Supporting Information for

Nanomolar Antimalarial Agents against Chloroquine-Resistant *Plasmodium falciparum* from Medicinal Plants and their Structure-Activity Relationships

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Table S1 The purities of compounds 1–44

Comounds	Method	Retention Time (min)	Purity (%)
1	A	12.27	95.65
2	A	17.35	98.00
3	A	16.97	98.10
4	A	12.54	96.99
5	A	12.28	98.98
6	A	18.74	94.77
7	A	7.16	94.79
8	A	14.89	95.61
9	A	10.35	97.98
10	A	8.99	94.56
11	A	19.49	98.75
12	A	19.19	98.06
13	A	5.23	97.74
14	A	14.35	98.84
15	B	18.84	99.28
16	A	13.06	97.36
17	A	15.94	98.96
18	A	16.35	98.79
19	A	17.35	96.33
20	A	10.77	98.27
21	A	10.76	97.87
22	A	12.65	98.91
23	B	18.99	96.84
24	A	14.08	98.15
25	A	19.01	99.06
26	A	12.14	97.87
27	A	15.24	98.38
28	A	16.34	96.49
29	A	16.46	98.30
30	A	18.25	99.78
31	A	13.15	97.98
32	A	17.09	96.89
33	A	17.05	99.02
34	A	17.04	99.53
35	A	11.71	95.45
36	A	12.23	99.51
37	A	9.20	99.39
38	A	17.06	98.29
39	A	9.83	99.36
40	A	11.84	97.32
41	A	10.15	95.18
42	A	8.36	96.68
43	B	18.30	96.15
44	A	15.46	96.62

The purities of compounds **1**–**44** were checked by reversed-phase HPLC, which was performed on an Aglient 1100 binary pump system with an Aglient 1100 detector (210 nm) using a YMC-Pack ODS-A (150×4.6 mm, *S*-5 μm).

Methods: A: 30–80% CH_3CN in H_2O for 20 min, 0.5 ml/min; B: 30–90% CH_3CN in H_2O for 20 min, 0.5 ml/min

Figure S1. ^{1}H NMR spectrum of fortunilide A (1) in $CDCl_3$

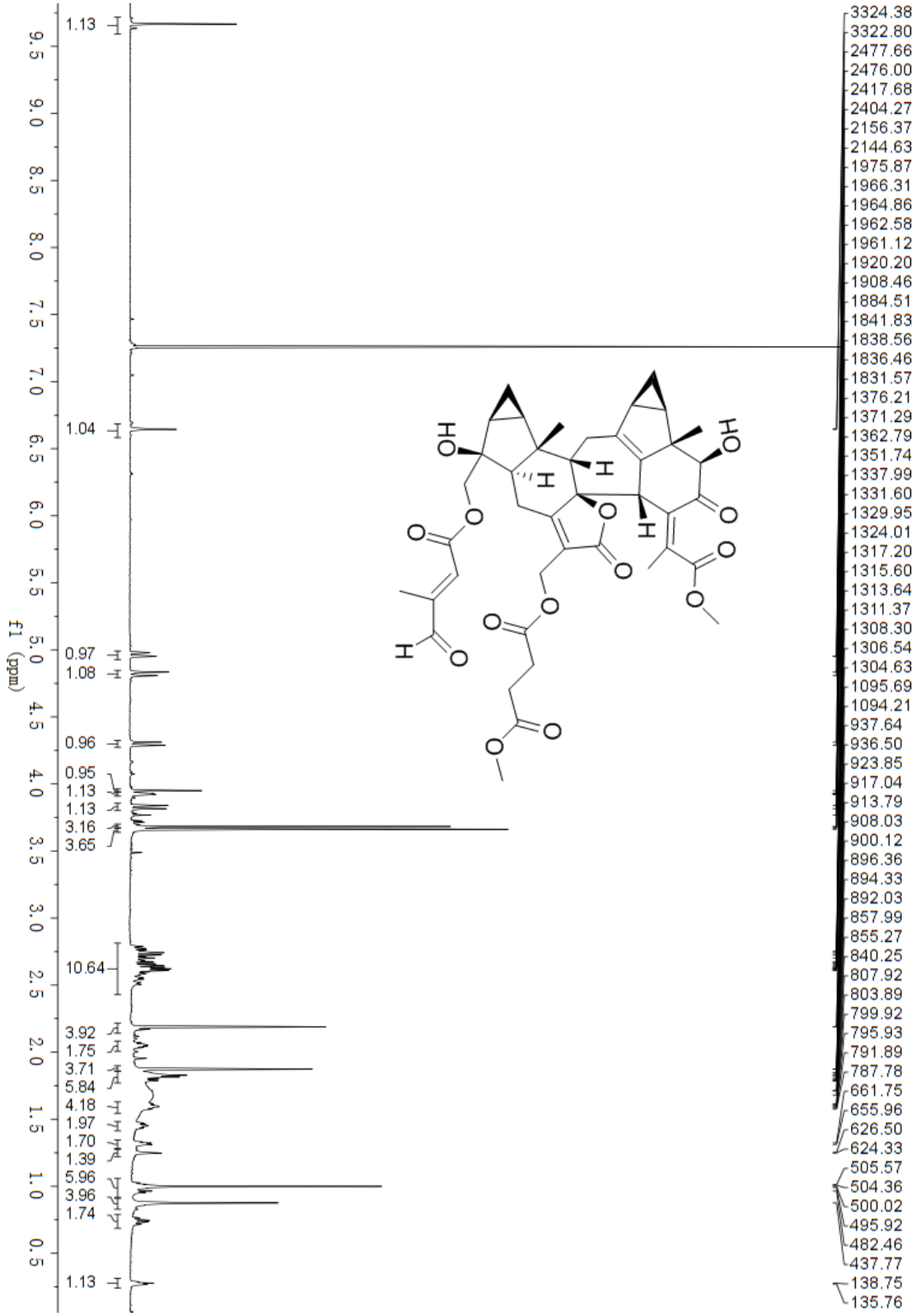


Figure S2. ^{13}C NMR spectrum of fortunilide A (1) in $CDCl_3$

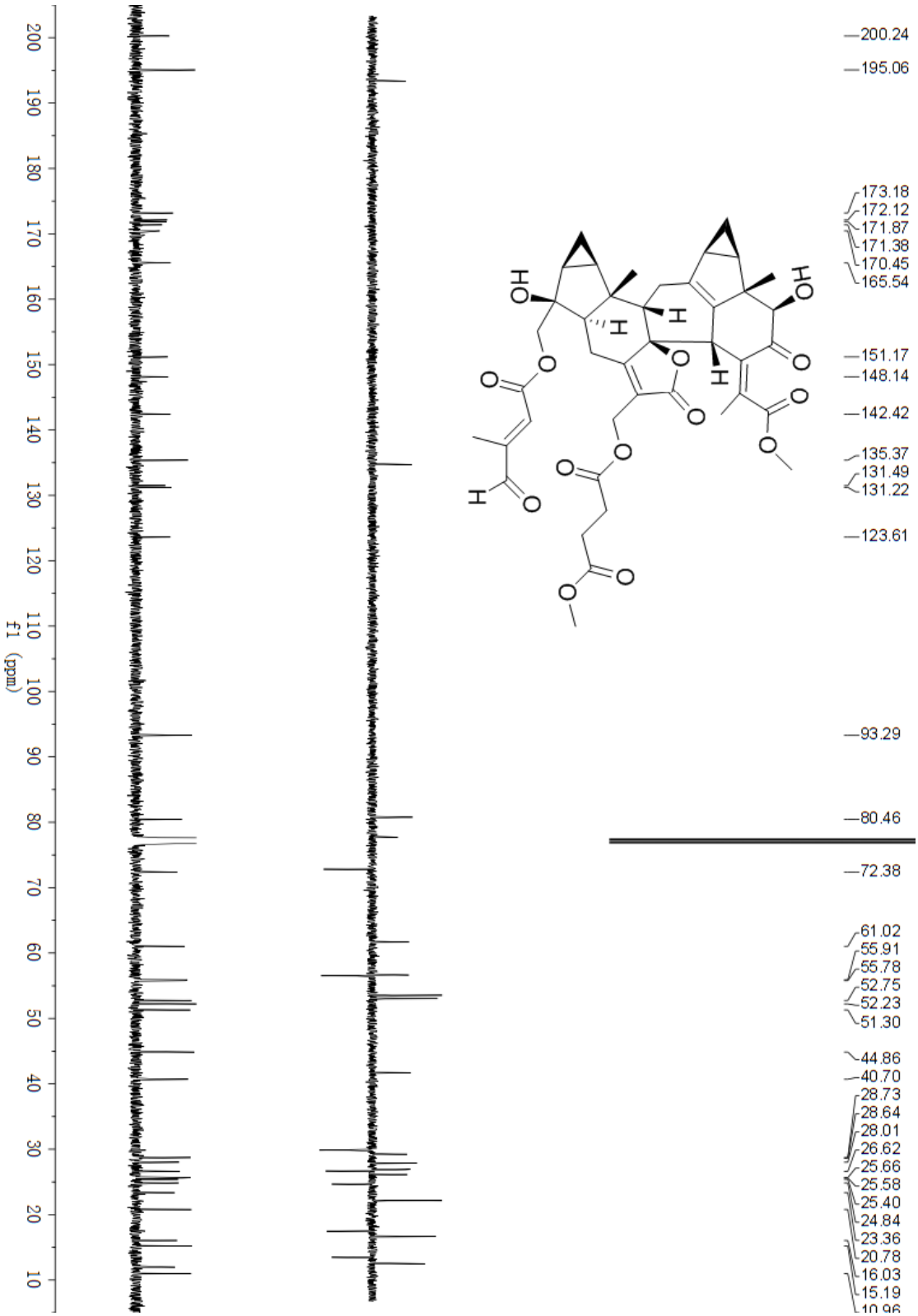


Figure S3. HSQC spectrum of fortunilide A (1) in $CDCl_3$

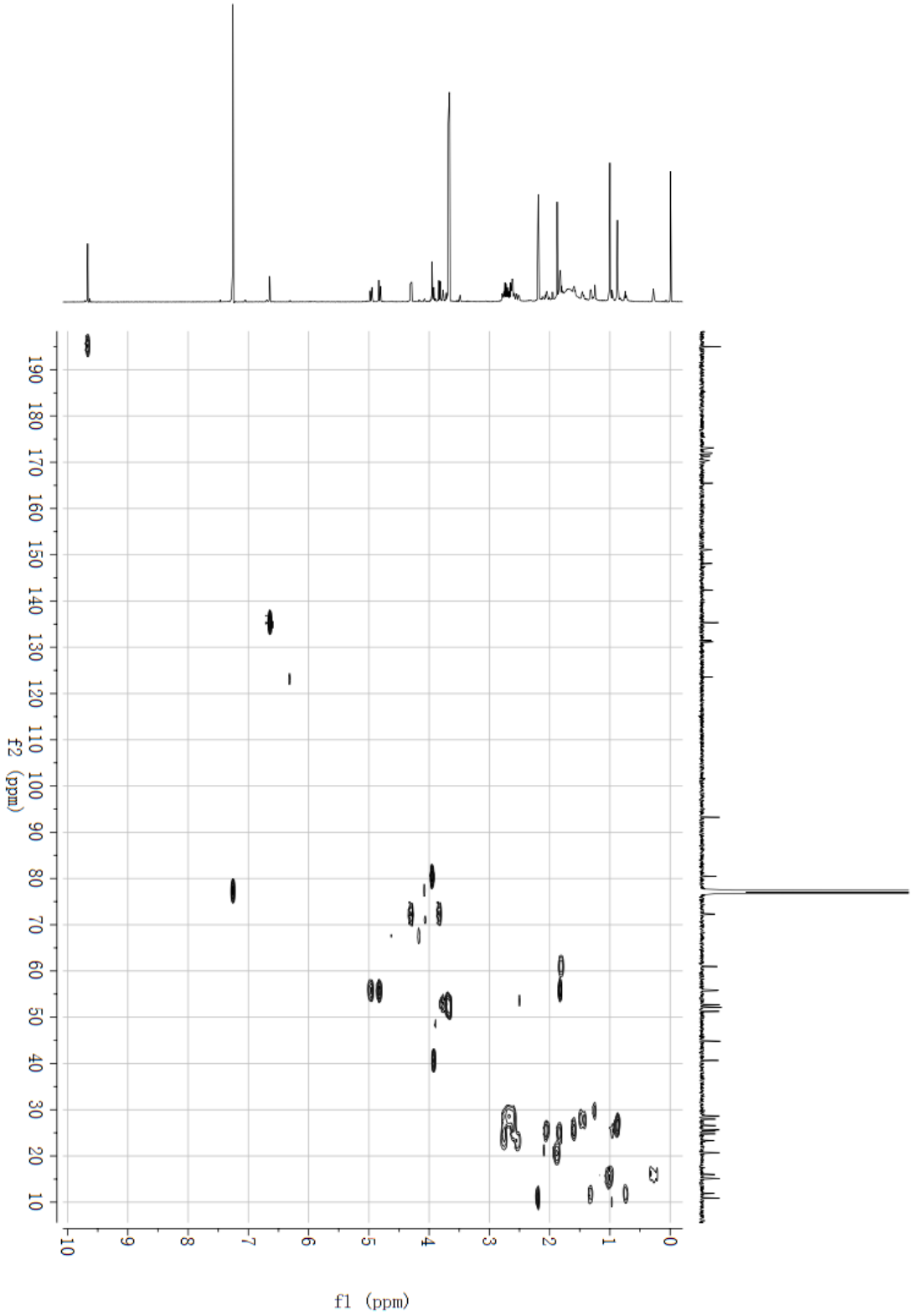


Figure S4. HMBC spectrum of fortunilide A (1) in $CDCl_3$

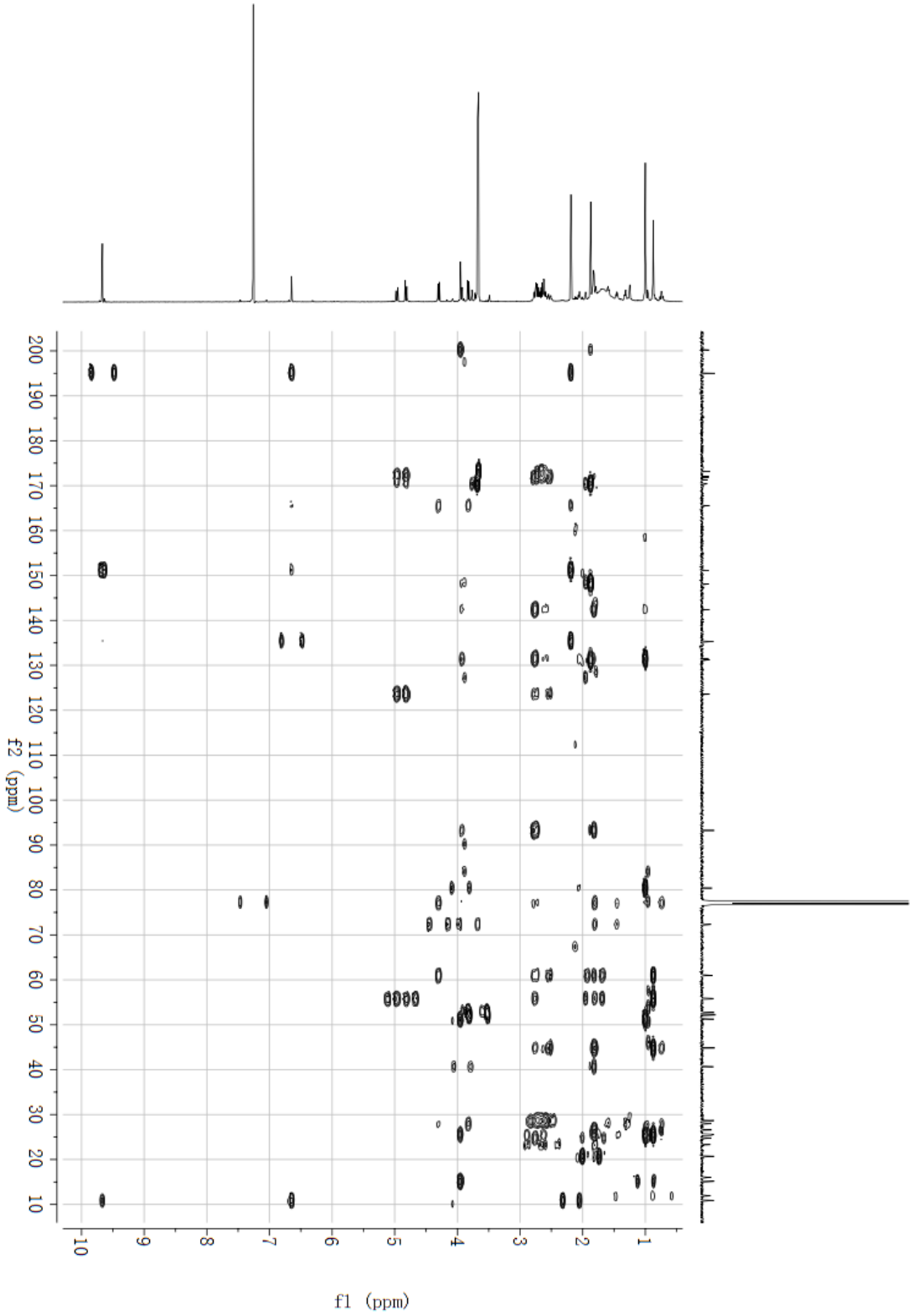


Figure S5. ROESY spectrum of fortunilide A (1) in $CDCl_3$

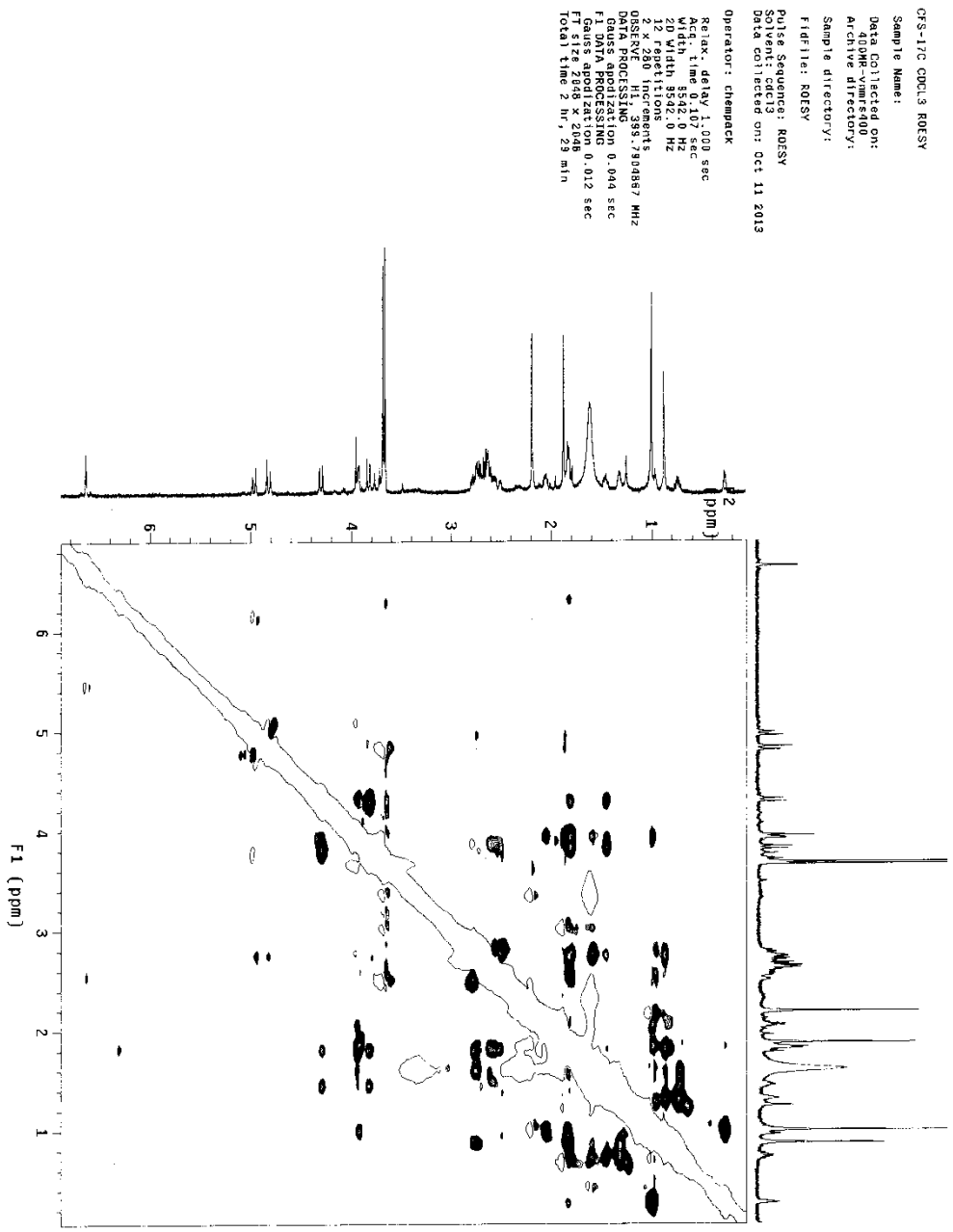


Figure S6. (+)-ESIMS of fortunilide A (1)

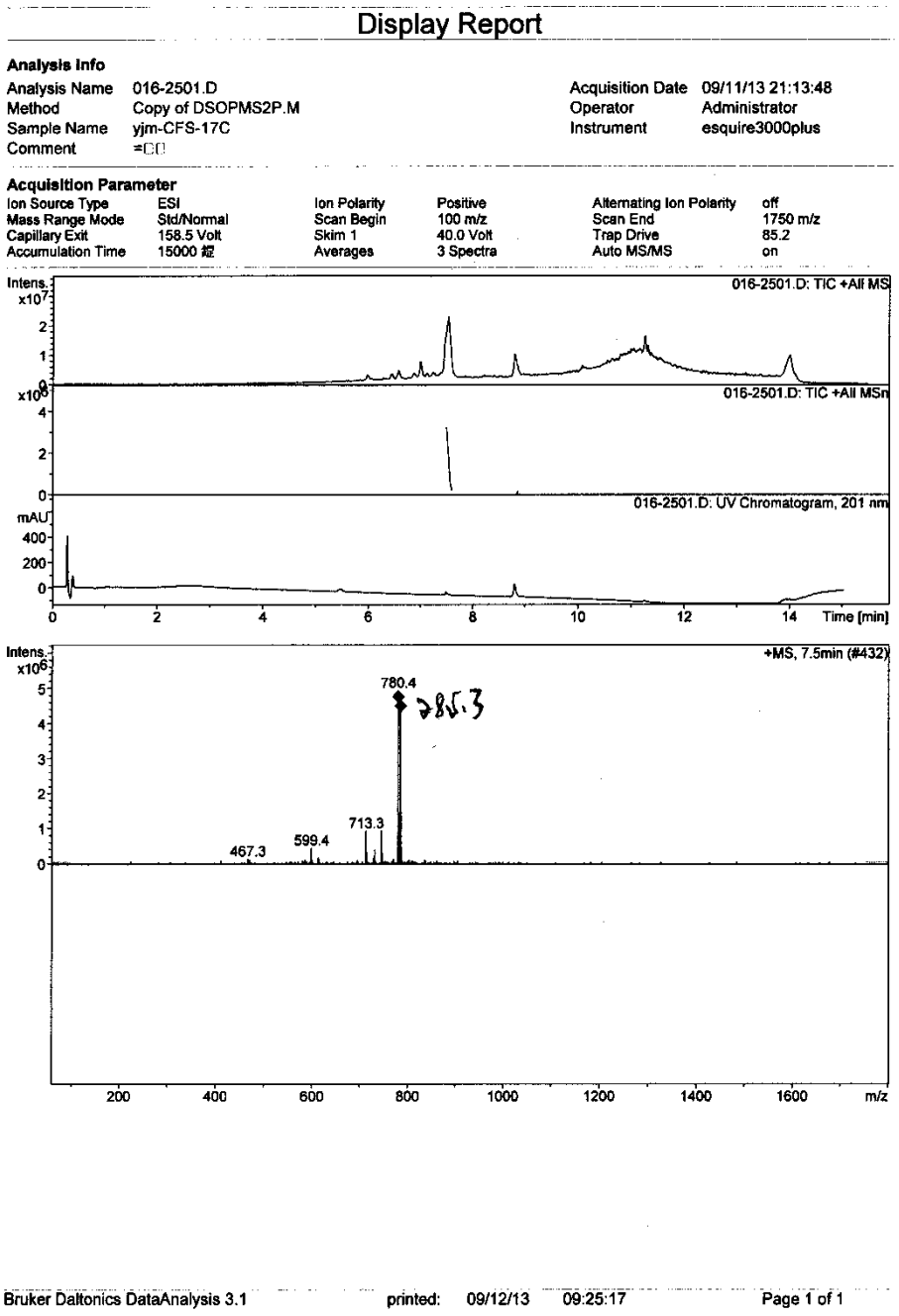


Figure S7. (–)-ESIMS of fortunilide A (1)

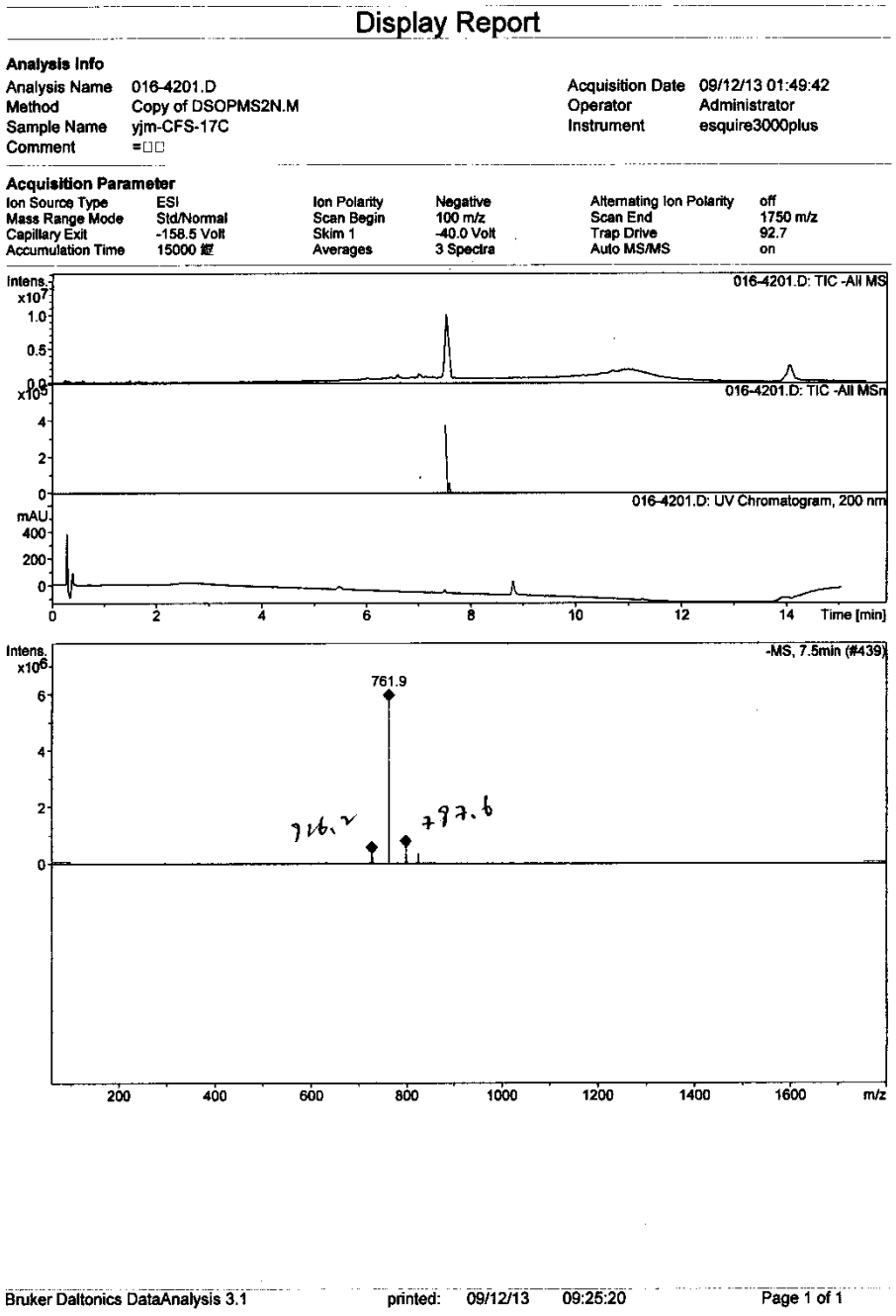


Figure S8. (+)-HRESIMS of fortunilide (1)

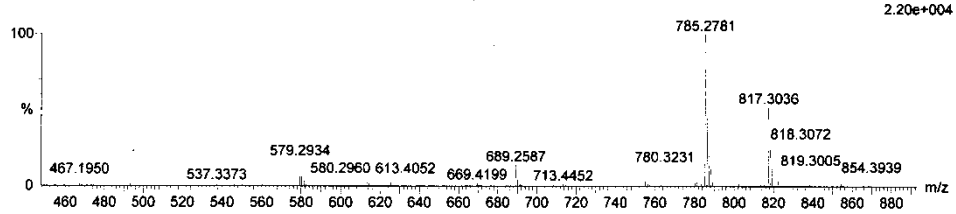
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
336 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 O: 0-20 Na: 0-1

CFS-17C LCT PXE KE324 13-Sep-2013 13:54:24

CFS-17C_0913 43 (0.935) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (27:45) 1: TOF MS ES+ 2.20e+004



Minimum:				-1.5						
Maximum:		3.0	5.0	50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
785.2781	785.2785	-0.4	-0.5	18.5	78.4	1.0	C41	H46	O14	Na
	785.2809	-2.8	-3.6	21.5	78.8	1.5	C43	H45	O14	
	785.2751	3.0	3.8	30.5	78.3	0.9	C50	H41	O9	

Figure S9. IR spectrum of fortunilide A (1)

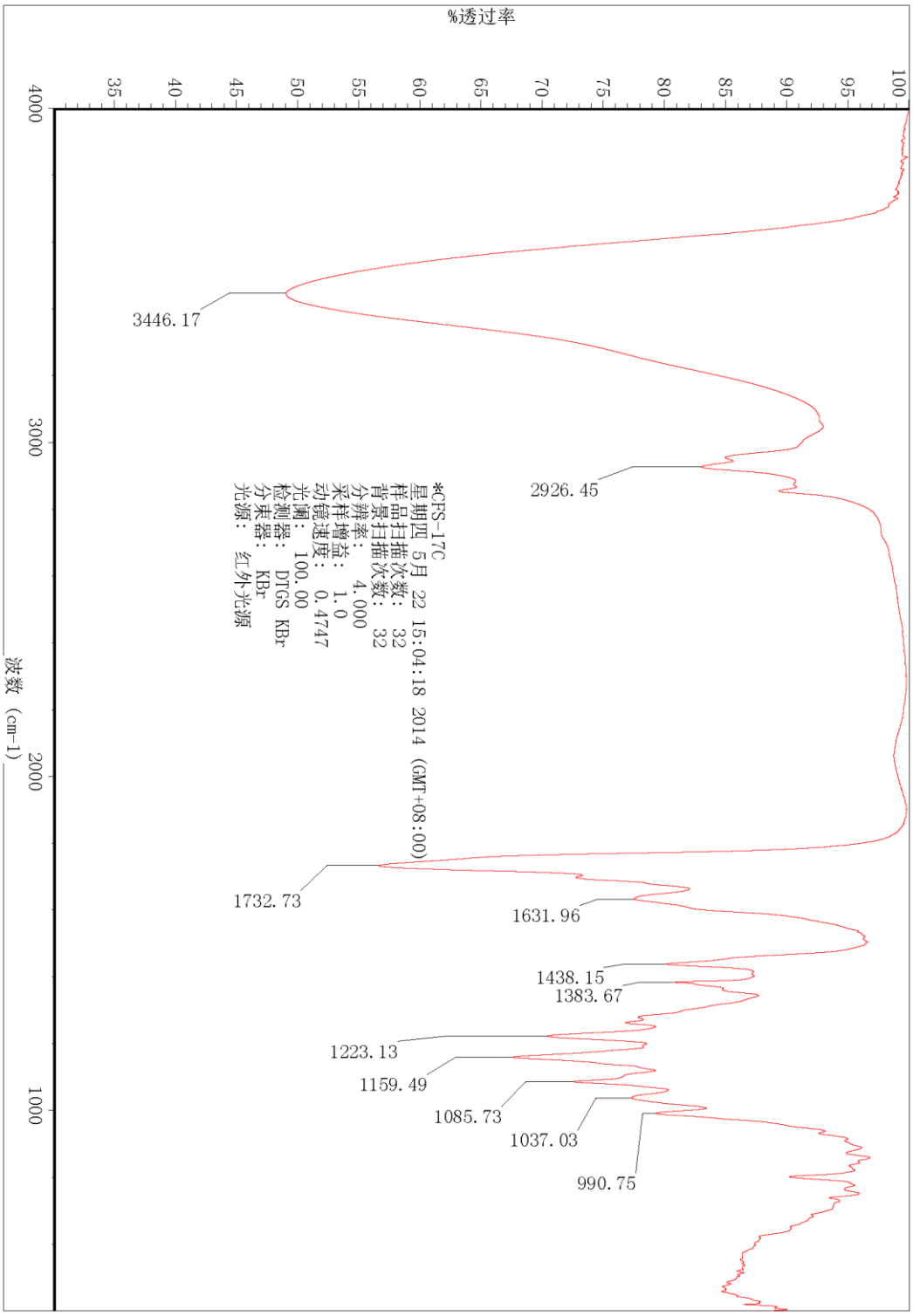


Figure S10. ^{1}H NMR spectrum of fortunilide B (2) in $CDCl_3$

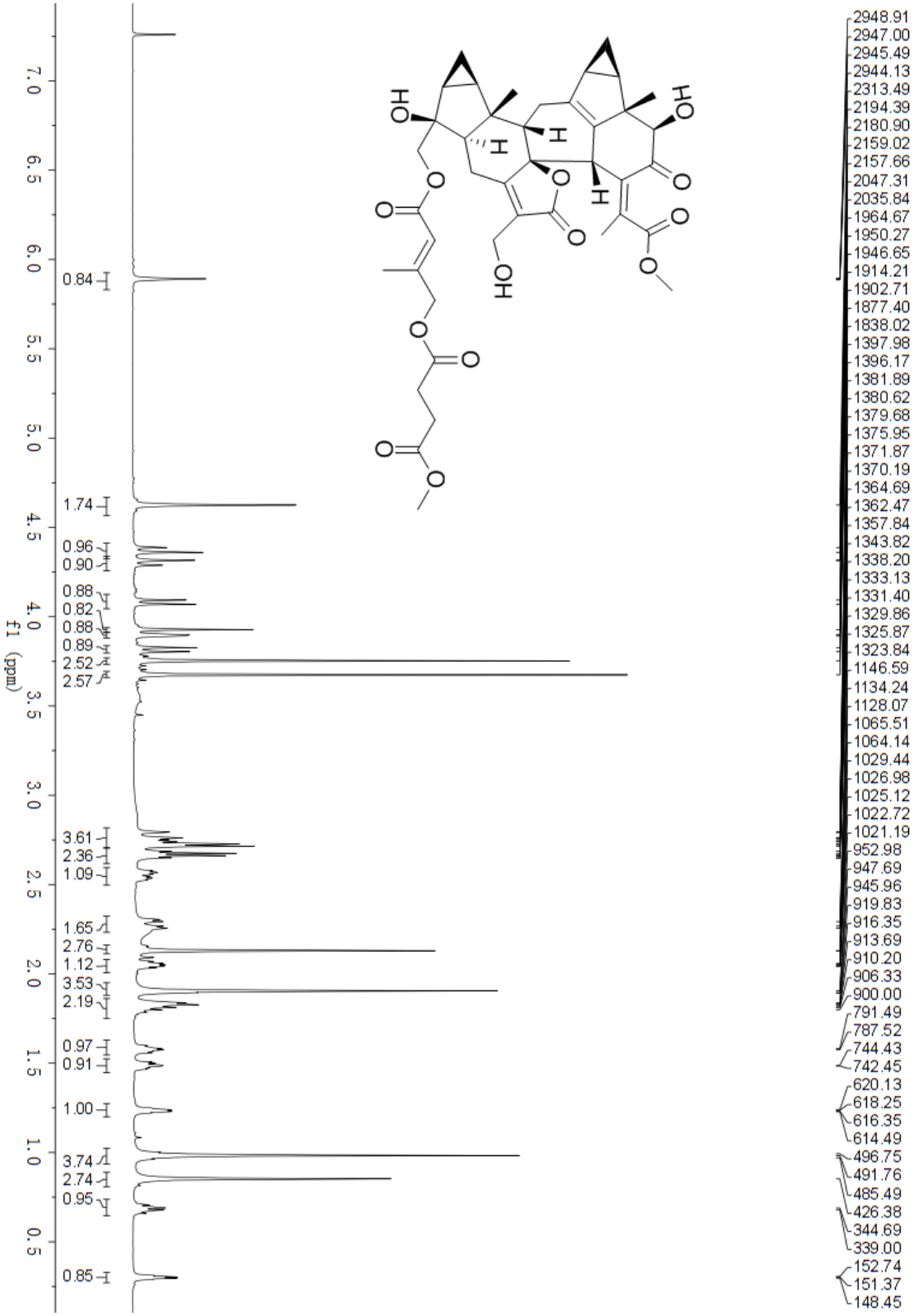


Figure S11. ^{13}C NMR spectrum of fortunilide B (2) in $CDCl_3$

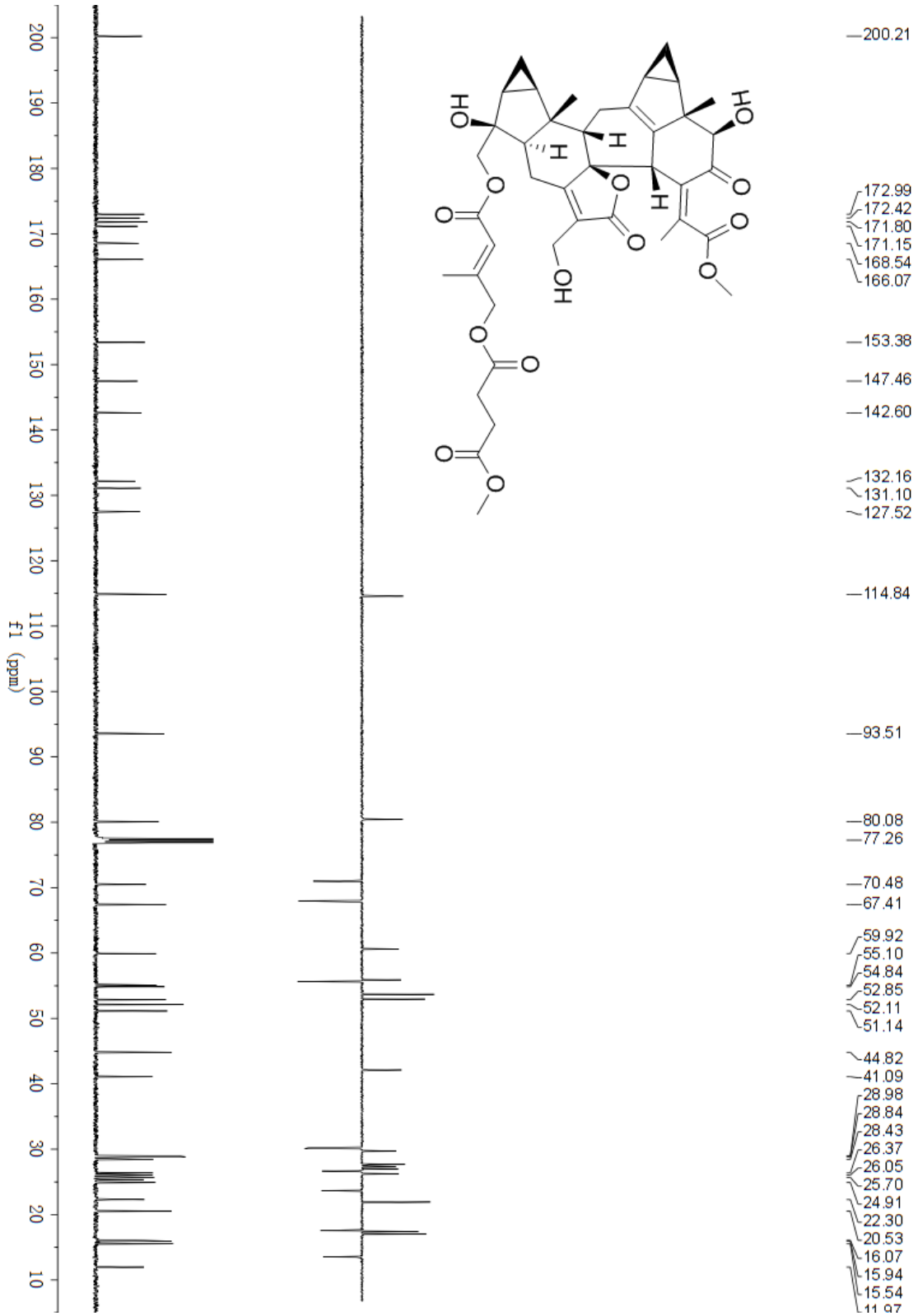


Figure S12. HSQC spectrum of fortunilide B (2) in $CDCl_3$

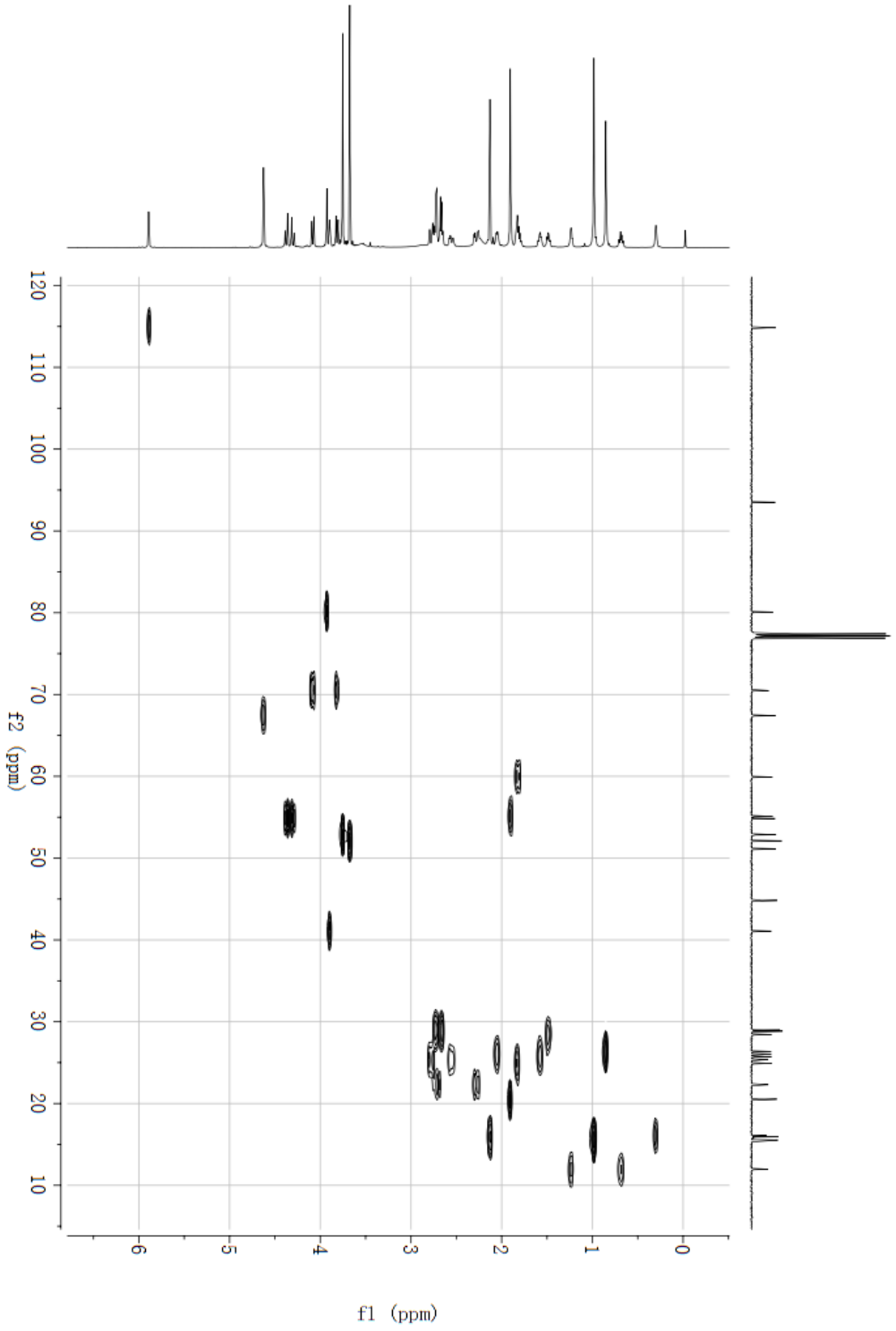


Figure S13. HMBC spectrum of fortunilide B (2) in $CDCl_3$

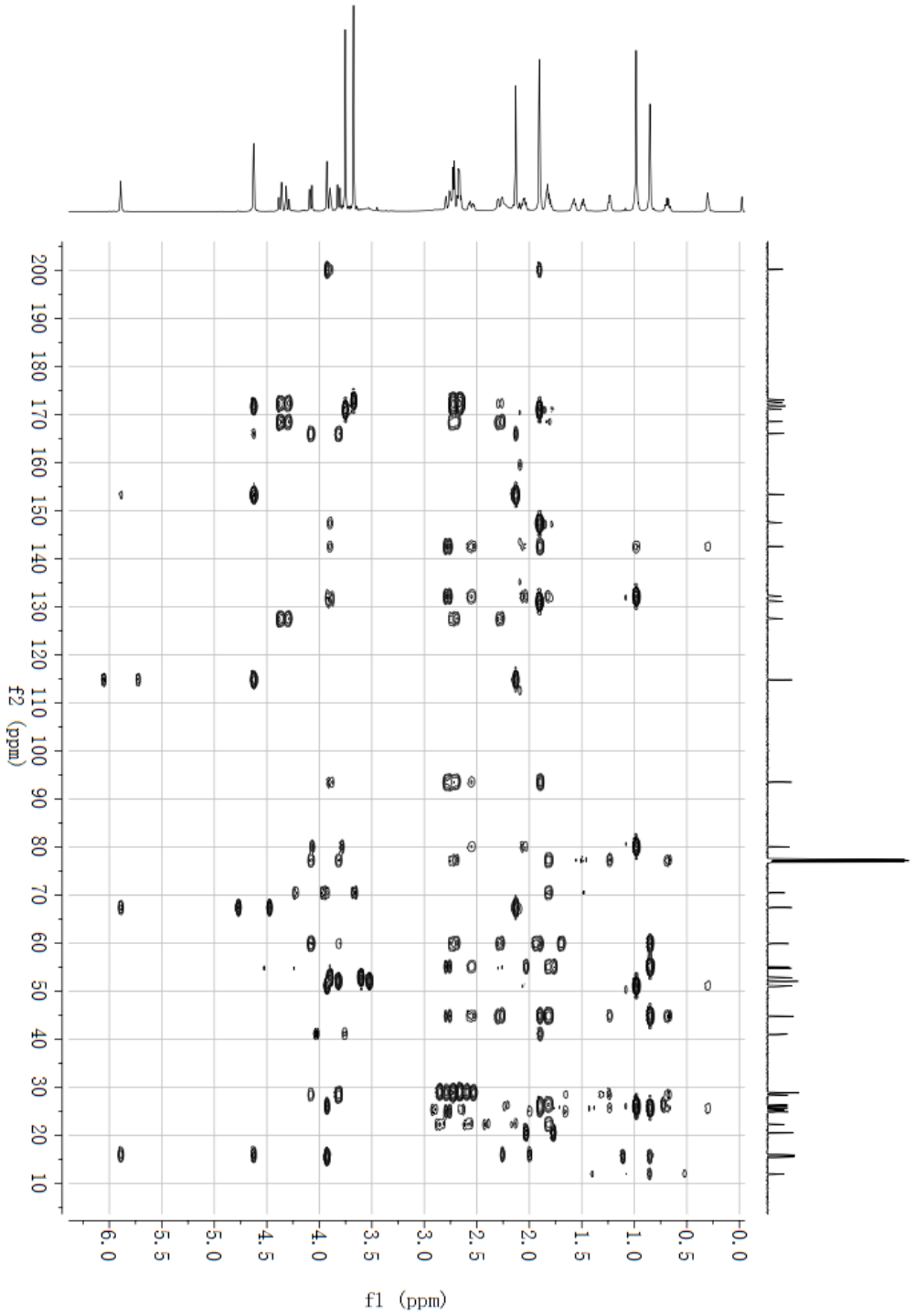


Figure S14. ROESY spectrum of fortunilide B (2) in $CDCl_3$

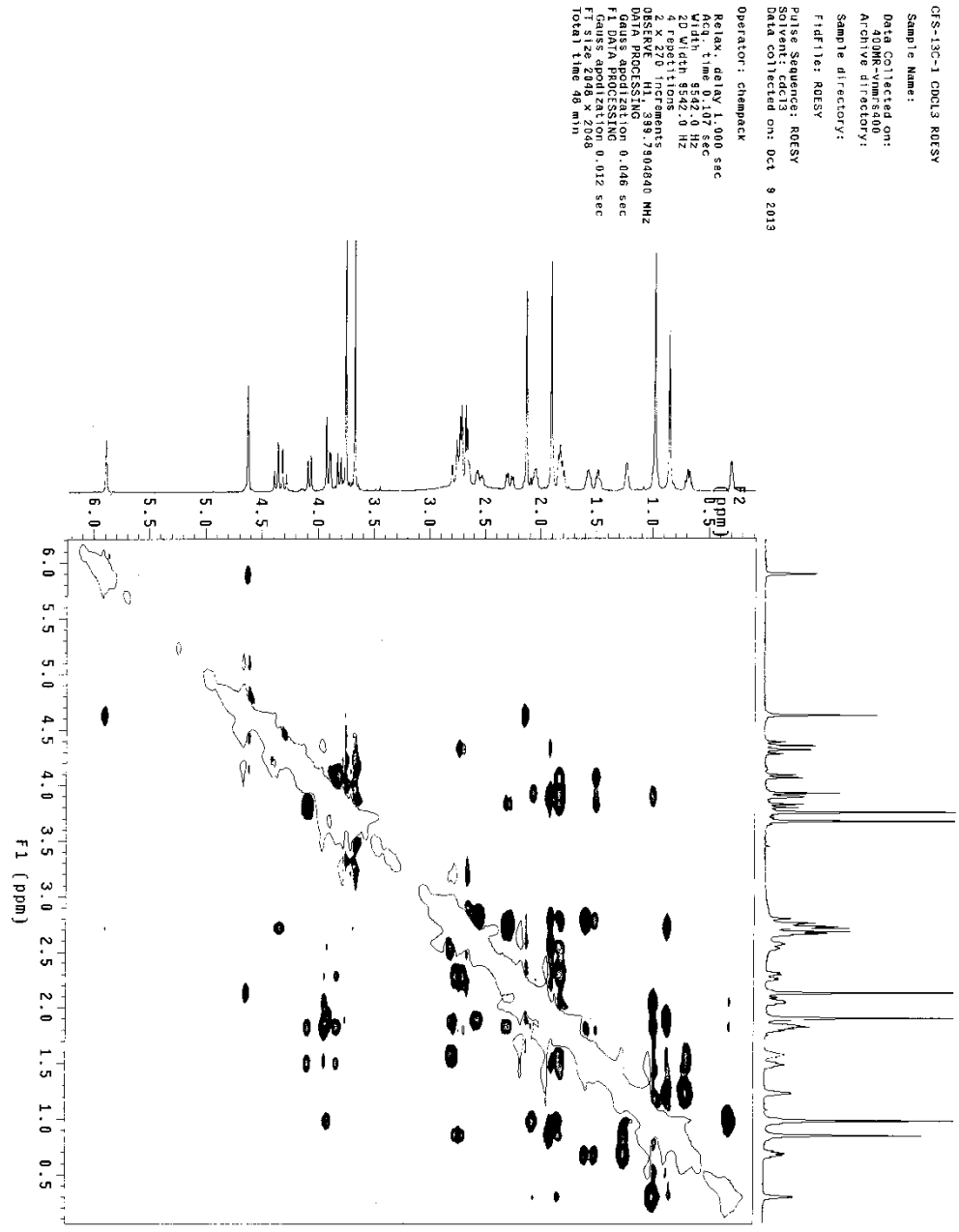


Figure S15. (+)-ESIMS of fortunilide B (2)

