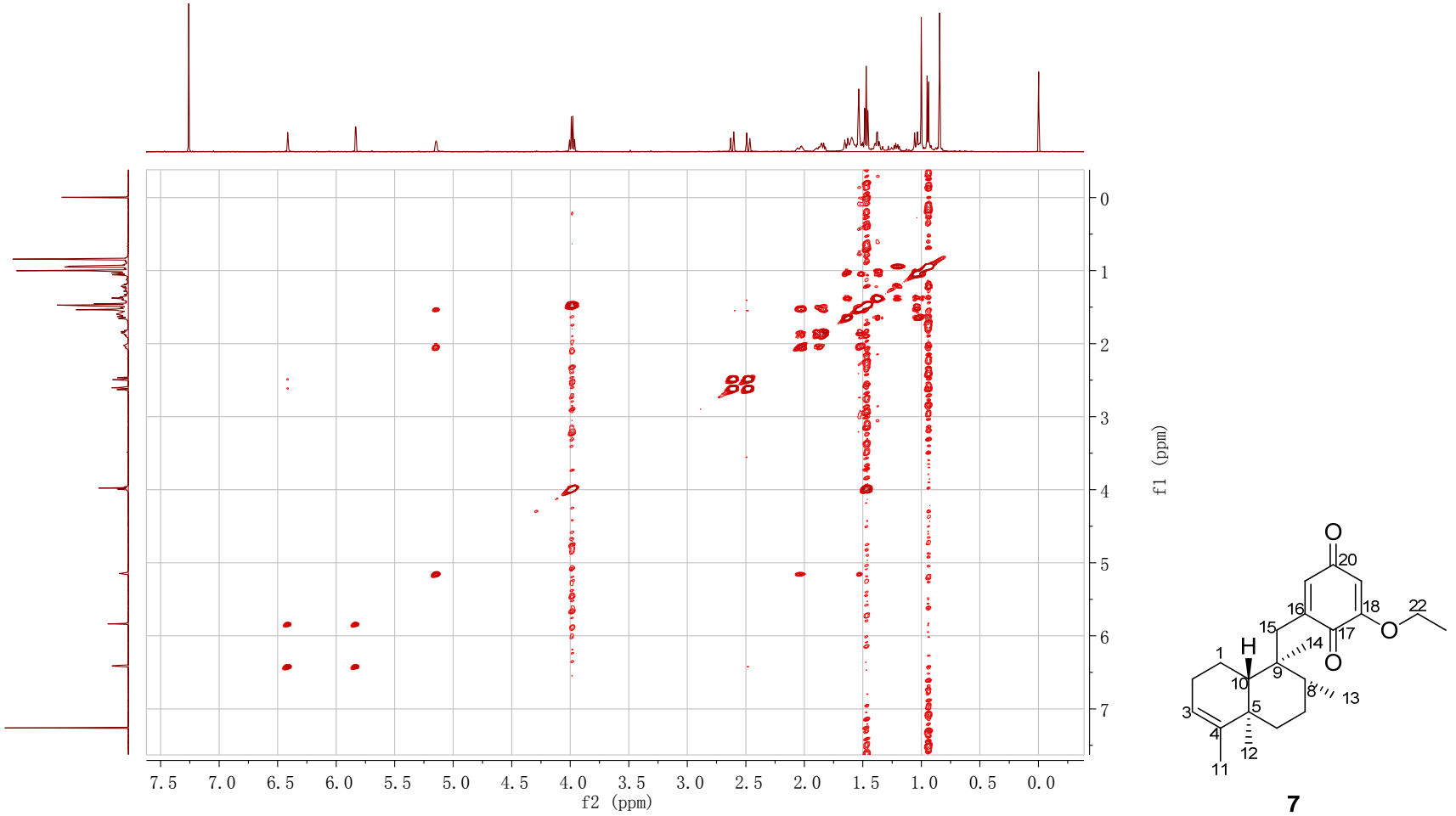
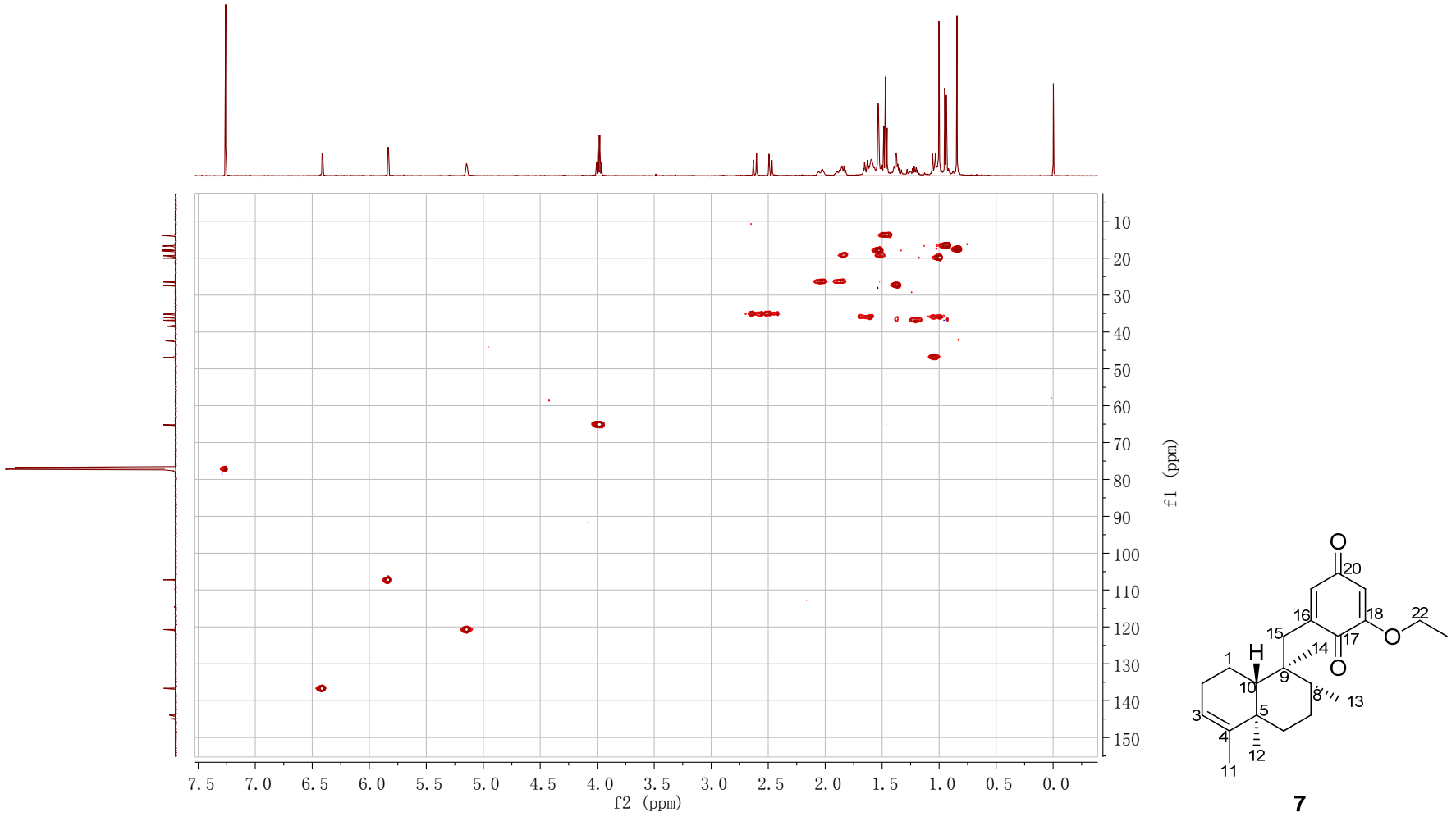


Figure S69. DEPT135 Spectrum of (5*R*,8*R*,9*S*,10*R*)-18-ethoxylavarone (**7**).



7

Figure S70. ^{1}H-^{1}H COSY Spectrum of (5*R*,8*R*,9*S*,10*R*)-18-ethoxylavarone (**7**).



7

Figure S71. HSQC Spectrum of (5*R*,8*R*,9*S*,10*R*)-18-ethoxylavarone (**7**).

