Electronic Supplementary Information for

New Rearranged Limonoids from *Walsura cochinchinensis*

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Figure S99. HRESI(+)MS spectrum of walsucochinoid N (**12**)
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Figure S101. ^{1}H NMR spectrum of walsucochinoid O (**13**) in $CDCl_3$
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Figure S103. HSQC spectrum of walsucochinoid O (**13**) in $CDCl_3$
Figure S104. HMBC spectrum of walsucochinoid O (**13**) in $CDCl_3$

Table S1. X-ray crystallographic data for walsucochinoid C (**1**).[a]

Empirical formula	$C_{27}H_{32}O_4$
Formula weight	420.53
Temperature	133(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	*a* = 5.96350 (10) Å, α = 90° *b* = 13.7471 (3) Å, β = 90° *c* = 28.1129 (6) Å, γ = 90°
Volume	2304.72(8) $Å^3$
Z	4
Calculated density	1.212 Mg/m^3
Absorption coefficient	0.636 mm^{-1}
F(000)	904
Crystal size	0.499 × 0.226 × 0.152 mm^3
Theta range for data collection	3.14 to 64.98°
Index ranges	-6<=h<=6, -16<=k<=16, -32<=l<=33
Reflections collected	17561
Independent collections	3887 [R(int) = 0.0362]
Completeness to theta = 66.32°	99.8 %
Absorption correction	Semi-empirical
Max. and min. transmission	0.7535 and 0.5818
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3887 / 0 / 287
Goodness-of-fit on F^2	1.086
Final R indices [I>2σ(I)]	R1 = 0.0419, wR2 = 0.1162
R indices (all data)	R1 = 0.0420, wR2 = 0.1163
Absolute structure parameter	0.0(2)
Largest diff. peak and hole	0.416 and –0.424 e. $Å^{-3}$

[a] **1** was crystallized from MeOH/H_2O (50:1)

Table S2. X-ray crystallographic data for walsucochinoid L (**10**).[a]

Empirical formula	$C_{27}H_{36}O_4$
Formula weight	424.56
Temperature	133(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 8.2016 (5) Å, α = 90° b = 10.1084 (6) Å, β = 90° c = 13.3847 (8) Å, γ = 90°
Volume	1109.36(12) $Å^3$
Z	2
Calculated density	1.271 Mg/m^3
Absorption coefficient	0.661 mm^{-1}
F(000)	460
Crystal size	0.15 × 0.12 × 0.10 mm^3
Theta range for data collection	3.30 to 64.98°
Index ranges	-8<=h<=9,-11<=k<=11,-15<=l<=15
Reflections collected	6271
Independent collections	3273 [R(int) = 0.0622]
Completeness to theta = 66.32°	94.4 %
Absorption correction	Semi-empirical
Max. and min. transmission	0.9368 and 0.9073
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3273 / 1 / 289
Goodness-of-fit on F^2	1.069
Final R indices [I>2σ(I)]	R1 = 0.0704, wR2 = 0.1858
R indices (all data)	R1 = 0.0725, wR2 = 0.1884
Absolute structure parameter	0.0(4)
Largest diff. peak and hole	0.395 and –0.319 e. $Å^{-3}$

[a] **10** was crystallized from MeOH/H_2O (100:1)

Figure S1. ^{1}H NMR spectrum of walsucochinoid C (**1**) in $CDCl_3$

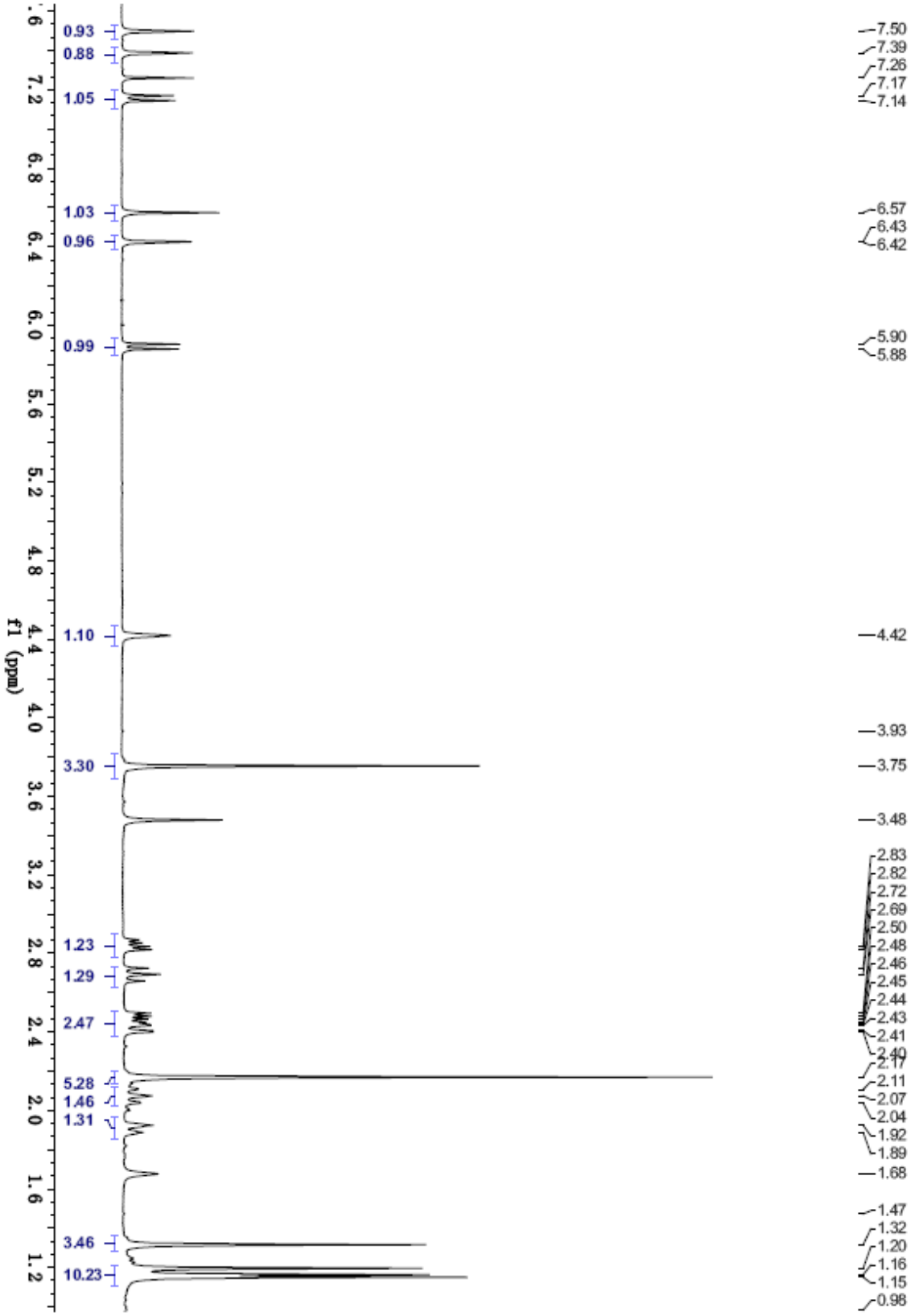


Figure S2. ^{13}C NMR spectrum of walsucochinoid C (**1**) in $CDCl_3$

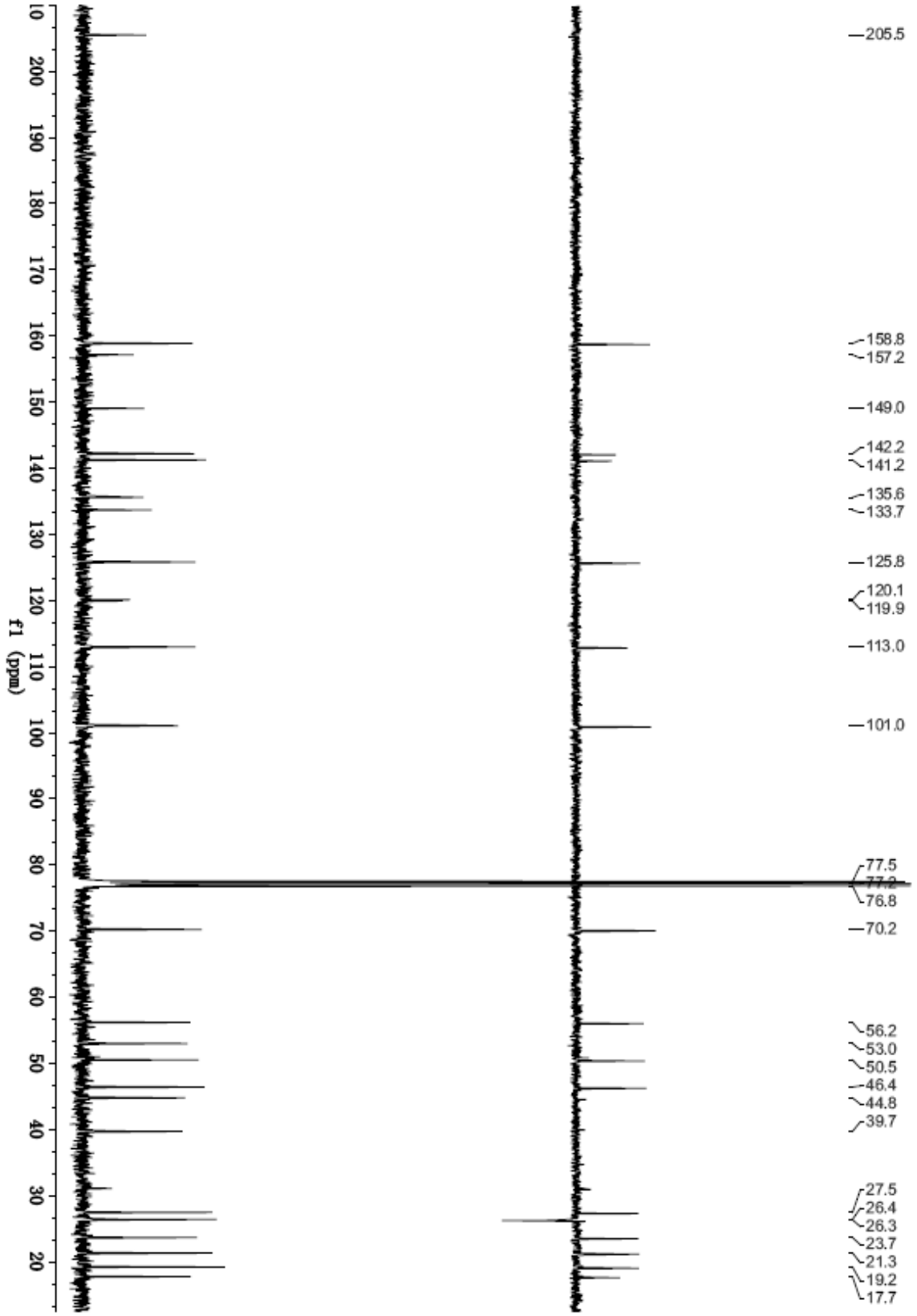


Figure S3. HSQC spectrum of walsucochinoid C (**1**) in $CDCl_3$

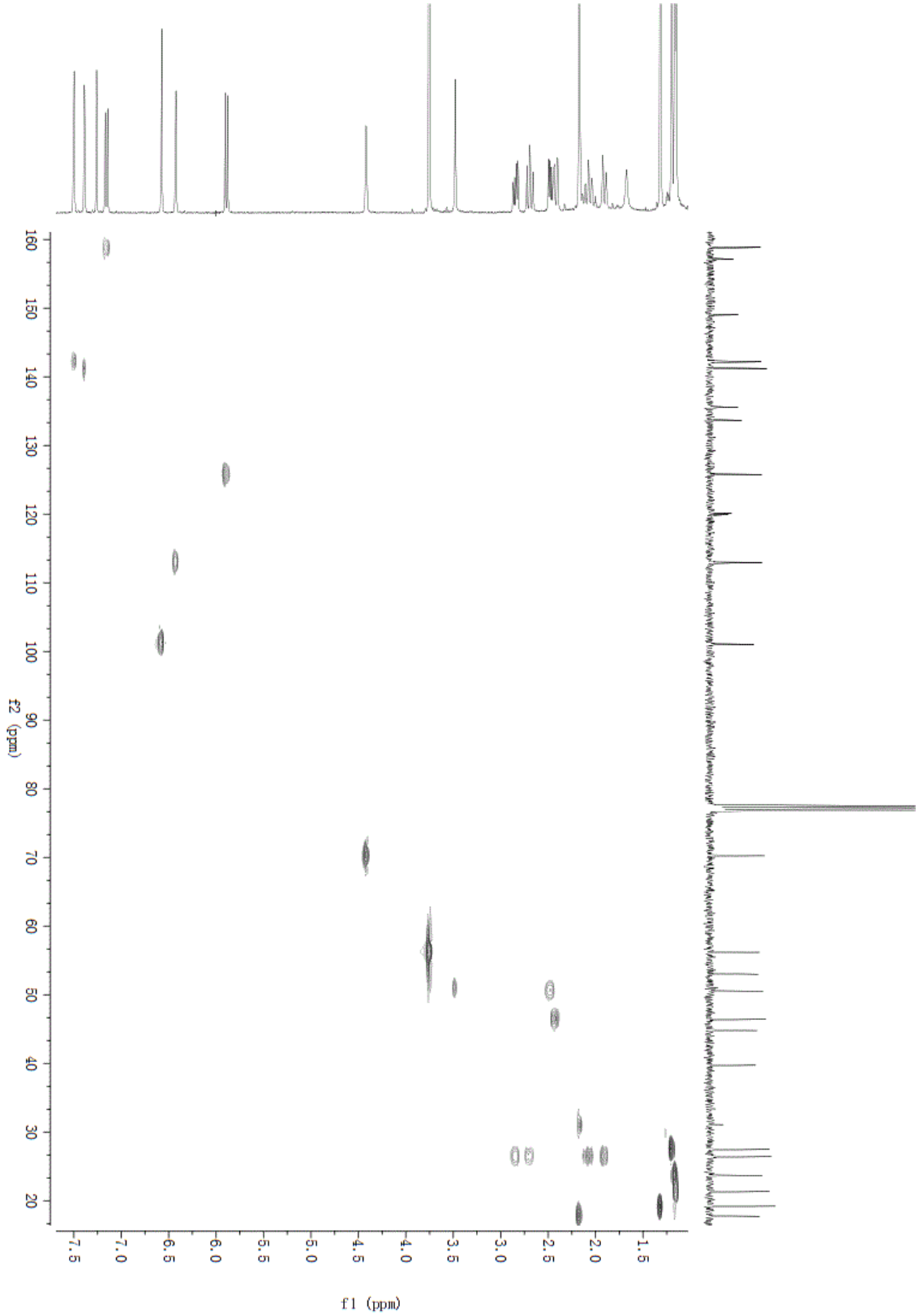


Figure S4. HMBC spectrum of walsucochinoid C (**1**) in $CDCl_3$

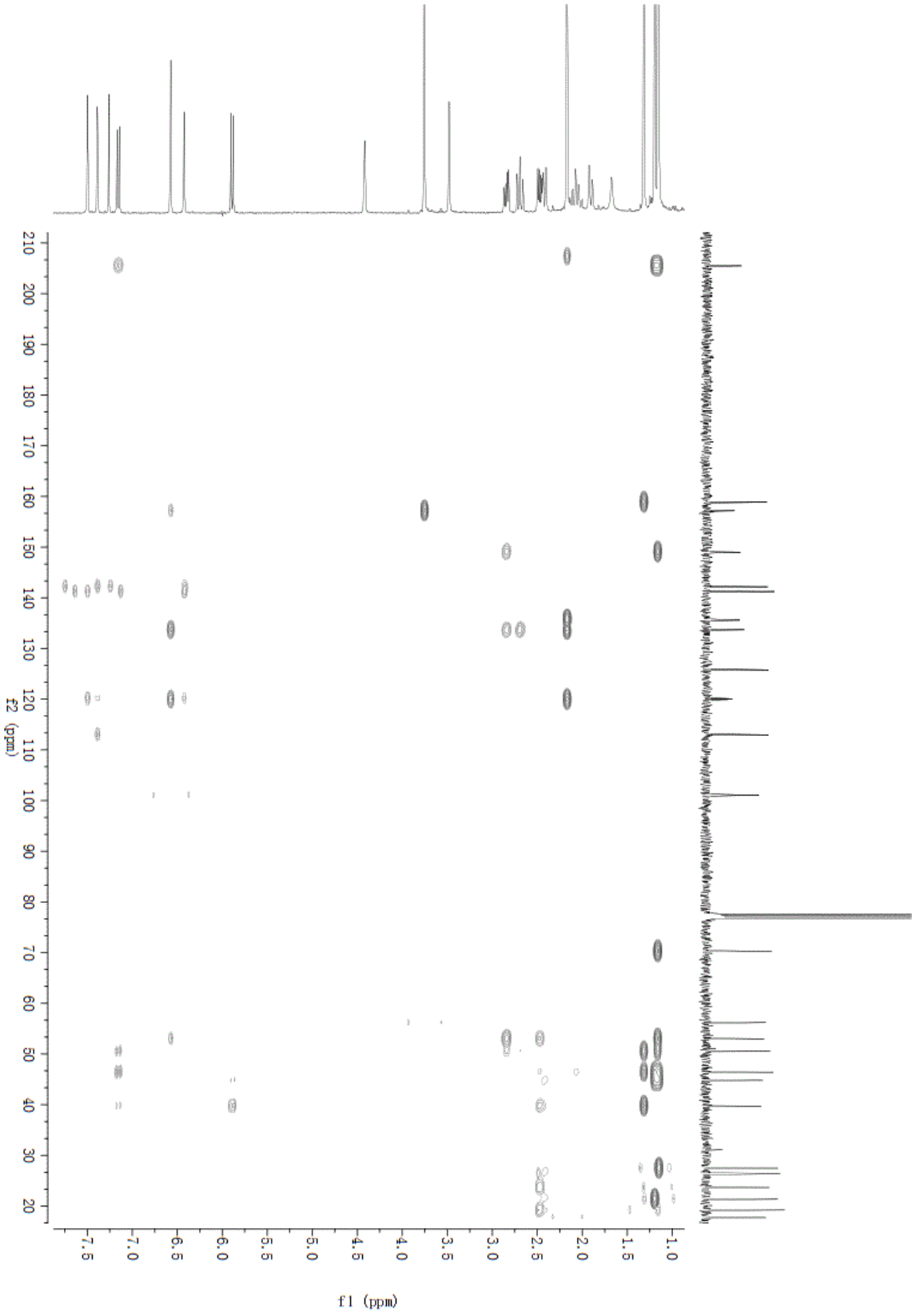


Figure S5. NOESY spectrum of walsucochinoid C (**1**) in $CDCl_3$

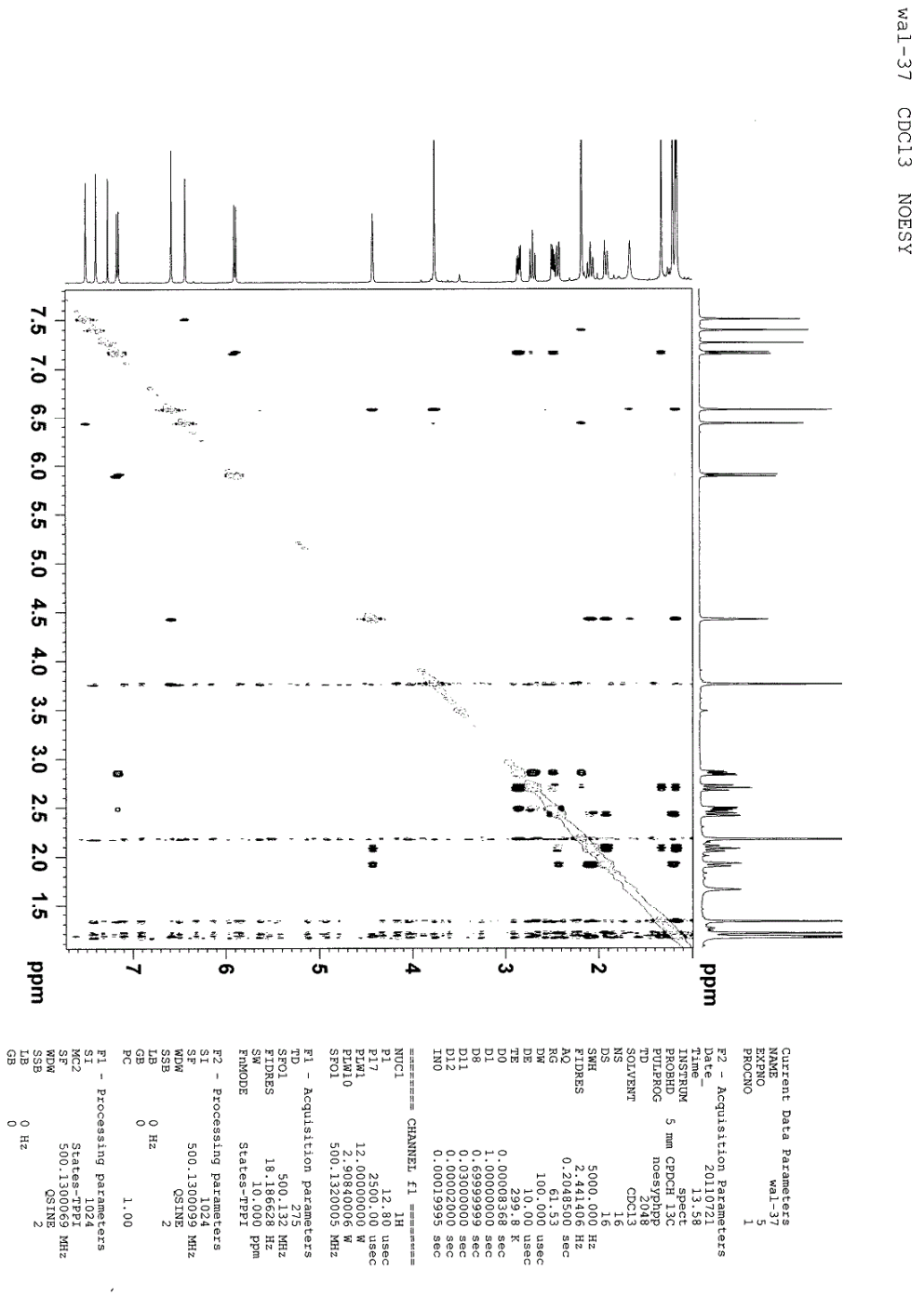


Figure S6. ESI(+)MS spectrum of walsucochinoid C (**1**)

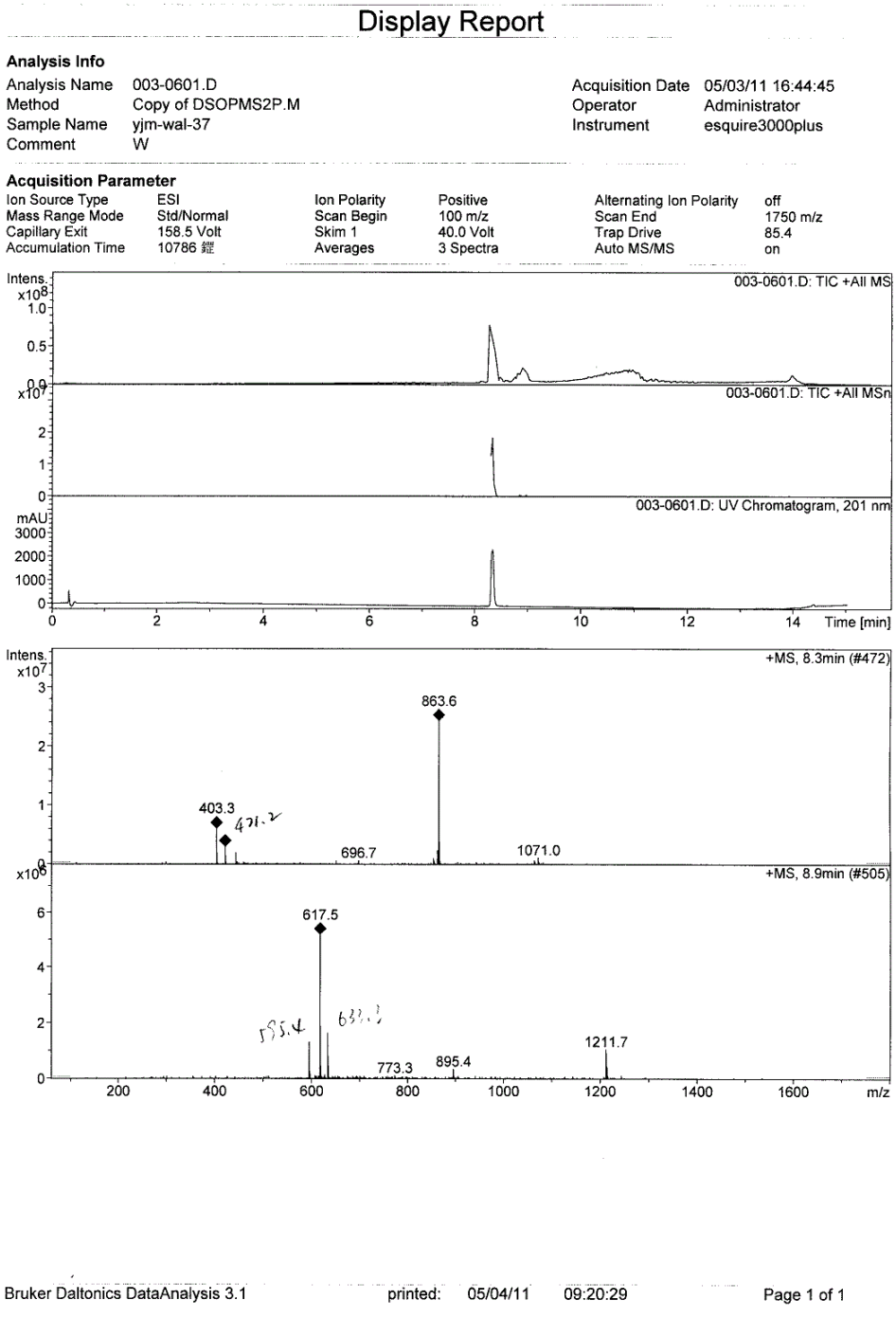


Figure S7. ESI(–)MS spectrum of walsucochinoid C (**1**)

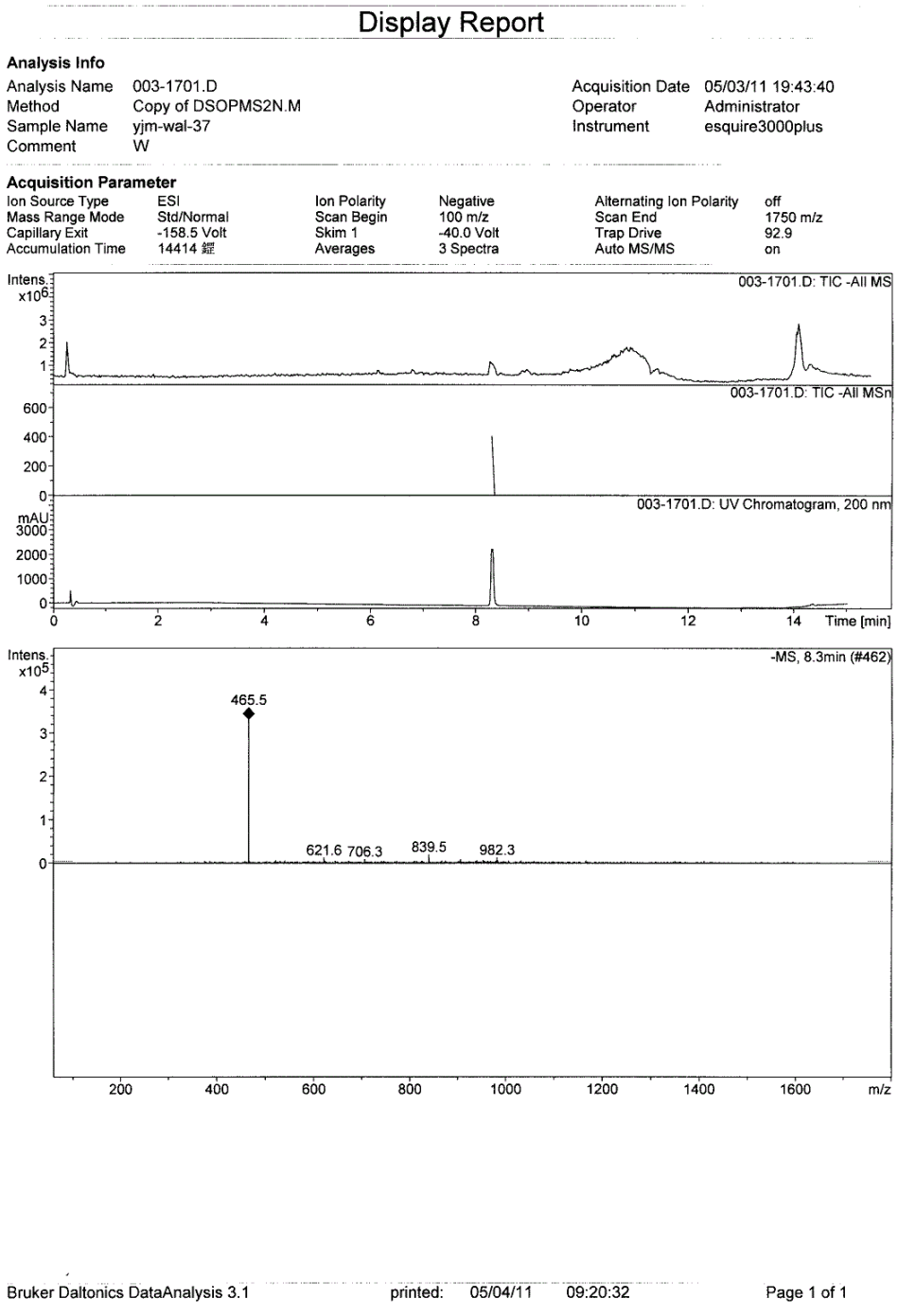


Figure S8. HRESI(–)MS spectrum of walsucochinoid C (**1**)

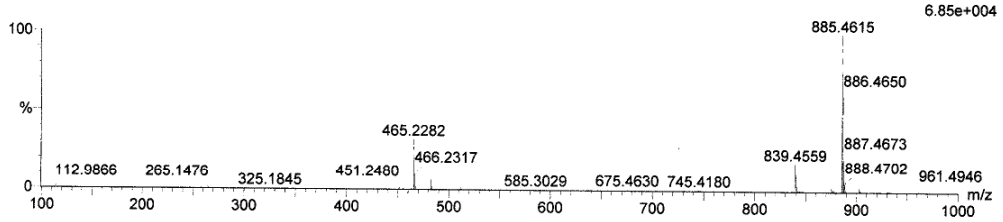
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
105 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30

WAL-37 LCT PXE KE324 04-Nov-2011 16:19:50

WAL-37_1104 13 (0.283) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (13:37) 1: TOF MS ES- 6.85e+004



Minimum:				-1.5			
Maximum:		2.0	2.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
465.2282	465.2277	0.5	1.1	12.5	117.3	0.0	C28 H33 O6

Figure S9. IR spectrum of walsucochinoid C (**1**)

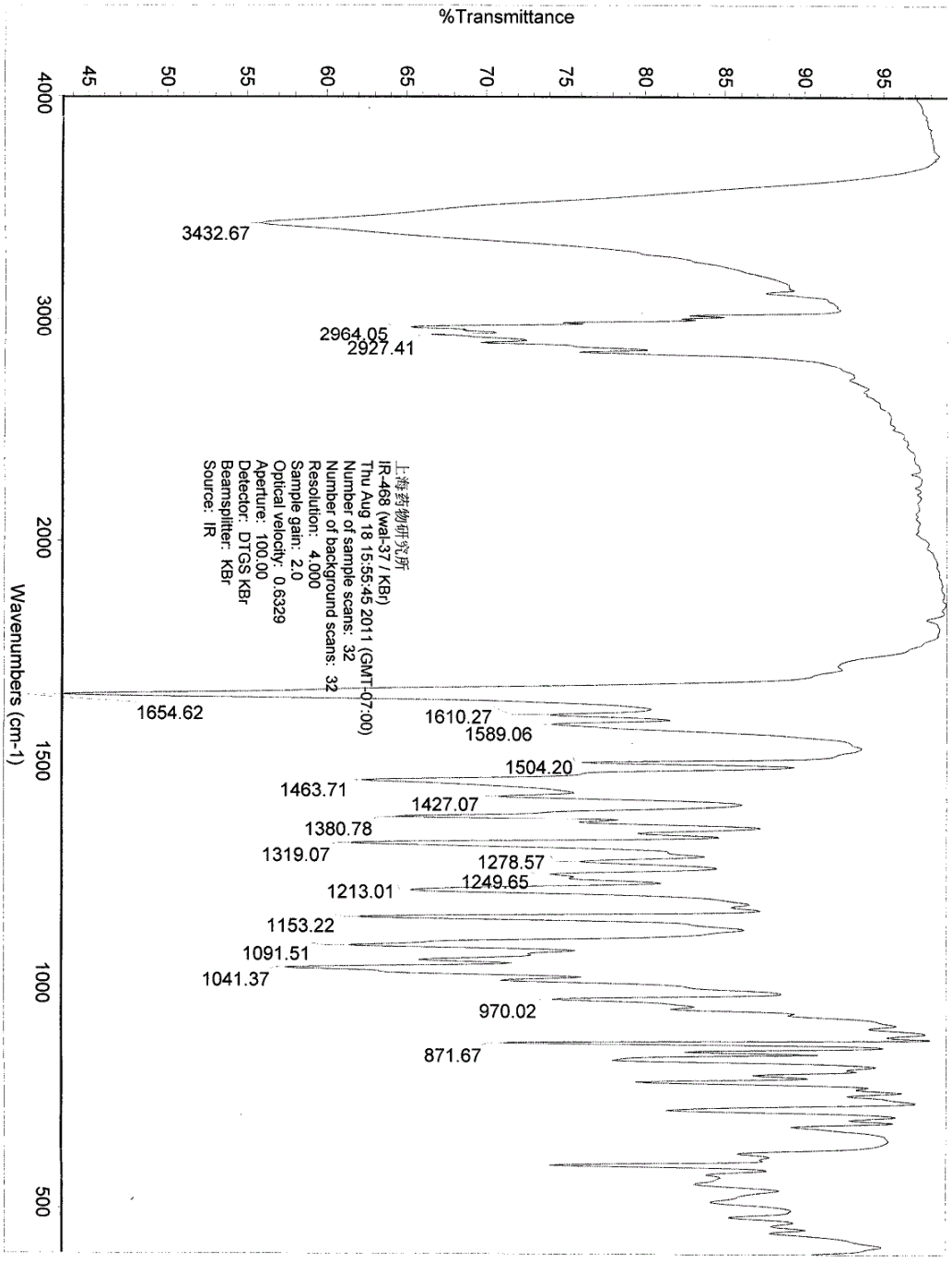


Figure S10. ^{1}H NMR spectrum of walsucochinoid D (**2**) in $CDCl_3$

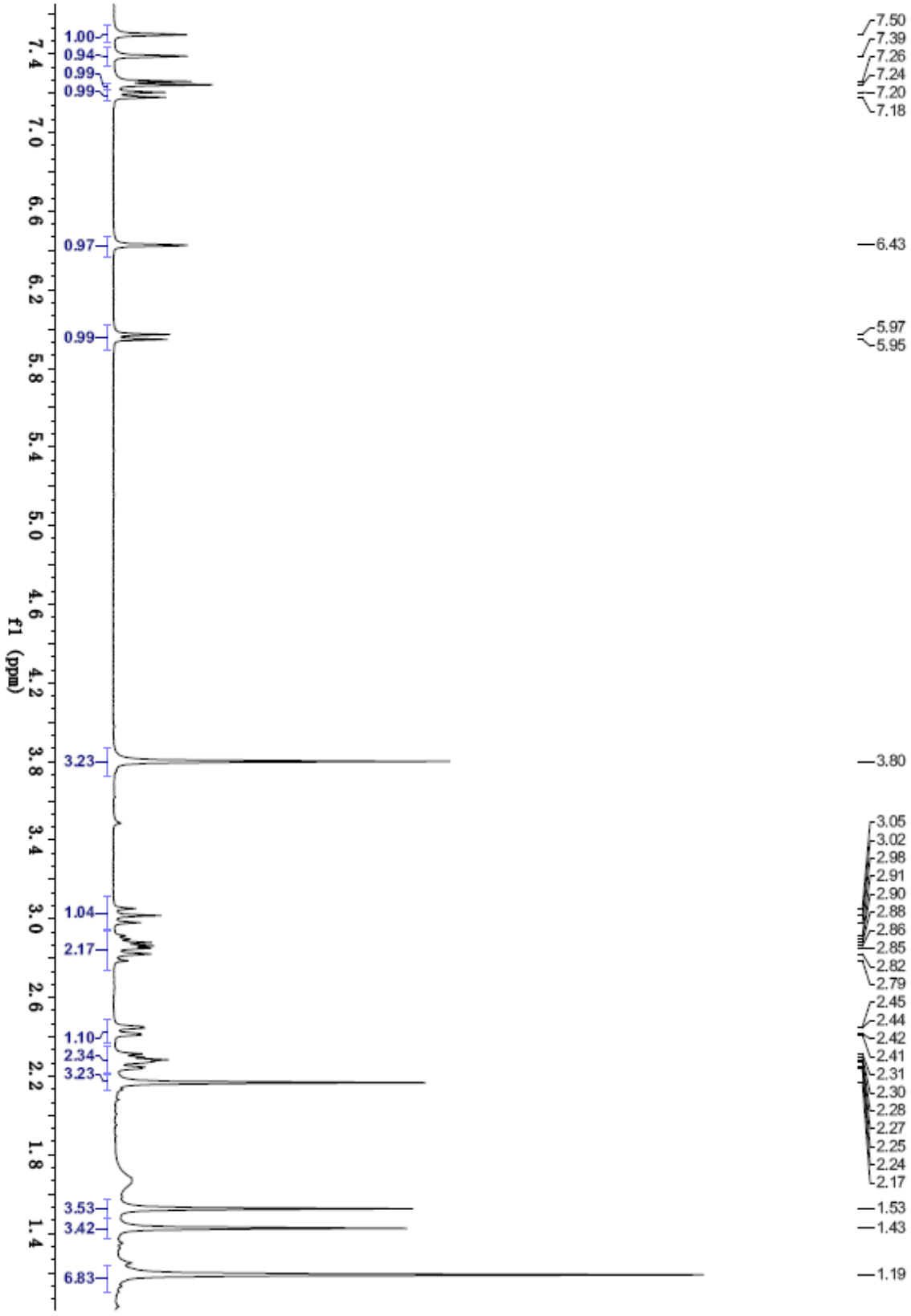


Figure S11. ^{13}C NMR spectrum of walsucochinoid D (**2**) in $CDCl_3$

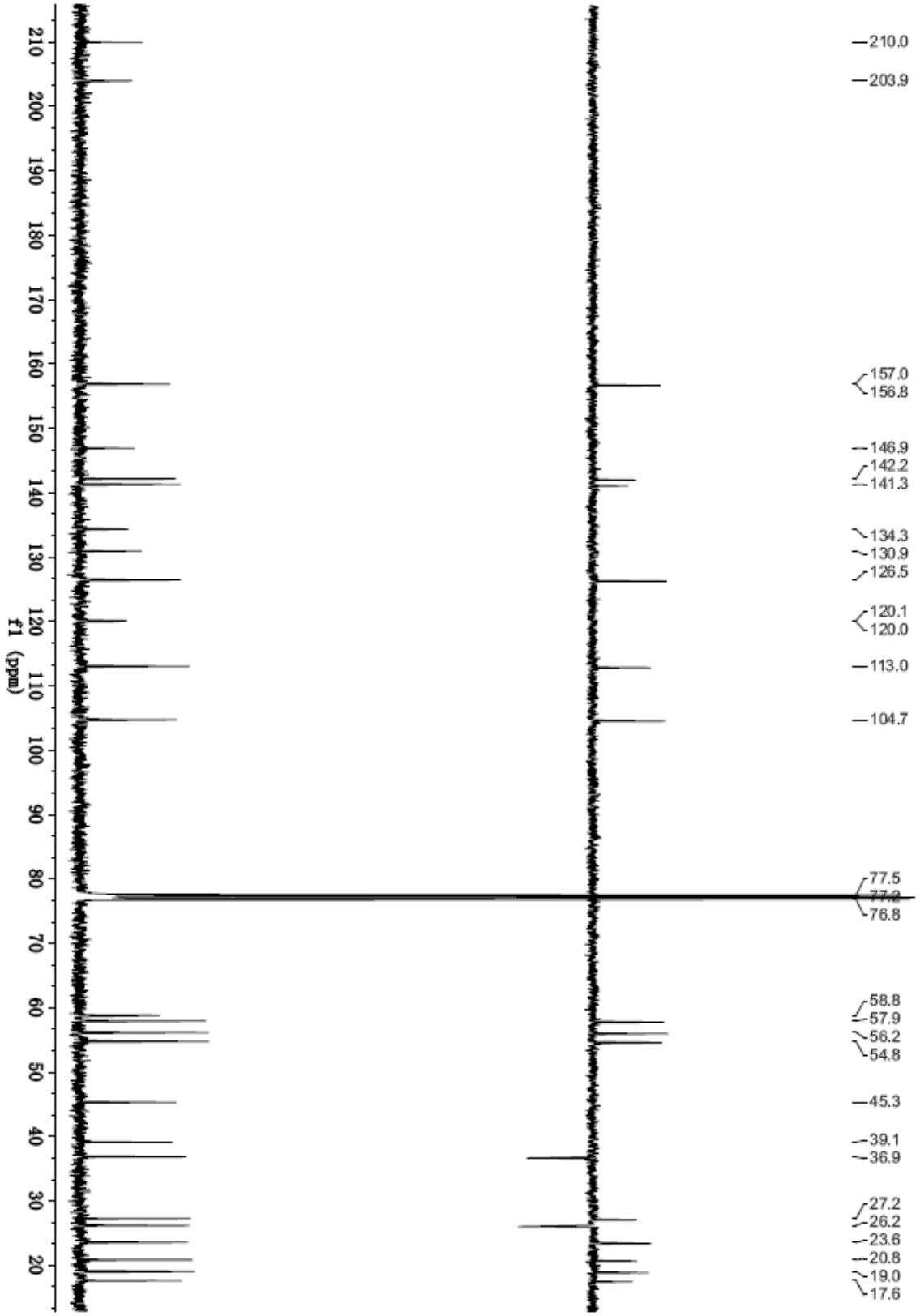


Figure S12. HMBC spectrum of walsucochinoid D (**2**) in $CDCl_3$

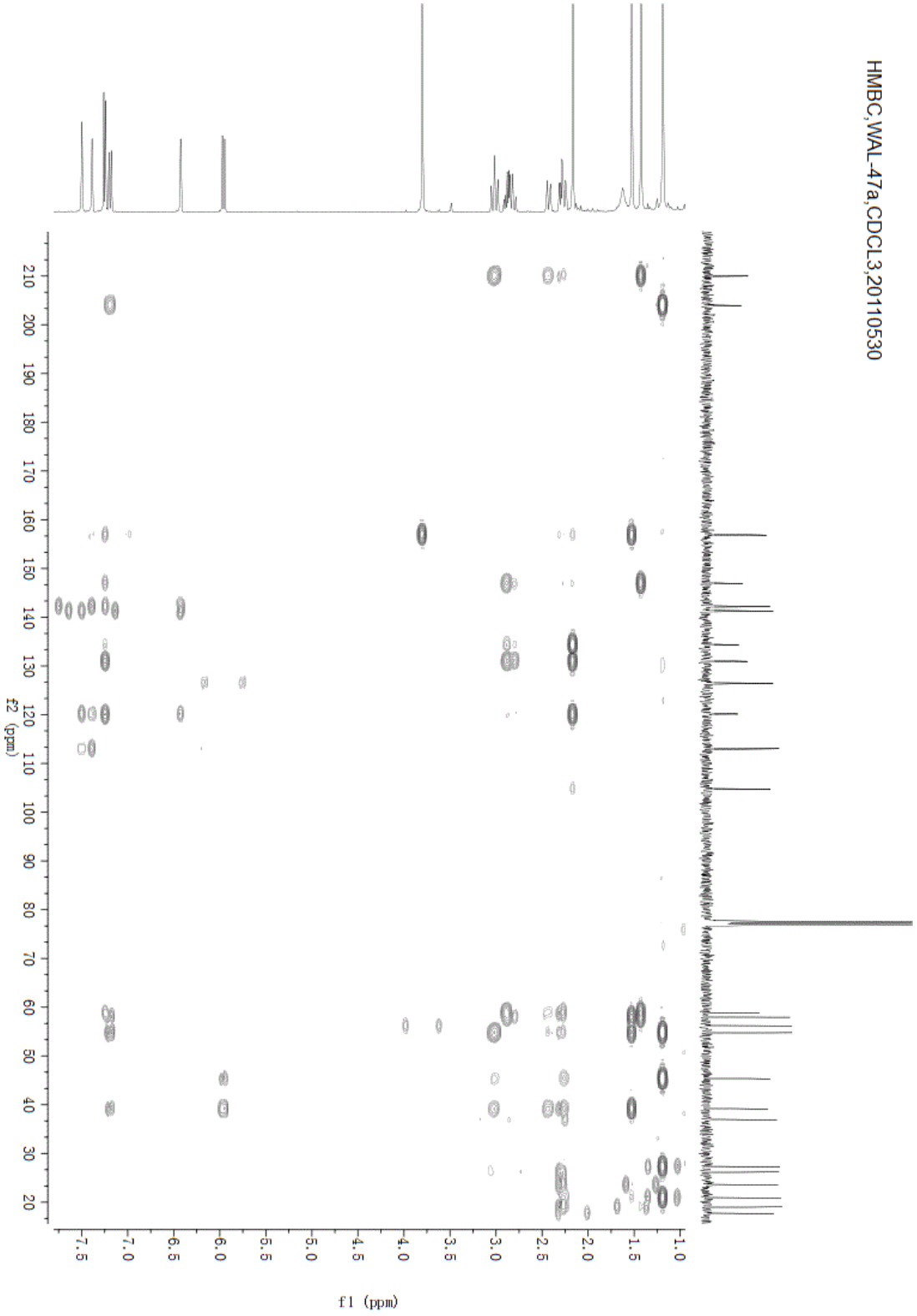


Figure S13. ROESY spectrum of walsucochinoid D (**2**) in $CDCl_3$

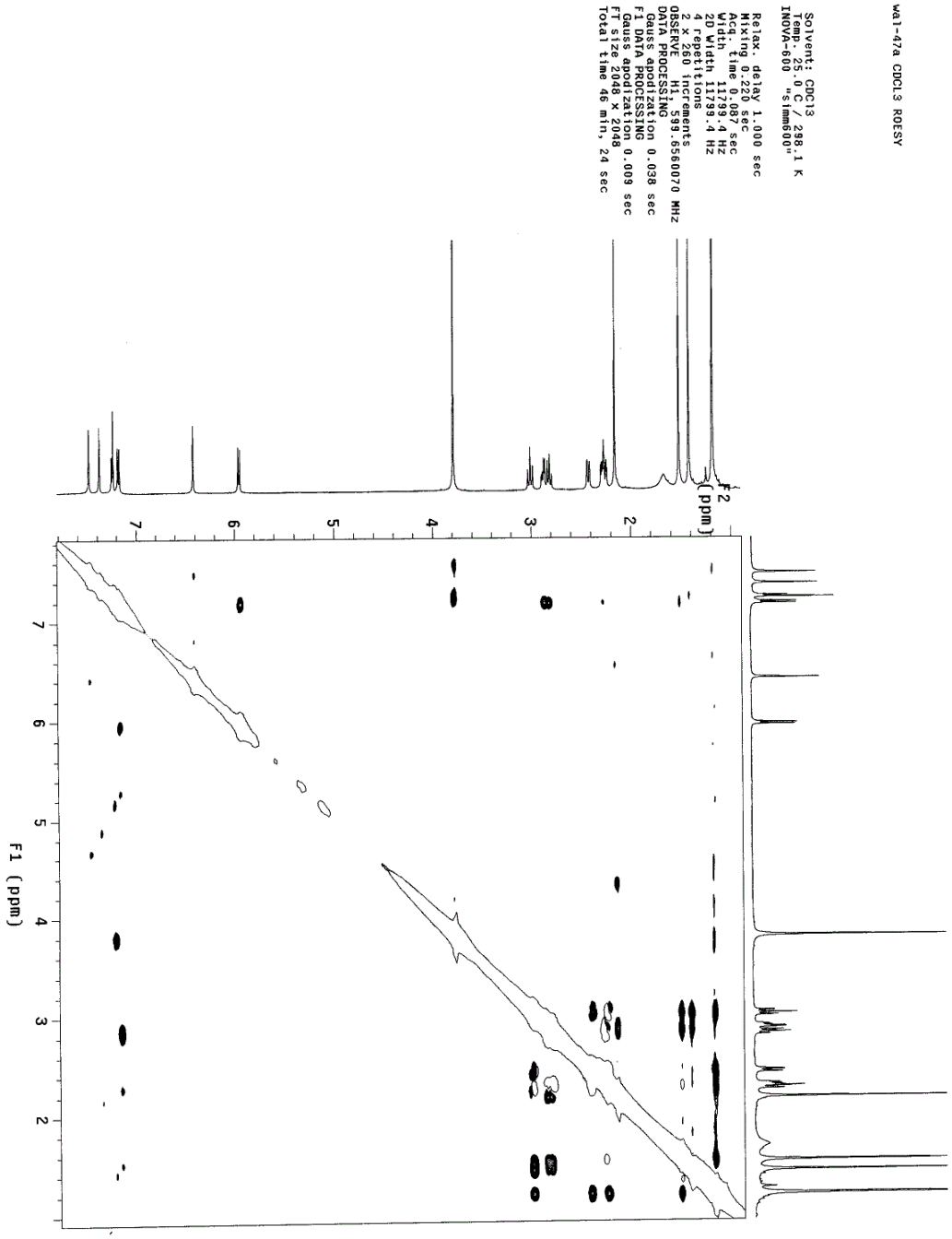


Figure S14. ESI(+)MS spectrum of walsucochinoid D (**2**)

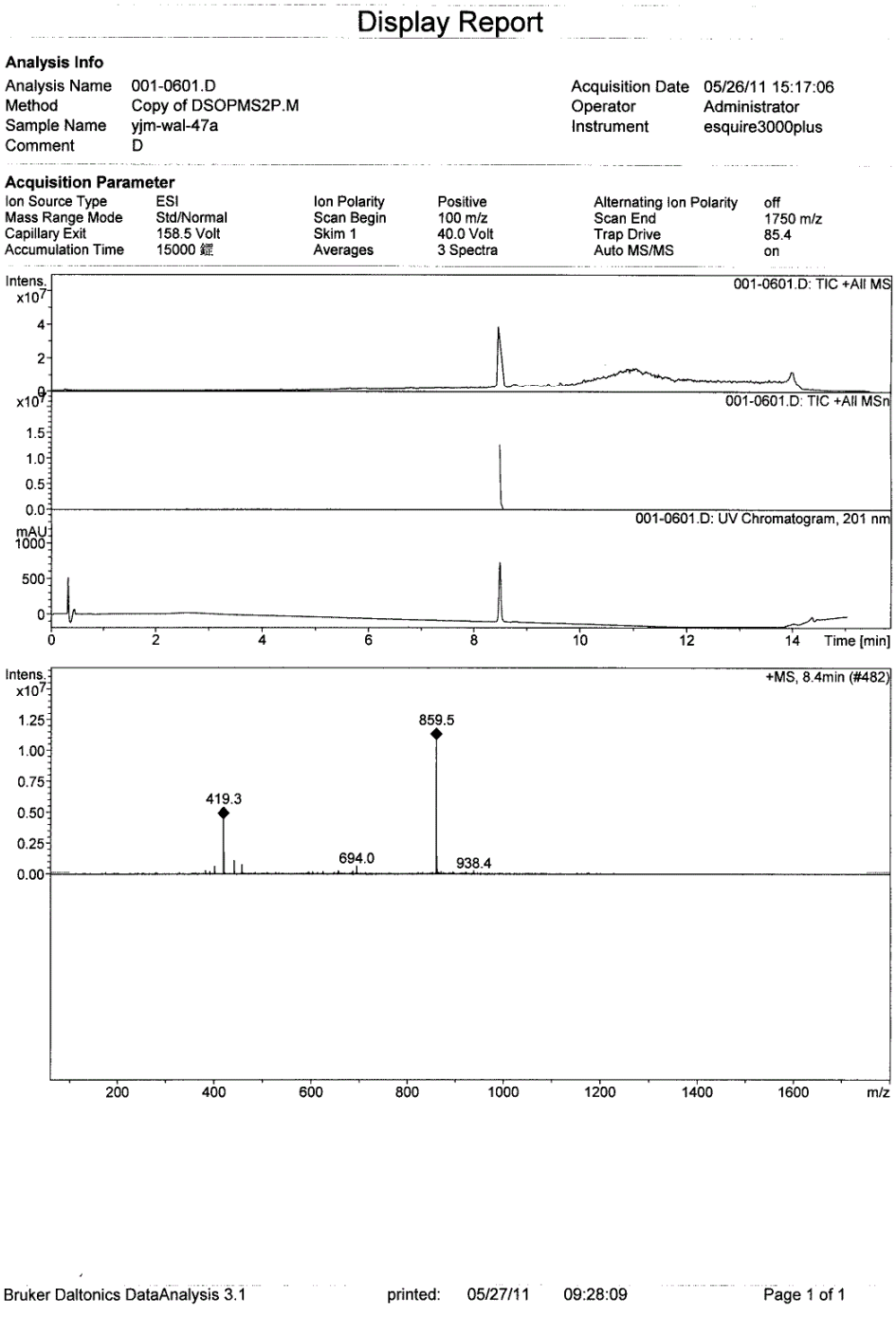


Figure S15. HRESI(+)MS spectrum of walsucochinoid D (**2**)

Elemental Composition Report **Page 1**

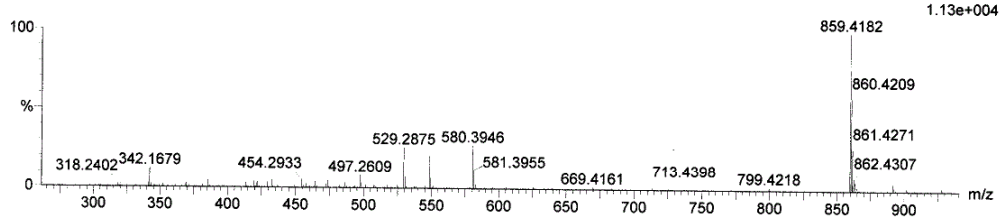
Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
418 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30 Na: 0-1
WAL-47a

LCT PXE KE324

04-Nov-2011
16:36:39
1: TOF MS ES+
1.13e+004

WAL-47a_1104 18 (0.389) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (5:27)



Minimum:				-1.5			
Maximum:		2.0	2.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
859.4182	859.4186	-0.4	-0.5	24.5	60.4	0.0	C54 H60 O8 Na
	859.4175	0.7	0.8	5.5	64.5	4.1	C38 H67 O21

Figure S16. IR spectrum of walsucochinoid D (**2**)