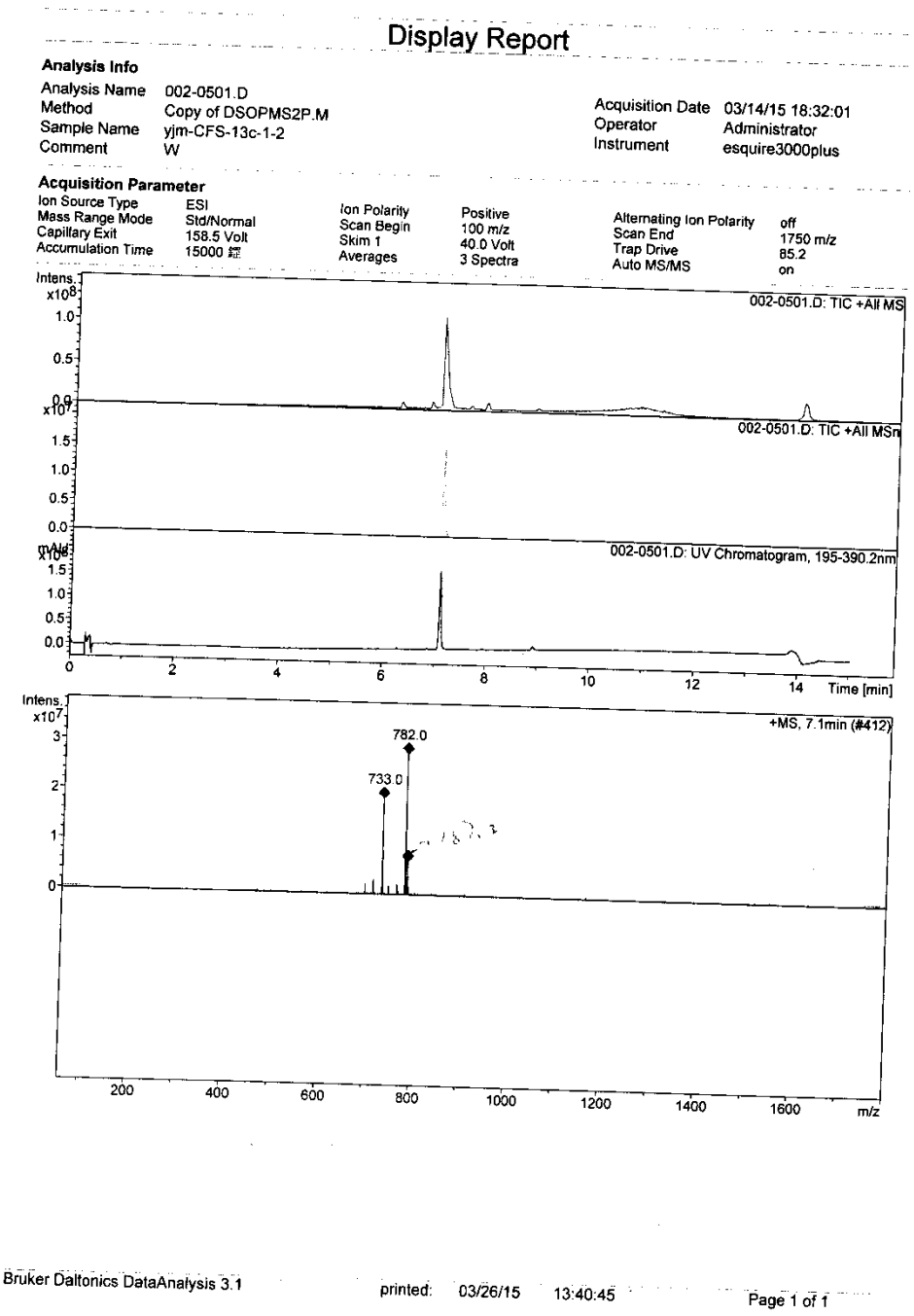


Figure S16. (–)-ESIMS of fortunilide B (2)

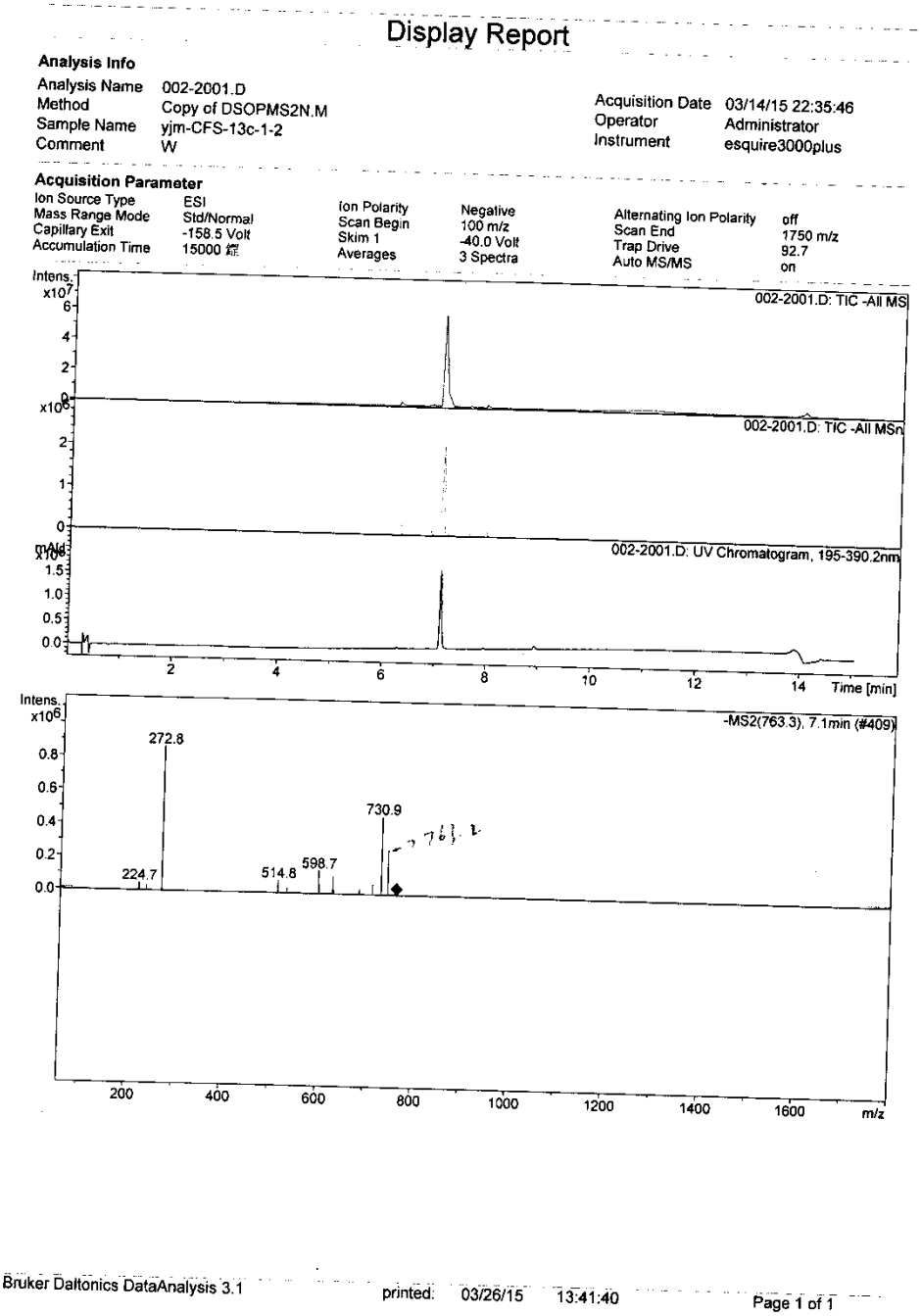


Figure S17. (+)-HRESIMS of fortunilide B (2)

Elemental Composition Report **Page 1**

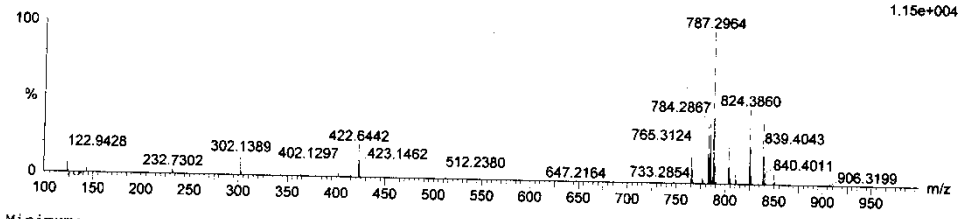
Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
337 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 O: 0-20 Na: 0-1
CFS-13C-1

LCT PXE KE324

03-Sep-2013
15:27:14
1: TOF MS ES+
1.15e+004

CFS-13C-1_0903 38 (0.831) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (22:38)



Minimum:				-1.5			
Maximum:		3.0	3.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
787.2964	787.2966	-0.2	-0.3	20.5	50.3	1.3	C43 H47 O14
	787.2977	-1.3	-1.7	39.5	56.5	7.5	C59 H40 O Na
	787.2942	2.2	2.8	17.5	49.4	0.3	C41 H48 O14 Na

Figure S18. IR spectrum of fortunilide B (2)

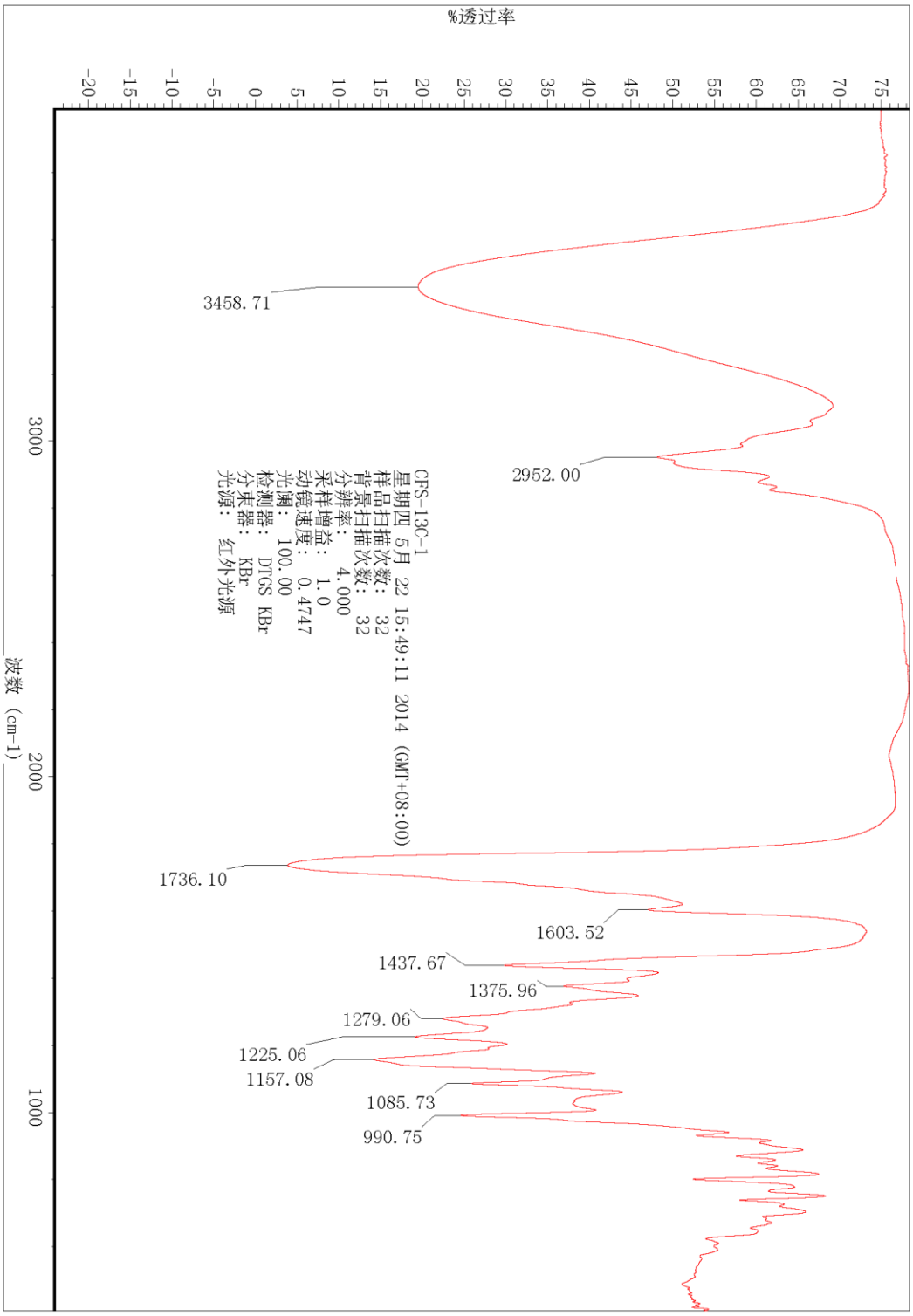


Figure S19. ^{1}H NMR spectrum of fortunilide C (3) in $CDCl_3$

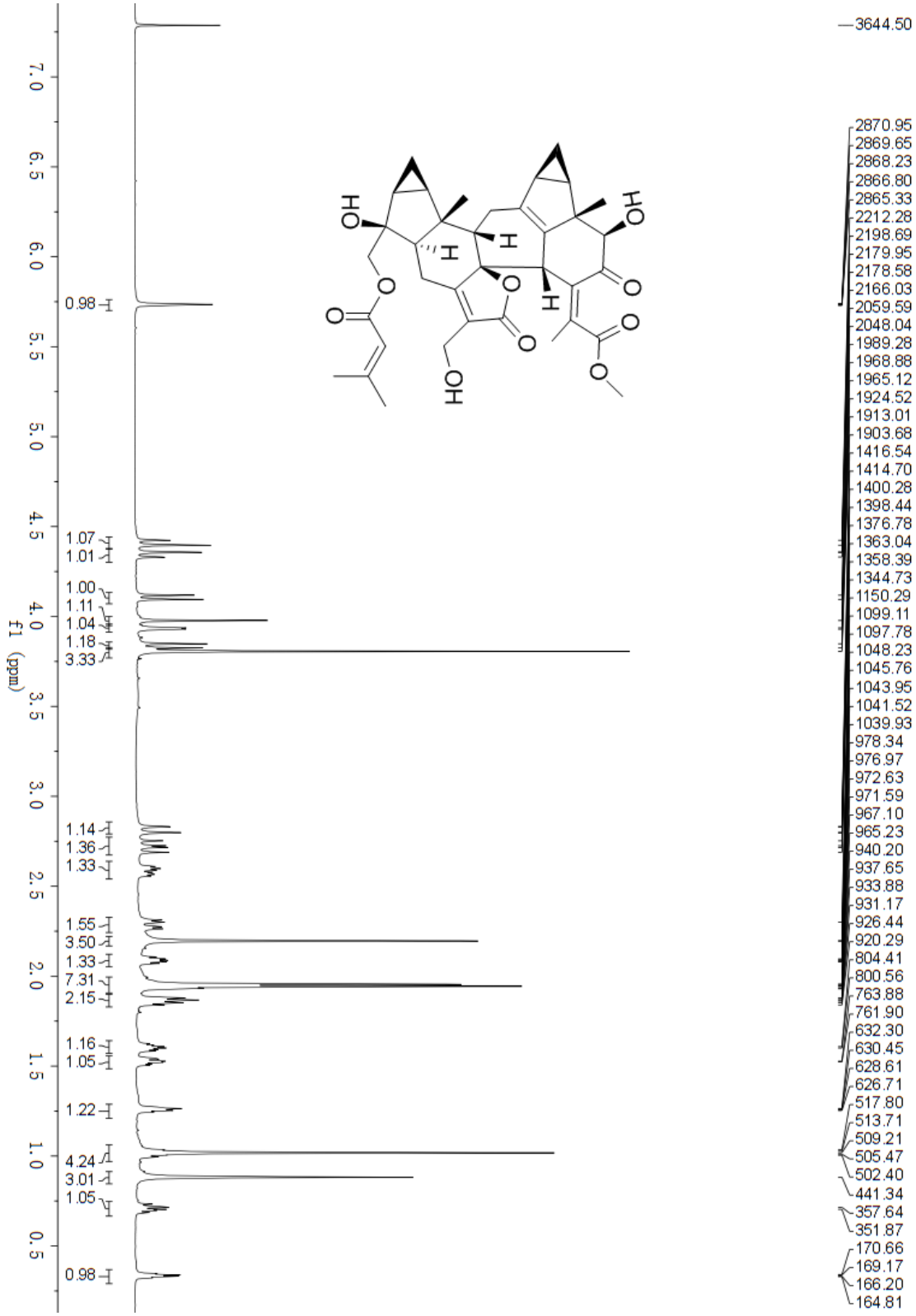


Figure S20. ^{13}C NMR spectrum of fortunilide C (3) in $CDCl_3$

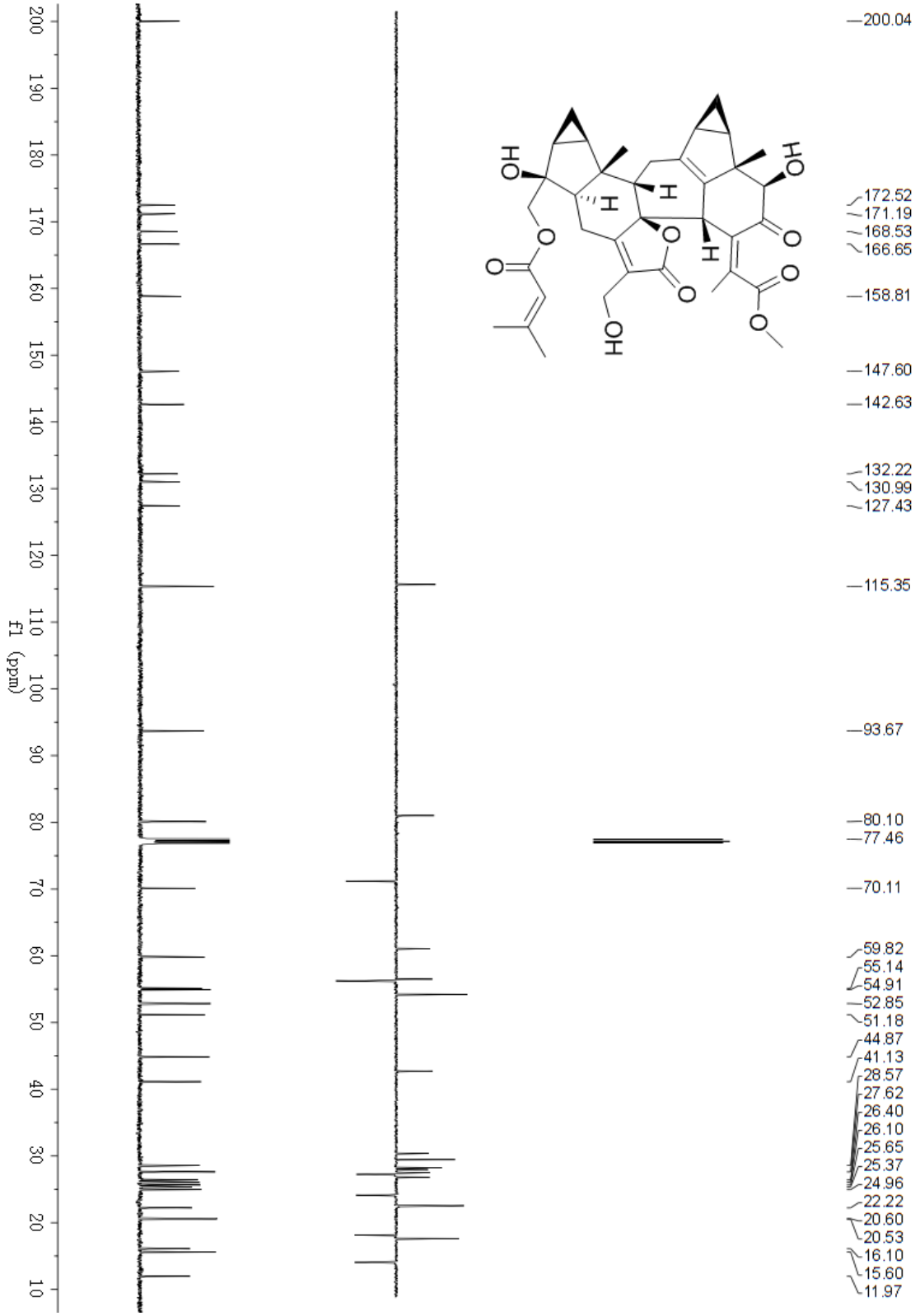


Figure S21. HSQC spectrum of fortunilide C (3) in $CDCl_3$

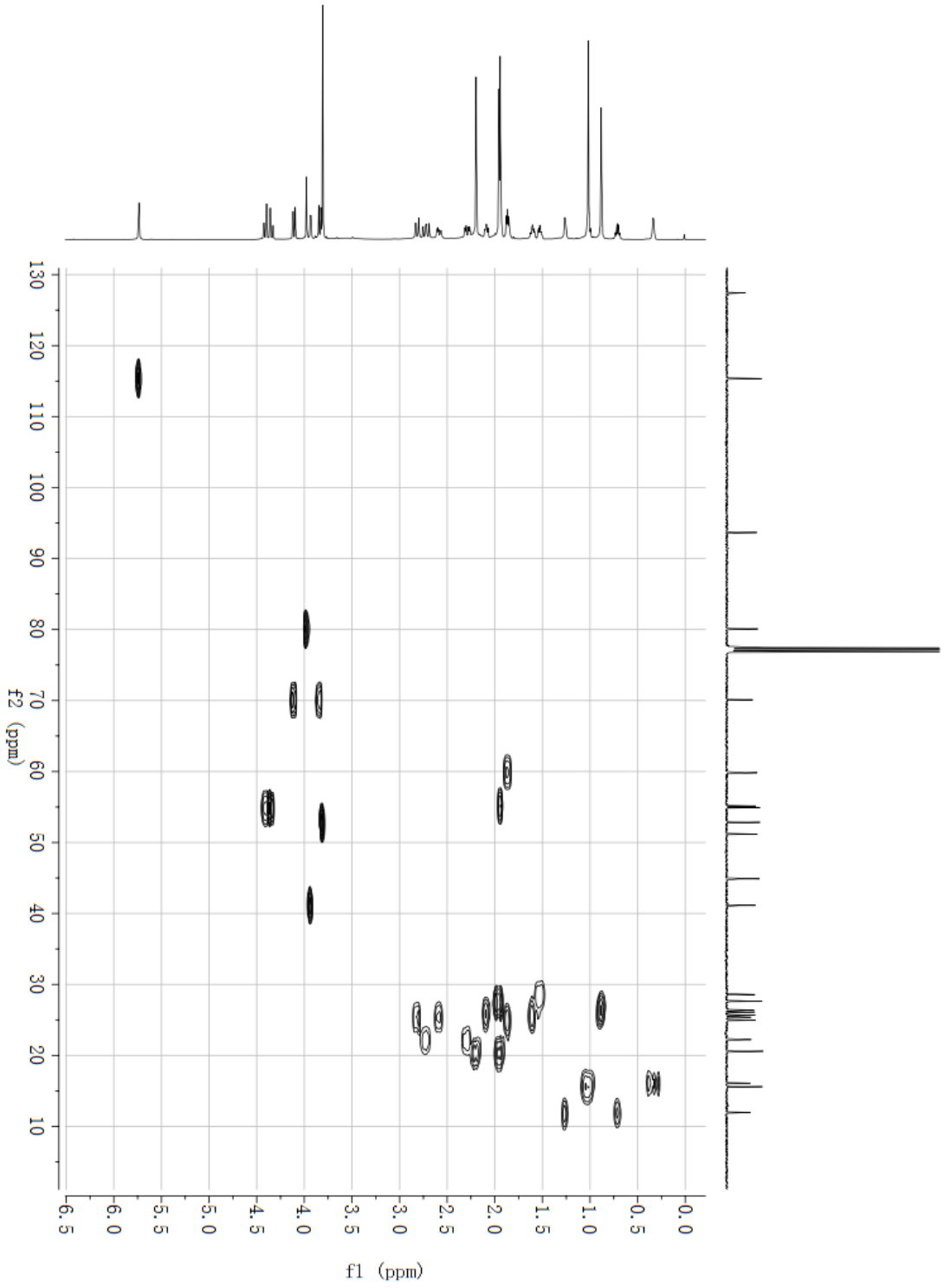


Figure S22. HMBC spectrum of fortunilide C (3) in $CDCl_3$

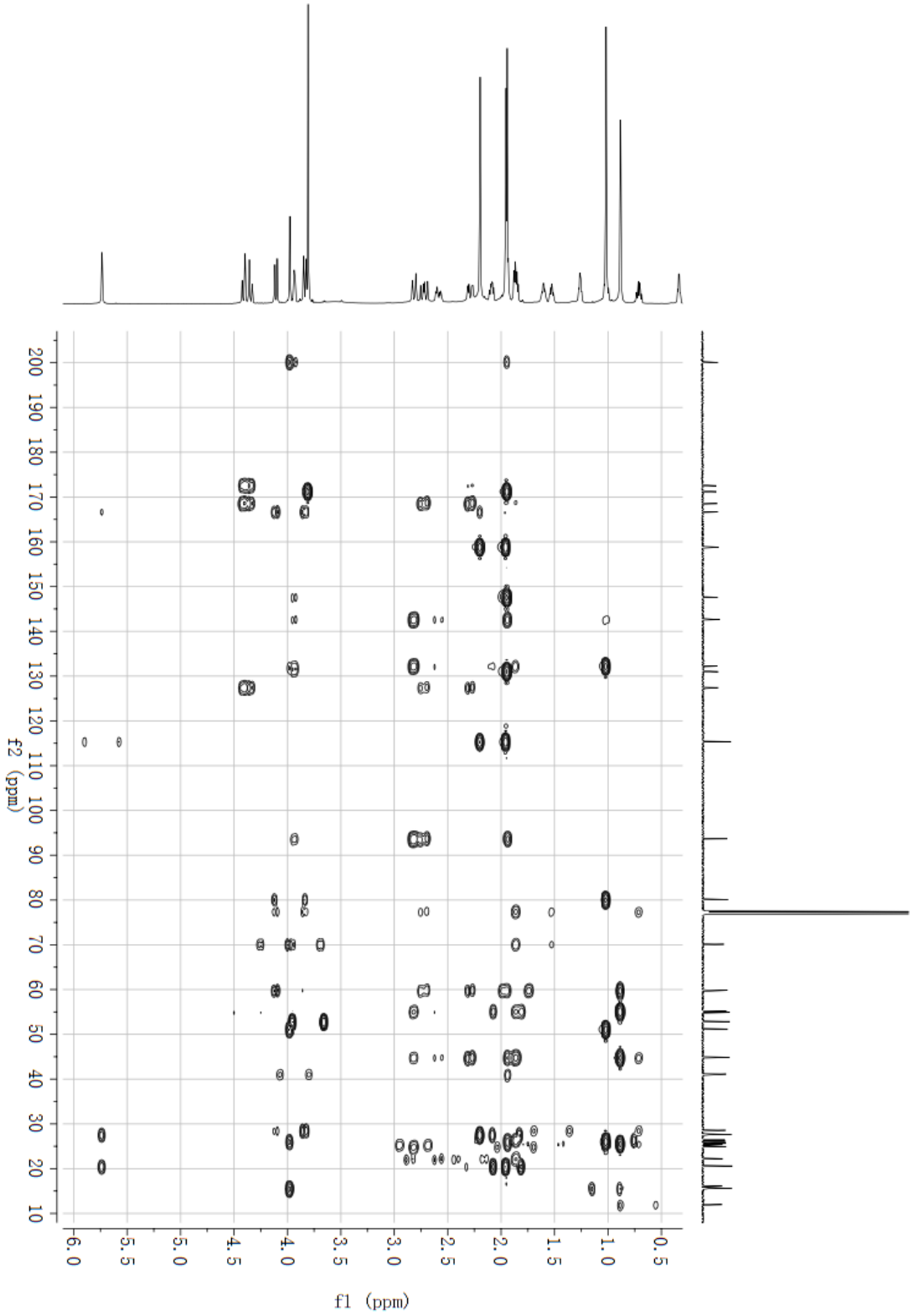


Figure S23. ROESY spectrum of fortunilide C (3)

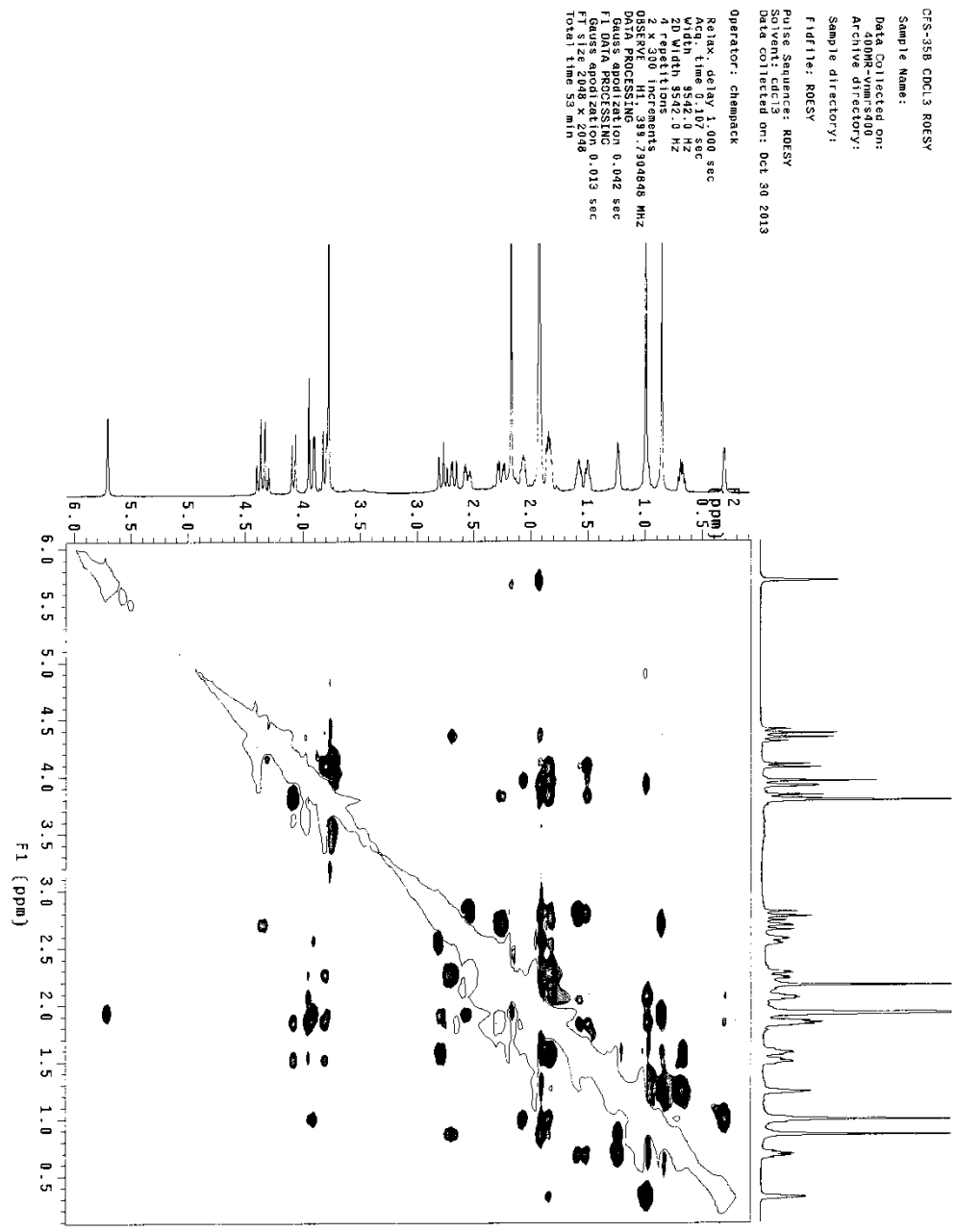


Figure S24. (+)-ESIMS spectrum of fortunilide C (3)

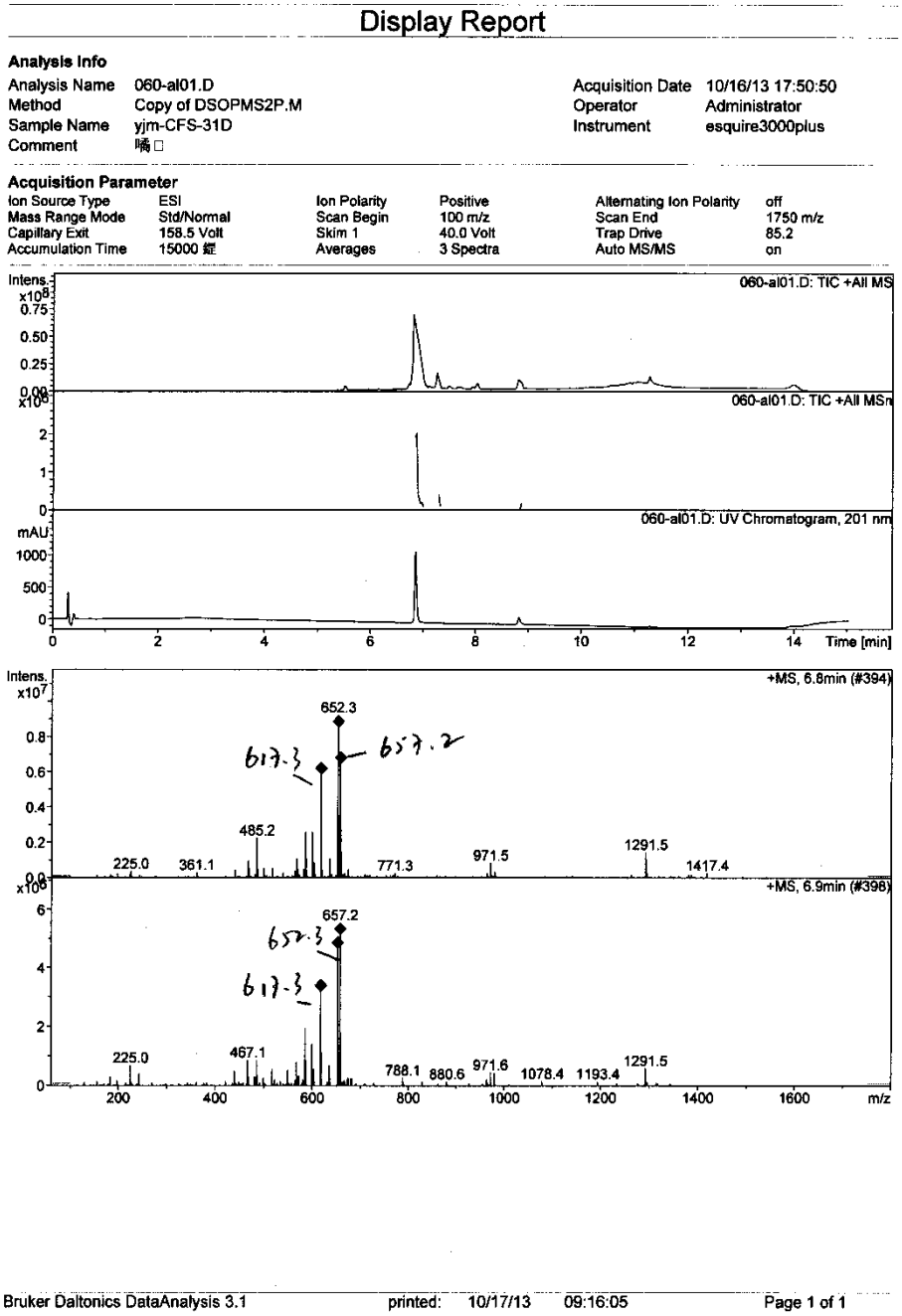


Figure S25. (–)-ESIMS spectrum of fortunilide C (3)

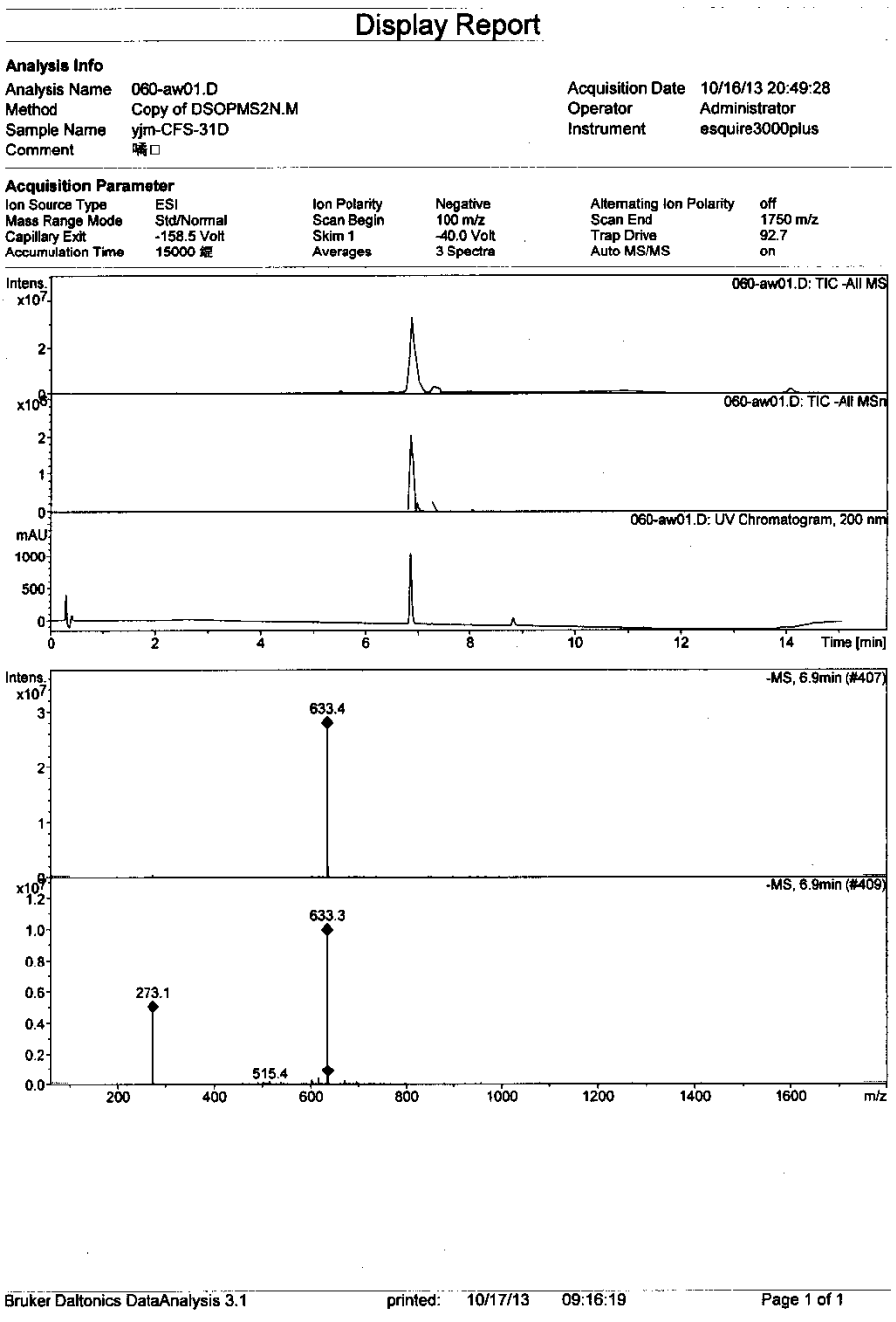


Figure S26. (+)-HRESIMS spectrum of fortunilide C (3)

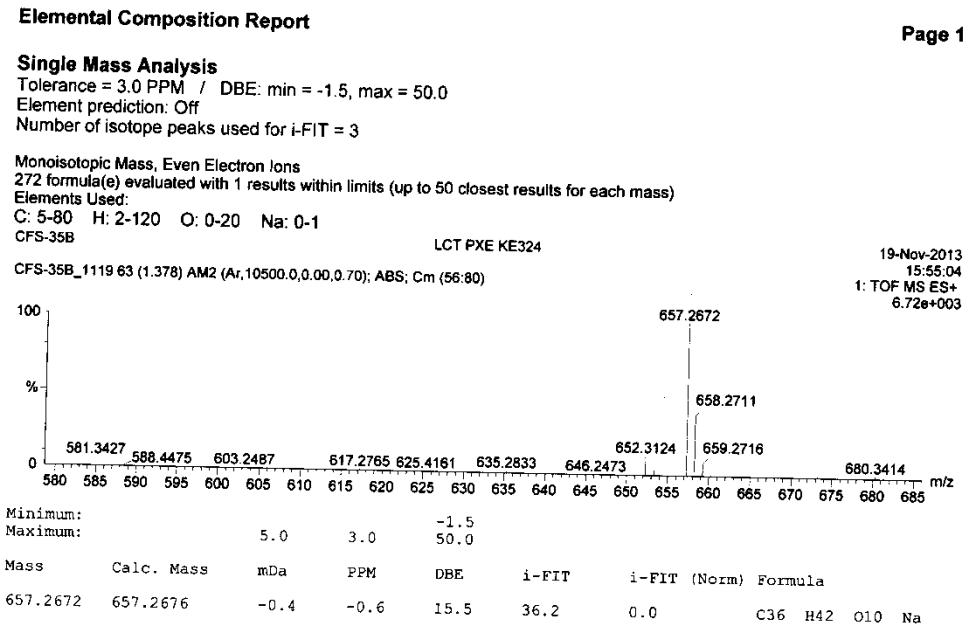


Figure S27. IR spectrum of fortunilide C (3)