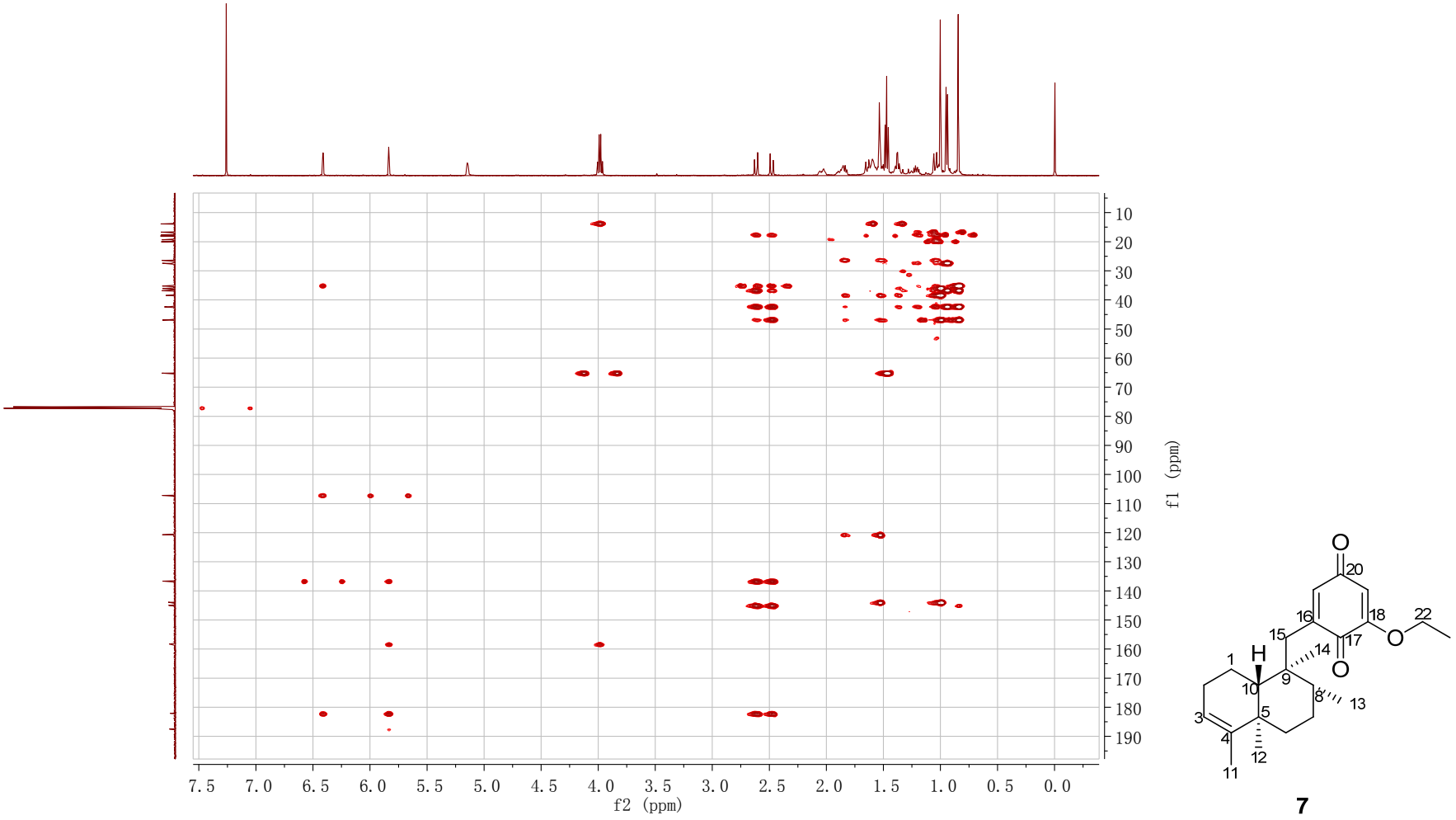
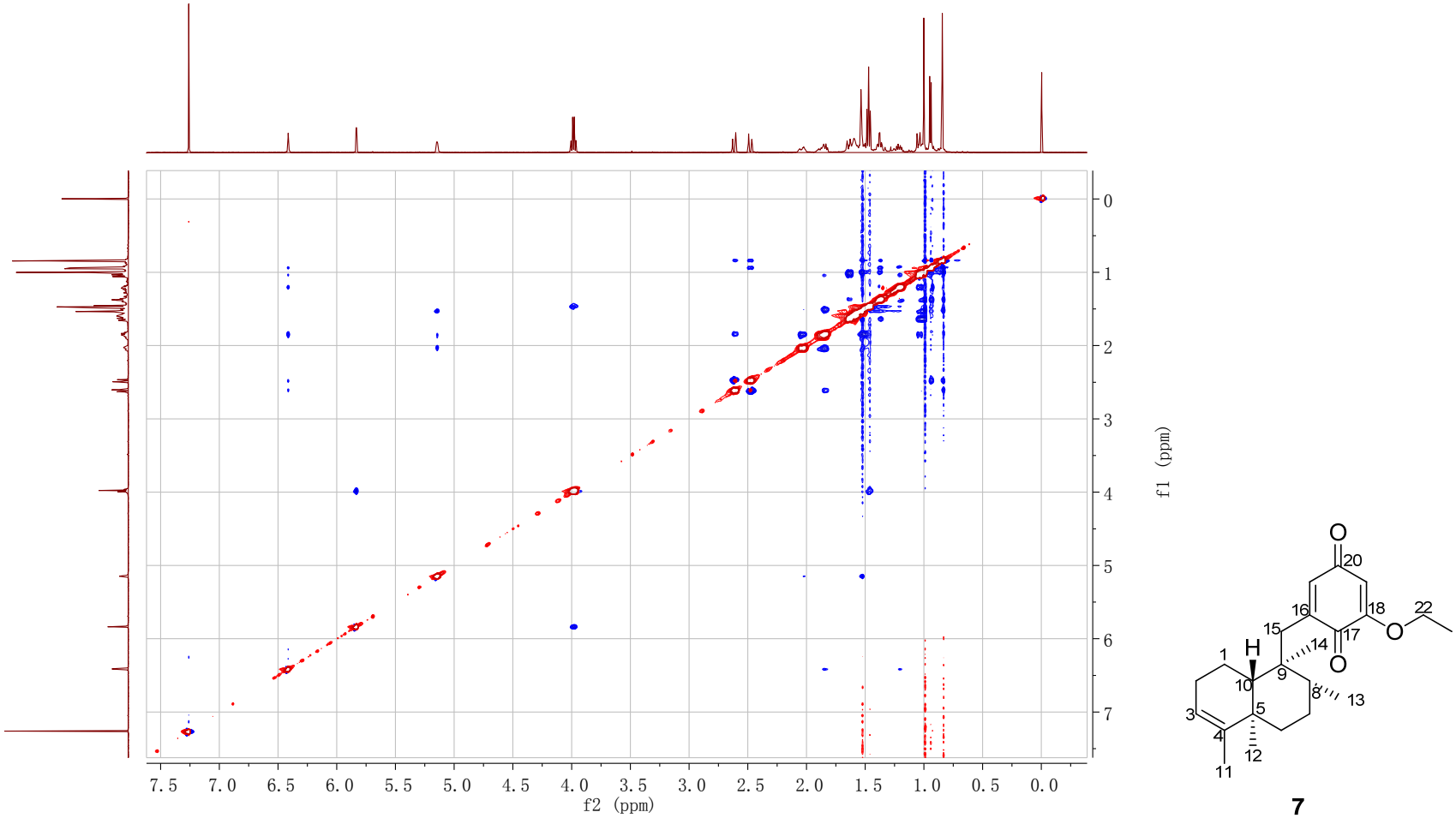


Figure S72. HMBC Spectrum of (5*R*,8*R*,9*S*,10*R*)-18-ethoxylavarone (**7**).



7

Figure S73. NOESY Spectrum of (5*R*,8*R*,9*S*,10*R*)-18-ethoxylavarone (**7**).

Elemental Composition Report XJ-12

Page 1

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

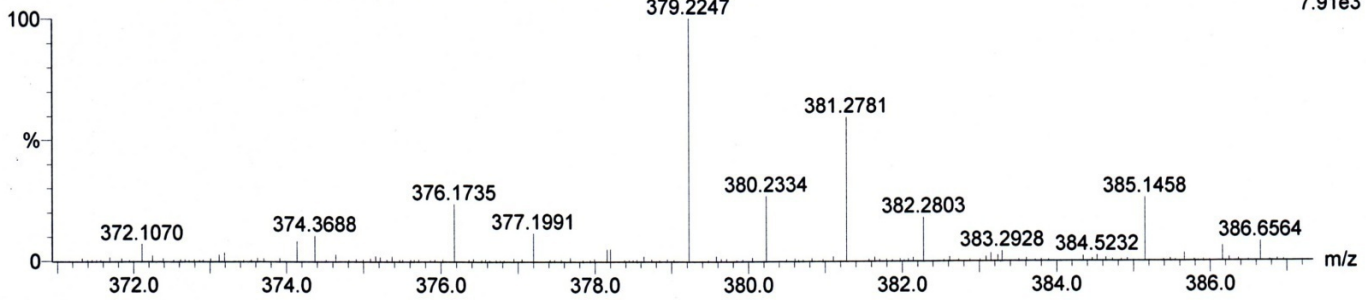
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 10-25 H: 10-40 O: 1-6 Na: 1-1

SIPI
XT-12 M.W=356
WQ12-327H2 81 (2.854) AM (Cen,4, 80.00, Ar,5000.0,384.13,0.70); Sm (SG, 2x1.00); Cm (63:81)