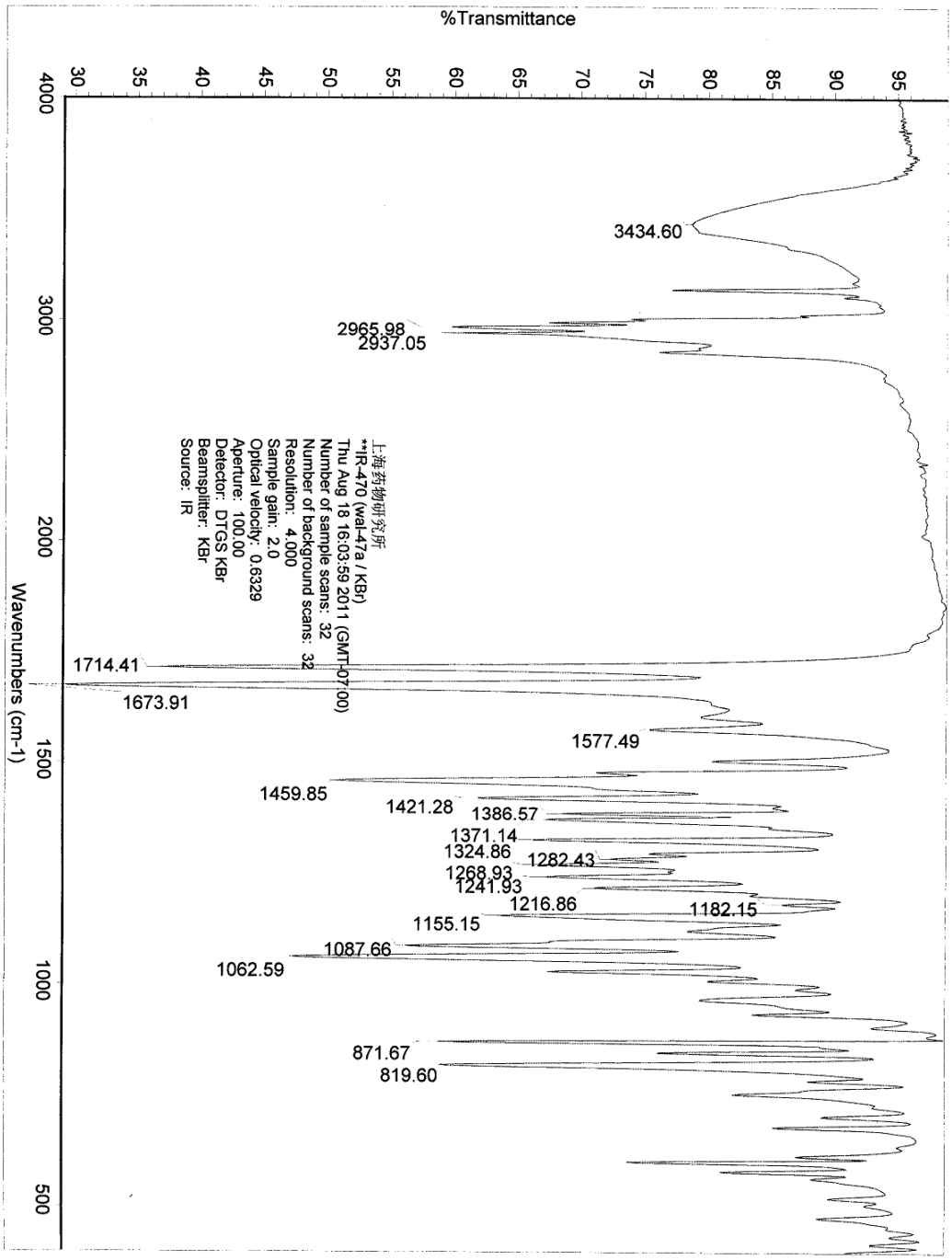


Figure S17. ^{1}H NMR spectrum of walsucochinoid E (**3**) in $CDCl_3$

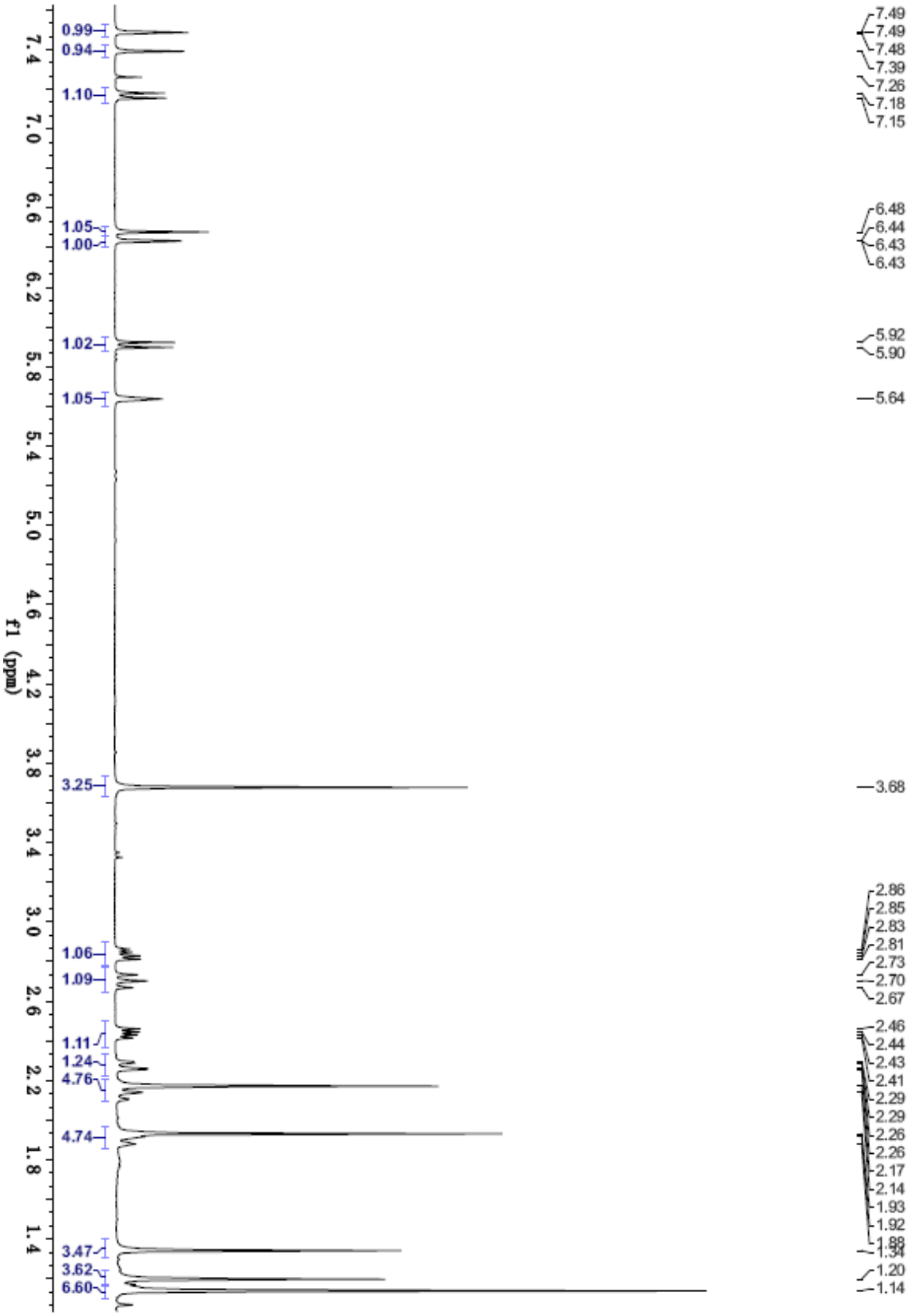


Figure S18. ^{13}C NMR spectrum of walsucochinoid E (**3**) in $CDCl_3$

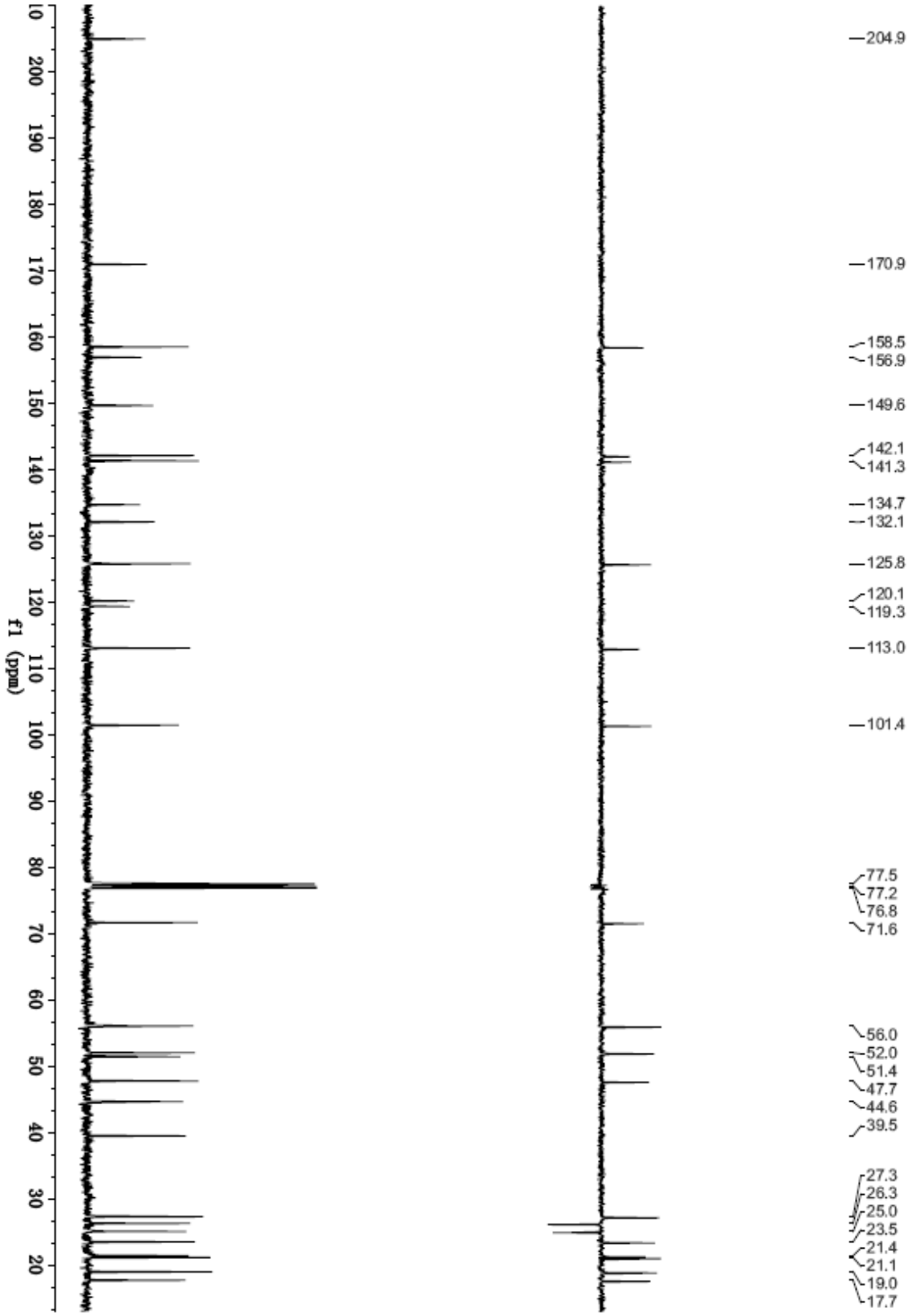


Figure S19. HMBC spectrum of walsucochinoid E (**3**) in $CDCl_3$

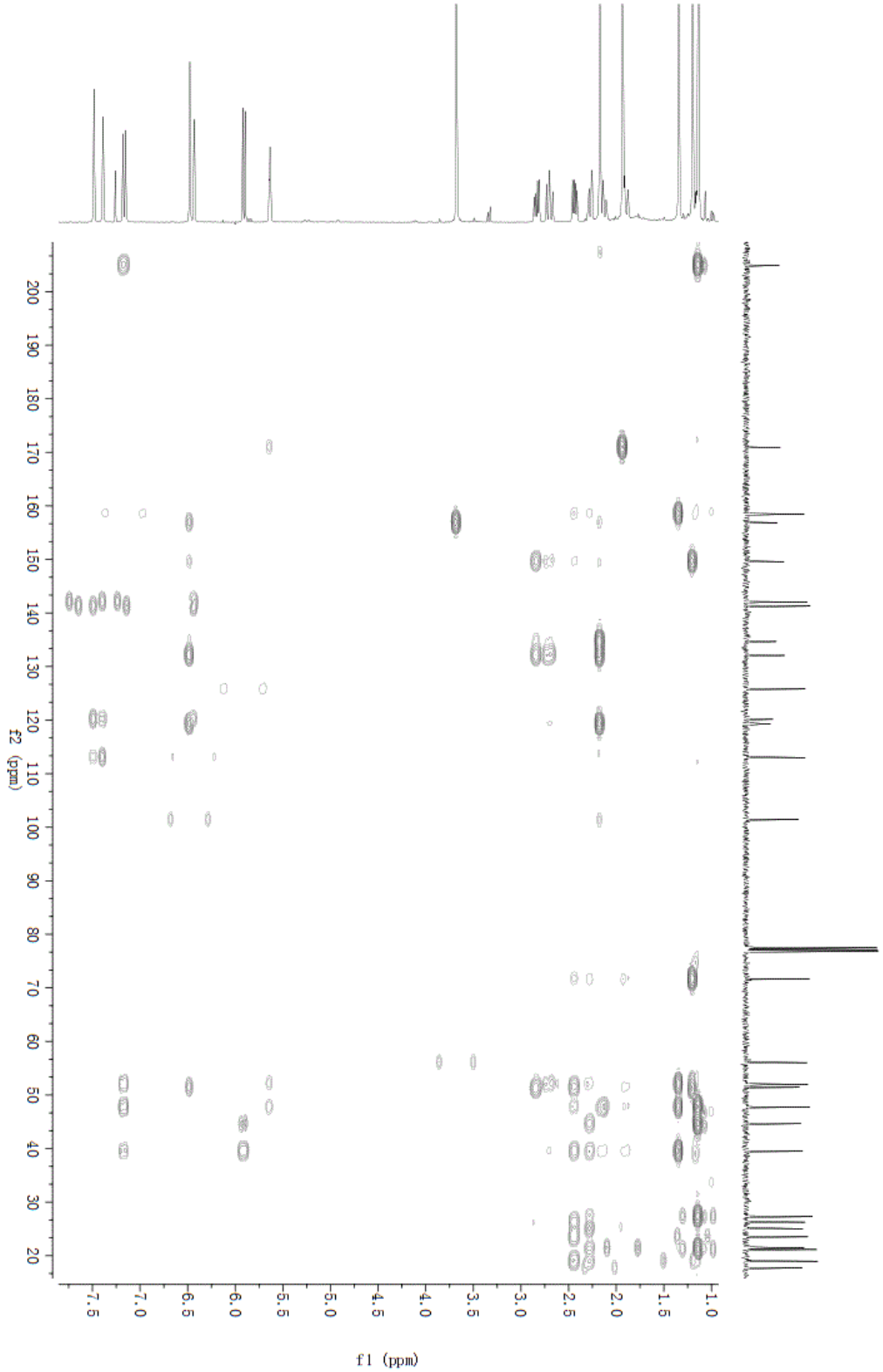


Figure S20. ROESY spectrum of walsucochinoid E (**3**) in $CDCl_3$

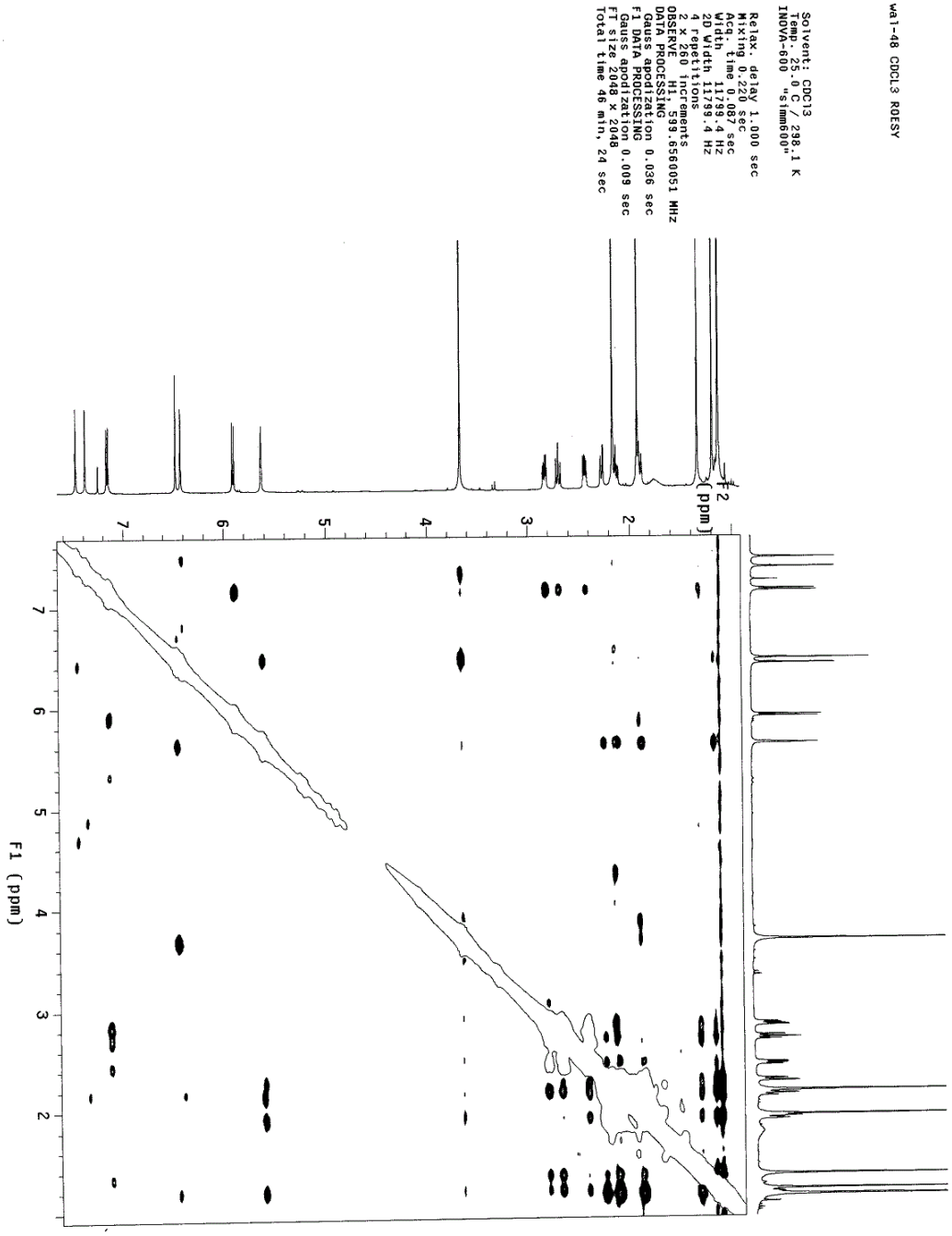


Figure S21. ESI(+)MS spectrum of walsucochinoid E (**3**)

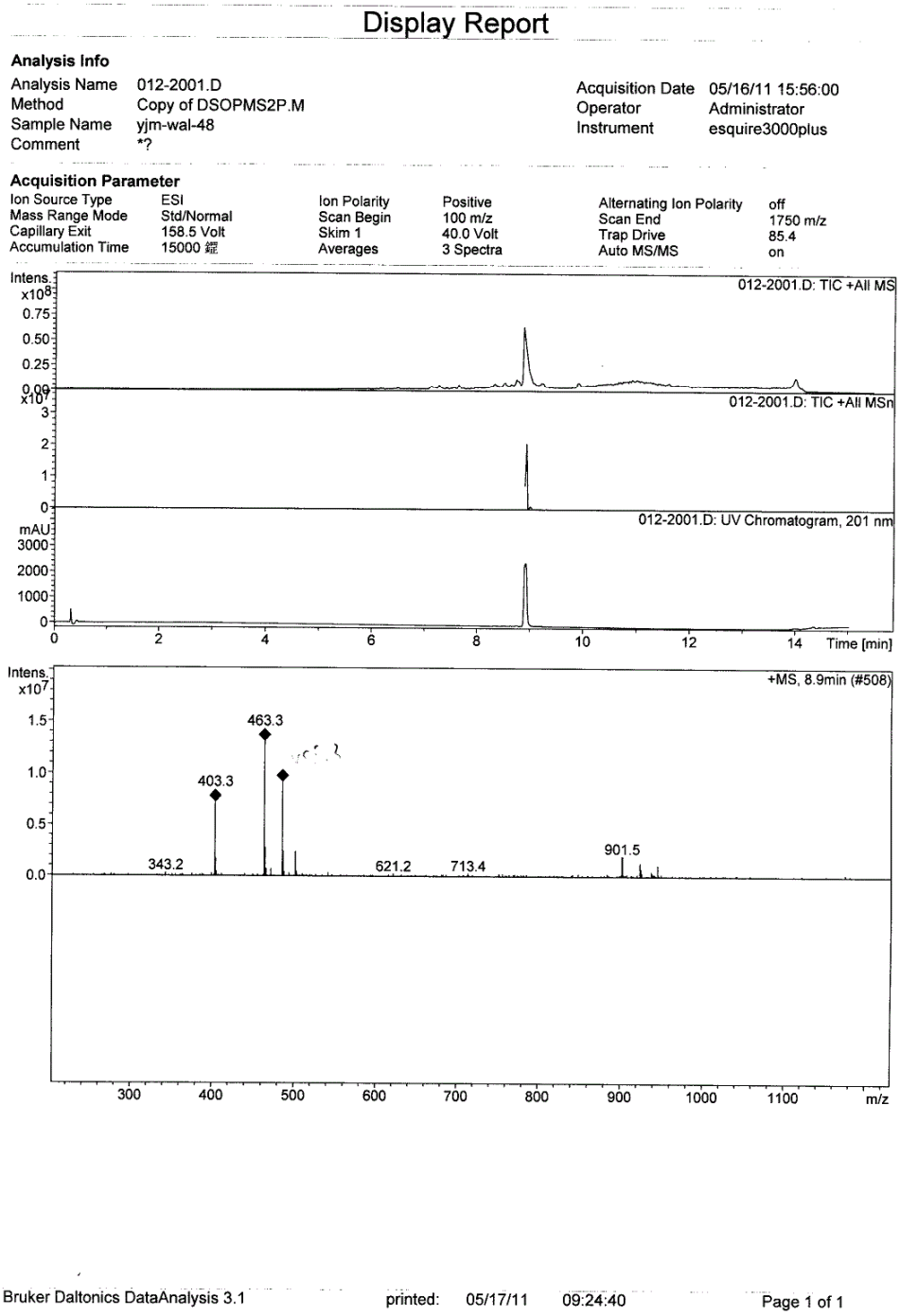


Figure S22. HRESI(+)MS spectrum of walsucochinoid E (**3**)

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
381 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30 Na: 0-1

WAL-48 LCT PXE KE324 09-Nov-2011 16:03:09

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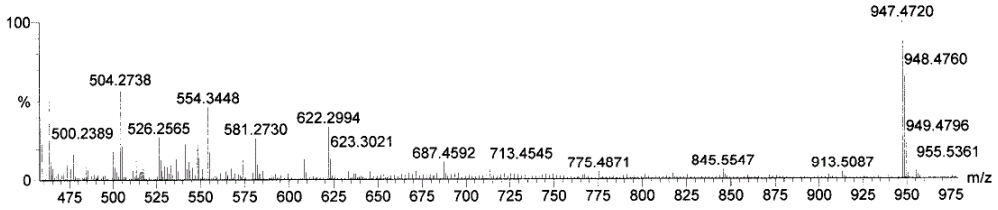

Minimum:				-1.5						
Maximum:		5.0	3.0	50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
947.4720	947.4710	1.0	1.1	24.5	42.9	0.0	C58	H68	O10	Na
	947.4734	-1.4	-1.5	27.5	46.1	3.2	C60	H67	O10	
	947.4699	2.1	2.2	5.5	53.9	11.1	C42	H75	O23	

Figure S23. IR spectrum of walsucochinoid E (**3**)

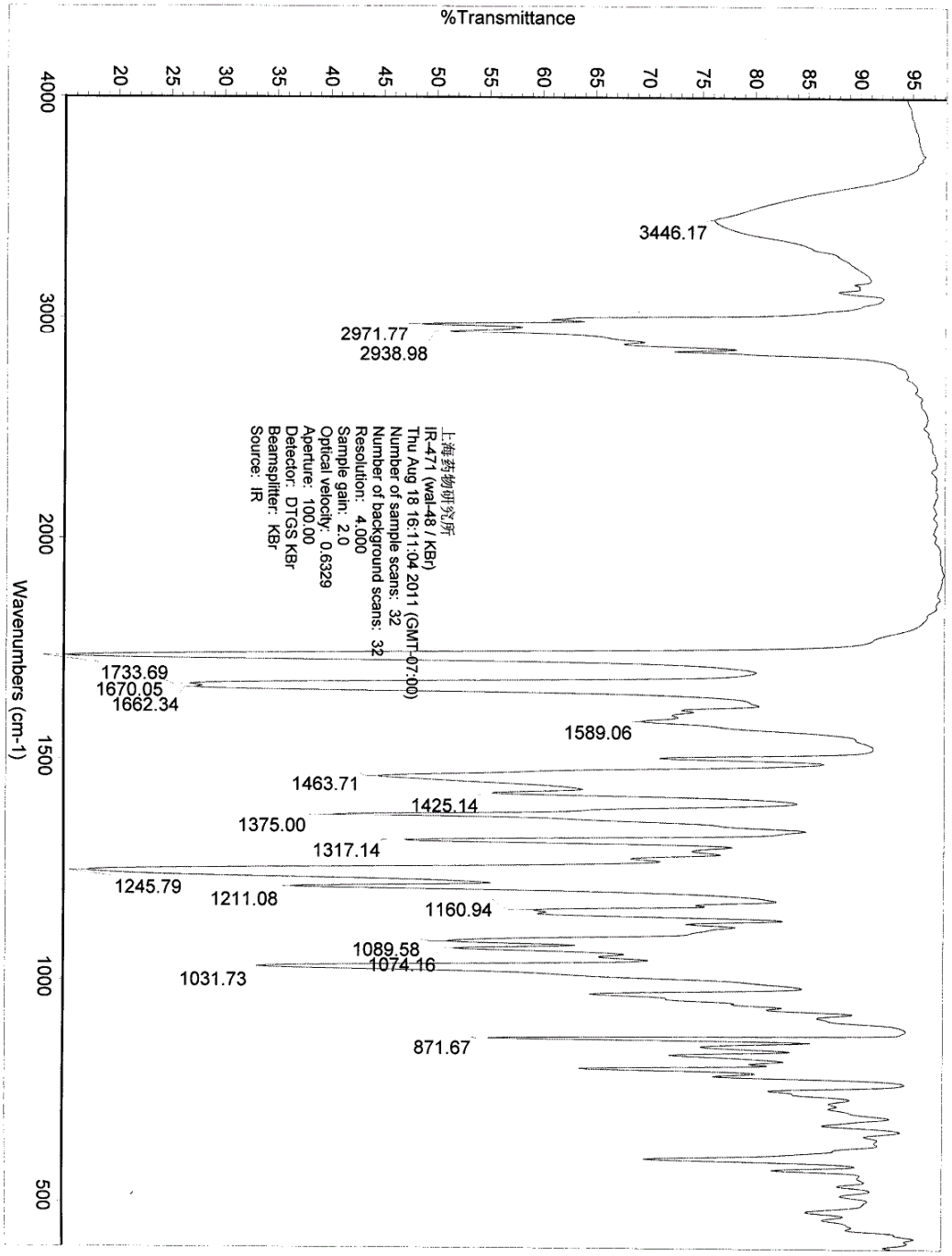

Figure S24. ^{1}H NMR spectrum of walsucochinoid F (**4**) in $CDCl_3$

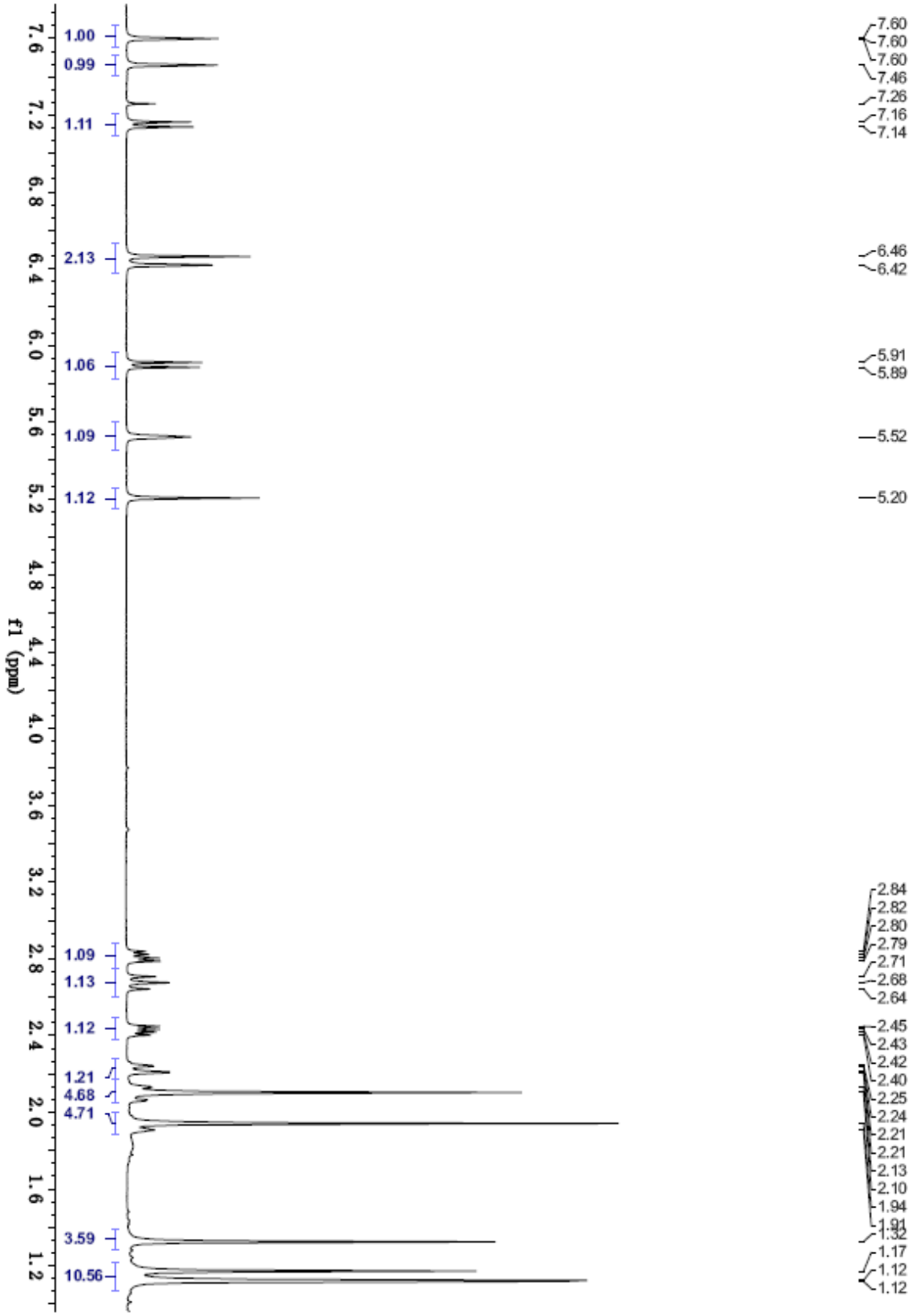

Figure S25. ^{13}C NMR spectrum of walsucochinoid F (**4**) in $CDCl_3$

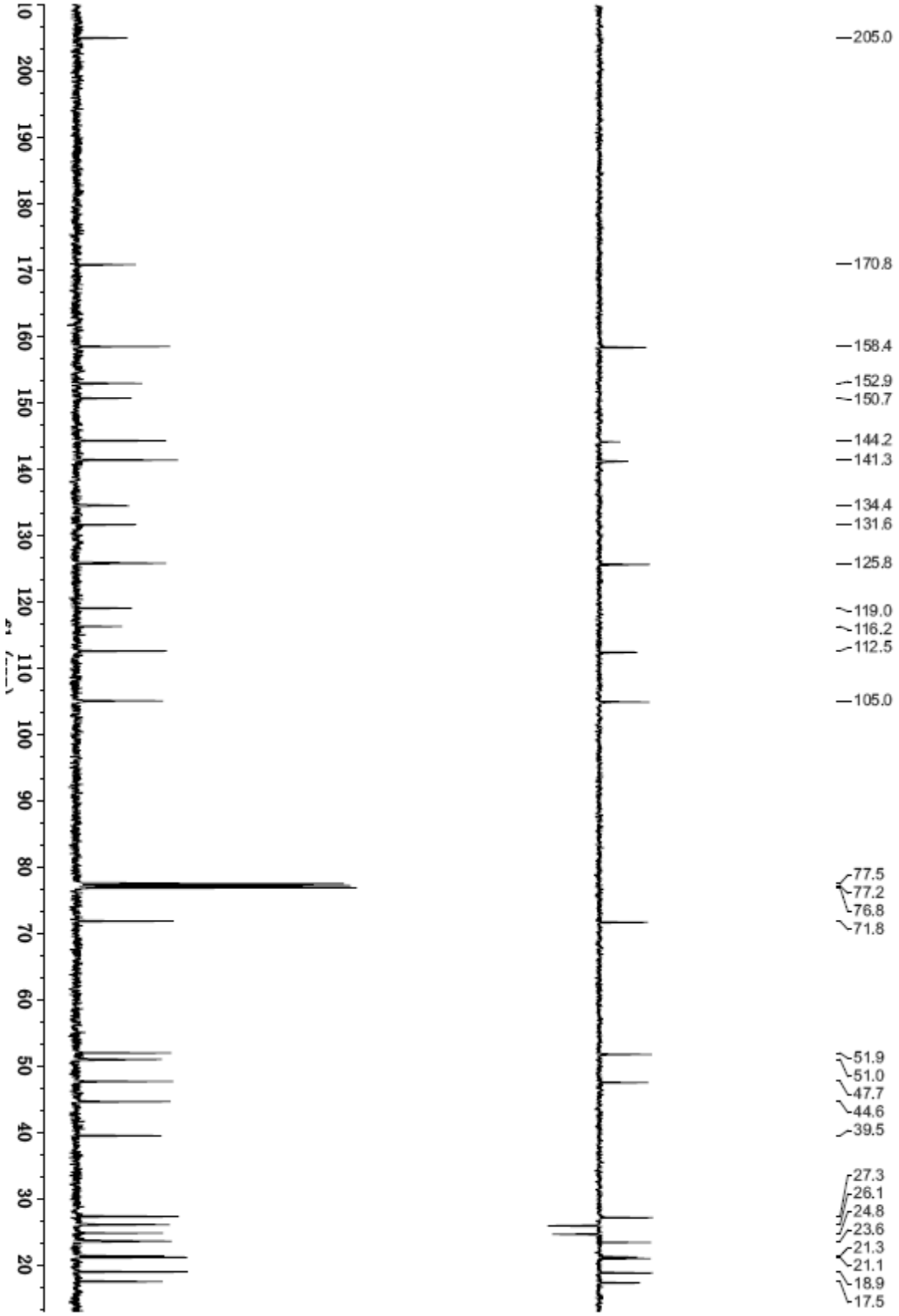

Figure S26. ROESY spectrum of walsucochinoid F (**4**) in $CDCl_3$

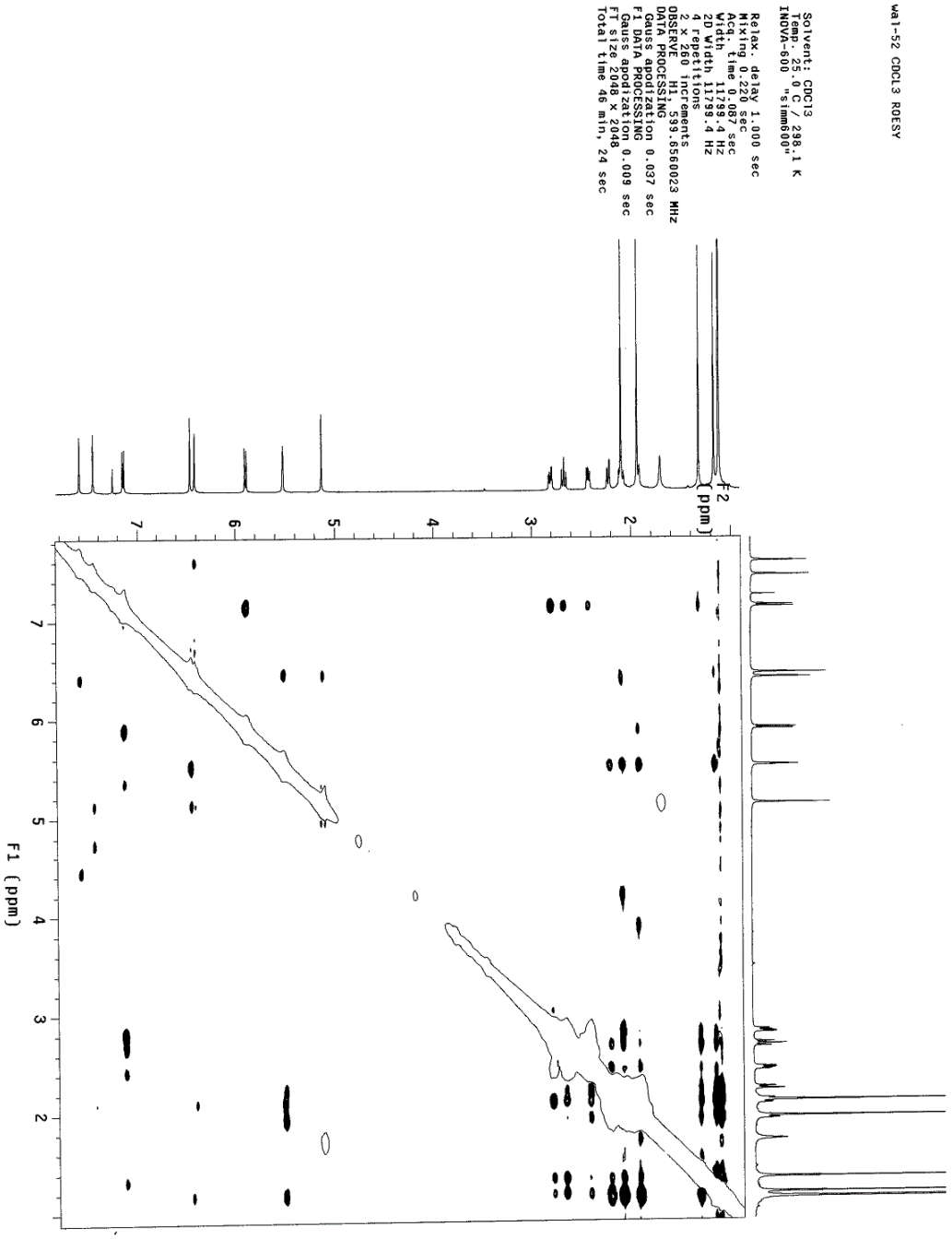

Figure S27. ESI(+)MS spectrum of walsucochinoid F (**4**)

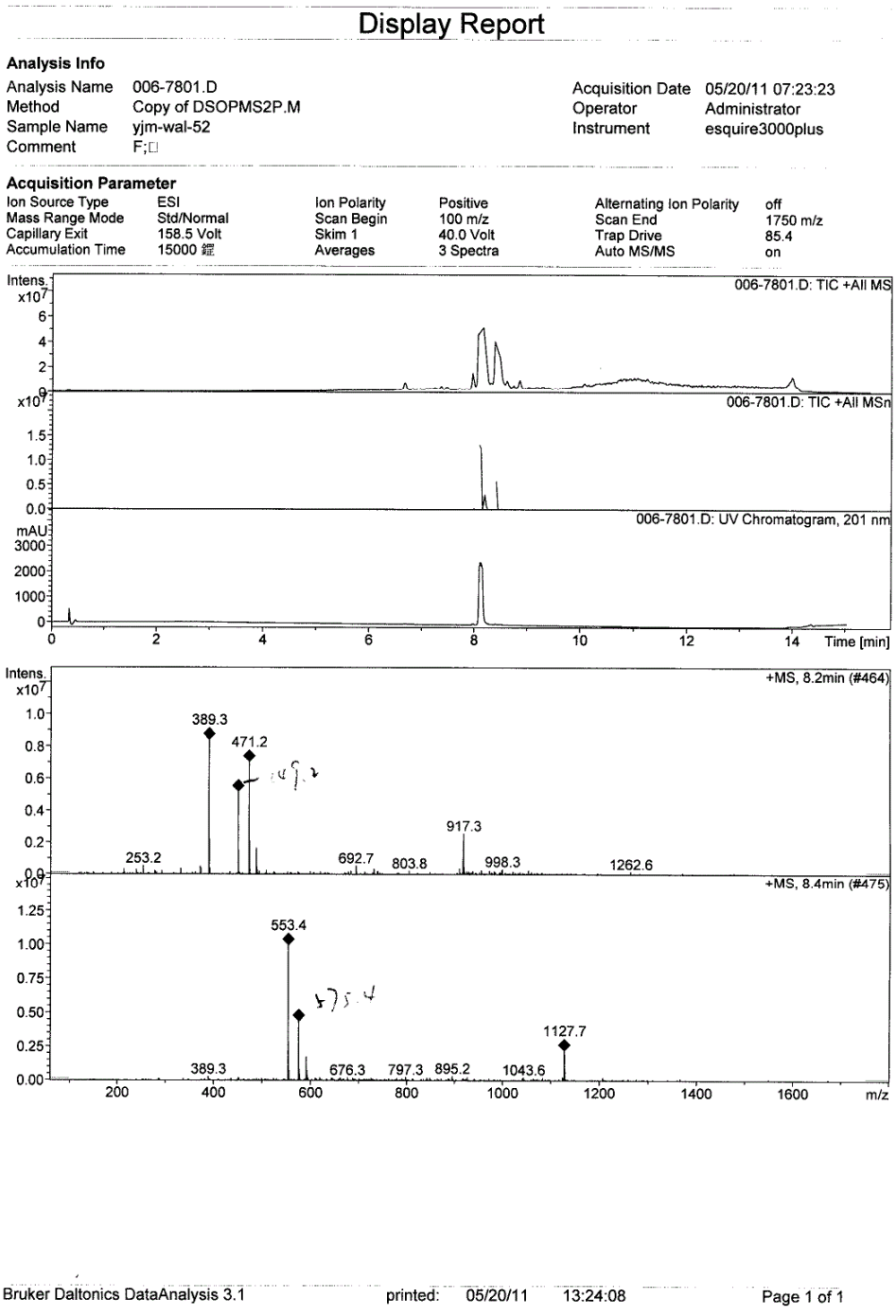

Figure S28. ESI(−)MS spectrum of walsucochinoid F (**4**)

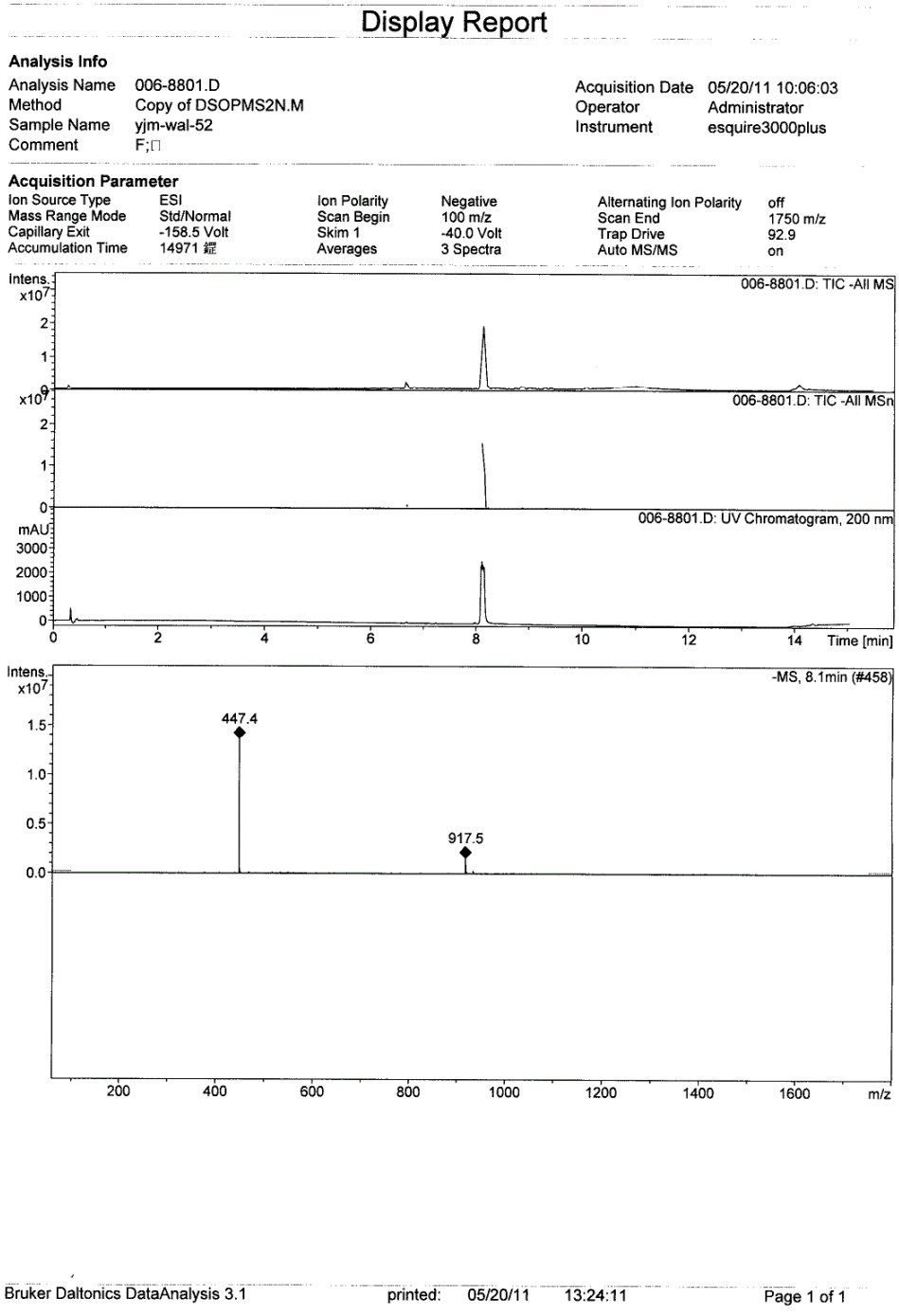

Figure S29. HRESI(–)MS spectrum of walsucochinoid F (**4**)

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
116 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30

WAL-52 LCT PXE KE324 09-Nov-2011 15:54:40

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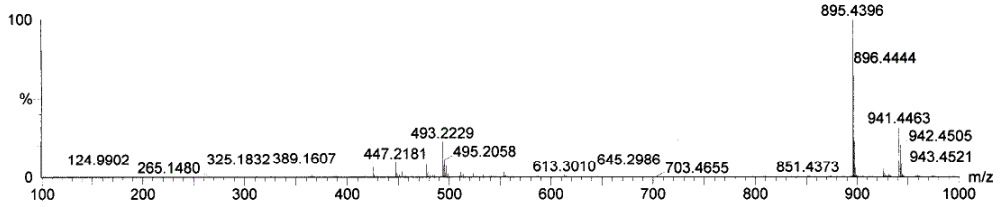


Minimum:				-1.5			
Maximum:		5.0	3.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
493.2229	493.2226	0.3	0.6	13.5	156.3	0.0	C29 H33 O7

Figure S30. IR spectrum of walsucochinoid F (**4**)