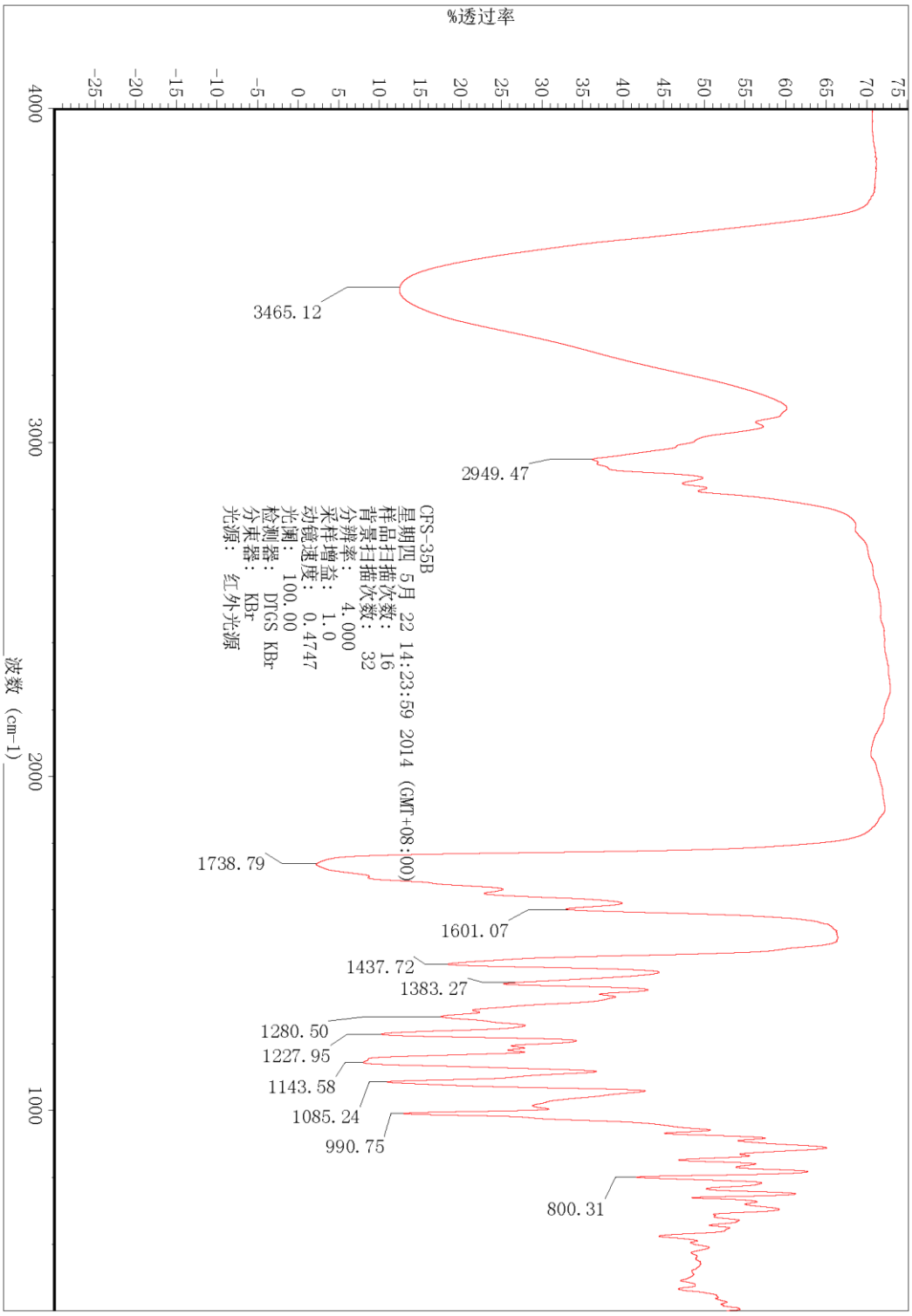


Figure S28. ^{1}H NMR spectrum of fortunilide D (4) in $CDCl_3$

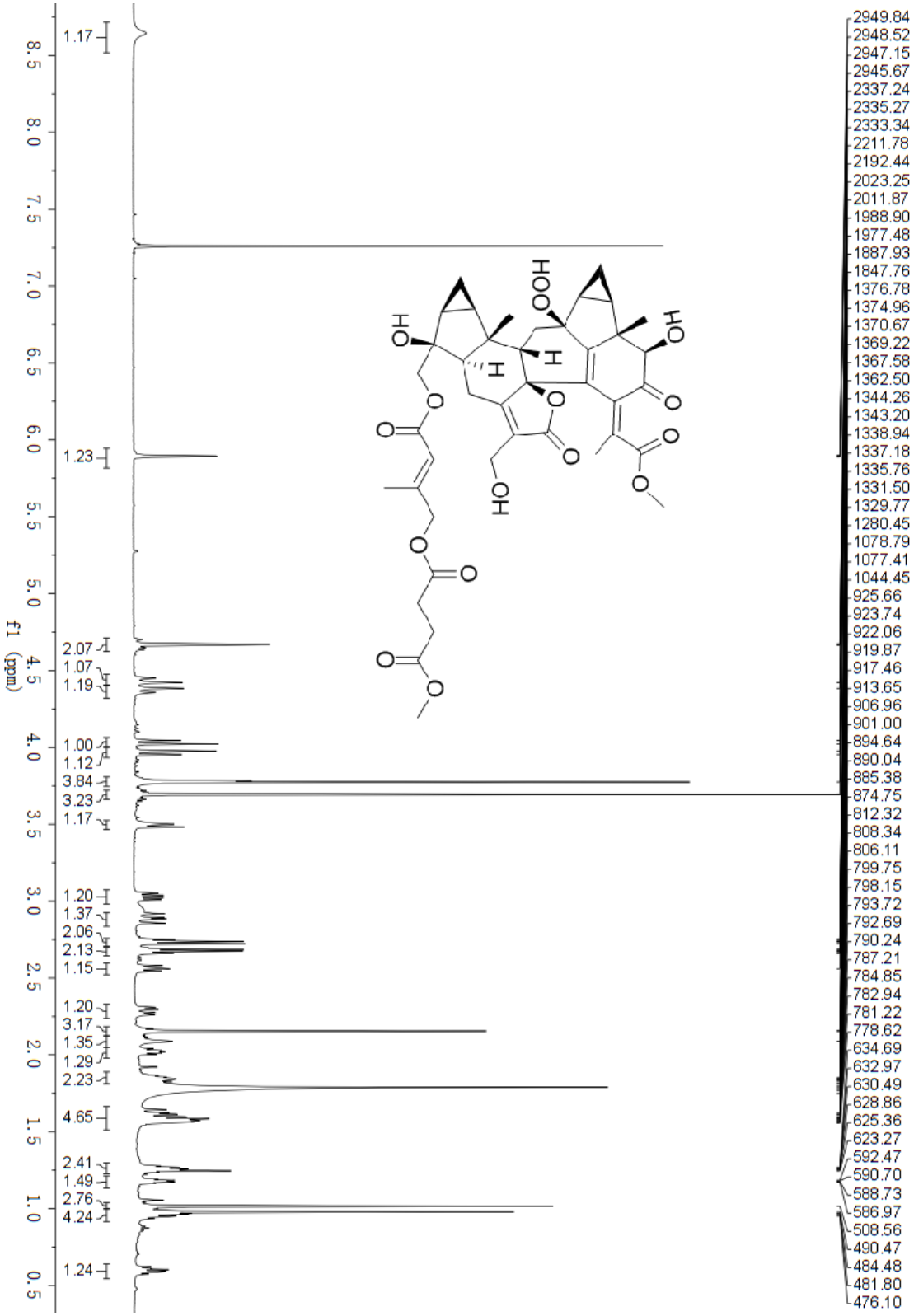


Figure S29. ^{13}C NMR spectrum of fortunilide D (4) in $CDCl_3$

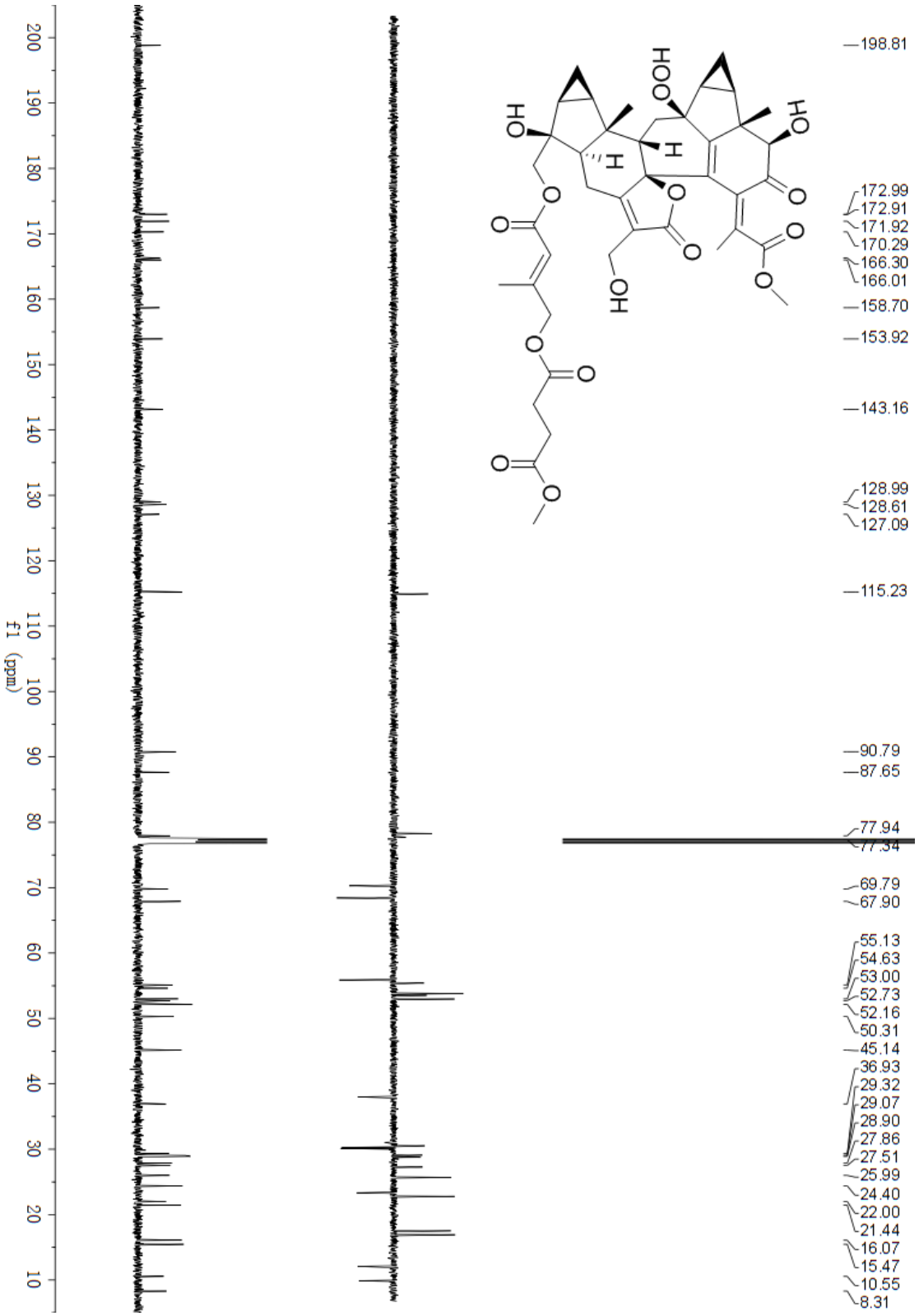


Figure S30. HSQC spectrum of fortunilide D (4) in $CDCl_3$

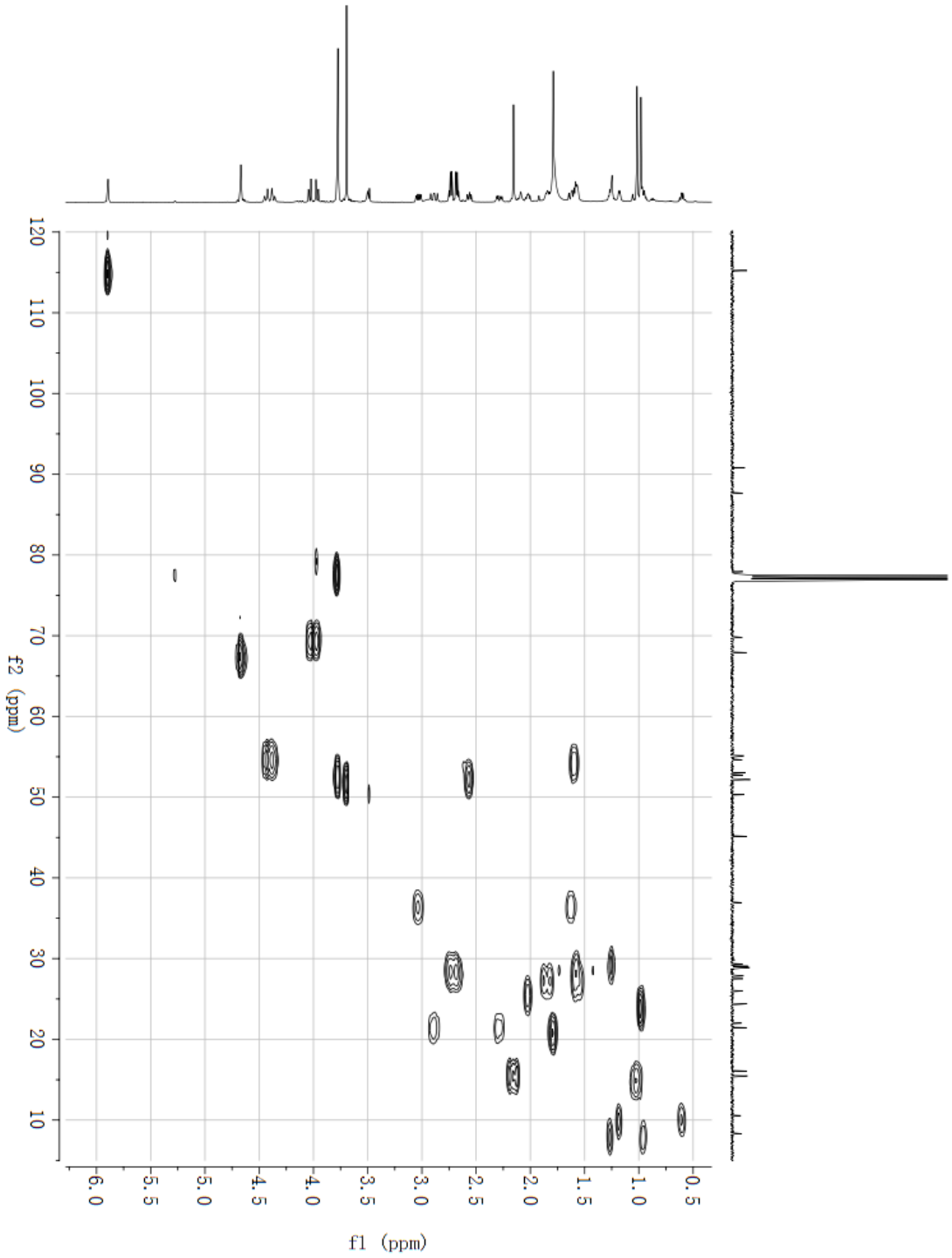


Figure S31. HMBC spectrum of fortunilide D (4) in $CDCl_3$

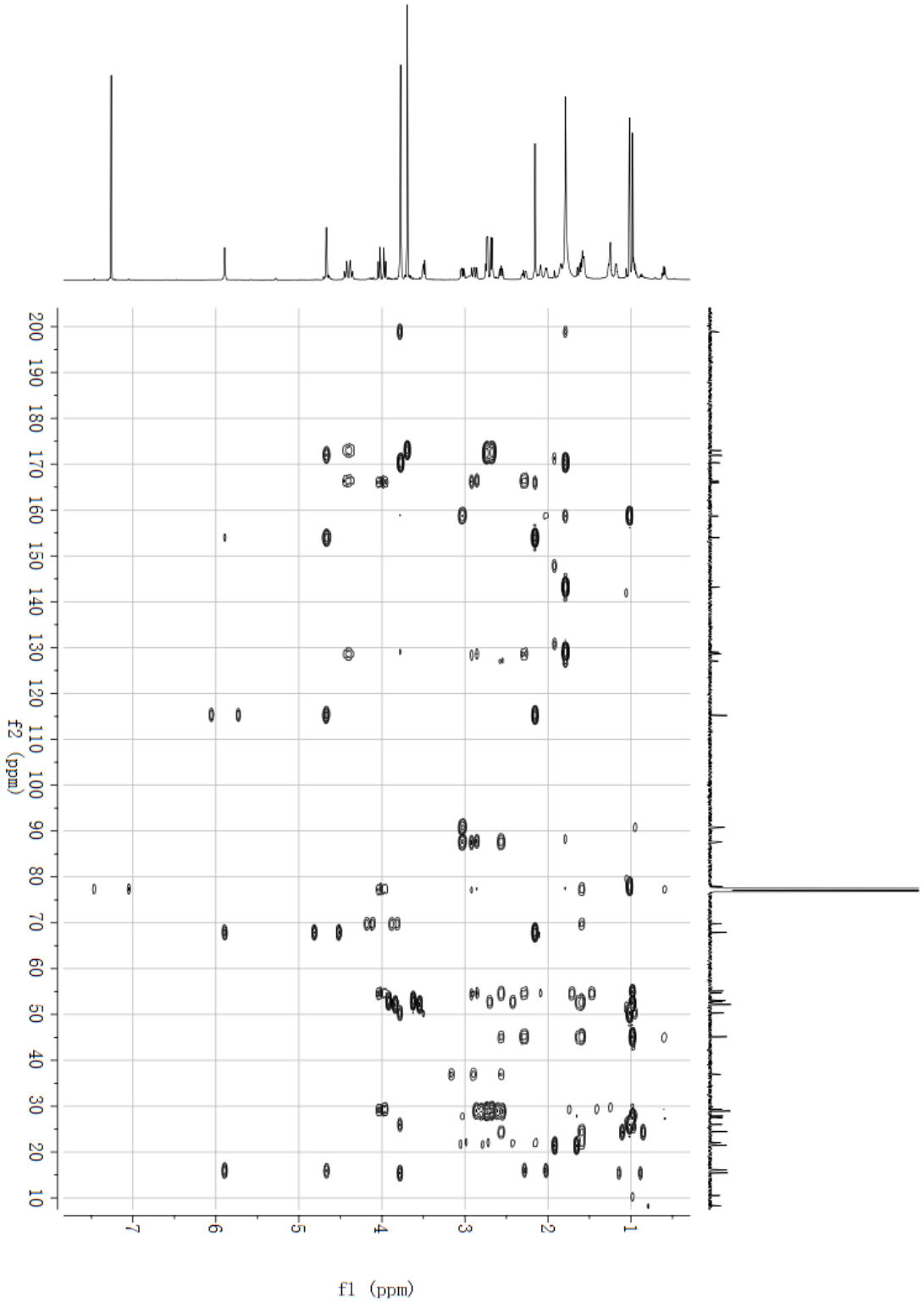


Figure S32. ROESY spectrum of fortunilide D (4)

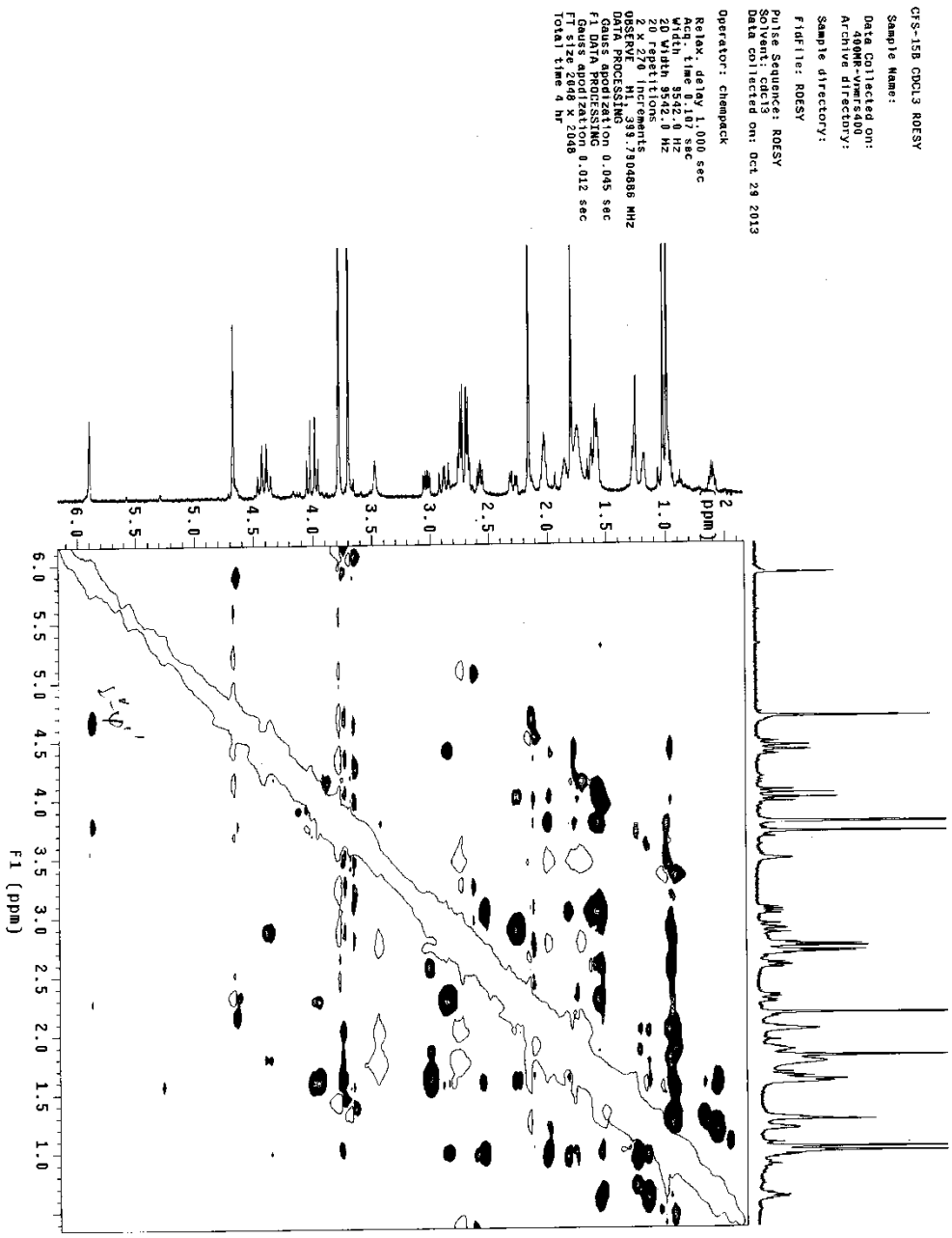


Figure S33. (+)-ESIMS spectrum of fortunilide D (4)

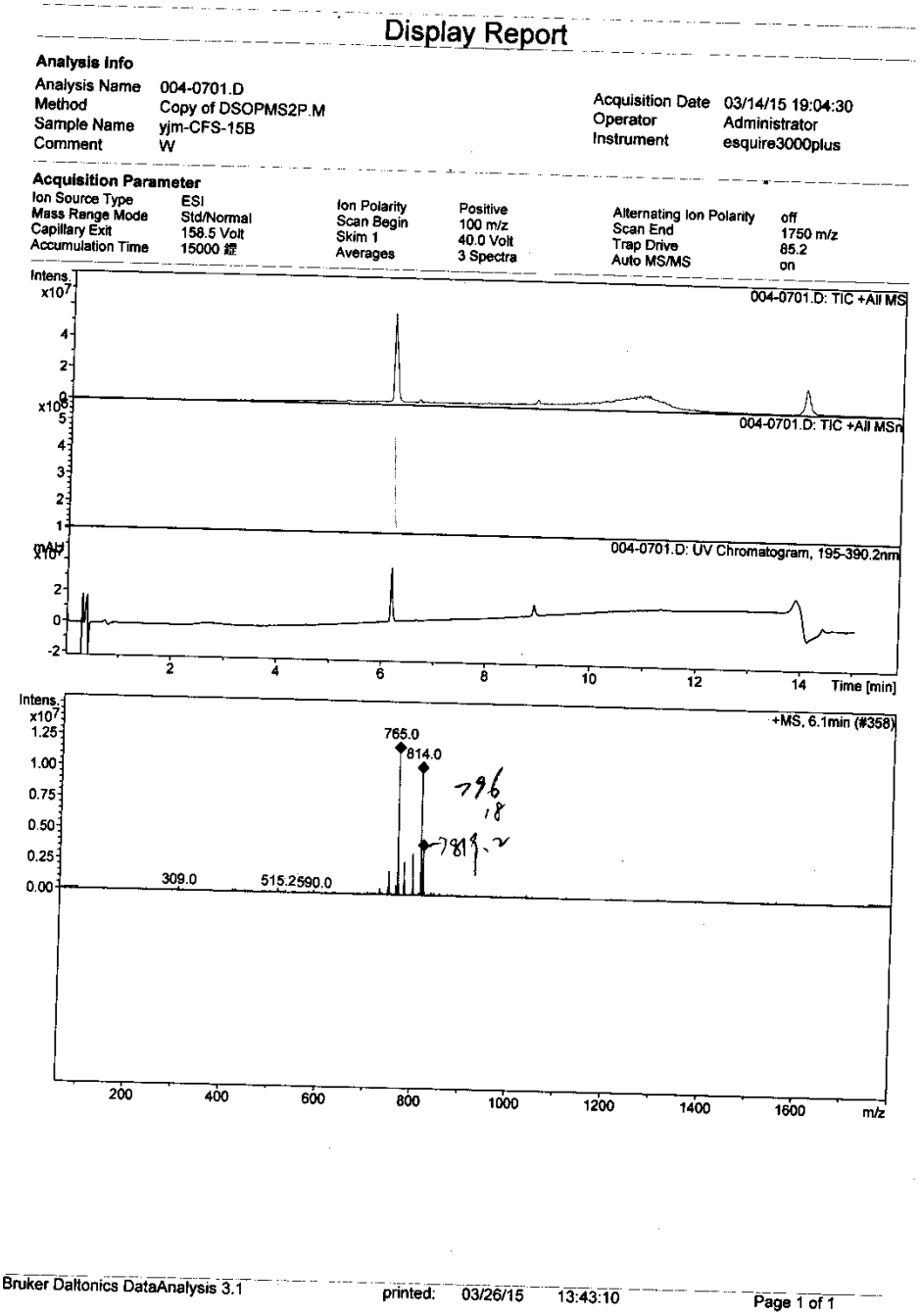


Figure S34. (–)-ESIMS spectrum of fortunilide D (4)

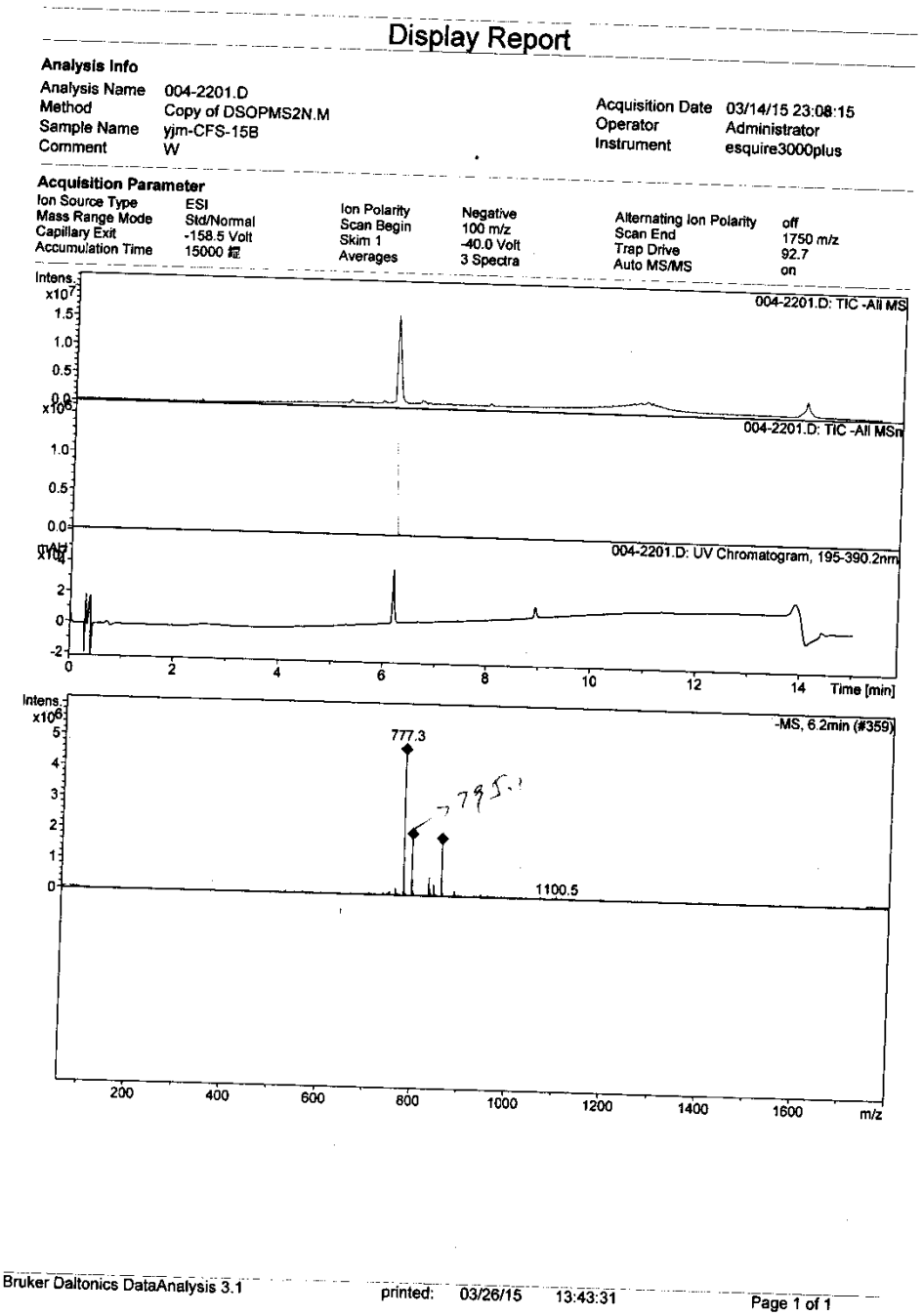


Figure S35. (+)-HRESIMS spectrum of fortunilide D (4)

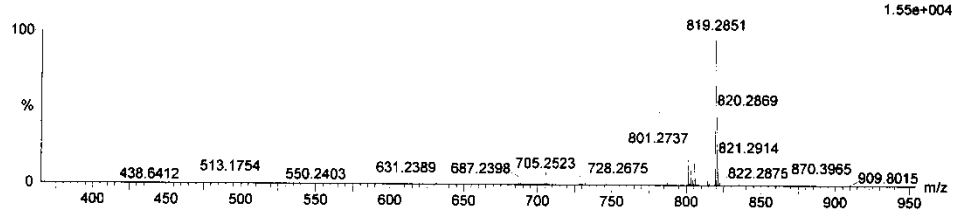
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 4.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
352 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 O: 0-20 Na: 0-1

CFS-15B LCT PXE KE324 13-Sep-2013 13:42:58

CFS-15B_0913 4 (0.070) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (4:21) 1: TOF MS ES+ 1.55e+004



Minimum:				-1.5						
Maximum:		3.0	4.0	50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
819.2851	819.2840	1.1	1.3	17.5	61.4	0.0	C41	H48	O16	Na
	819.2864	-1.3	-1.6	20.5	65.7	4.3	C43	H47	O16	
	819.2875	-2.4	-2.9	39.5	73.4	11.9	C59	H40	O3	Na

Figure S36. IR spectrum of fortunilide D (4)

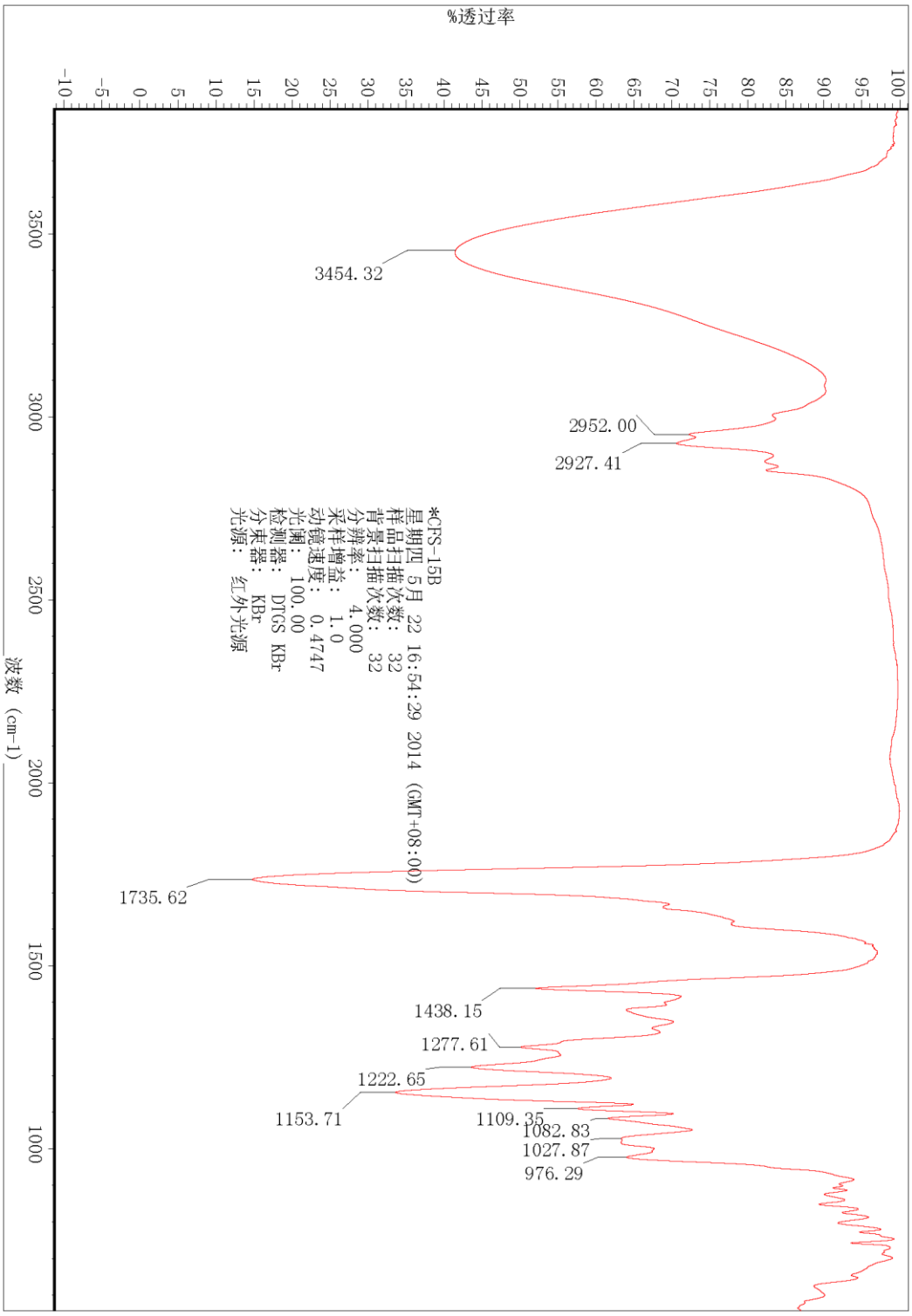


Figure S37. ^{1}H NMR spectrum of fortunilide E (5) in $CDCl_3$

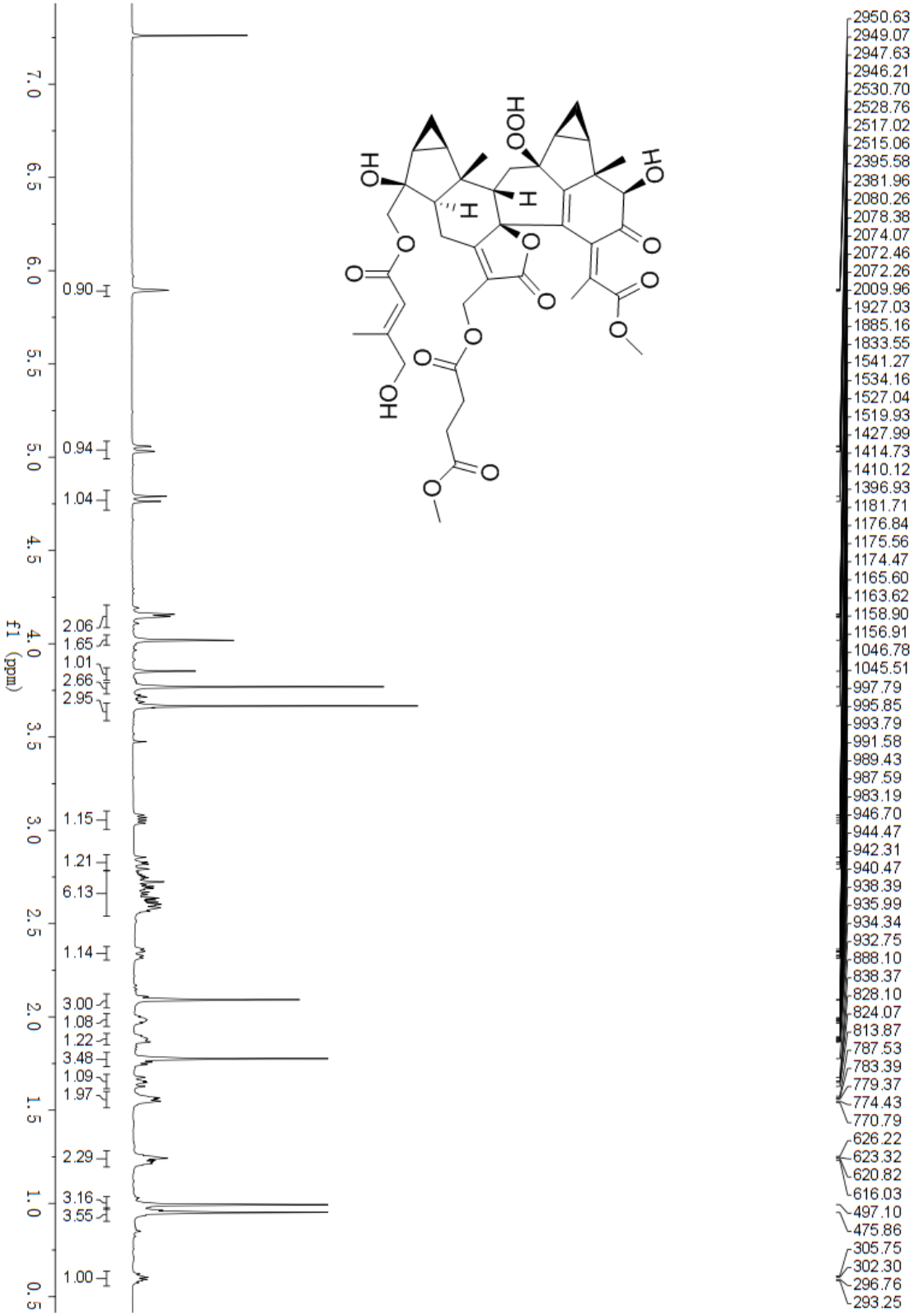


Figure S38. ^{13}C NMR spectrum of fortunilide E (5) in $CDCl_3$

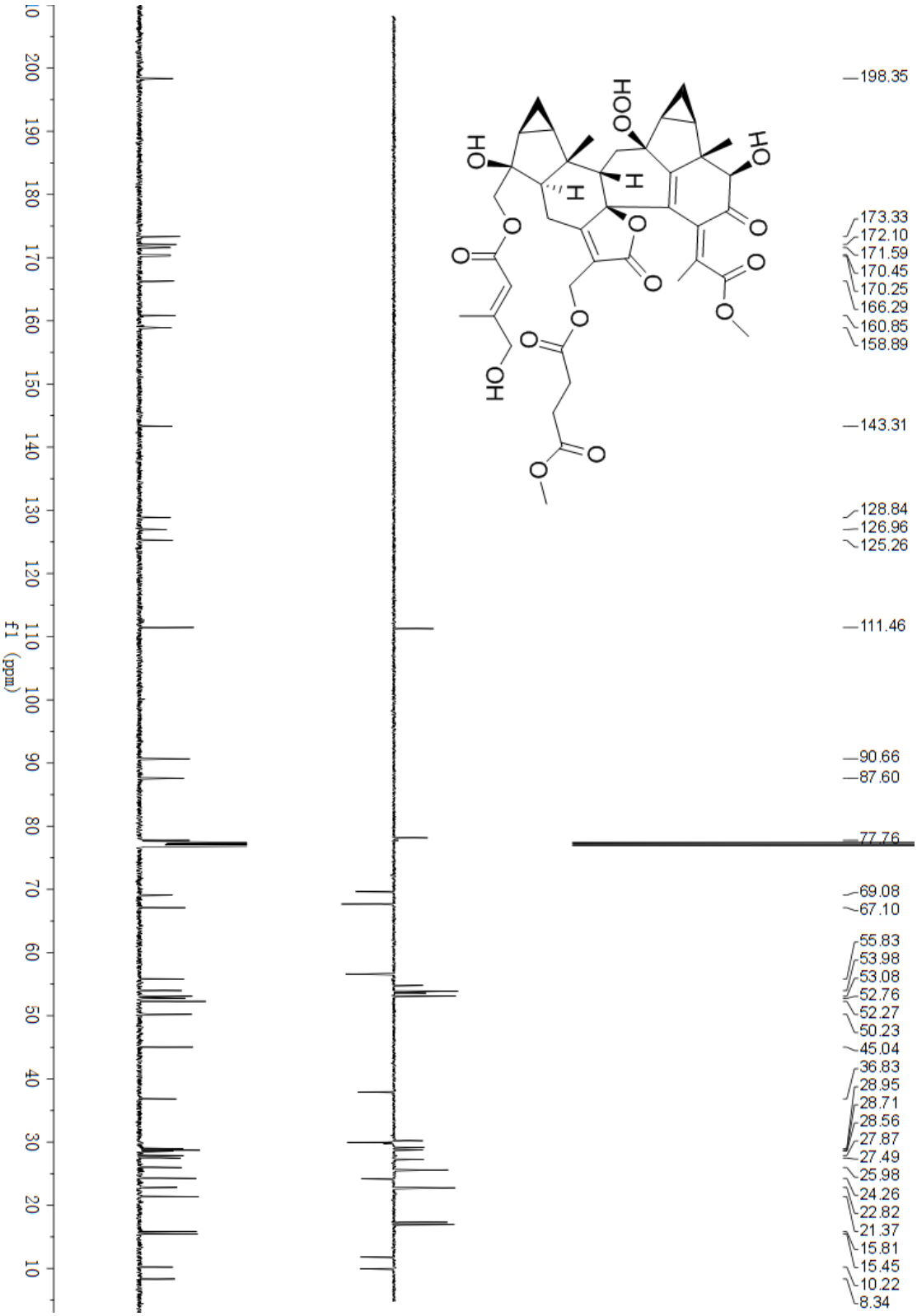


Figure S39. HSQC spectrum of fortunilide E (5) in $CDCl_3$

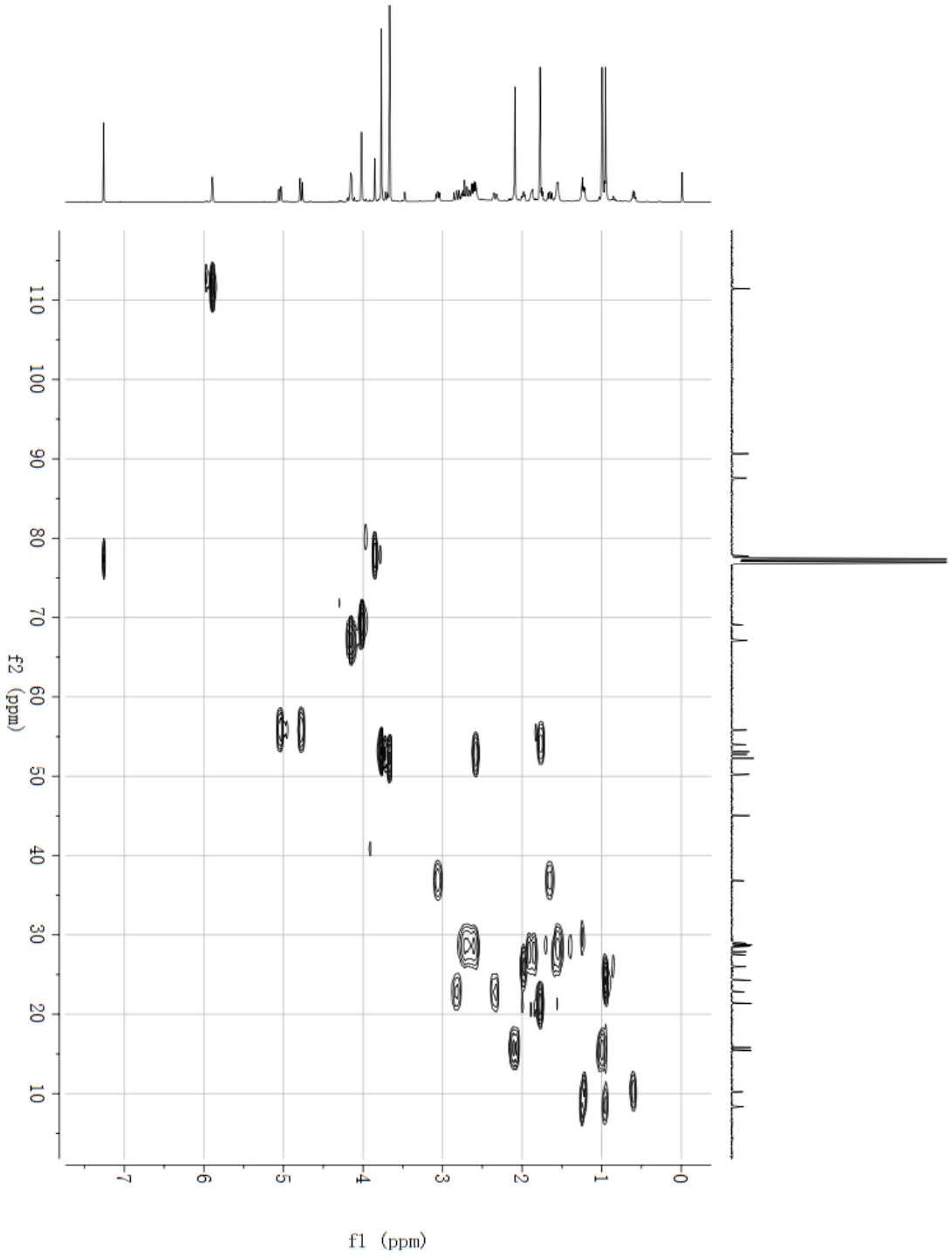


Figure S40. HMBC spectrum of fortunilide E (5) in $CDCl_3$

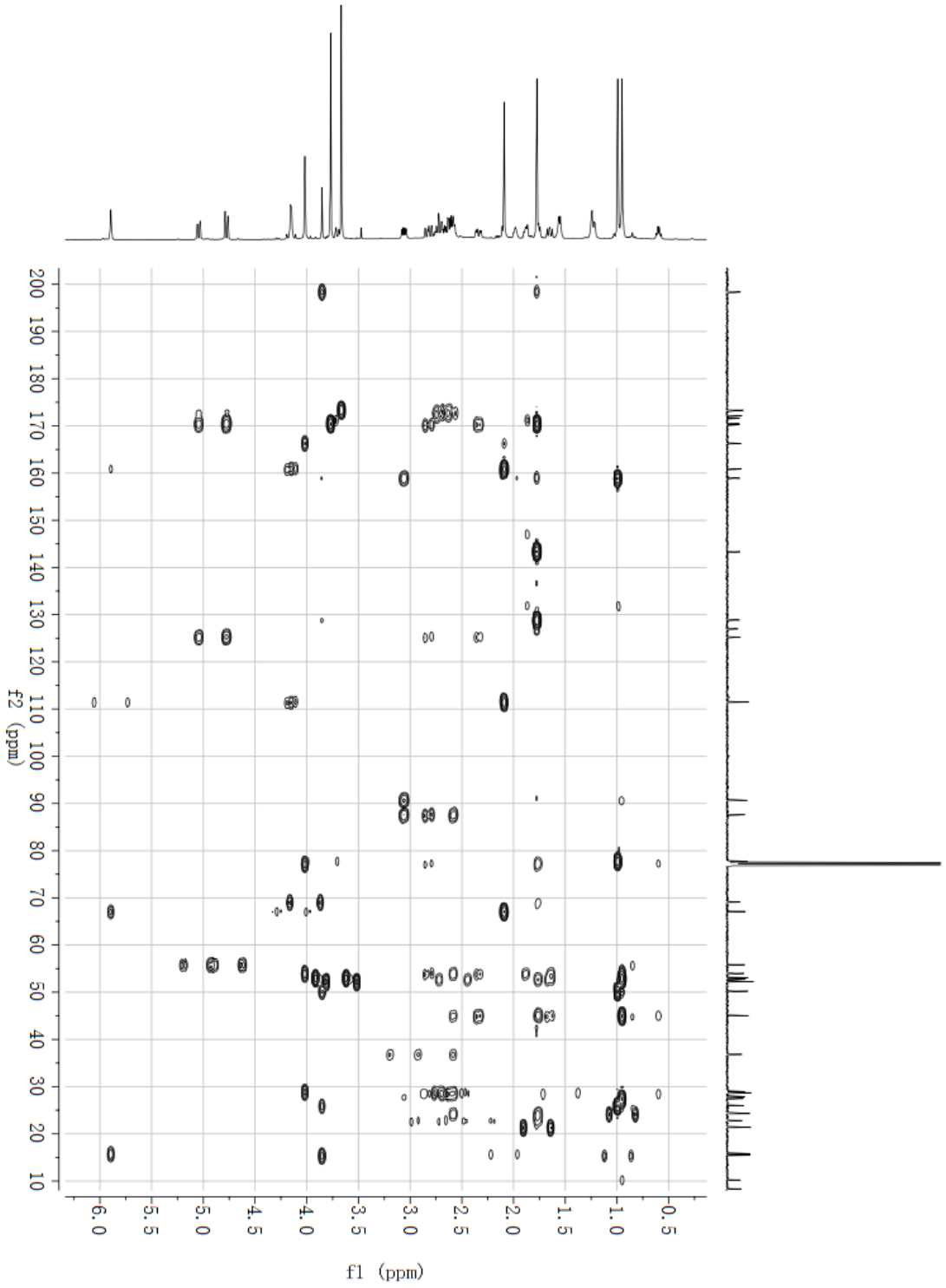


Figure S41. ROESY spectrum of fortunilide E (5)