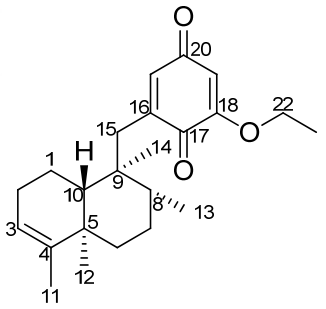
Q-Tof micro
YA019

17-Jul-2012,13:43:54

TOF MS ES+
7.91e3

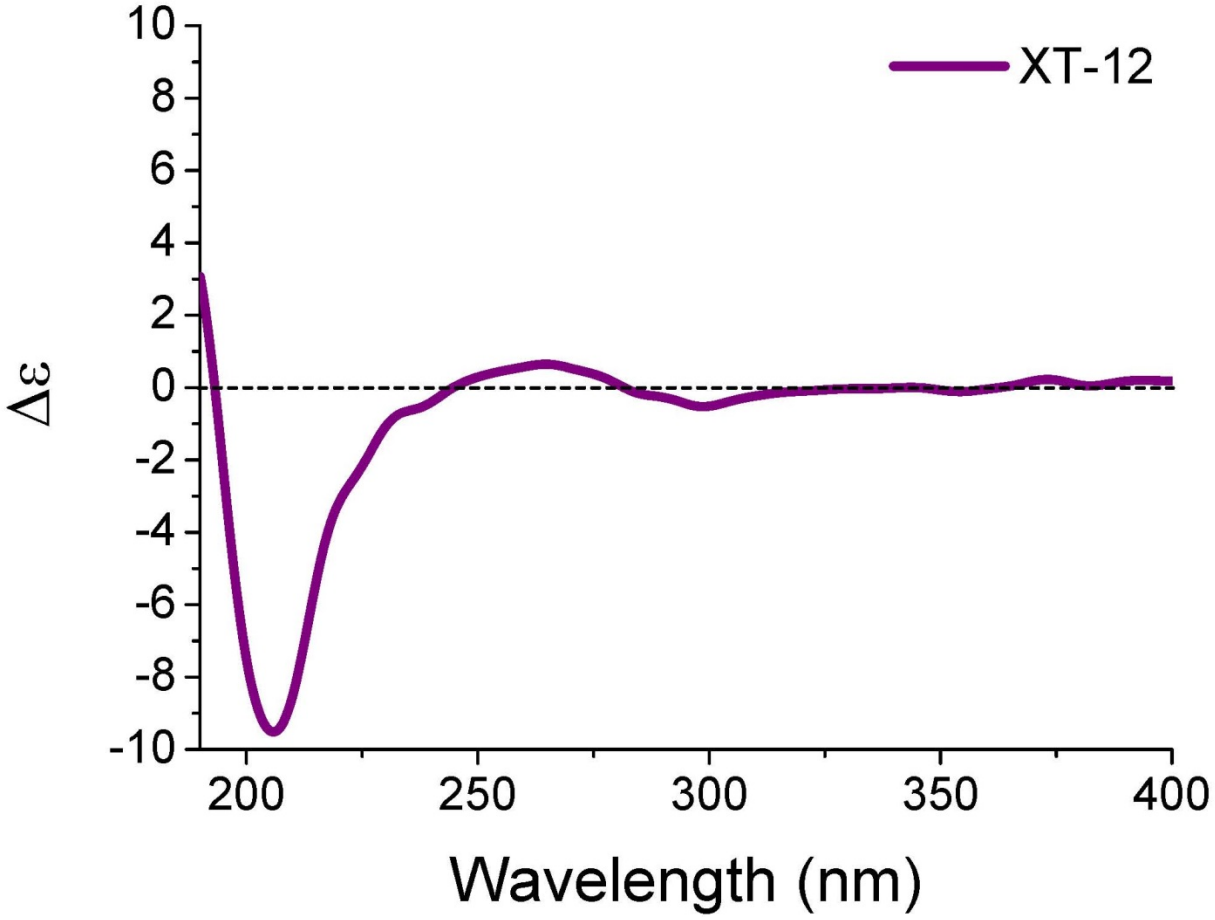


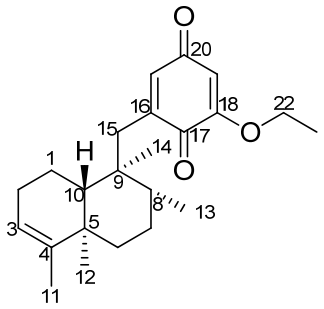
Minimum:	70.00				-1.5		
Maximum:	100.00		5.0	20.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
379.2247	100.00	379.2249	-0.2	-0.5	7.5	2244.6	C23 H32 O3 Na



7

Figure S74. HRESIMS of (5*R*,8*R*,9*S*,10*R*)-18-ethoxylavarone (**7**).





7

Figure S75. CD Spectrum of (5*R*,8*R*,9*S*,10*R*)-18-ethoxylavarone (**7**) in MeOH.

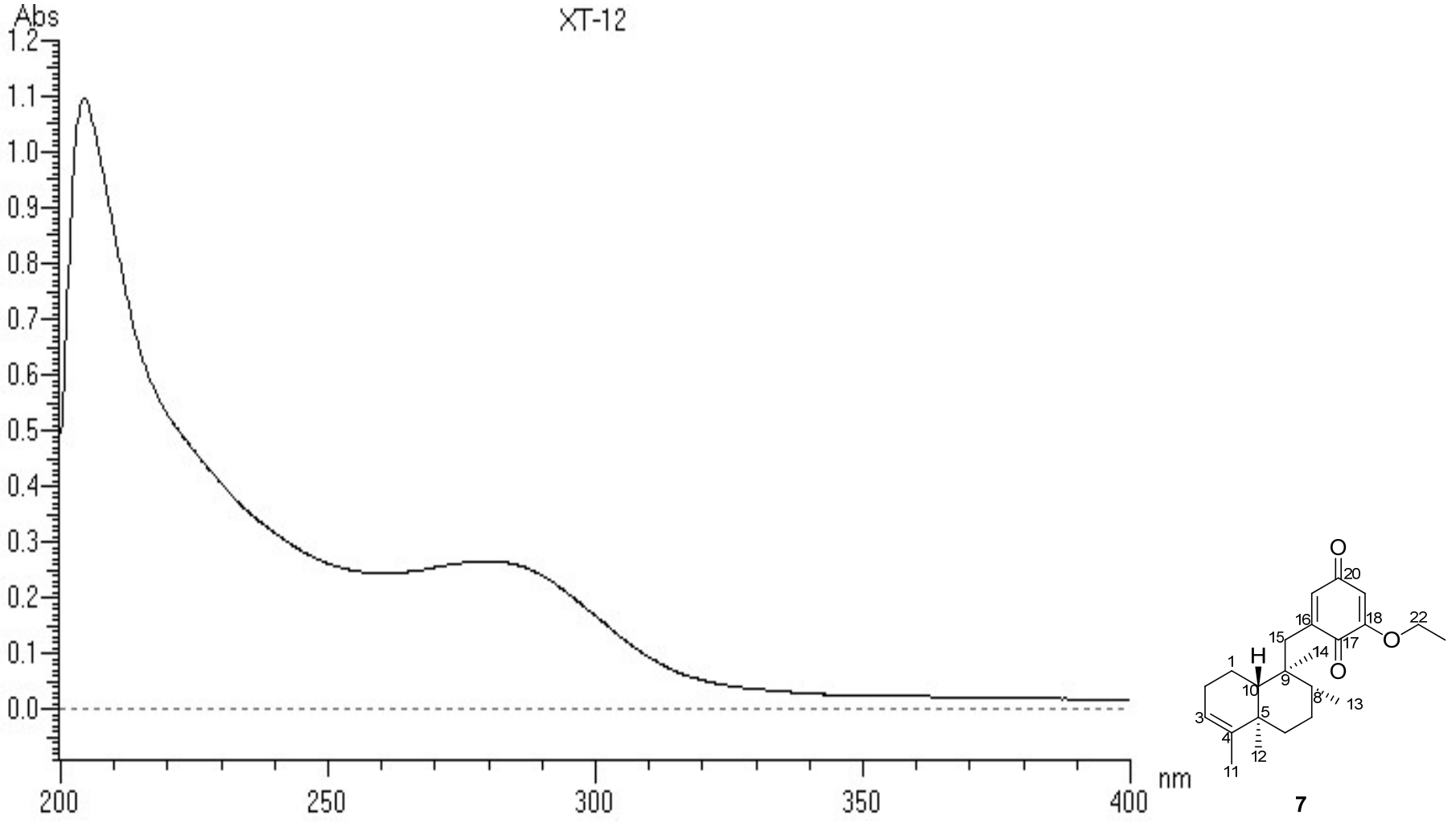
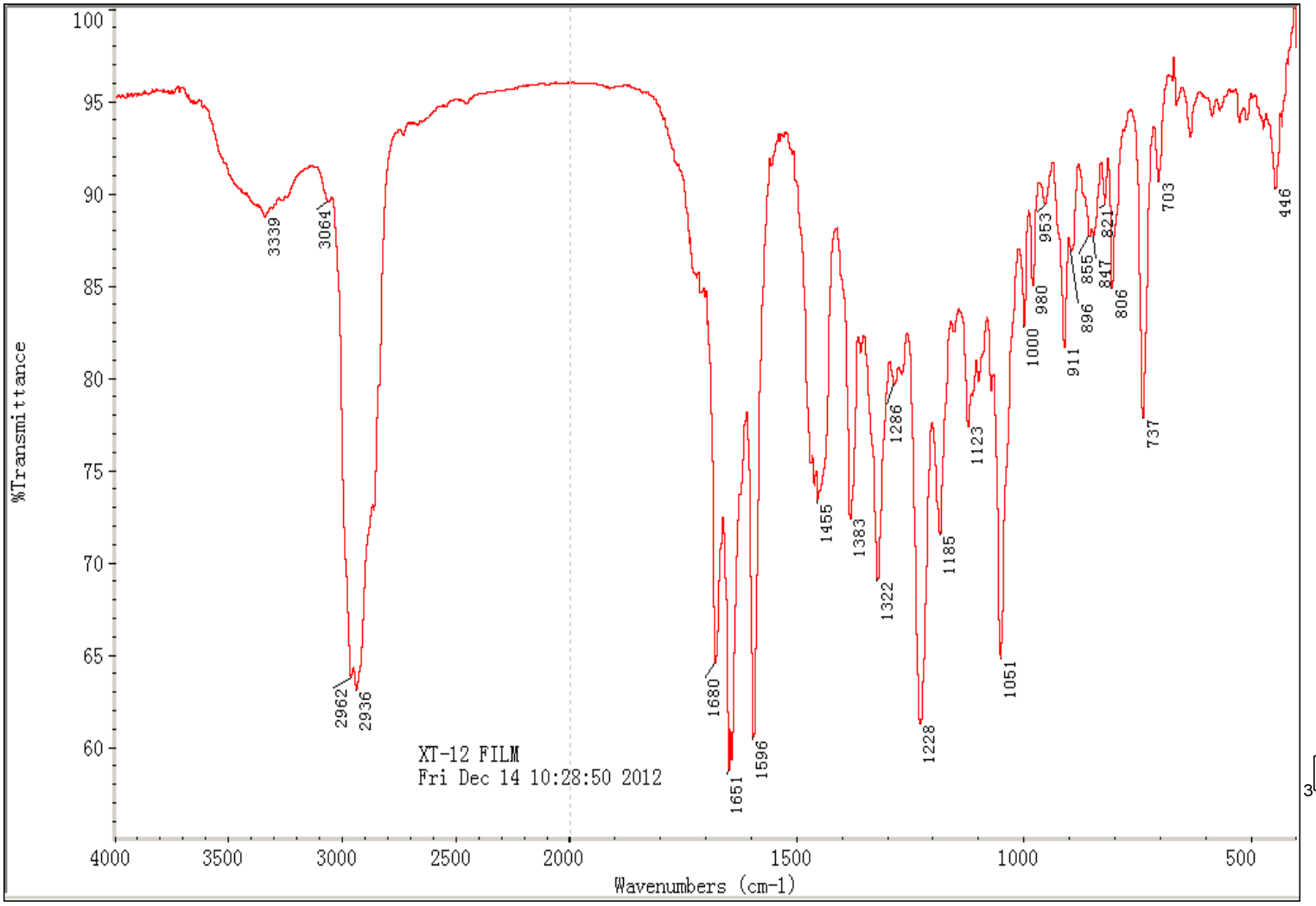
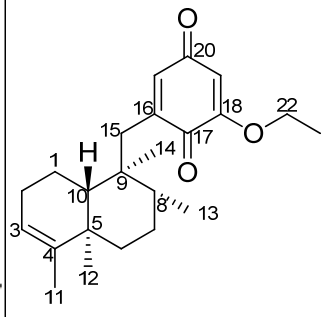