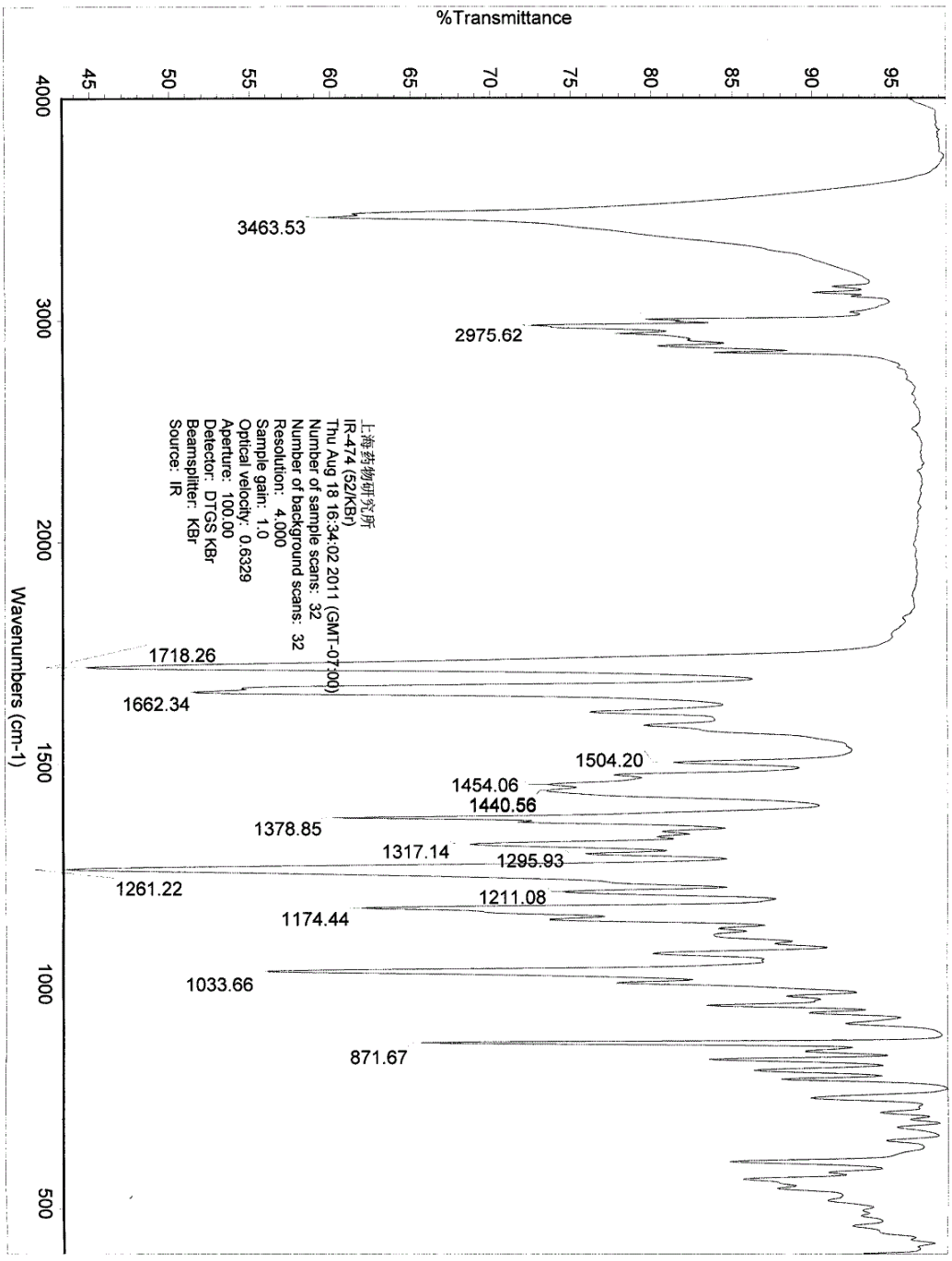


Figure S31. ^{1}H NMR spectrum of walsucochinoid G (**5**) in $CDCl_3$

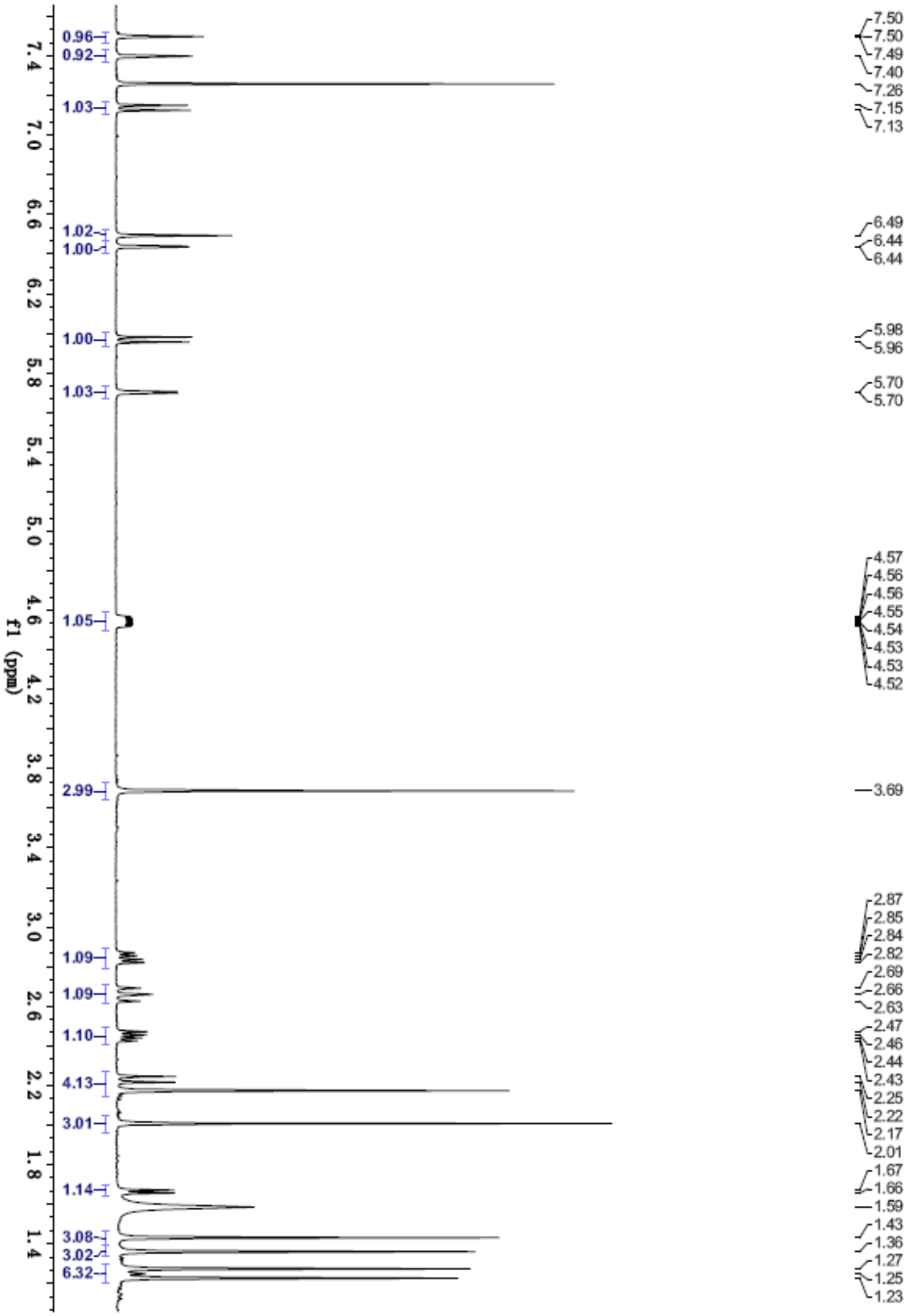


Figure S32. ^{13}C NMR spectrum of walsucochinoid G (**5**) in $CDCl_3$

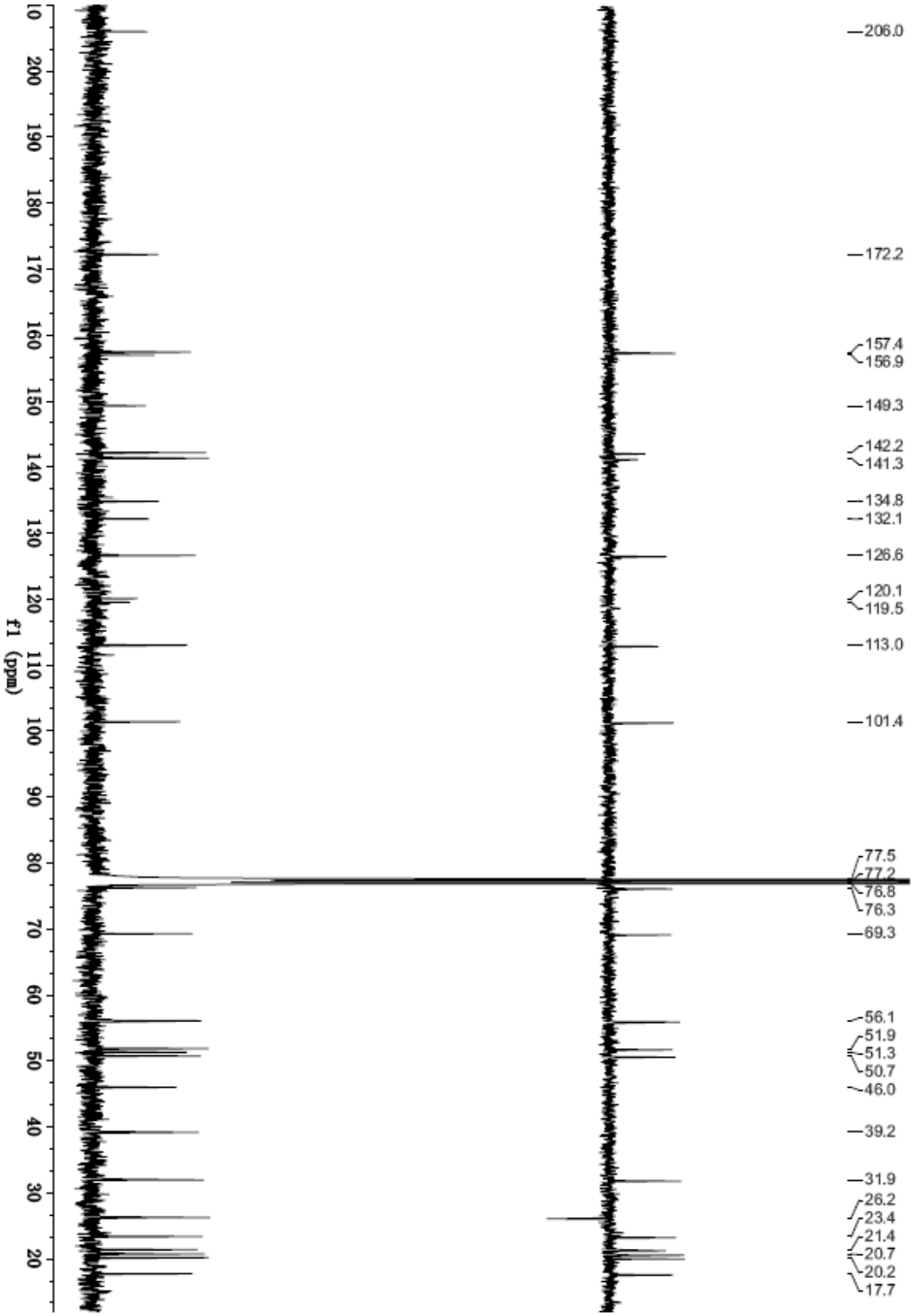


Figure S33. HSQC spectrum of walsucochinoid G (**5**) in $CDCl_3$

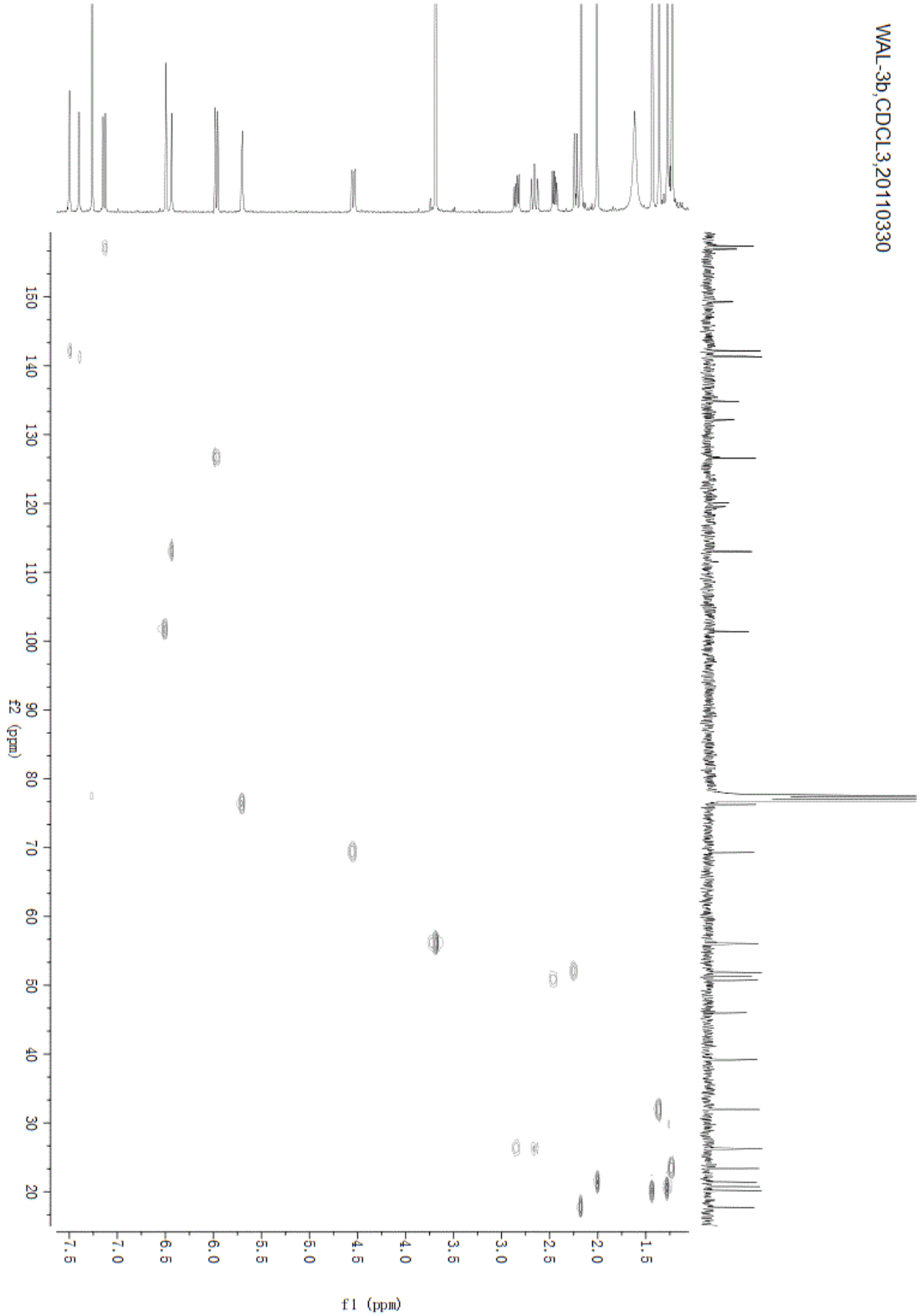


Figure S34. HMBC spectrum of walsucochinoid G (**5**) in $CDCl_3$

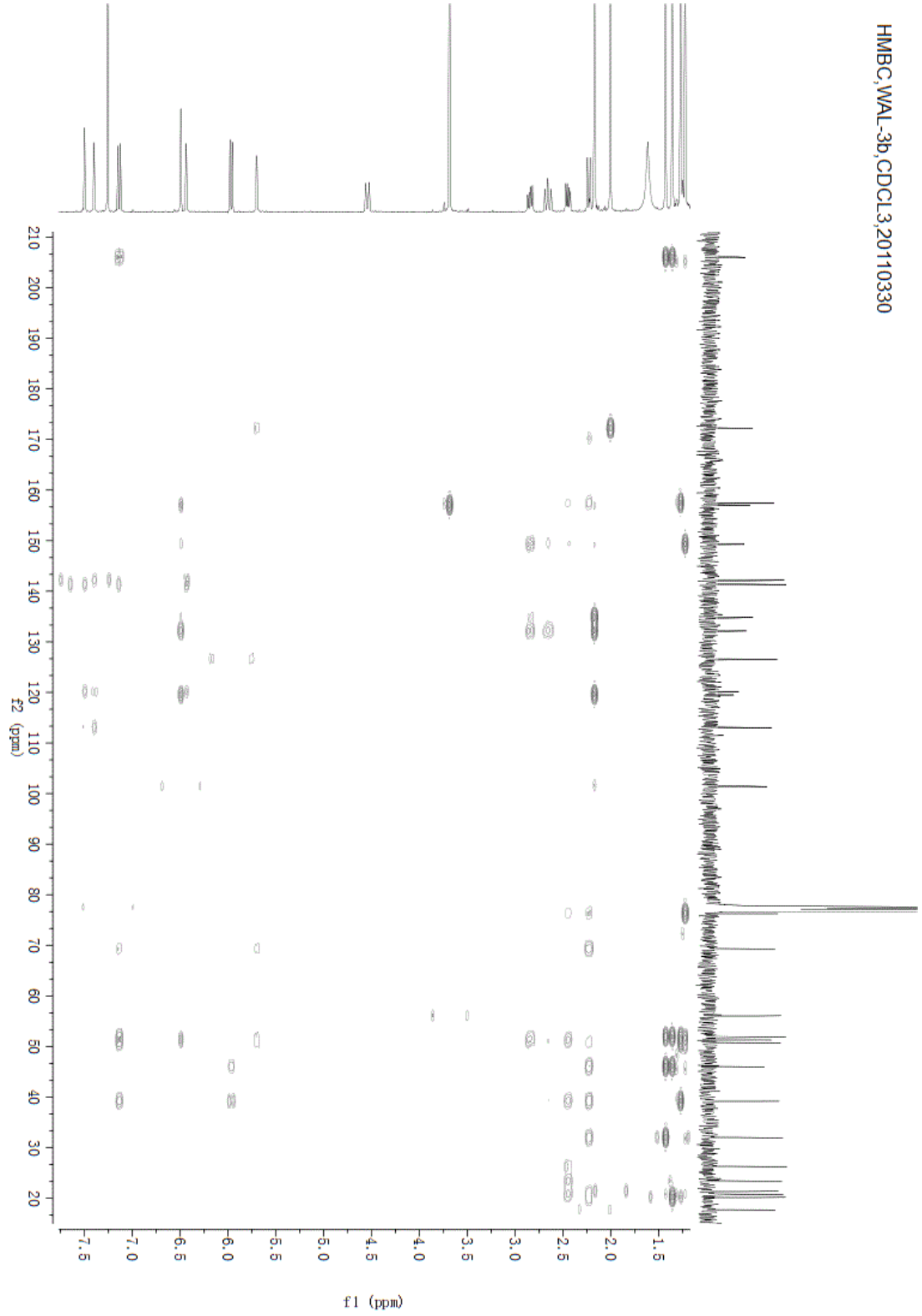


Figure S35. ROESY spectrum of walsucochinoid G (**5**) in $CDCl_3$

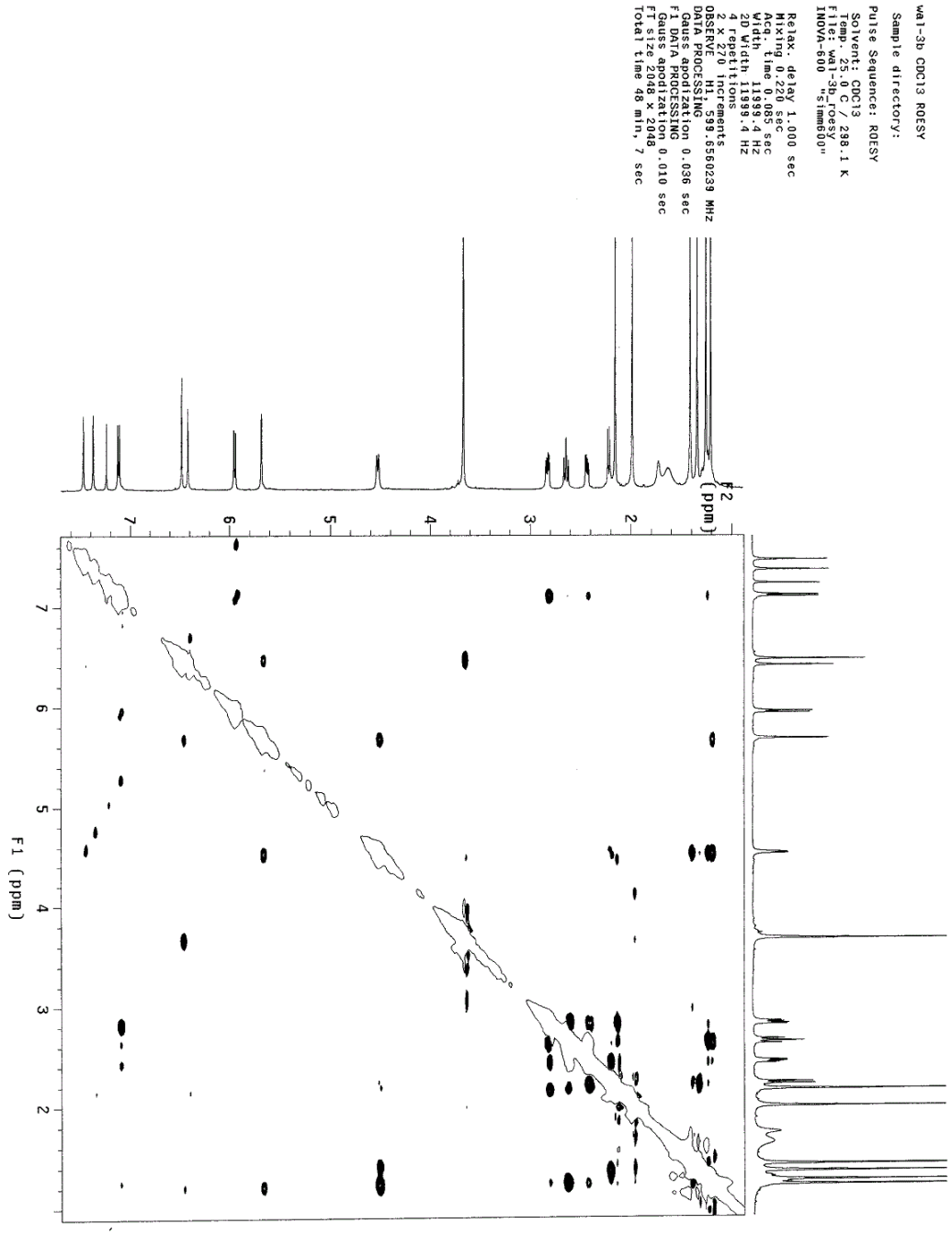


Figure S36. ESI(+)MS spectrum of walsucochinoid G (**5**)

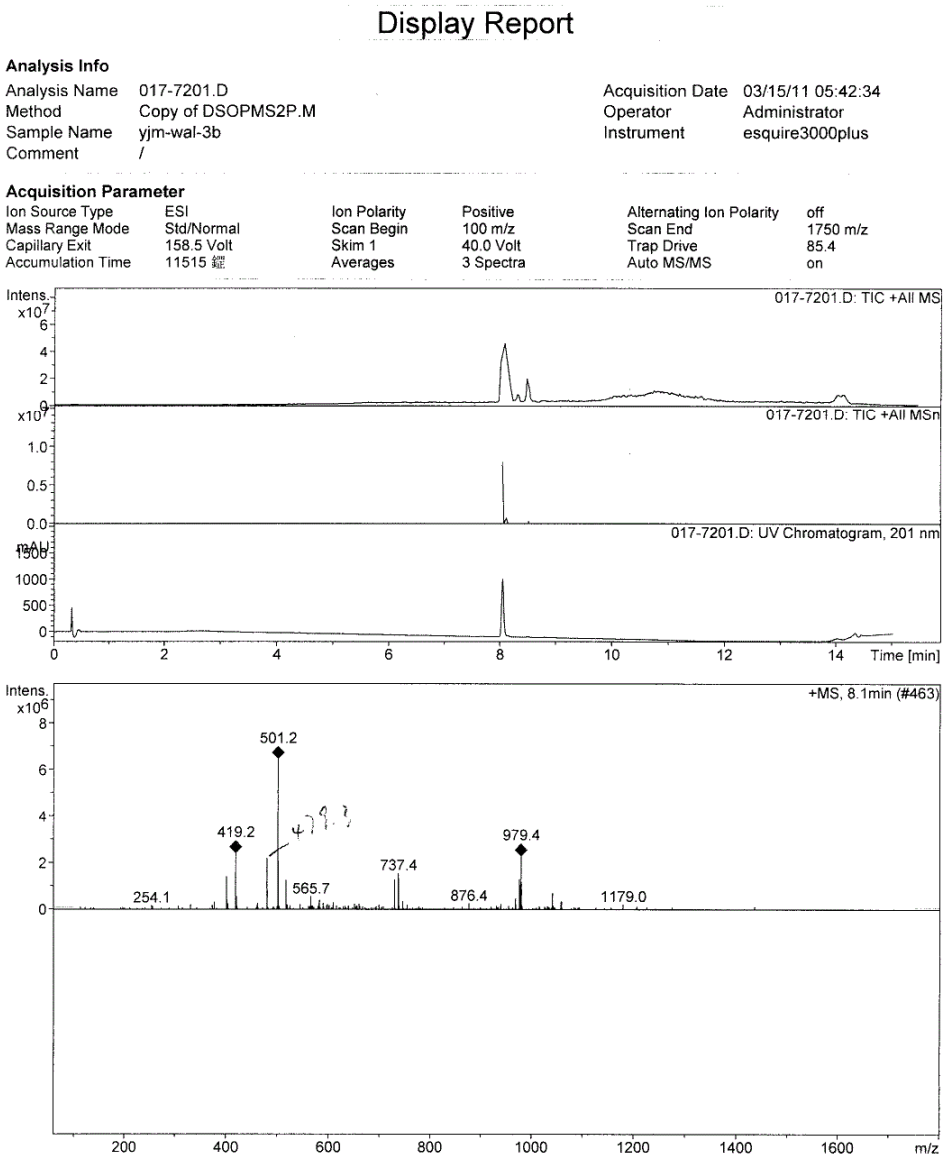


Figure S37. ESI(−)MS spectrum of walsucochinoid G (**5**)

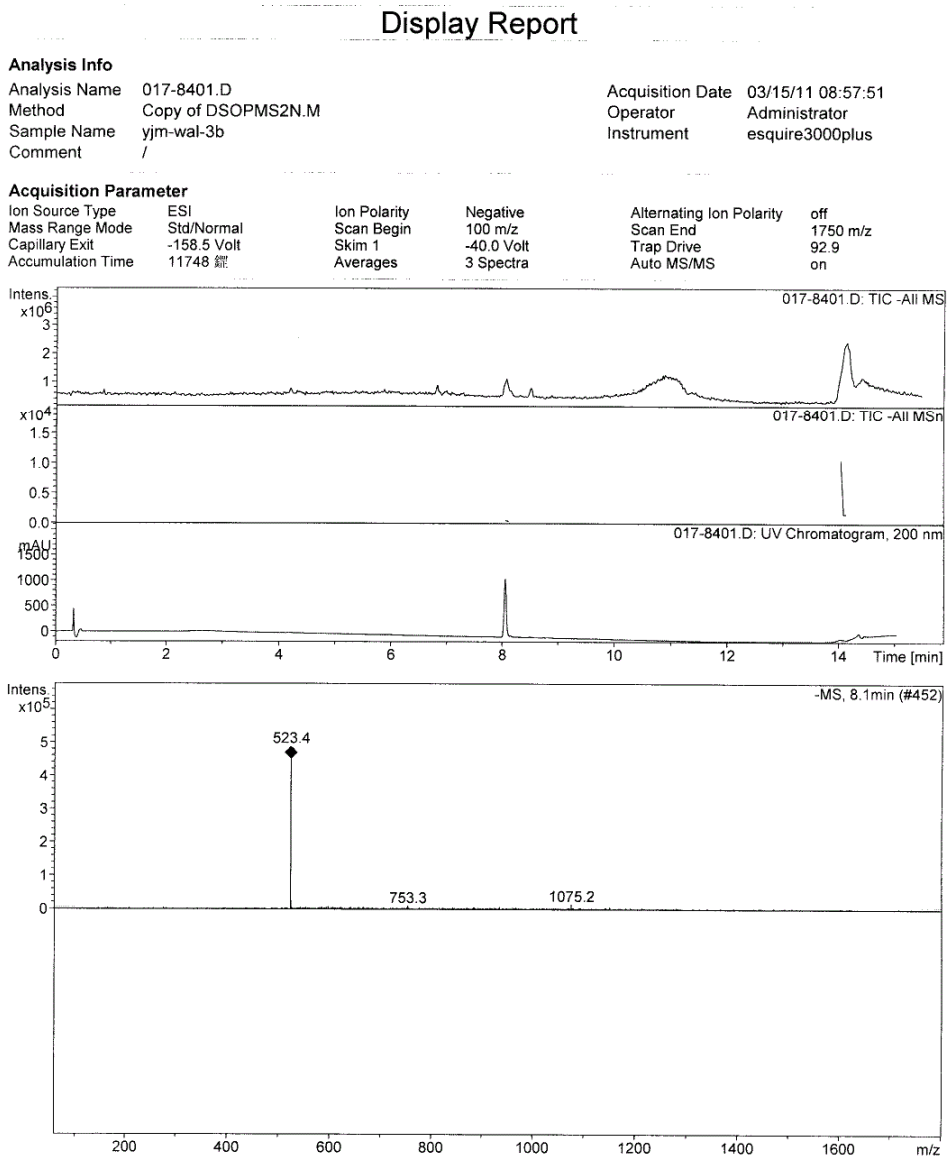


Figure S38. HRESI(–)MS spectrum of walsucochinoid G (**5**)

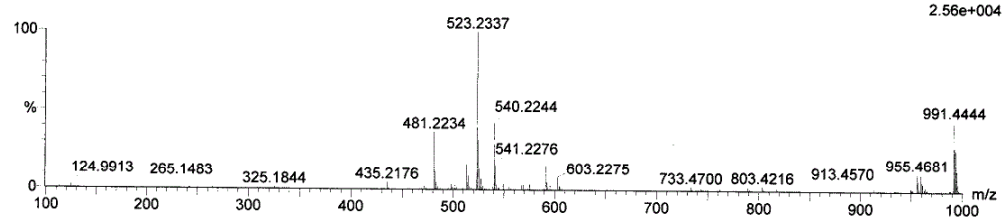
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
131 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30

WAL-3b LCT PXE KE324 04-Nov-2011 14:33:22

WAL-3b_1104 12 (0.247) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (6:21) 1: TOF MS ES- 2.56e+004



Minimum:				-1.5			
Maximum:		2.0	2.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
523.2337	523.2332	0.5	1.0	13.5	137.8	0.0	C30 H35 O8

Figure S39. IR spectrum of walsucochinoid G (**5**)

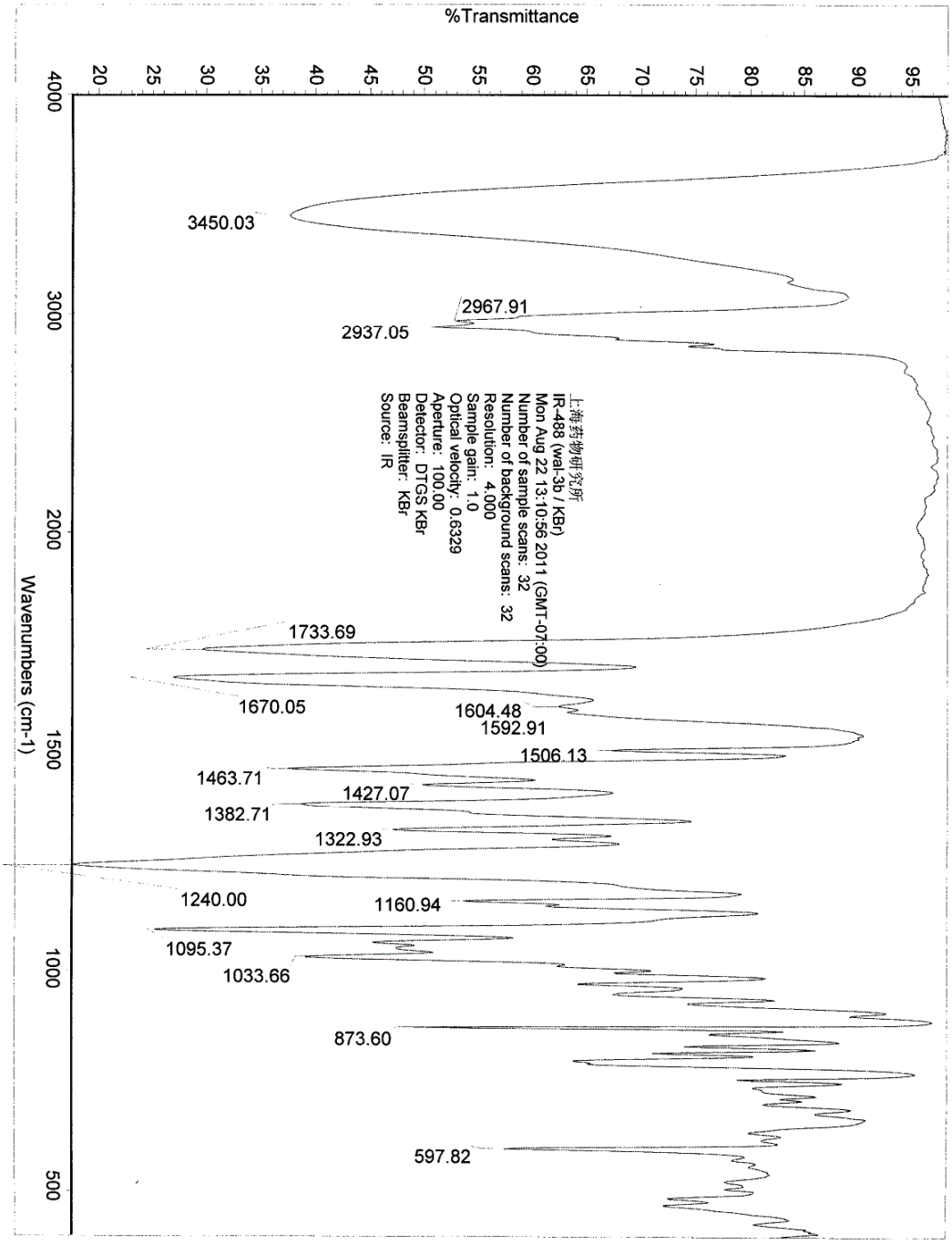


Figure S40. ^{1}H NMR spectrum of walsucochinoid H (**6**) in $CDCl_3$

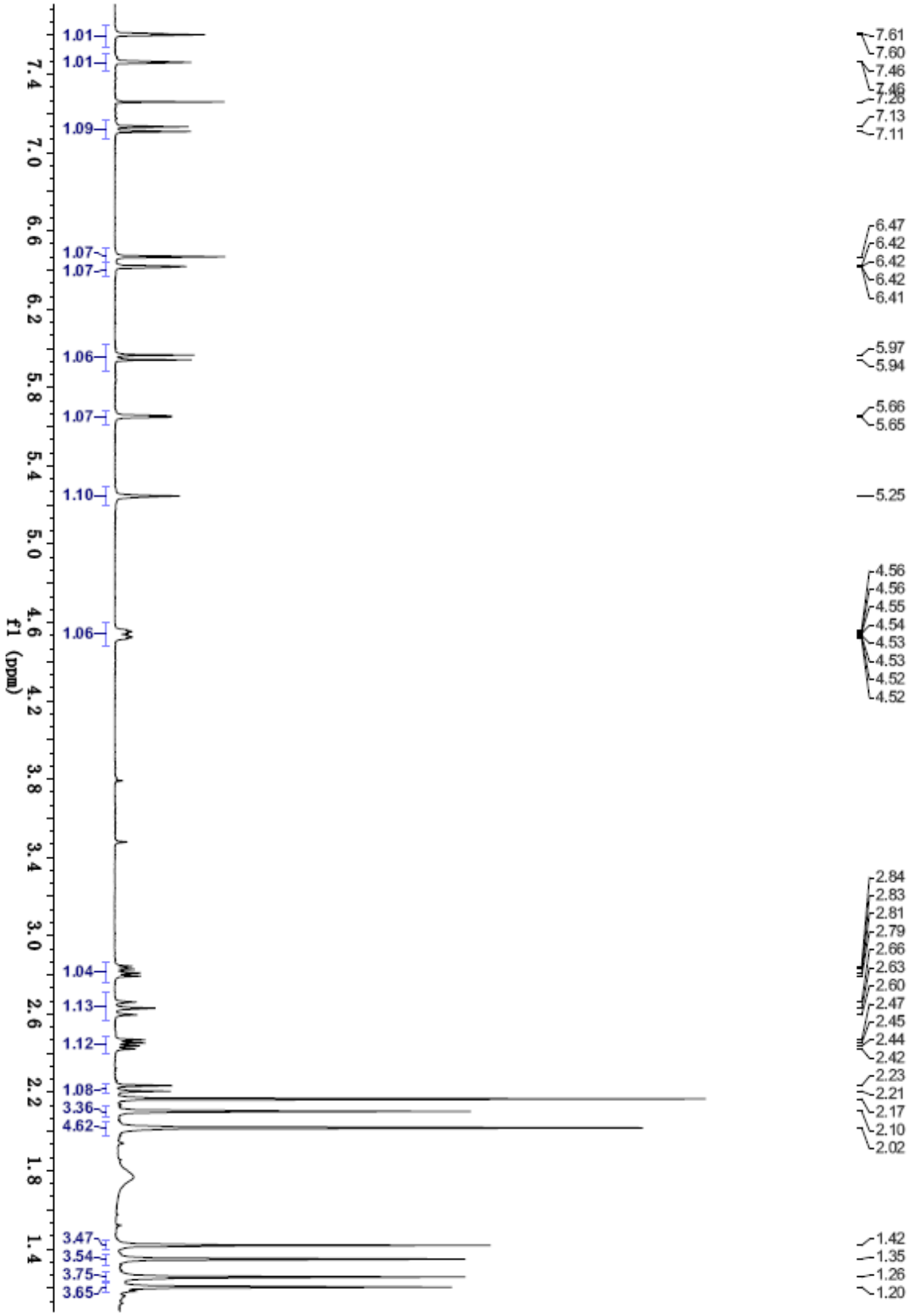


Figure S41. ^{13}C NMR spectrum of walsucochinoid H (**6**) in $CDCl_3$

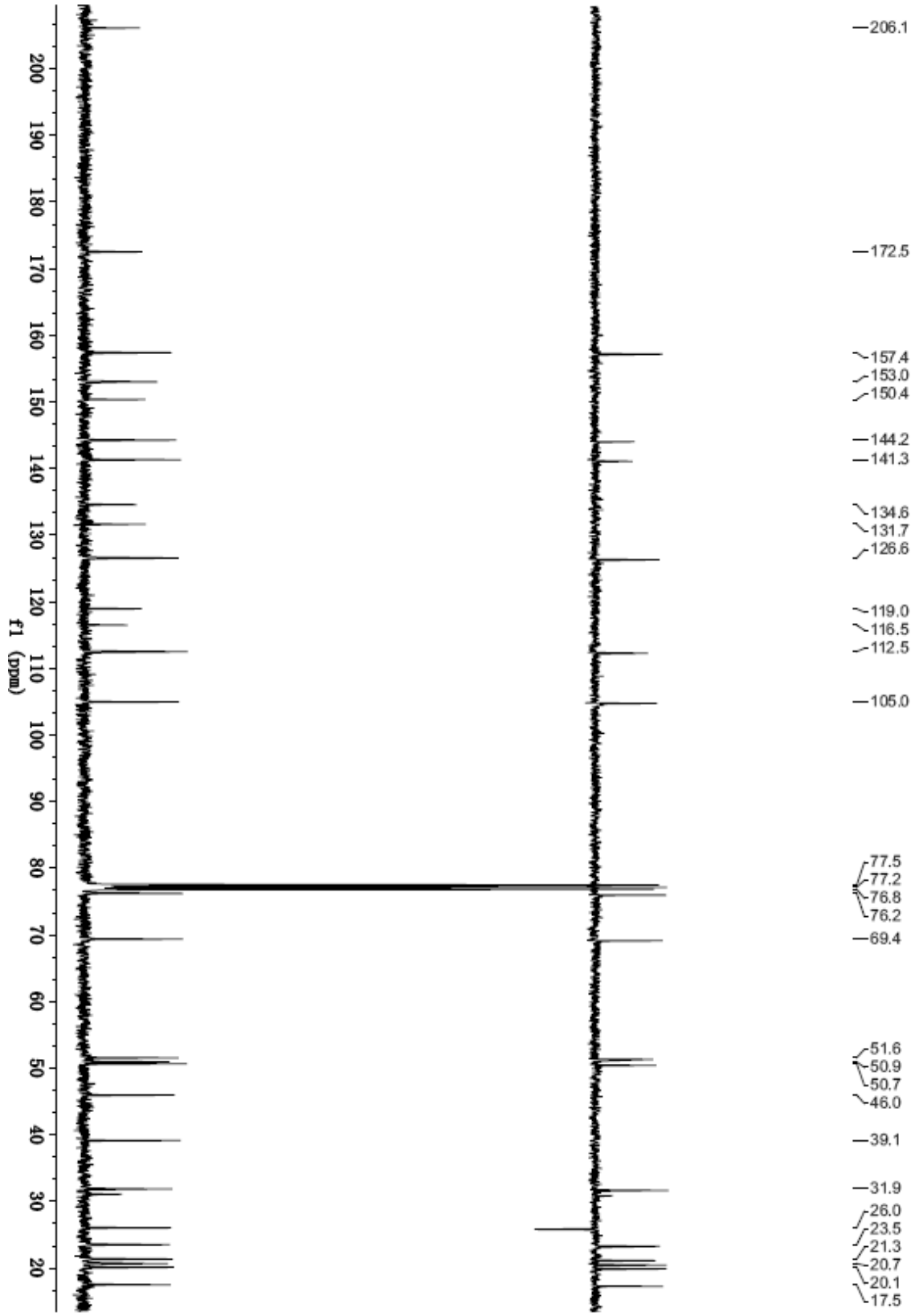


Figure S42. HSQC spectrum of walsucochinoid H (**6**) in $CDCl_3$

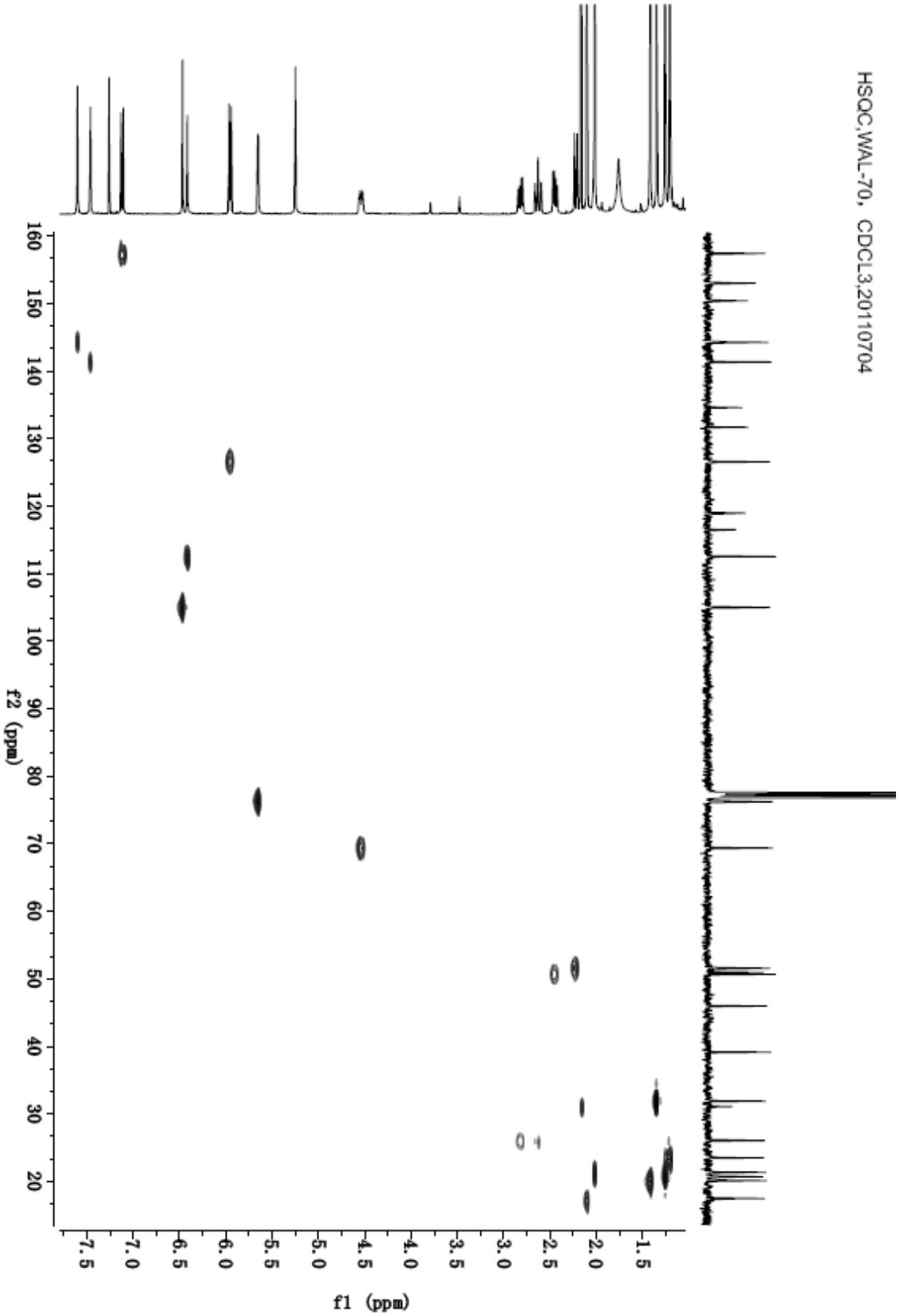


Figure S43. HMBC spectrum of walsucochinoid H (**6**) in $CDCl_3$

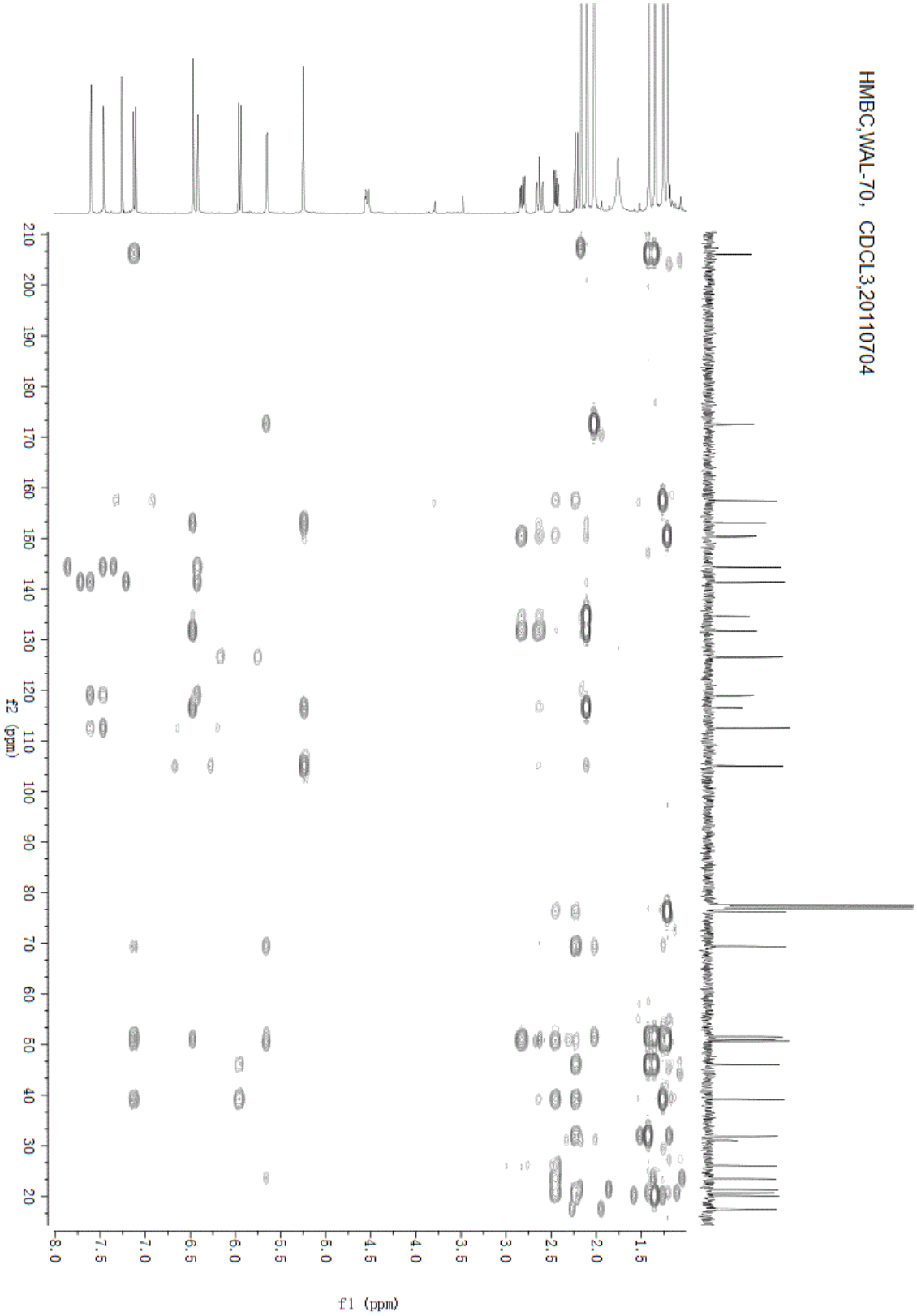


Figure S44. NOESY spectrum of walsucochinoid H (**6**) in $CDCl_3$

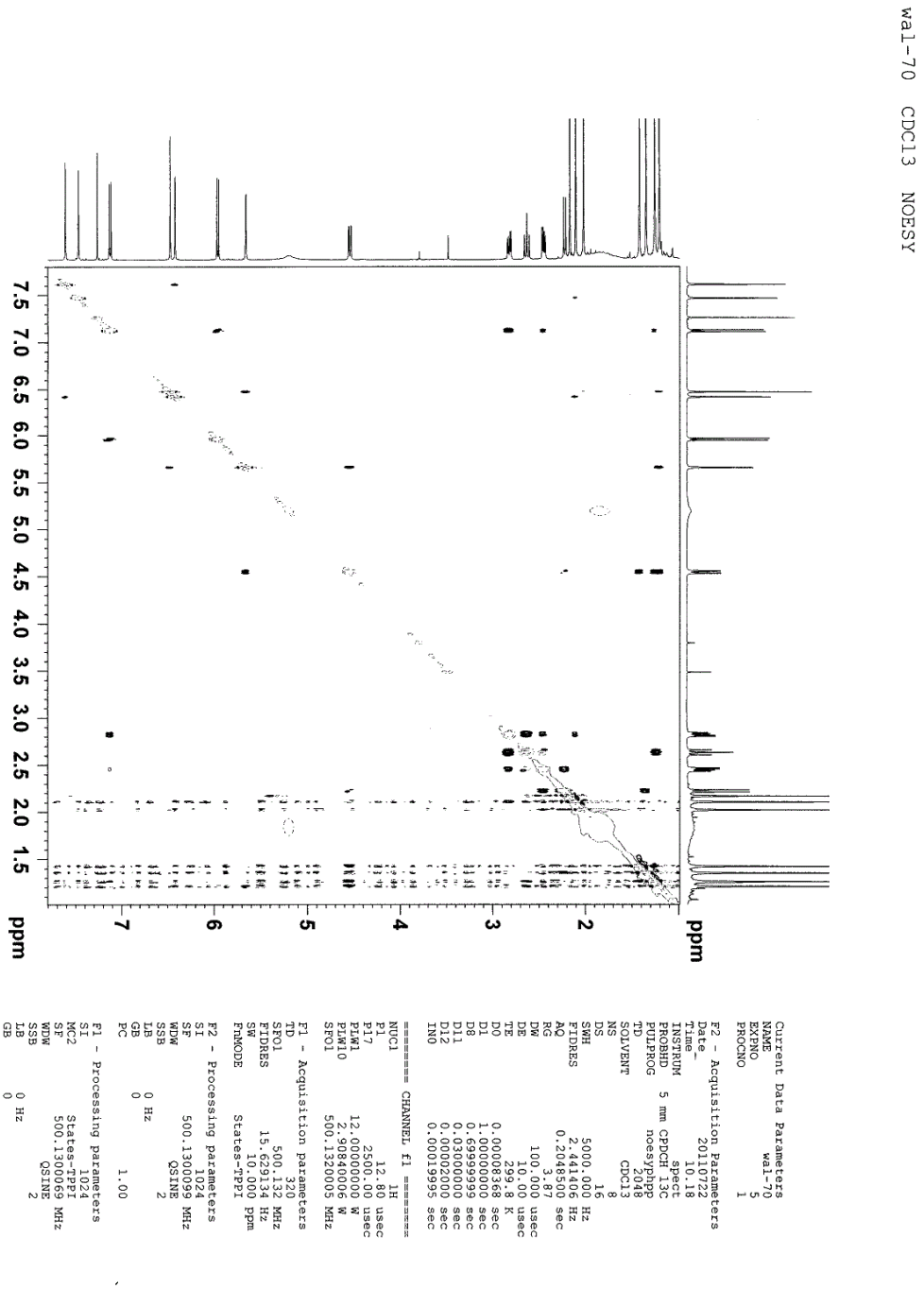


Figure S45. ESI(+)MS spectrum of walsucochinoid H (**6**)

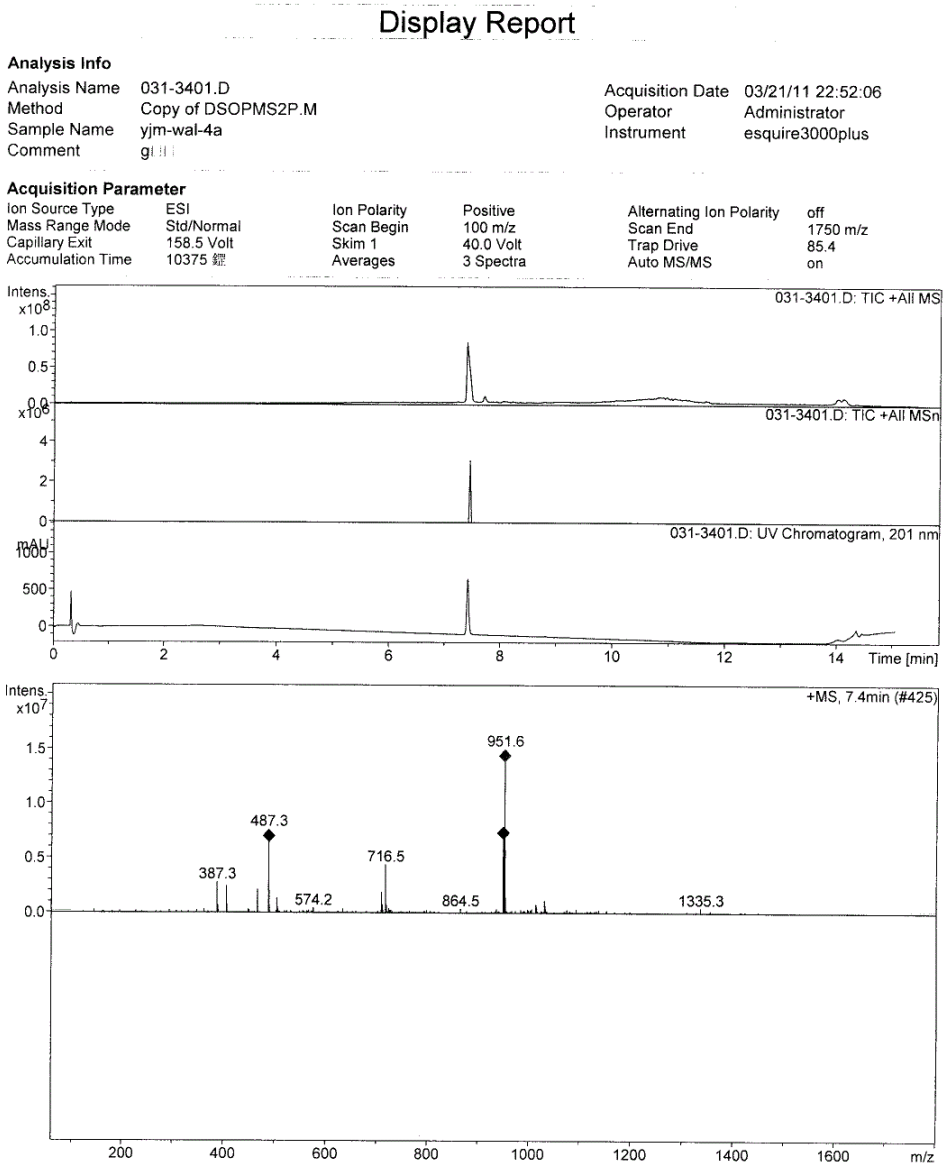


Figure S46. ESI(–)MS spectrum of walsucochinoid H (**6**)

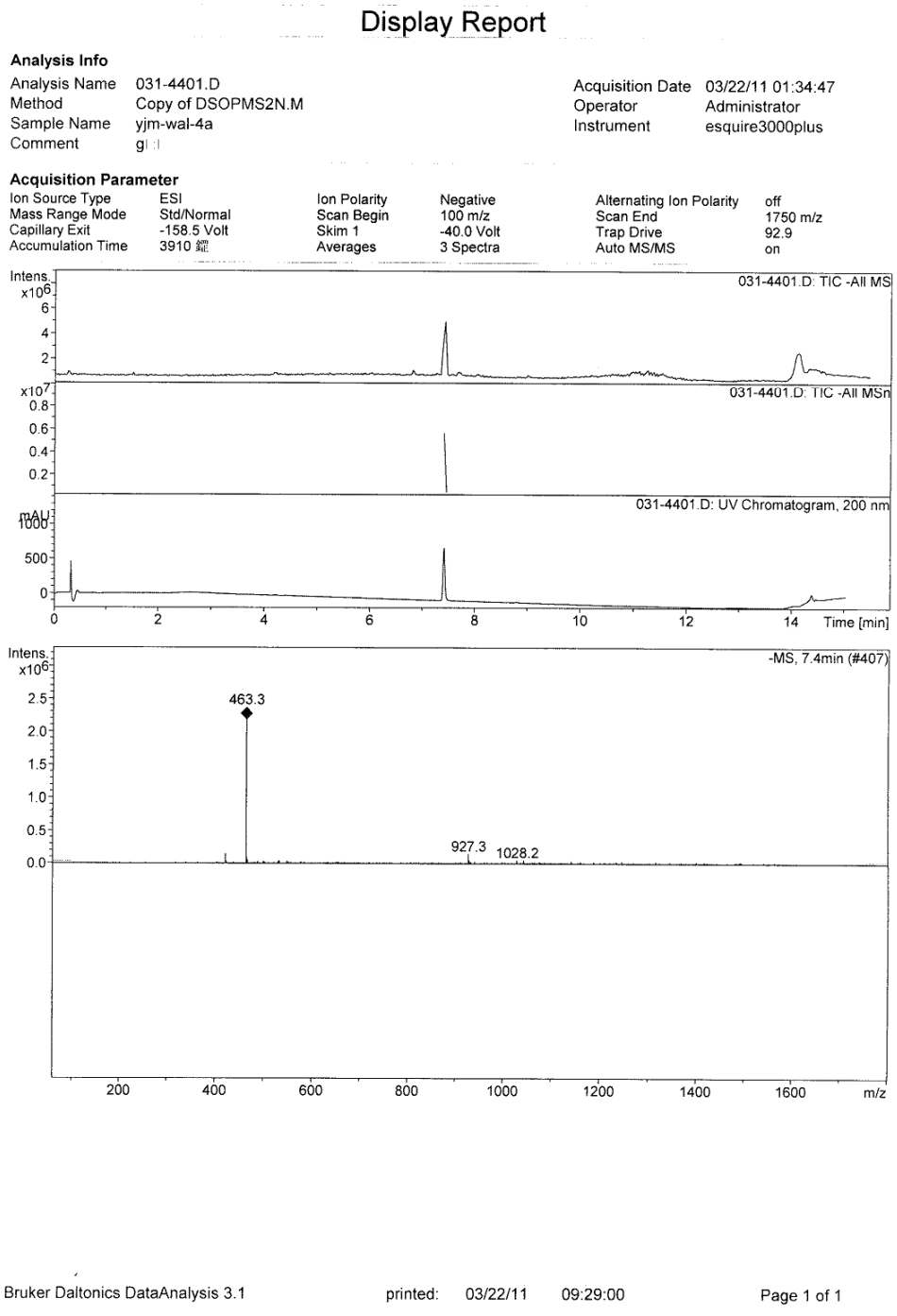


Figure S47. HRESI(–)MS spectrum of walsucochinoid H (**6**)

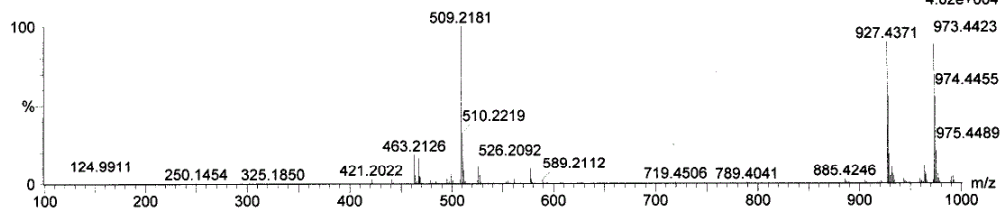
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
232 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30 Na: 0-1

WAL-4a LCT PXE KE324 04-Nov-2011 15:09:16

WAL-4a_1104 24 (0.528) AM2 (Ar,12000.0,0.00,0.70); ABS; Cm (22:36) 1: TOF MS ES- 4.02e+004



Minimum:				-1.5			
Maximum:		2.0	2.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
509.2181	509.2175	0.6	1.2	13.5	178.7	0.0	C29 H33 O8

Figure S48. IR spectrum of walsucochinoid H (**6**)