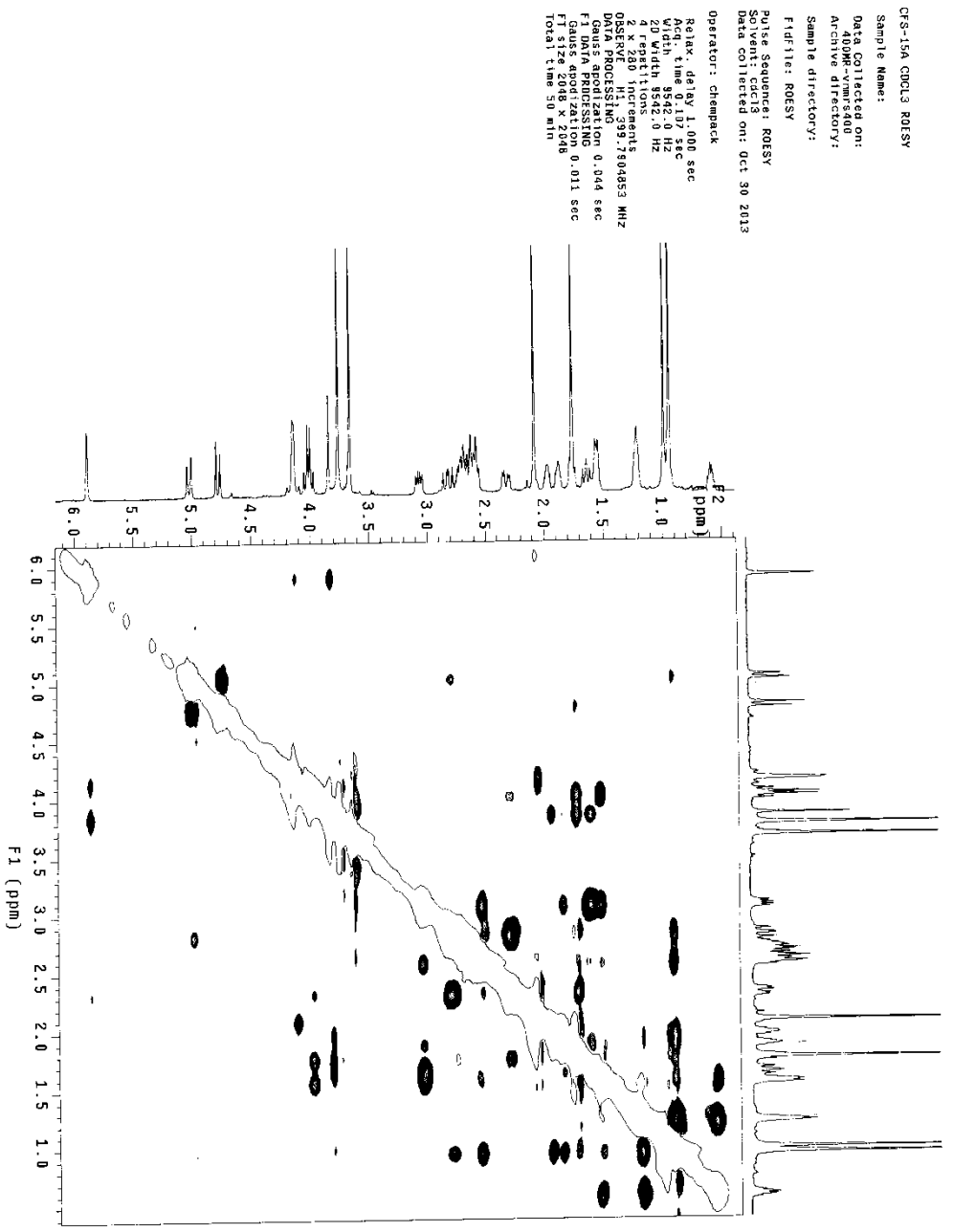


Figure S42. (+)-ESIMS spectrum of fortunilide E (5)

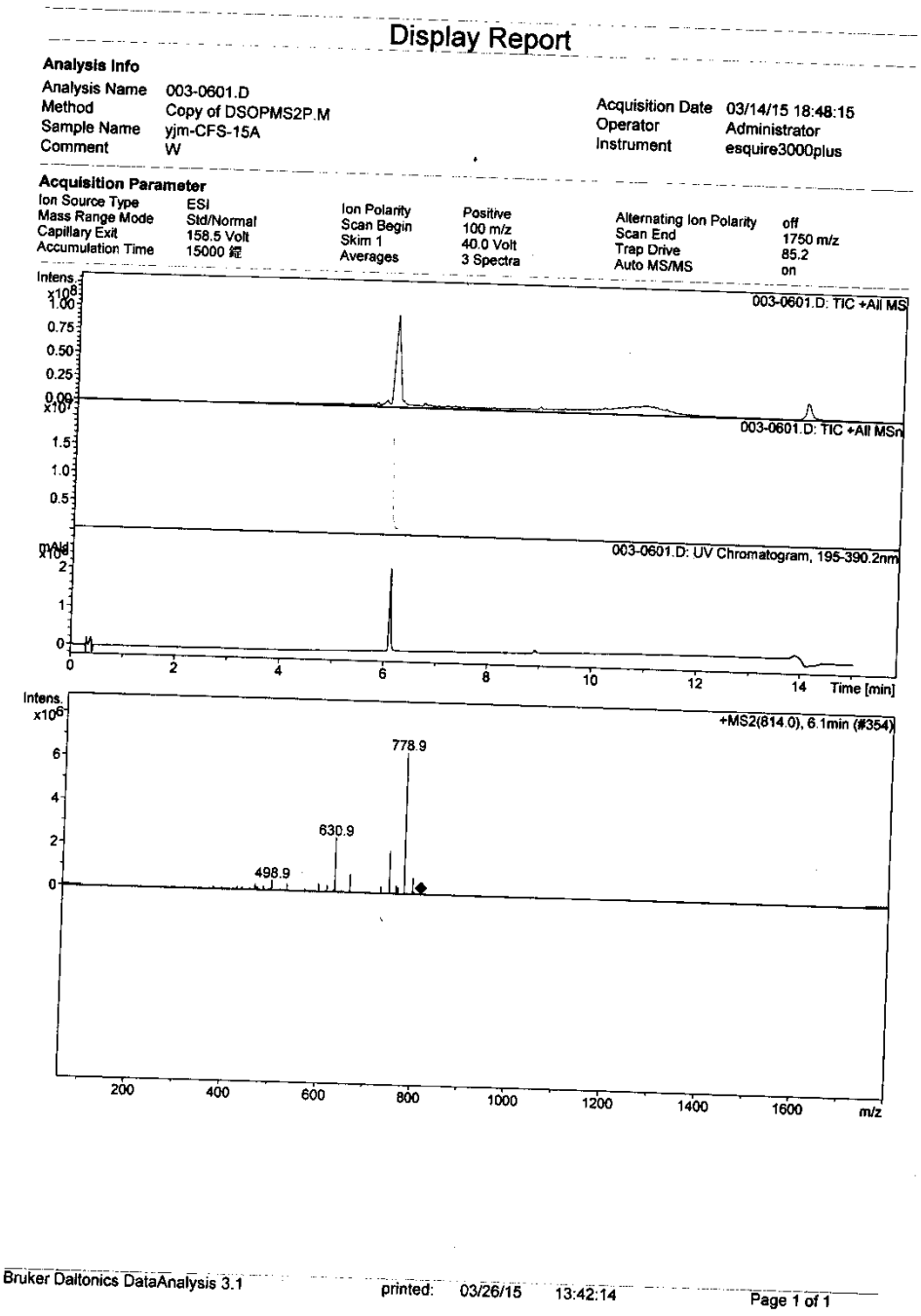


Figure S43. (–)-ESIMS spectrum of fortunilide E (5)

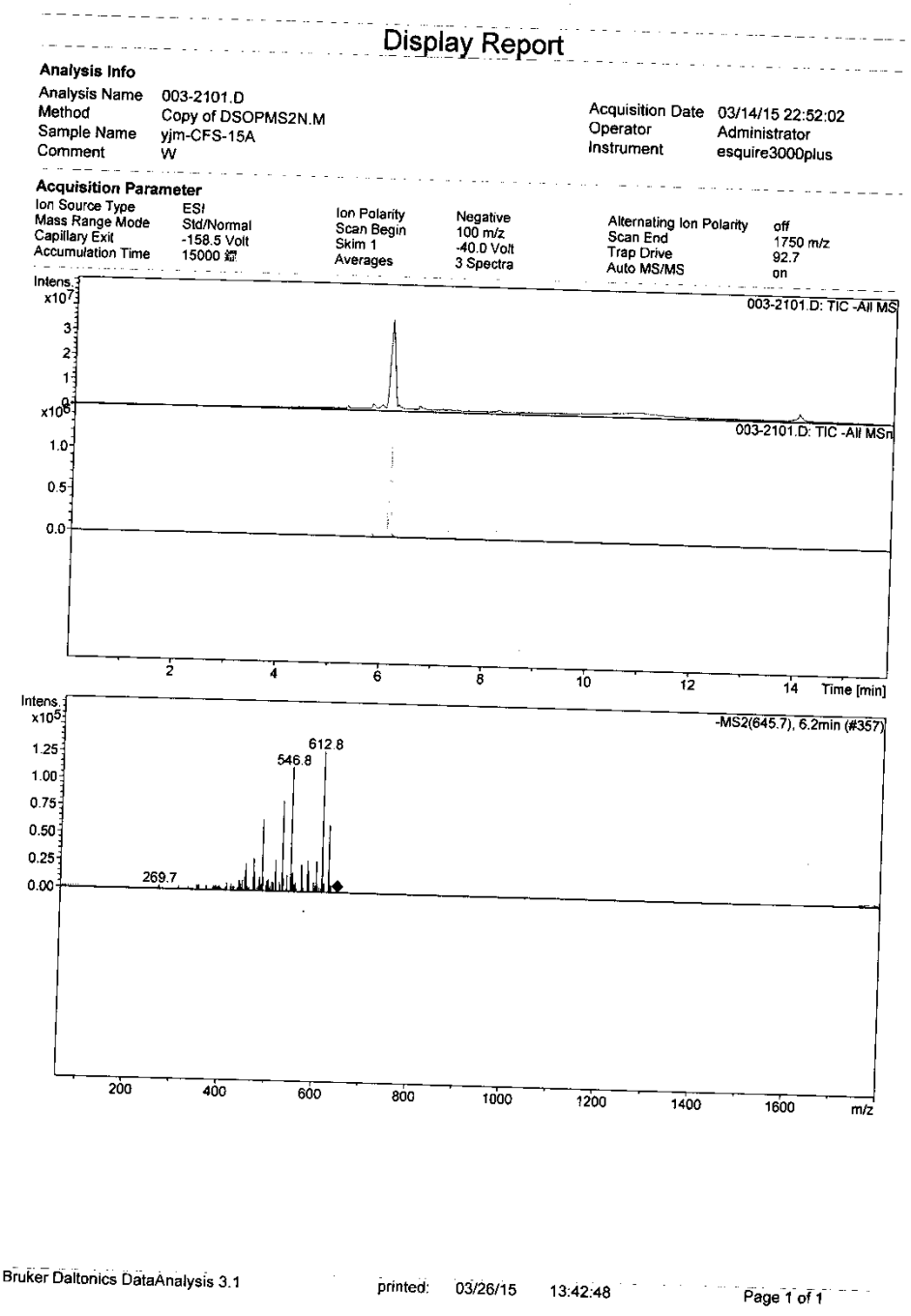


Figure S44. (+)-HRESIMS spectrum of fortunilide E (5)

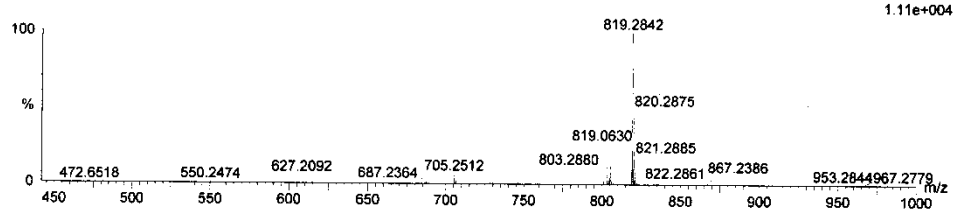
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 4.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
352 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 O: 0-20 Na: 0-1

CFS-15A LCT PXE KE324 13-Sep-2013 13:38:06

CFS-15A_0913 4 (0.070) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (2:19) 1: TOF MS ES+ 1.11e+004



Minimum:				-1.5			
Maximum:		3.0	4.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
819.2842	819.2840	0.2	0.2	17.5	61.1	0.0	C41 H48 O16 Na
	819.2864	-2.2	-2.7	20.5	65.5	4.4	C43 H47 O16

Figure S45. IR spectrum of fortunilide E (5)

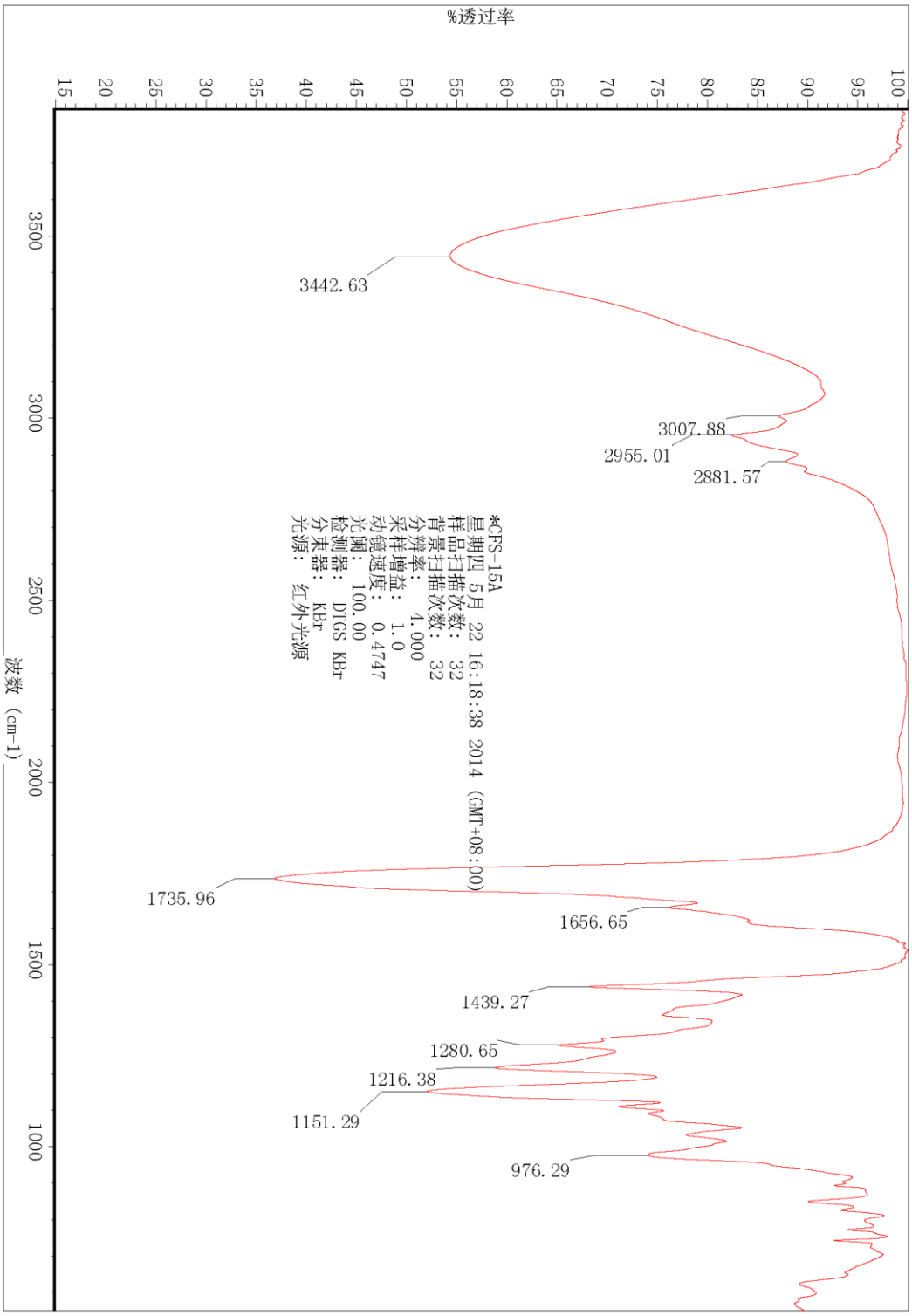


Figure S46. ^{1}H NMR spectrum of fortunilide F (6) in CD_3OD

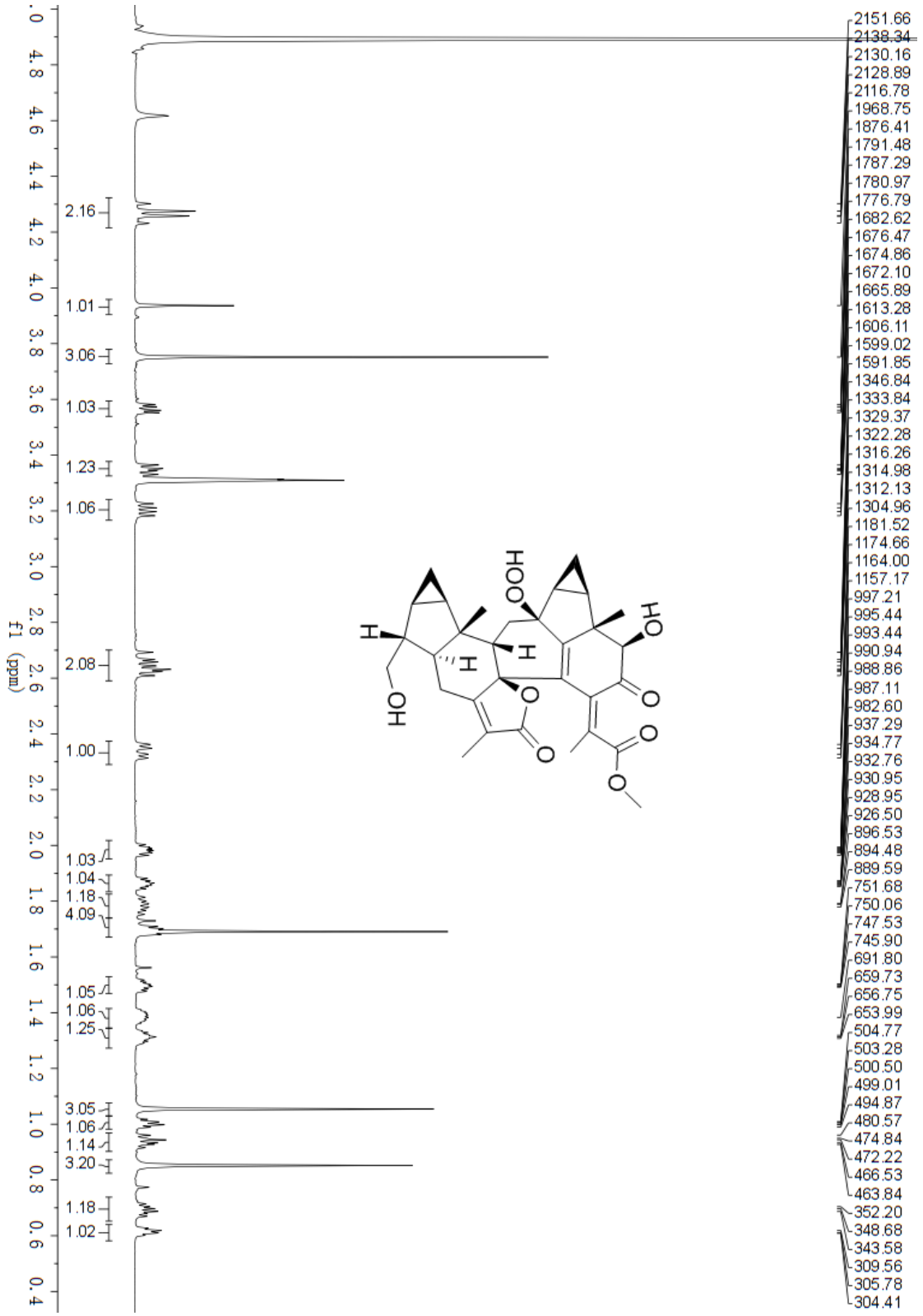


Figure S47. ^{13}C NMR spectrum of fortunilide F (6) in CD_3OD

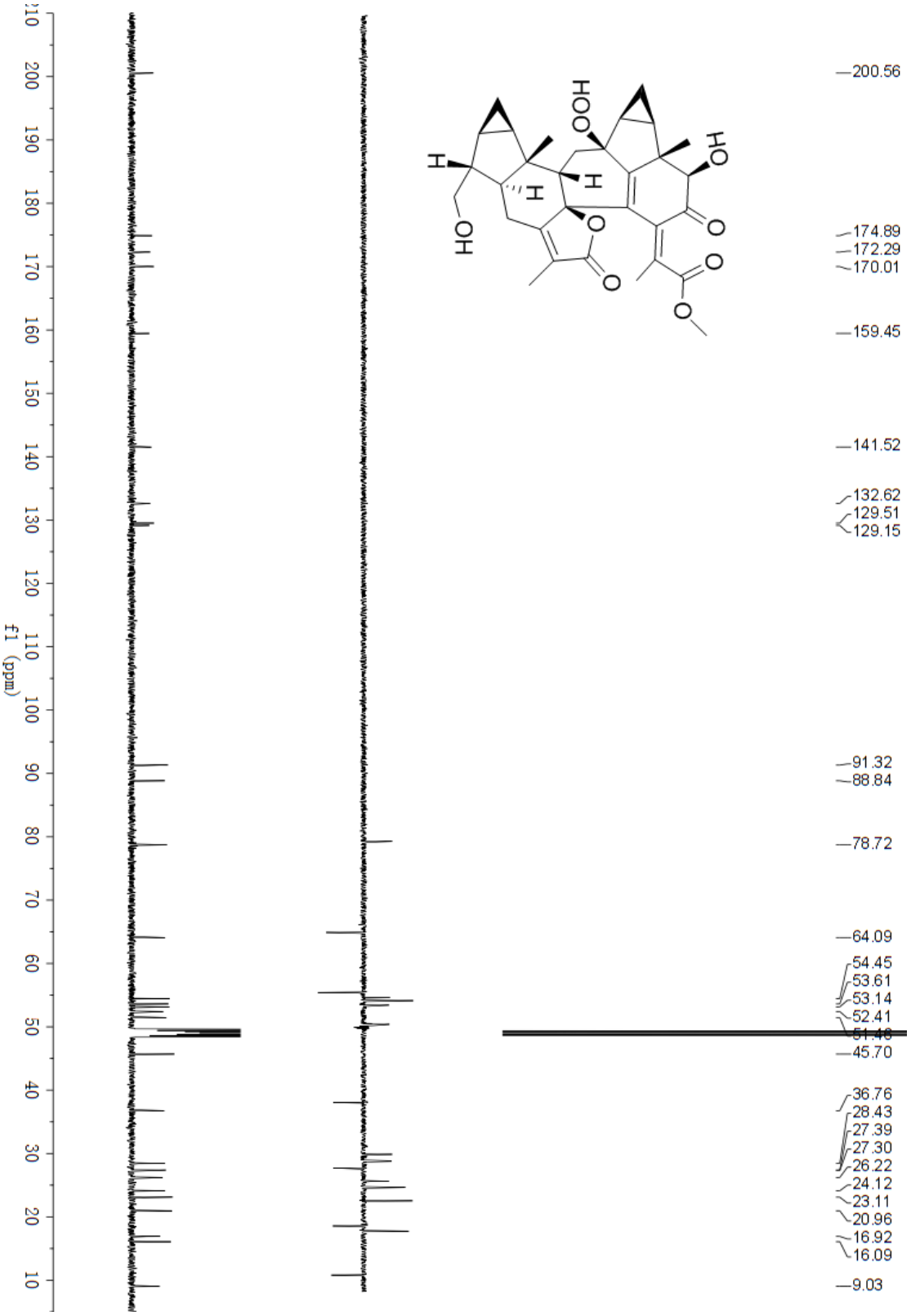


Figure S48. HSQC spectrum of fortunilide F (6) in CD_3OD

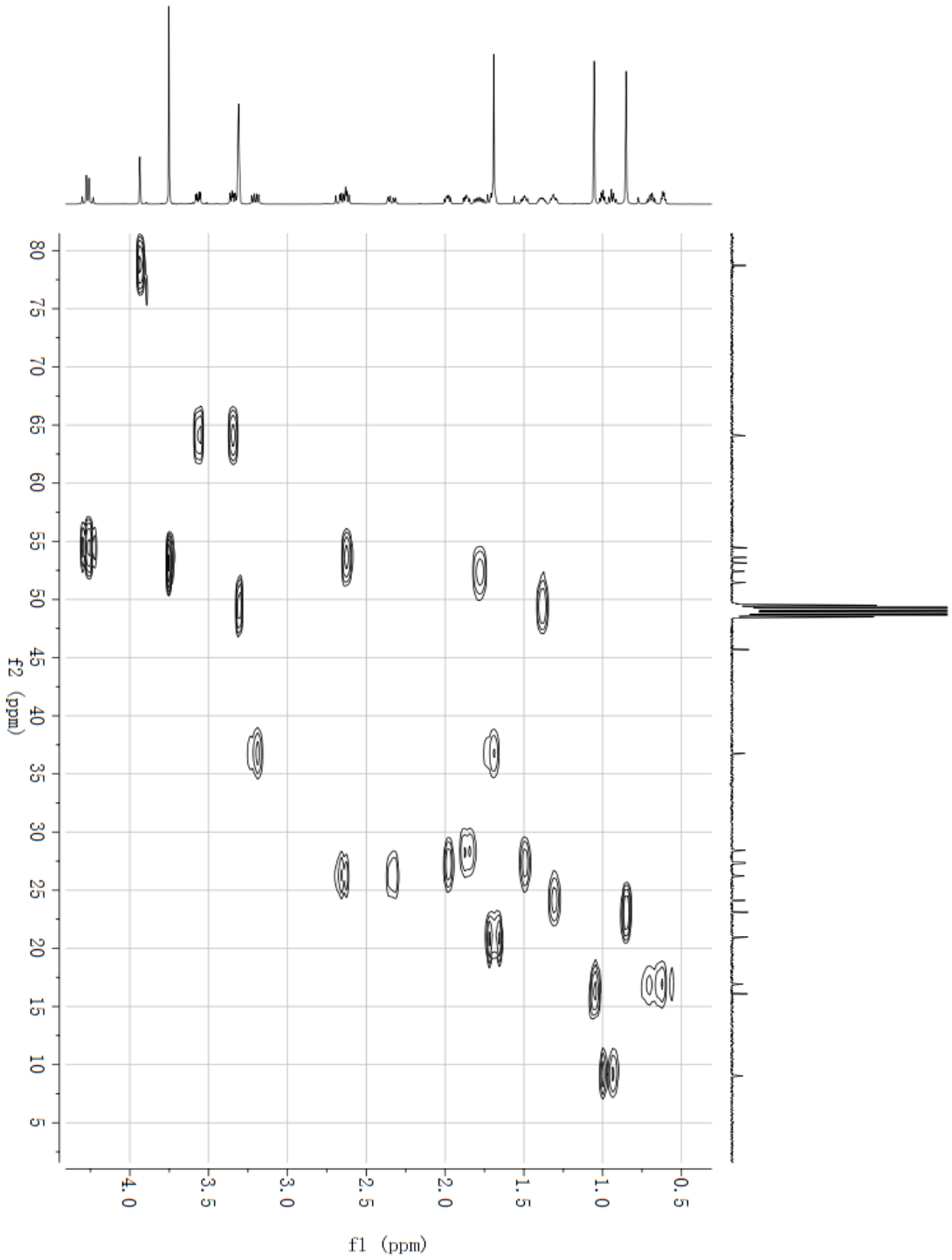


Figure S49. HMBC spectrum of fortunilide F (6) in CD_3OD

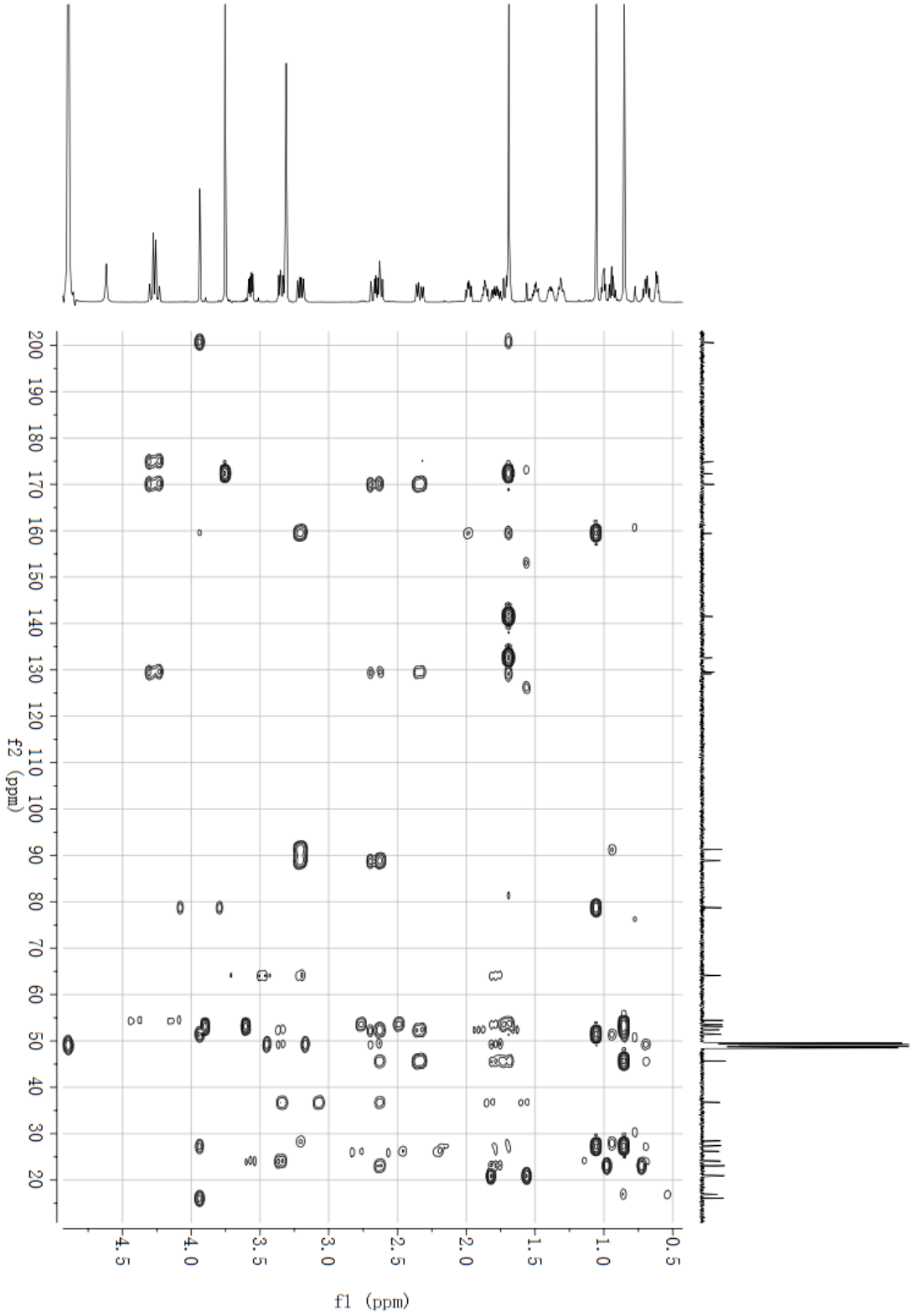


Figure S50. ROESY spectrum of fortunilide F (6)

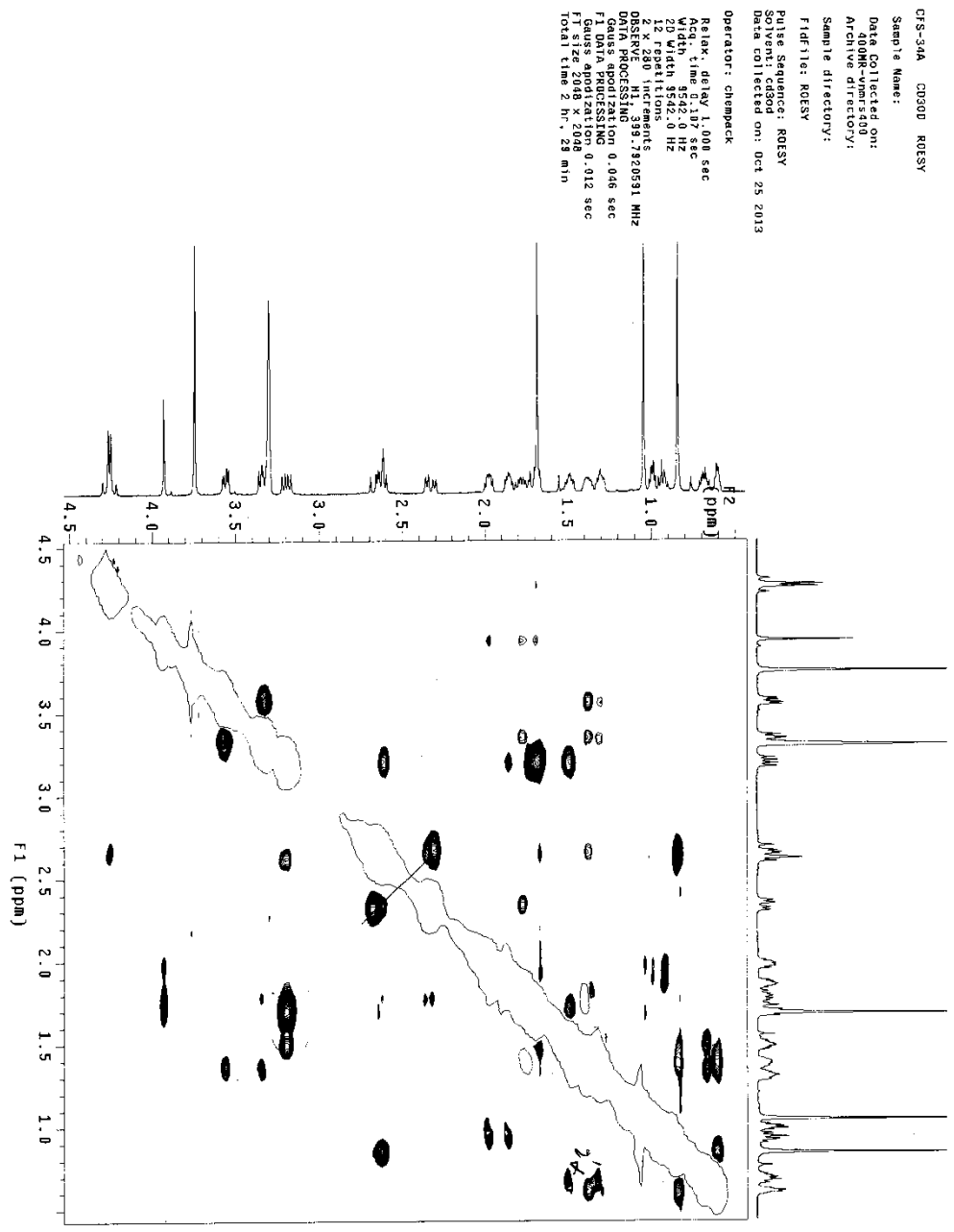


Figure S51. (+)-ESIMS spectrum of fortunilide F (6)

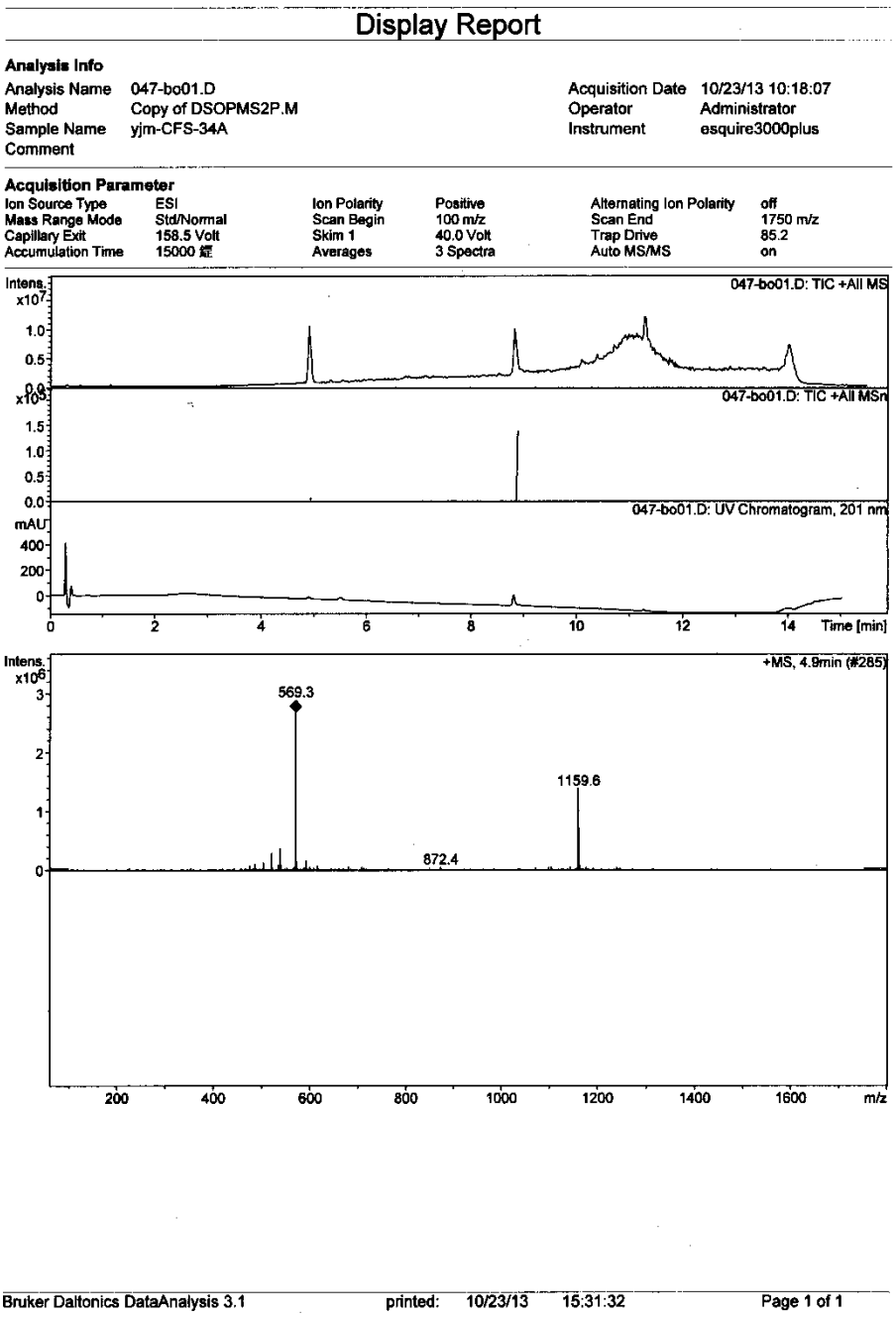


Figure S52. (–)-ESIMS spectrum of fortunilide F (6)

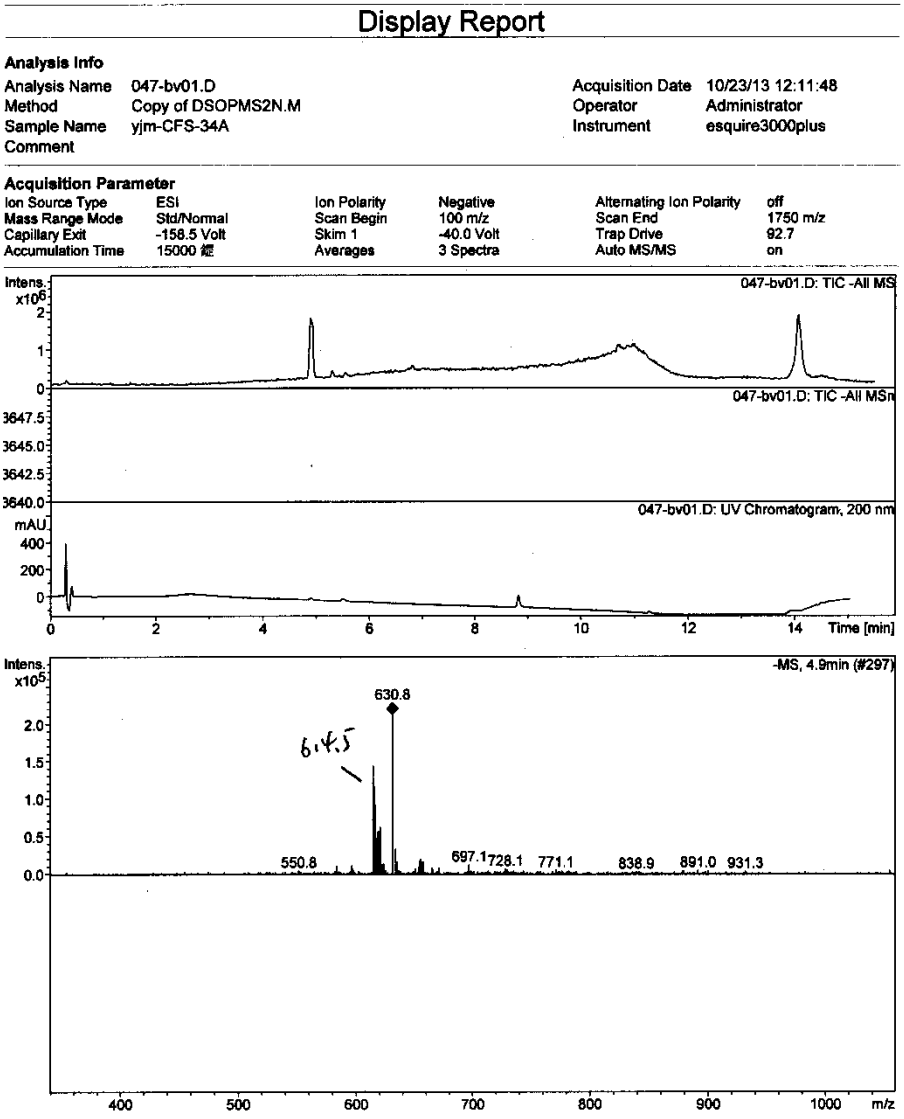


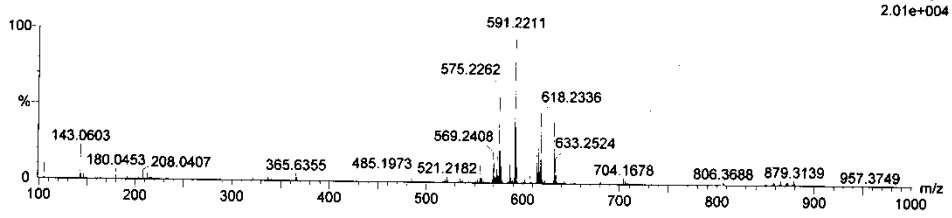
Figure S53. (+)-HRESIMS spectrum of fortunilide F (6)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
239 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 O: 0-20 Na: 0-1
CFS-34A LCT PXE KE324 31-Oct-2013 14:40:52

CFS-34A_1031 37 (0.776) AM2 (Ar,10500.0,0.00,0.70); ABS; Cm (30:51) 1: TOF MS ES+ 2.01e+004



Minimum:				-1.5			
Maximum:		5.0	3.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
591.2211	591.2206	0.5	0.8	13.5	108.9	0.0	C31 H36 O10 Na

Figure S54. IR spectrum of fortunilide F (6)