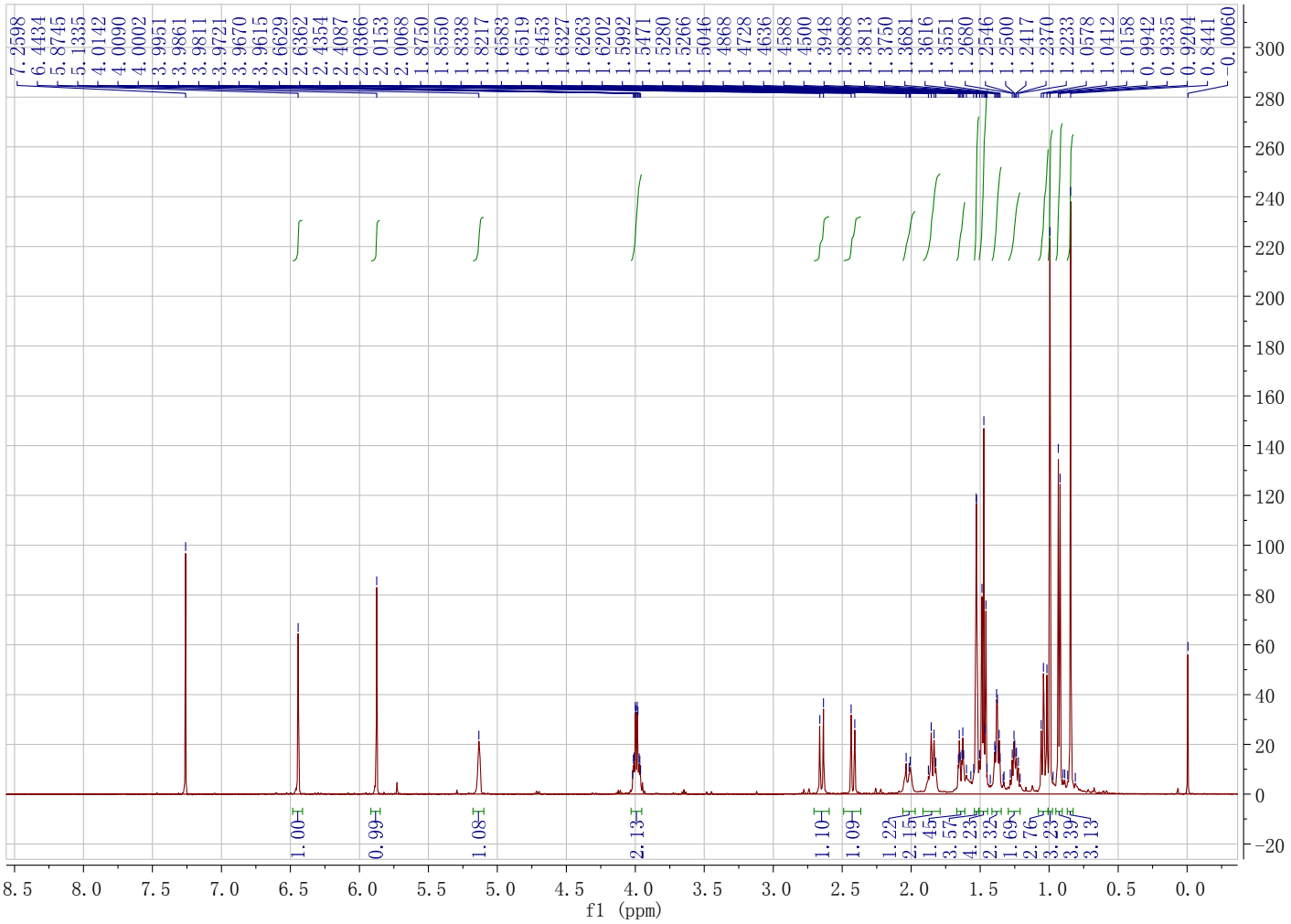
Figure S76. UV Spectrum of (5*R*,8*R*,9*S*,10*R*)-18-ethoxylavarone (**7**).

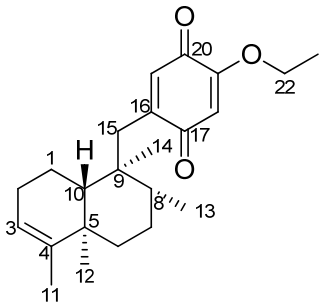




7

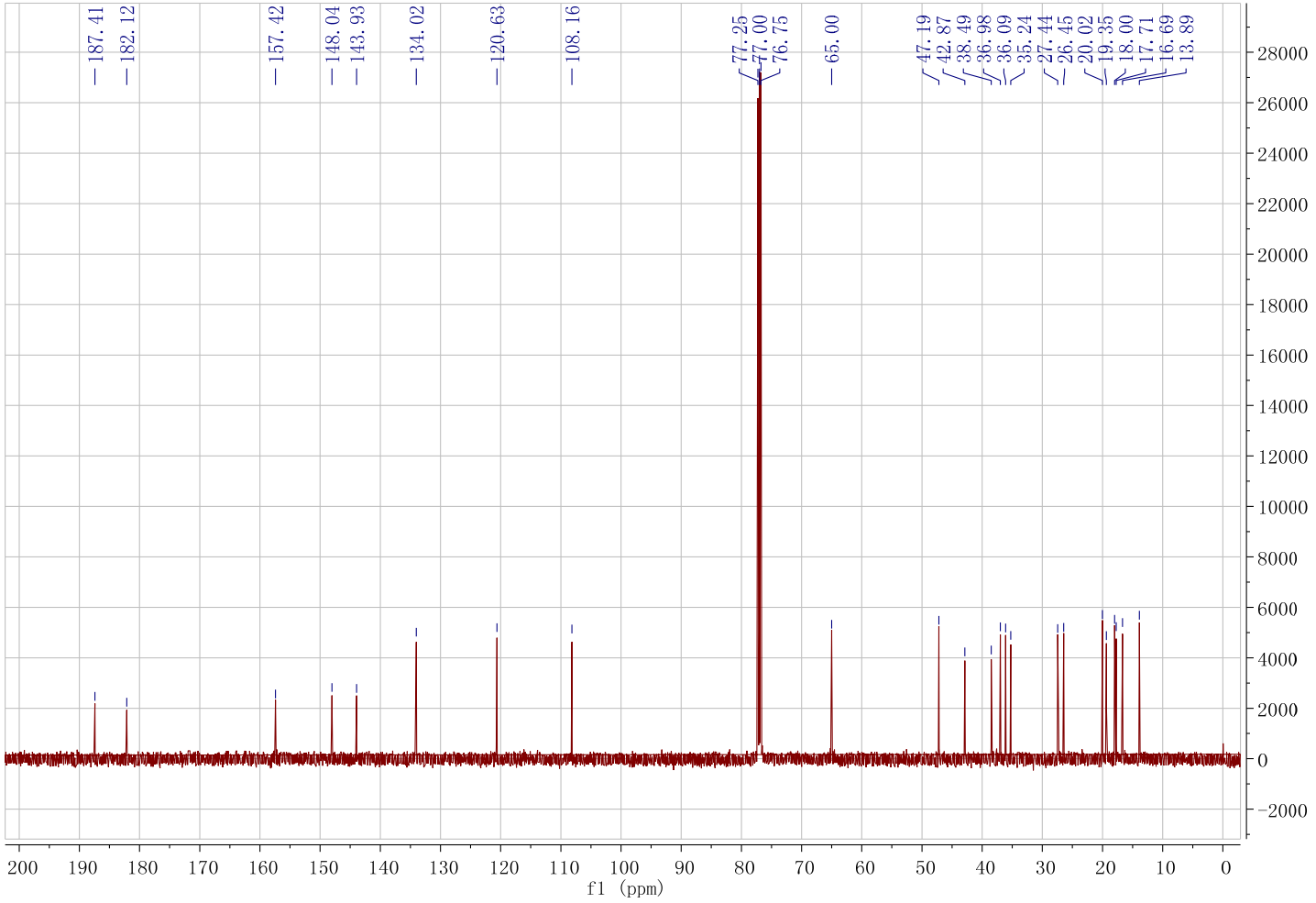
Figure S77. IR Spectrum of (5*R*,8*R*,9*S*,10*R*)-18-ethoxylavarone (**7**).