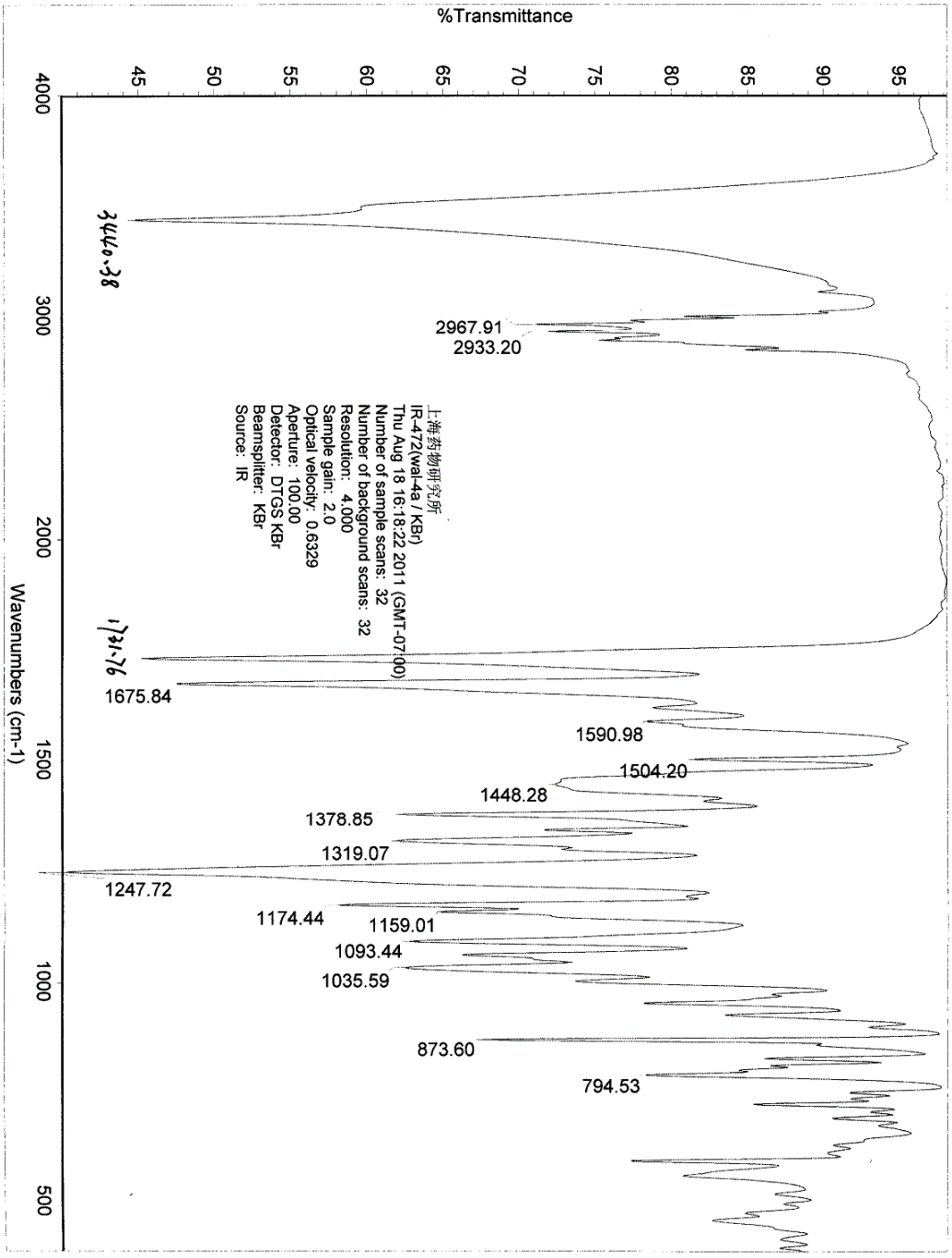


Figure S49. ^{1}H NMR spectrum of walsucochinoid I (**7**) in $CDCl_3$

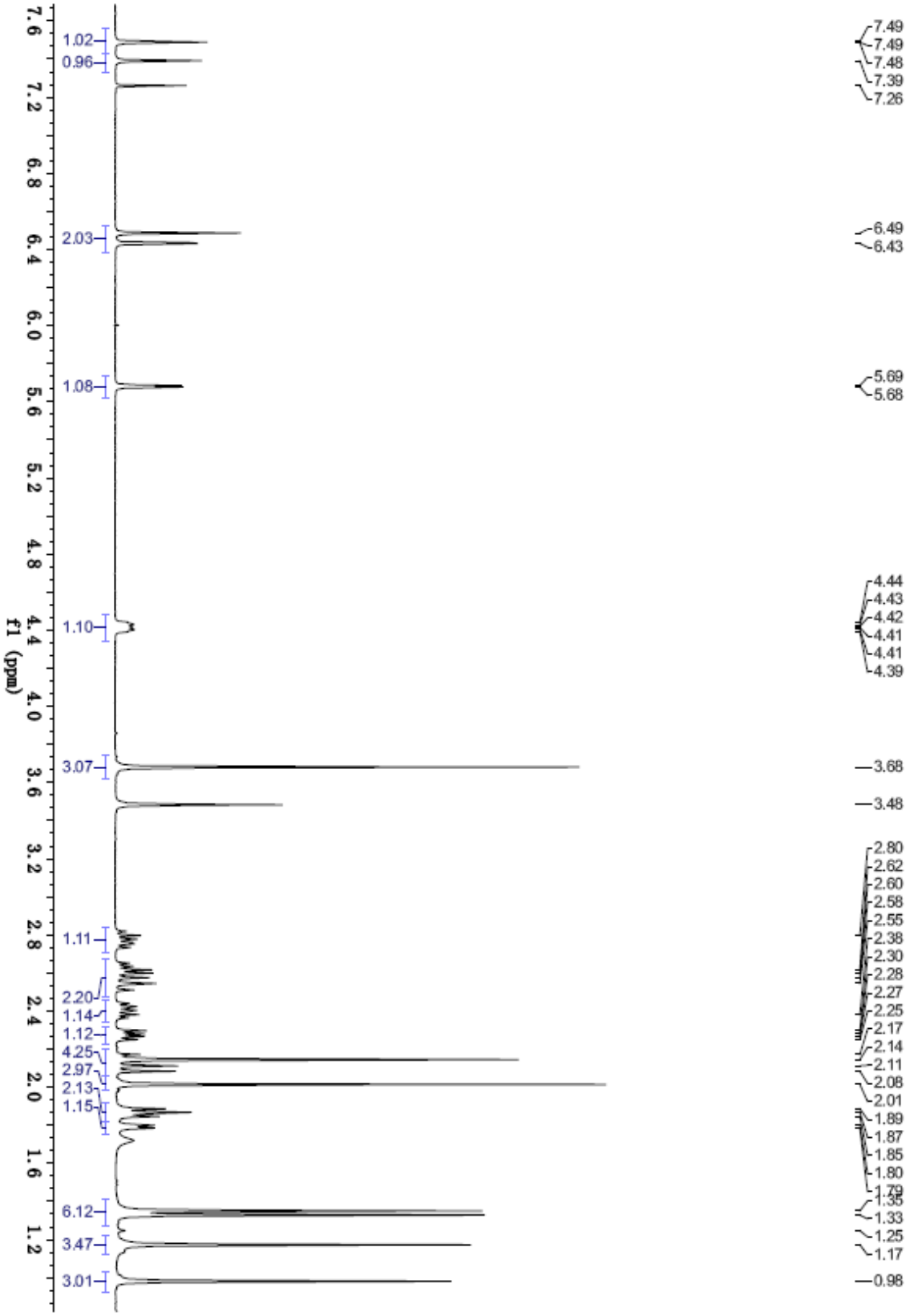


Figure S50. ^{13}C NMR spectrum of walsucochinoid I (**7**) in $CDCl_3$

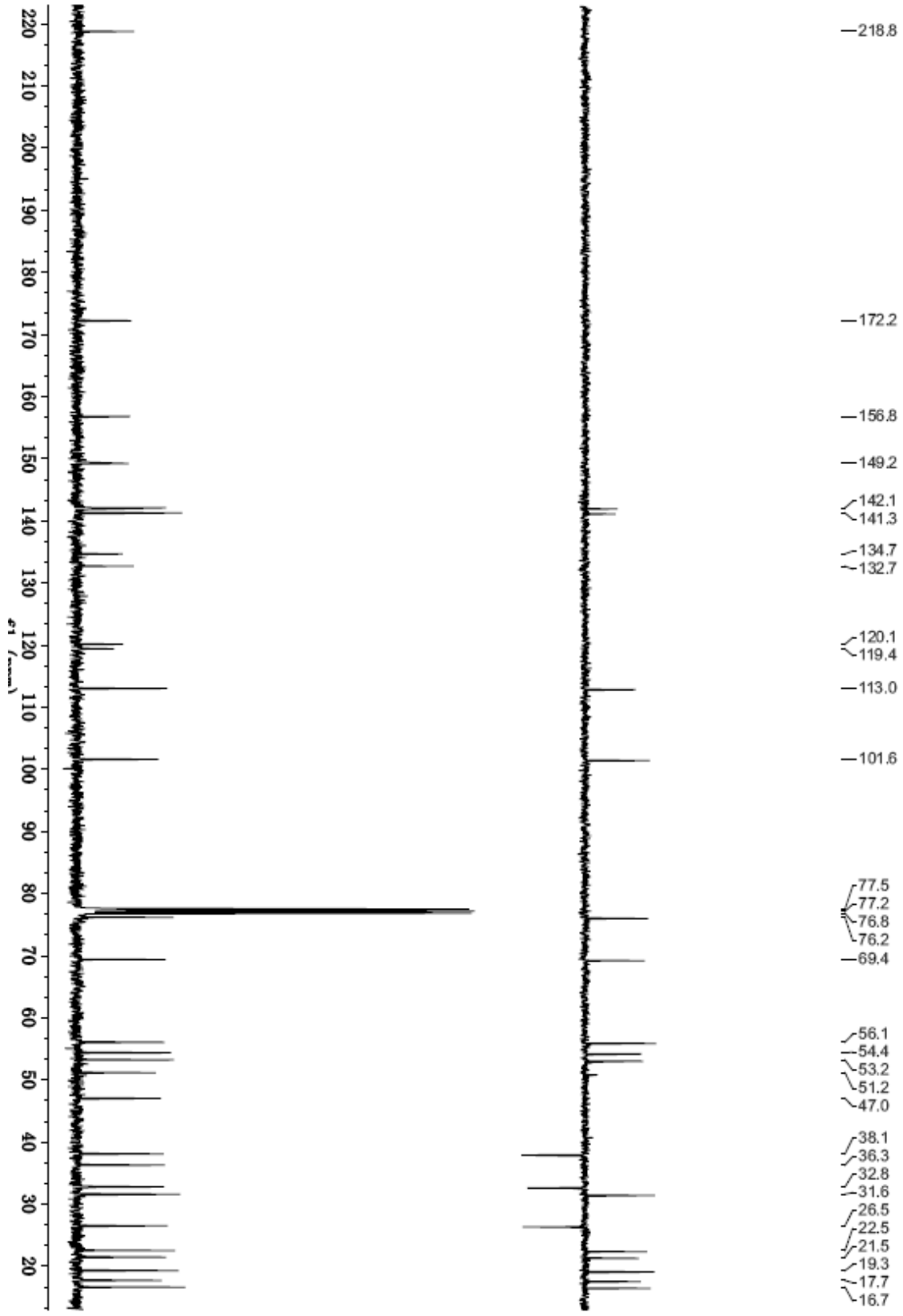


Figure S51. HSQC spectrum of walsucochinoid I (**7**) in $CDCl_3$

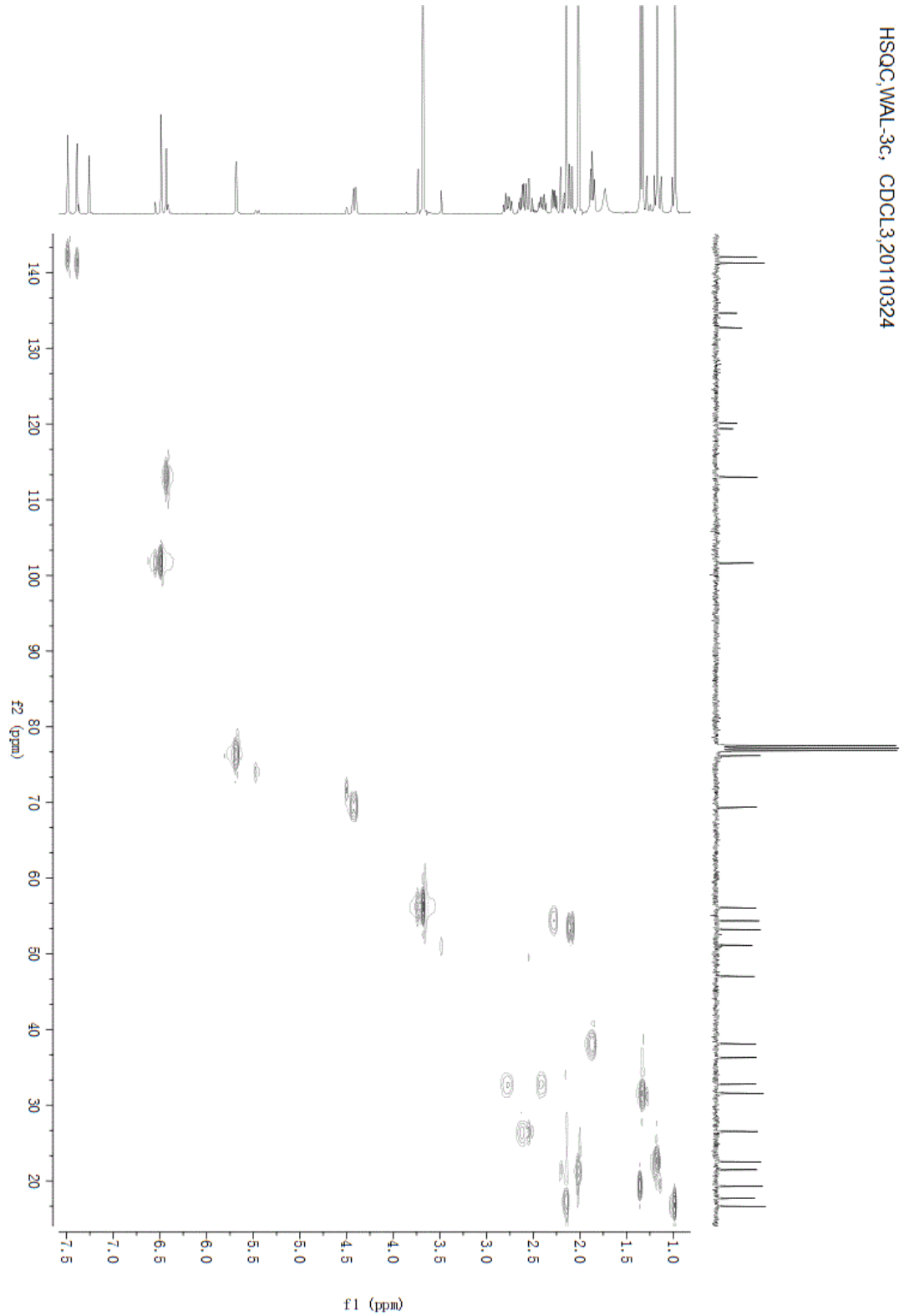


Figure S52. HMBC spectrum of walsucochinoid I (**7**) in $CDCl_3$

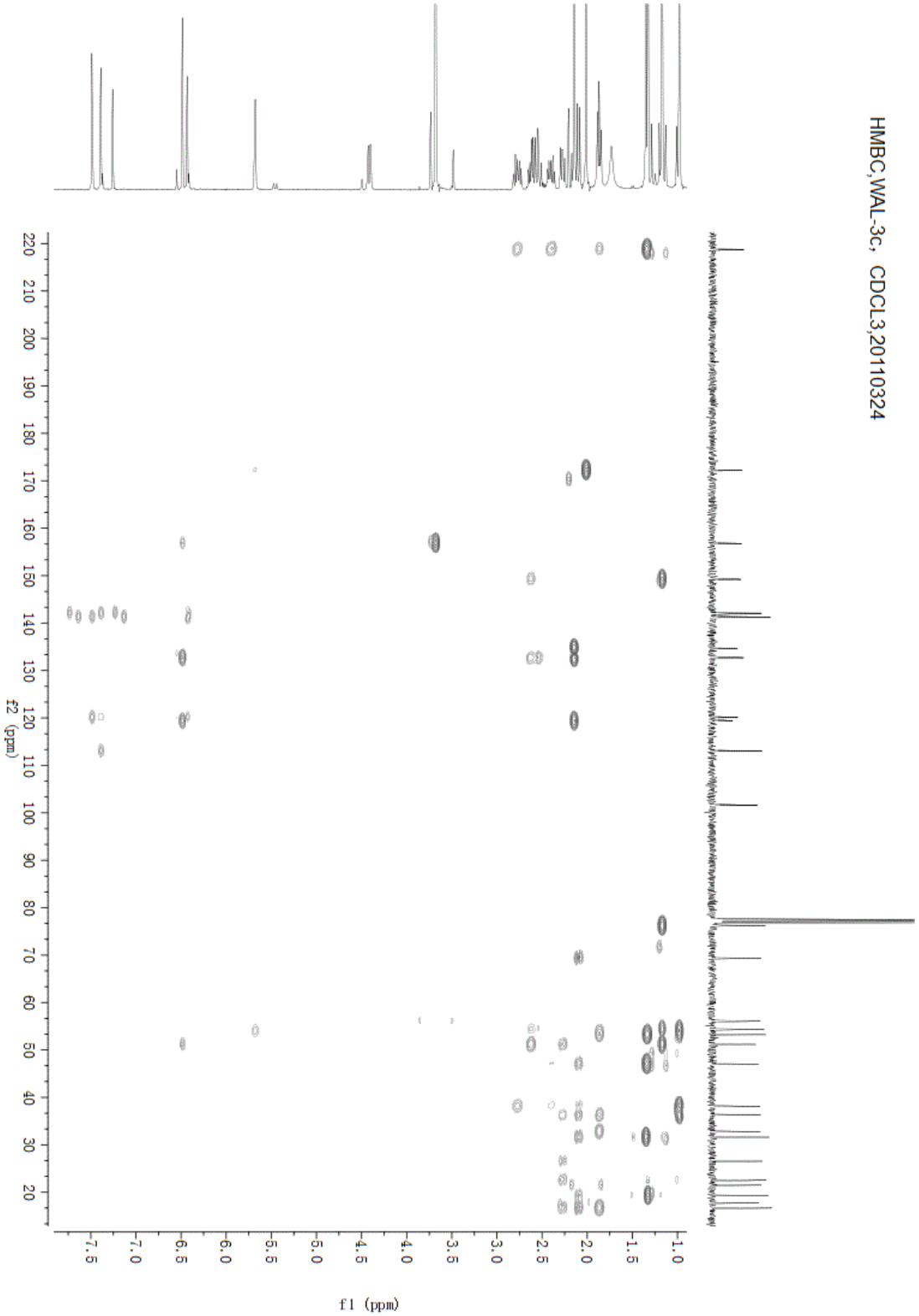


Figure S53. ROESY spectrum of walsucochinoid I (**7**) in $CDCl_3$

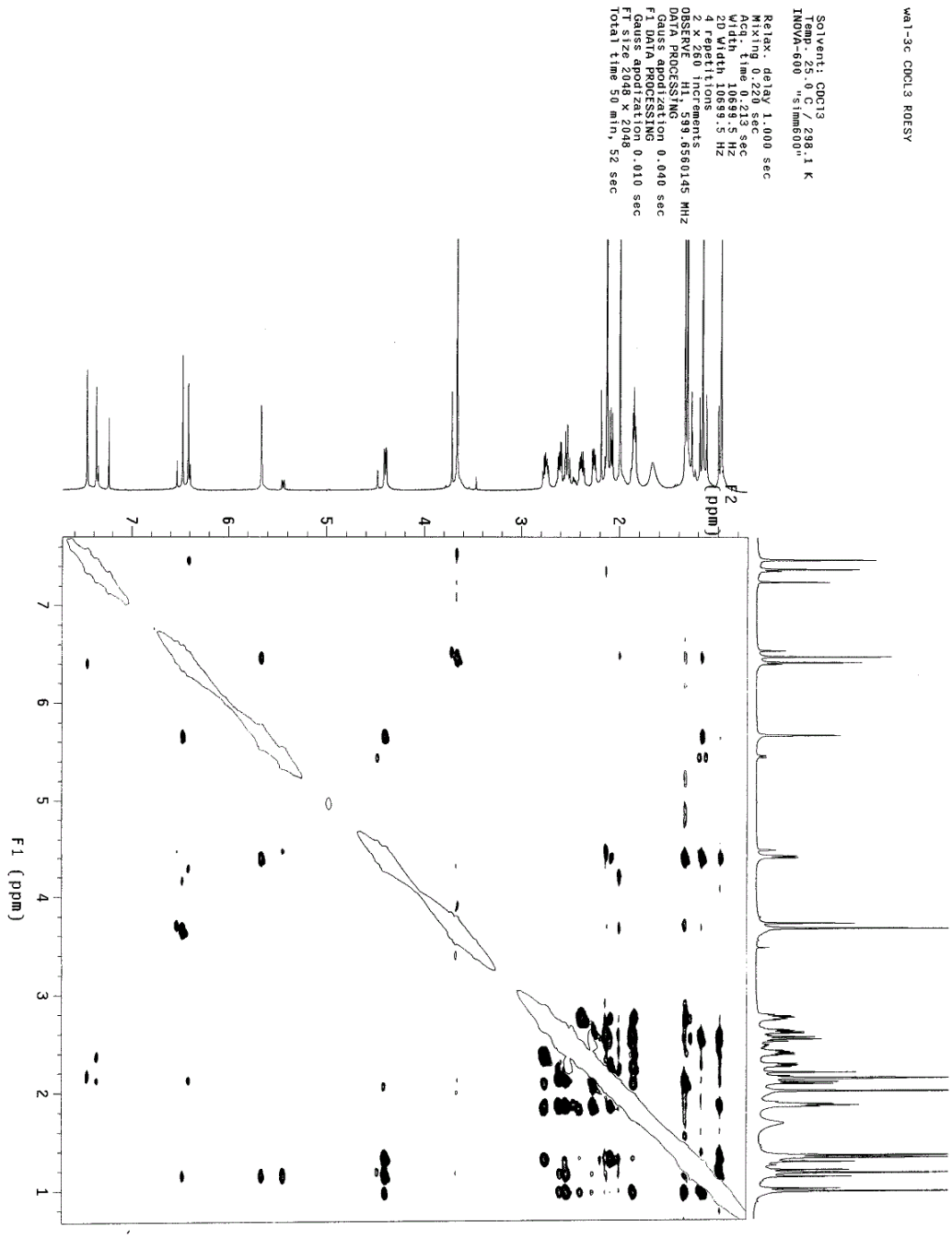


Figure S54. ESI(+)MS spectrum of walsucochinoid I (**7**)

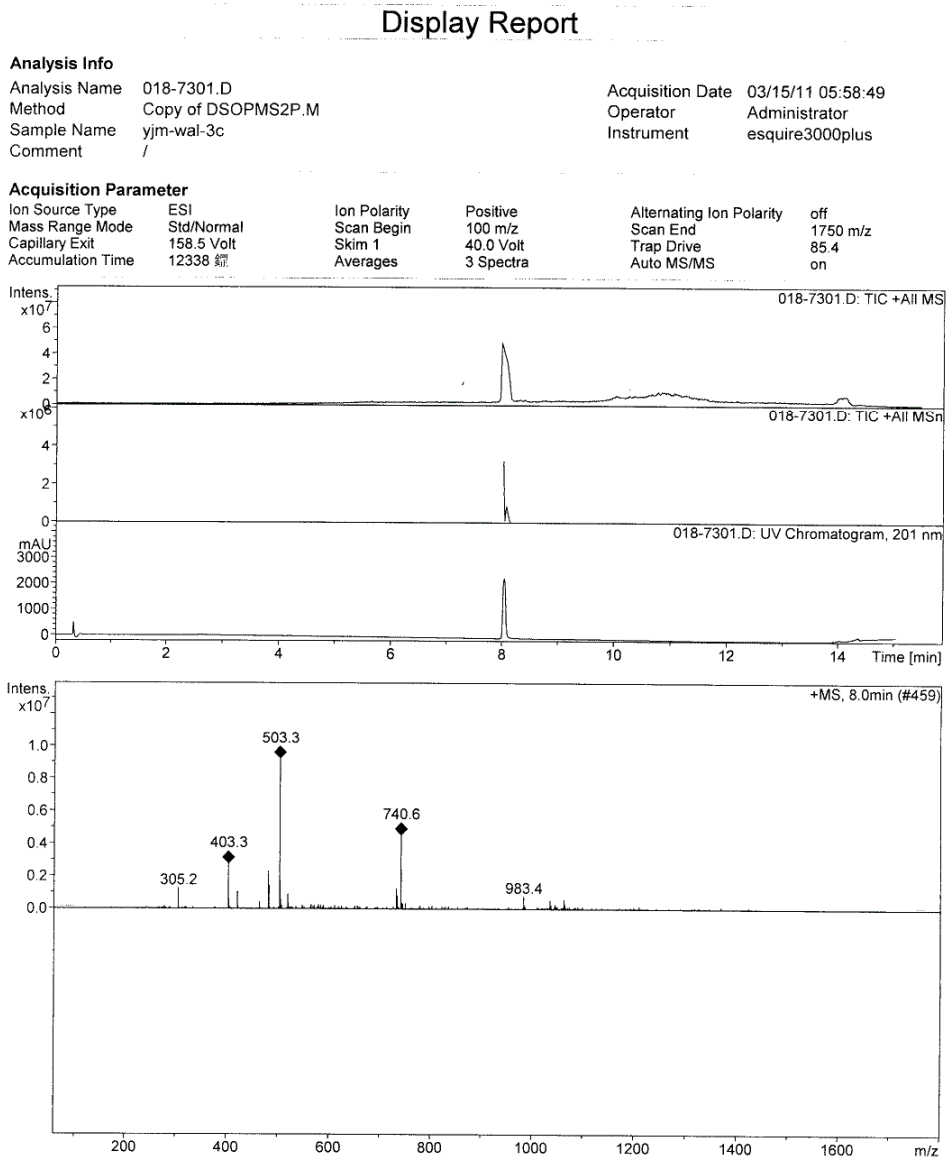


Figure S55. ESI(−)MS spectrum of walsucochinoid I (**7**)

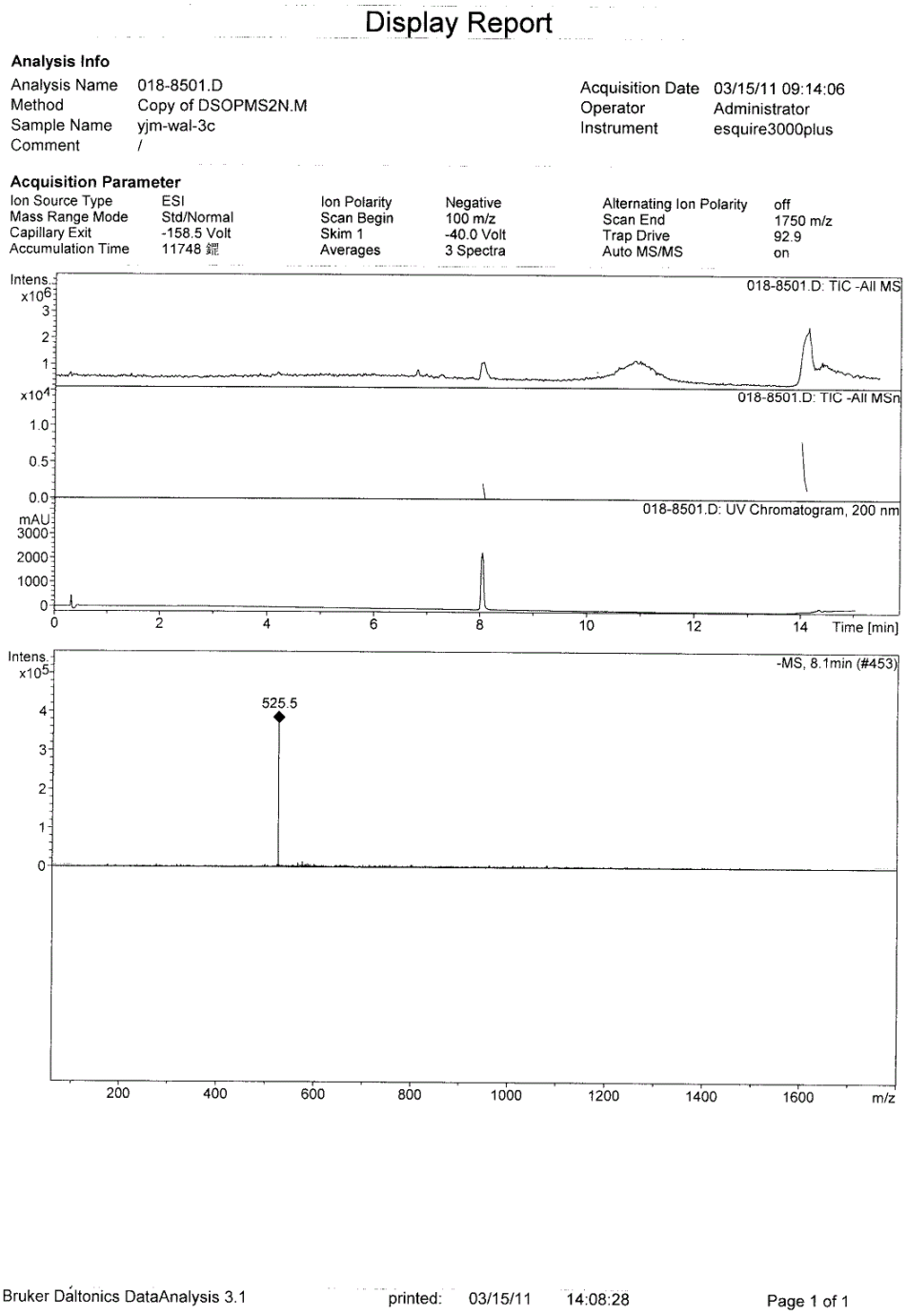


Figure S56. HRESI(–)MS spectrum of walsucochinoid I (**7**)

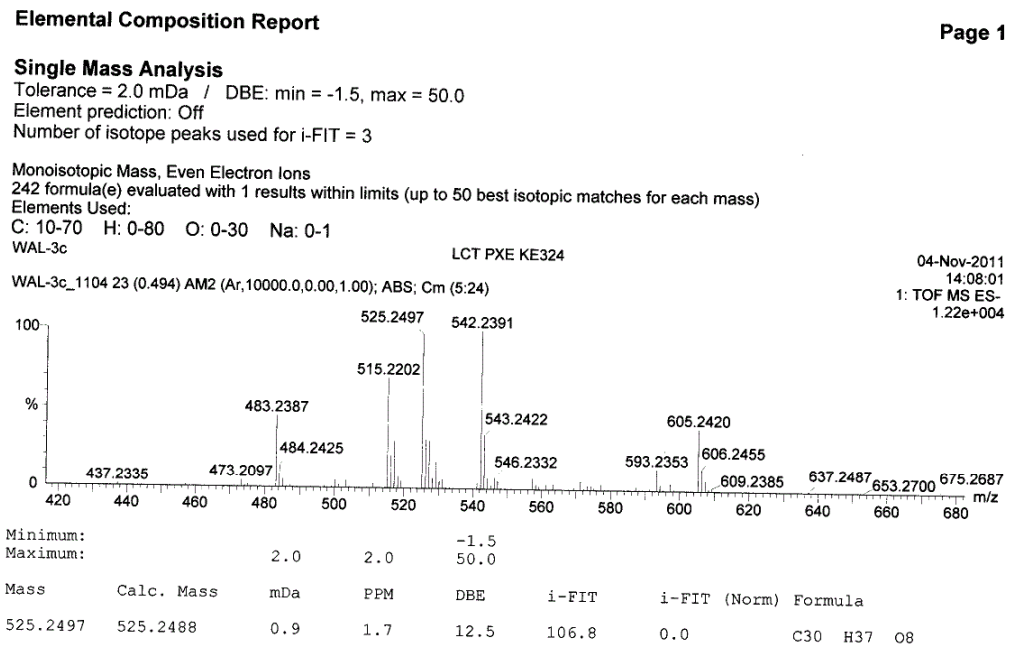


Figure S57. IR spectrum of walsucochinoid I (**7**)

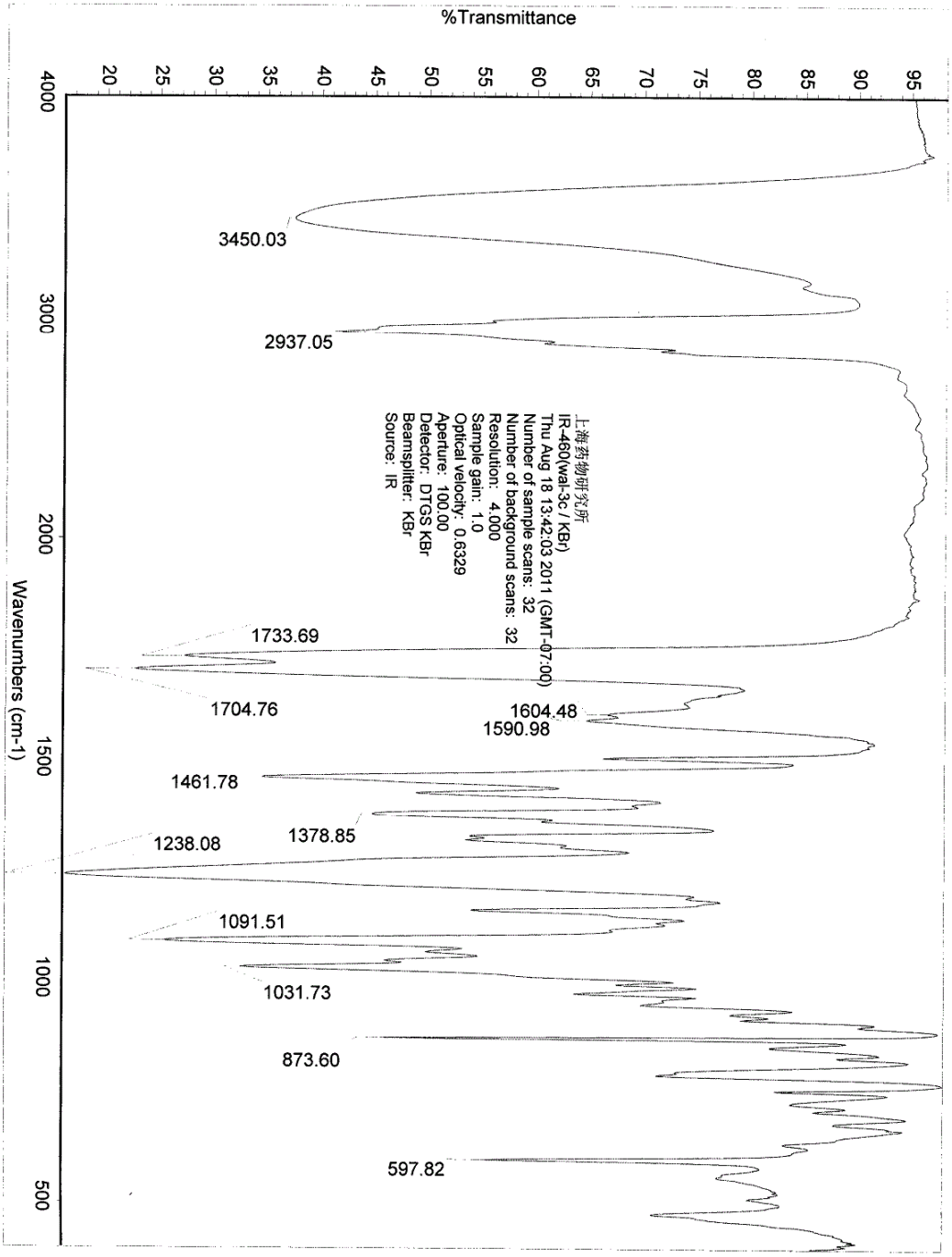


Figure S58. ^{1}H NMR spectrum of walsucochinoid J (**8**) in $CDCl_3$

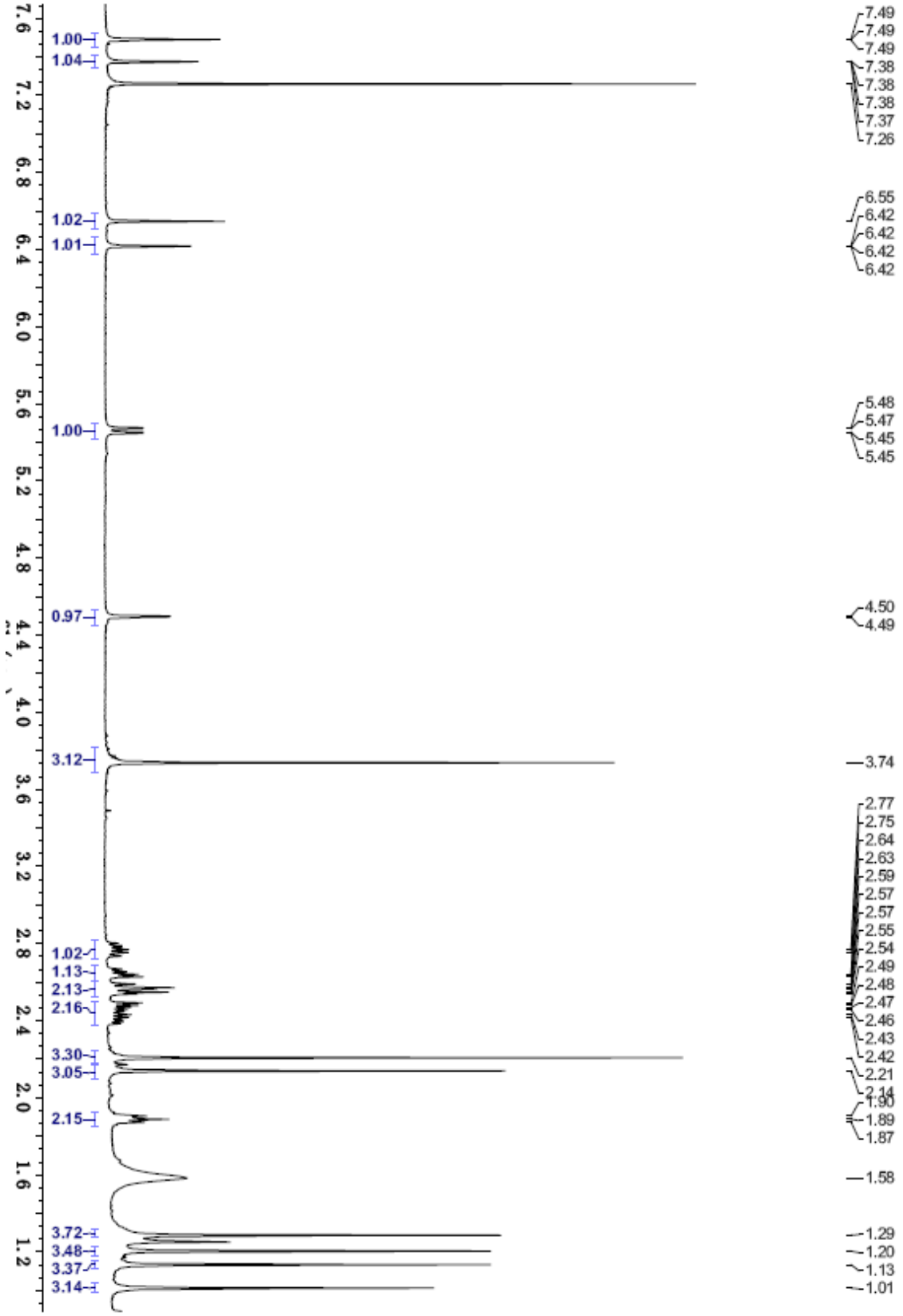


Figure S59. ^{13}C NMR spectrum of walsucochinoid J (**8**) in $CDCl_3$

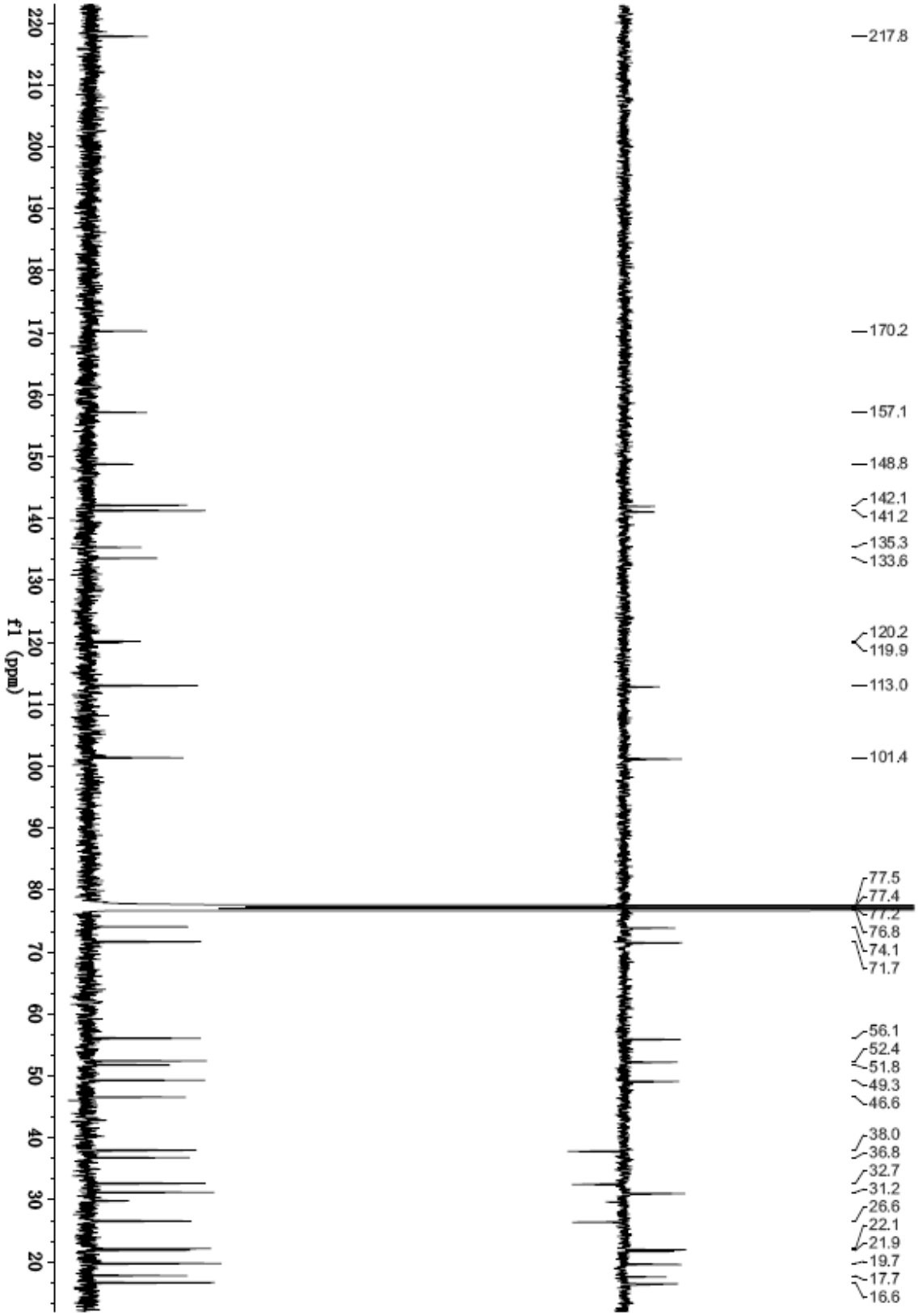


Figure S60. HSQC spectrum of walsucochinoid J (**8**) in $CDCl_3$

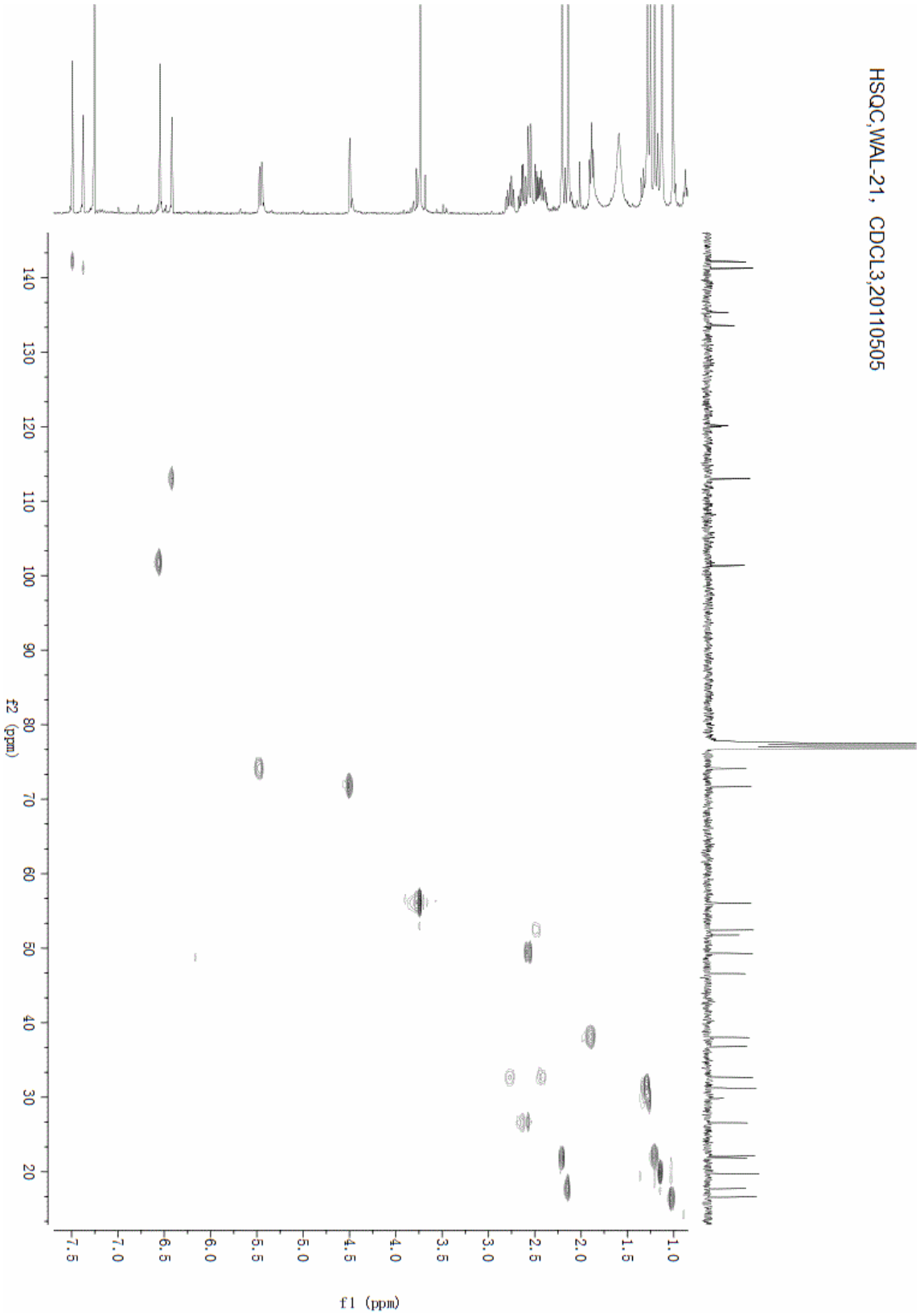


Figure S61.HMBC spectrum of walsucochinoid J (**8**) in $CDCl_3$

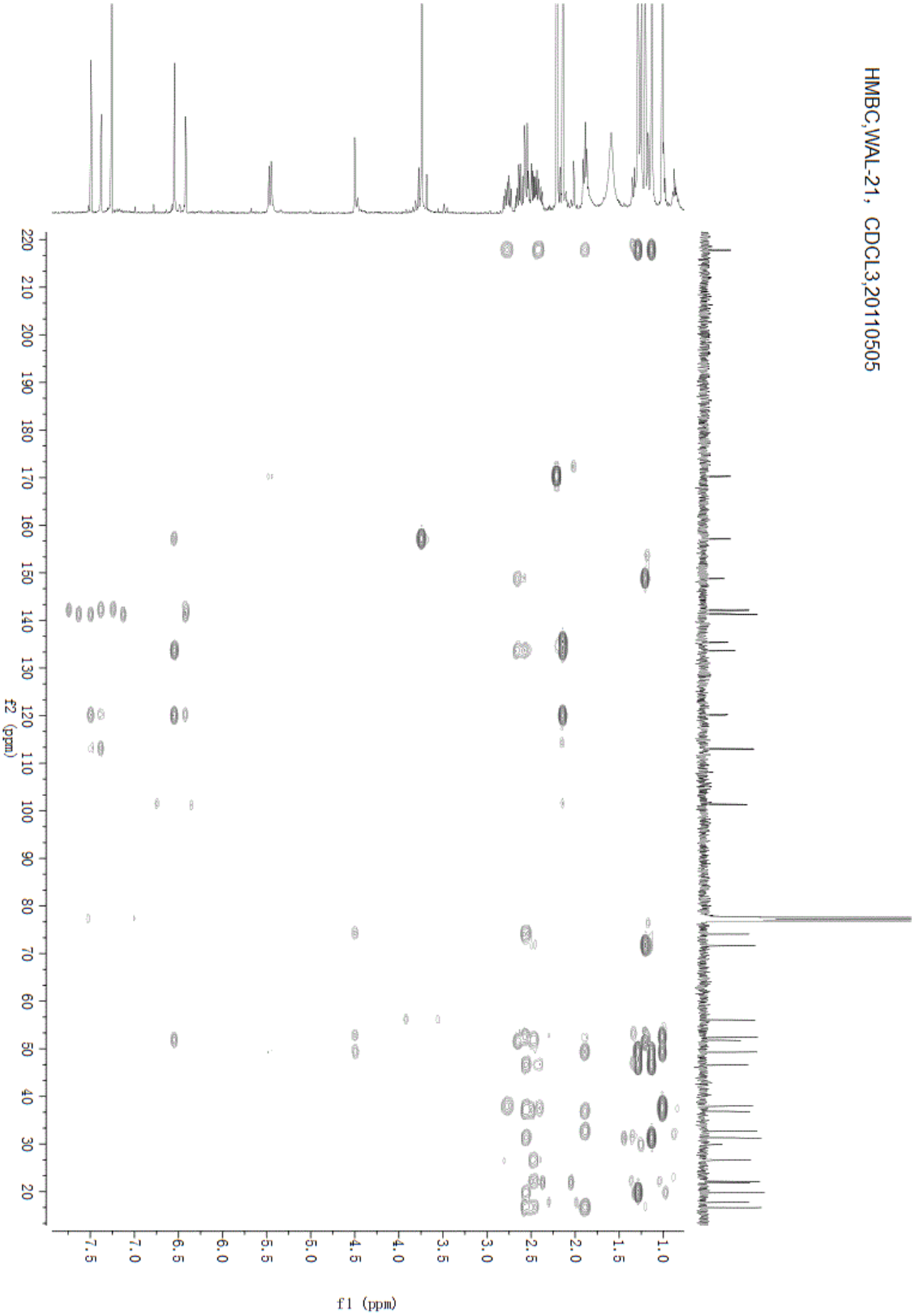


Figure S62. ROESY spectrum of walsucochinoid J (**8**) in $CDCl_3$

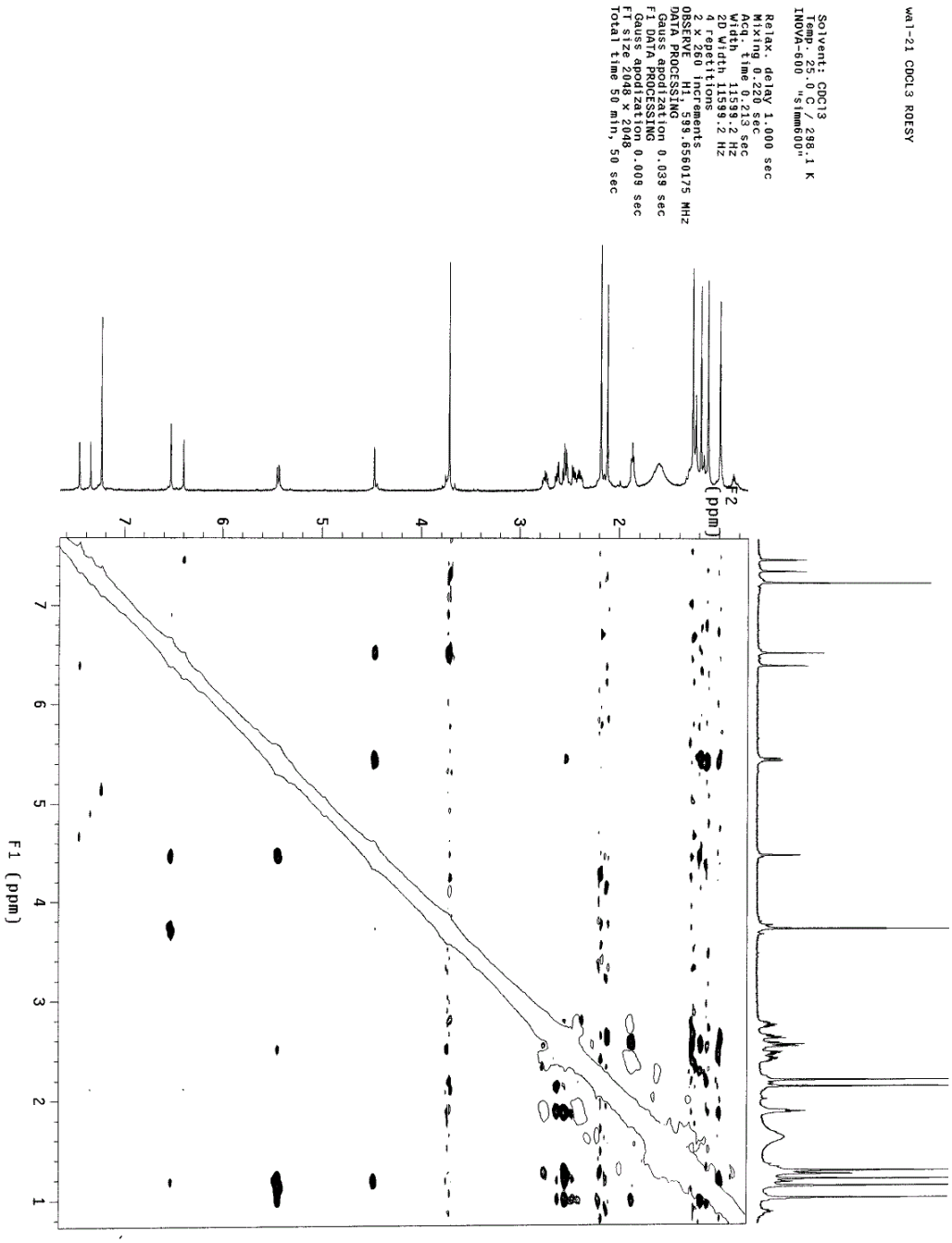


Figure S63. ESI(+)MS spectrum of walsucochinoid J (**8**)

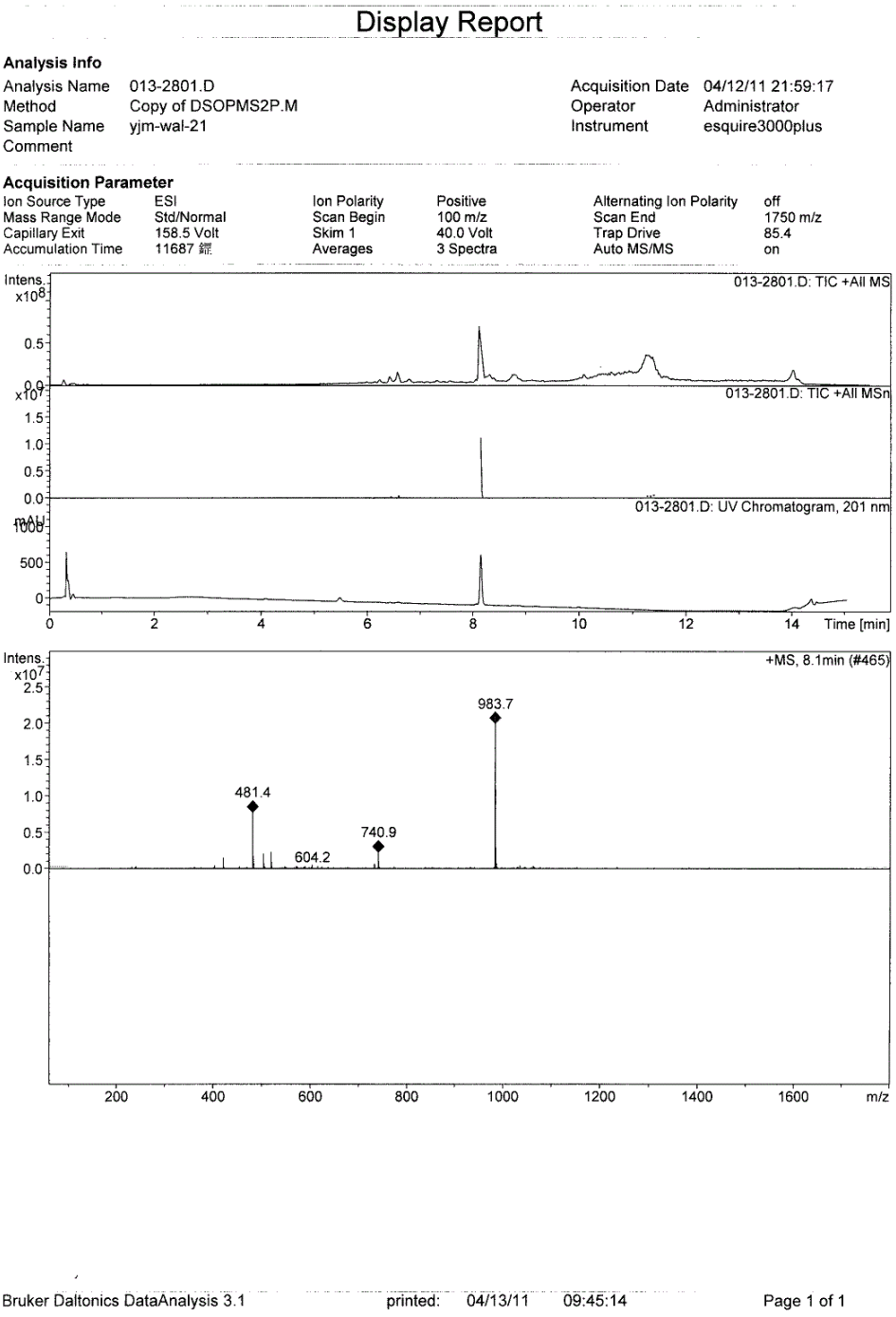


Figure S64. ESI(−)MS spectrum of walsucochinoid J (**8**)

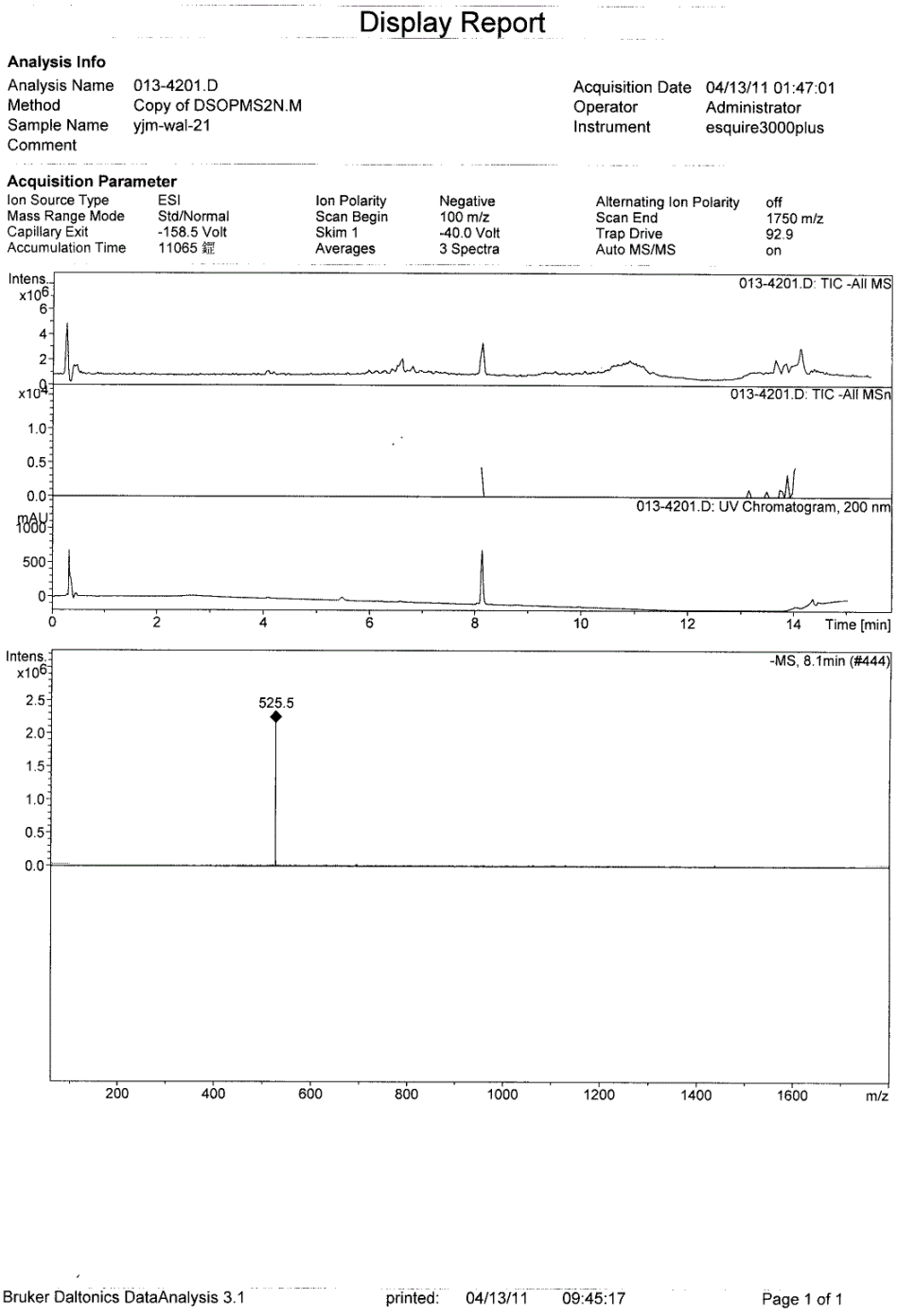


Figure S65. HRESI(–)MS spectrum of walsucochinoid J (**8**)

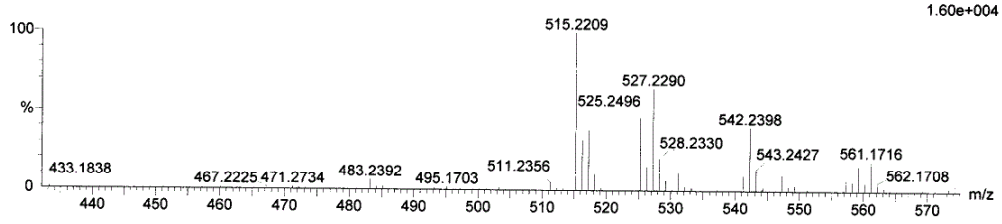
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
242 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30 Na: 0-1

WAL-21 LCT PXE KE324 04-Nov-2011 16:02:56

WAL-21_1104 7 (0.124) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (6:18) 1: TOF MS ES- 1.60e+004



Minimum:				-1.5			
Maximum:		2.0	2.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
525.2496	525.2488	0.8	1.5	12.5	125.7	0.0	C30 H37 O8

Figure S66. IR spectrum of walsucochinoid J (**8**)