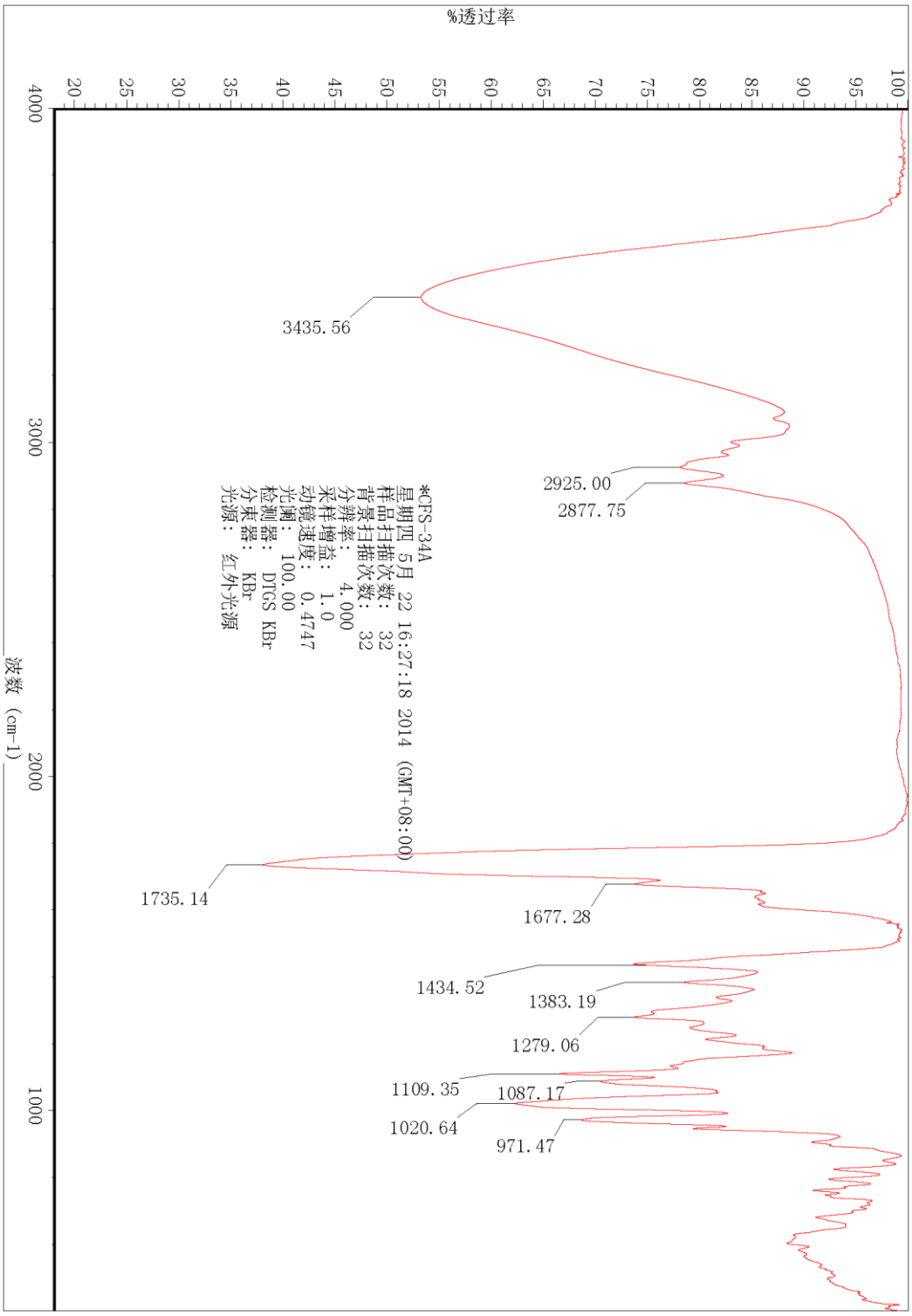


Figure S55. ^{1}H NMR spectrum of fortunilide G (7) in $CDCl_3$

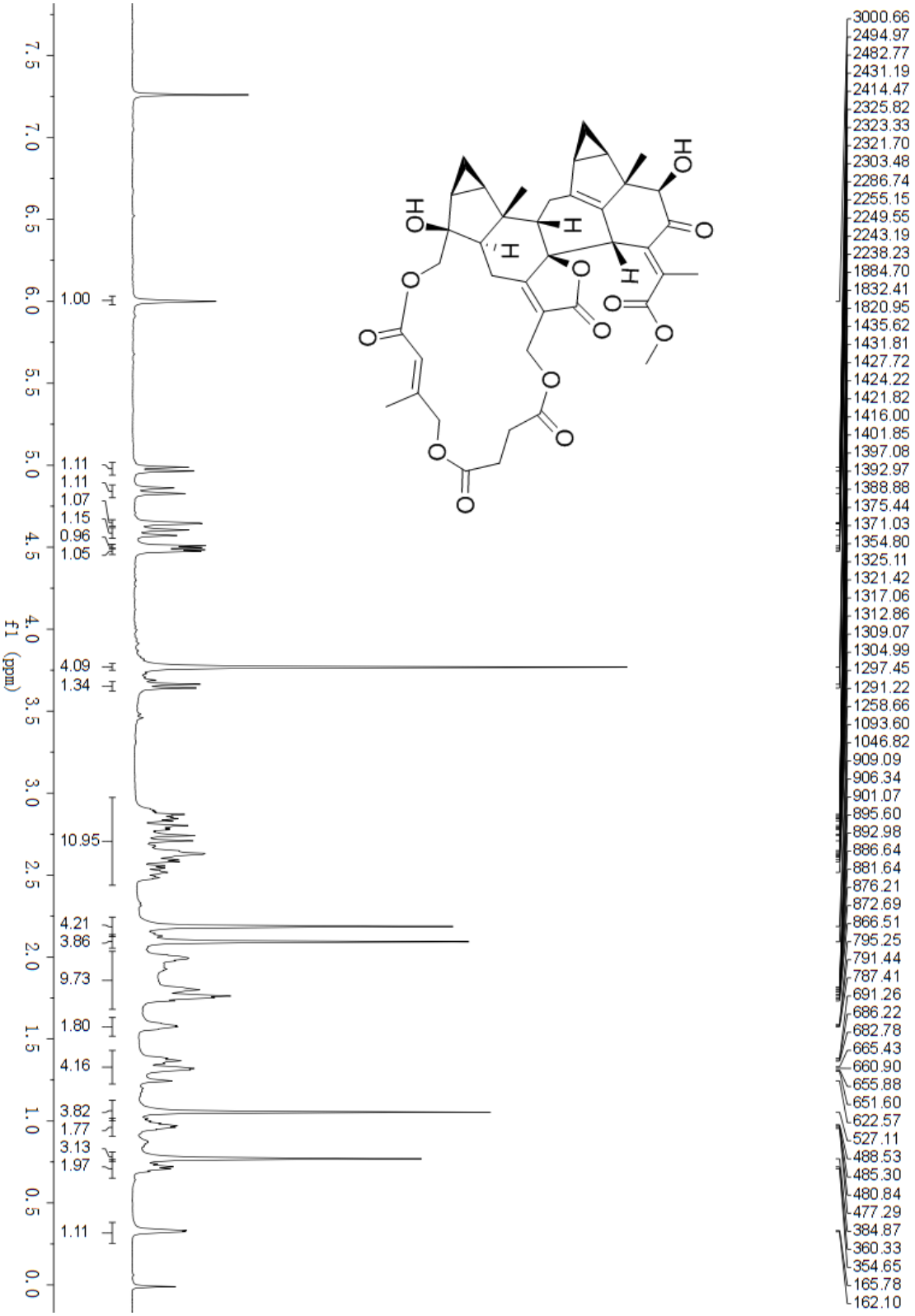


Figure S56. ^{13}C NMR spectrum of fortunilide G (7) in $CDCl_3$

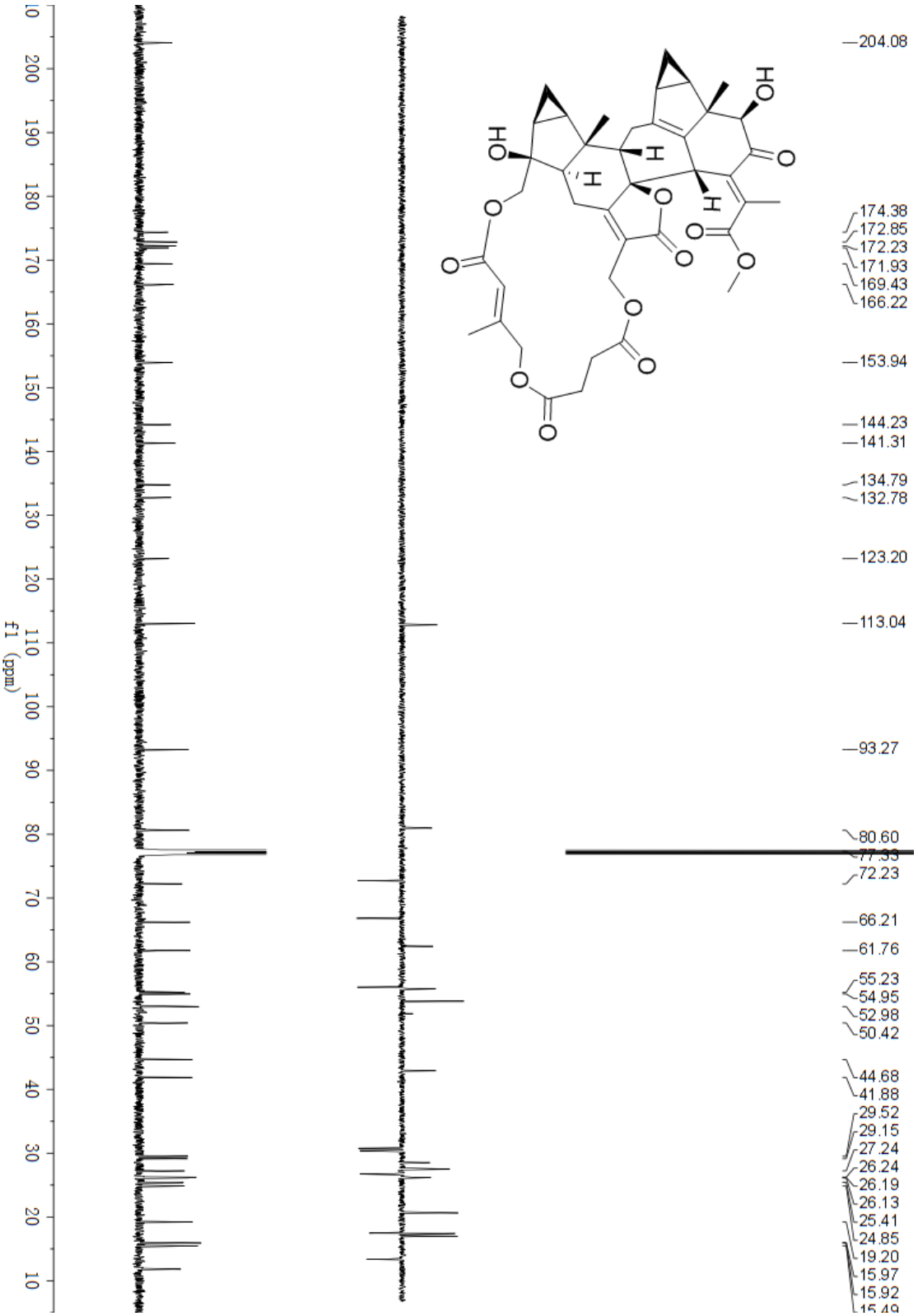


Figure S57. HSQC spectrum of fortunilide G (7) in $CDCl_3$

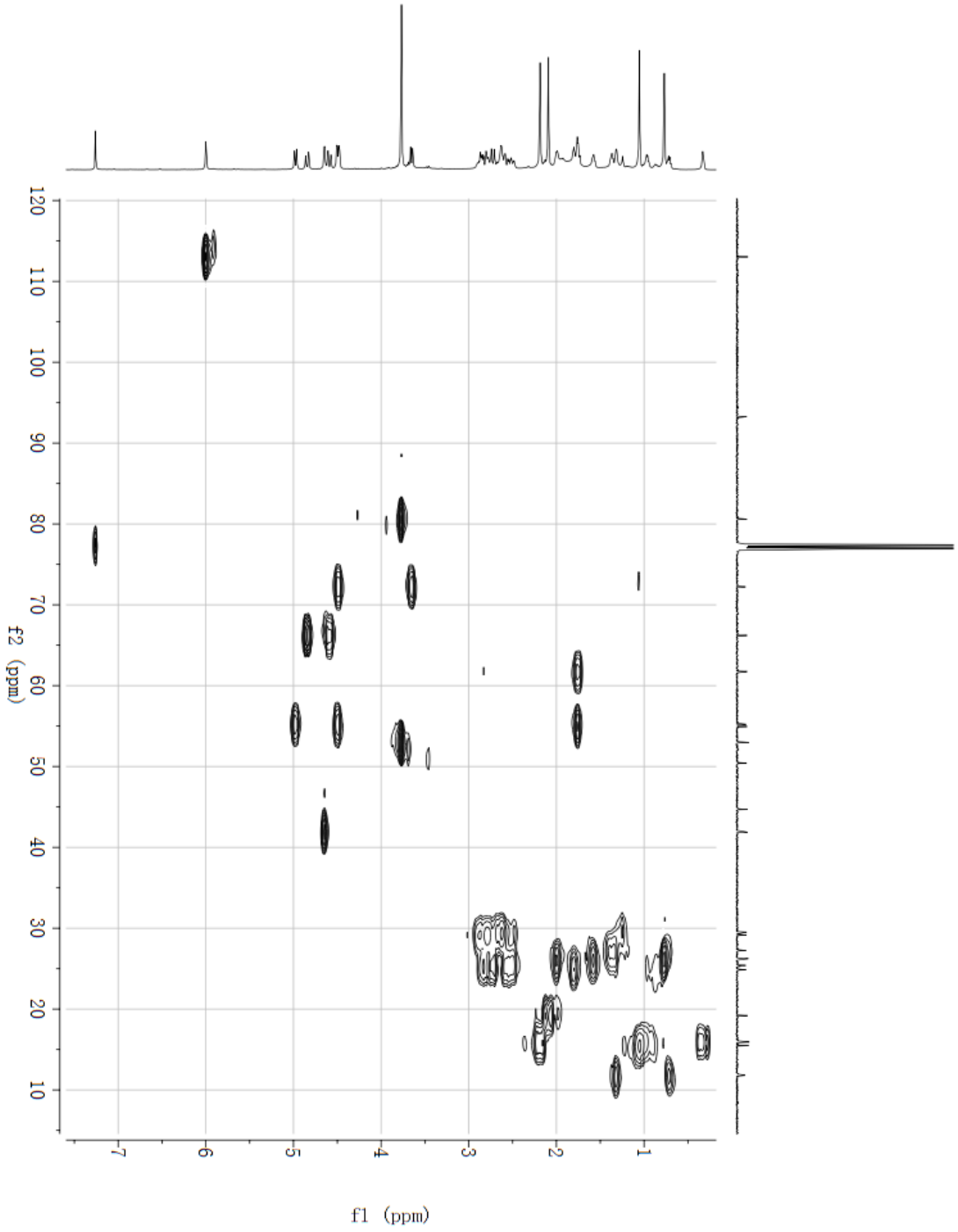


Figure S58. HMBC spectrum of fortunilide G (7) in $CDCl_3$

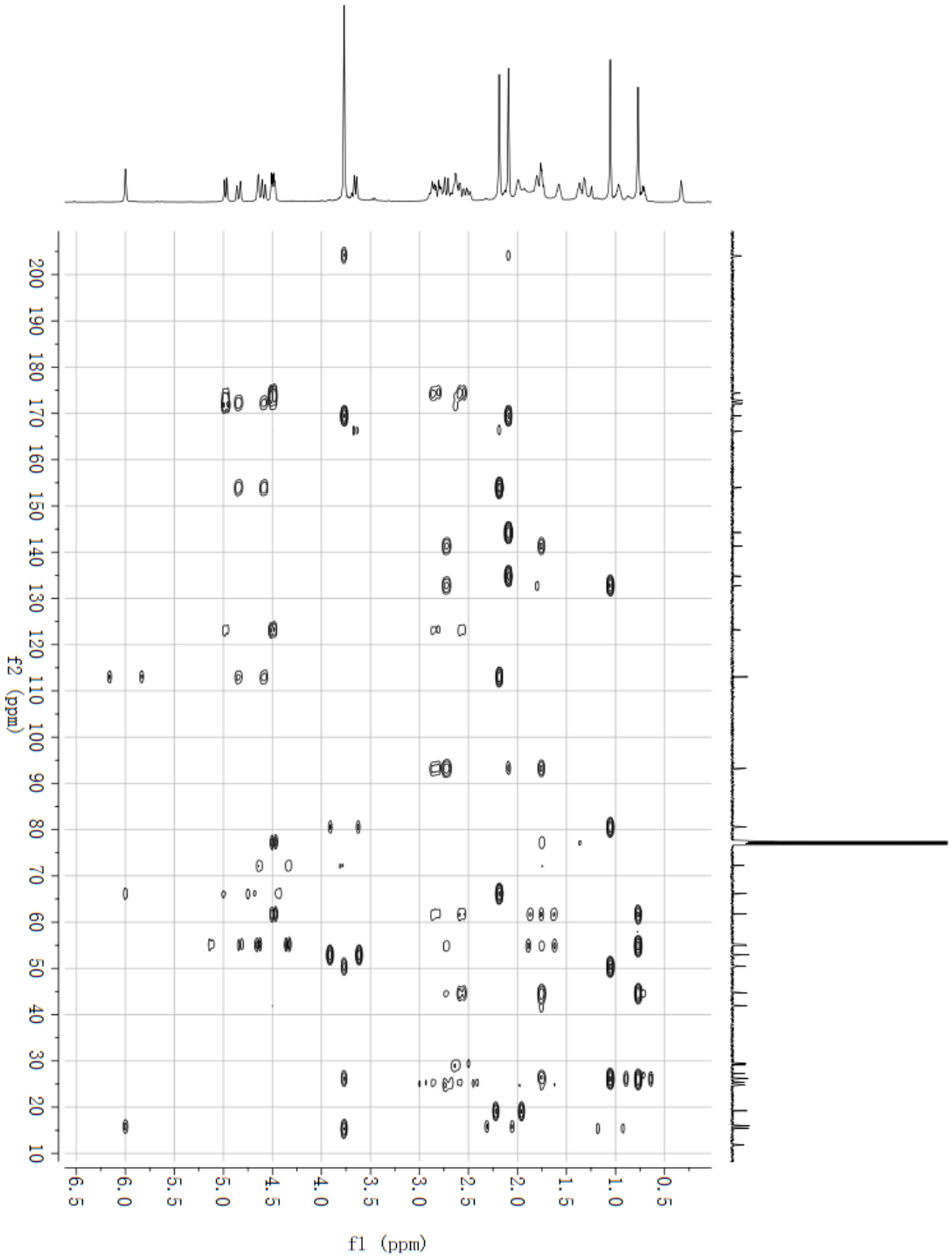


Figure S59. ROESY spectrum of fortunilide G (7)

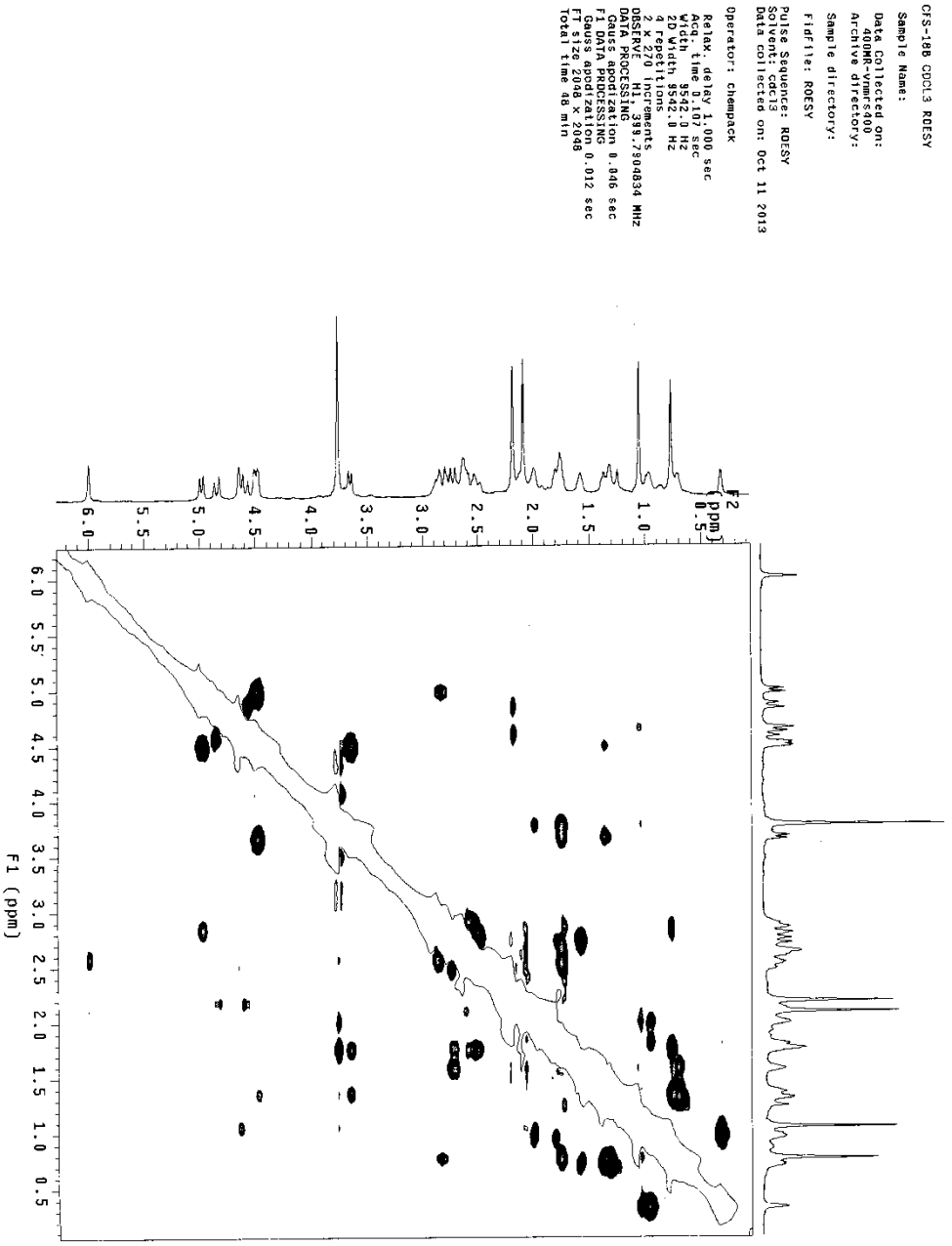


Figure S60. (+)-ESIMS spectrum of fortunilide G (7)

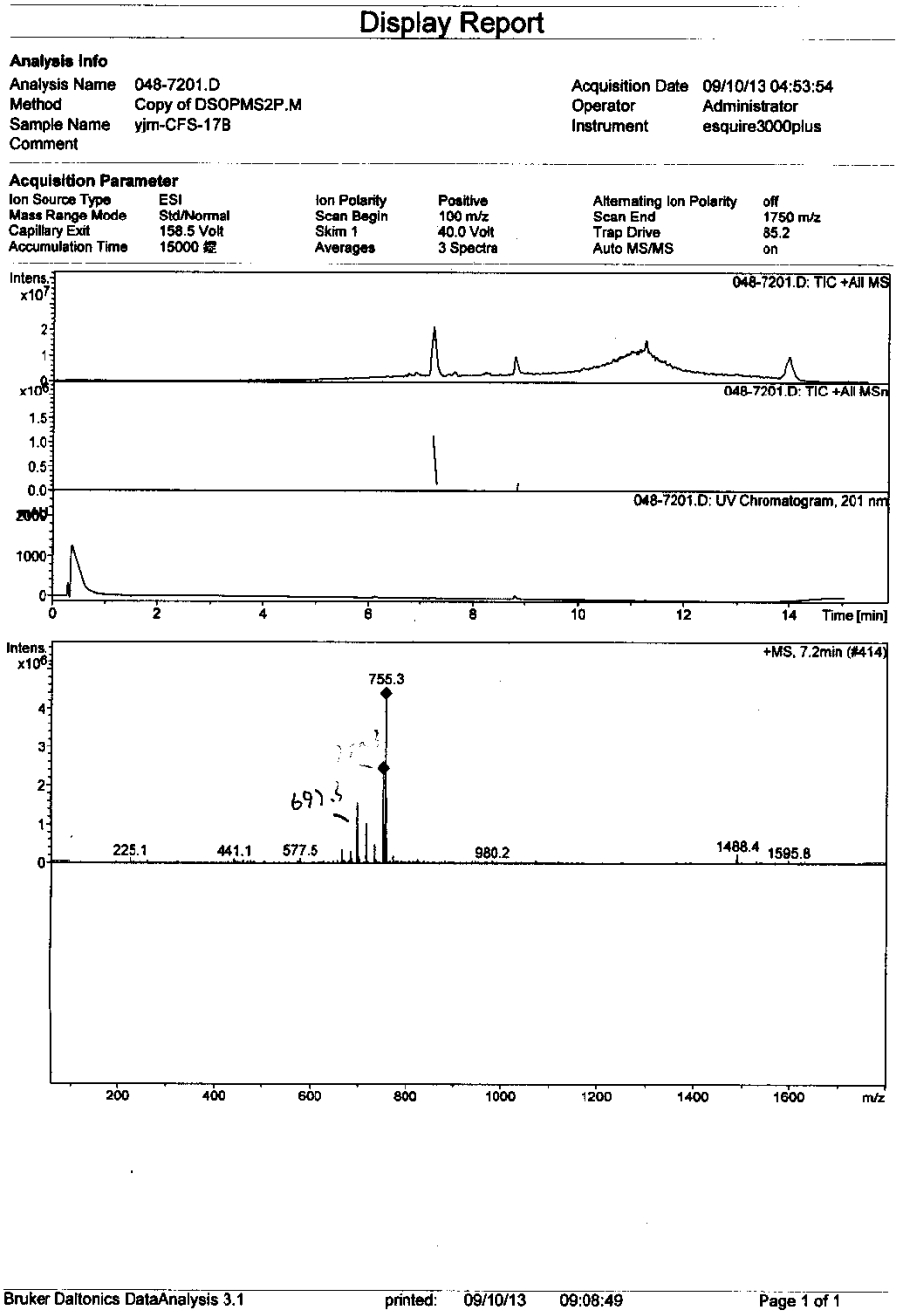


Figure S61. (–)-ESIMS spectrum of fortunilide G (7)

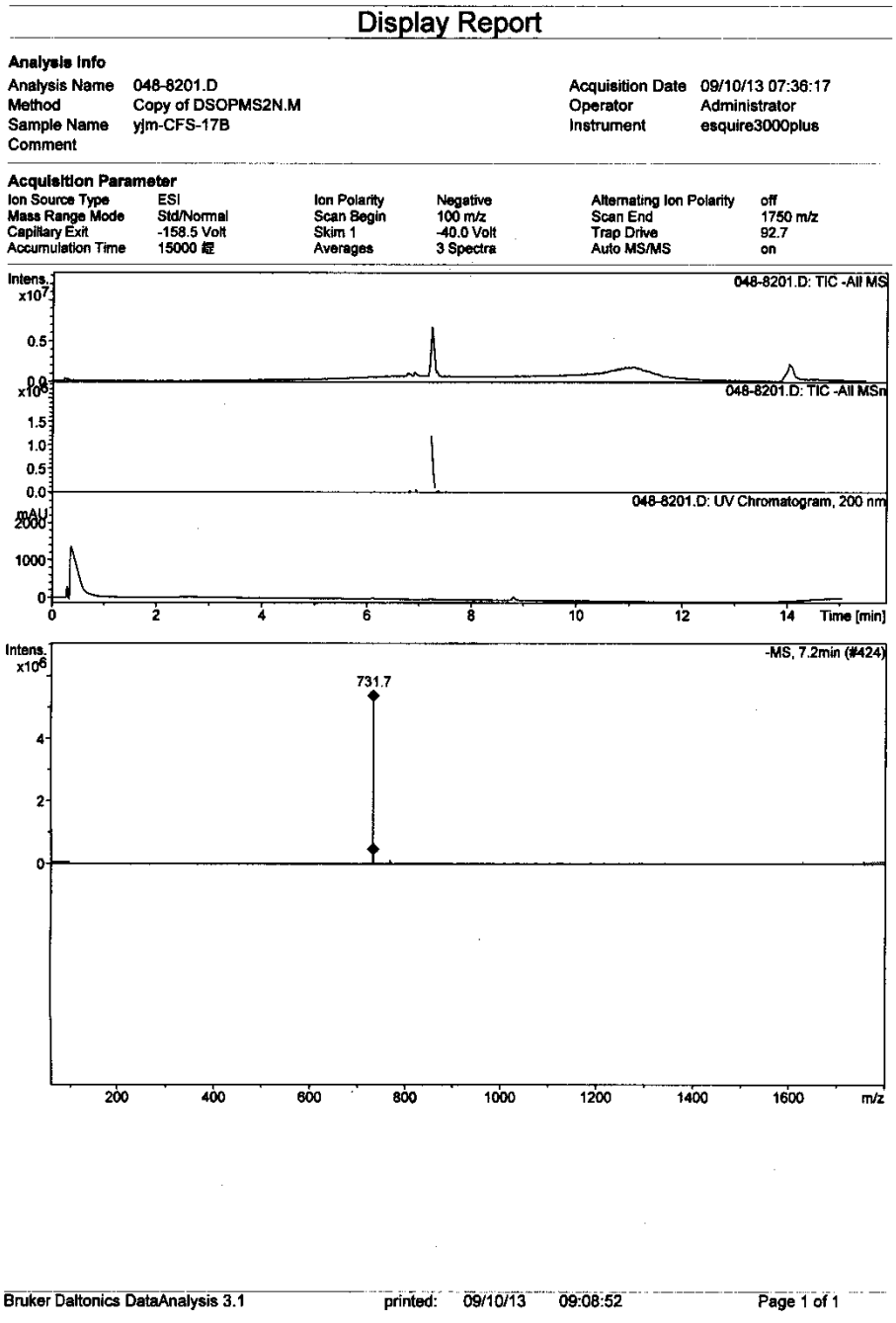


Figure S62. (+)-HRESIMS spectrum of fortunilide G (7)

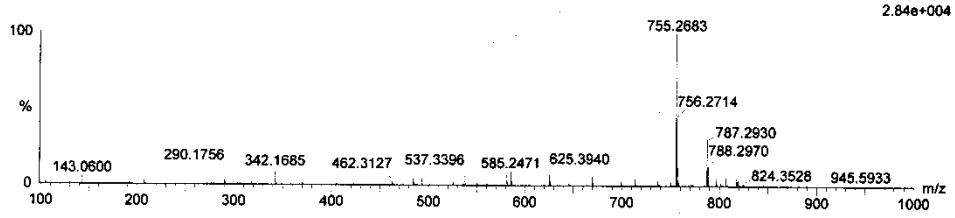
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
321 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 O: 0-20 Na: 0-1

CFS-17B LCT PXE KE324 13-Sep-2013 14:07:16

CFS-17B_0913 42 (0.902) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (26:44) 1: TOF MS ES+ 2.84e+004



Minimum:				-1.5						
Maximum:		3.0	3.0	50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
755.2683	755.2680	0.3	0.4	18.5	80.6	0.0	C40	H44	O13	Na
	755.2704	-2.1	-2.8	21.5	86.9	6.3	C42	H43	O13	

Figure S63. IR spectrum of fortunilide G (7)

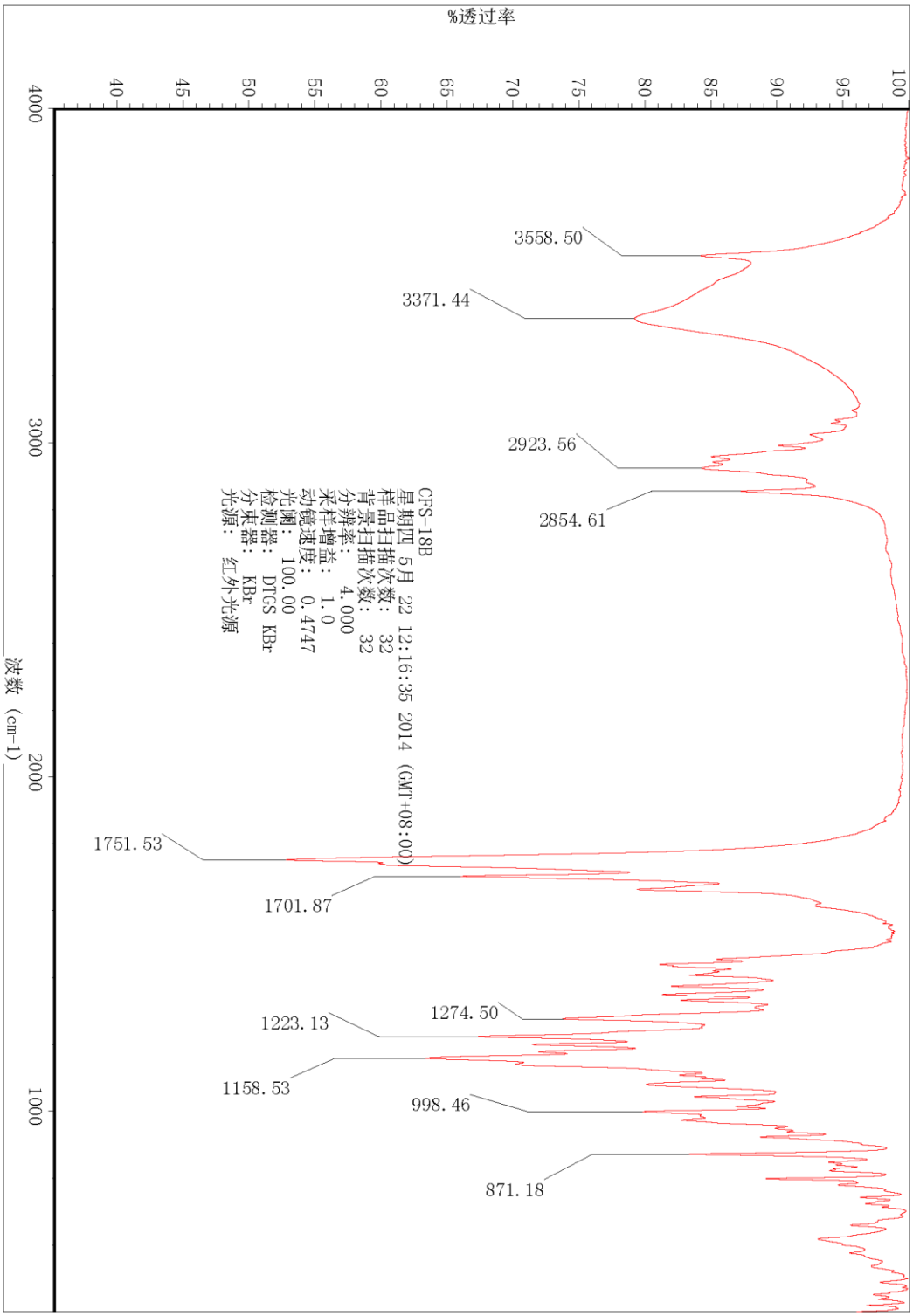


Figure S64. ^{1}H NMR spectrum of fortunilide H (8) in $CDCl_3$

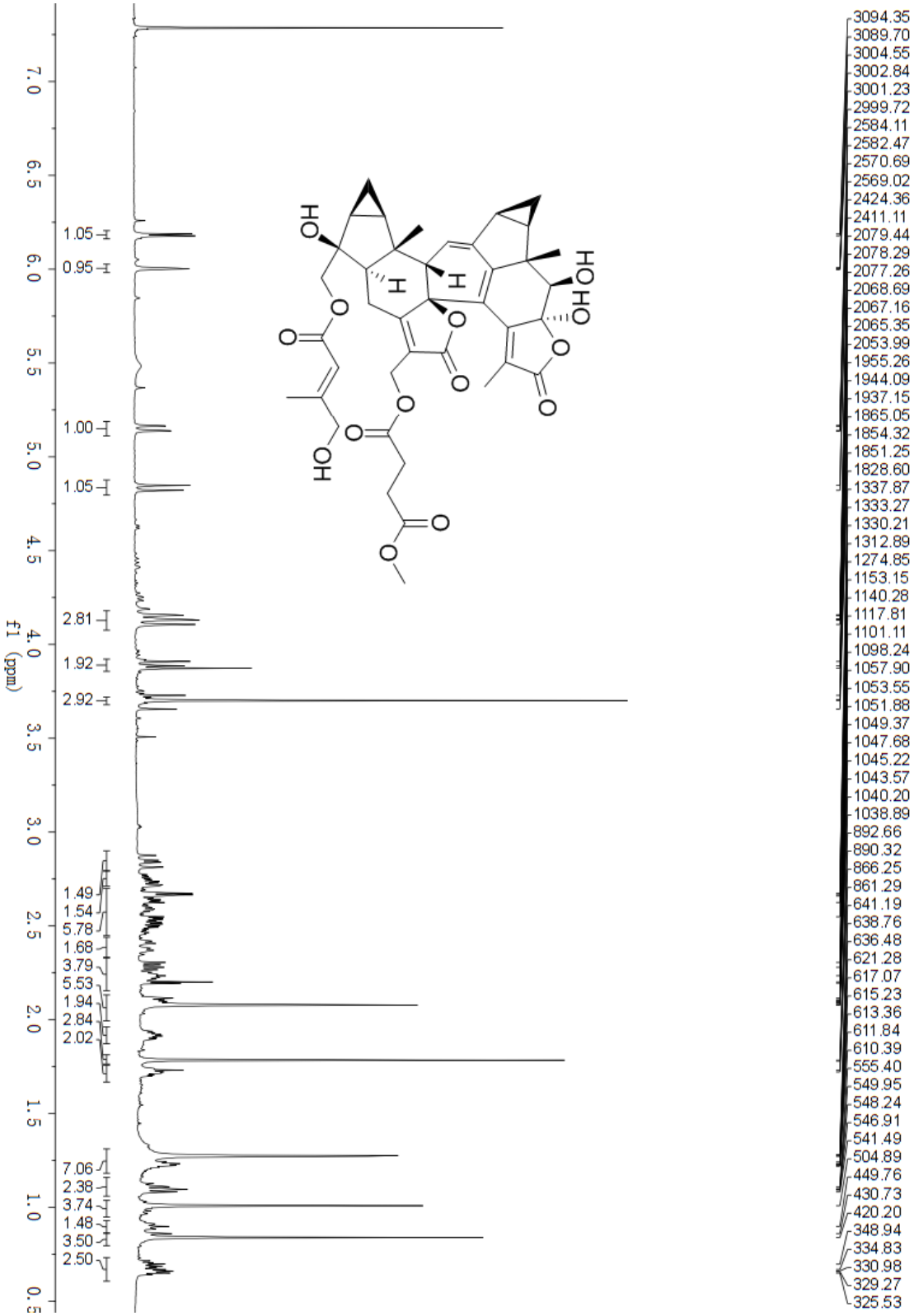


Figure S65. ^{13}C NMR spectrum of fortunilide H (8) in $CDCl_3$

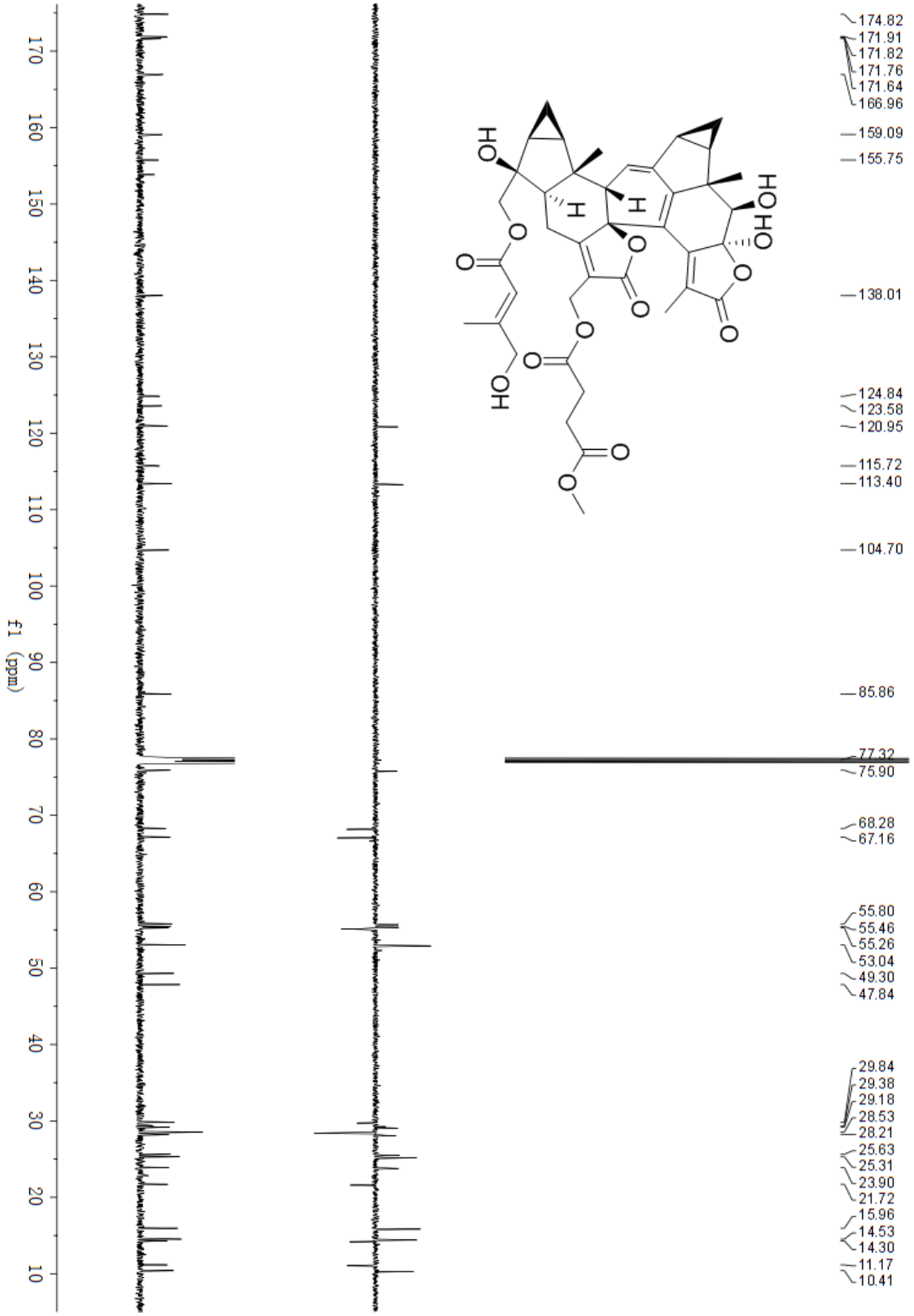


Figure S66. HSQC spectrum of fortunilide H (8) in $CDCl_3$

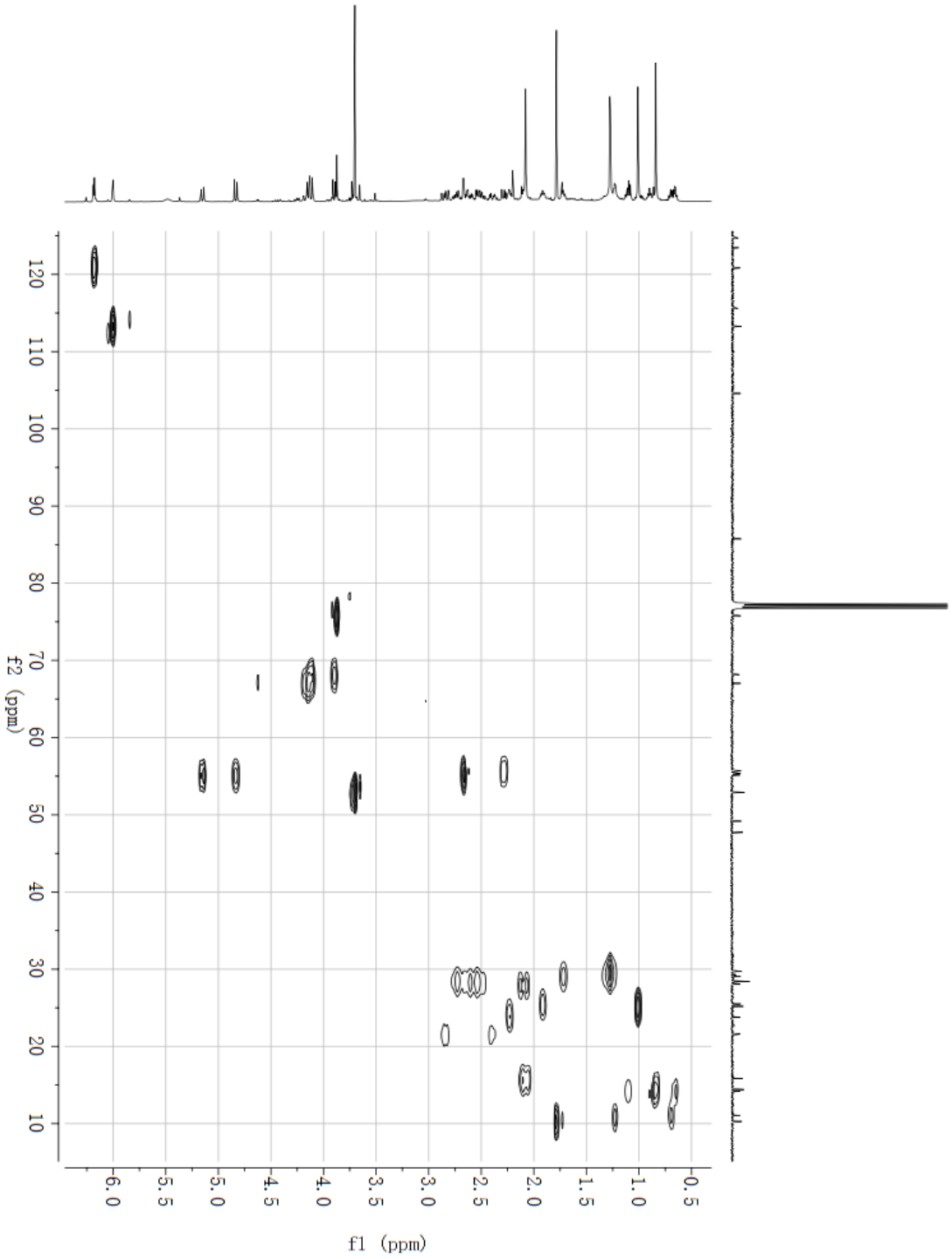


Figure S67. HMBC spectrum of fortunilide H (8) in $CDCl_3$

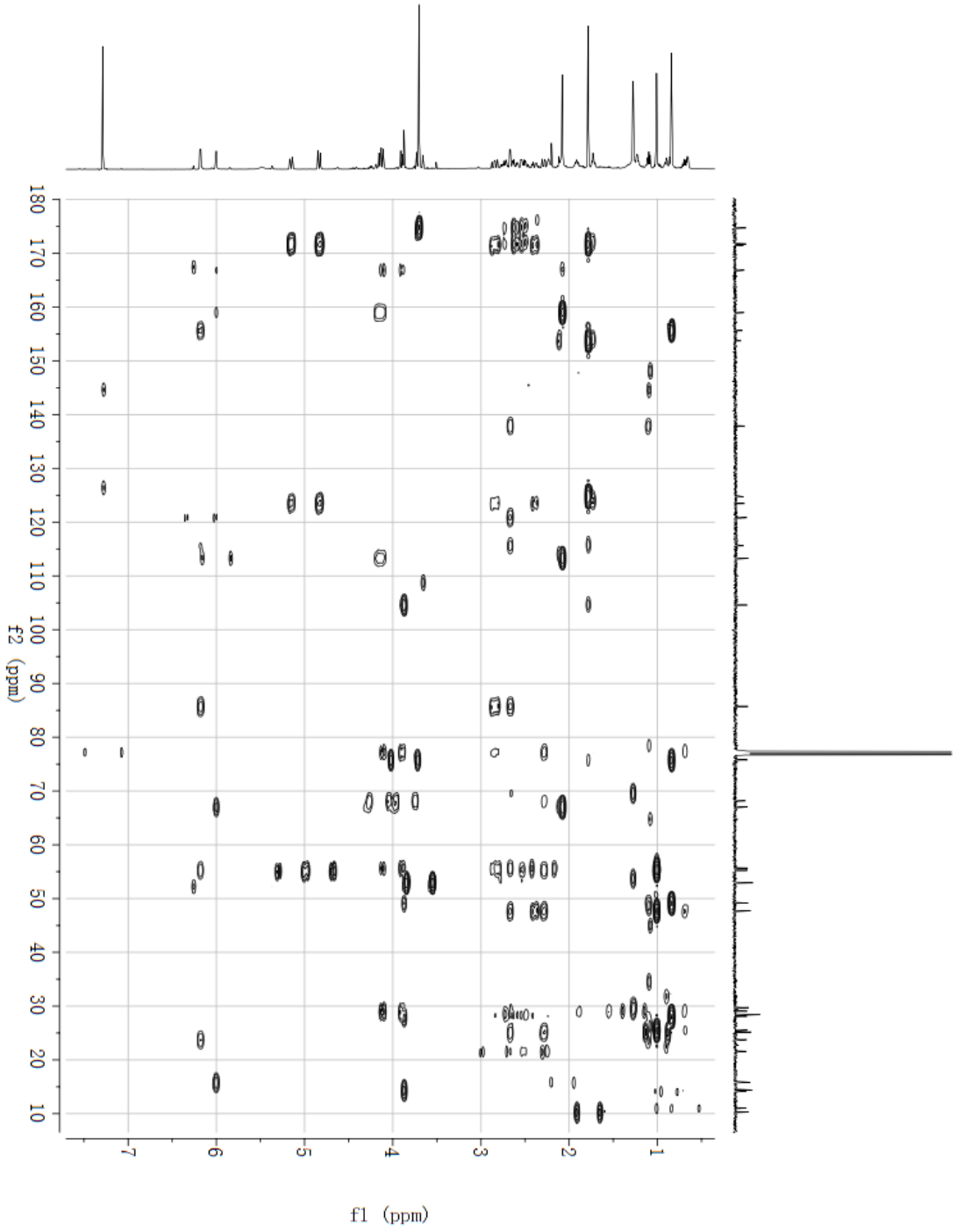


Figure S68. ROESY spectrum of fortunilide H (8)