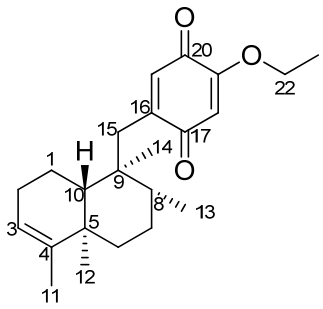




8

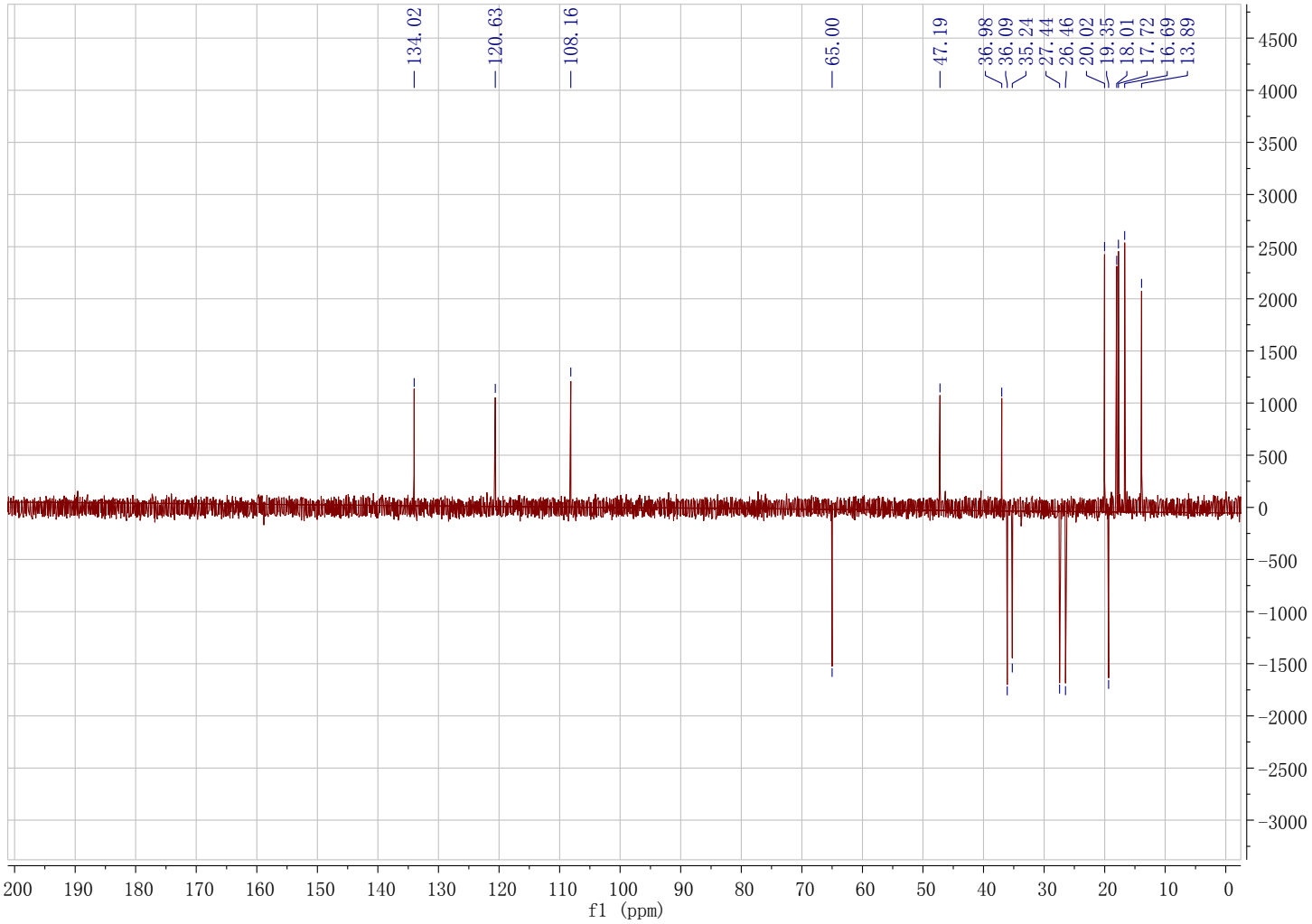
Figure S78. ^{1}H NMR Spectrum of (5*R*,8*R*,9*S*,10*R*)-19-ethoxylavarone (**8**).

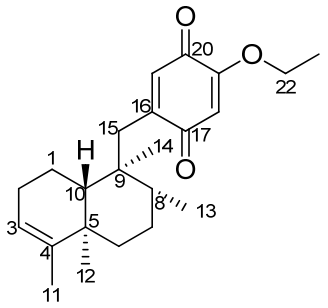




8

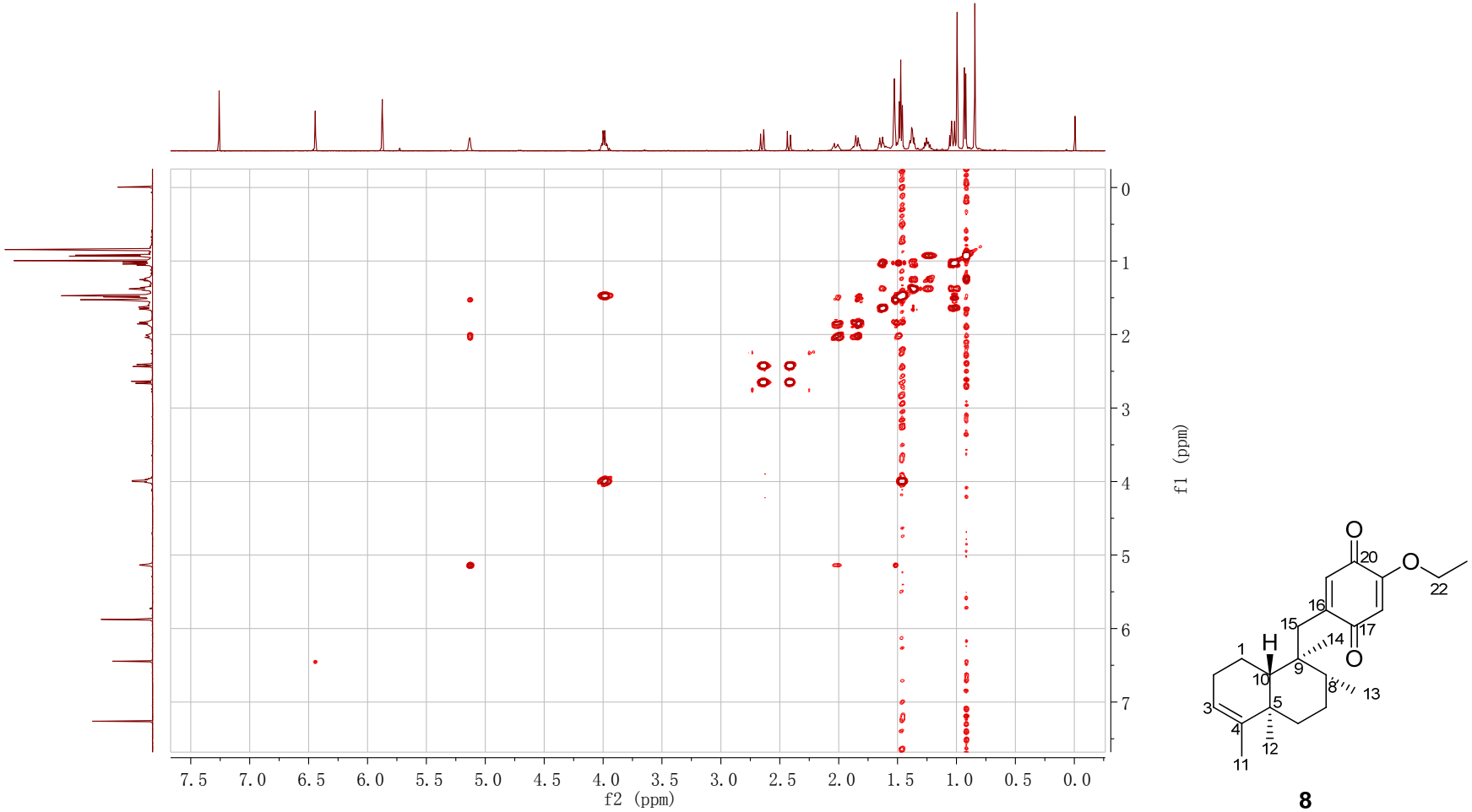
Figure S79. ^{13}C NMR Spectrum of (5*R*,8*R*,9*S*,10*R*)-19-ethoxylavarone (**8**).