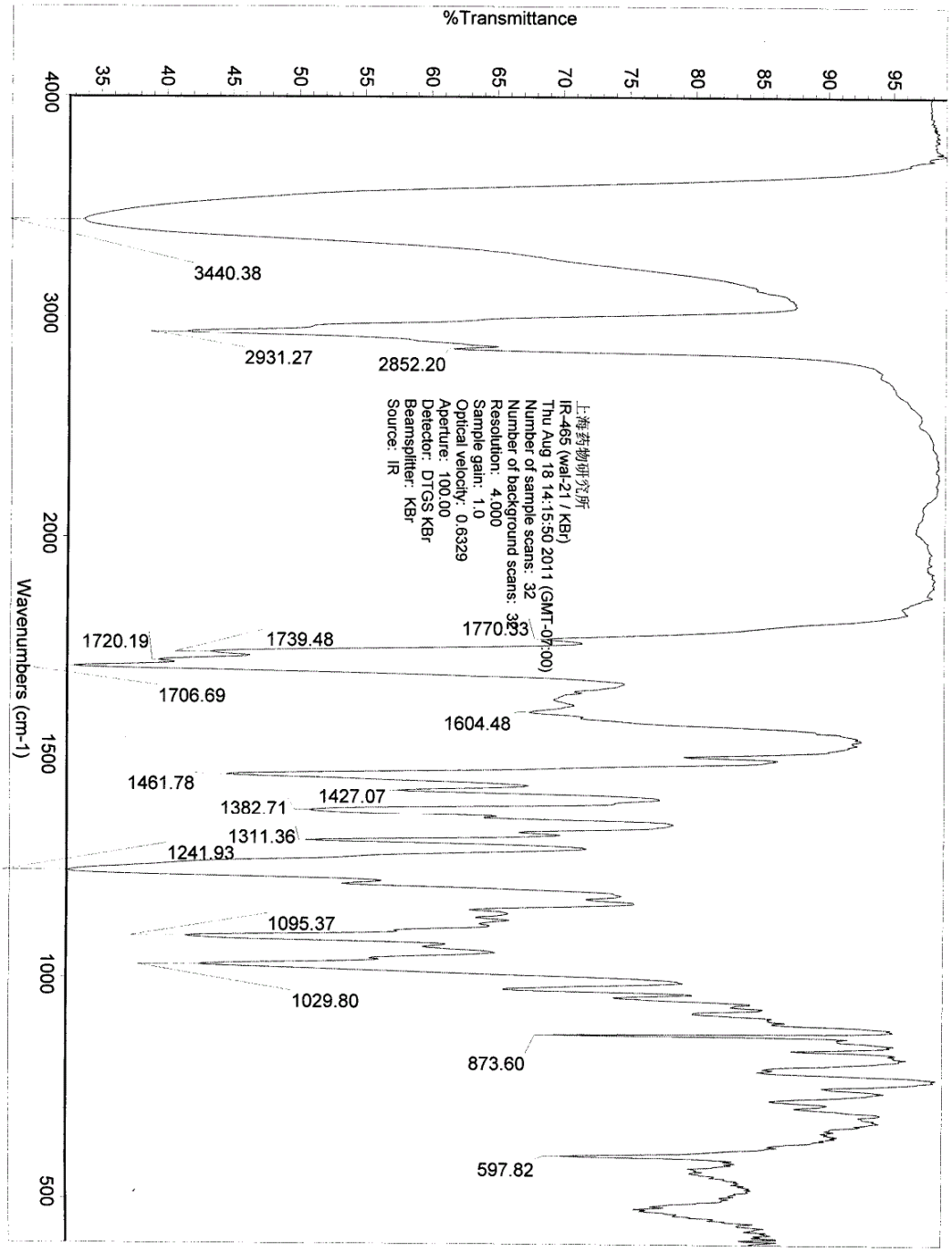


Figure S67. ^{1}H NMR spectrum of walsucochinoid K (**9**) in $CDCl_3$

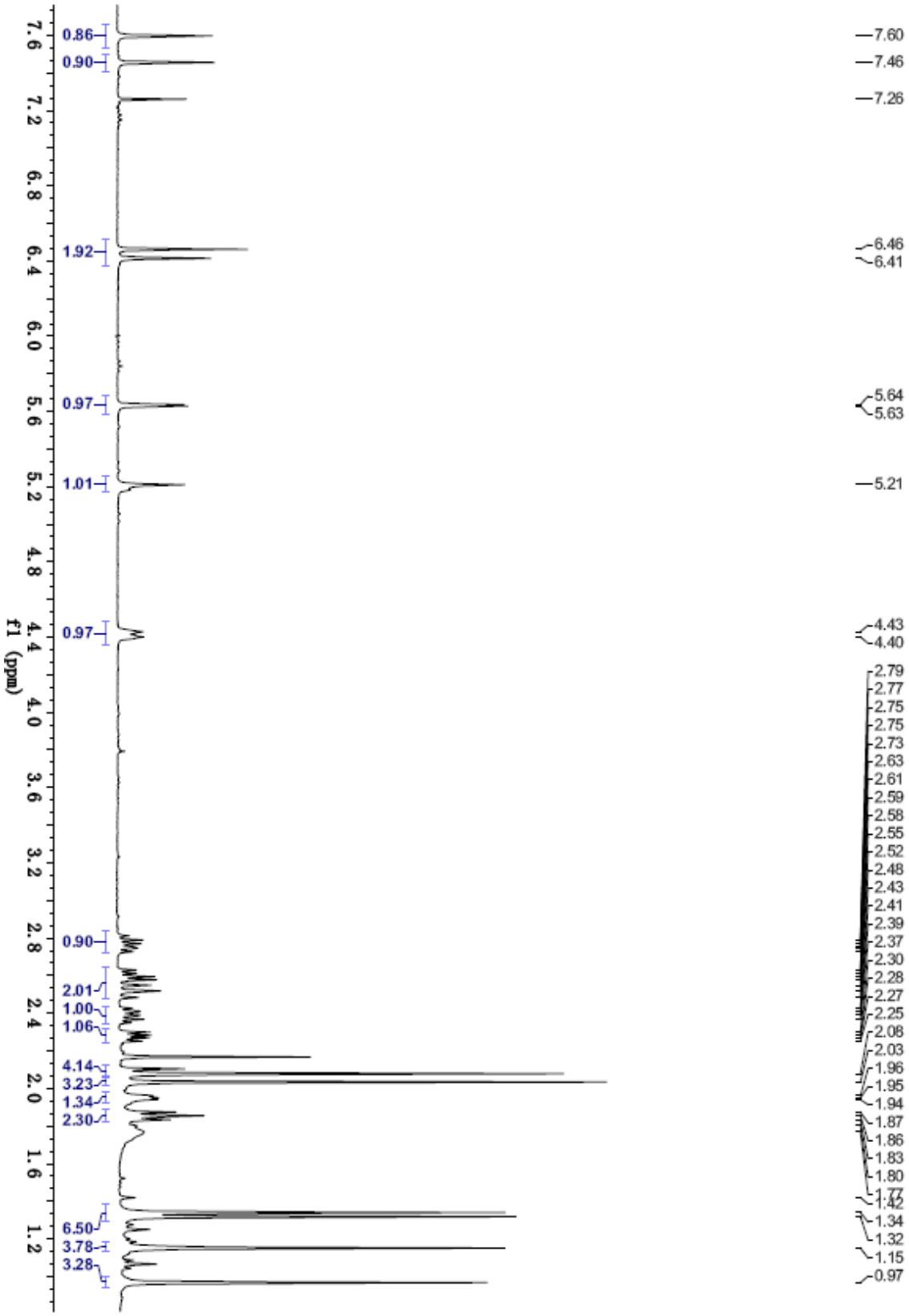


Figure S68. ^{13}C NMR spectrum of walsucochinoid K (**9**) in $CDCl_3$

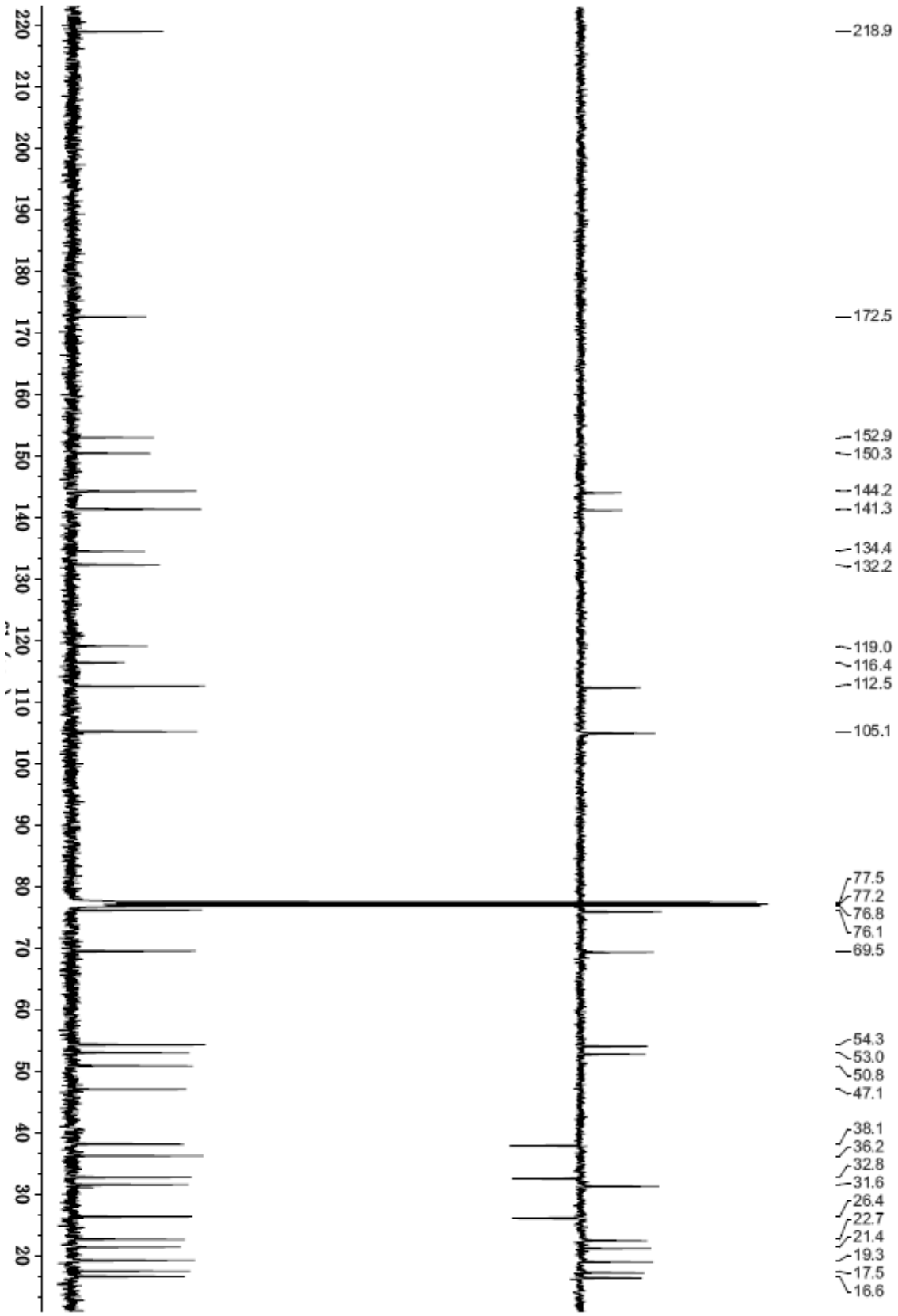


Figure S69. HSQC spectrum of walsucochinoid K (**9**) in $CDCl_3$

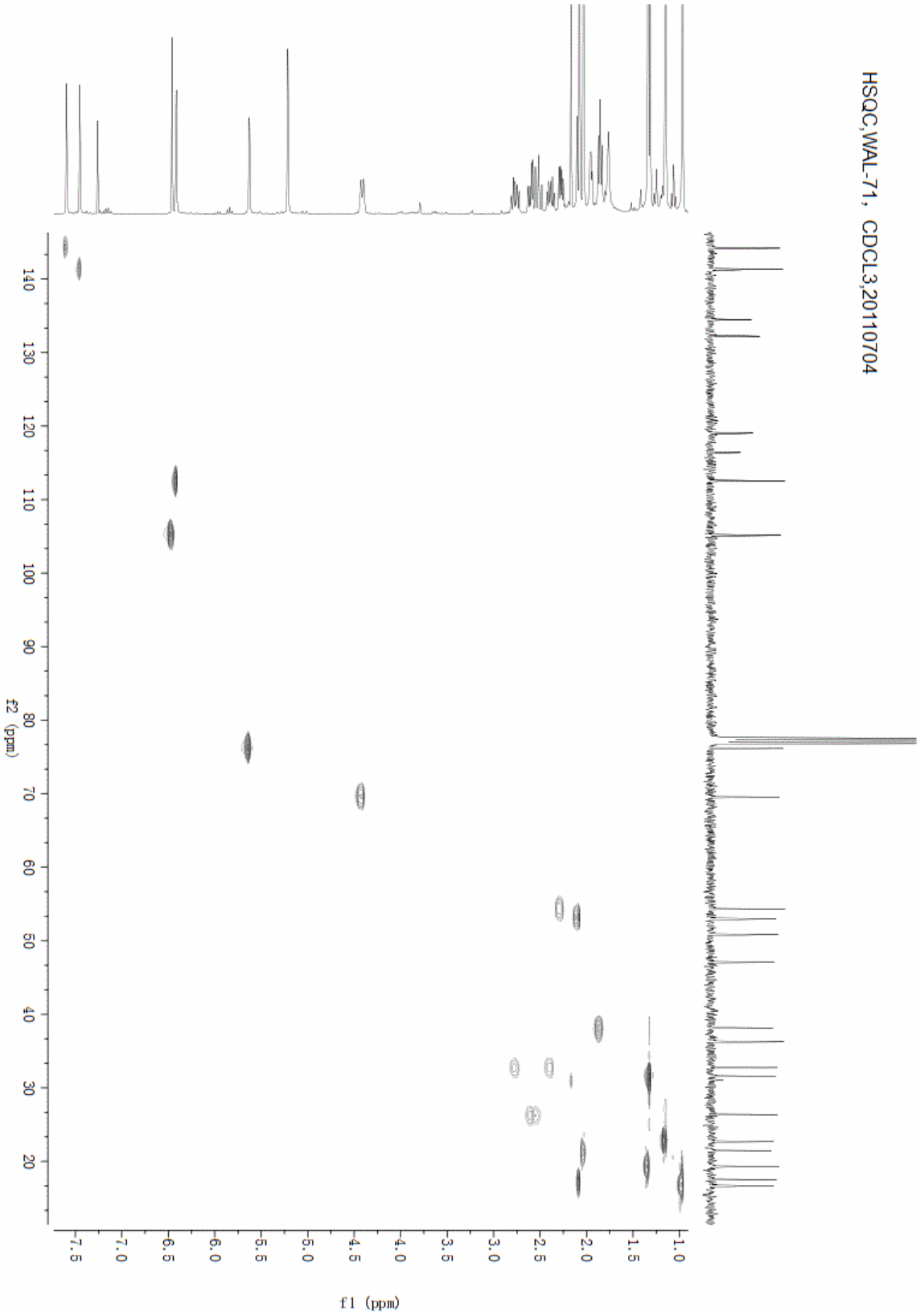


Figure S70. HMBC spectrum of walsucochinoid K (**9**) in $CDCl_3$

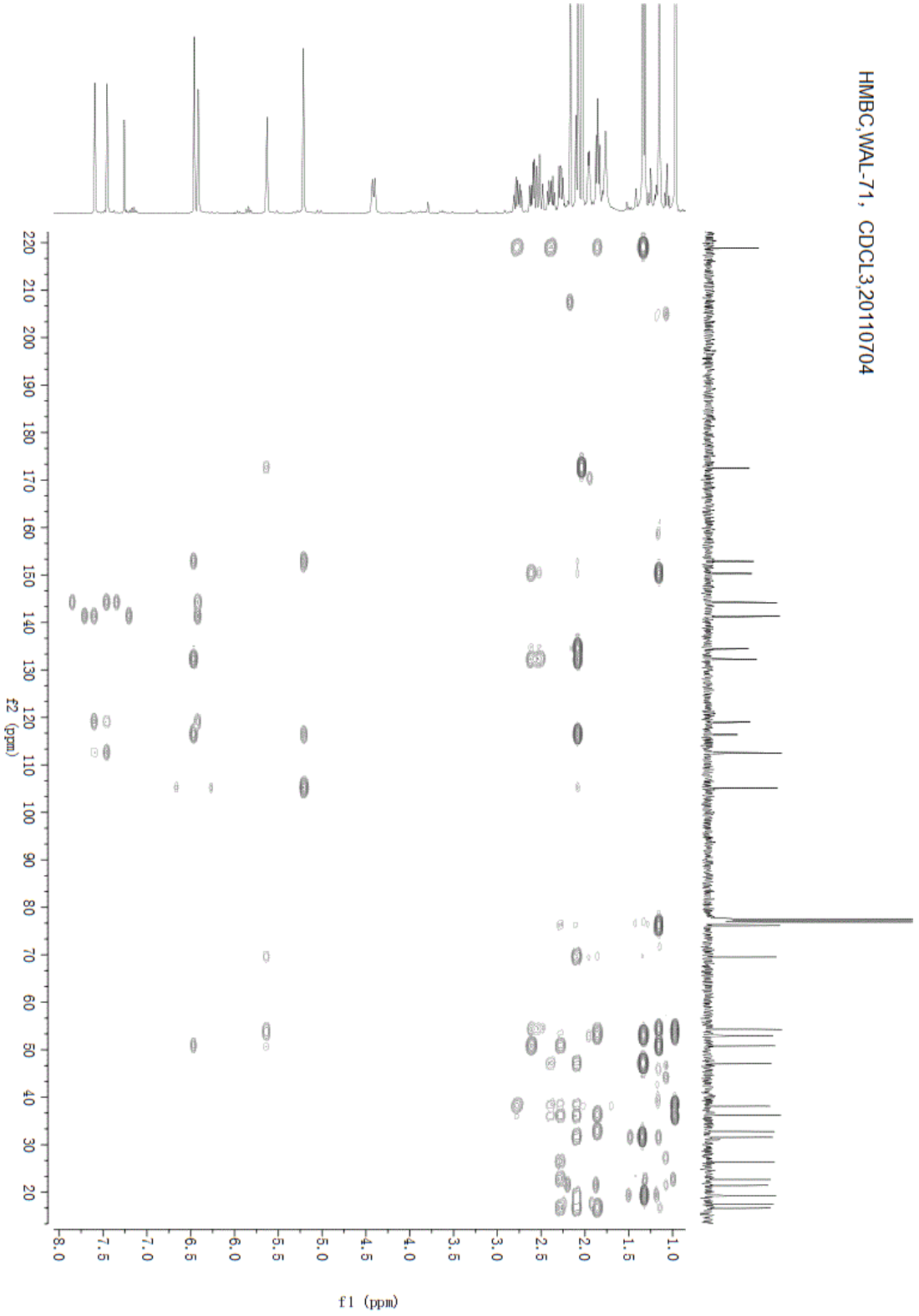


Figure S71. ROESY spectrum of walsucochinoid K (**9**) in $CDCl_3$

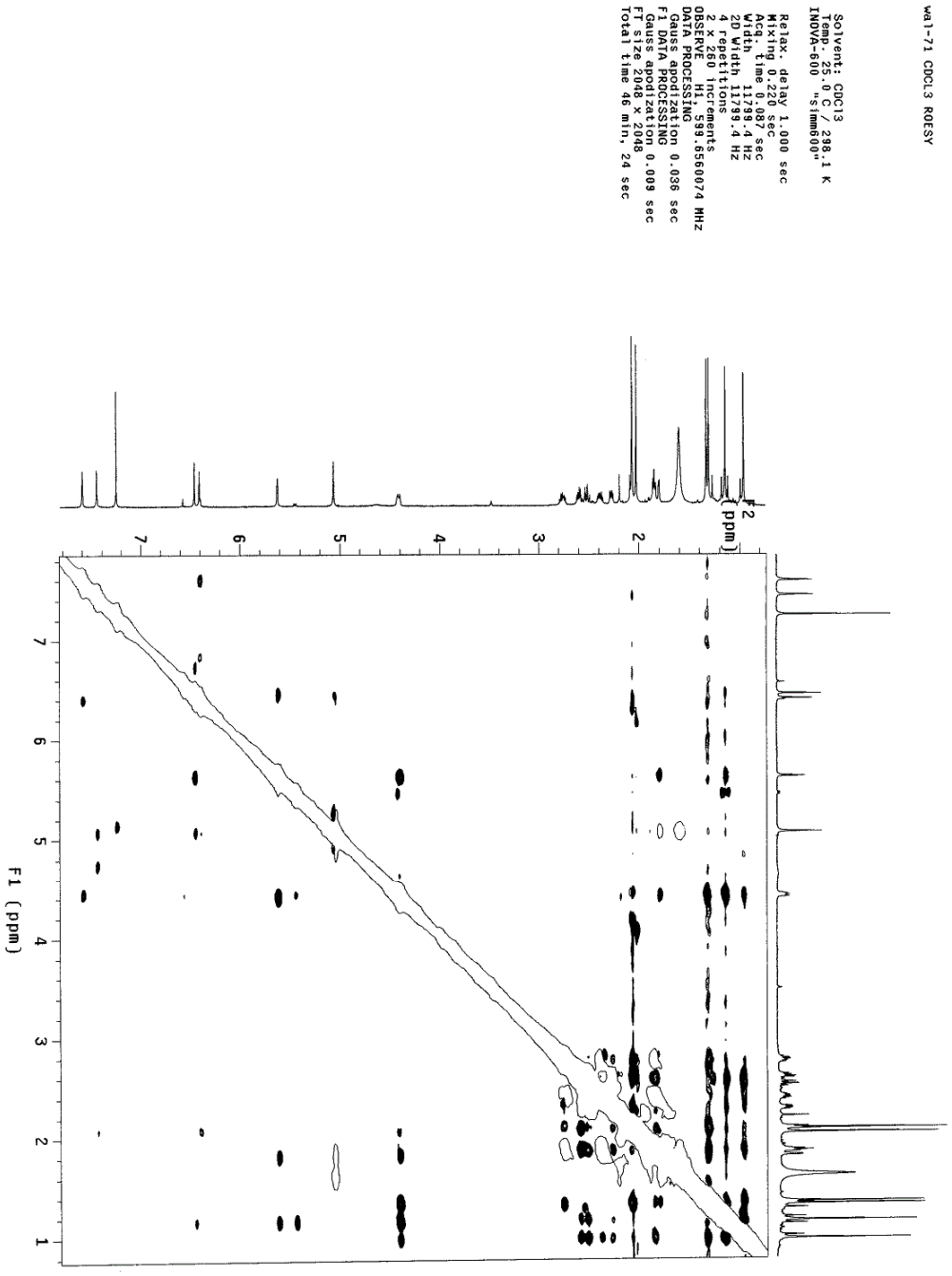


Figure S72. ESI(+)MS spectrum of walsucochinoid K (**9**)

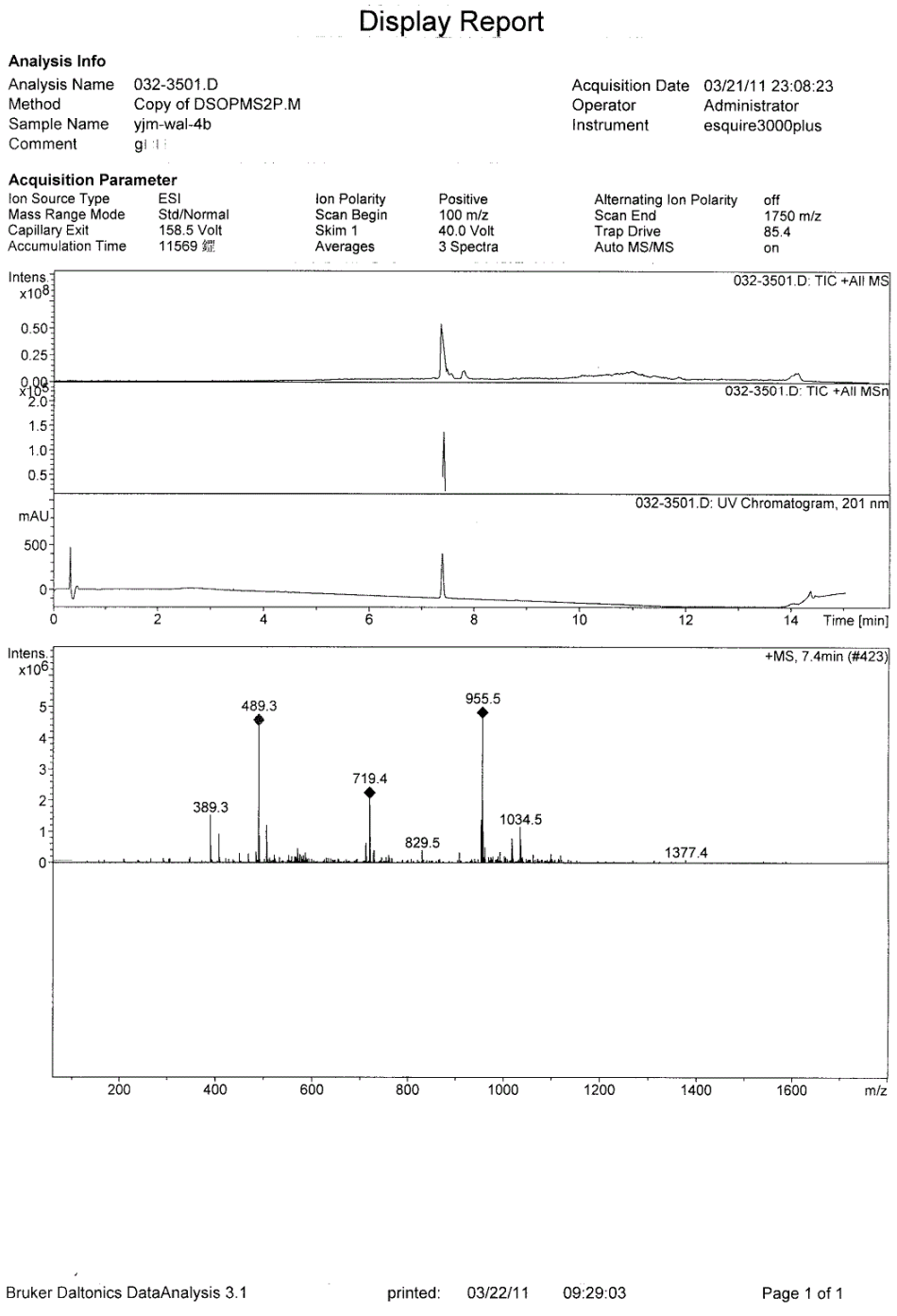


Figure S73. ESI(−)MS spectrum of walsucochinoid K (**9**)

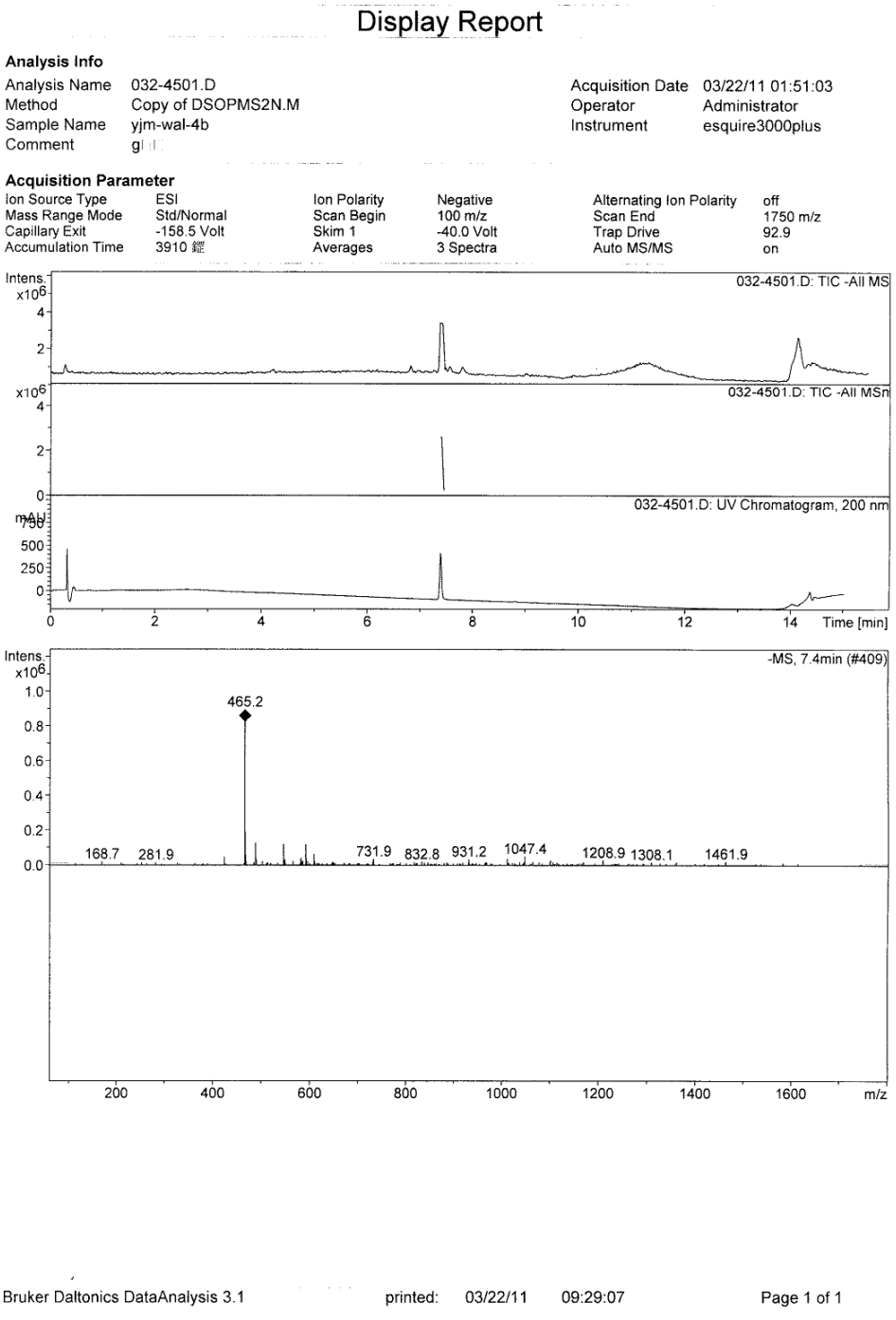


Figure S74. HRESI(–)MS spectrum of walsucochinoid K (**9**)

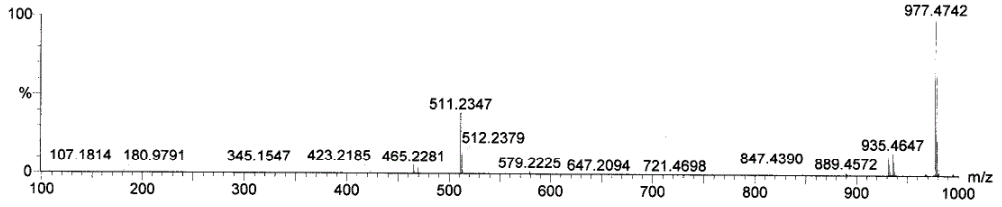
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
241 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30 Na: 0-1

WAL-4b LCT PXE KE324 04-Nov-2011 15:16:49

WAL-4b_1104 25 (0.548) AM2 (Ar,12000.0,0.00,0.70); ABS; Cm (9:41) 1: TOF MS ES- 1.08e+005



Minimum:				-1.5						
Maximum:		2.0	2.0	50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
511.2347	511.2332	1.5	2.9	12.5	143.9	0.0	C29	H35	O8	
	511.2367	-2.0	-3.9	0.5	152.3	8.4	C20	H40	O13	Na

Figure S75. IR spectrum of walsucochinoid K (**9**)

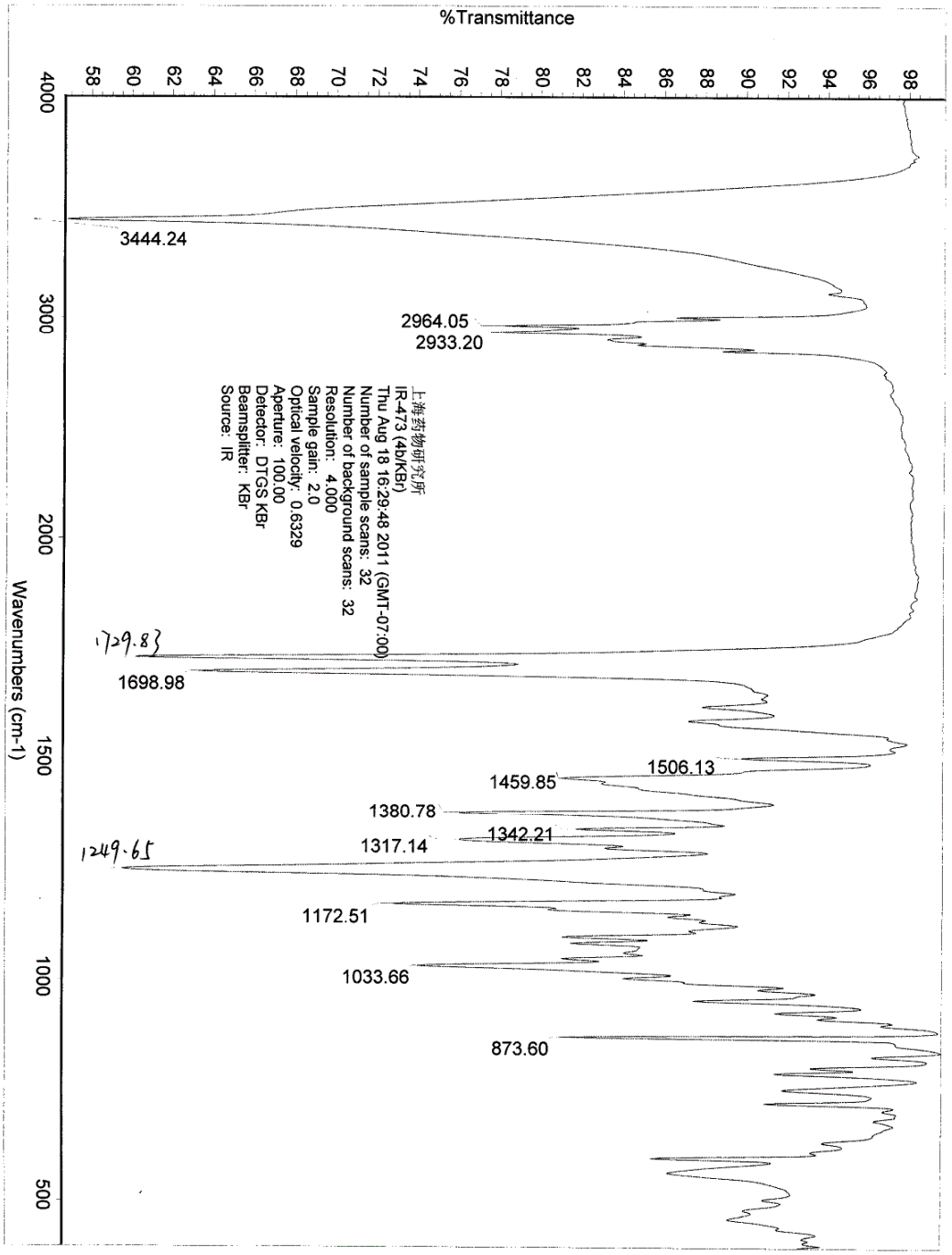


Figure S76. ^{1}H NMR spectrum of walsucochinoid L (**10**) in $CDCl_3$

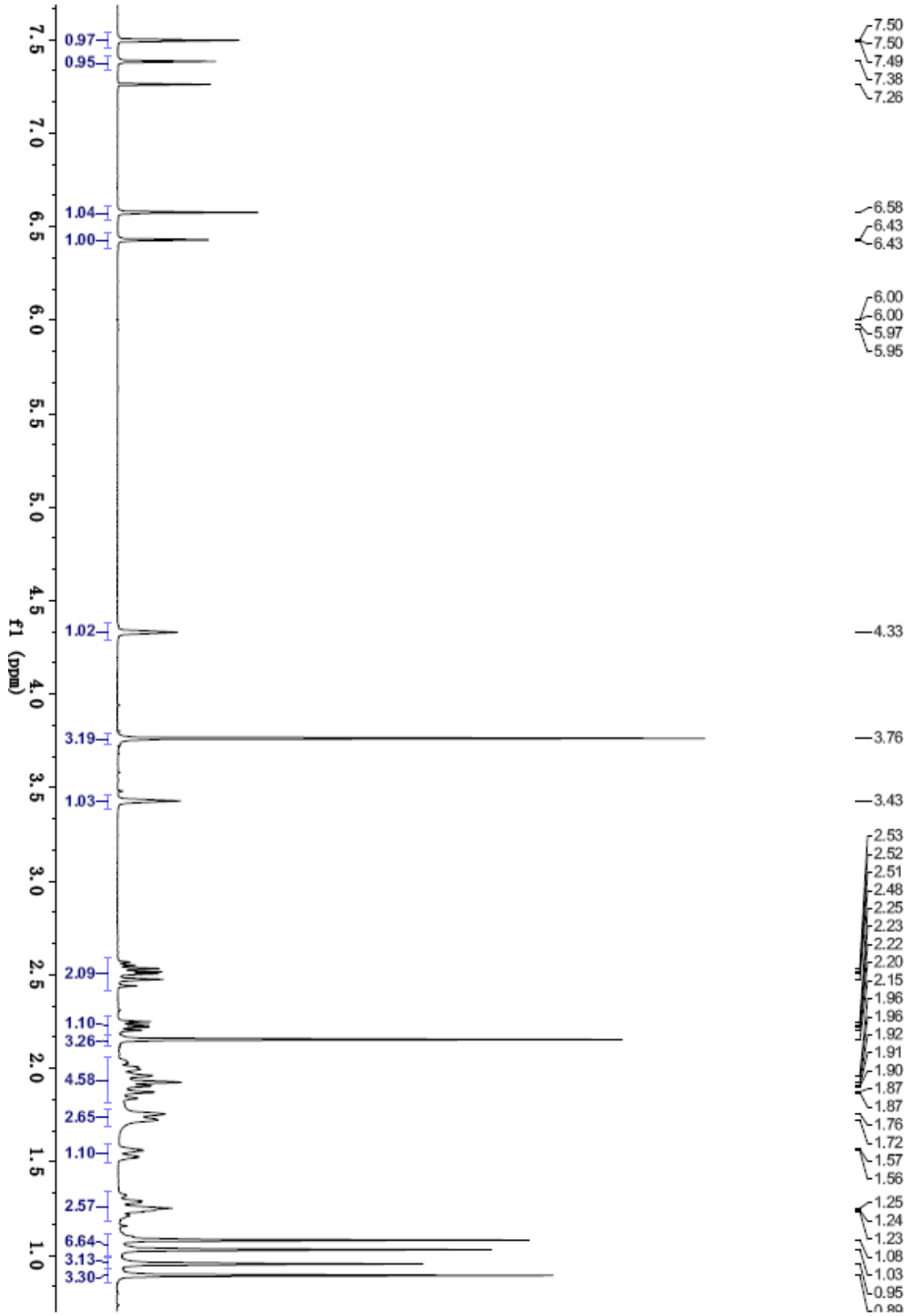


Figure S77. ^{13}C NMR spectrum of walsucochinoid L (**10**) in $CDCl_3$

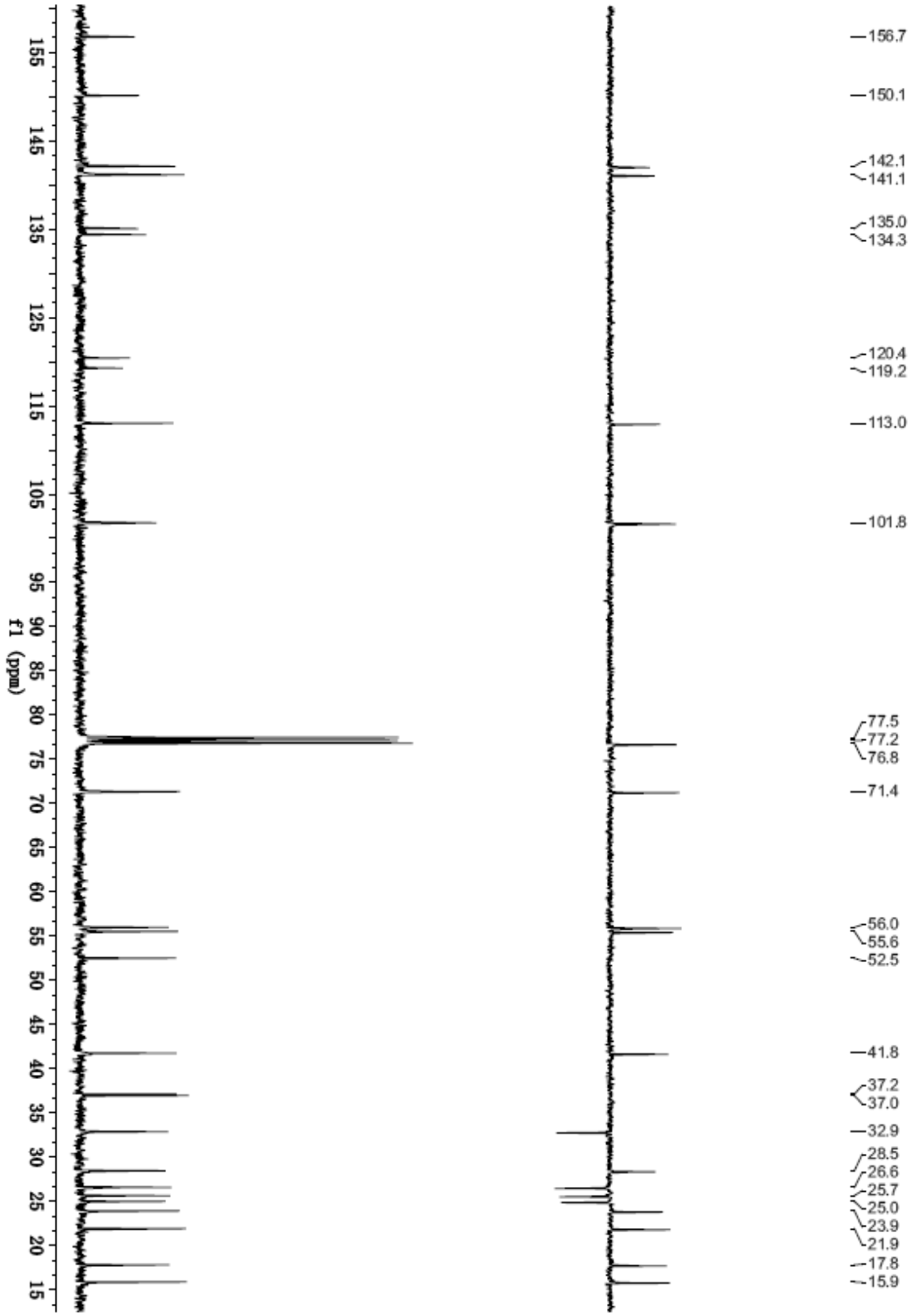


Figure S78. HSQC spectrum of walsucochinoid L (**10**) in $CDCl_3$

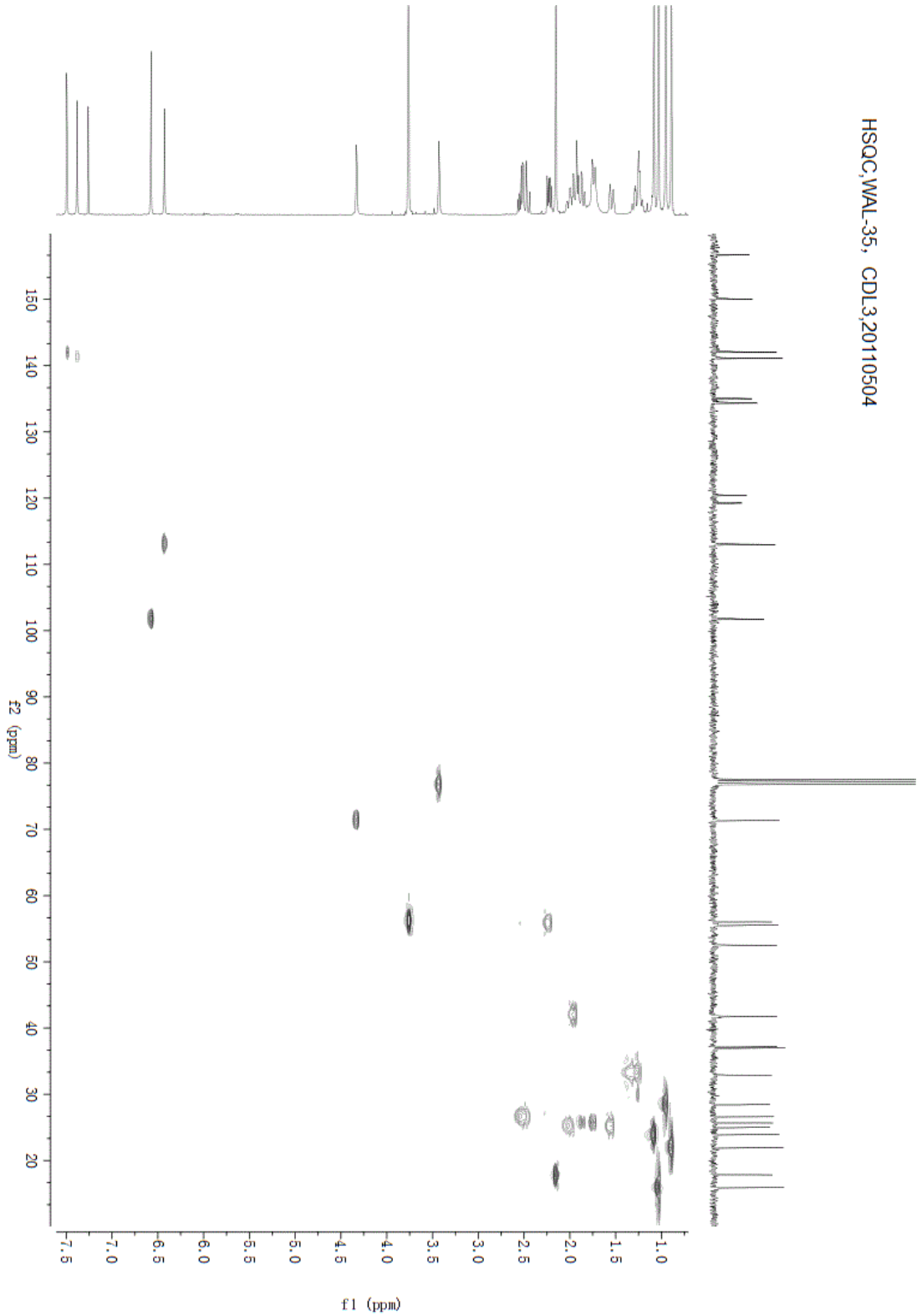


Figure S79. HMBC spectrum of walsucochinoid L (**10**) in $CDCl_3$

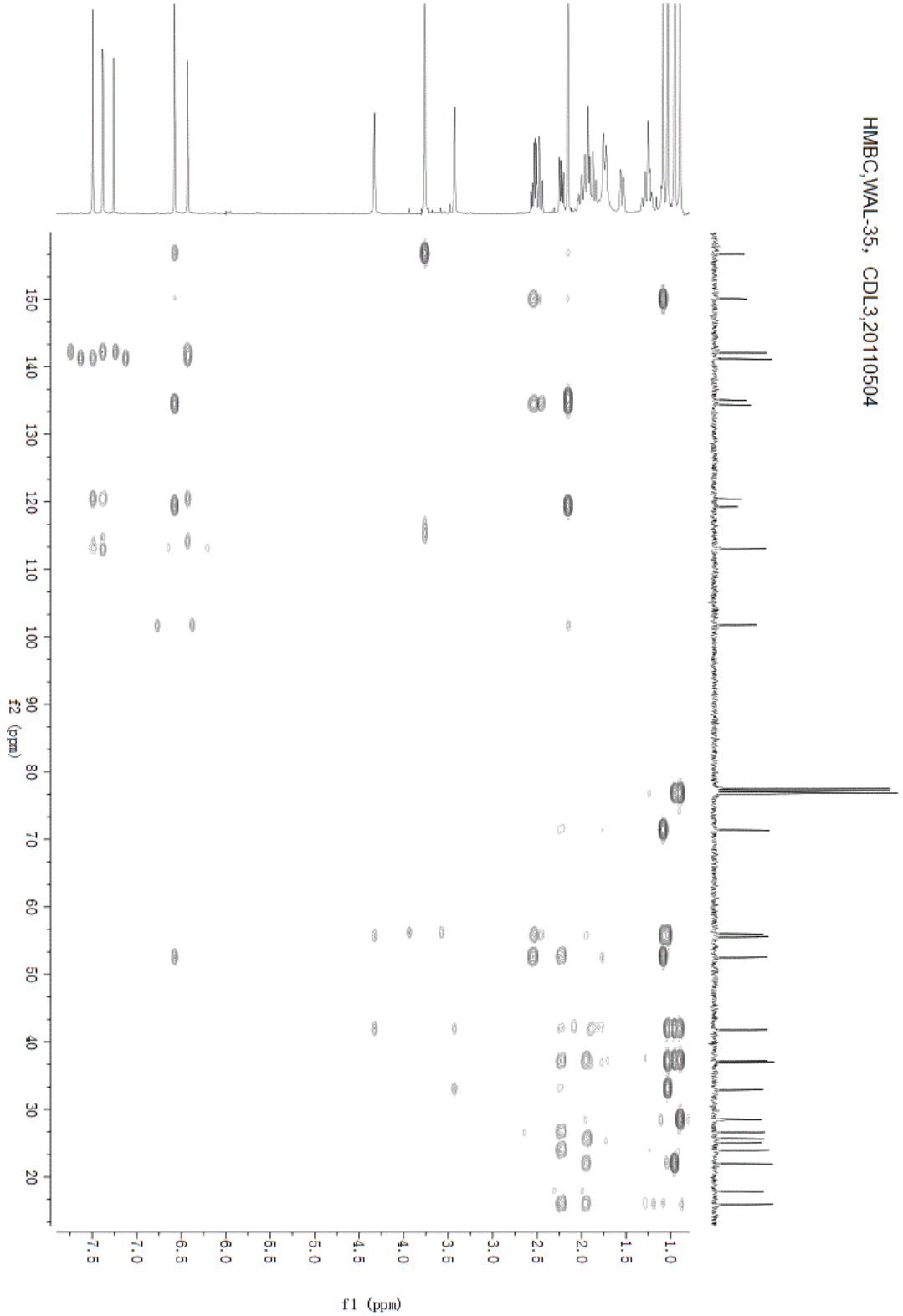


Figure S80. ROESY spectrum of walsucochinoid L (**10**) in $CDCl_3$

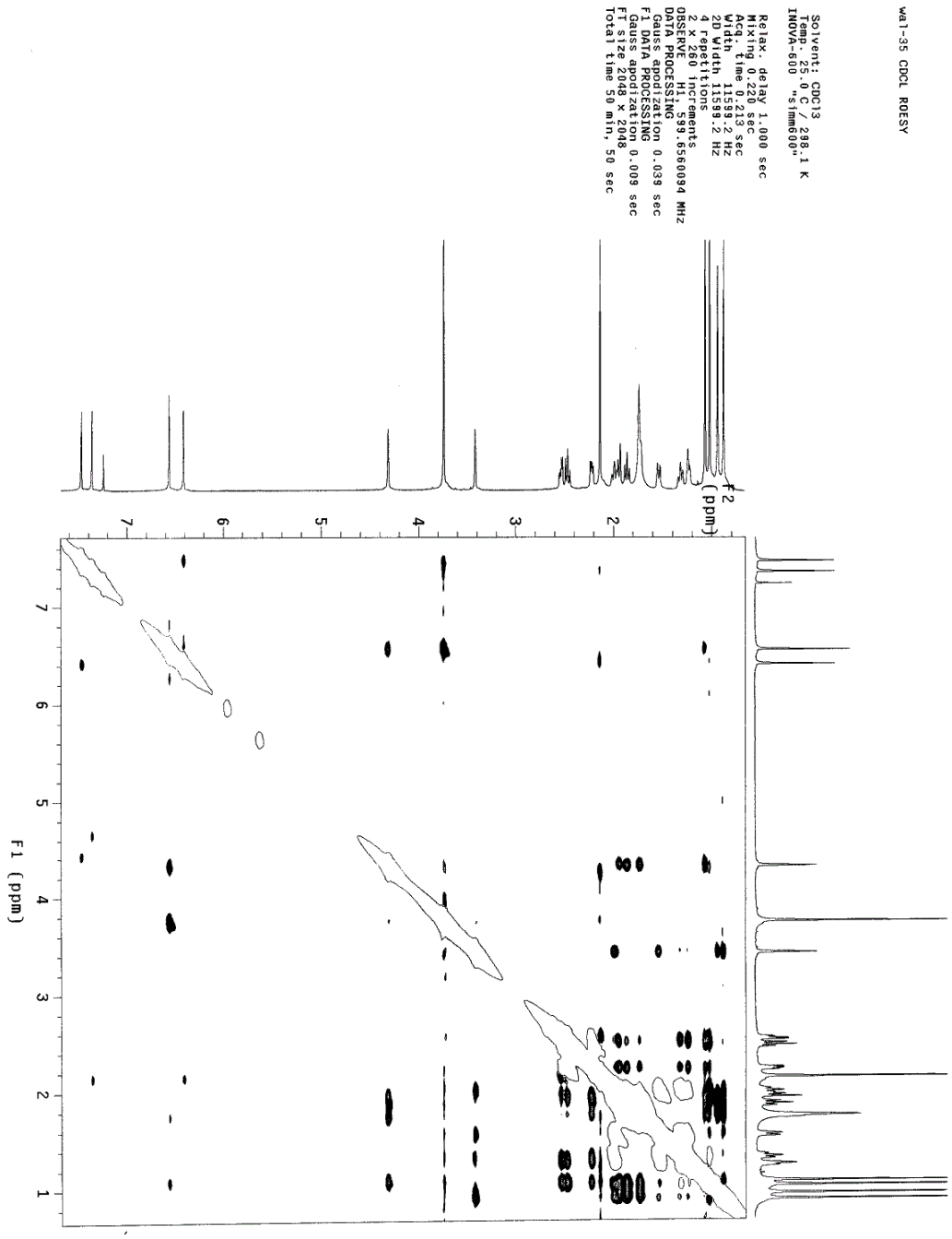


Figure S81. ESI(+)MS spectrum of walsucochinoid L (**10**)

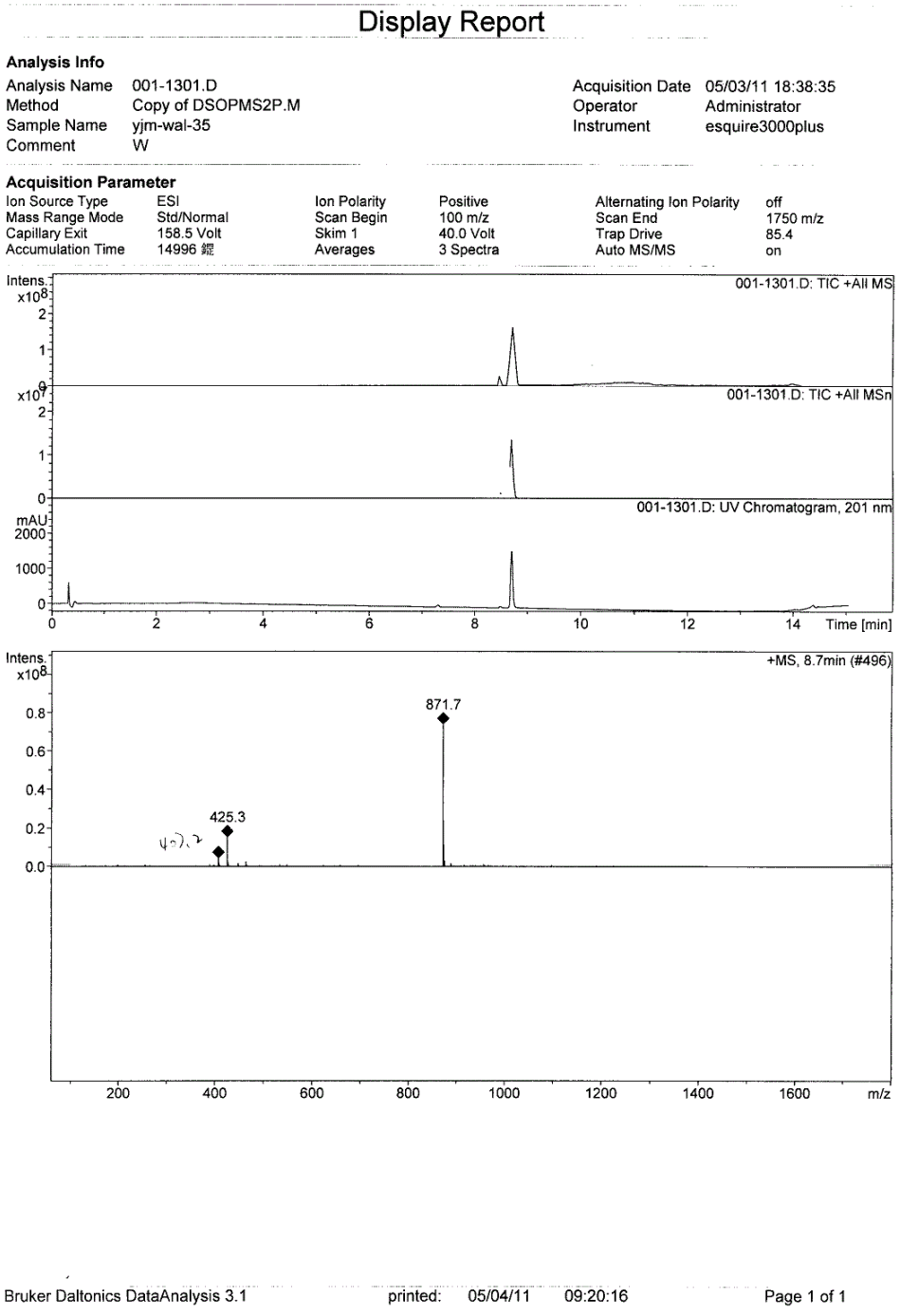


Figure S82. ESI(−)MS spectrum of walsucochinoid L (**10**)

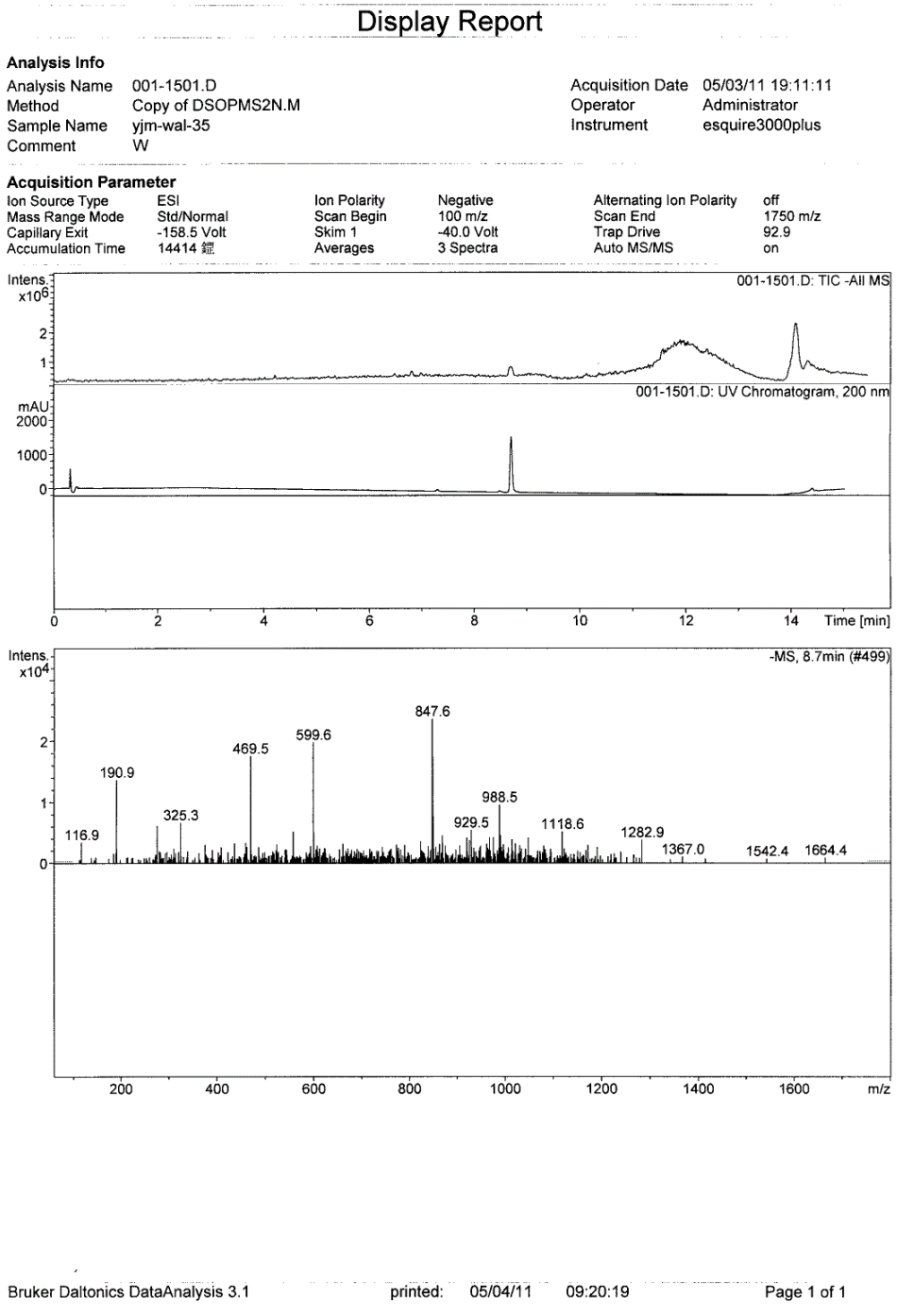


Figure S83. HRESI(–)MS spectrum of walsucochinoid L (**10**)