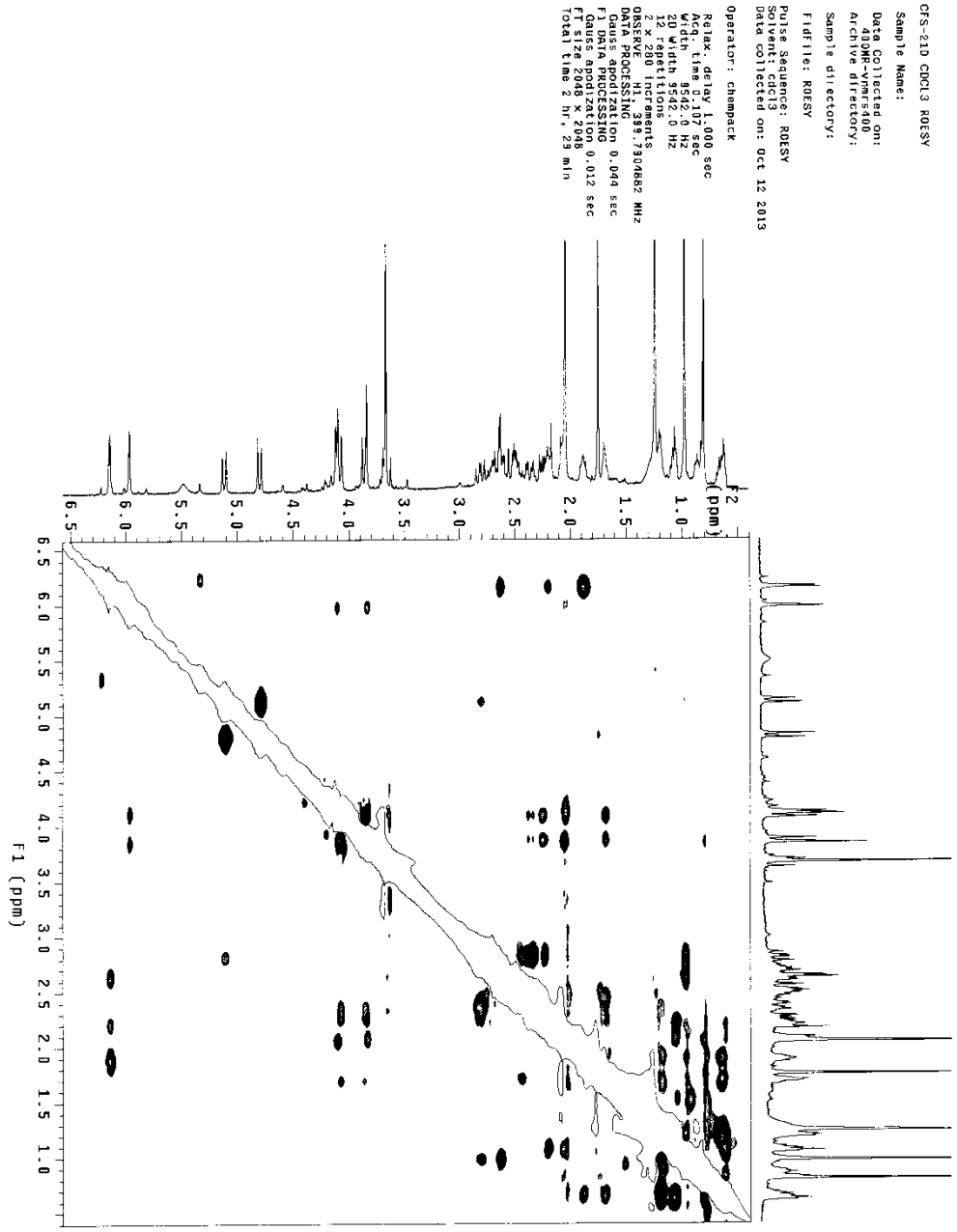


Figure S69. (+)-ESIMS spectrum of fortunilide H (8)

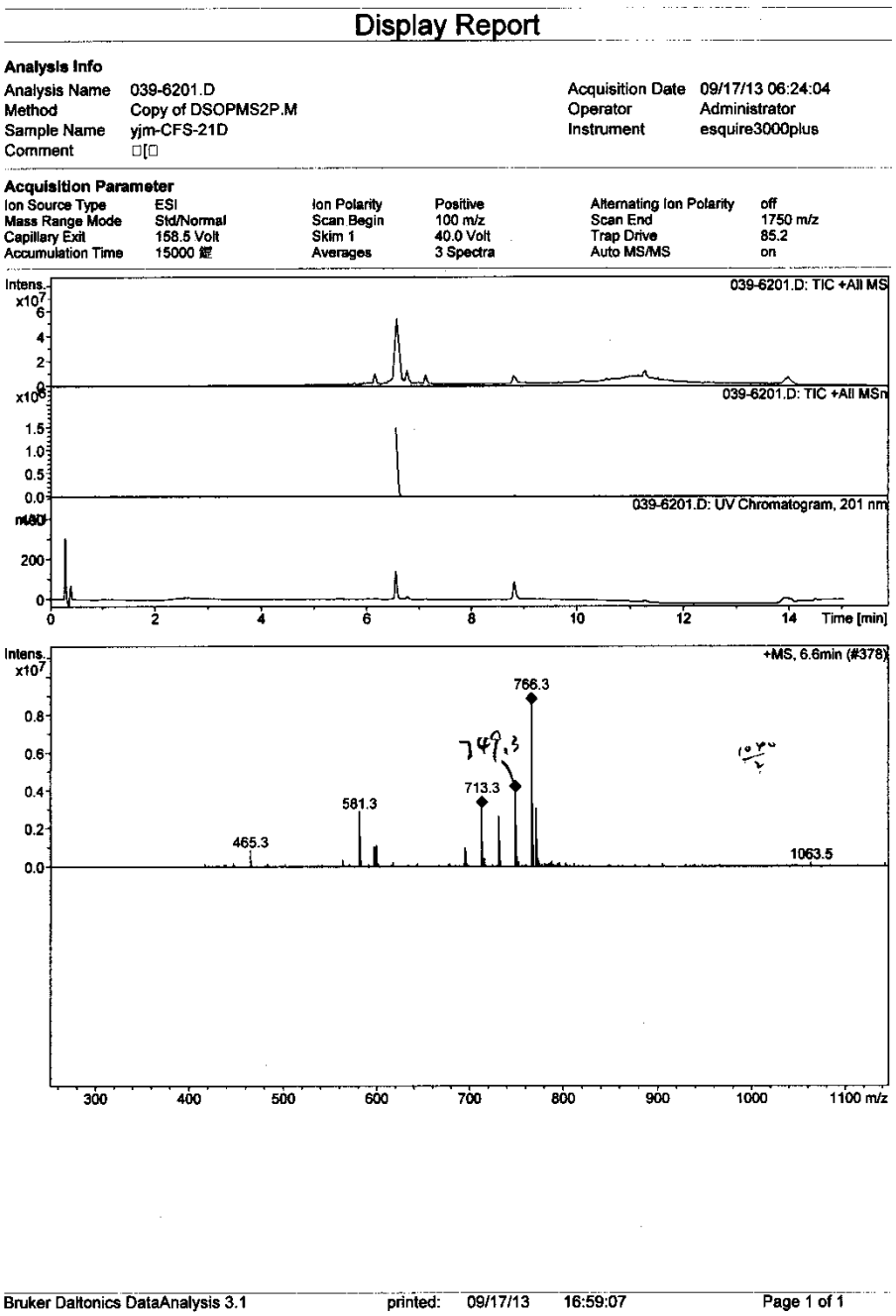


Figure S70. (–)-ESIMS spectrum of fortunilide H (8)

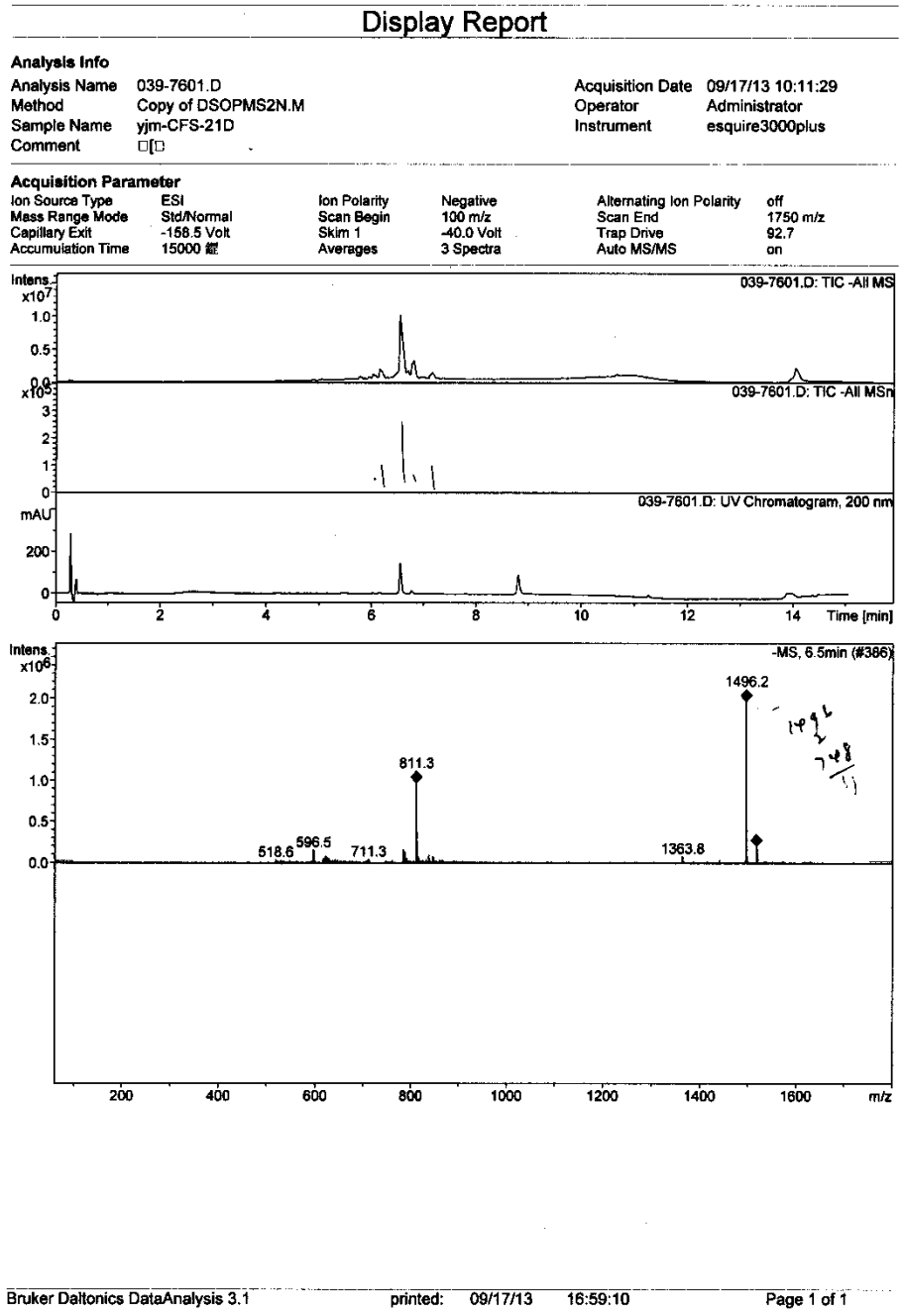


Figure S71. (+)-HRESIMS spectrum of fortunilide H (8)

Elemental Composition Report **Page 1**

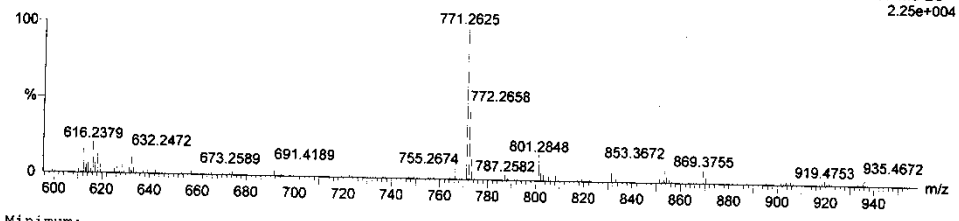
Single Mass Analysis
Tolerance = 4.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
329 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 O: 0-20 Na: 0-1
CFS-21D

LCT PXE KE324

31-Oct-2013
14:45:51
1: TOF MS ES+
2.25e+004

CFS-21D_1031 45 (0.989) AM2 (Ar,10500.0,0.00,0.70); ABS; Cm (27:46)



Minimum:				-1.5						
Maximum:		5.0	4.0	50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
771.2625	771.2629	-0.4	-0.5	18.5	76.1	0.0	C40	H44	O14	Na
	771.2653	-2.8	-3.6	21.5	81.9	5.8	C42	H43	O14	

Figure S72. IR spectrum of fortunilide H (8)

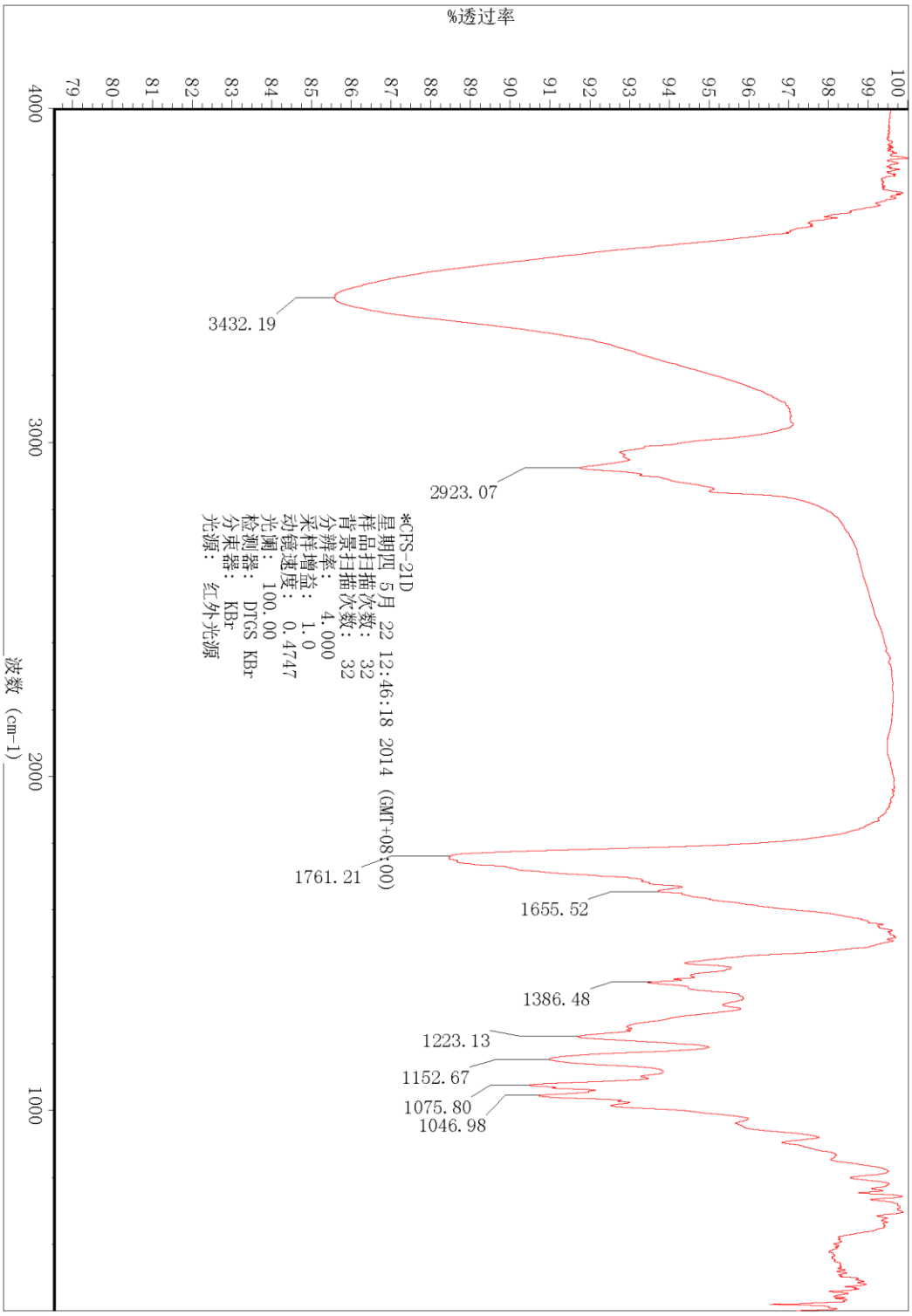


Figure S73. ^{1}H NMR spectrum of fortunilide I (9) in CD_3OD

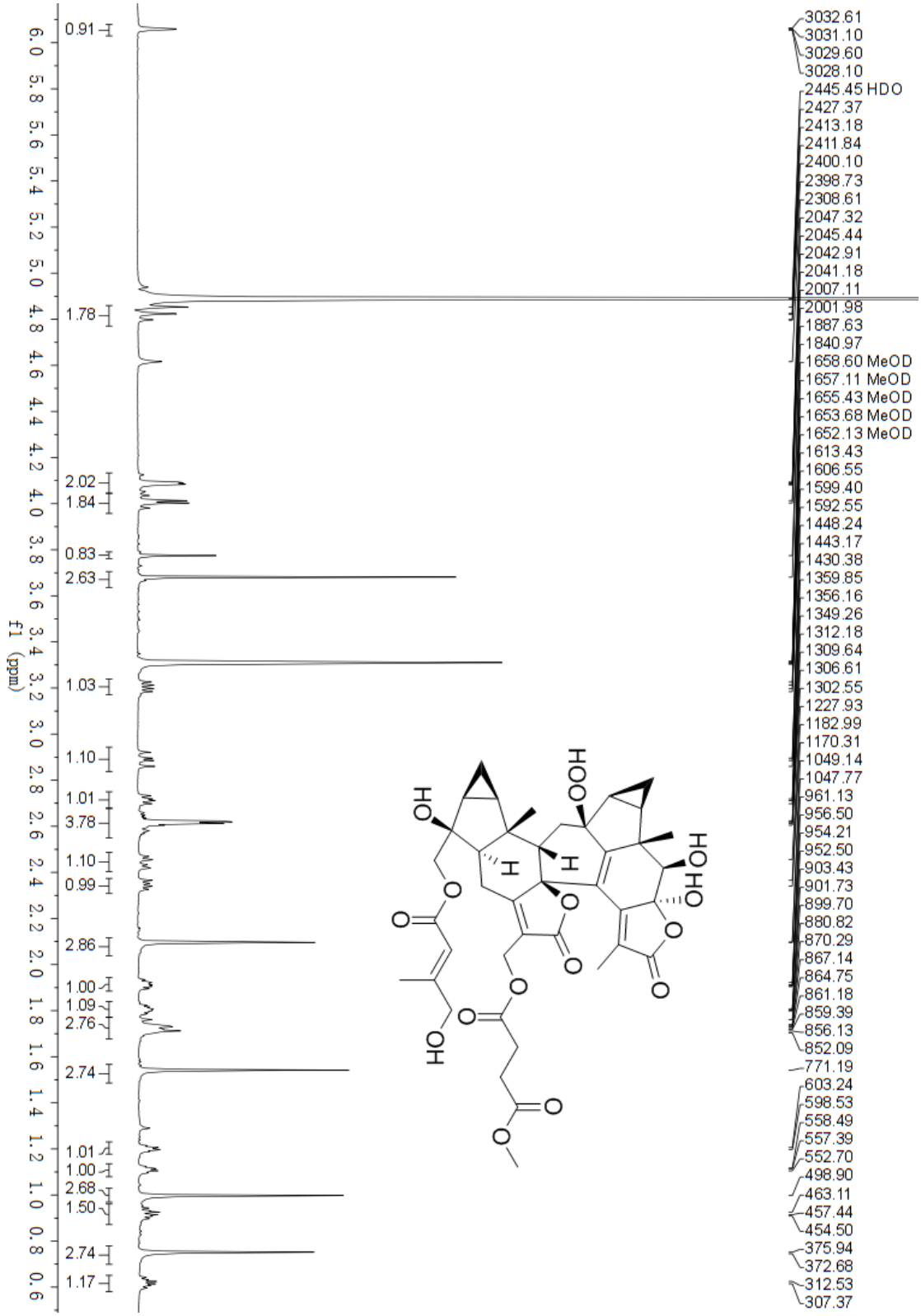


Figure S74. ^{13}C NMR spectrum of fortunilide I (9) in CD_3OD

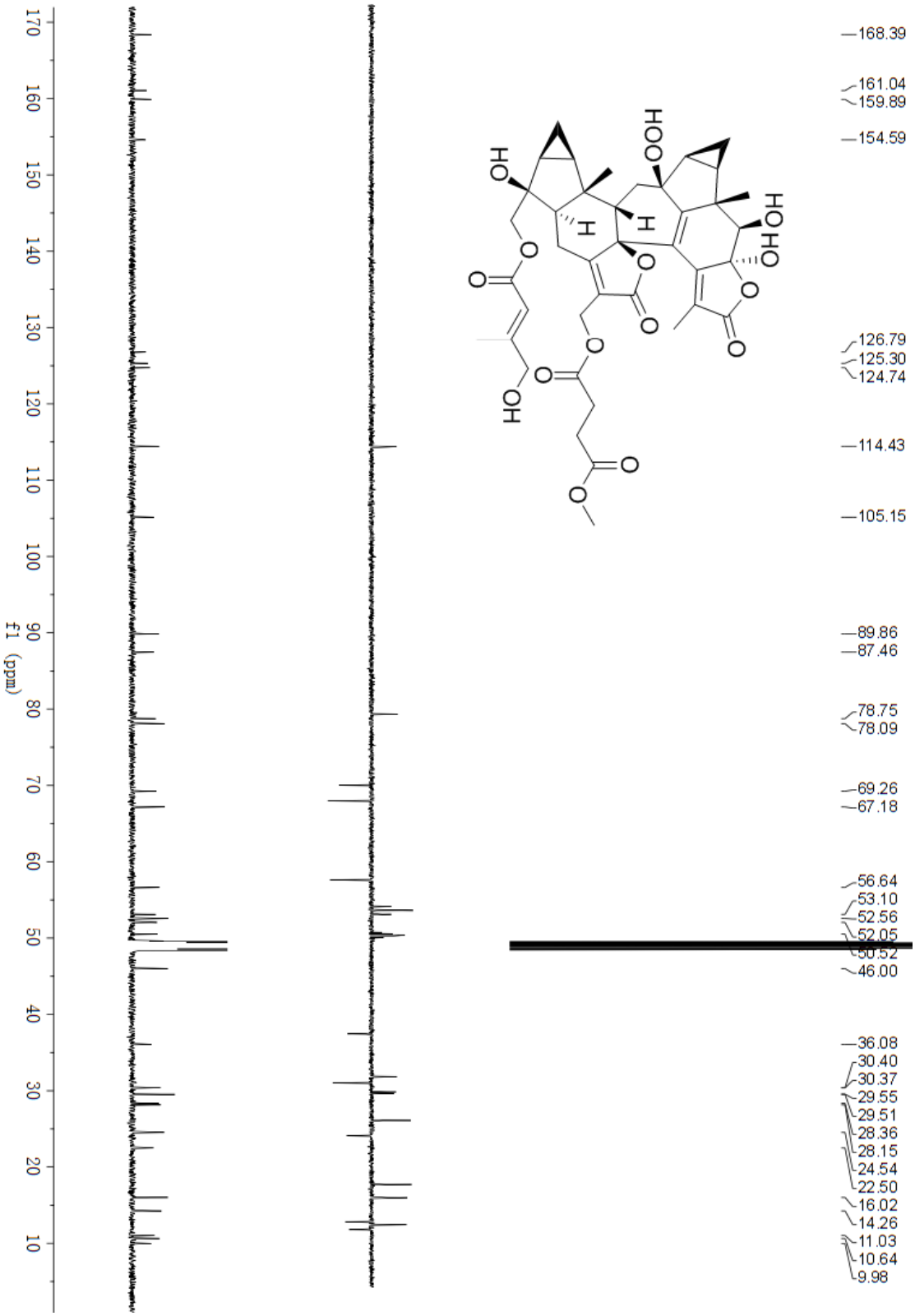


Figure S75. HSQC spectrum of fortunilide I (9) in CD_3OD

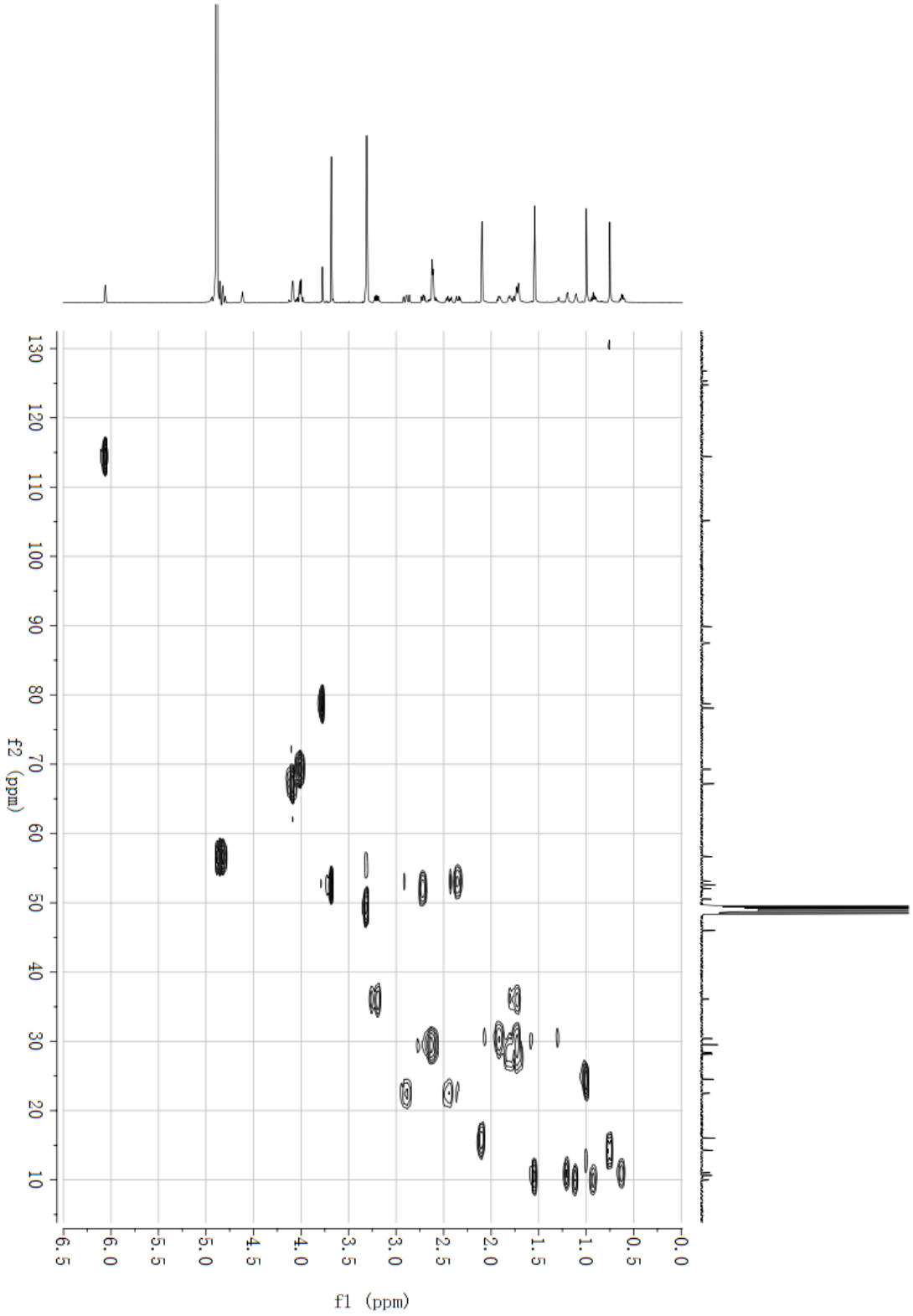


Figure S76. HMBC spectrum of fortunilide I (9) in CD_3OD

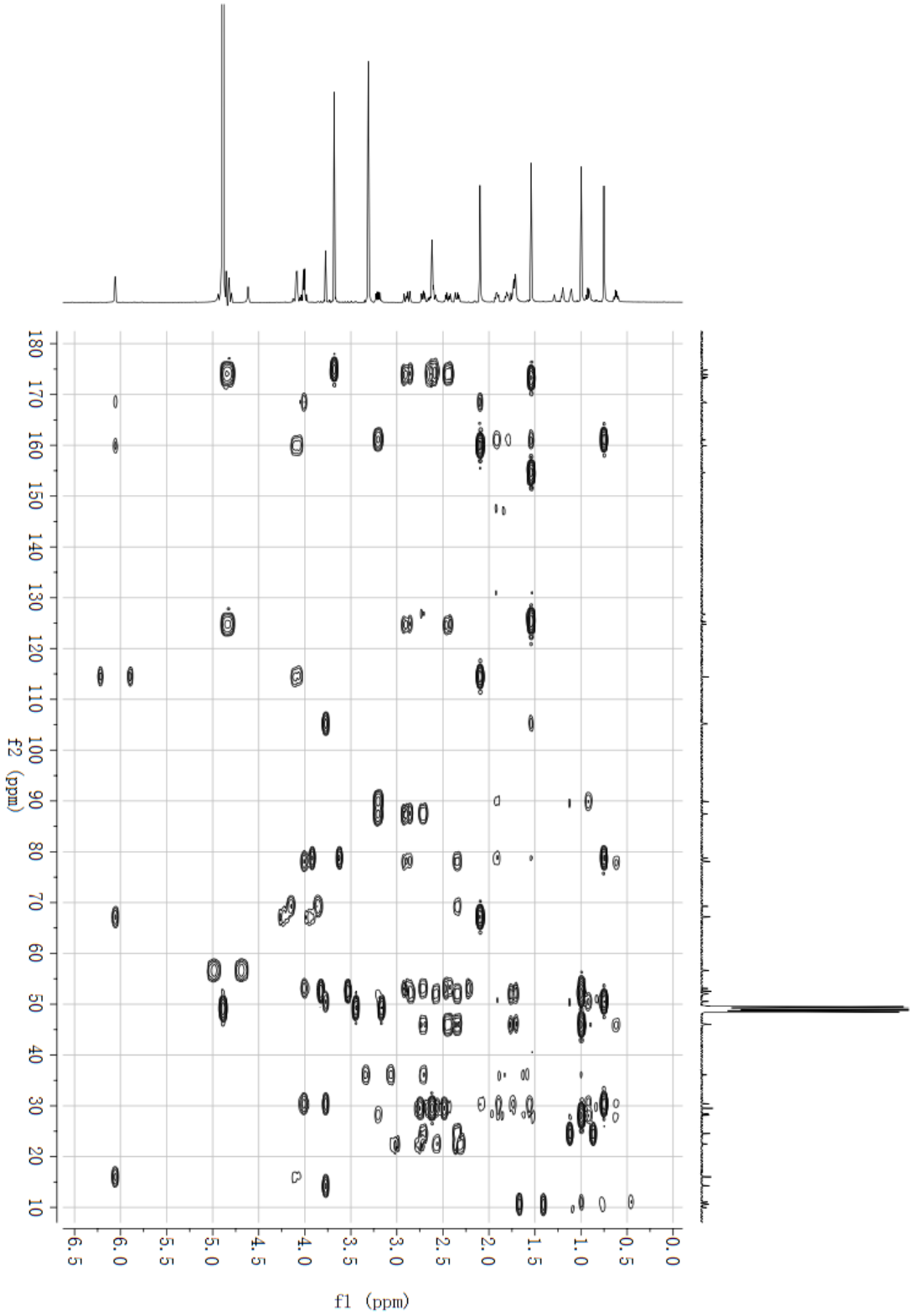


Figure S77. ROESY spectrum of fortunilide I (9)

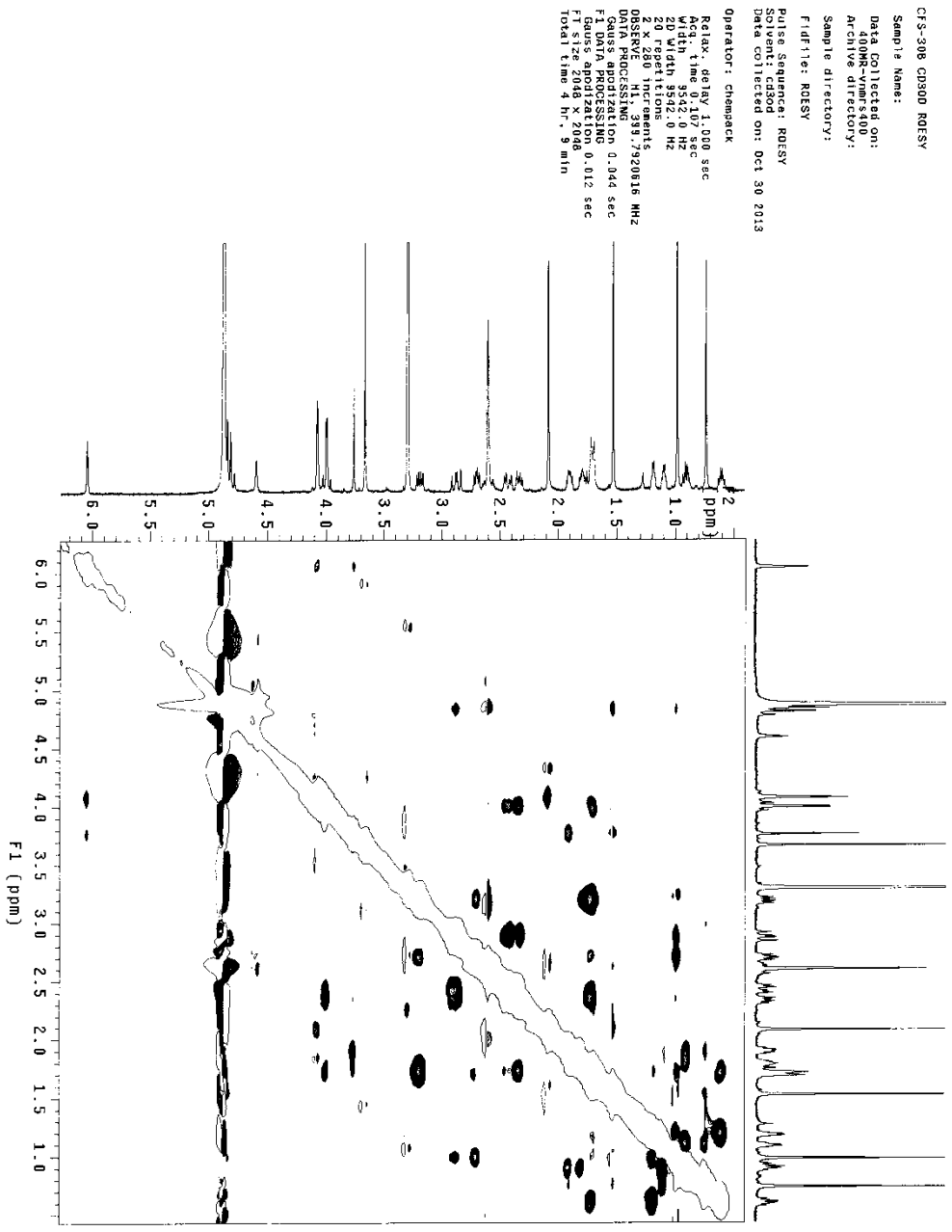


Figure S78. (+)-ESIMS spectrum of fortunilide I (9)

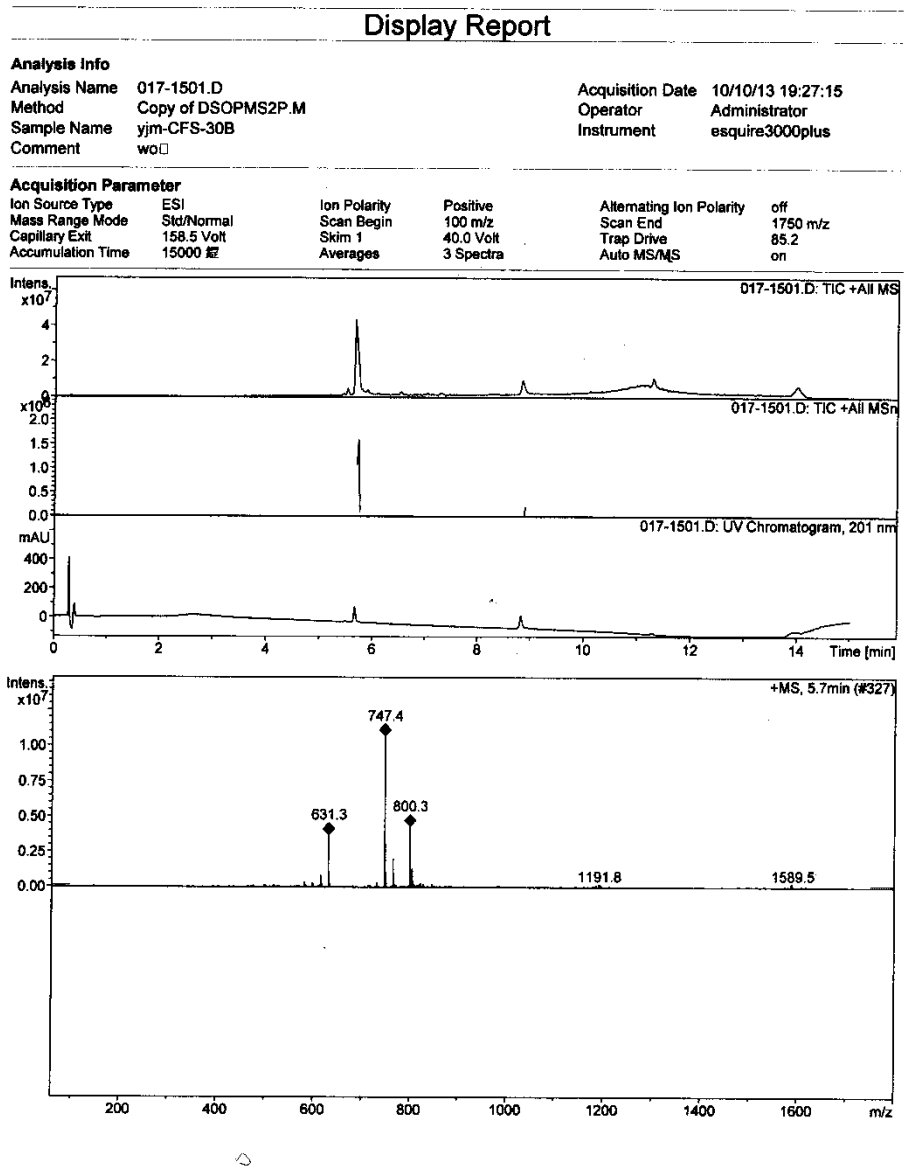


Figure S79. (–)-ESIMS spectrum of fortunilide I (9)

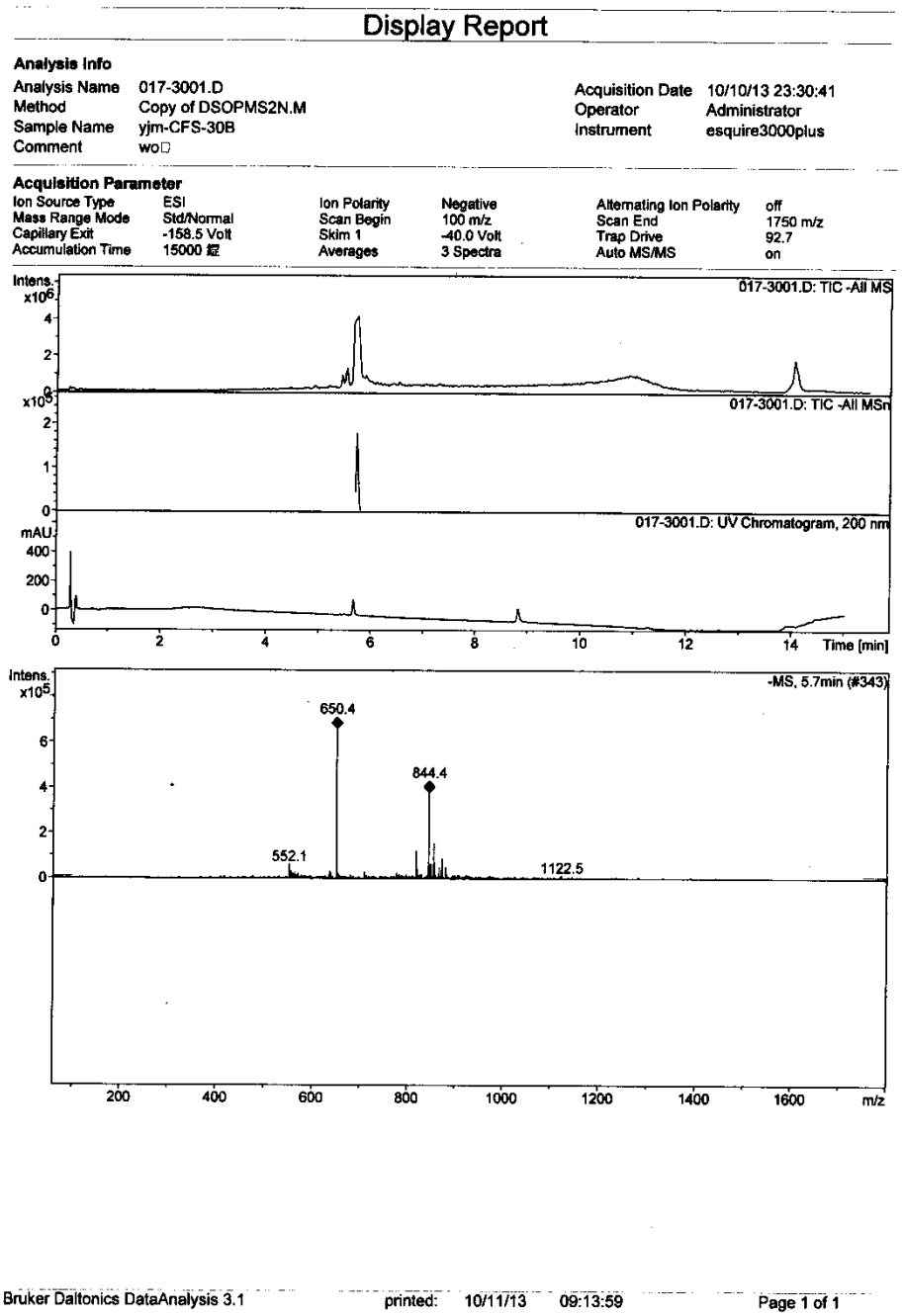


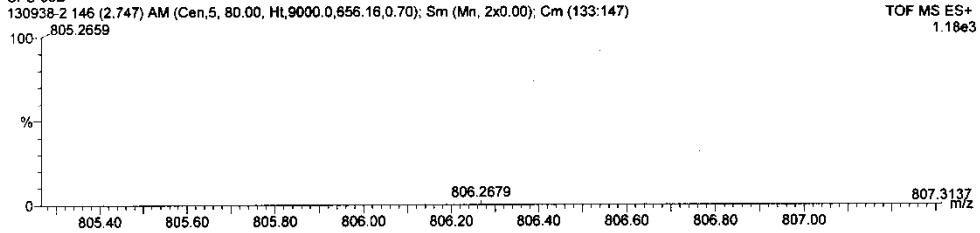
Figure S80. (+)-HRESIMS spectrum of fortunilide I (9)

Elemental Composition Report **Page 1**

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
32 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

SIMM-Mass Spec Q-Tof Ultima 23-Oct-201314:53:44
CFS-30B
130938-2 146 (2.747) AM (Cen,5, 80.00, Ht,9000.0,656.16,0.70); Sm (Mn, 2x0.00); Cm (133:147) TOF MS ES+
1.18e3



Minimum:	50.00				-1.5		
Maximum:	100.00		200.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
805.2659	100.00	805.2684	-2.5	-3.0	17.5	1	C40 H46 O16 Na

Figure S81. IR spectrum of fortunilide I (9)