8

Figure S80. DEPT Spectrum of (5*R*,8*R*,9*S*,10*R*)-19-ethoxylavarone (**8**).



8

Figure S81. ^{1}H-^{1}H COSY Spectrum of (5*R*,8*R*,9*S*,10*R*)-19-ethoxylavarone (**8**).

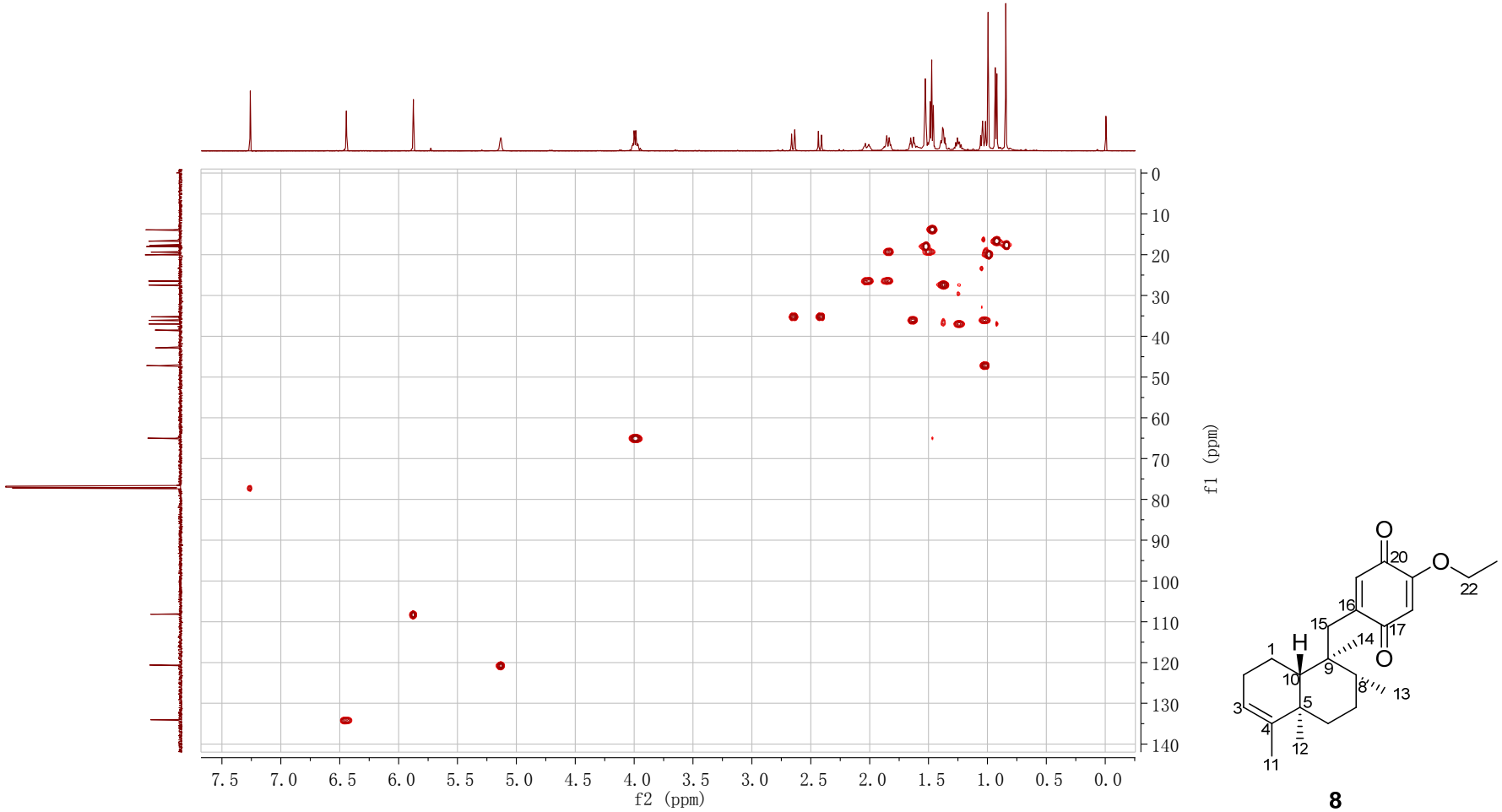
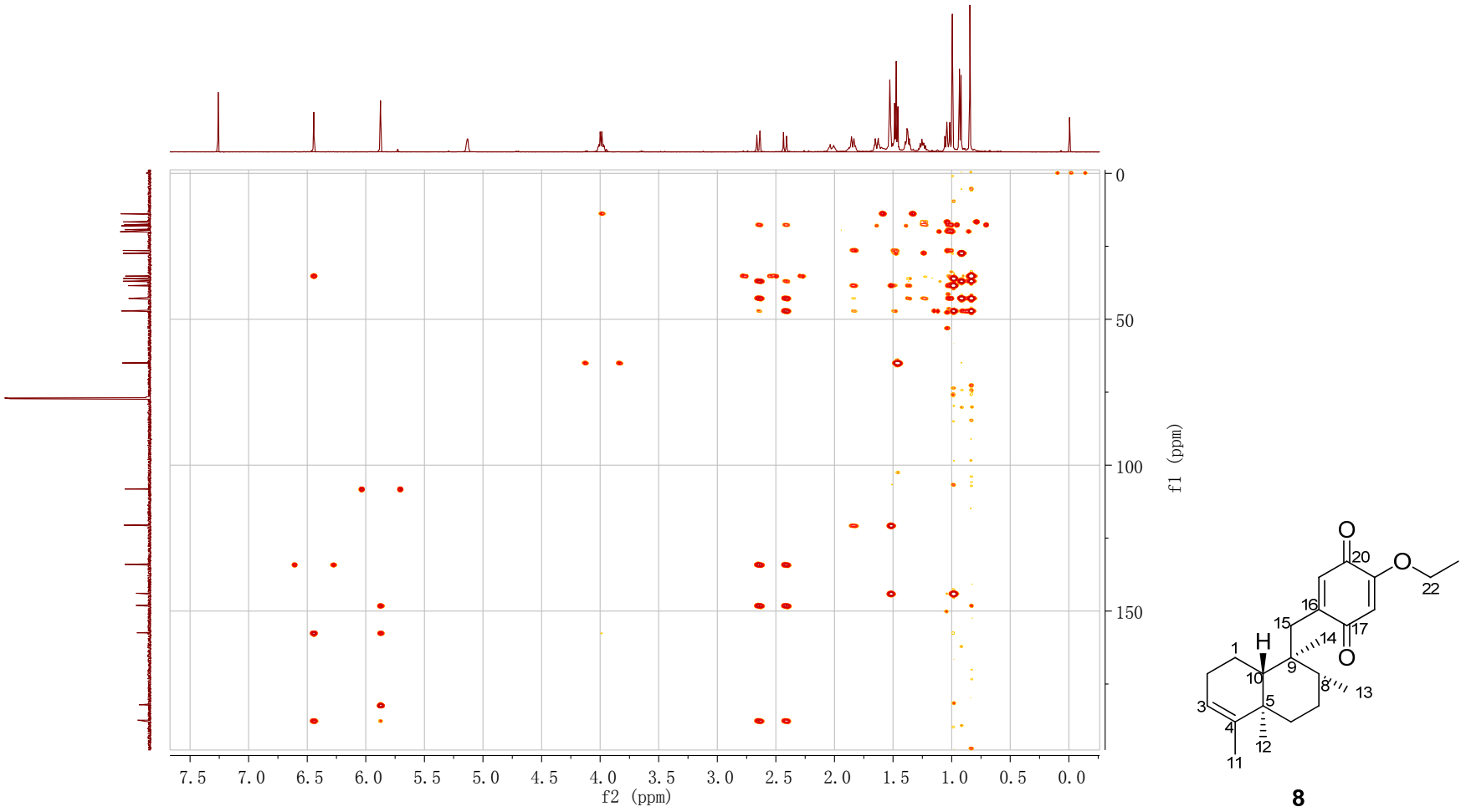
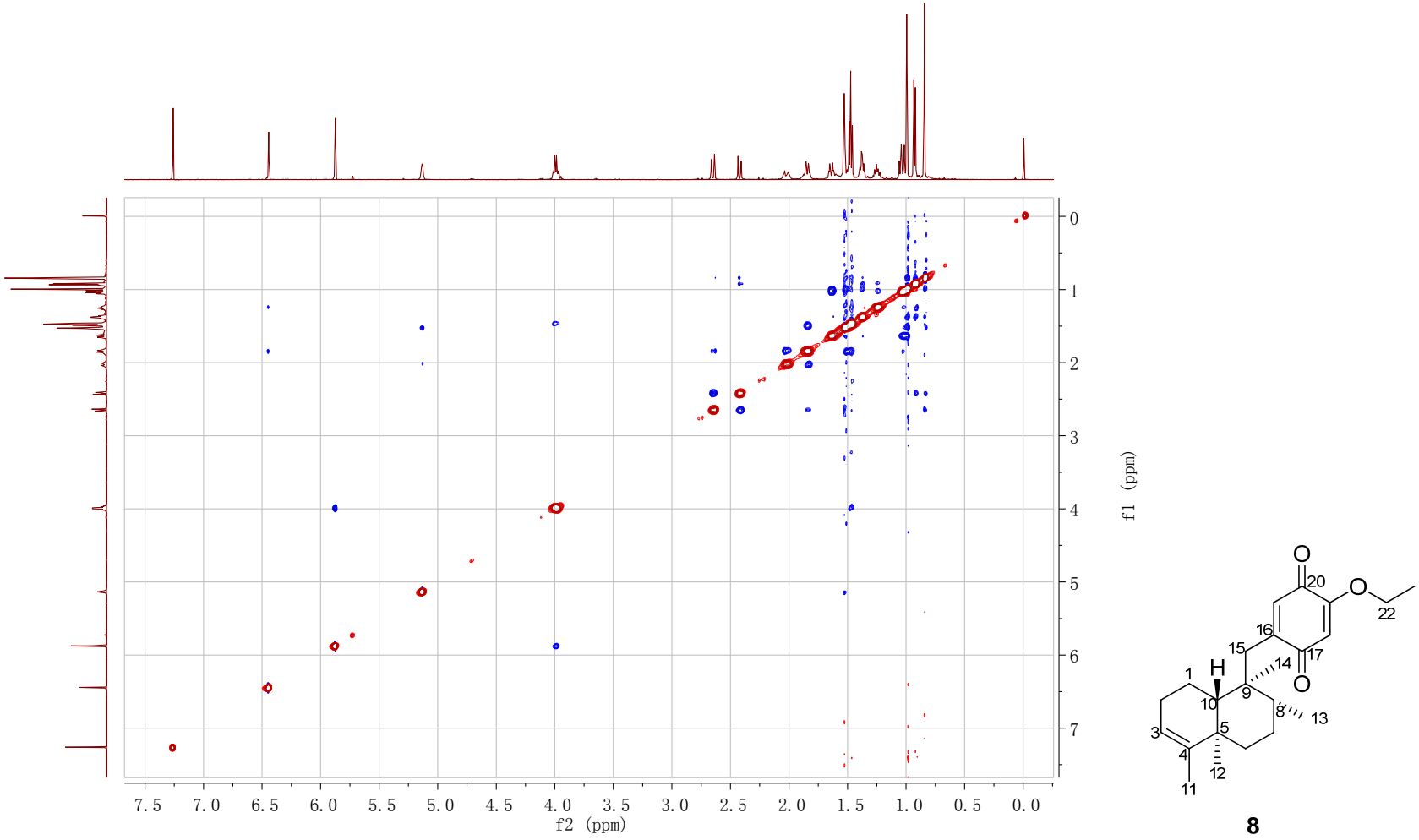