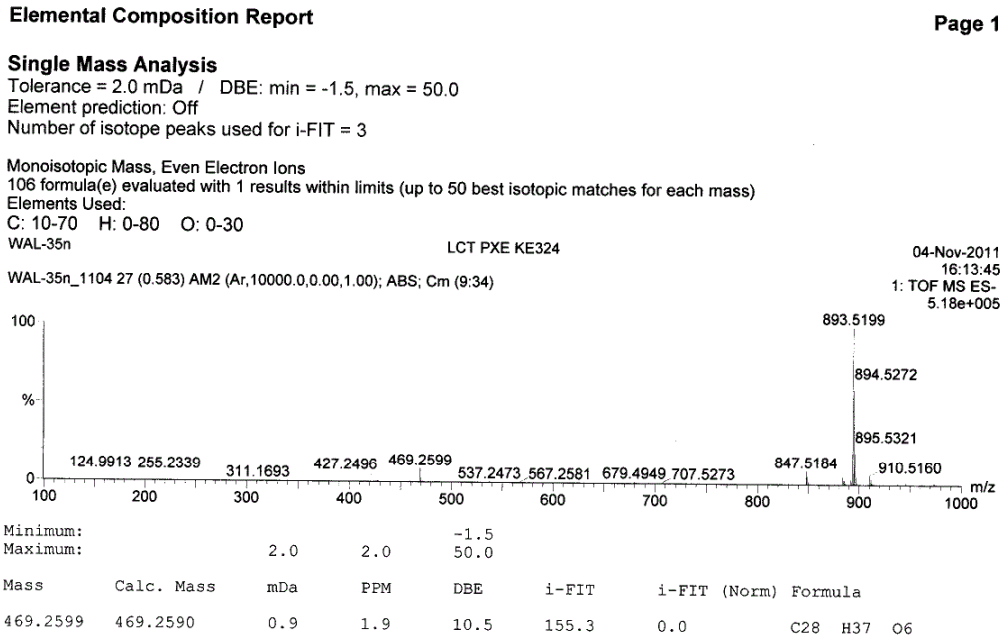


Figure S84. IR spectrum of walsucochinoid L (**10**)

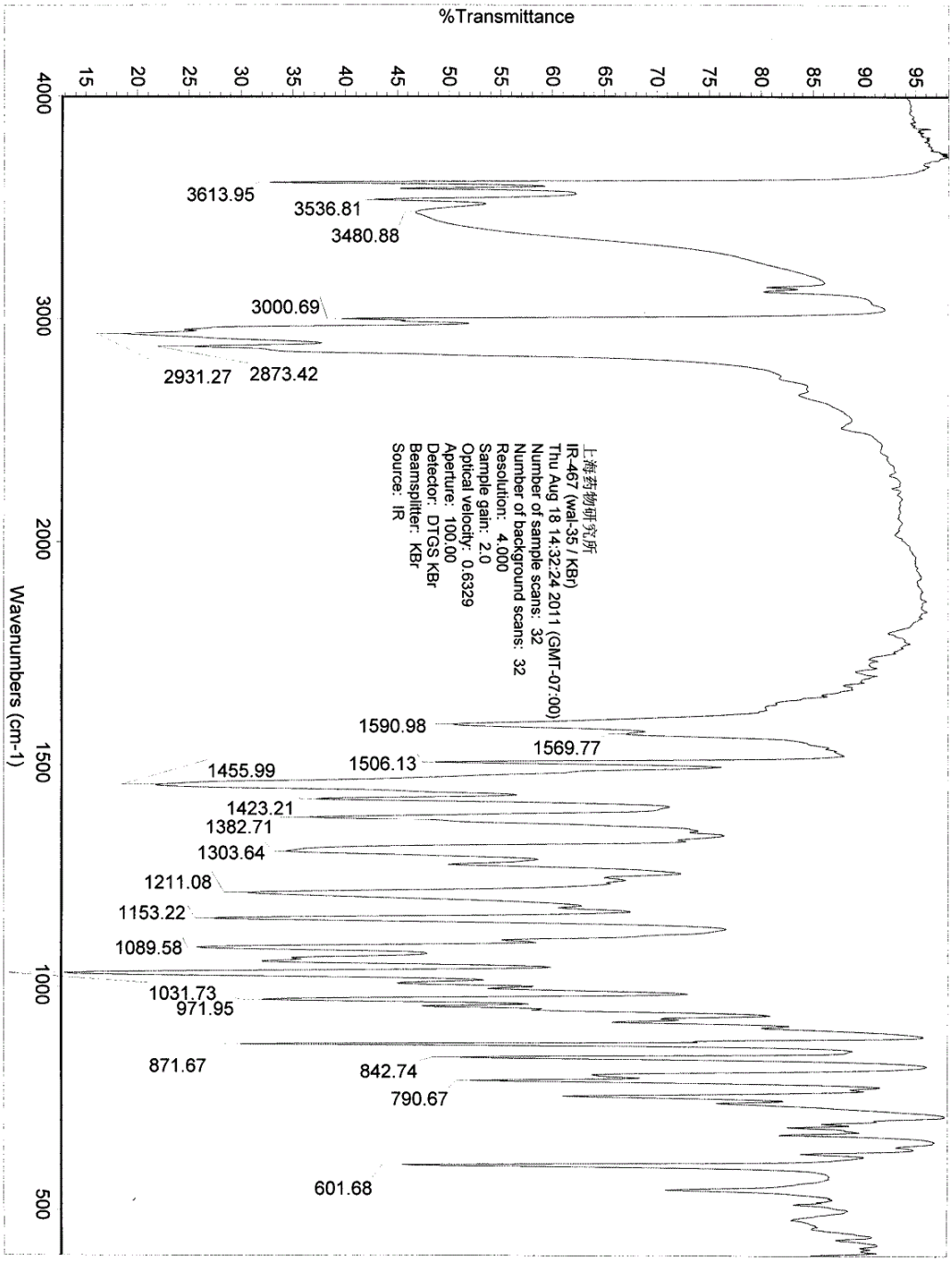


Figure S85. ^{1}H NMR spectrum of walsucochinoid M (**11**) in $CDCl_3$

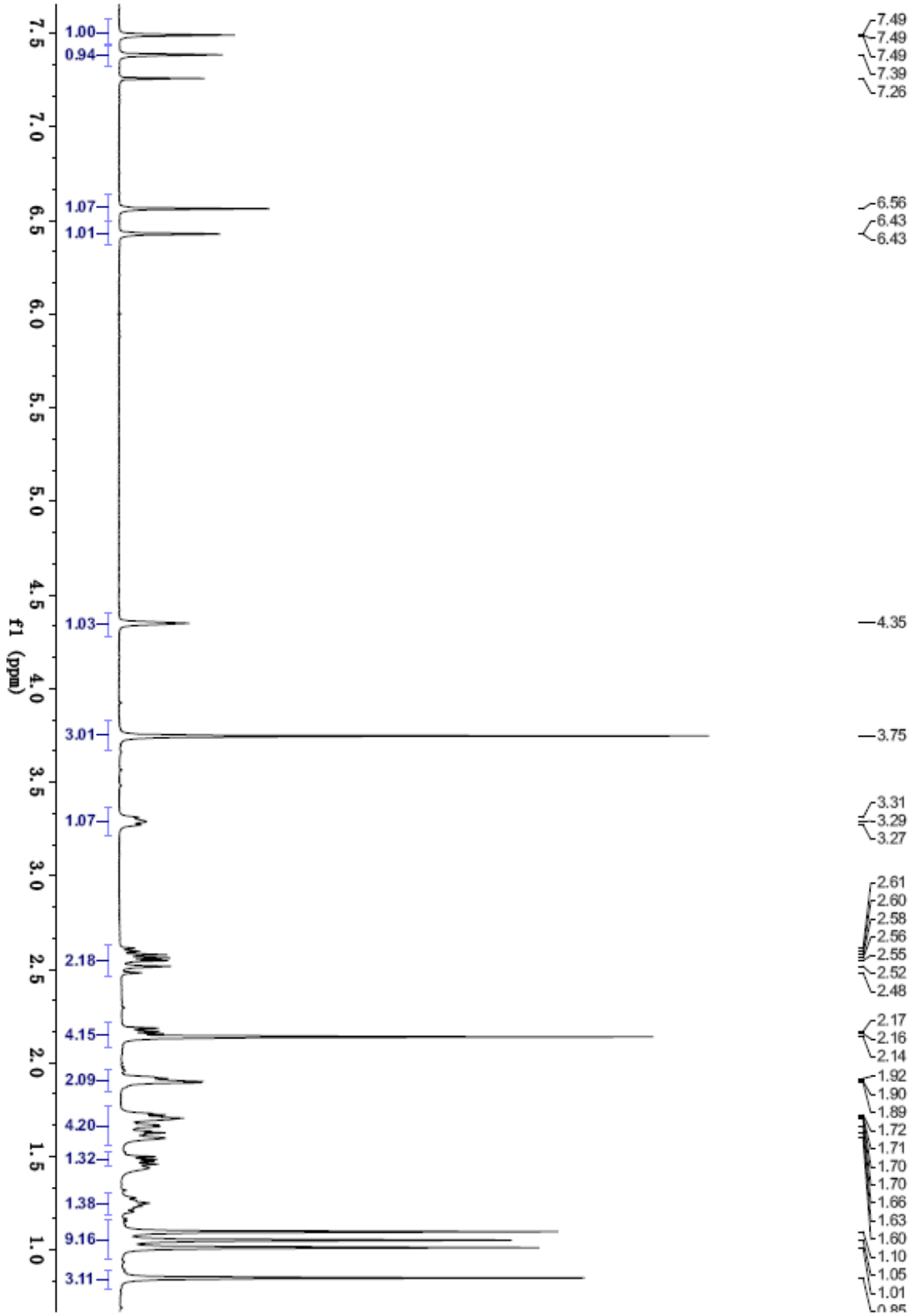


Figure S86. ^{13}C NMR spectrum of walsucochinoid M (**11**) in $CDCl_3$

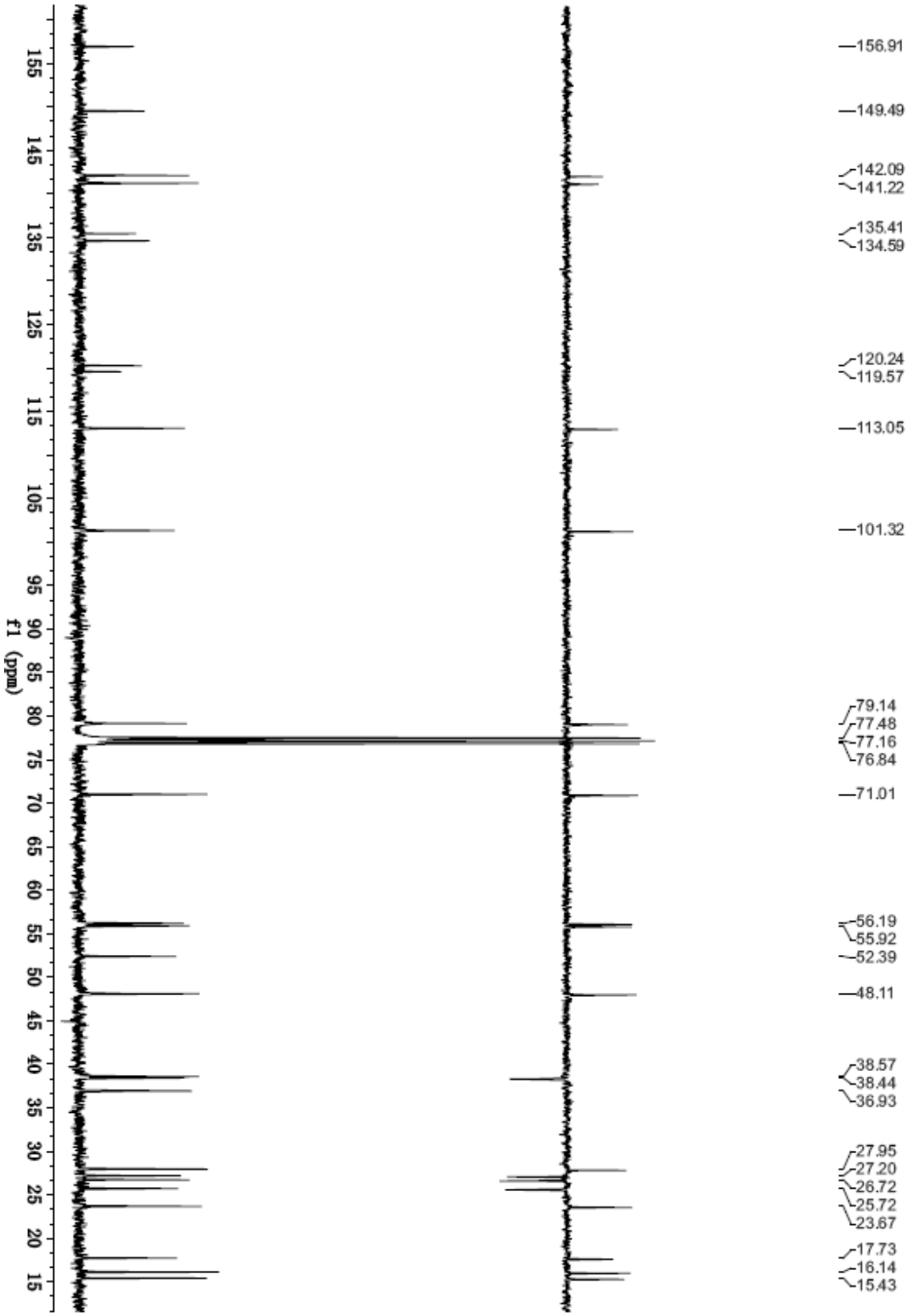


Figure S87. HSQC spectrum of walsucochinoid M (**11**) in $CDCl_3$

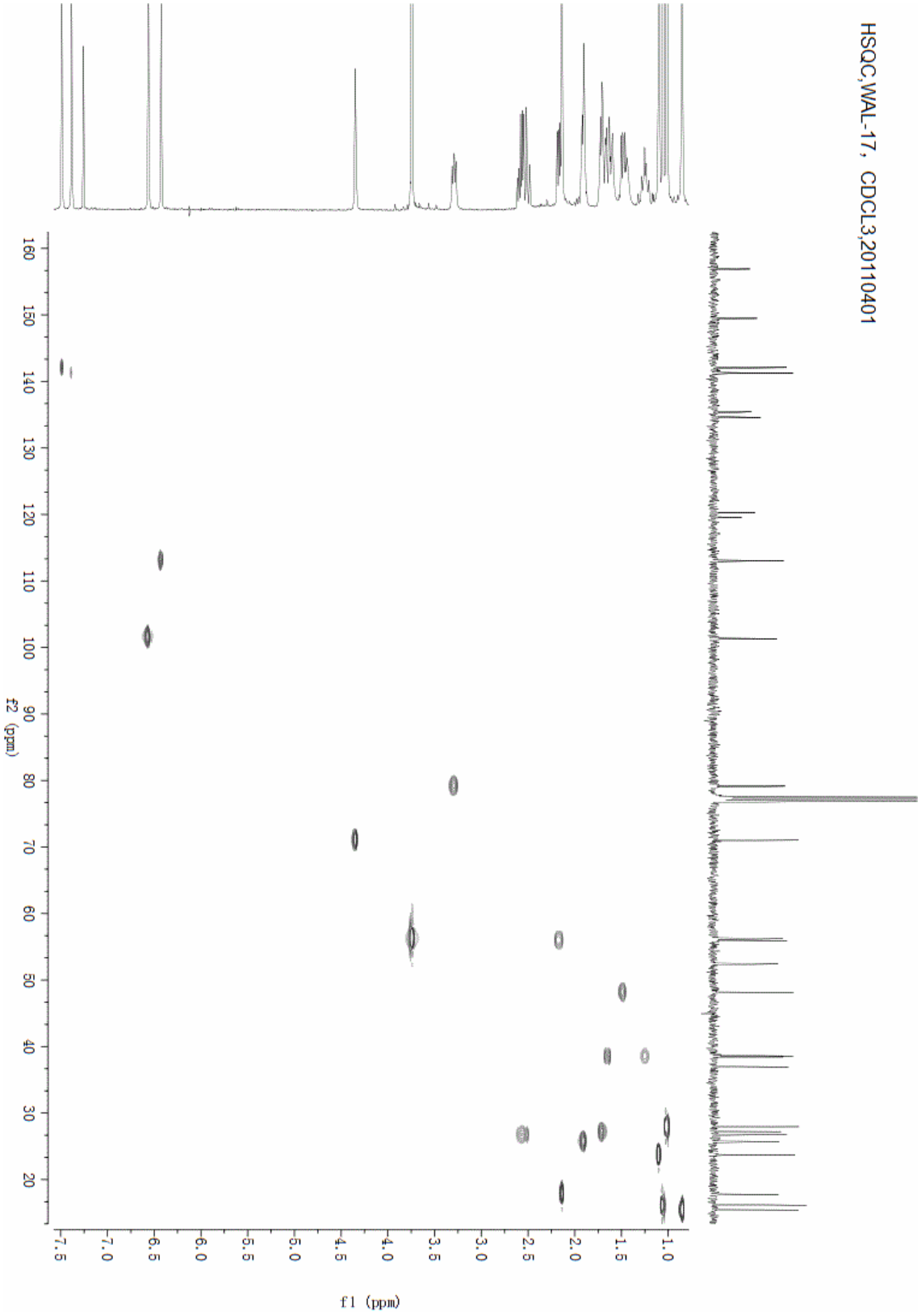


Figure S88. HMBC spectrum of walsucochinoid M (**11**) in $CDCl_3$

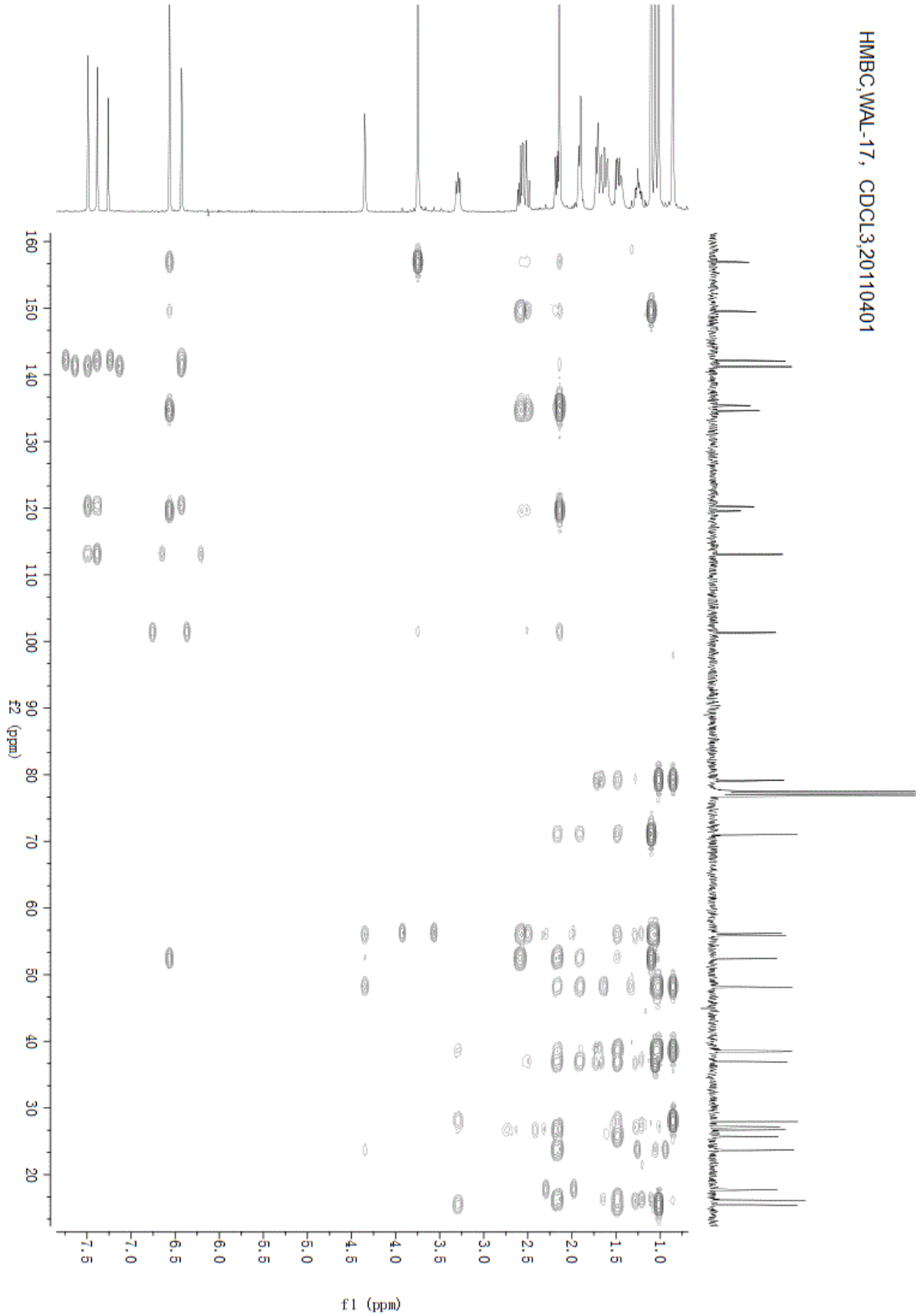


Figure S89. ROESY spectrum of walsucochinoid M (**11**) in $CDCl_3$

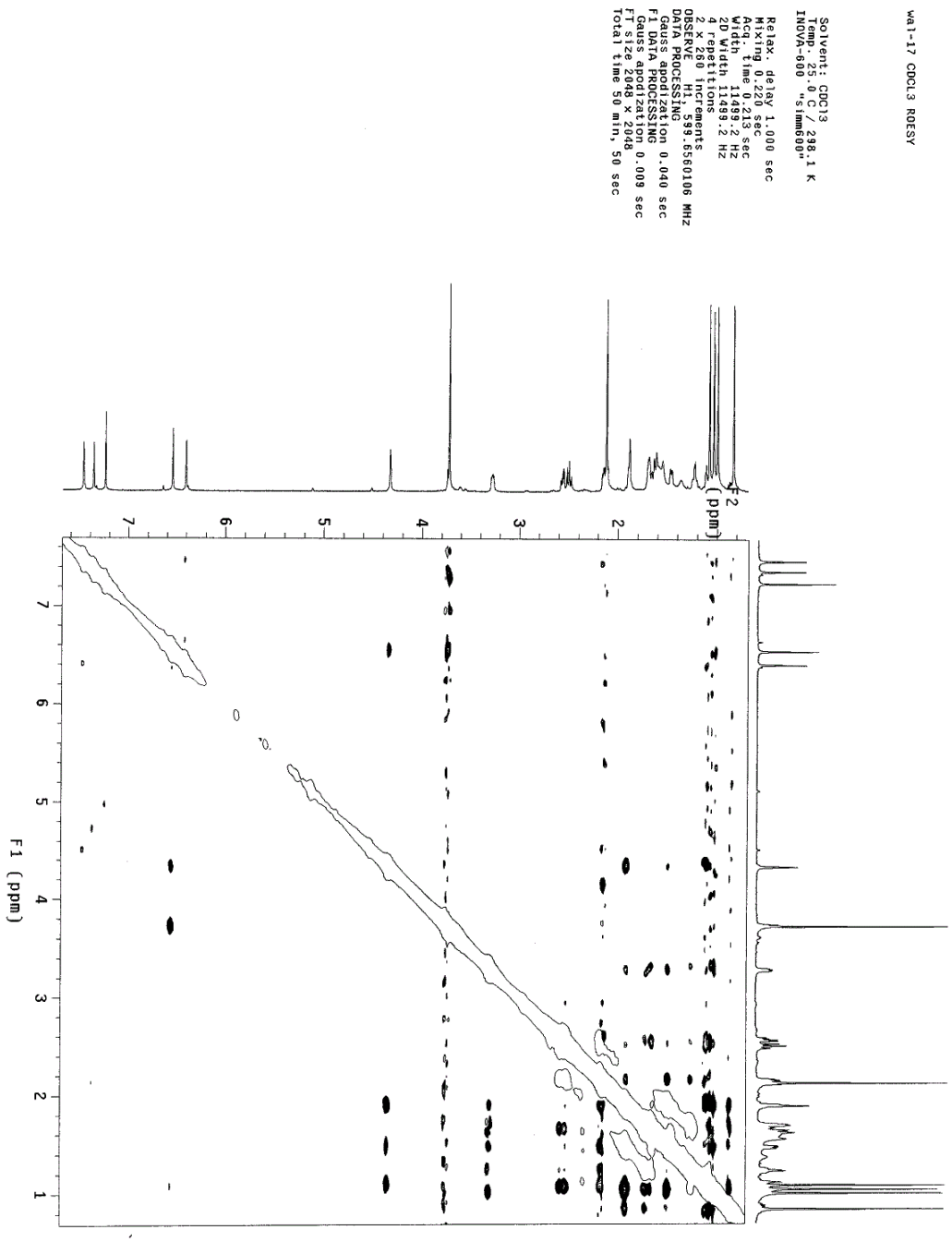


Figure S90. ESI(+)MS spectrum of walsucochinoid M (**11**)

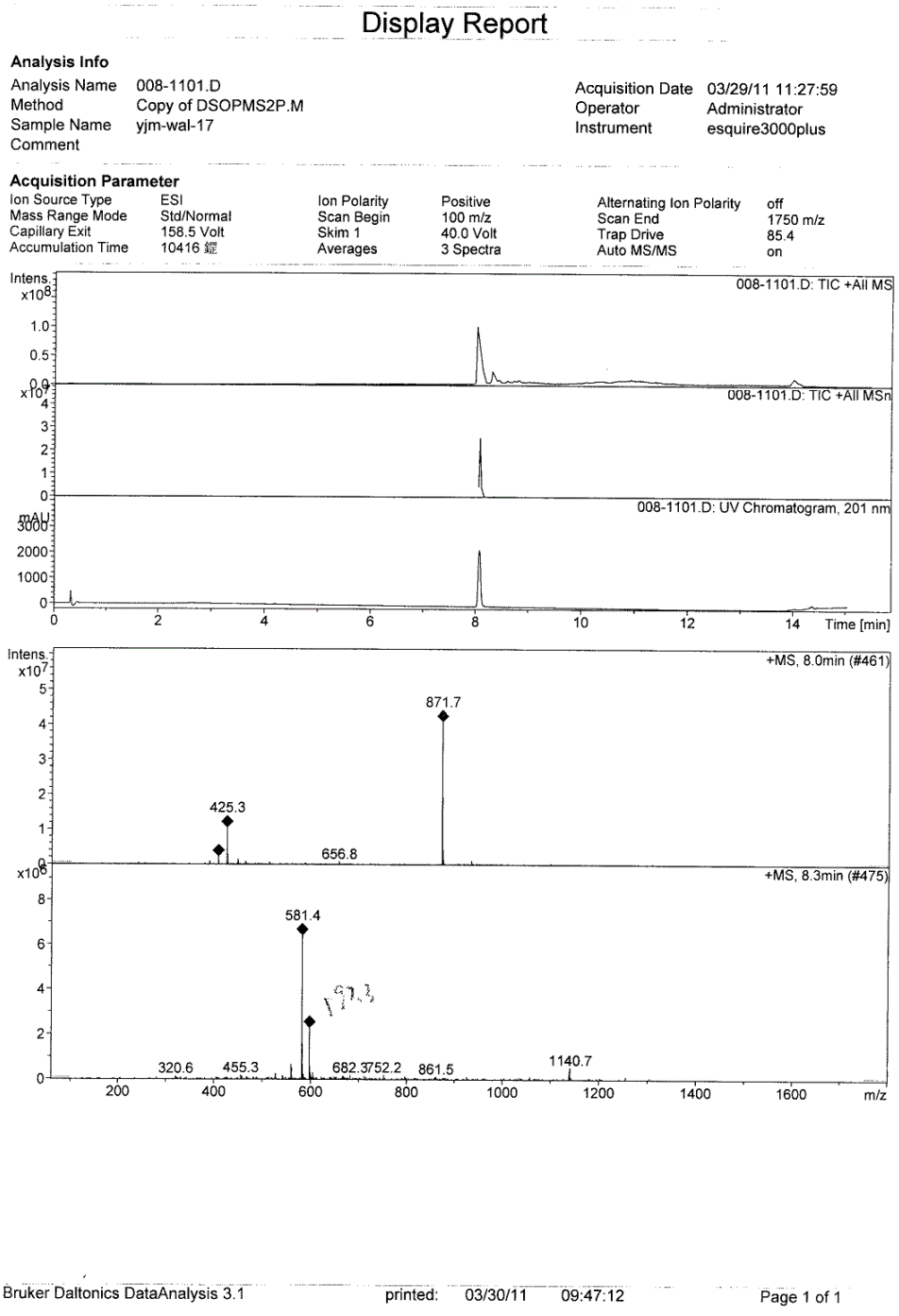


Figure S91. HRESI(+)MS spectrum of walsucochinoid M (**11**)

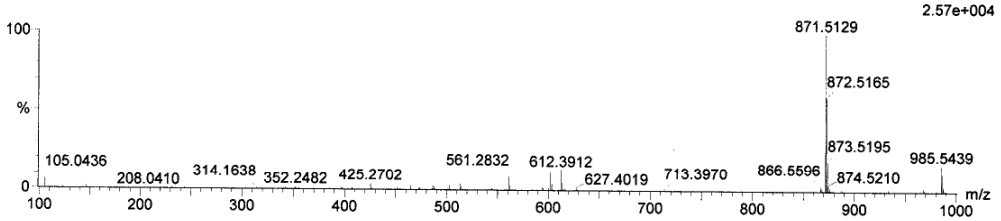
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
418 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30 Na: 0-1

WAL-17 LCT PXE KE324 04-Nov-2011 15:34:38

WAL-17_1104 23 (0.494) AM2 (Ar,13000.0,0.00,0.70); ABS; Cm (9:26) 1: TOF MS ES+ 2.57e+004



Minimum:				-1.5						
Maximum:		2.0	2.0	50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
871.5129	871.5125	0.4	0.5	18.5	80.7	0.0	C54	H72	O8	Na
	871.5149	-2.0	-2.3	21.5	85.9	5.2	C56	H71	O8	
	871.5114	1.5	1.7	-0.5	90.4	9.7	C38	H79	O21	

Figure S92. IR spectrum of walsucochinoid M (**11**)

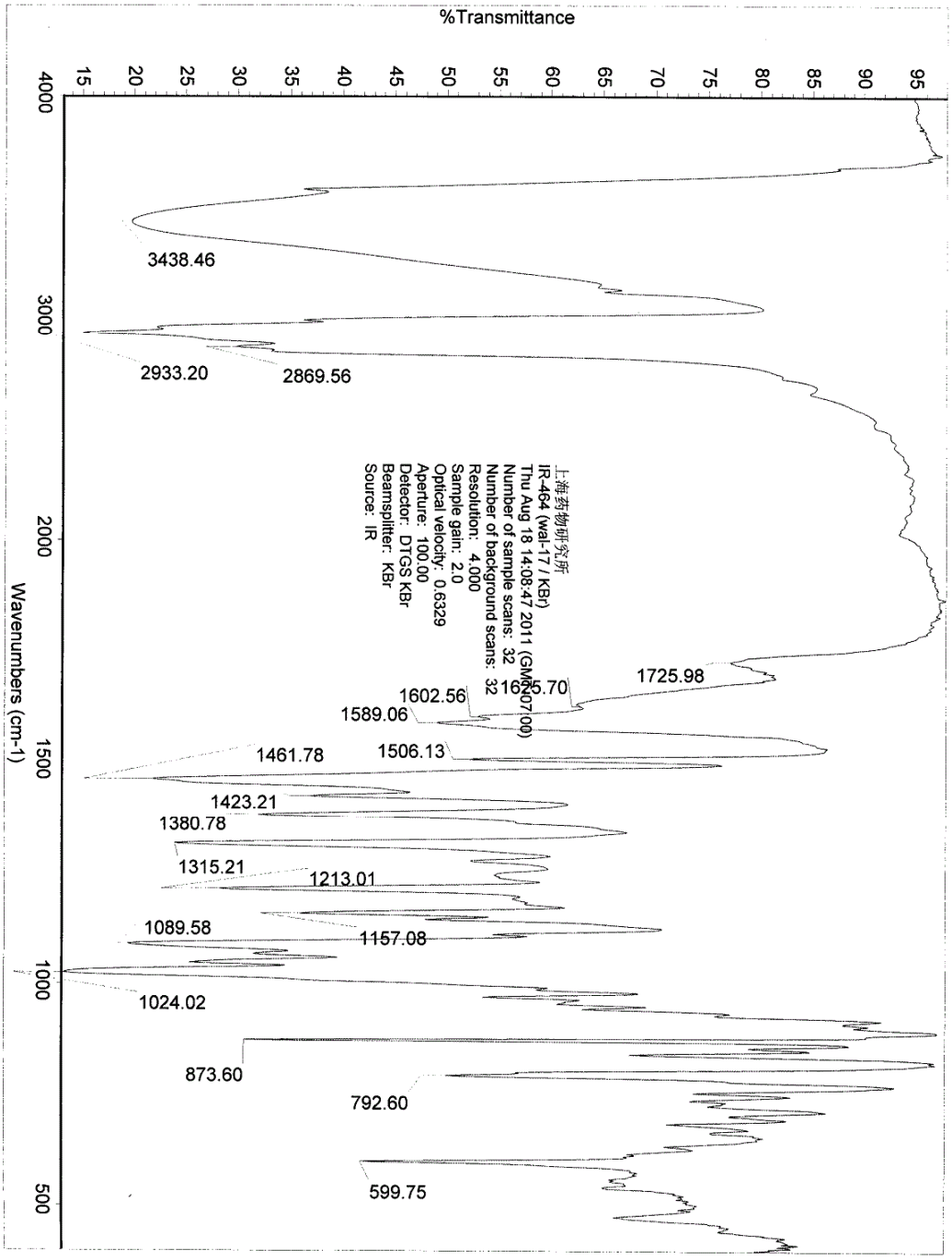


Figure S93. ^{1}H NMR spectrum of walsucochinoid N (**12**) in $CDCl_3$

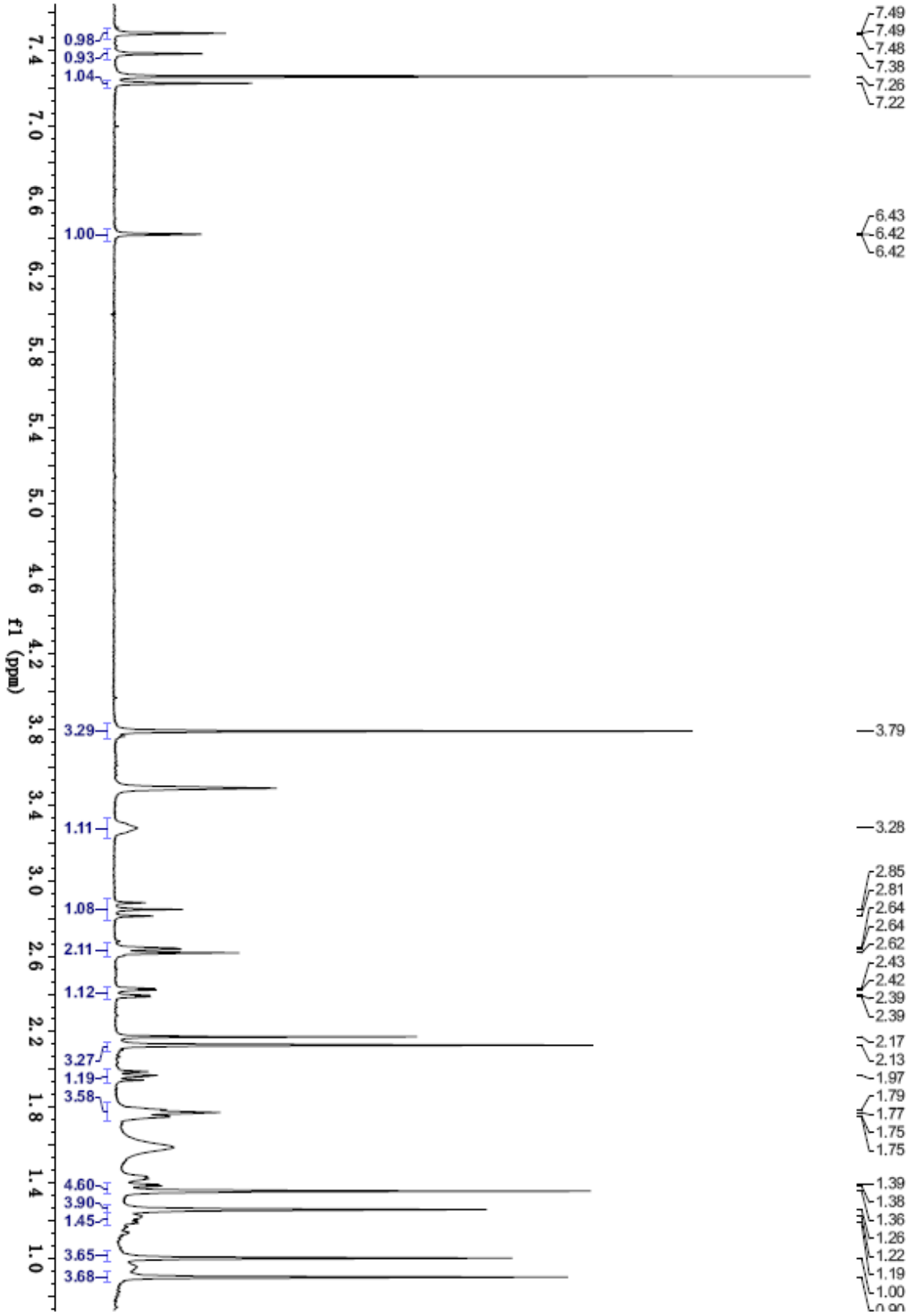


Figure S94. ^{13}C NMR spectrum of walsucochinoid N (**12**) in $CDCl_3$

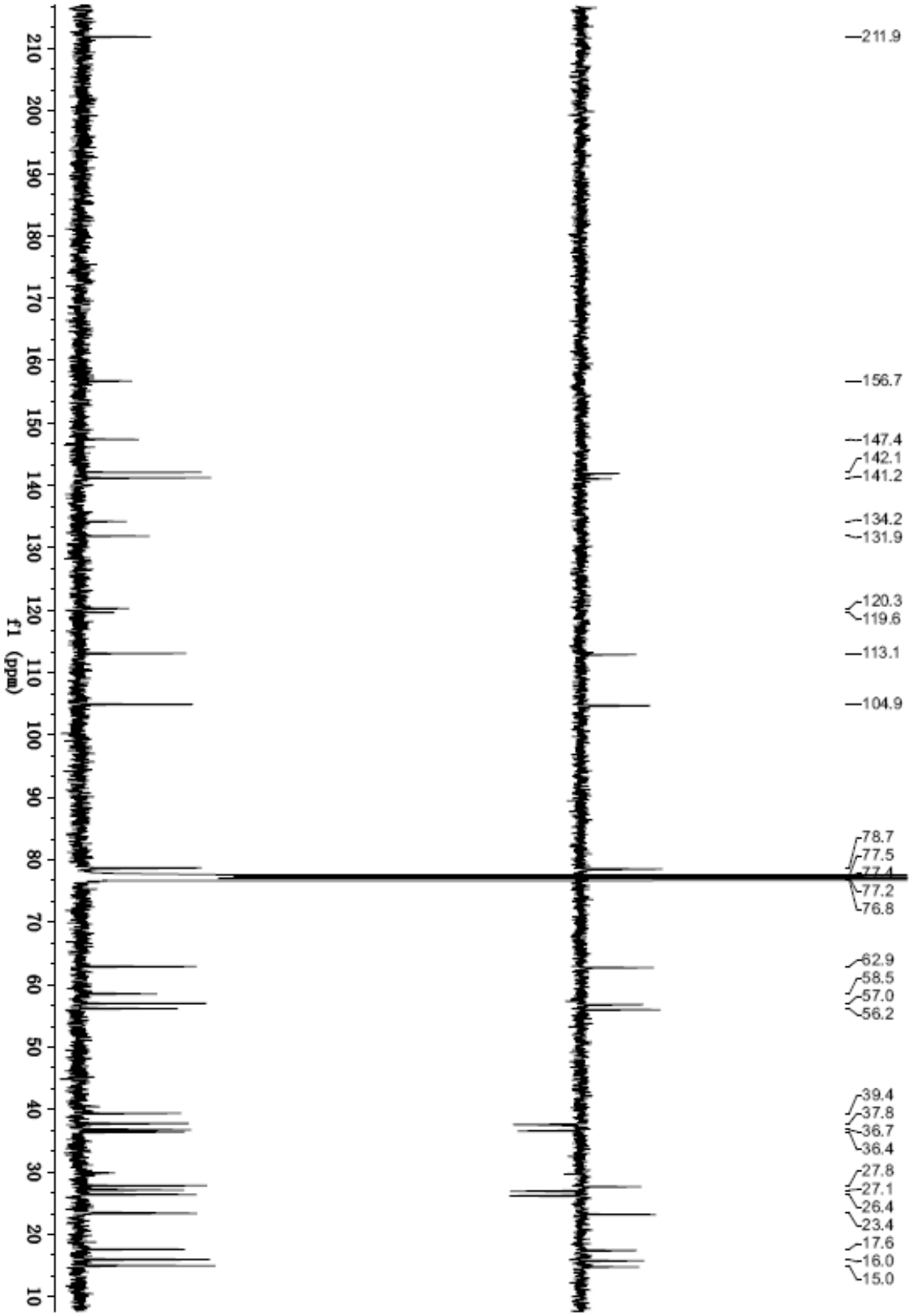


Figure S95. HSQC spectrum of walsucochinoid N (**12**) in $CDCl_3$

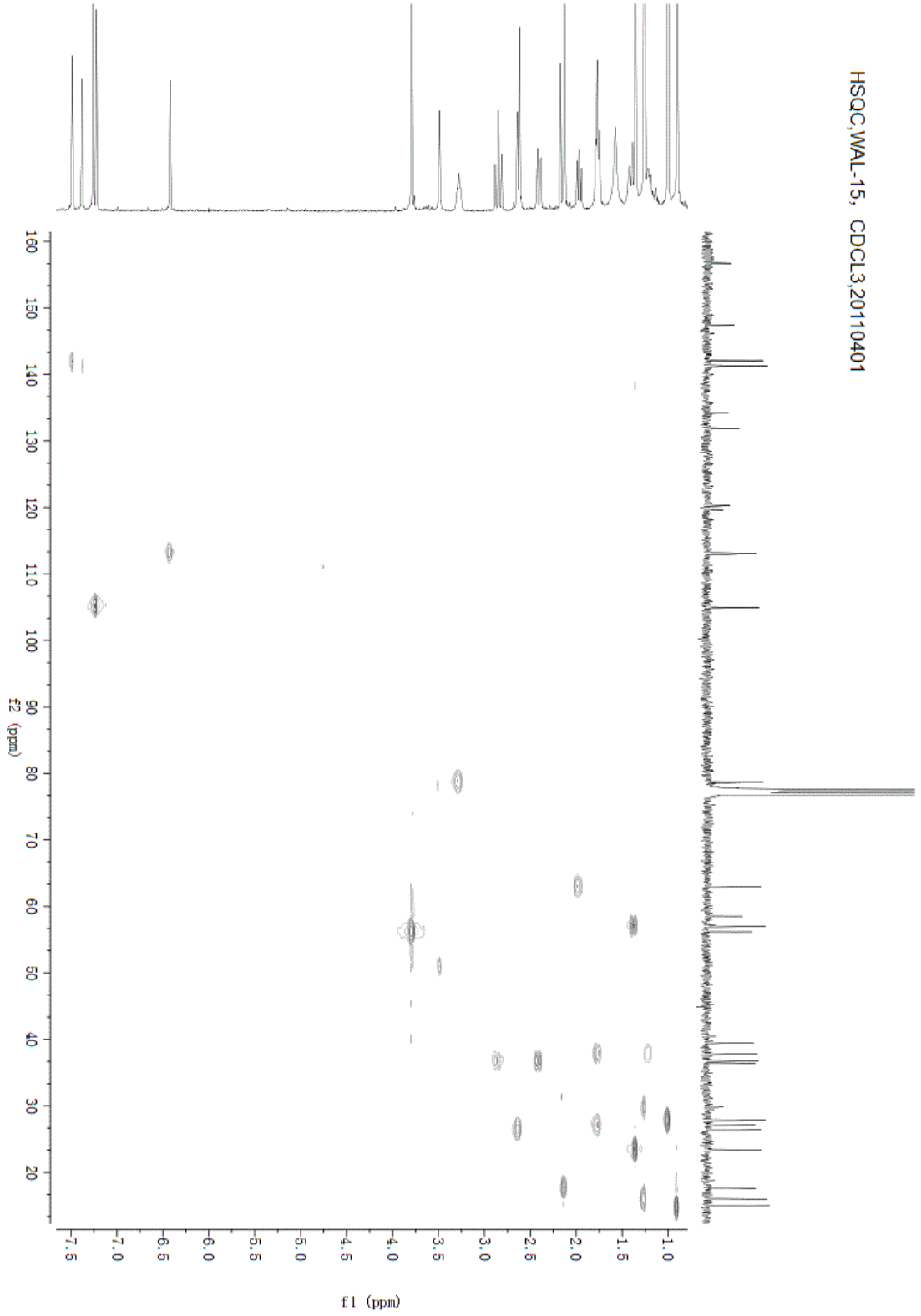


Figure S96. HMBC spectrum of walsucochinoid N (**12**) in $CDCl_3$

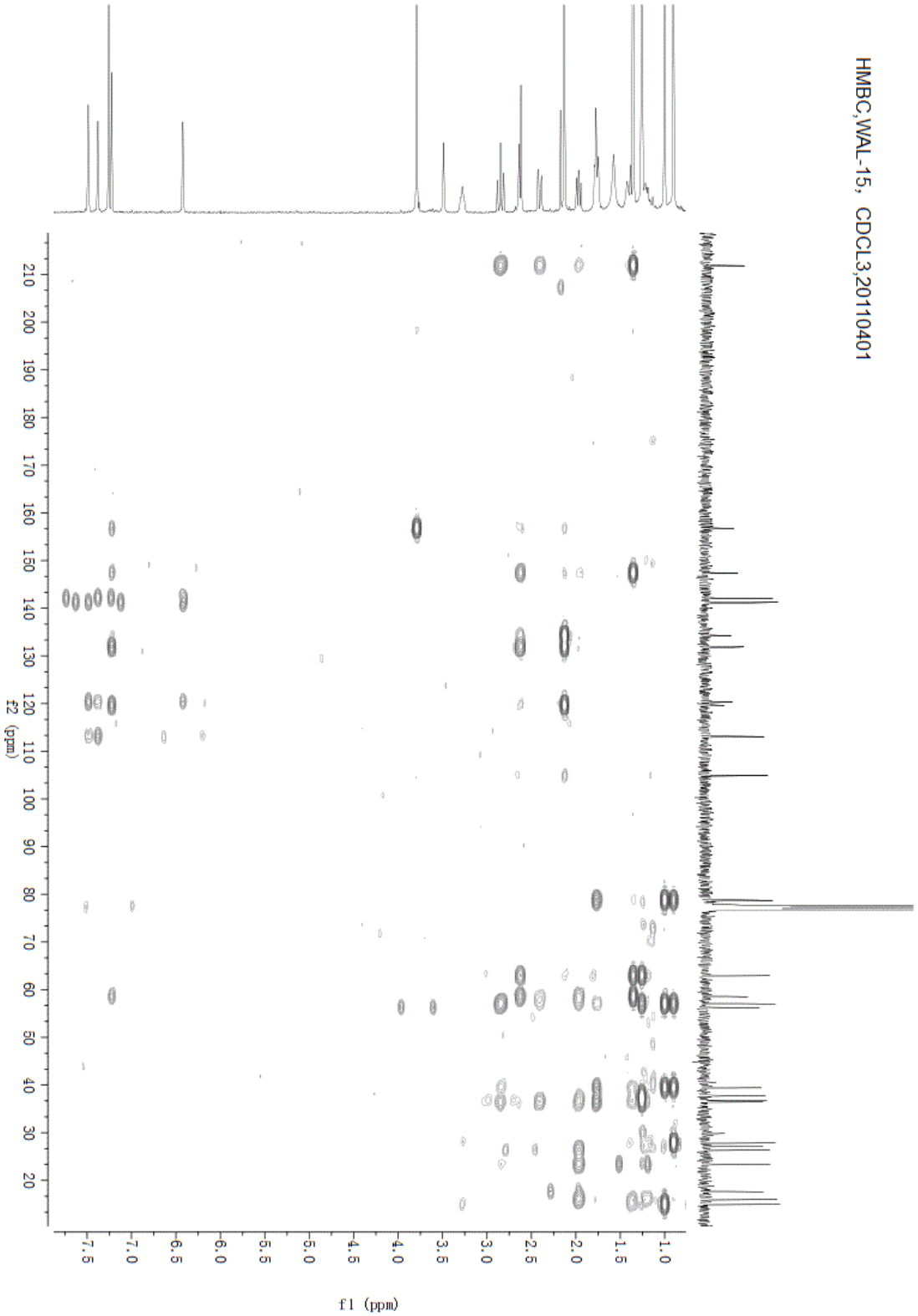


Figure S97. ROESY spectrum of walsucochinoid N (**12**) in $CDCl_3$

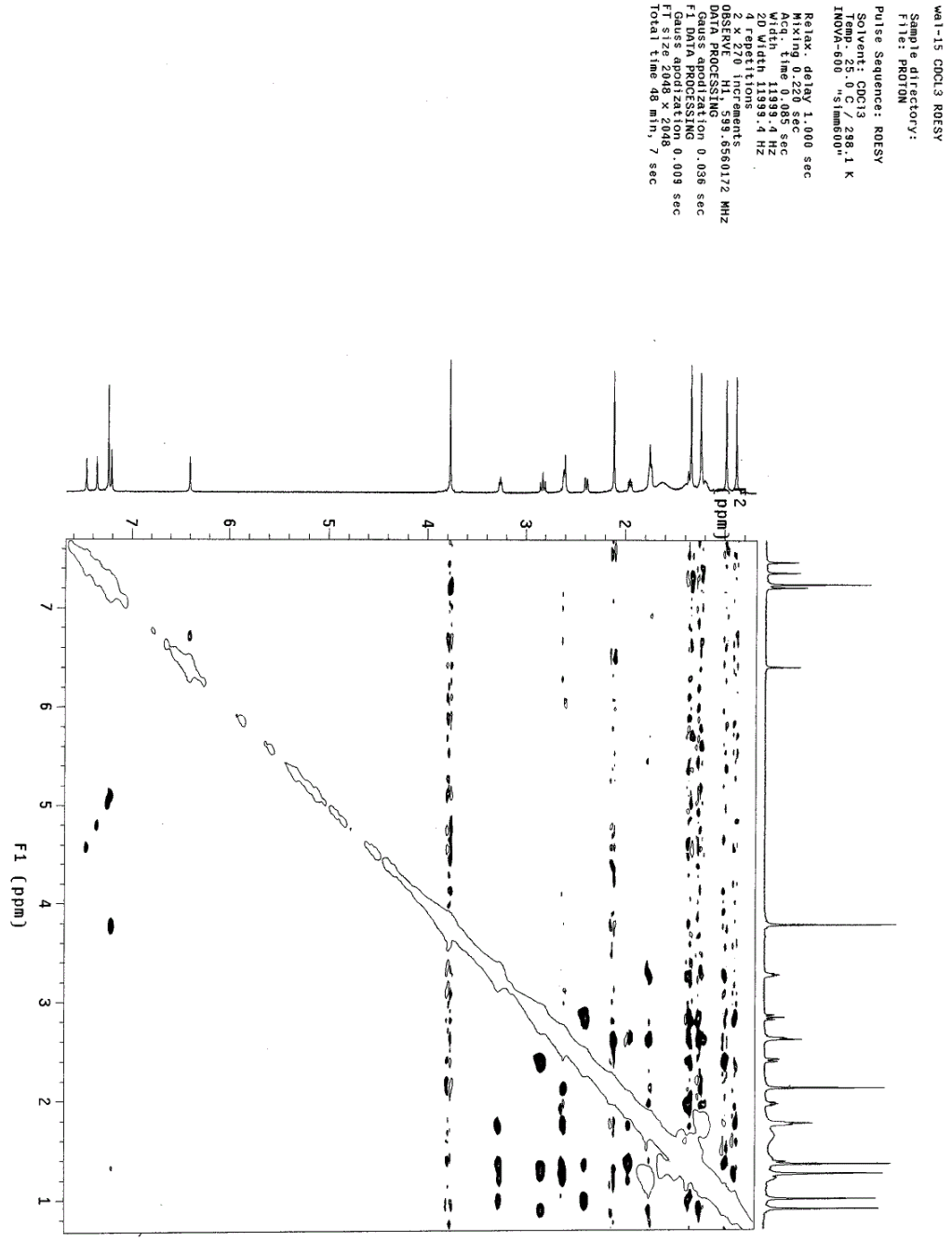


Figure S98. ESI(+)MS spectrum of walsucochinoid N (**12**)

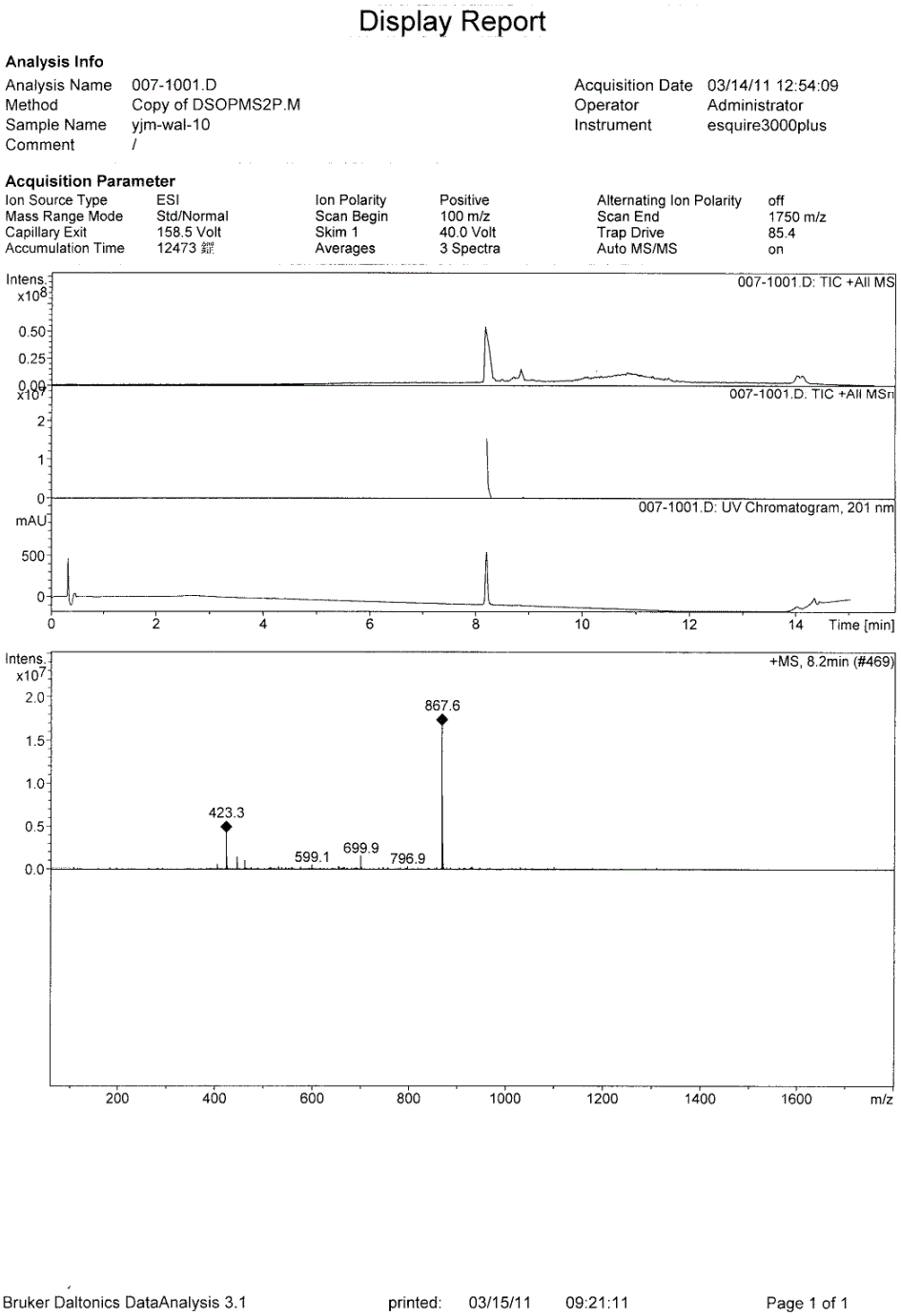


Figure S99. HRESI(+)MS spectrum of walsucochinoid N (**12**)

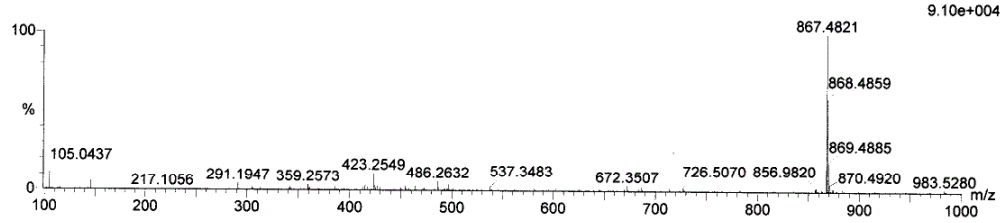
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
417 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30 Na: 0-1

WAL-15 LCT PXE KE324 04-Nov-2011 15:00:17

WAL-15_1104 30 (0.654) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (17:53) 1: TOF MS ES+ 9.10e+004



Minimum:				-1.5			
Maximum:		2.0	2.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
867.4821	867.4812	0.9	1.0	20.5	74.4	0.0	C54 H68 O8 Na
	867.4836	-1.5	-1.7	23.5	77.7	3.3	C56 H67 O8

Figure S100. IR spectrum of walsucochinoid N (**12**)