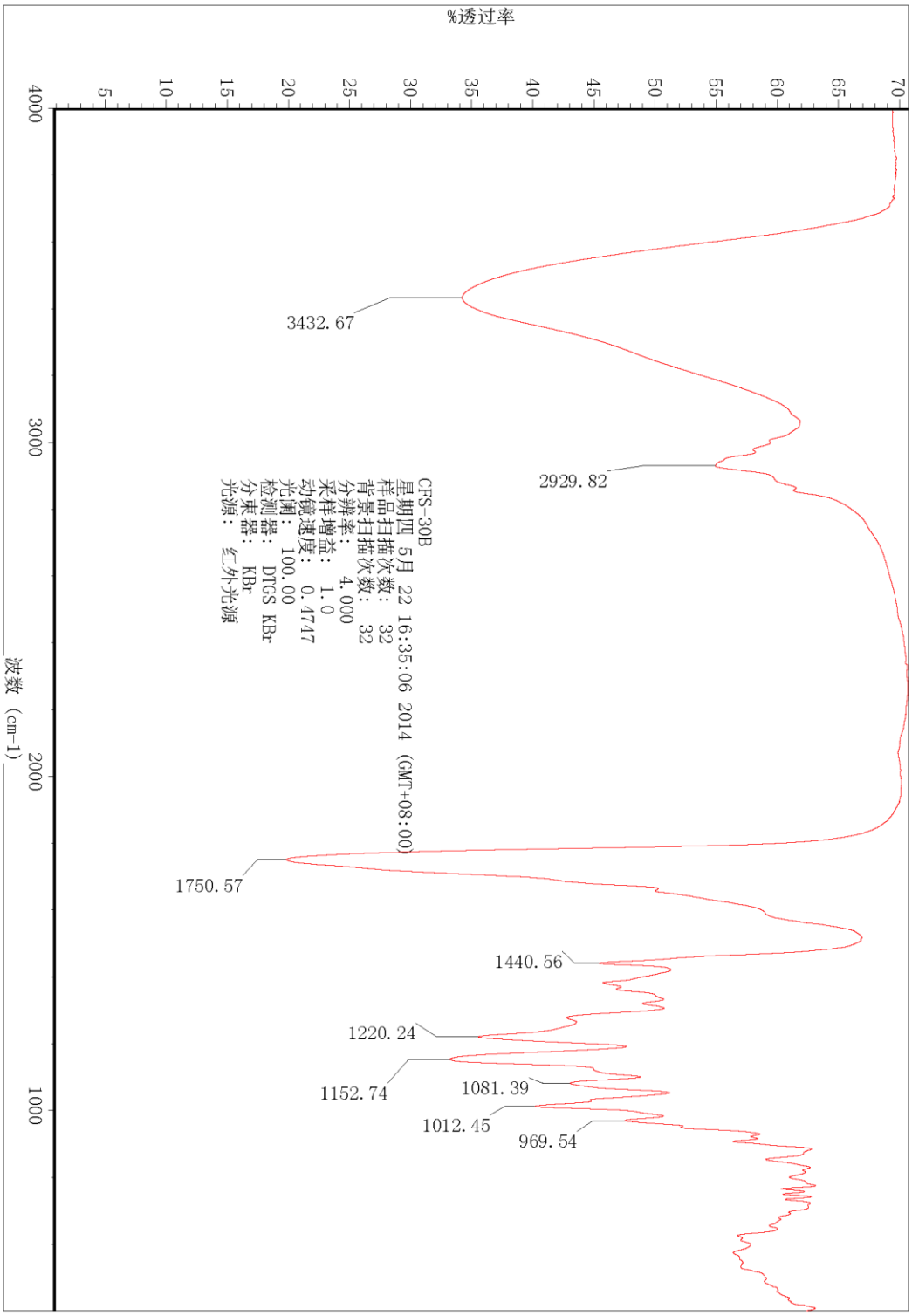


Figure S82. ^{1}H NMR spectrum of fortunilide J (10) in CD_3OD

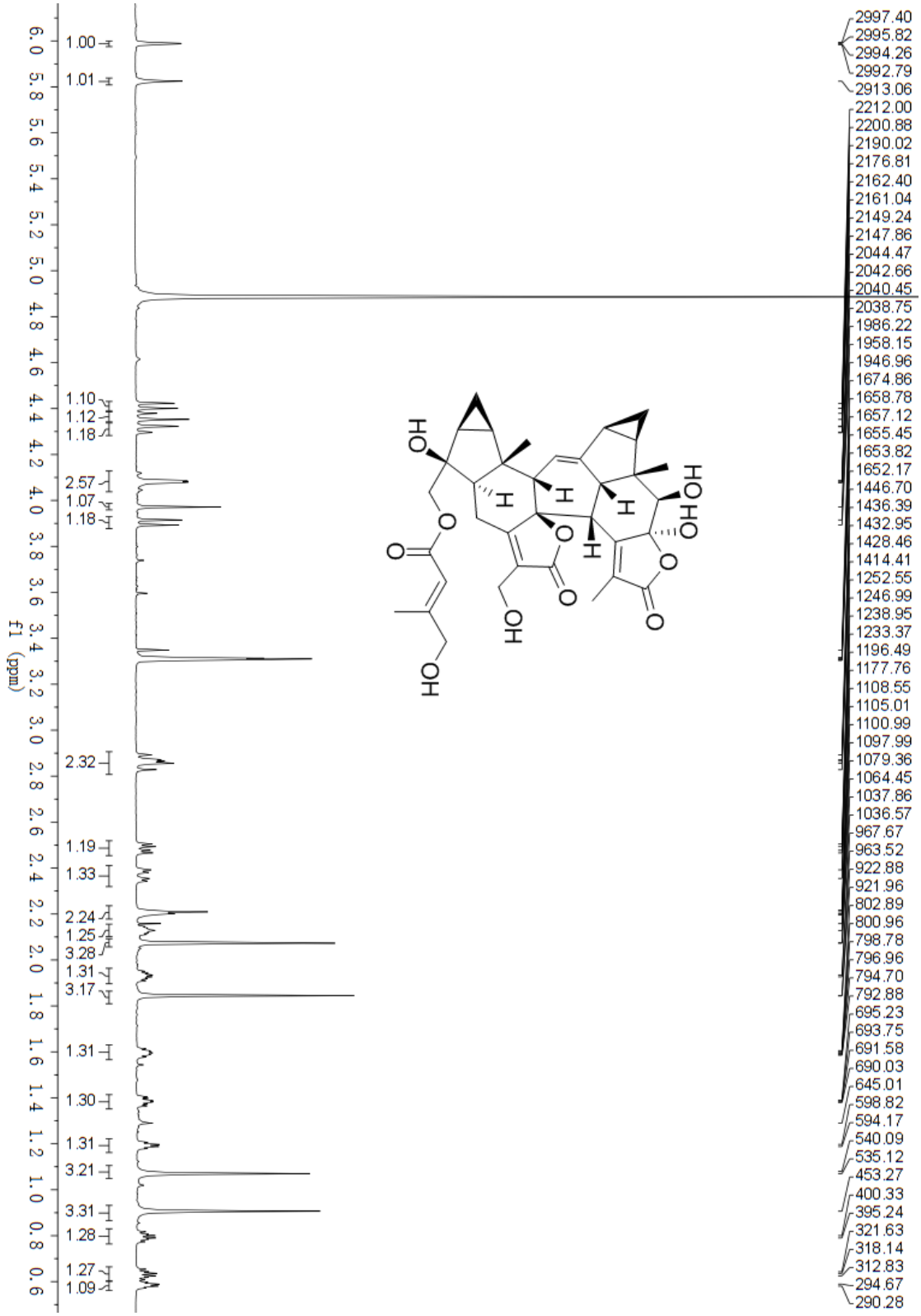


Figure S83. ^{13}C NMR spectrum of fortunilide J (10) in CD_3OD

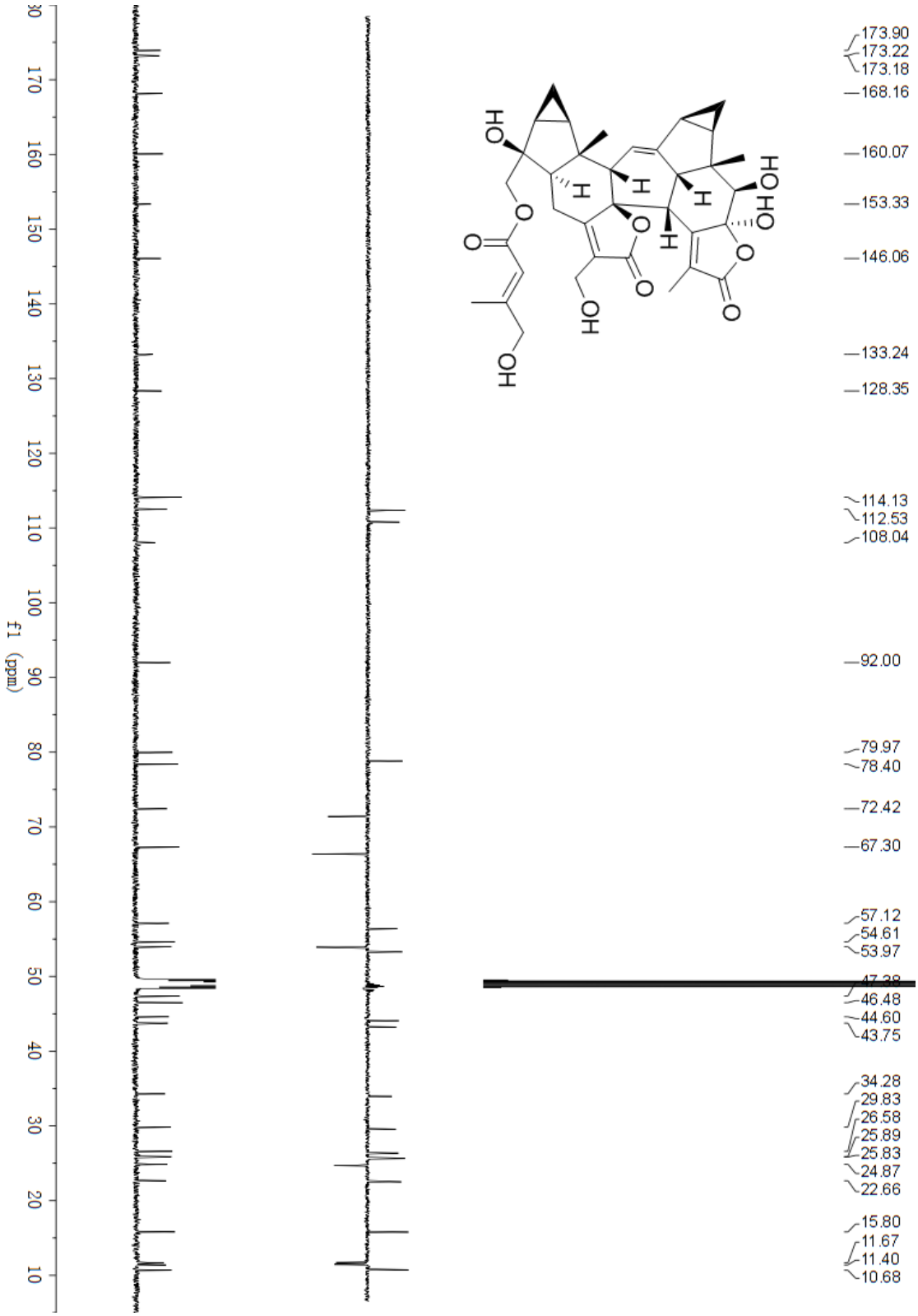


Figure S84. HSQC spectrum of fortunilide J (10) in CD_3OD

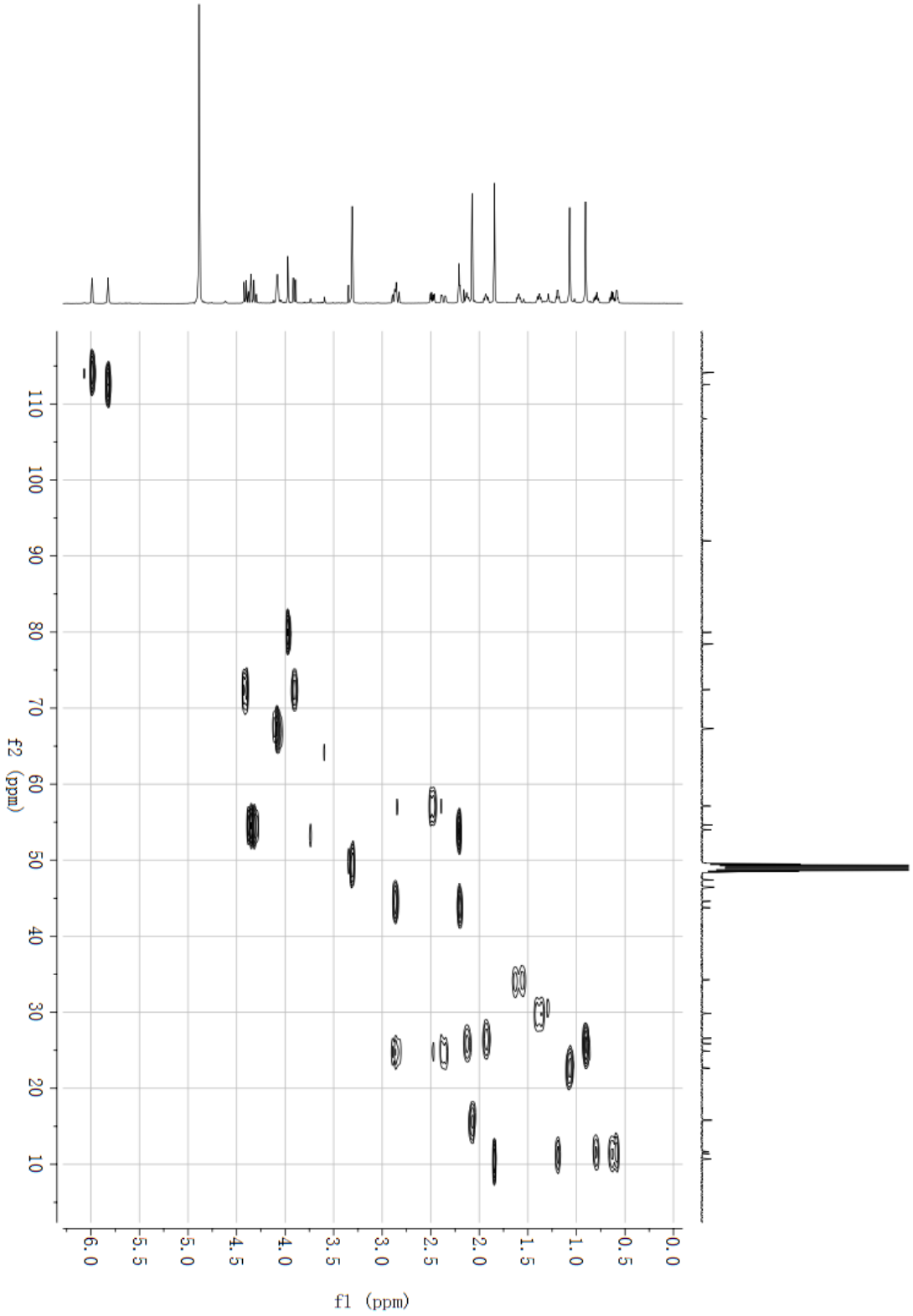


Figure S85. HMBC spectrum of fortunilide J (10) in CD_3OD

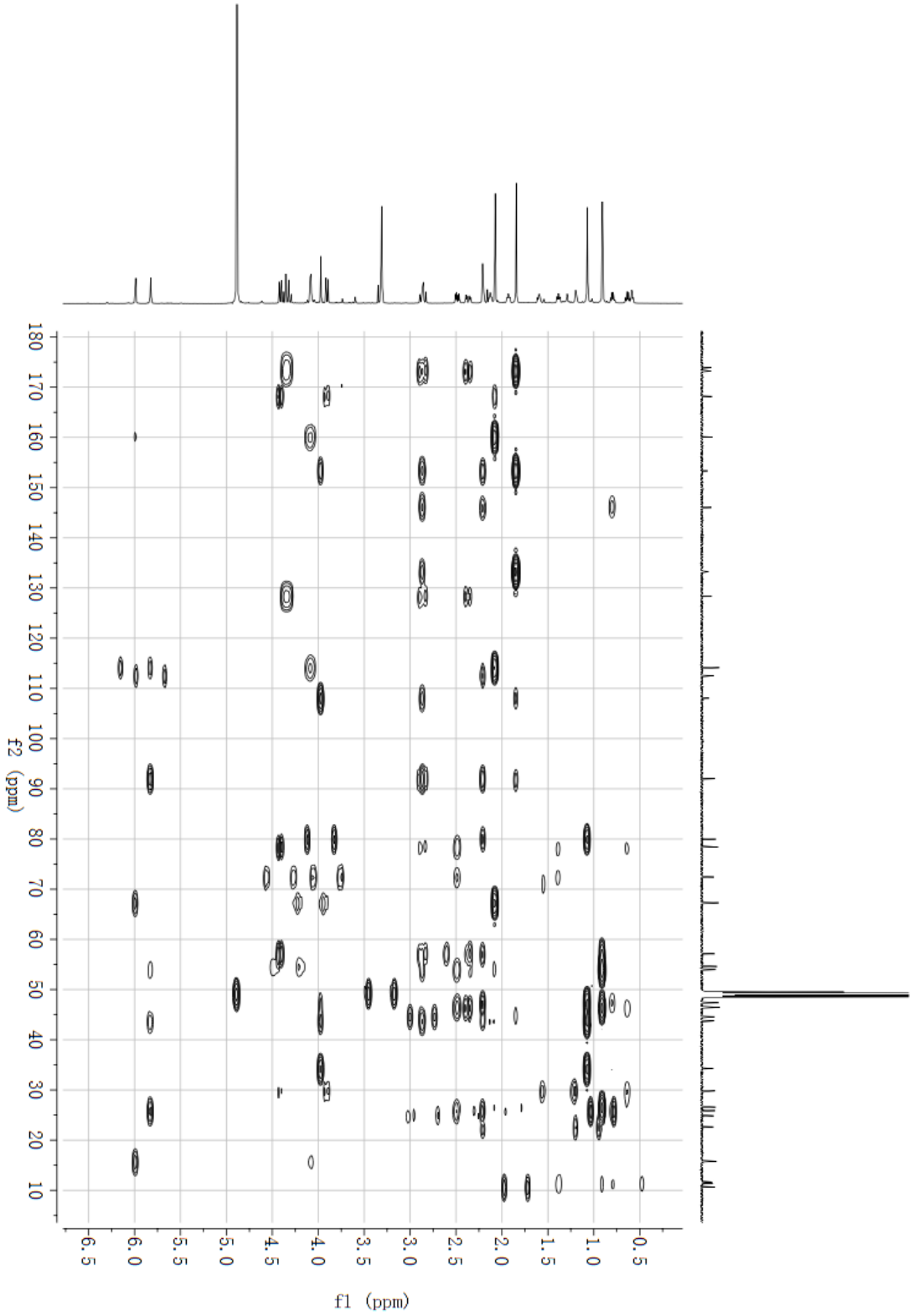


Figure S86. ROESY spectrum of fortunilide J (10)

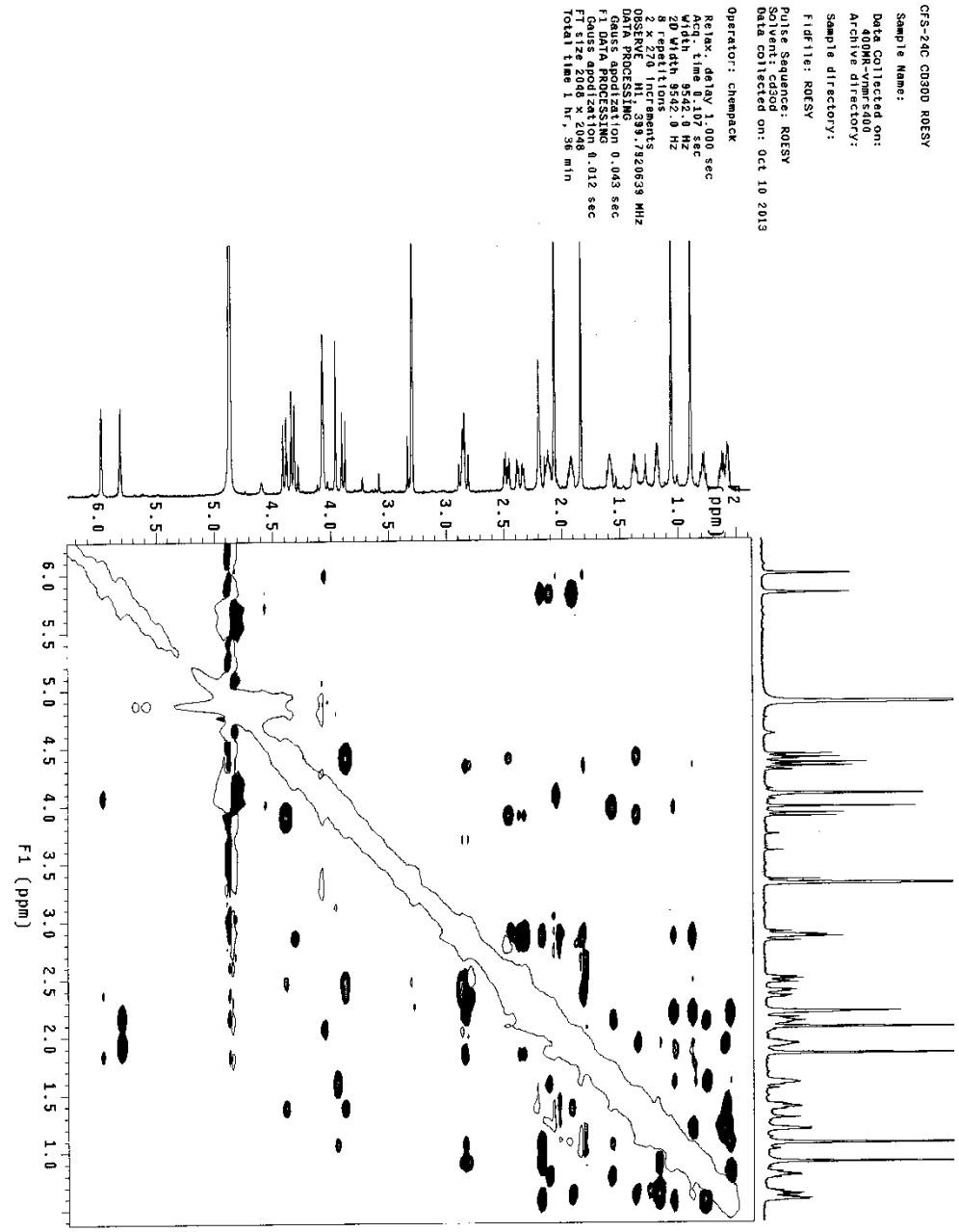


Figure S87. (+)-ESIMS spectrum of fortunilide J (10)

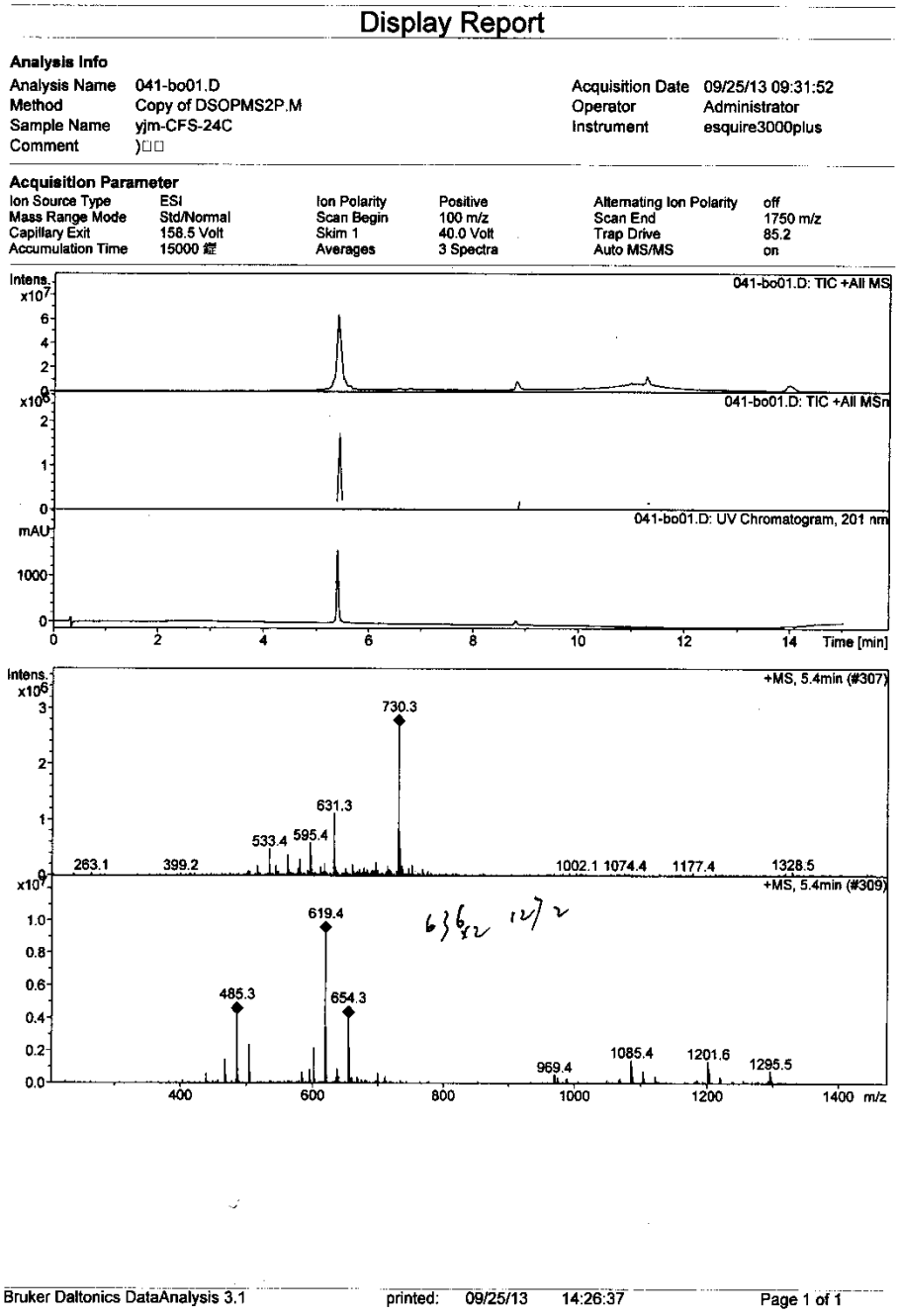


Figure S88. (–)-ESIMS spectrum of fortunilide J (10)

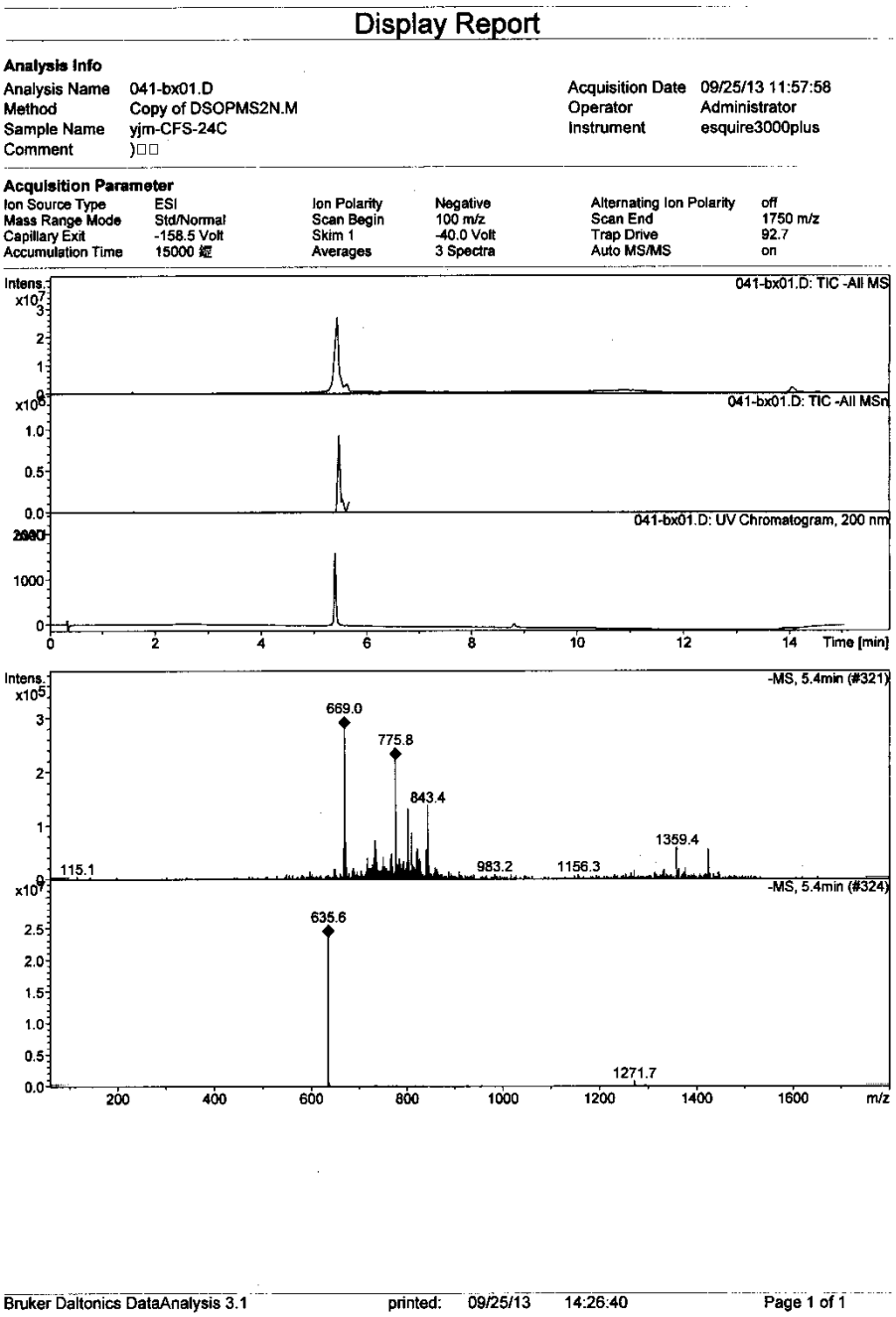


Figure S89. (–)-HRESIMS spectrum of fortunilide J (10)

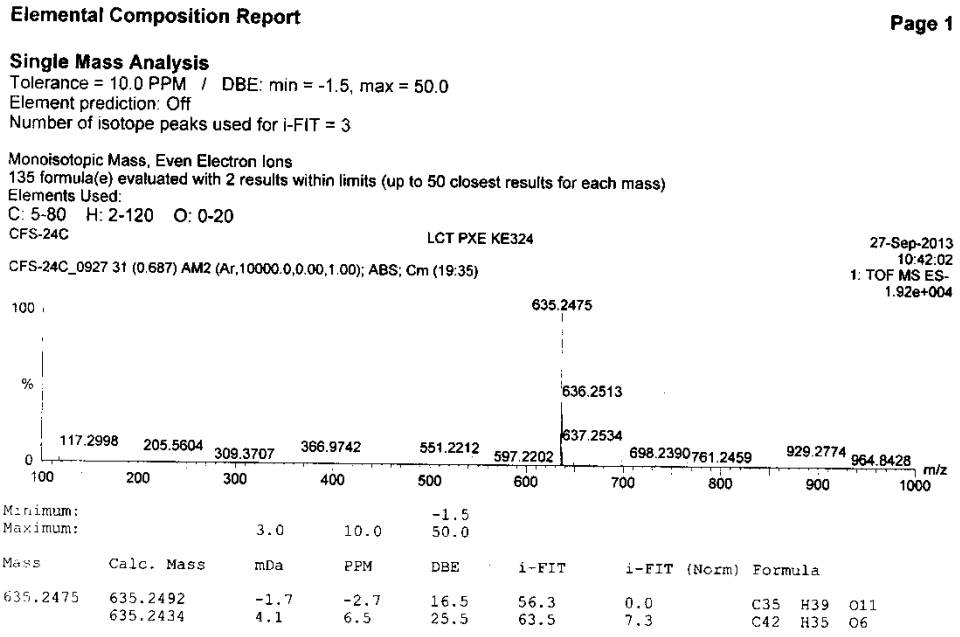


Figure S90. IR spectrum of fortunilide J (10)

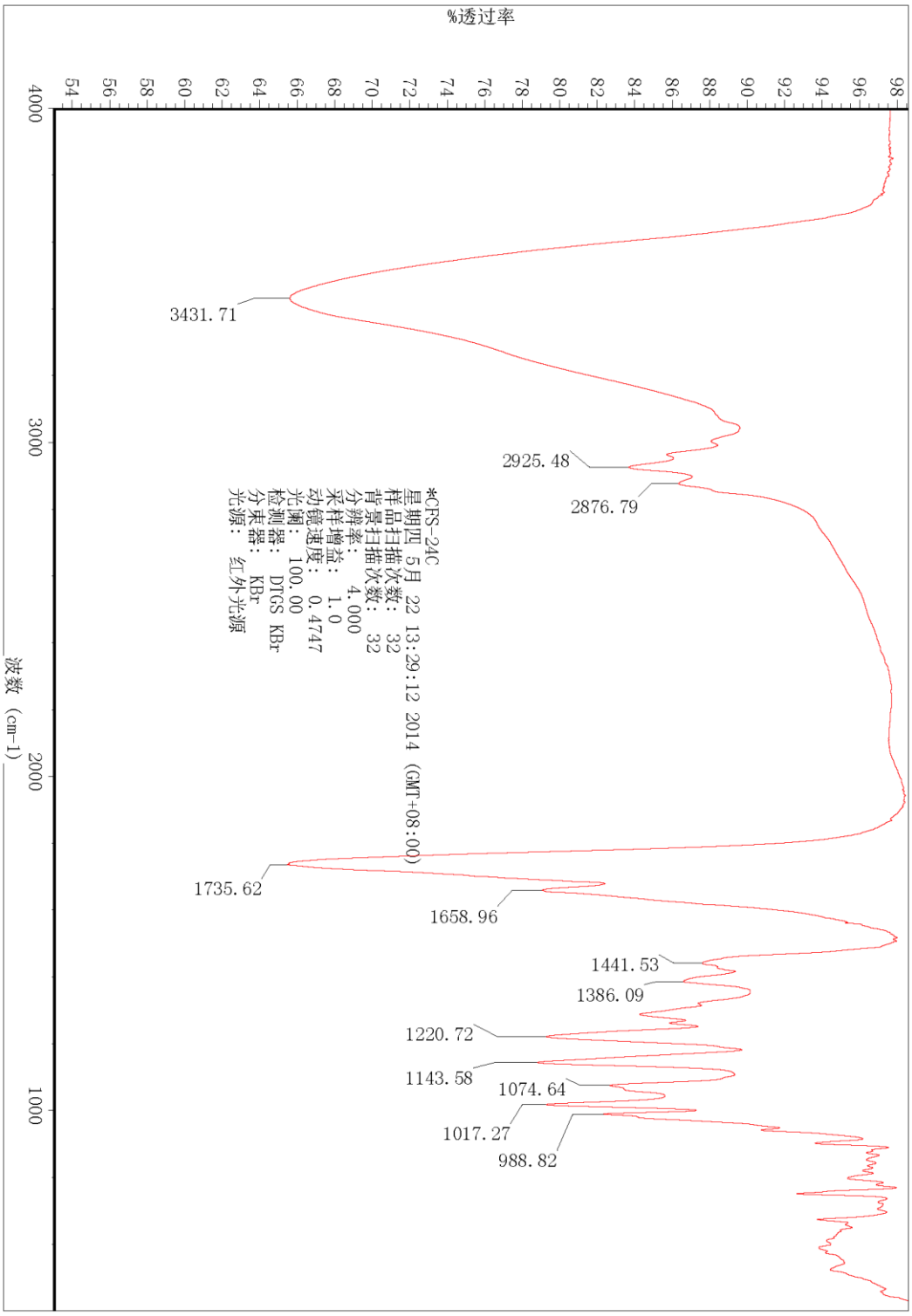


Figure S91. ^{1}H NMR spectrum of fortunilide K (11) in $CDCl_3$

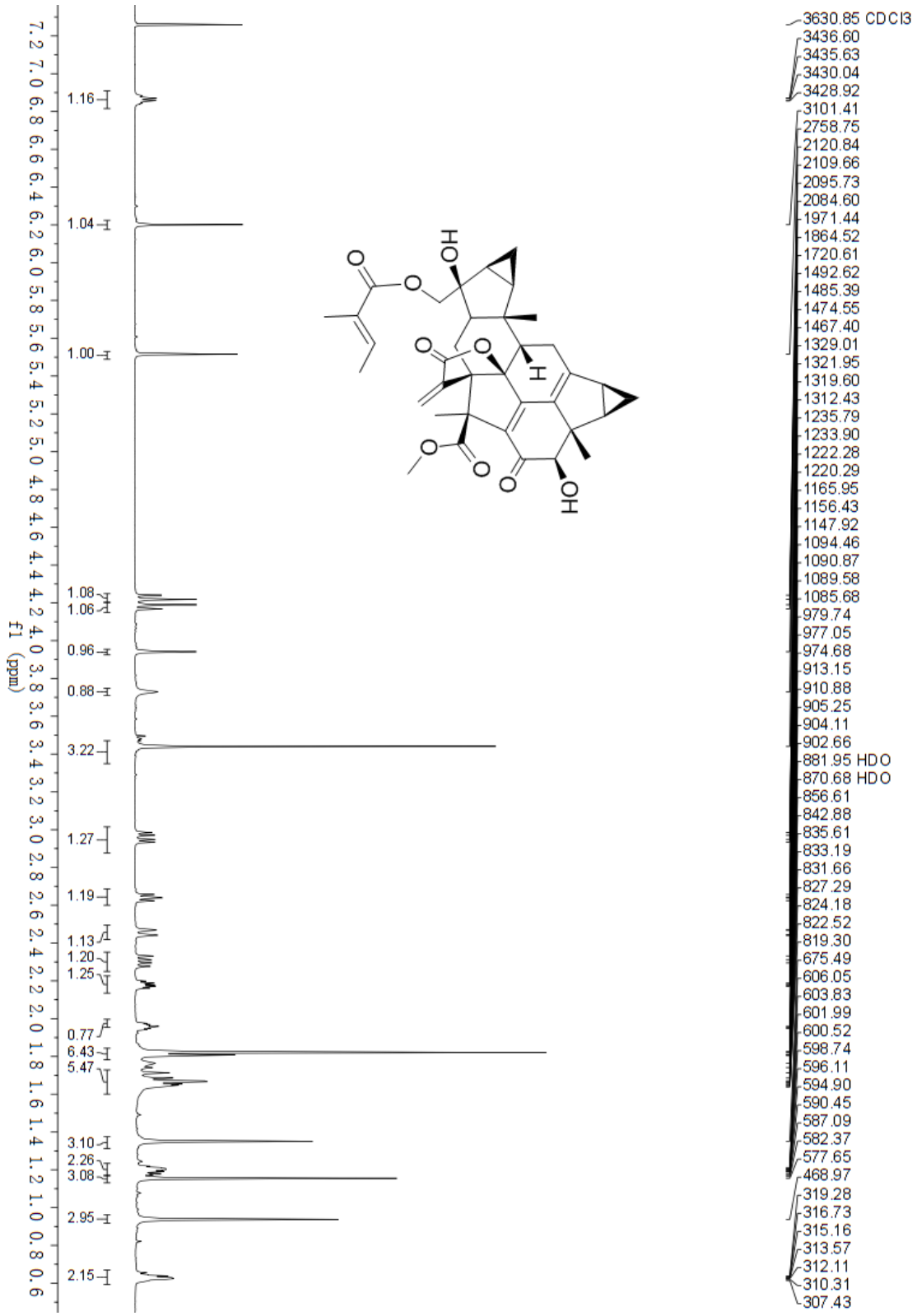


Figure S92. ^{13}C NMR spectrum of fortunilide K (11) in $CDCl_3$

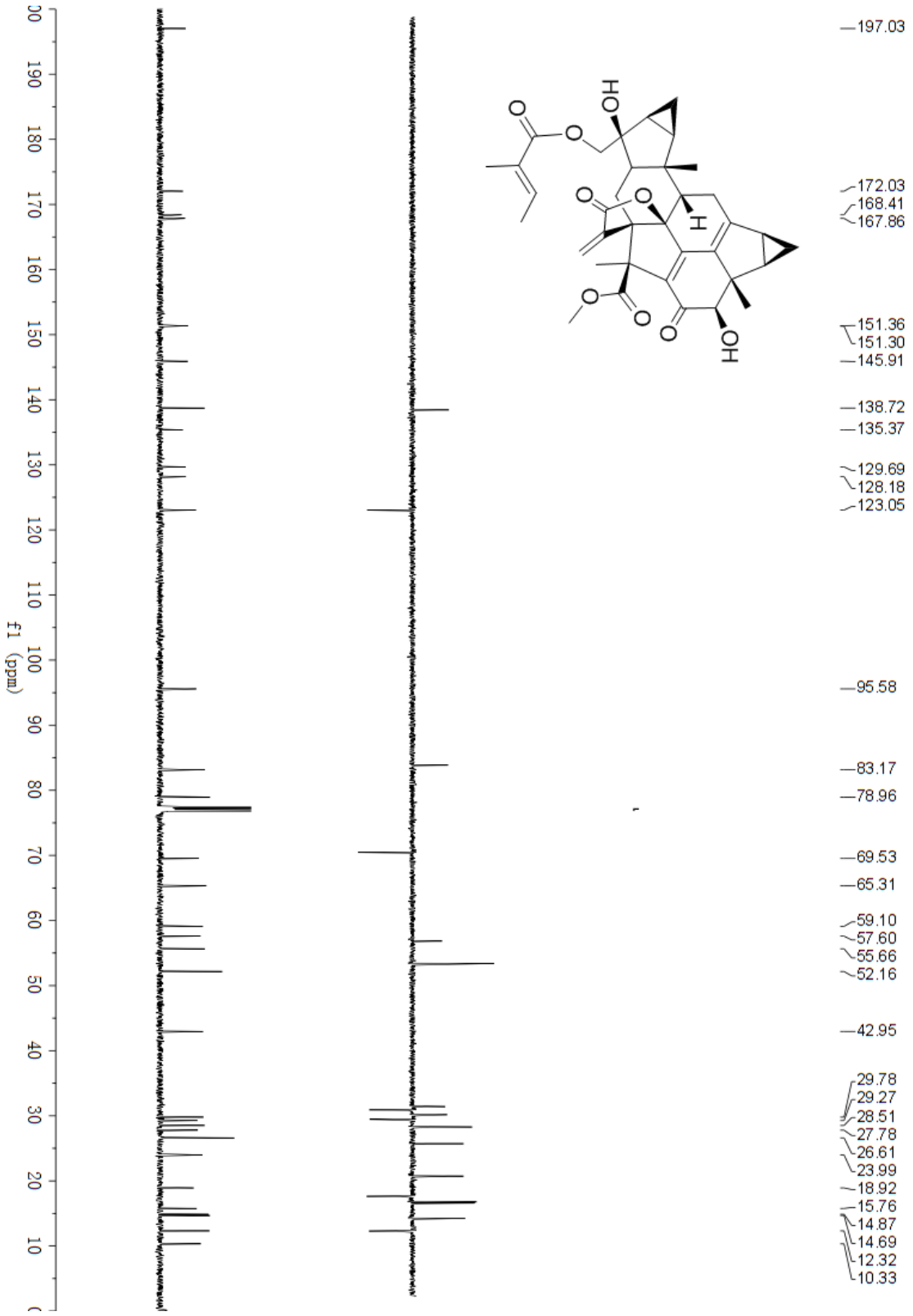


Figure S93. H–H COSY spectrum of fortunilide K (11) in $CDCl_3$

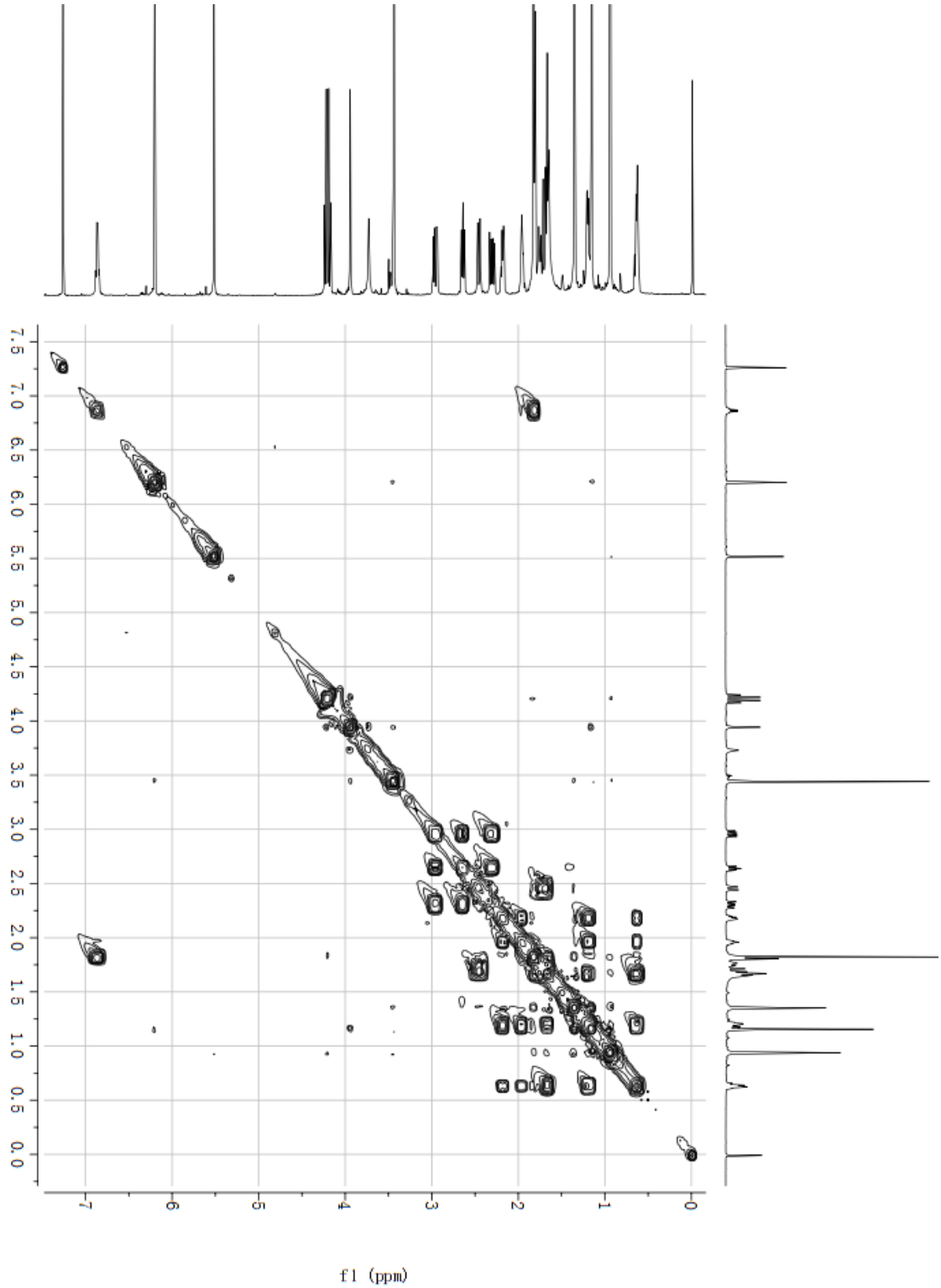


Figure S94. HSQC spectrum of fortunilide K (11) in $CDCl_3$

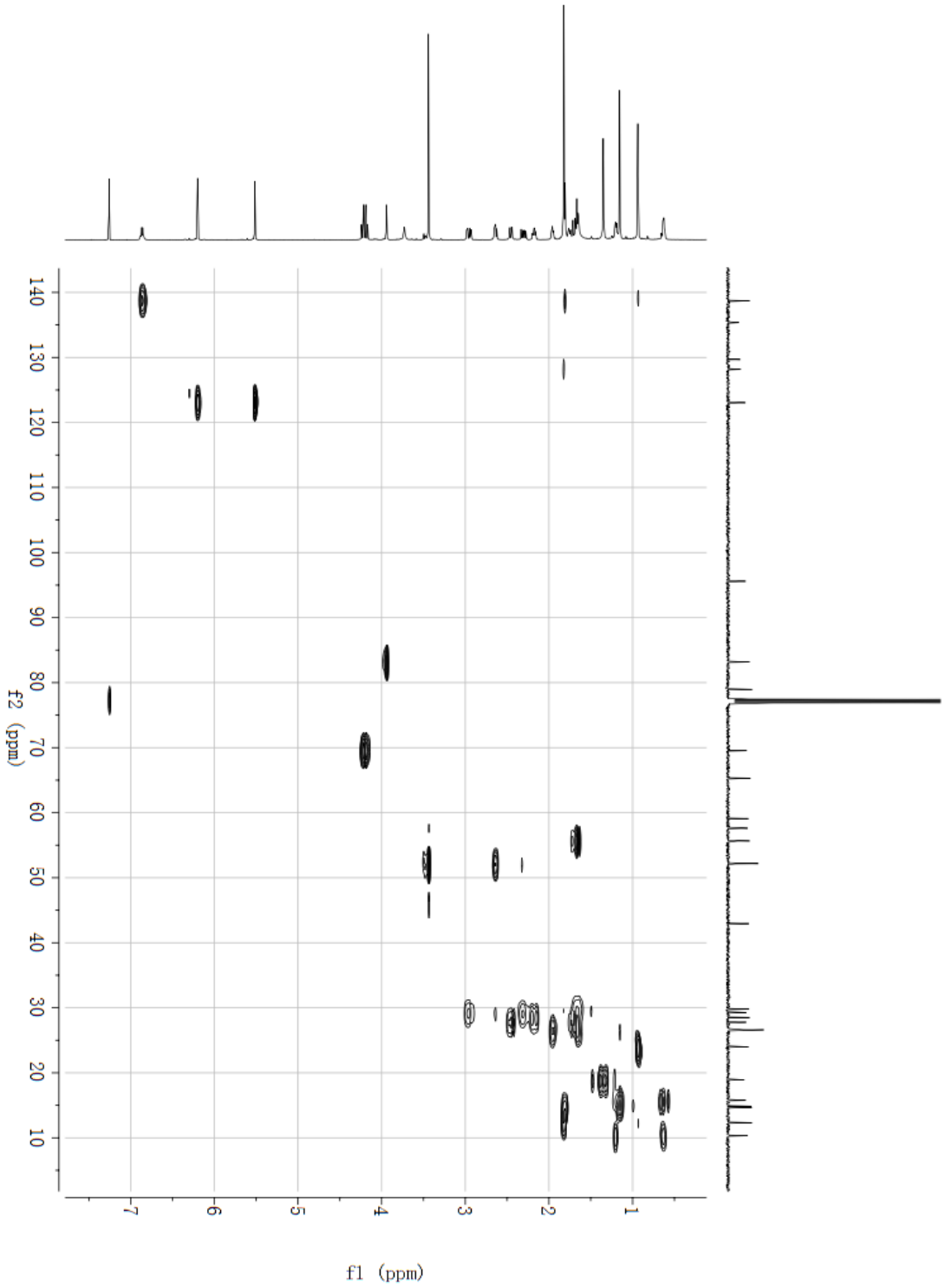


Figure S95. HMBC spectrum of fortunilid K (11) in $CDCl_3$

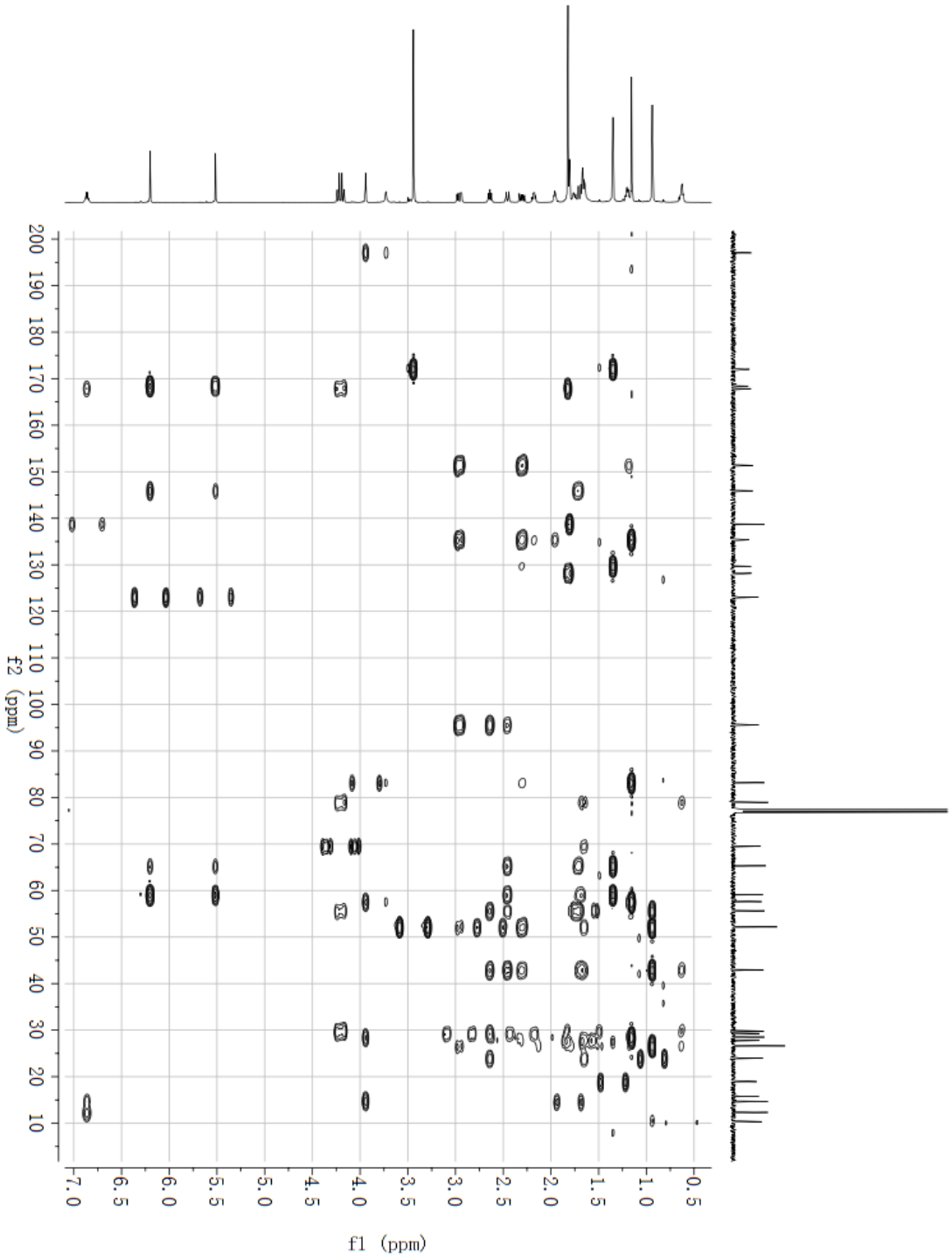


Figure S96. ROESY spectrum of fortunilide K (11)