Figure S82. HSQC Spectrum of (5*R*,8*R*,9*S*,10*R*)-19-ethoxylavarone (**8**).



8

Figure S83. HMBC Spectrum of (5*R*,8*R*,9*S*,10*R*)-19-ethoxylavarone (**8**).



8

Figure S84. NOESY Spectrum of (5*R*,8*R*,9*S*,10*R*)-19-ethoxylavarone (**8**).

Elemental Composition Report XT-6

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

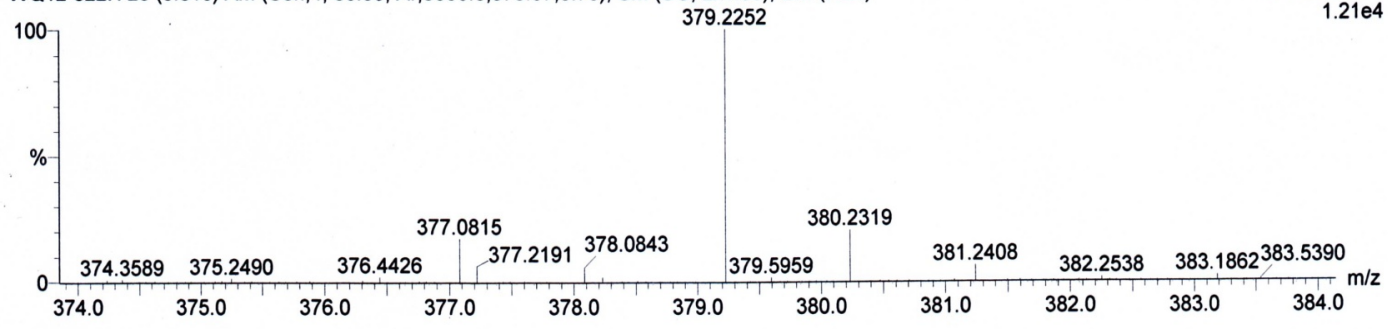
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 10-25 H: 10-40 O: 1-6 Na: 1-1

SIPI
XT-6 M.W=356
WQ12-322H 23 (0.810) AM (Cen,4, 80.00, Ar,5000.0,376.07,0.70); Sm (SG, 2x1.00); Cm (7:24)

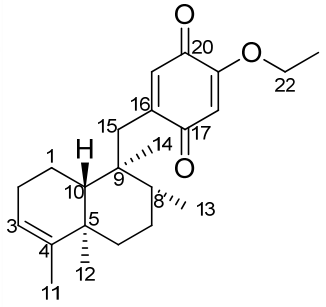
Q-Tof micro
YA019

16-Jul-2012,14:52:04

TOF MS ES+
1.21e4

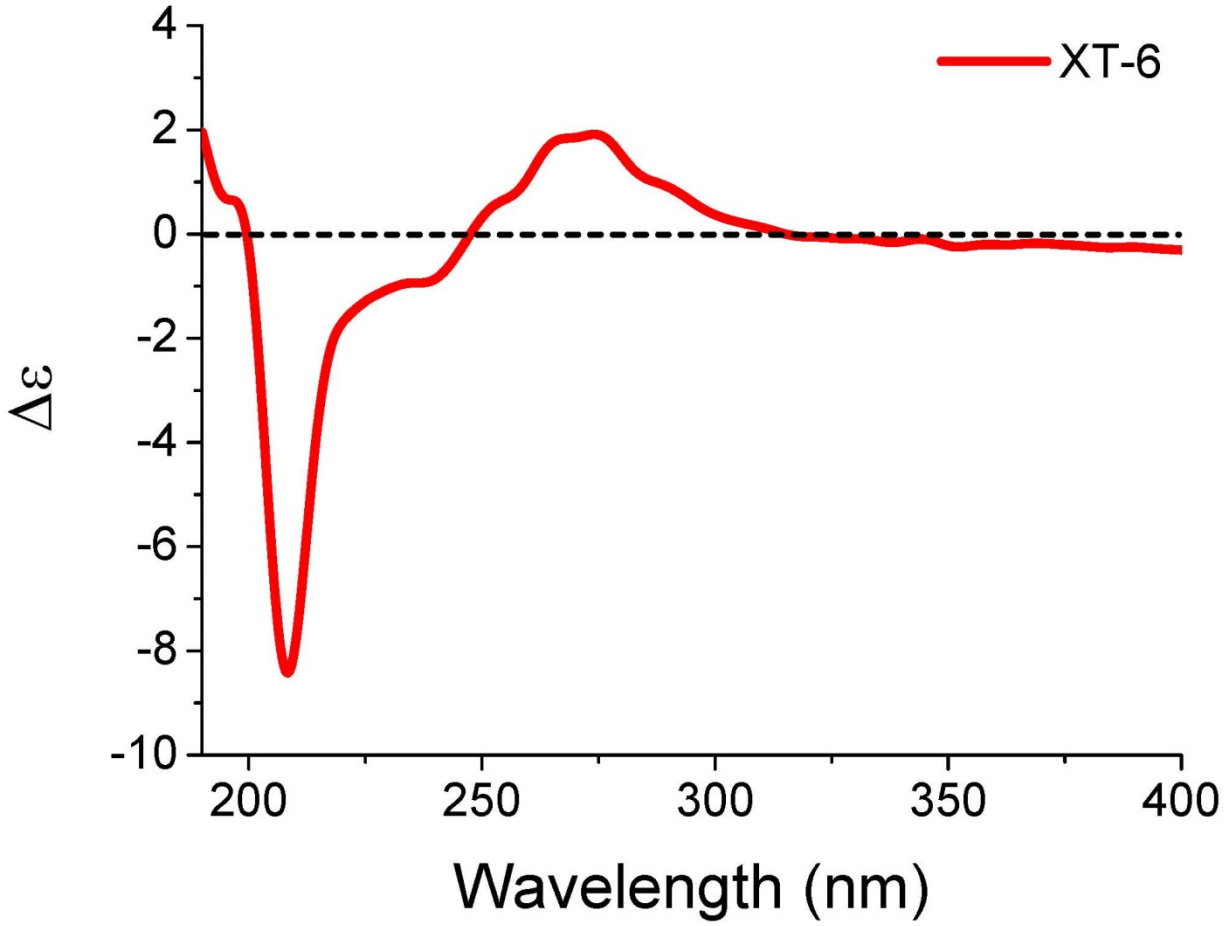


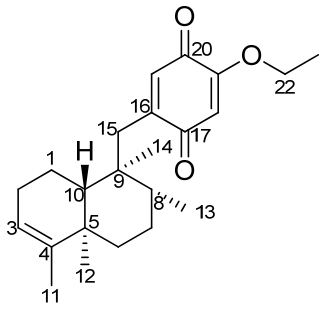
Minimum:	70.00				-1.5		
Maximum:	100.00		5.0	20.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
379.2252	100.00	379.2249	0.3	0.8	7.5	138.3	C23 H32 O3 Na