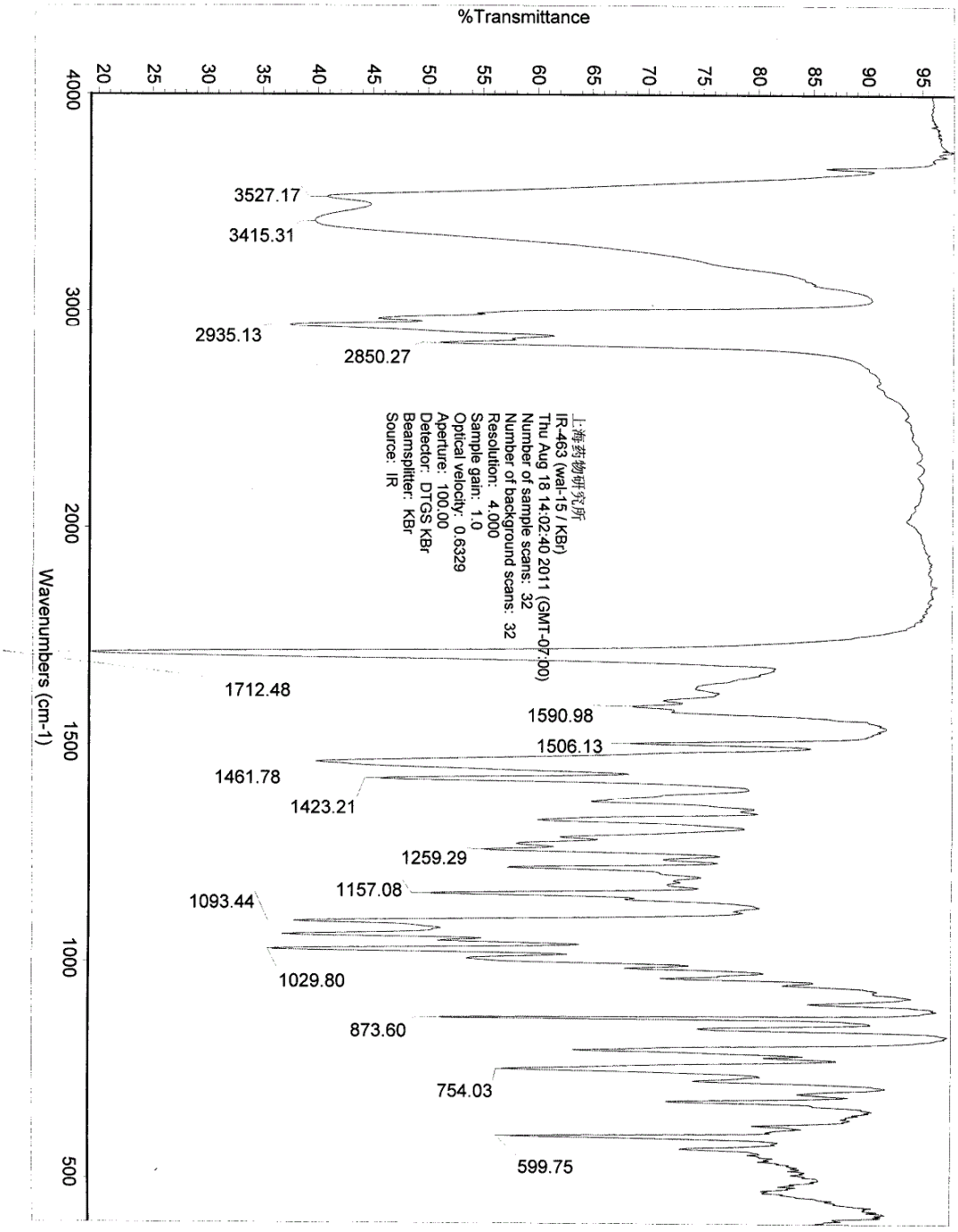


Figure S101. ^{1}H NMR spectrum of walsucochinoid O (**13**) in $CDCl_3$

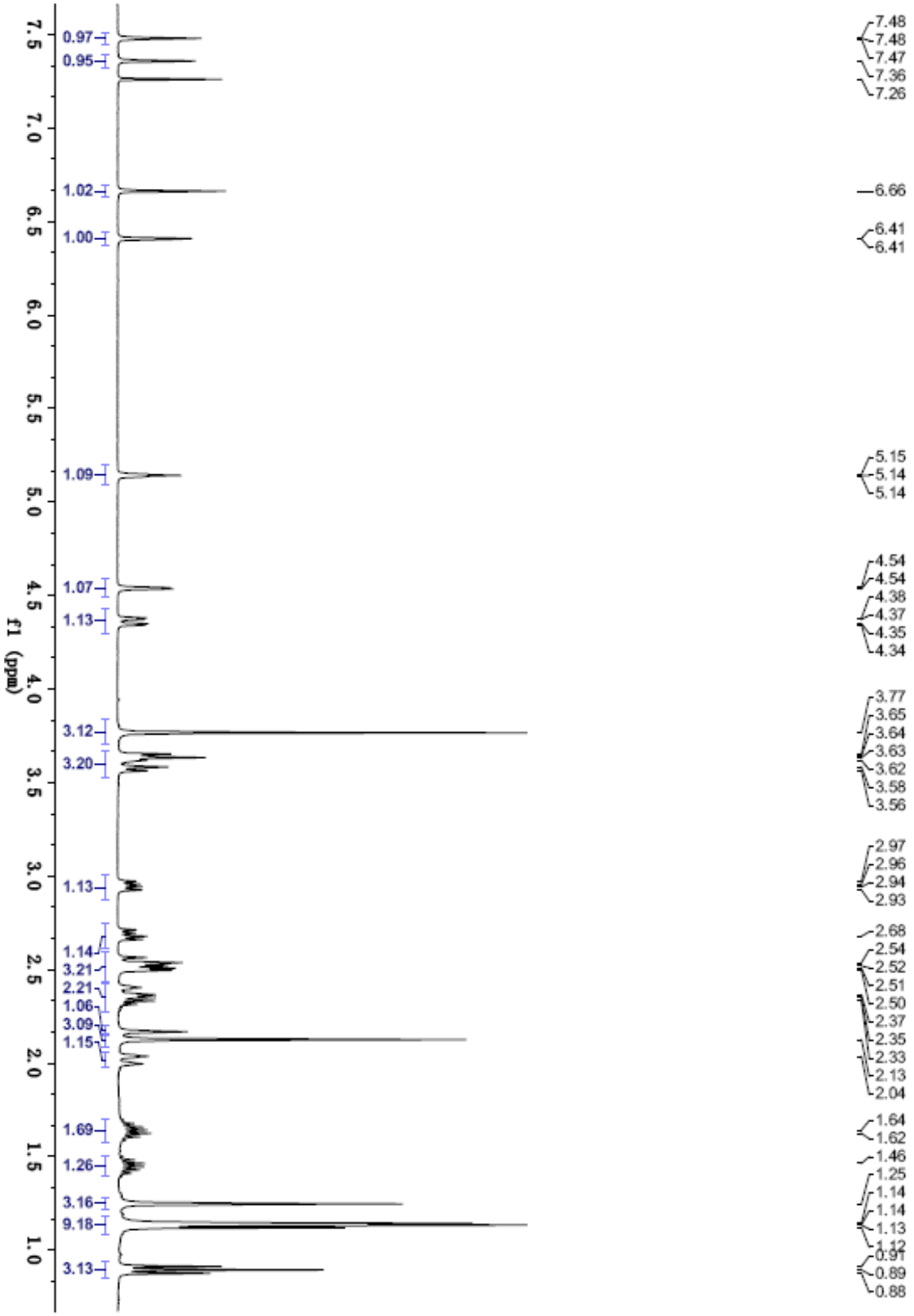


Figure S102. ^{13}C NMR spectrum of walsucochinoid O (**13**) in $CDCl_3$

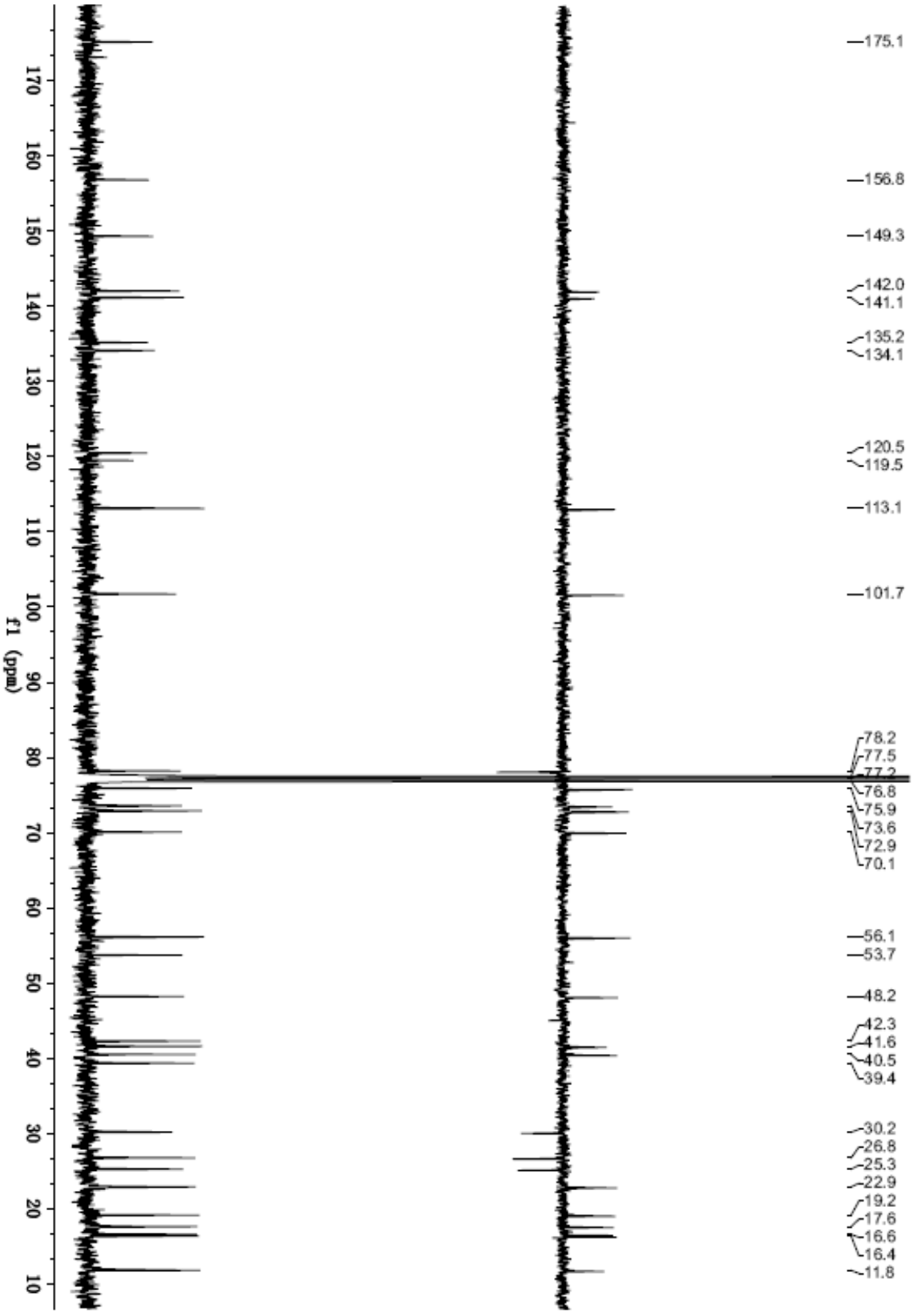


Figure S103. HSQC spectrum of walsucochinoid O (**13**) in $CDCl_3$

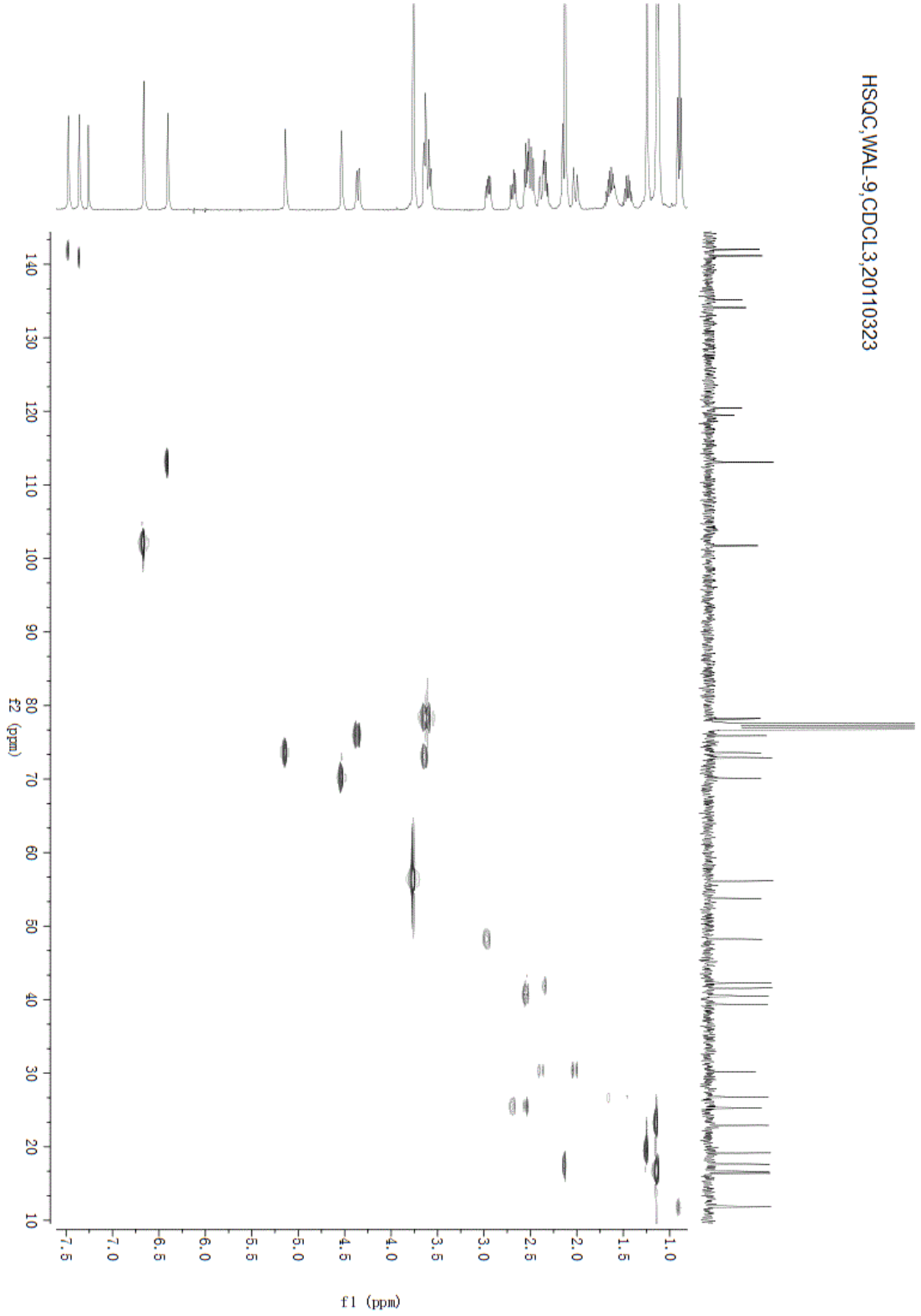


Figure S104. HMBC spectrum of walsucochinoid O (**13**) in $CDCl_3$

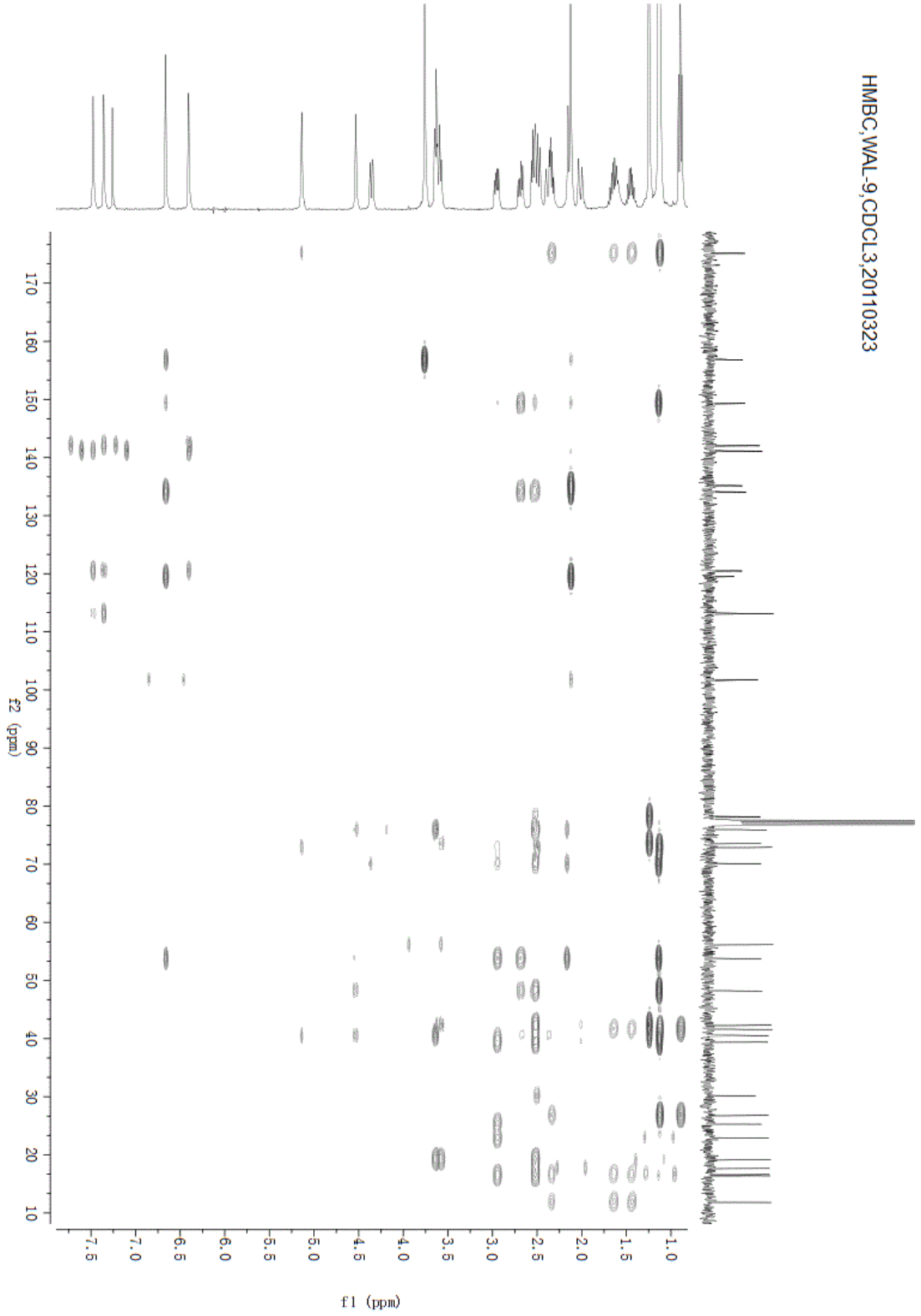


Figure S105. ROESY spectrum of walsucochinoid O (**13**) in $CDCl_3$

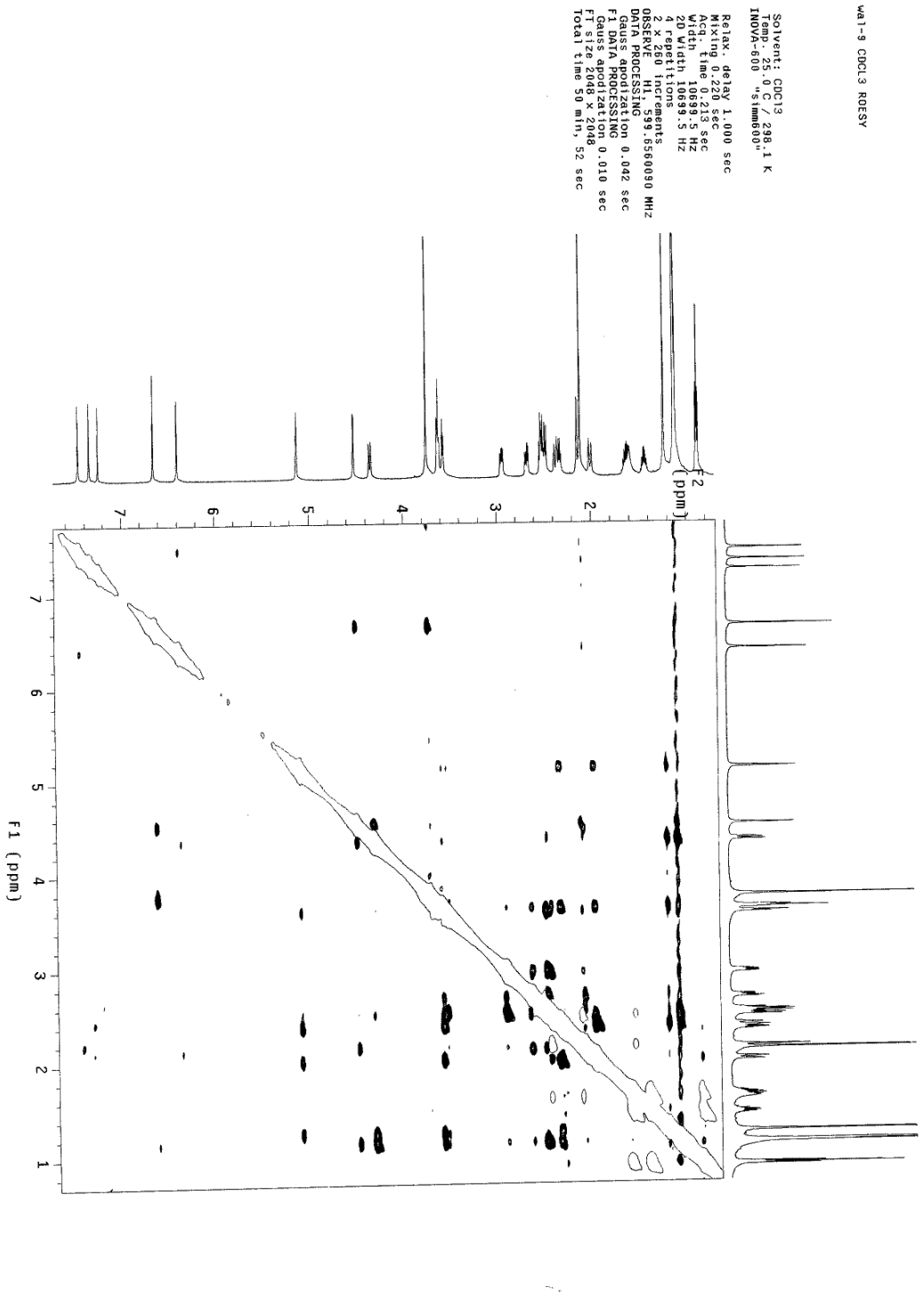


Figure S106. ESI(+)MS spectrum of walsucochinoid O (**13**)

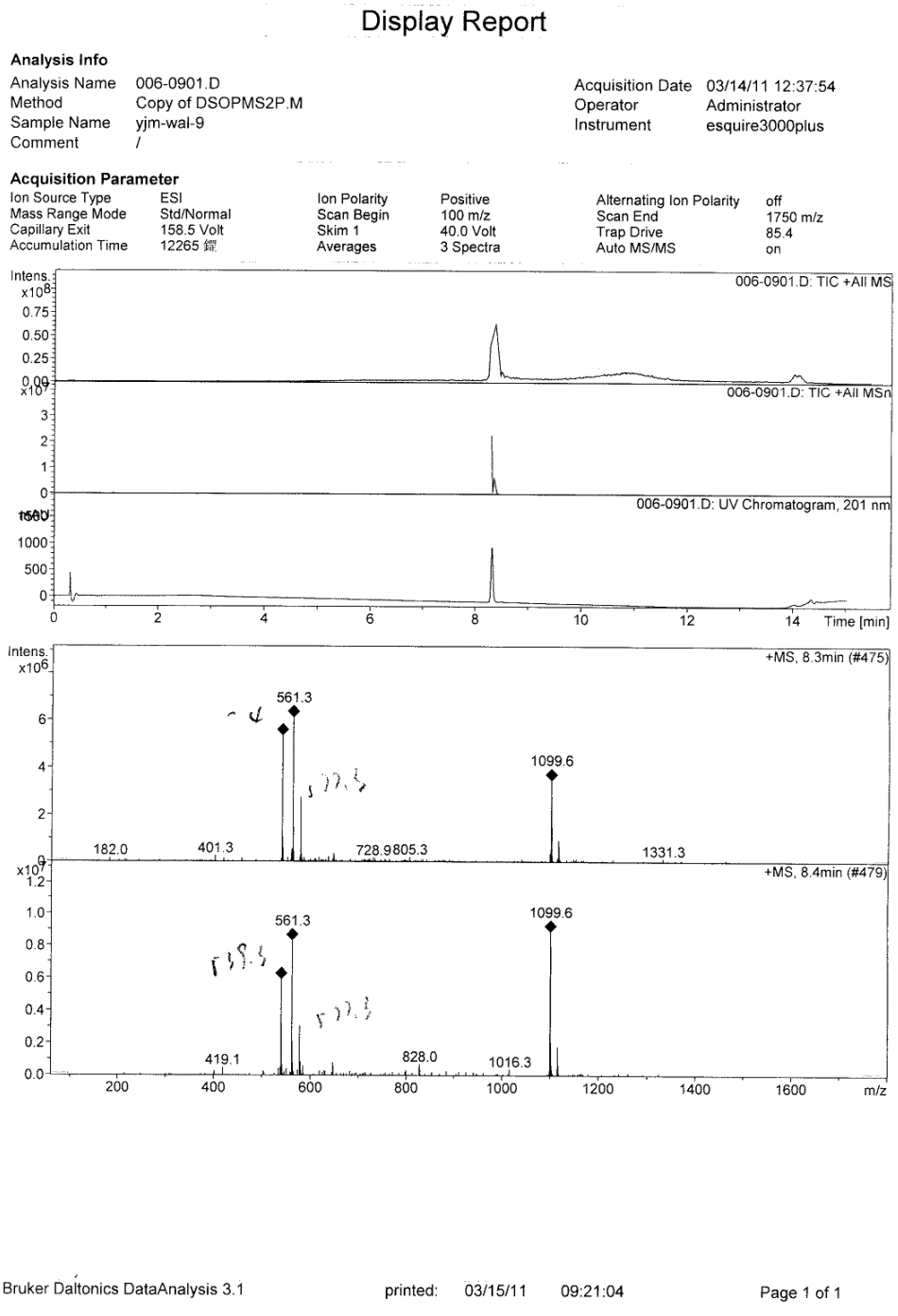


Figure S107. ESI(–)MS spectrum of walsucochinoid O (**13**)

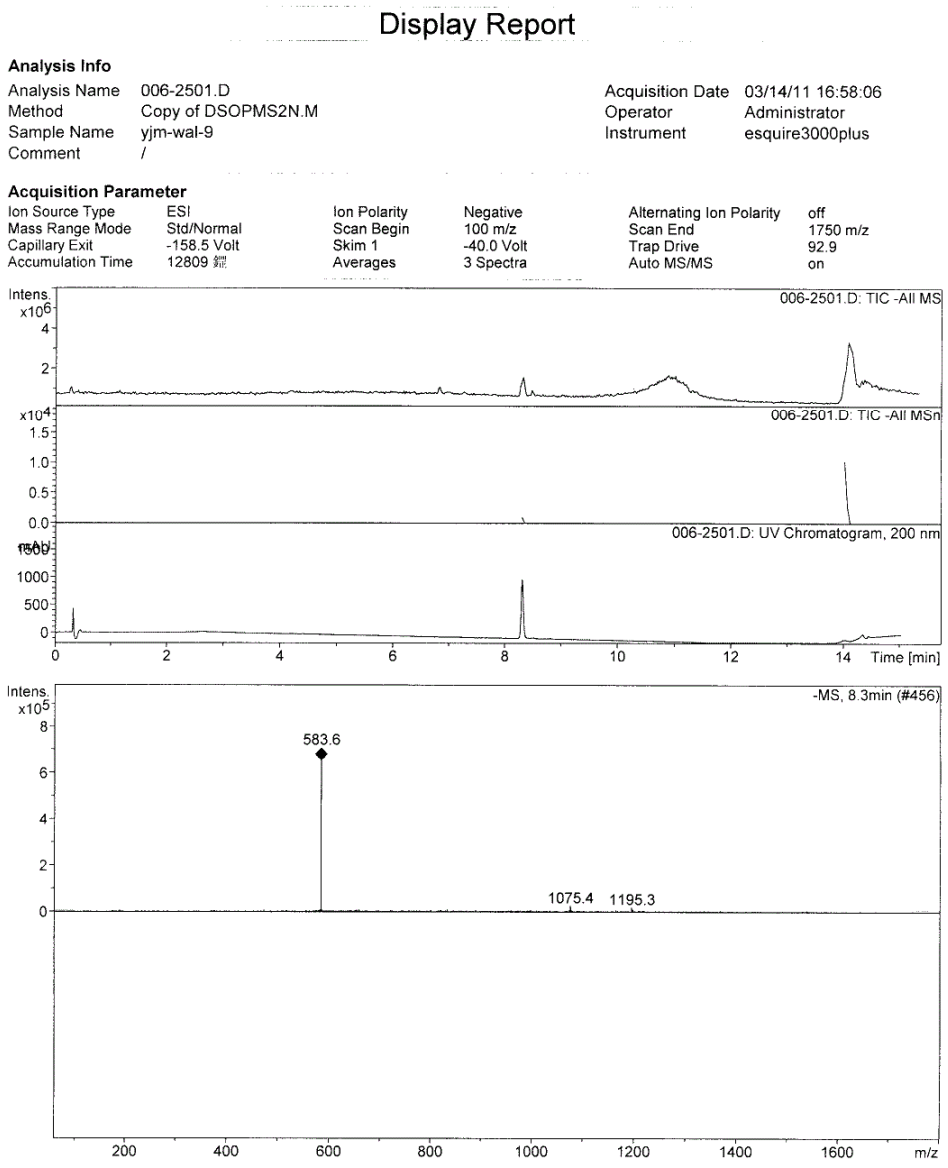


Figure S108. HRESI(+)MS spectrum of walsucochinoid O (**13**)

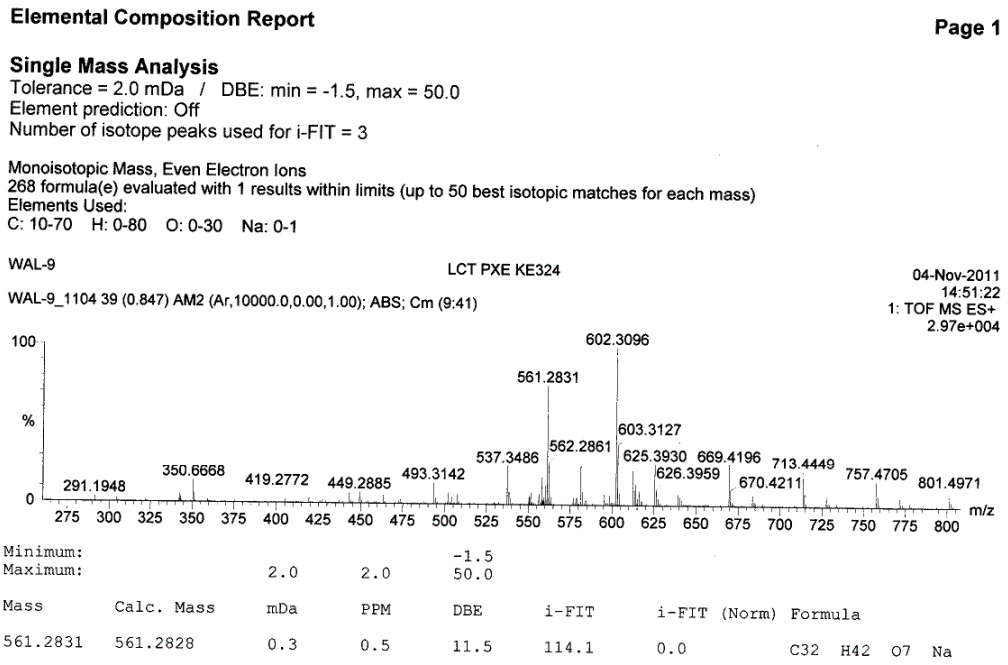


Figure S109. IR spectrum of walsucochinoid O (**13**)

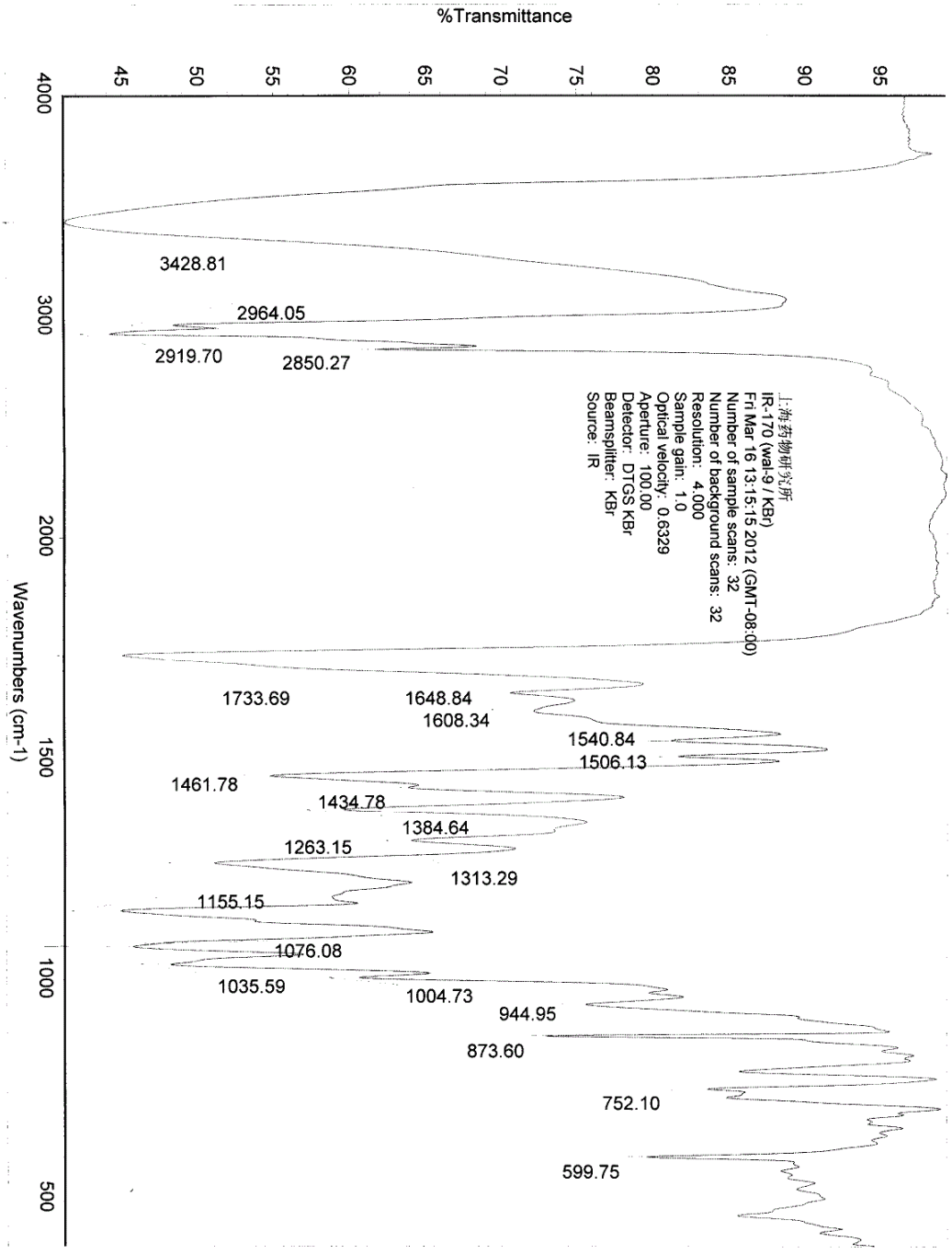


Figure S110. ^{1}H NMR spectrum of walsucochinoid P (**14**) in $CDCl_3$

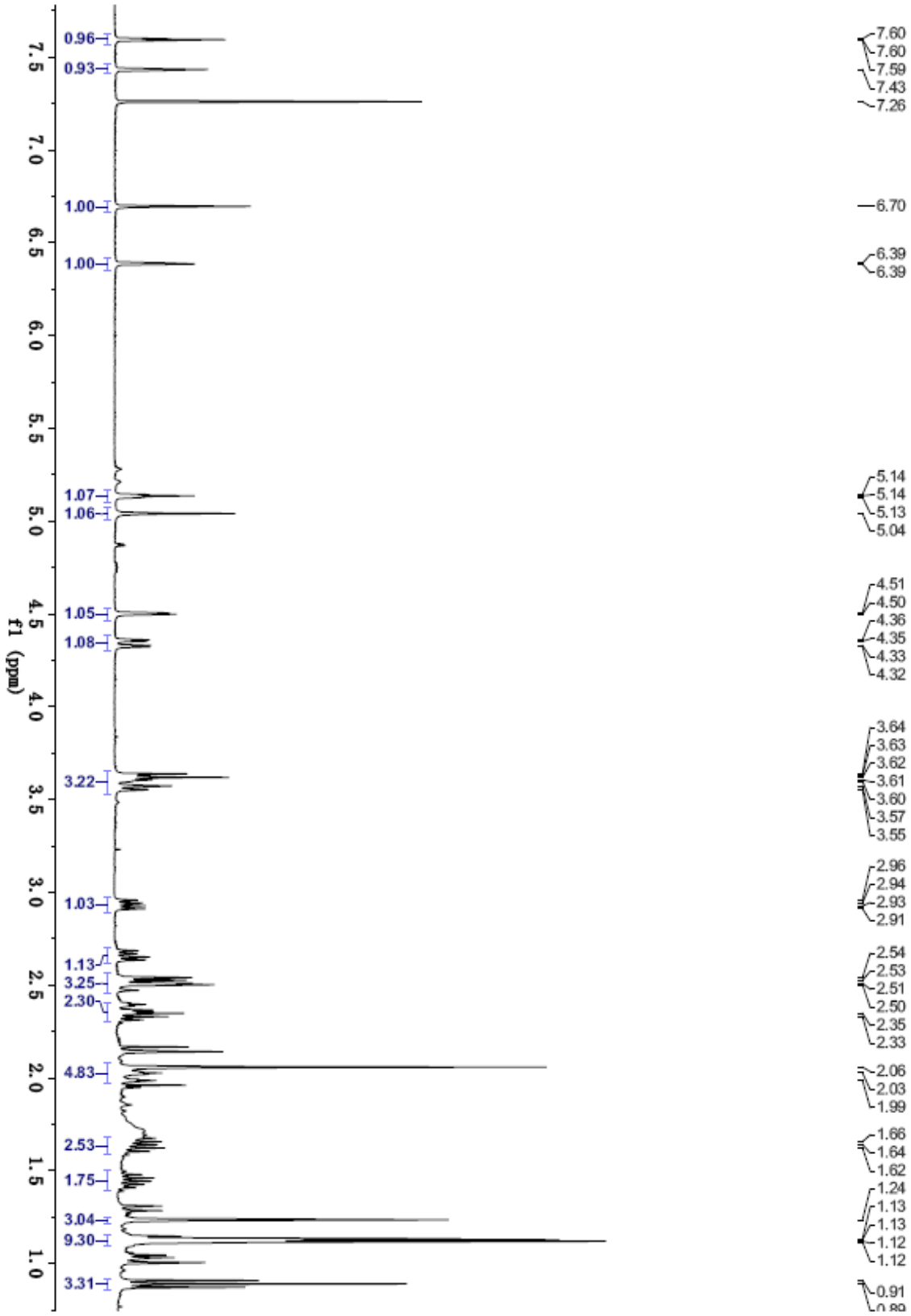


Figure S111. ^{13}C NMR spectrum of walsucochinoid P (**14**) in $CDCl_3$

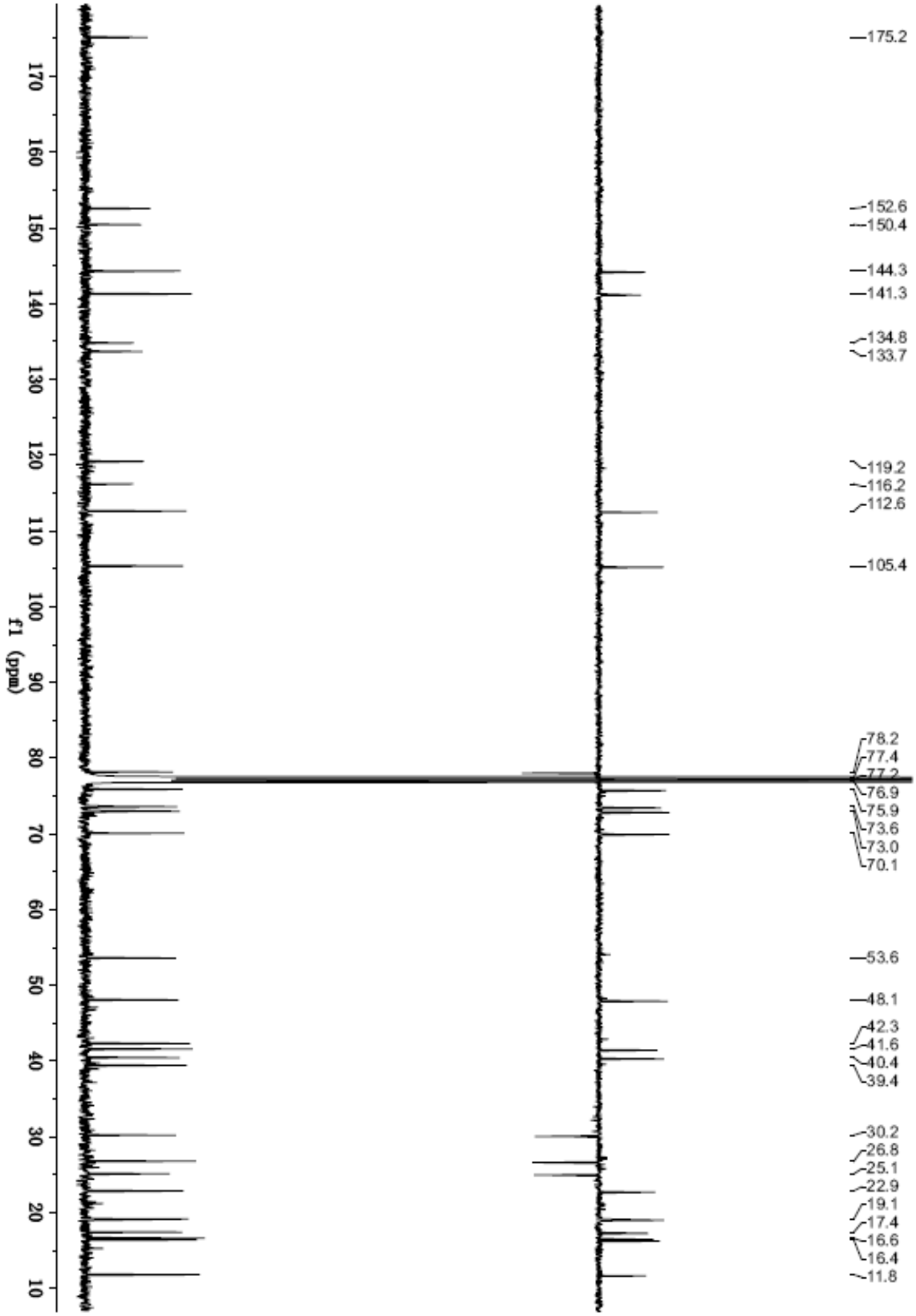


Figure S112. HSQC spectrum of walsucochinoid P (**14**) in $CDCl_3$

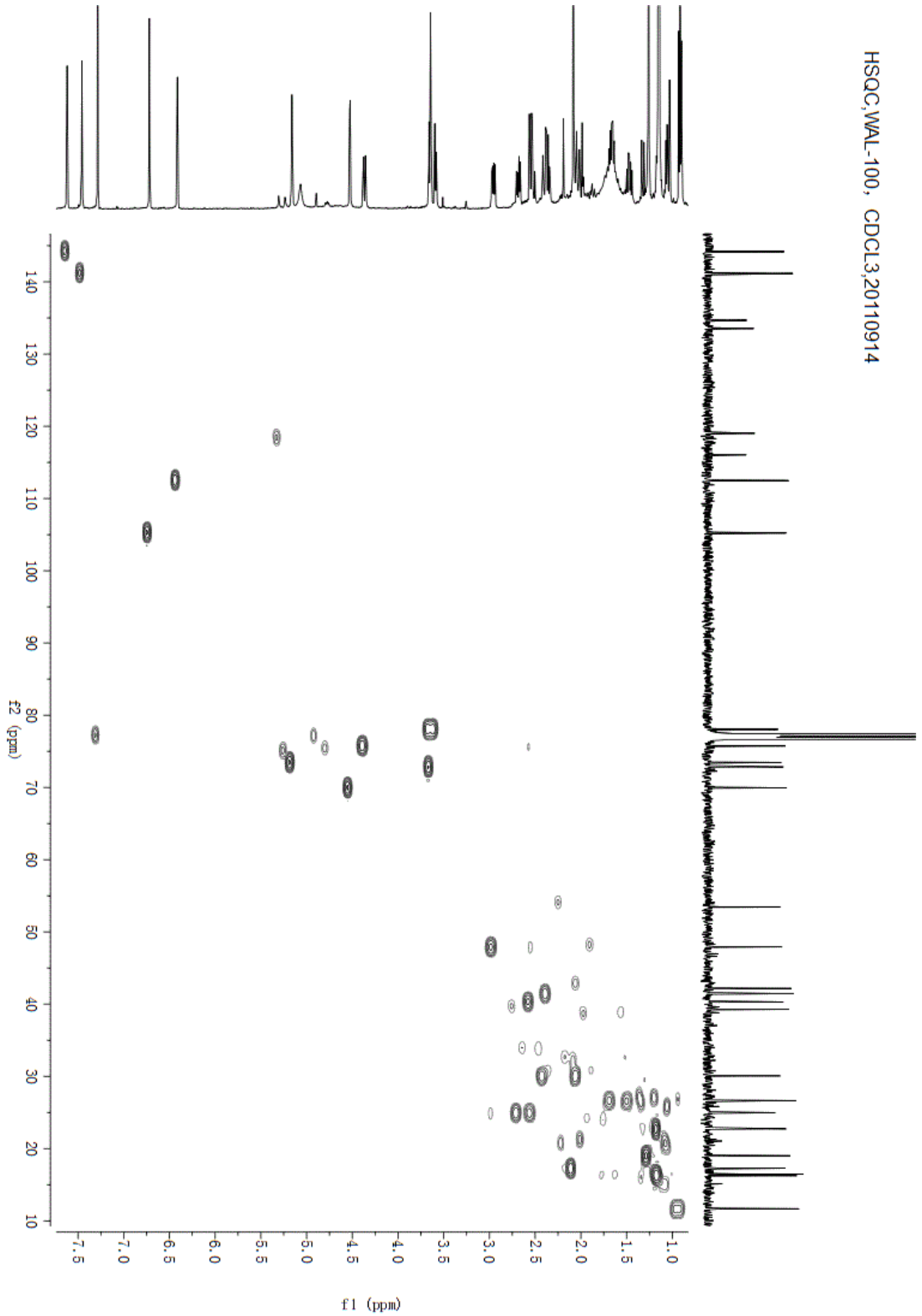


Figure S113. ROESY spectrum of walsucochinoid P (**14**) in $CDCl_3$

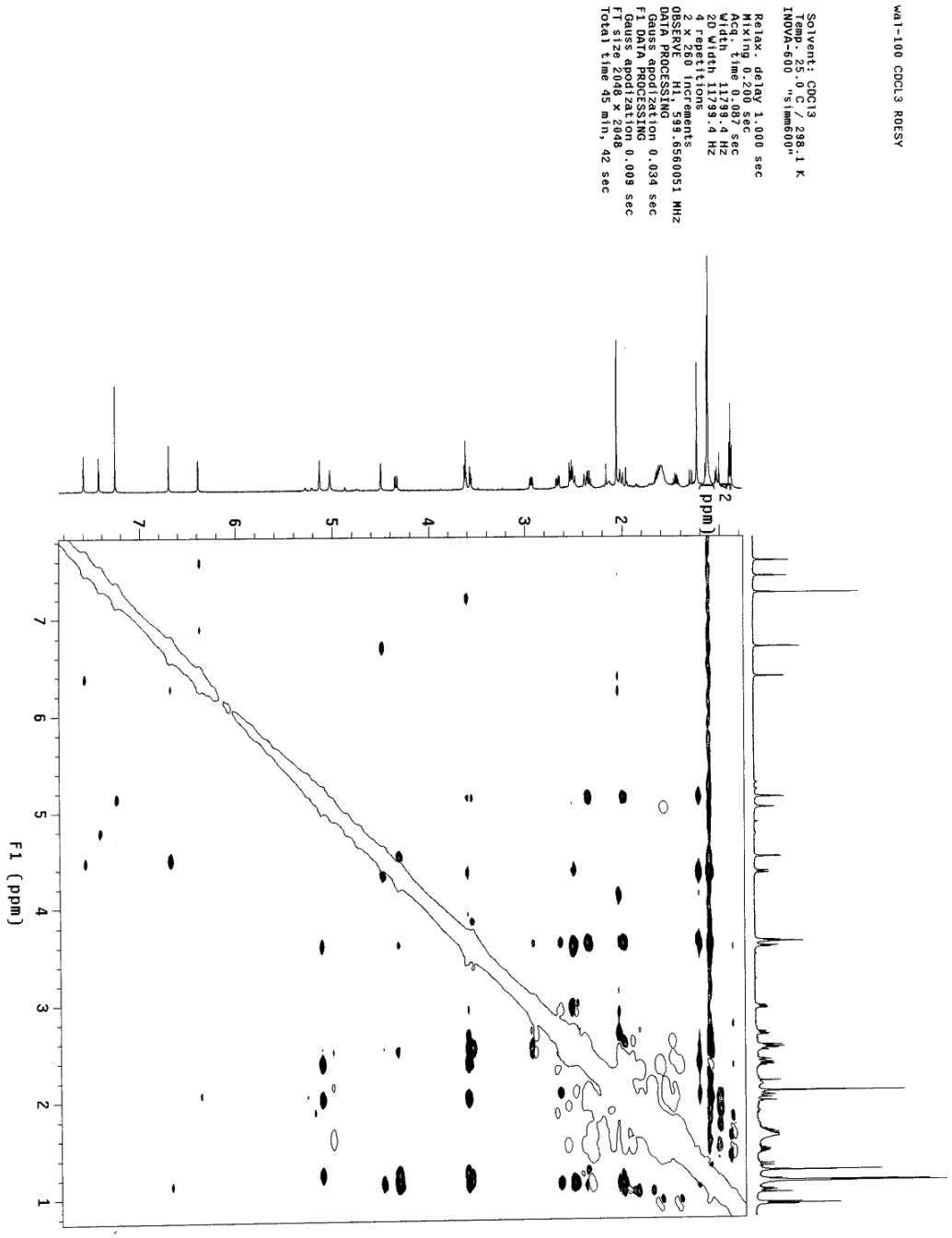


Figure S114. ESI(+)MS spectrum of walsucochinoid P (**14**)

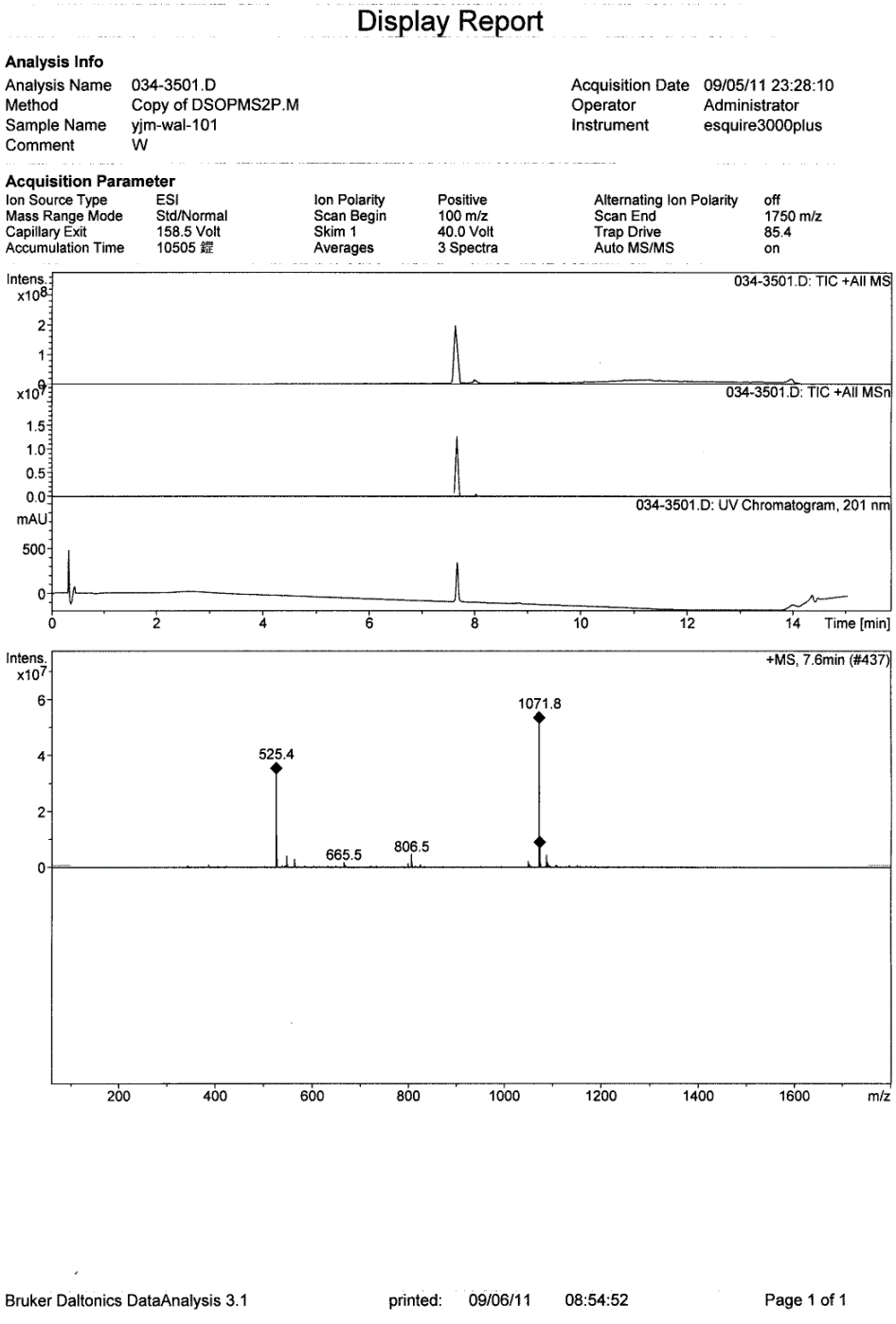


Figure S115. ESI(–)MS spectrum of walsucochinoid P (**14**)

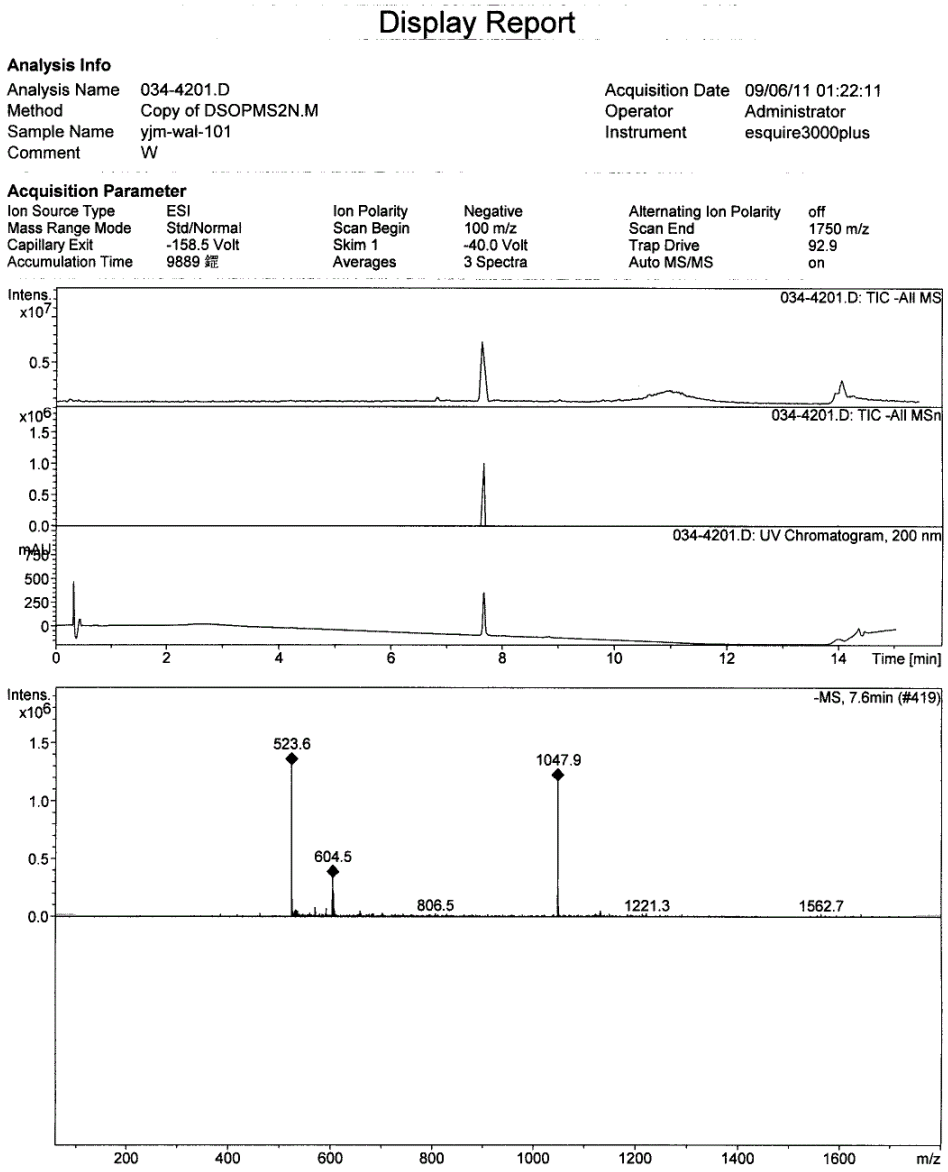


Figure S116. HRESI(+)MS spectrum of walsucochinoid P (**14**)

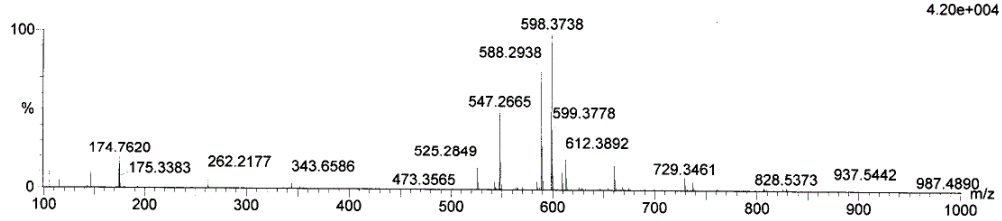
Elemental Composition Report **Page 1**

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
268 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30 Na: 0-1

WAL-100 LCT PXE KE324 09-Nov-2011 14:39:04

WAL-100_1109 28 (0.600) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (17:45) 1: TOF MS ES+ 4.20e+004



Minimum:				-1.5			
Maximum:		5.0	3.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
547.2665	547.2672	-0.7	-1.3	11.5	97.0	0.0	C31 H40 O7 Na