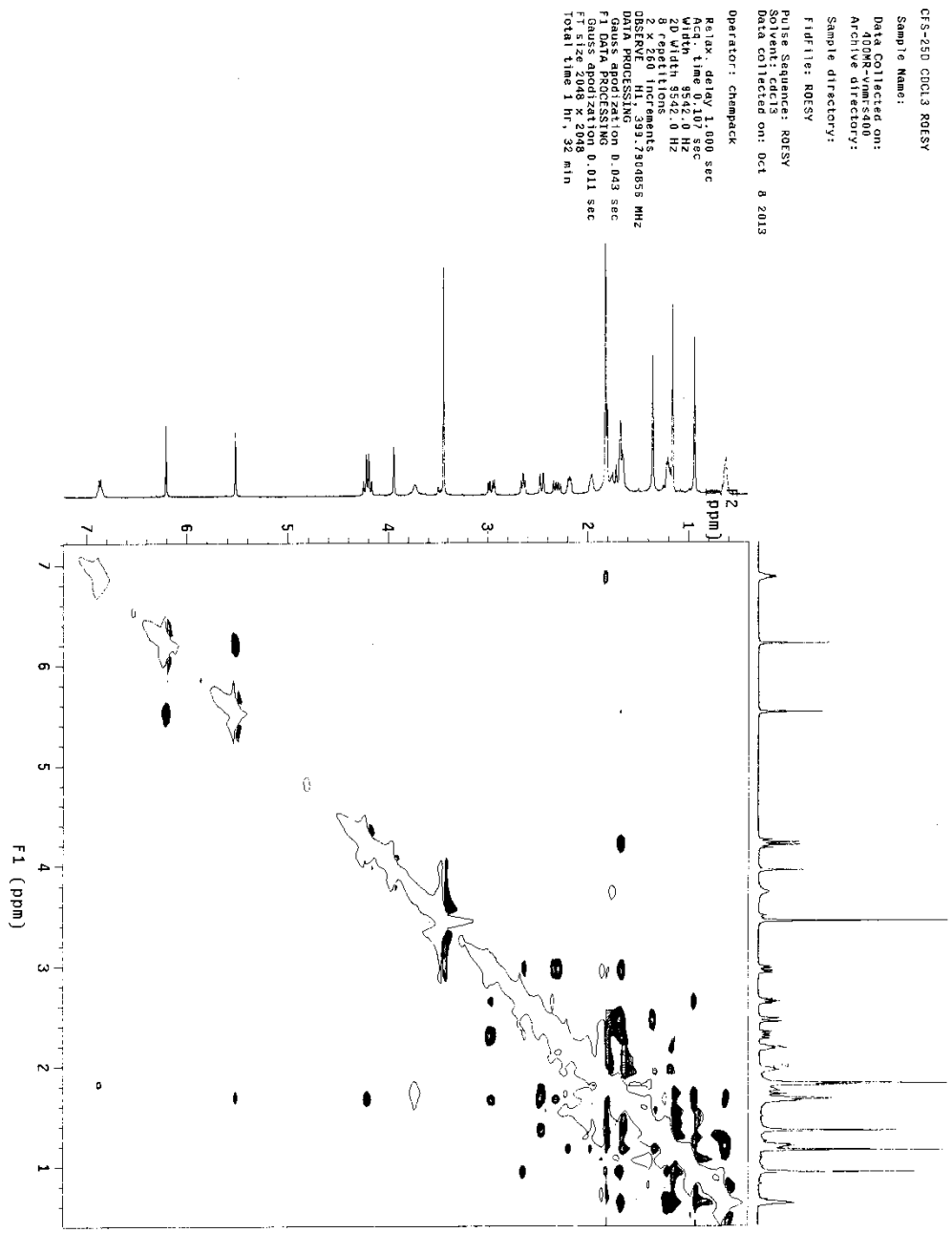


Figure S97. (+)-ESIMS spectrum of fortunilide K (11)

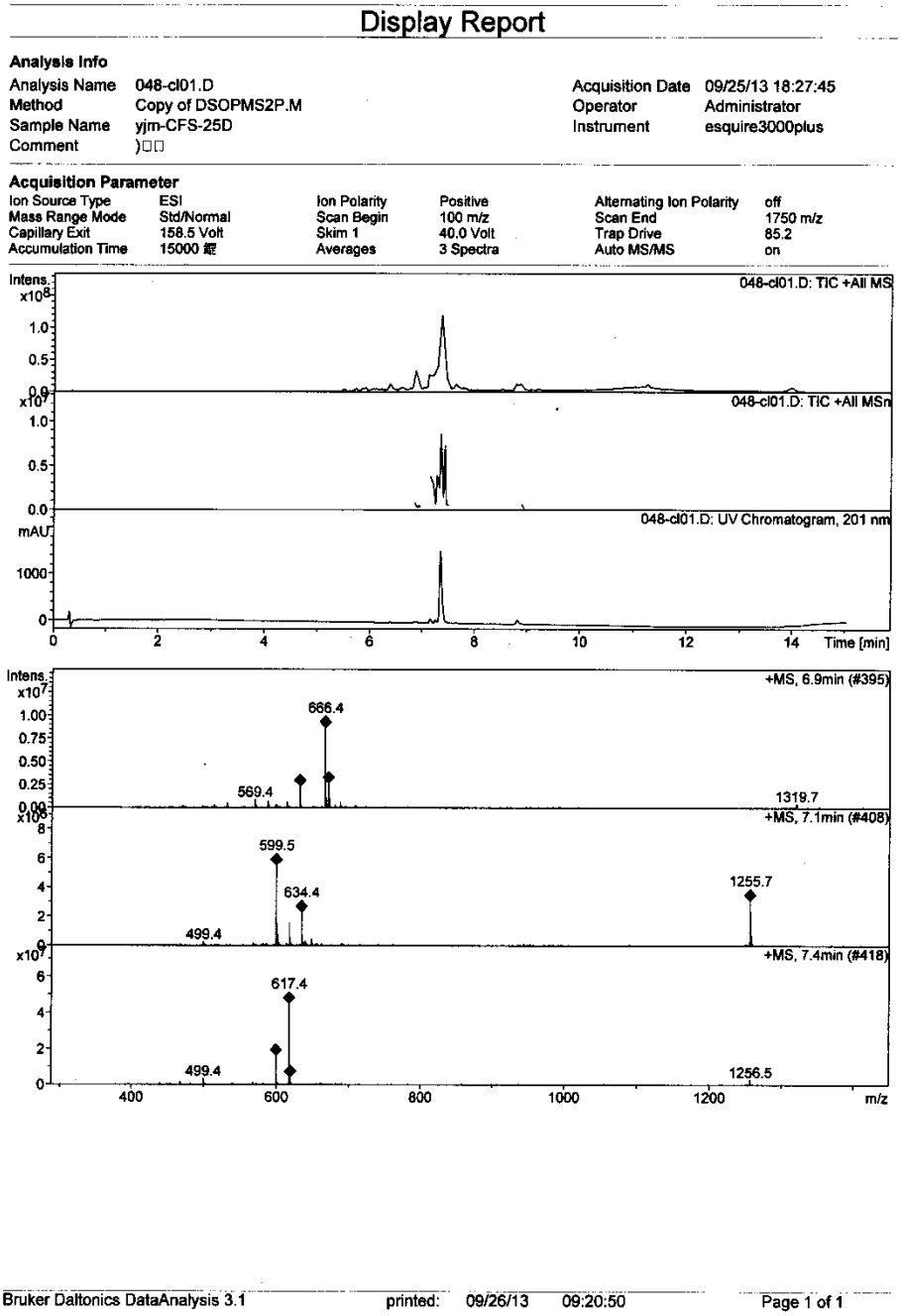


Figure S98. (–)-ESIMS spectrum of fortunilide K (11)

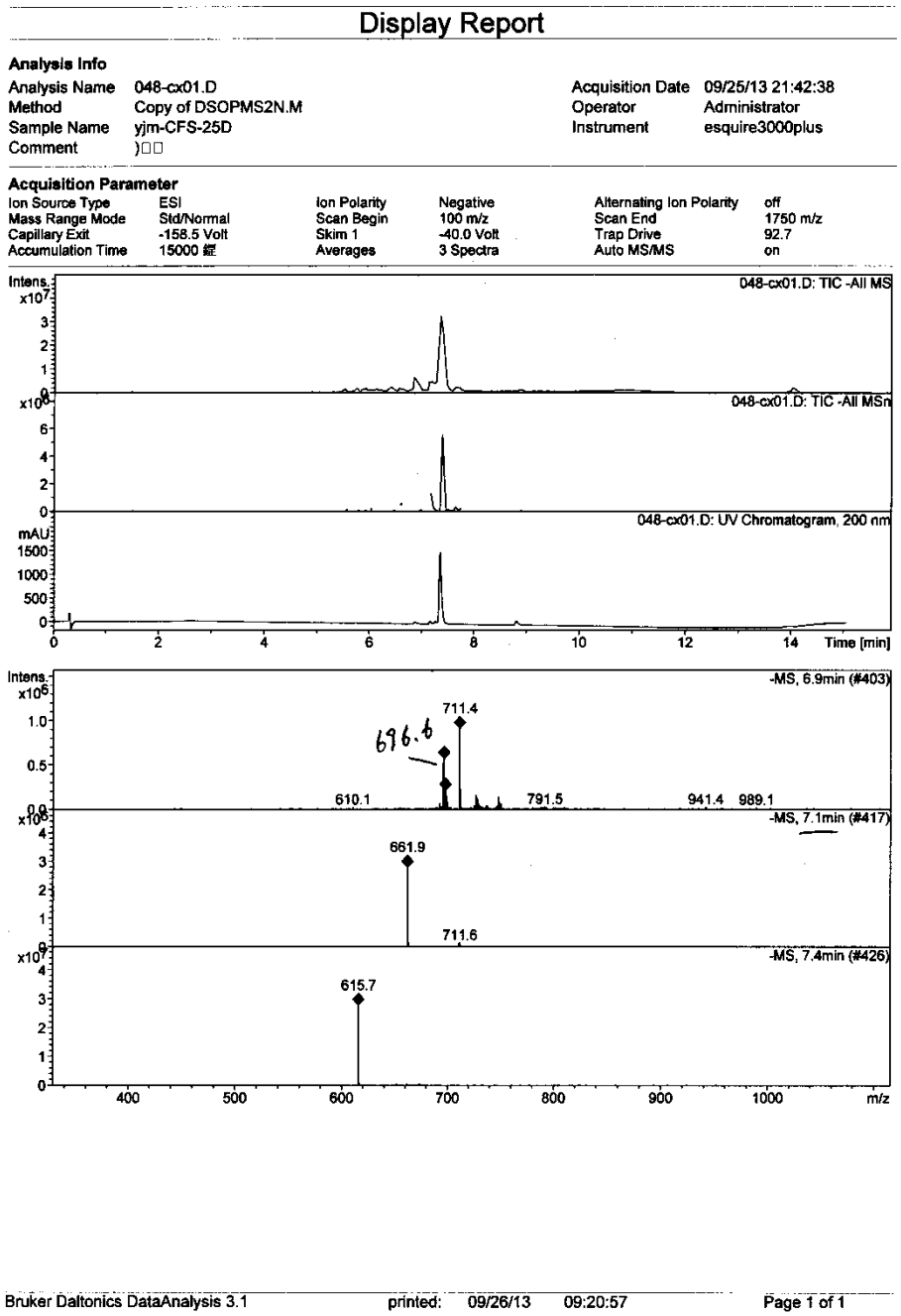


Figure S99. (+)-HRESIMS spectrum of fortunilide K (11)

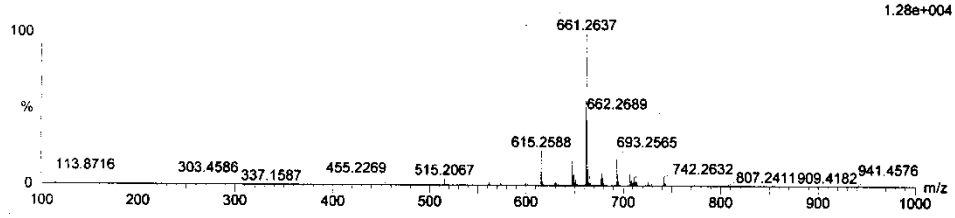
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
130 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-80 H: 2-120 O: 0-20

CFS-25D LCT PXE KE324 27-Sep-2013 10:26:44

CFS-25D_0927 24 (0.528) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (18:32) 1: TOF MS ES- 1.28e+004



Minimum:				-1.5			
Maximum:		3.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
615.2588	615.2594	-0.6	-1.0	17.5	50.6	0.2	C36 H39 O9
	615.2535	5.3	8.6	26.5	52.4	2.0	C43 H35 O4

Figure S100. IR spectrum of fortunilide K (11)

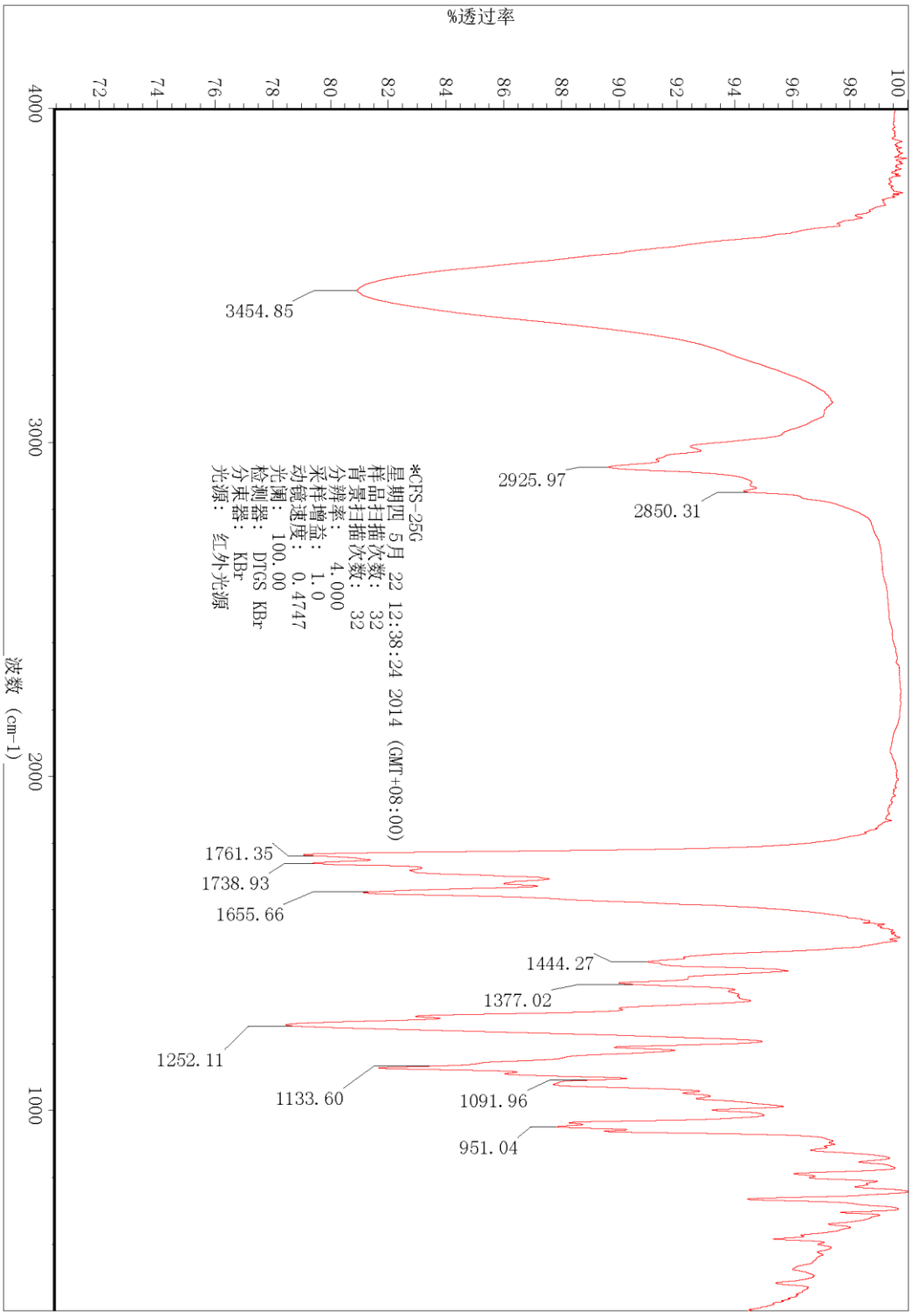


Figure S101. ^{1}H NMR spectrum of fortunilide L (12) in $CDCl_3$

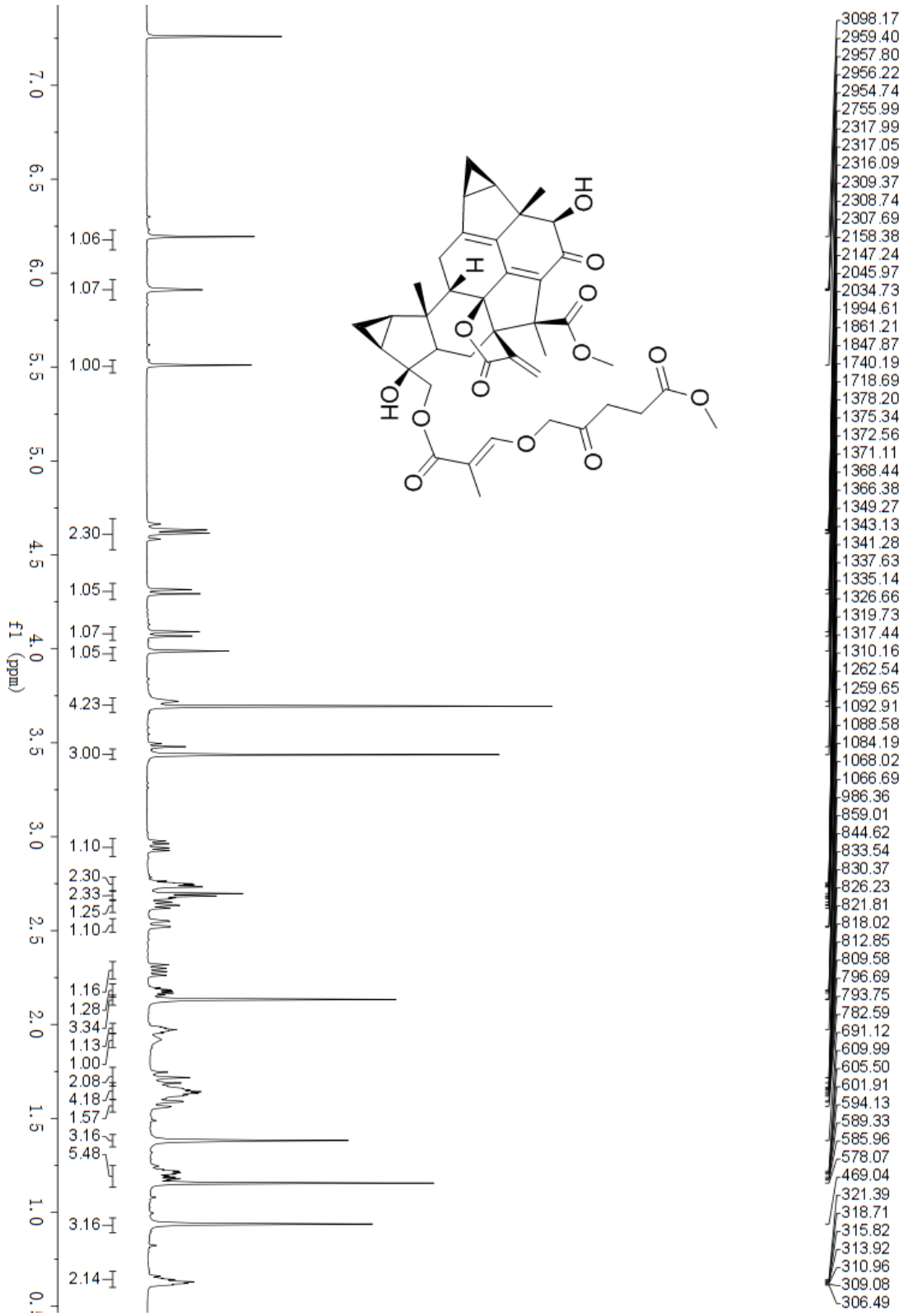


Figure S102. ^{13}C NMR spectrum of fortunilide L (12) in $CDCl_3$

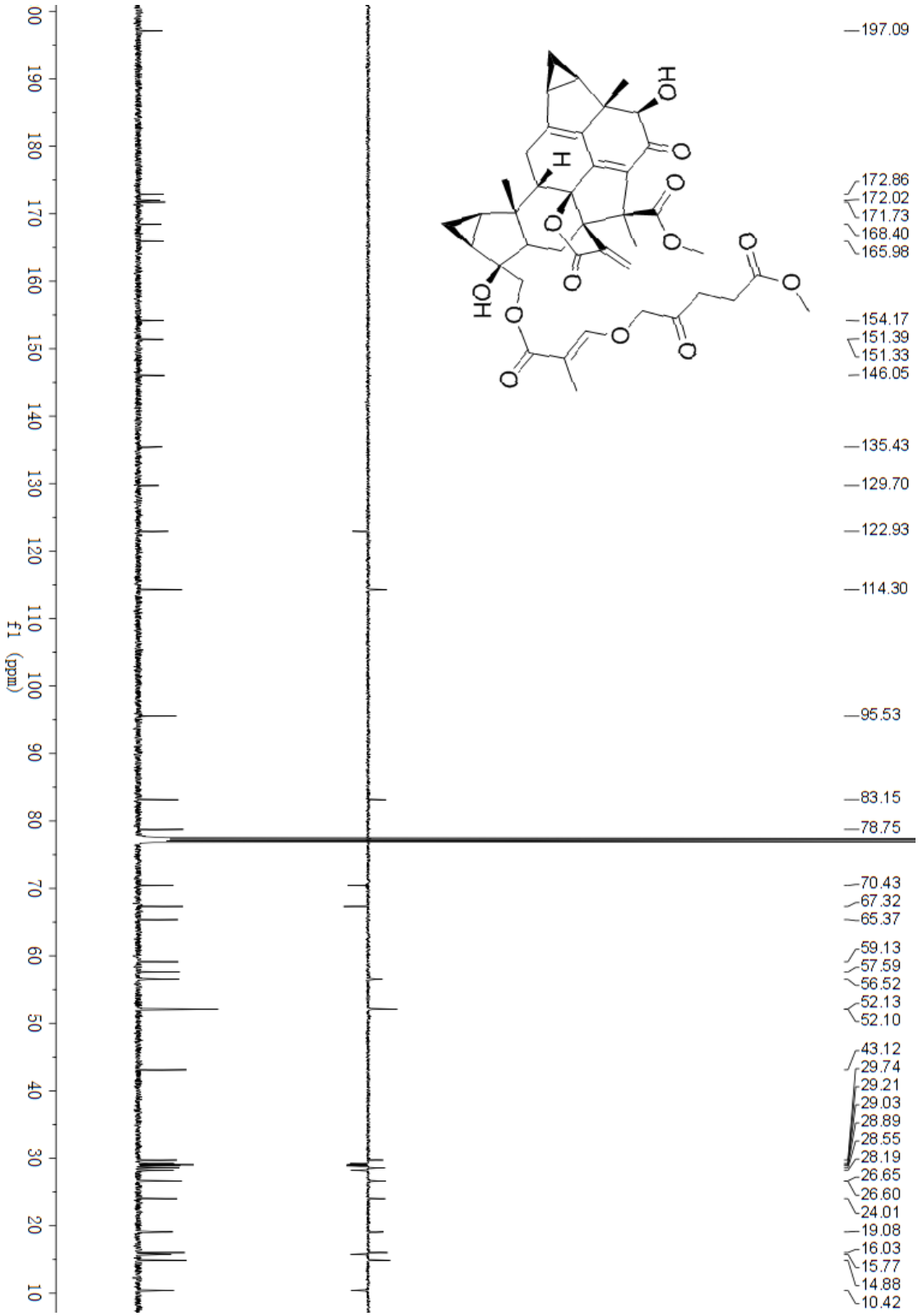


Figure S103. HSQC spectrum of fortunilide L (12) in $CDCl_3$

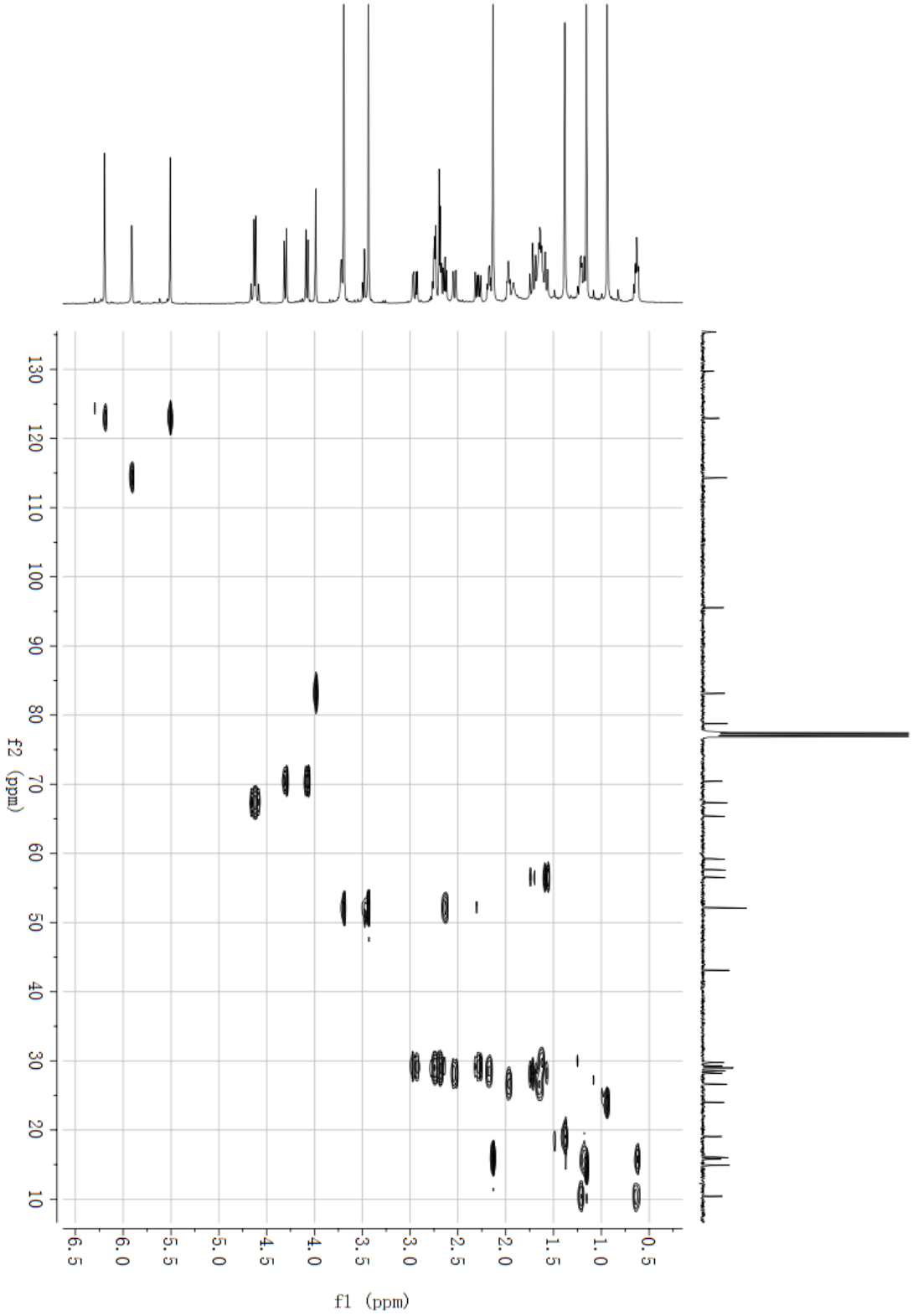


Figure S104. HMBC spectrum of fortunilid L (12) in $CDCl_3$

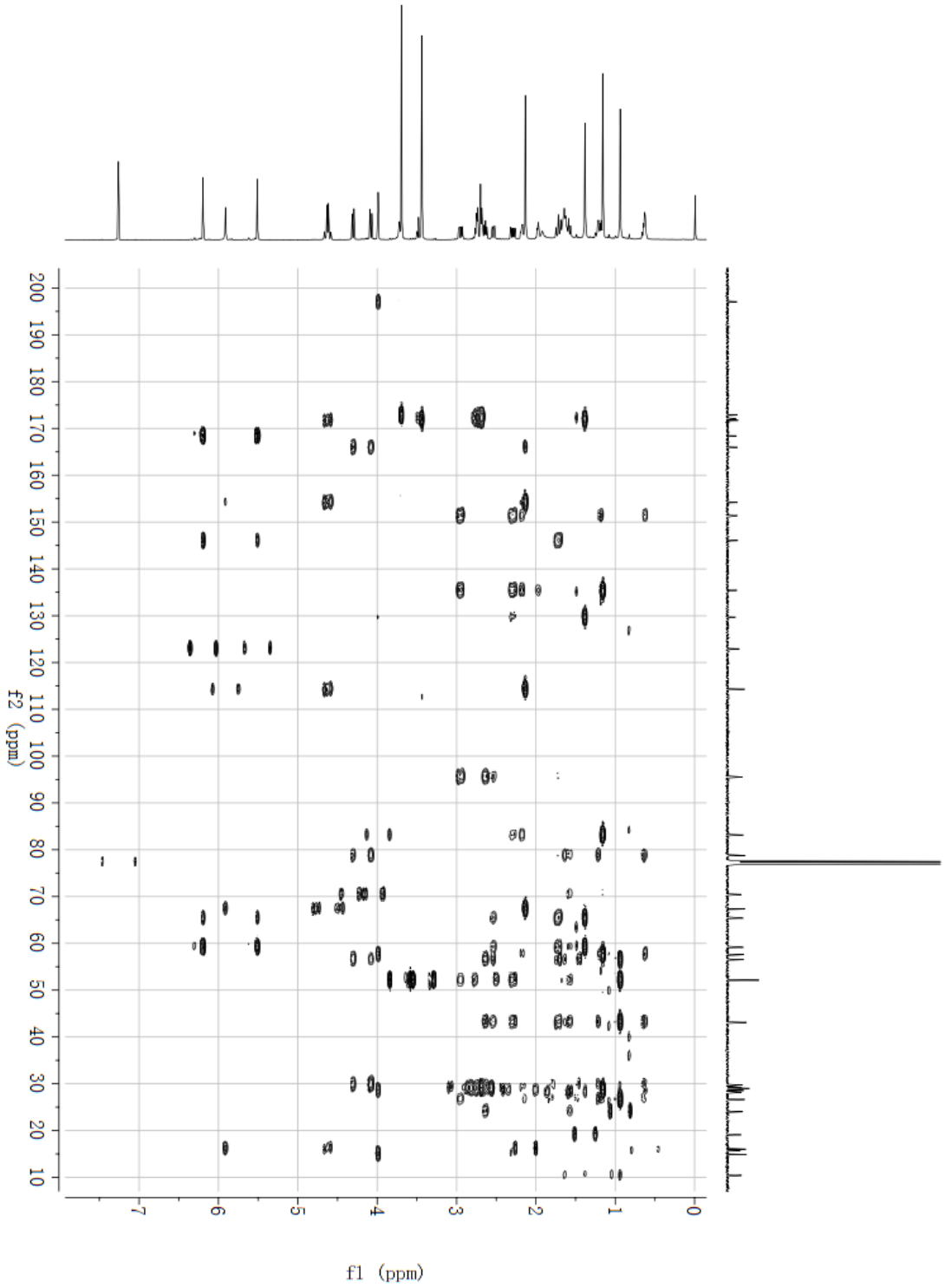


Figure S105. ROESY spectrum of fortunilide L (12)

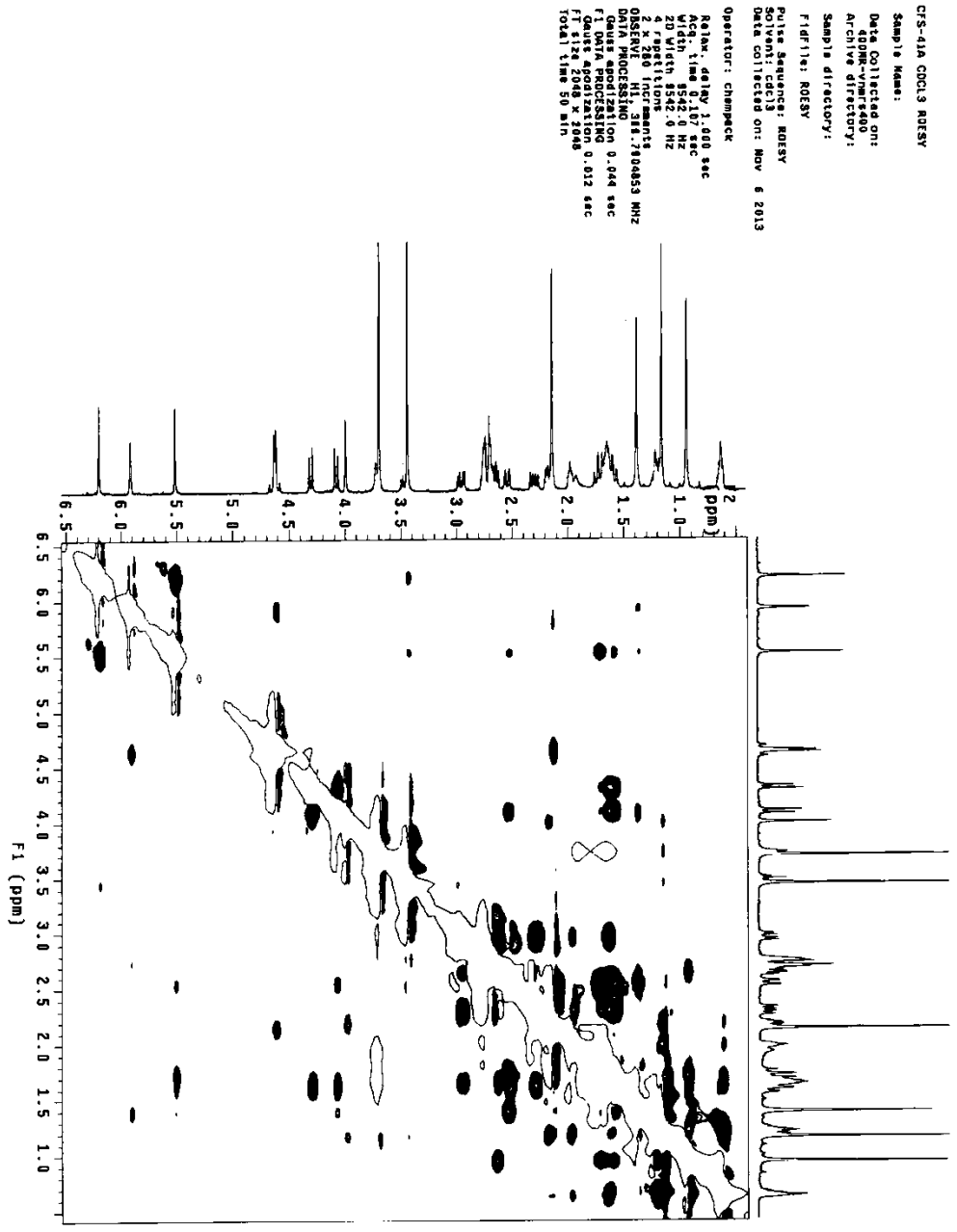


Figure S106. (+)-ESIMS spectrum of fortunilide L (12)

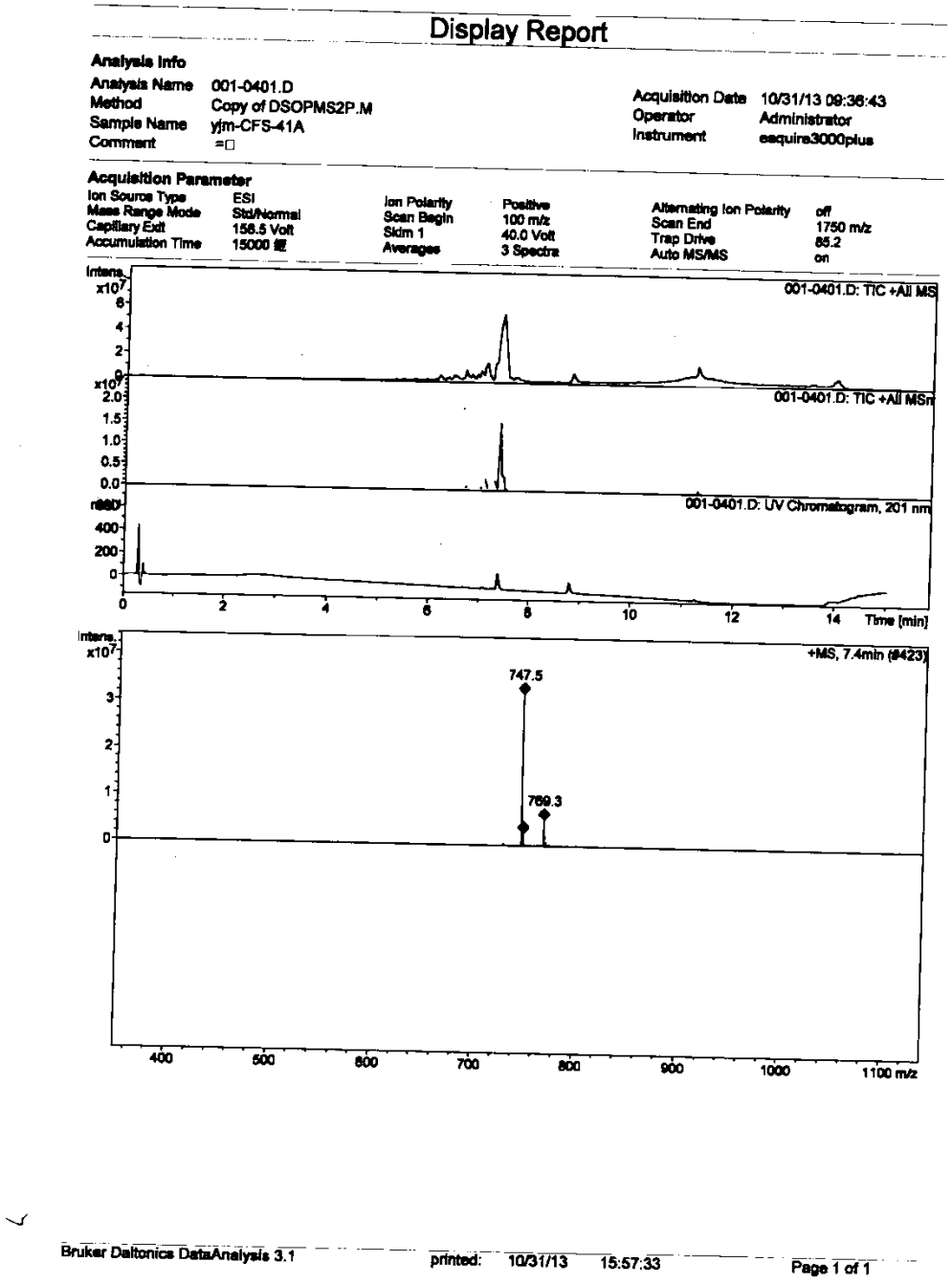


Figure S107. (–)-ESIMS spectrum of fortunilide L (12)

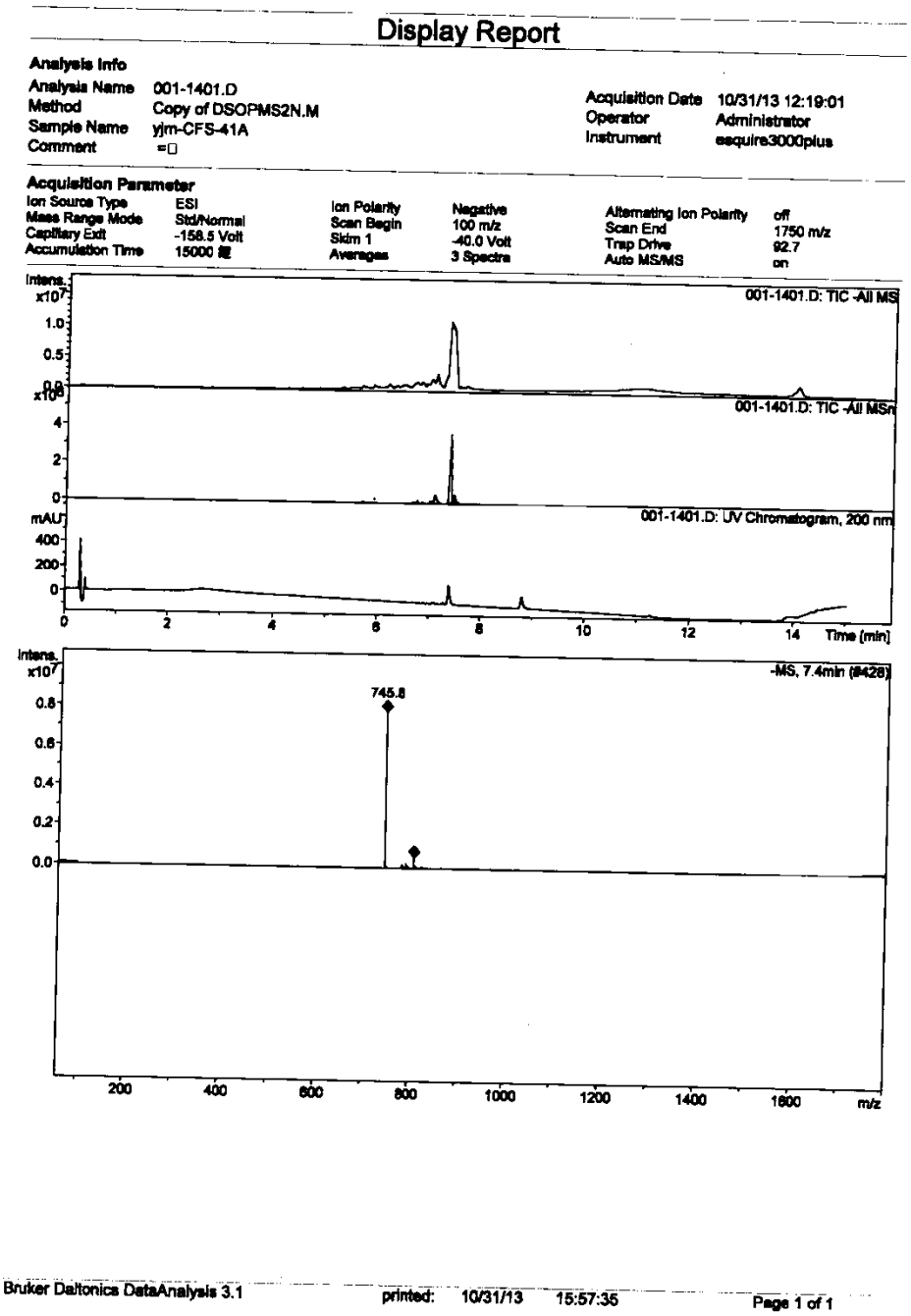


Figure S108. (+)-HRESIMS spectrum of fortunilide L (12)

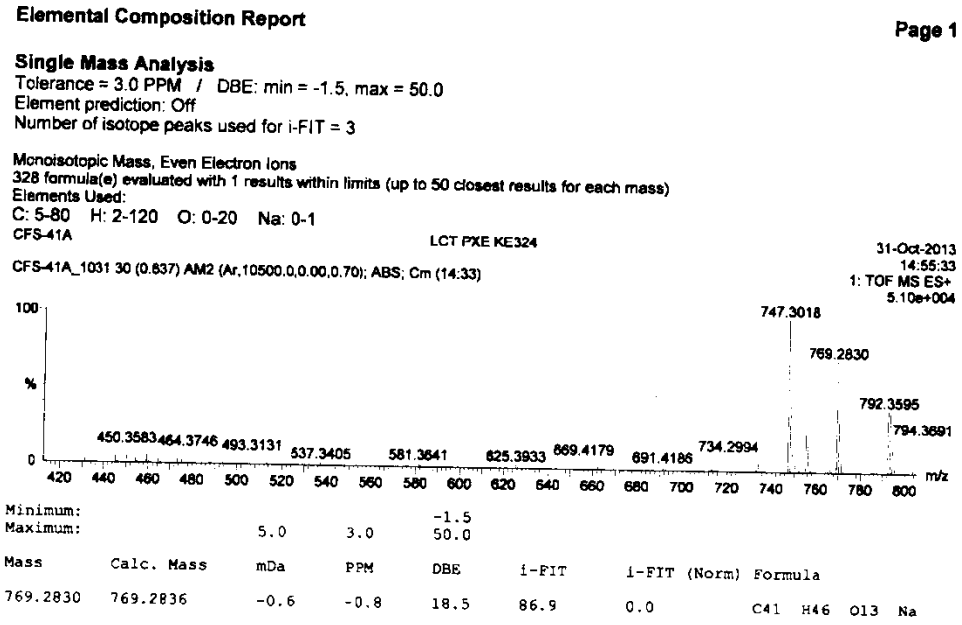


Figure S109. IR spectrum of fortunilide L (12)