8

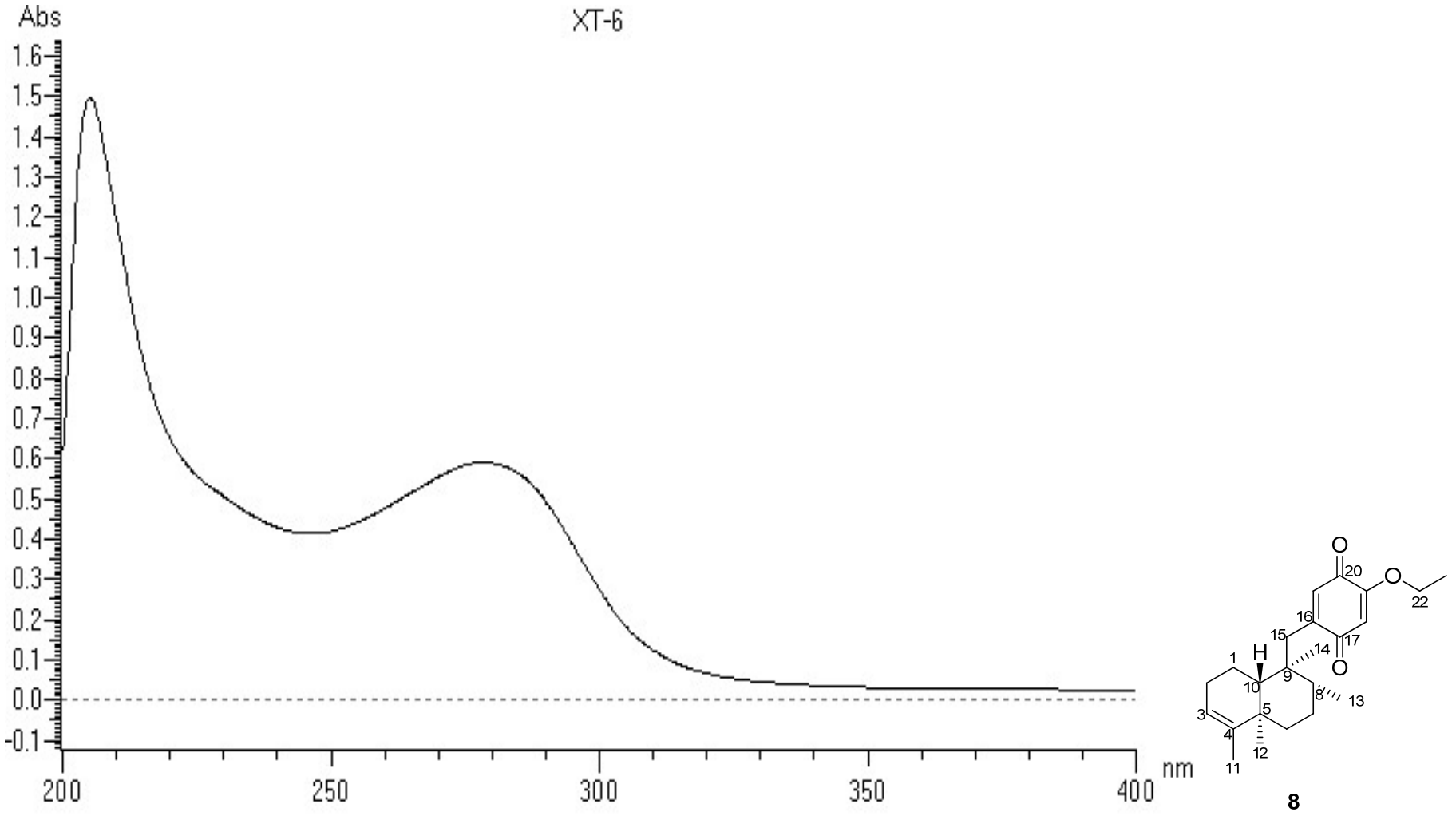
Figure S85. HRESIMS of (5*R*,8*R*,9*S*,10*R*)-19-ethoxylavarone (**8**).





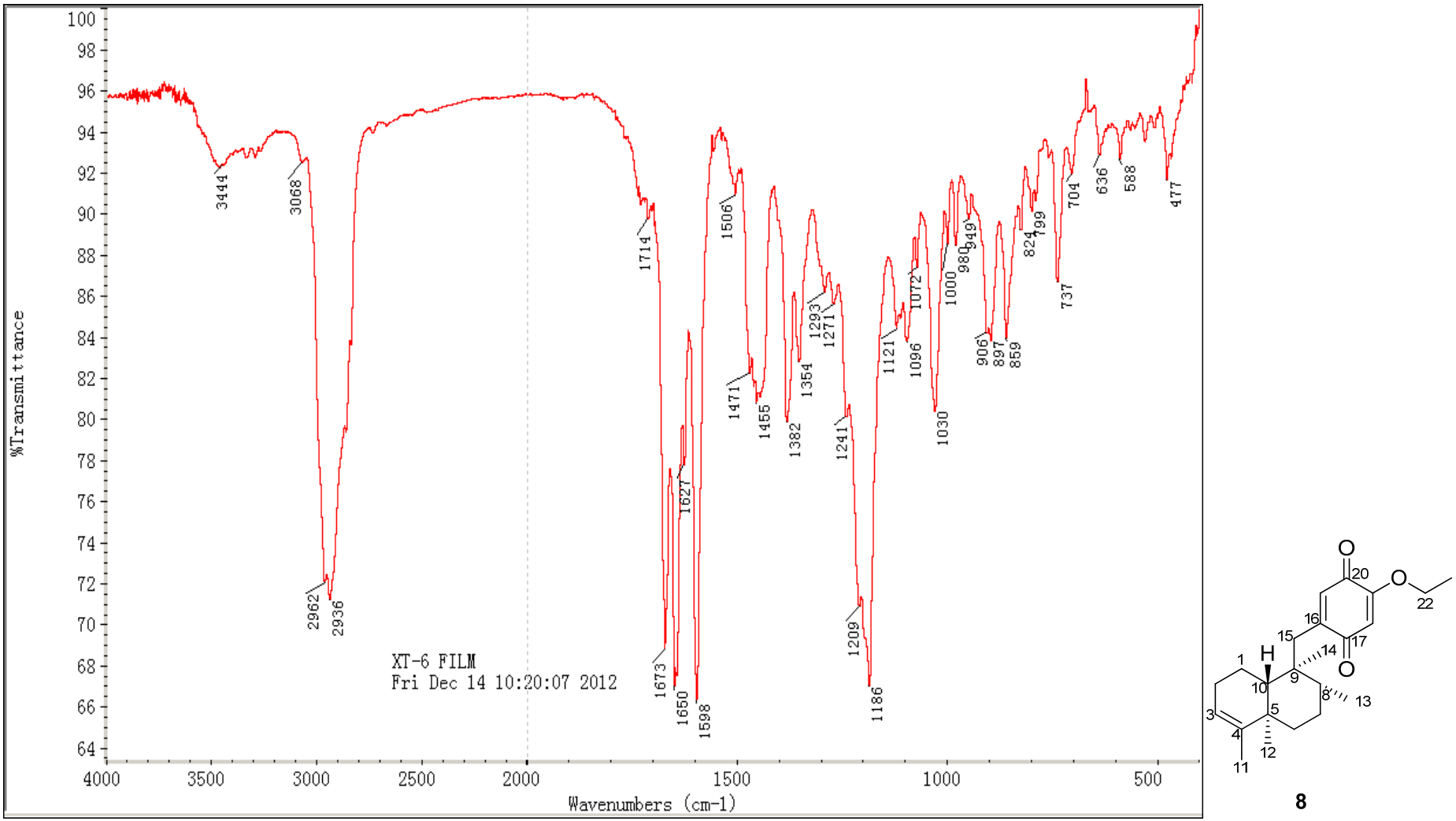
8

Figure S86. CD Spectrum of (5*R*,8*R*,9*S*,10*R*)-19-ethoxylavarone (**8**) in MeOH.



8

Figure S87. UV Spectrum of (5*R*,8*R*,9*S*,10*R*)-19-ethoxylavarone (**8**).



8

Figure S88. IR Spectrum of (5*R*,8*R*,9*S*,10*R*)-19-ethoxylavarone (**8**).