Figure S117. IR spectrum of walsucochinoid P (**14**)

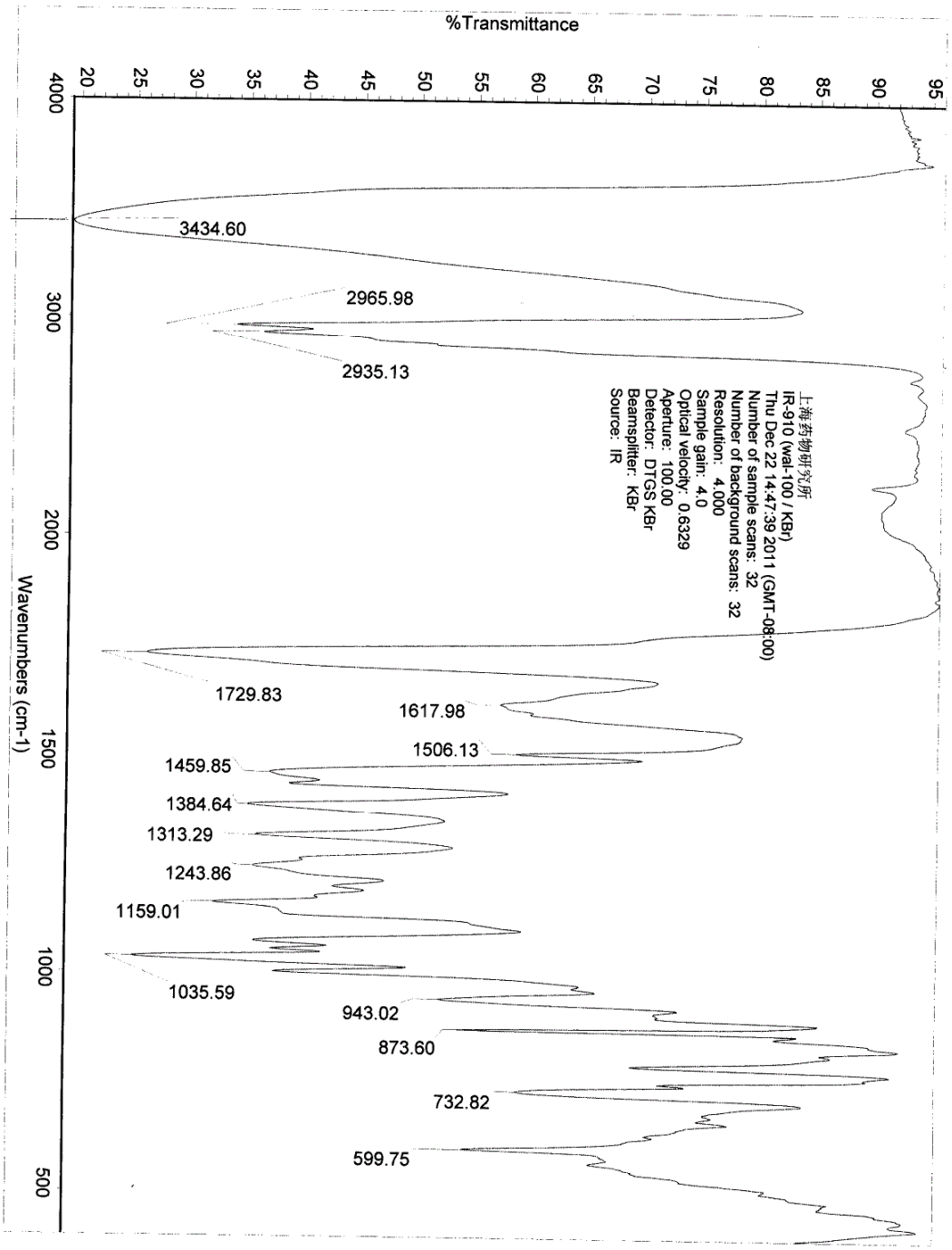


Figure S118. ^{1}H NMR spectrum of walsucochinoid Q (**15**) in $CDCl_3$

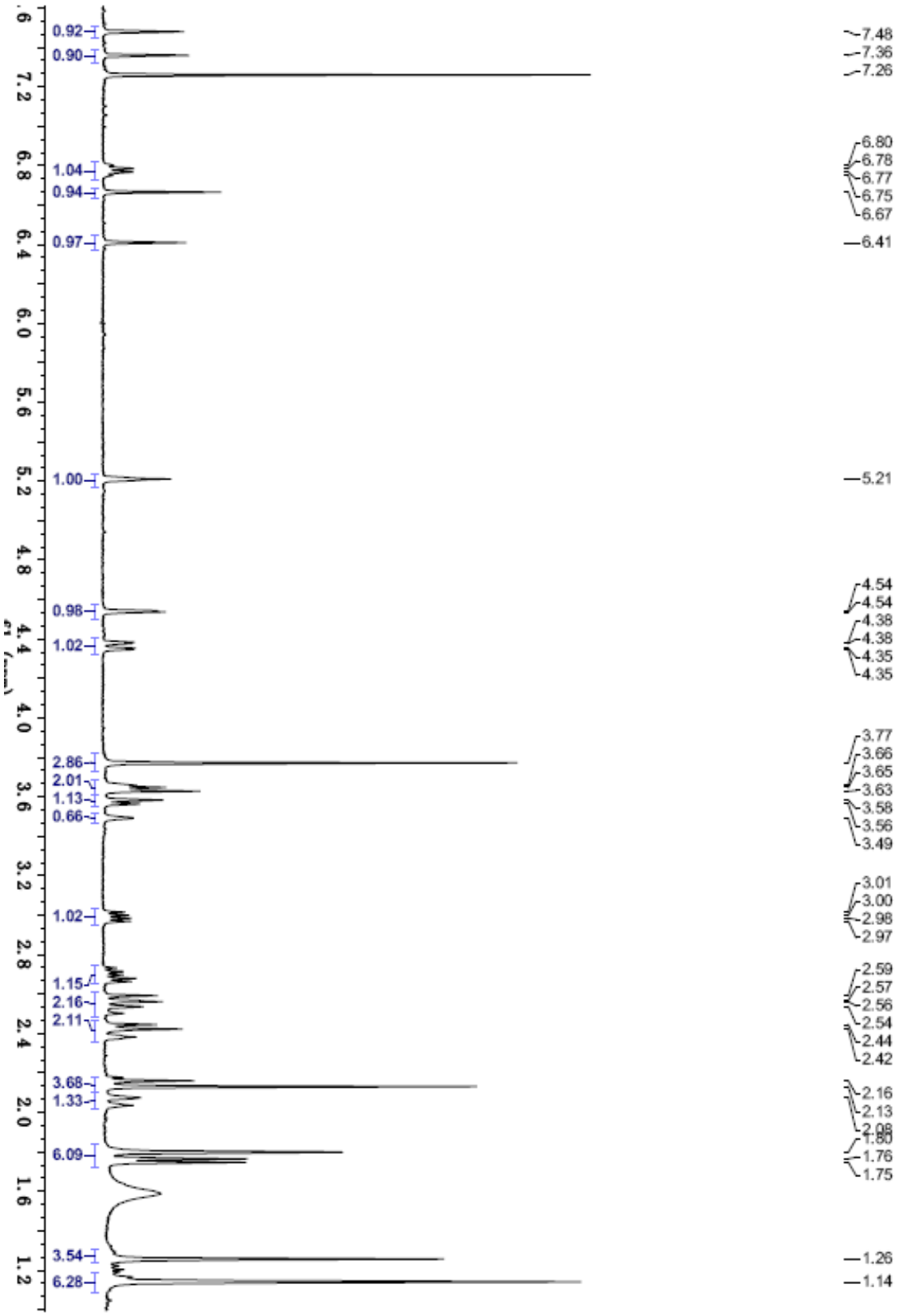


Figure S119. ^{13}C NMR spectrum of walsucochinoid Q (**15**) in $CDCl_3$

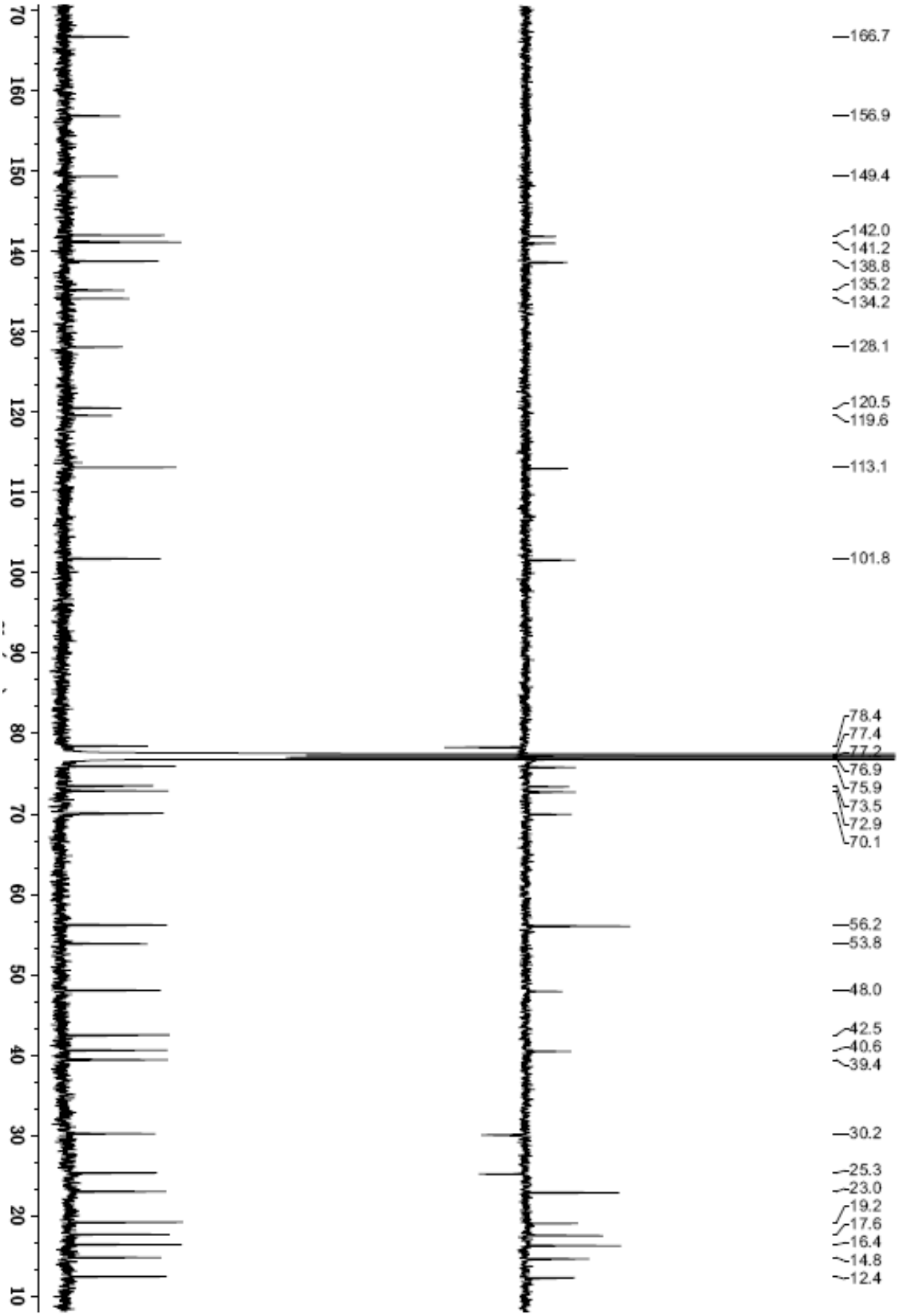


Figure S120. HSQC spectrum of walsucochinoid Q (**15**) in $CDCl_3$

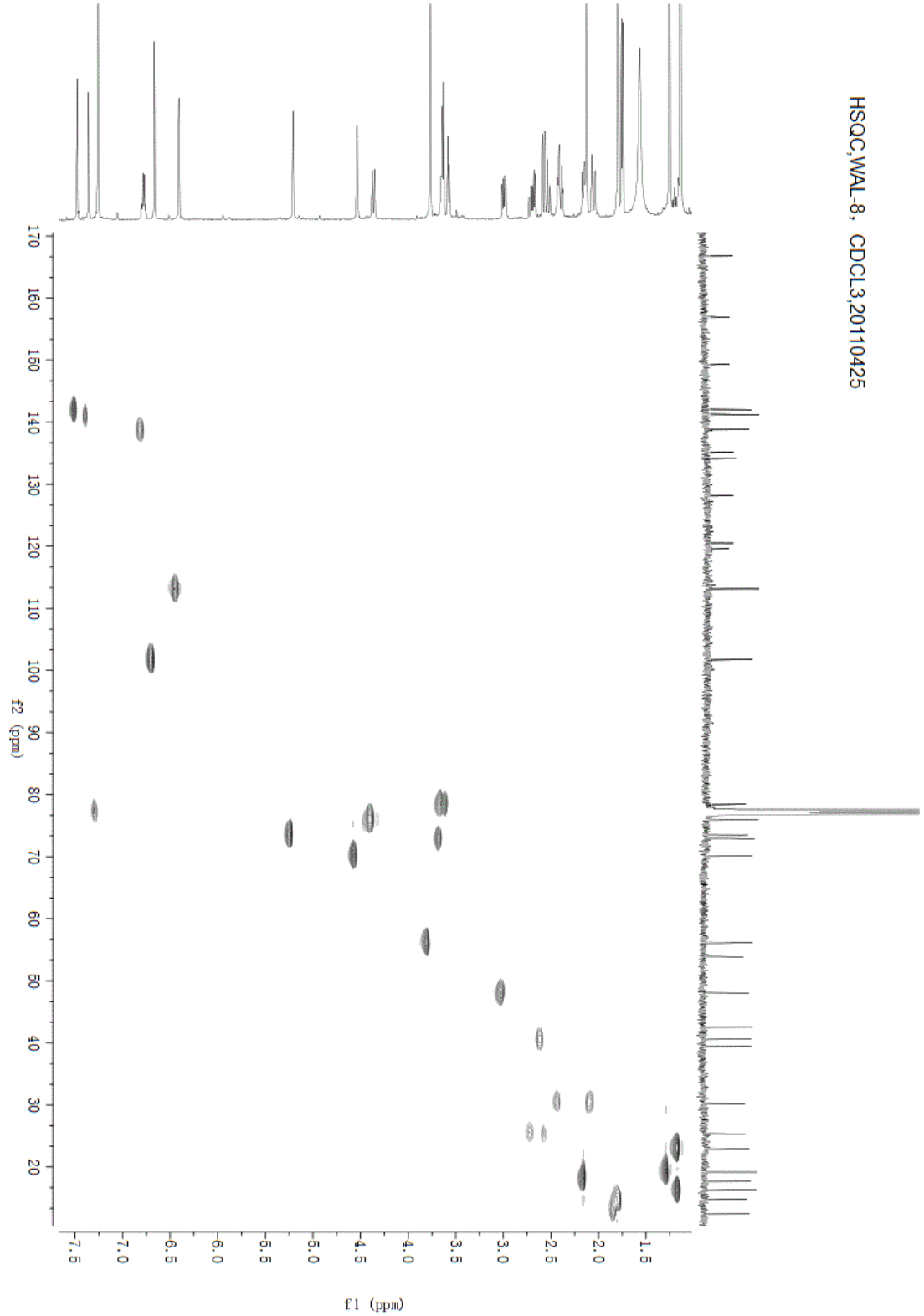


Figure S121. HMBC spectrum of walsucochinoid Q (**15**) in $CDCl_3$

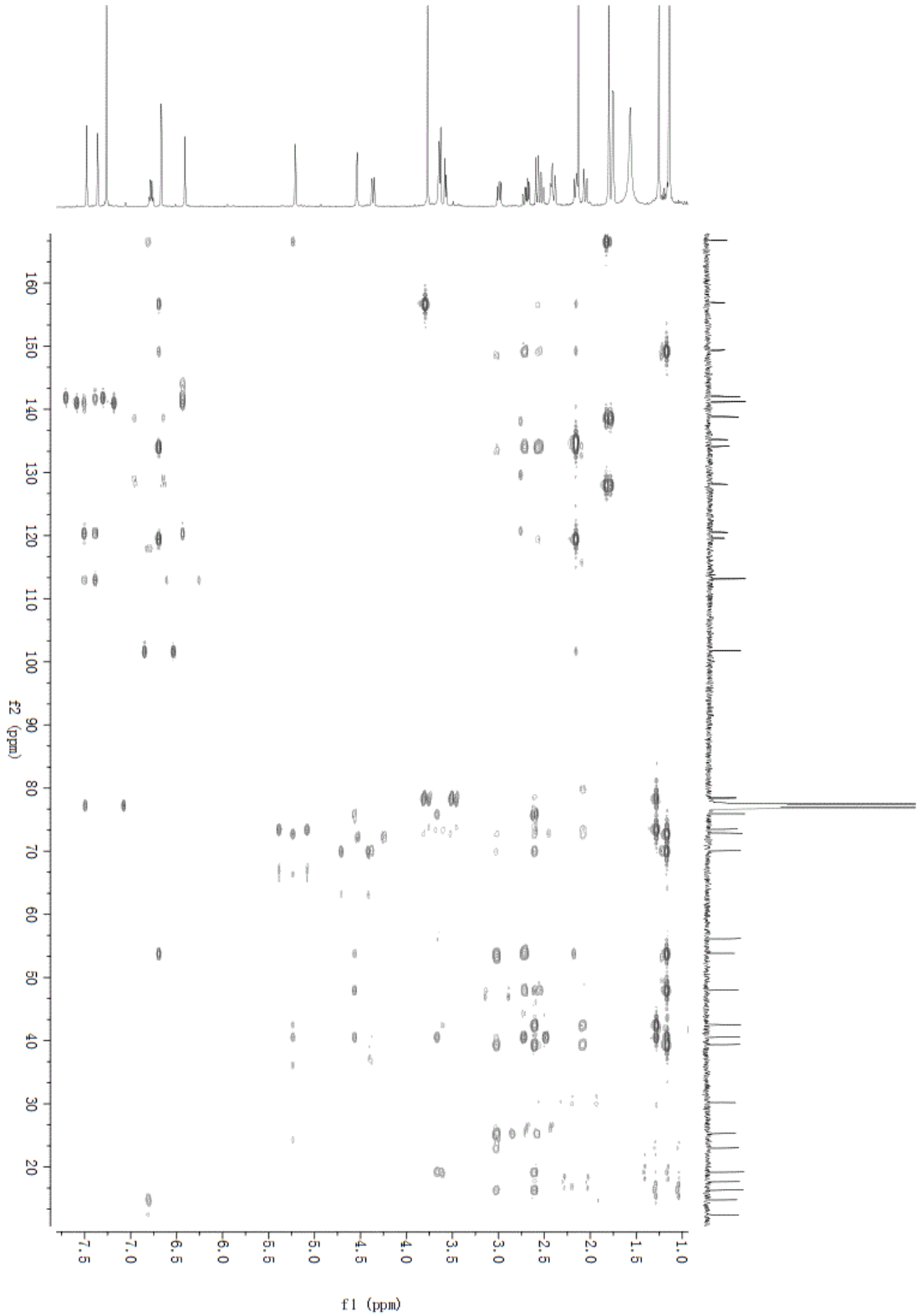


Figure S122. ROESY spectrum of walsucochinoid Q (**15**) in $CDCl_3$

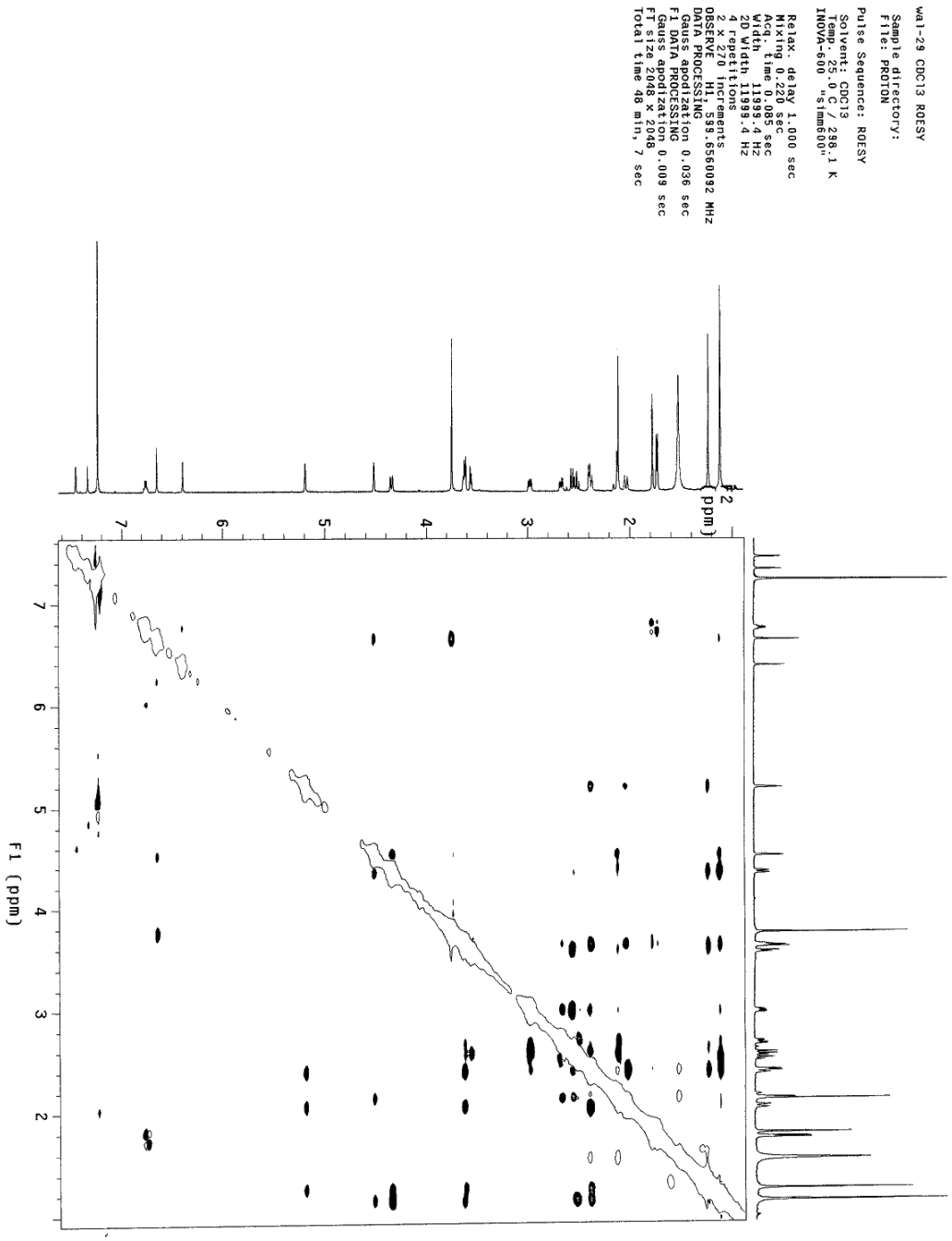


Figure S123. ESI(+)MS spectrum of walsucochinoid Q (**15**)

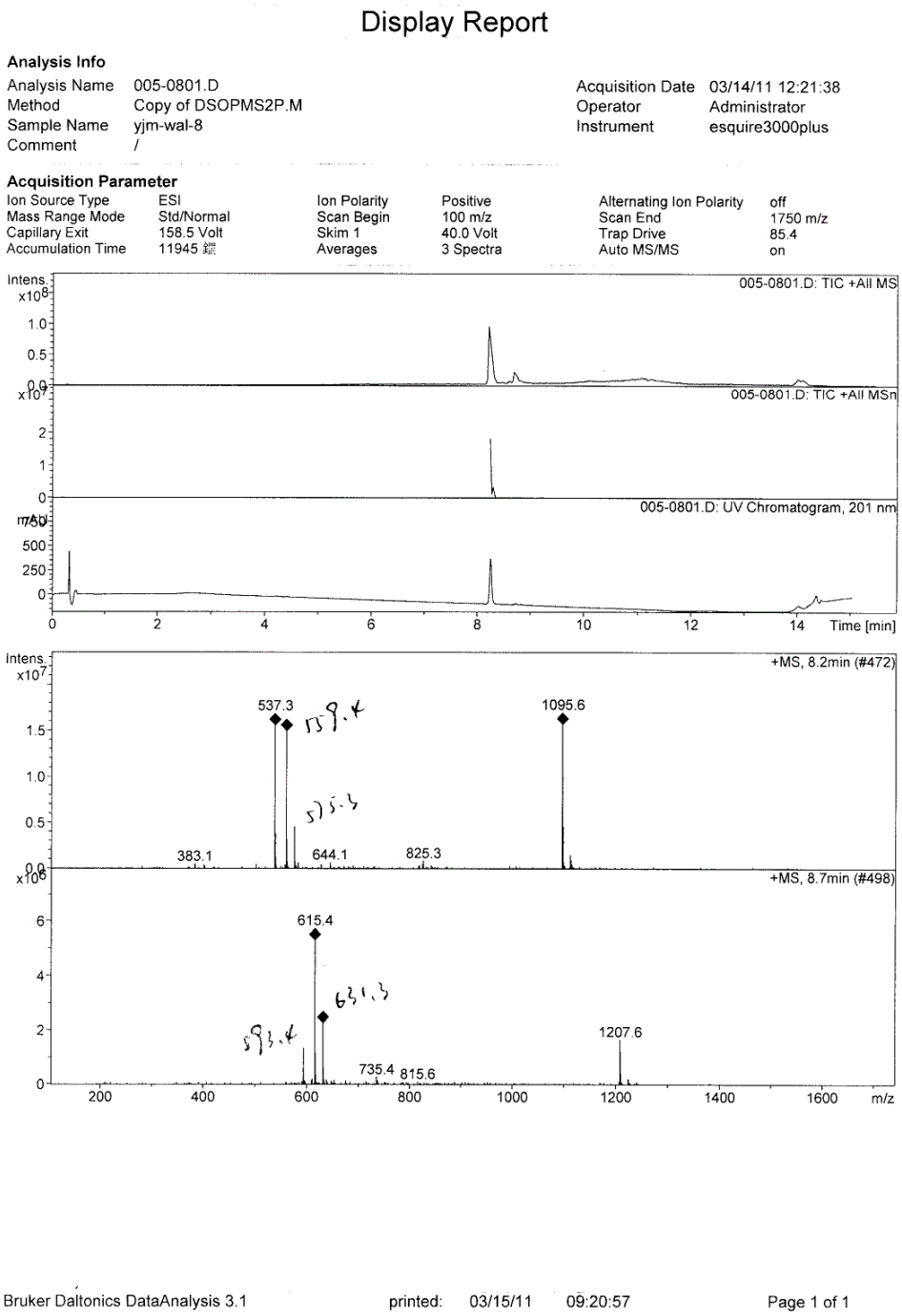


Figure S124. ESI(–)MS spectrum of walsucochinoid Q (**15**)

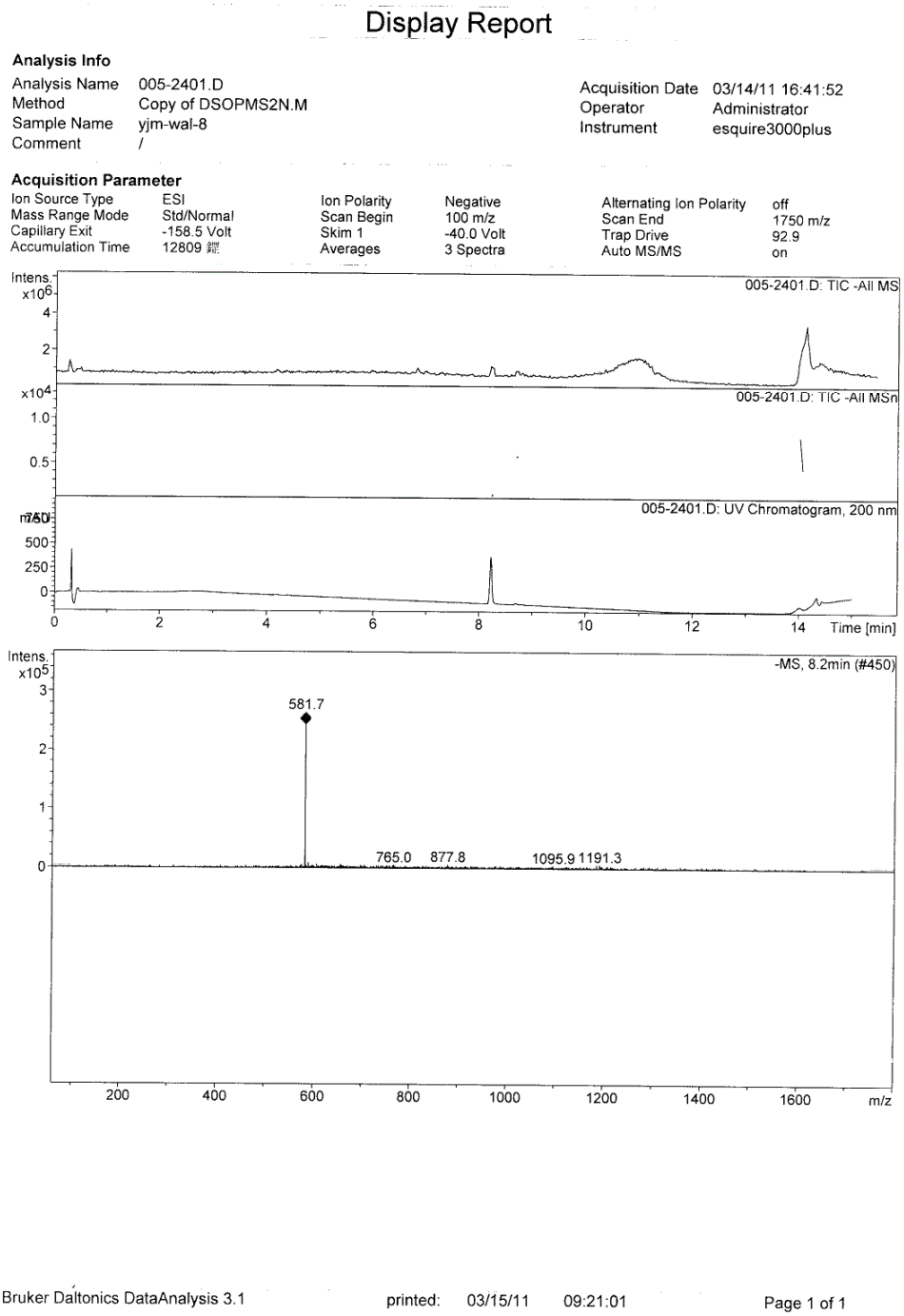
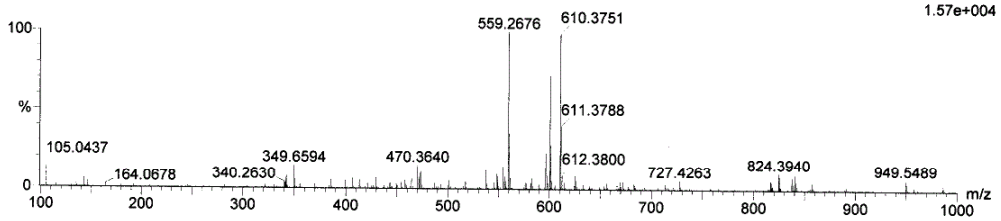


Figure S125. HRESI(+)MS spectrum of walsucochinoid Q (**15**)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
277 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30 Na: 0-1
WAL-8 LCT PXE KE324 04-Nov-2011 15:27:30
WAL-8_1104 19 (0.405) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (5:28) 1: TOF MS ES+ 1.57e+004



Minimum:				-1.5			
Maximum:		2.0	2.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
559.2676	559.2672	0.4	0.7	12.5	113.3	0.0	C32 H40 O7 Na
	559.2696	-2.0	-3.6	15.5	118.1	4.8	C34 H39 O7

Figure S126. IR spectrum of walsucochinoid Q (**15**)

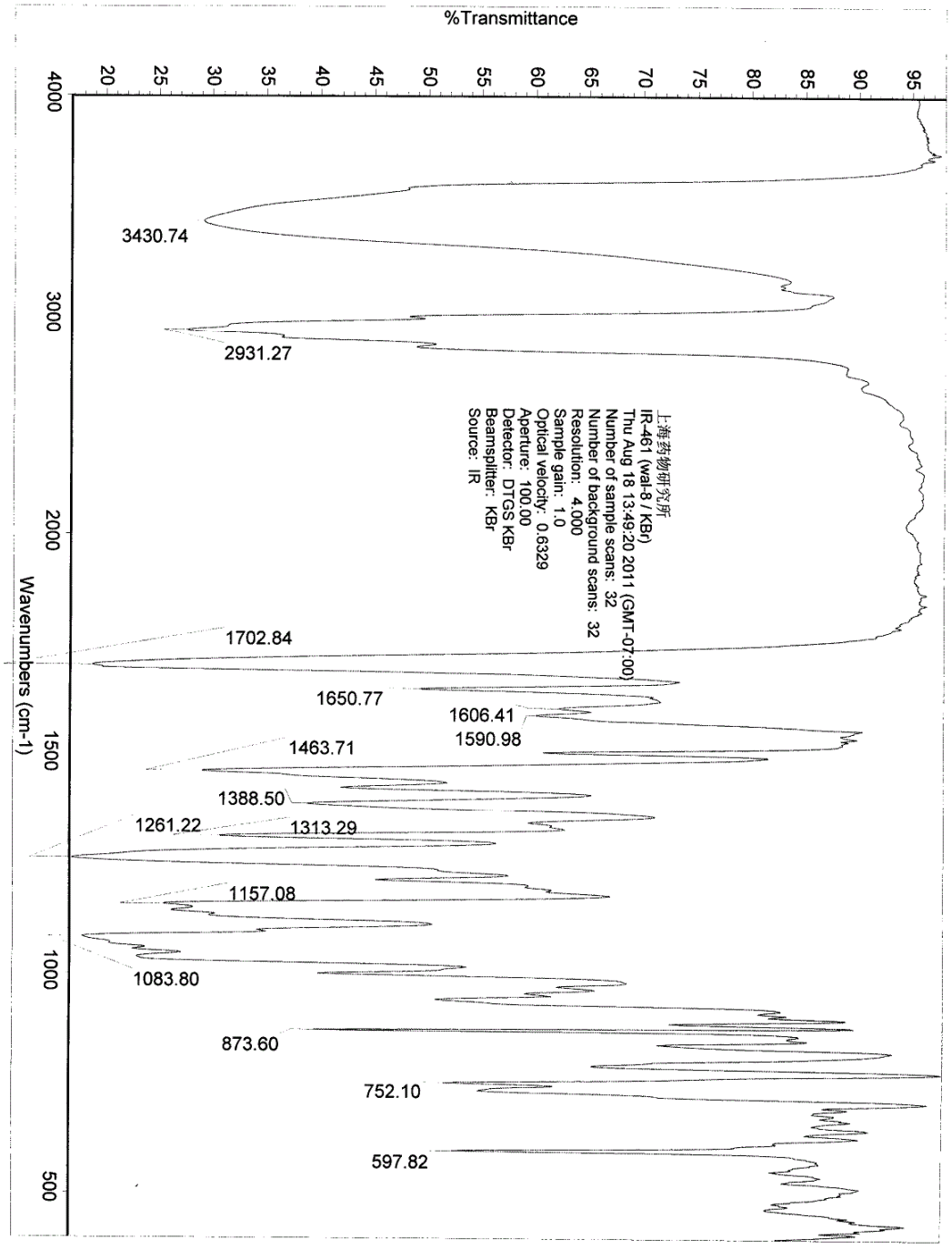


Figure S127. ^{1}H NMR spectrum of walsucochinoid R (**16**) in $CDCl_3$

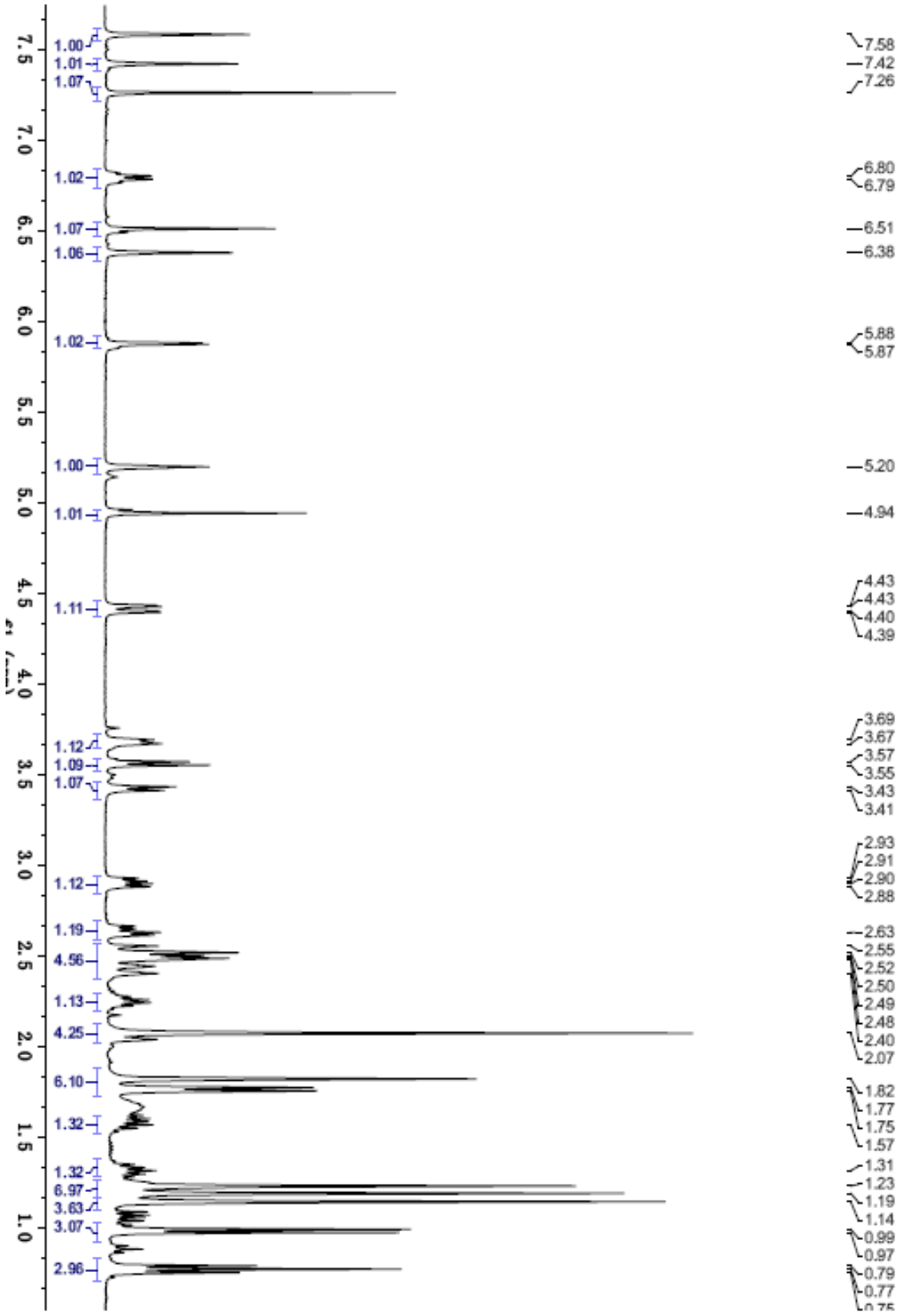


Figure S128. ^{13}C NMR spectrum of walsucochinoid R (**16**) in $CDCl_3$

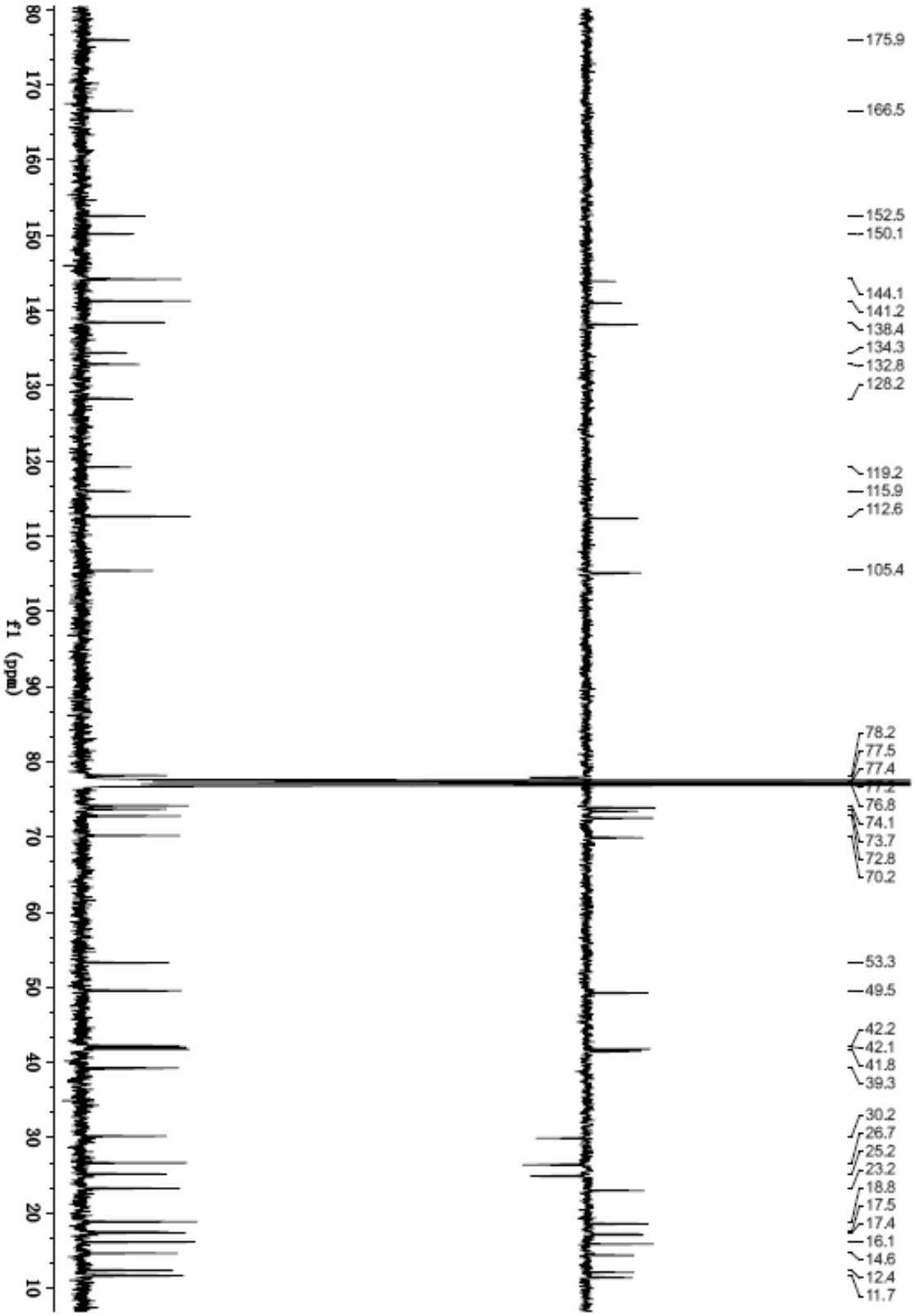


Figure S129. HSQC spectrum of walsucochinoid R (**16**) in $CDCl_3$

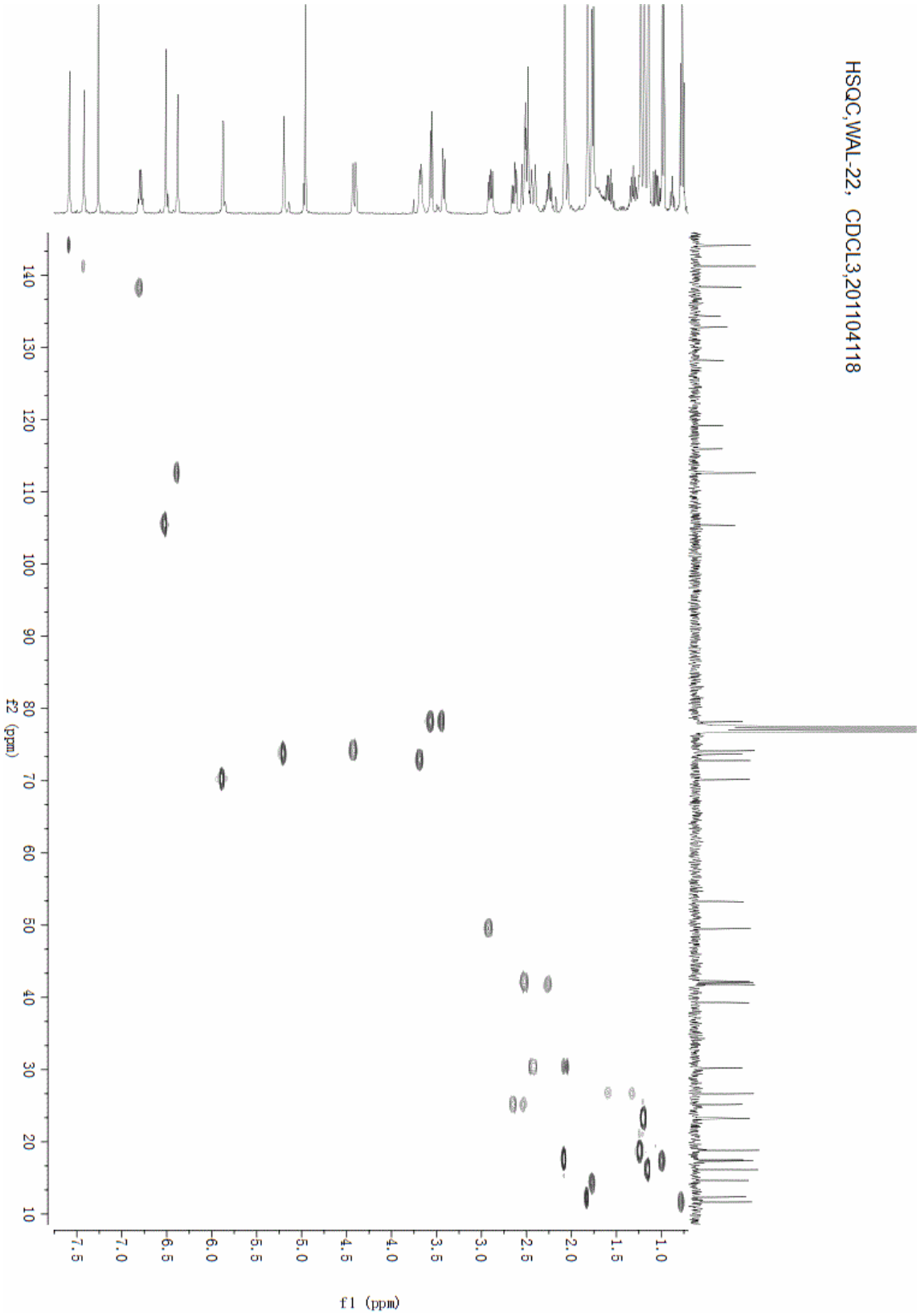


Figure S130. HMBC spectrum of walsucochinoid R (**16**) in $CDCl_3$

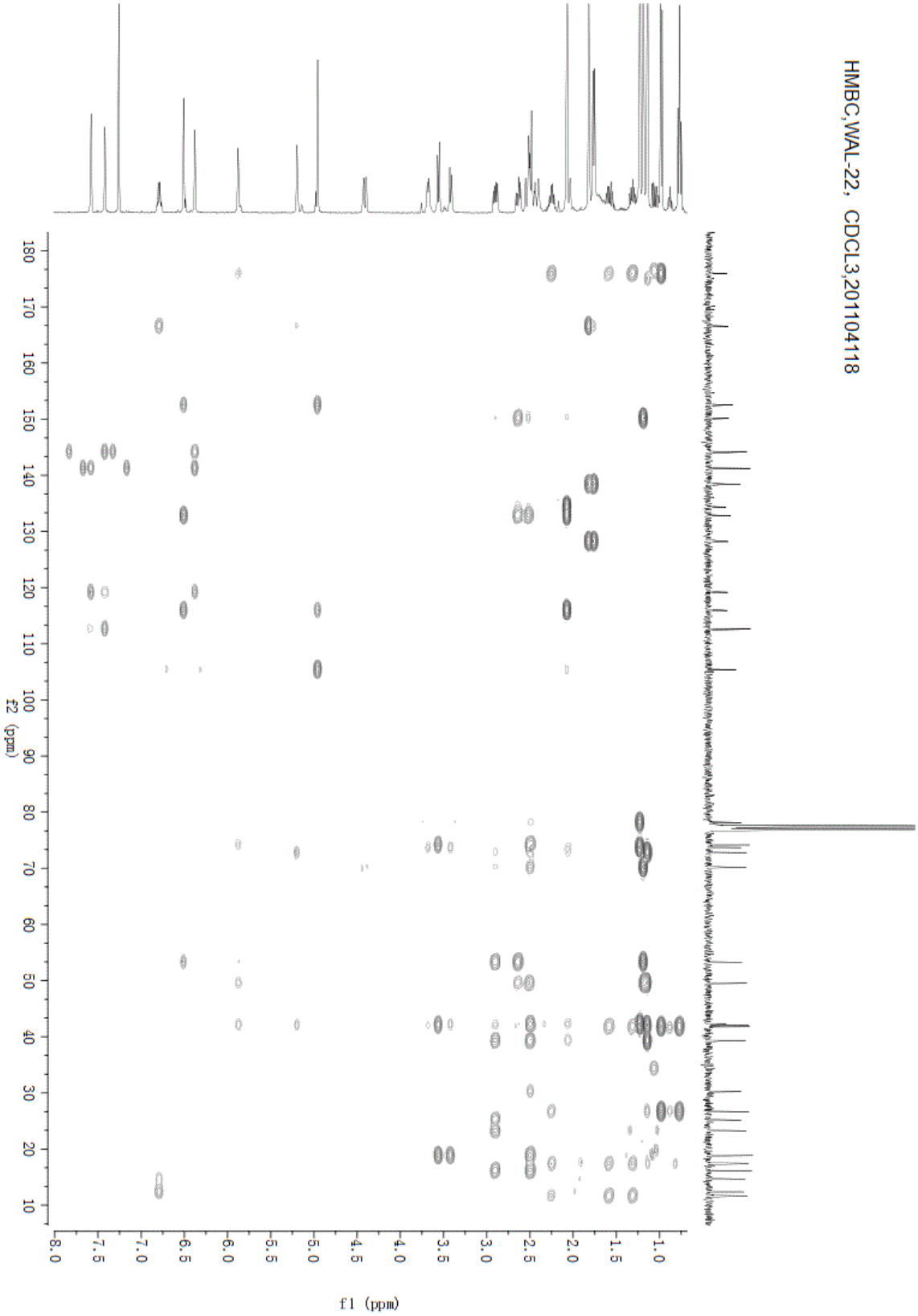


Figure S131. ROESY spectrum of walsucochinoid R (**16**) in $CDCl_3$

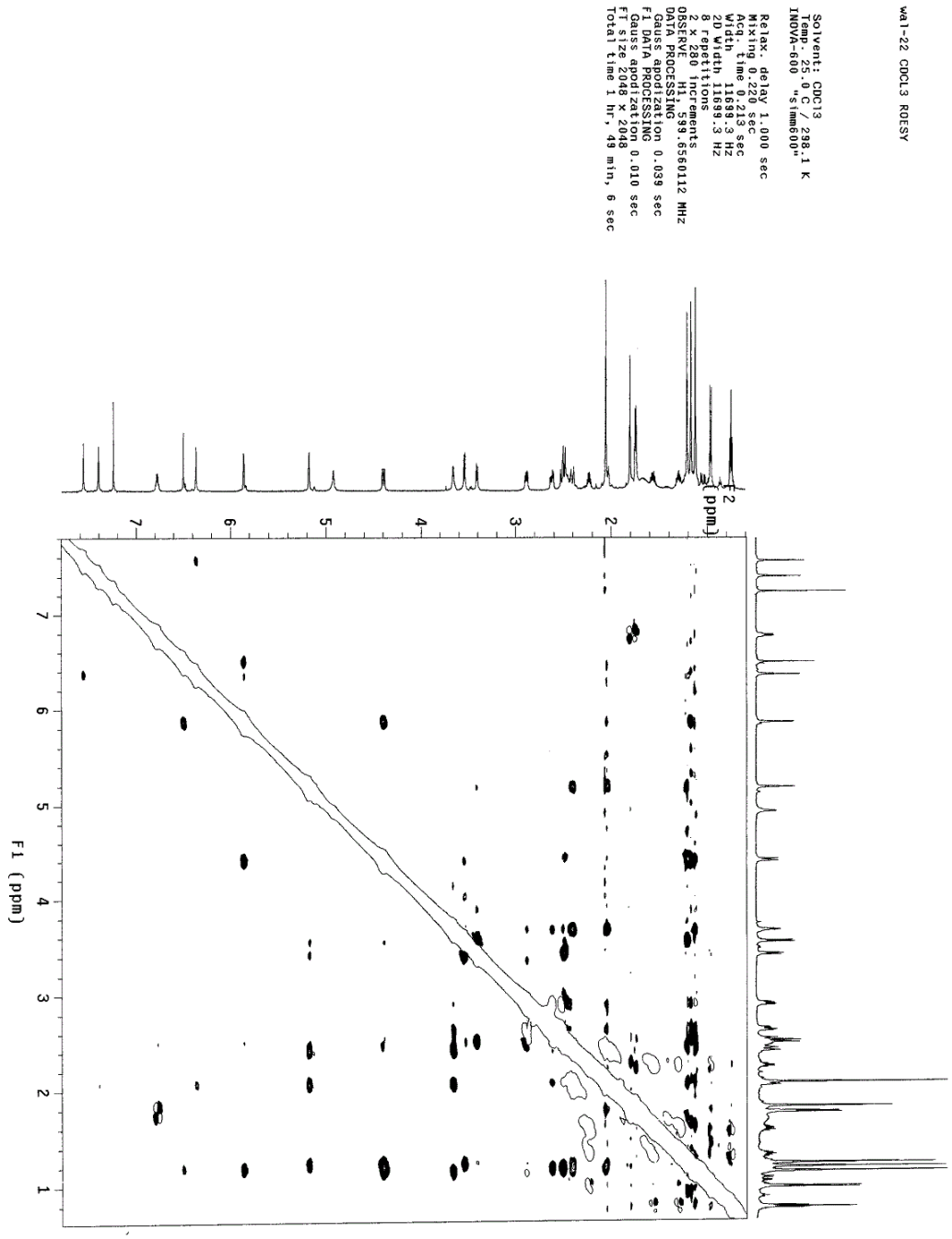


Figure S132. ESI(+)MS spectrum of walsucochinoid R (**16**)

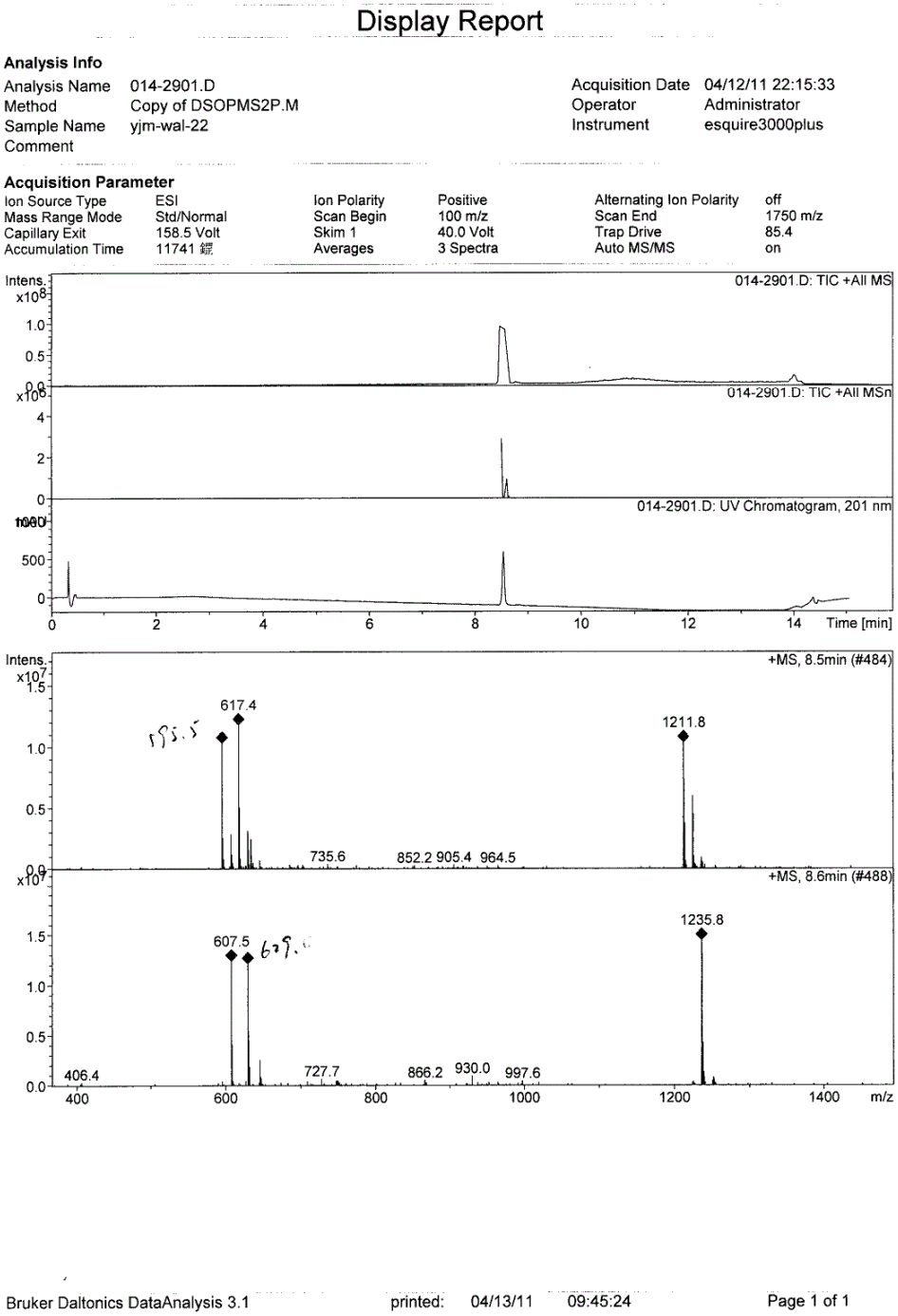


Figure S133. HRESI(+)MS spectrum of walsucochinoid R (**16**)

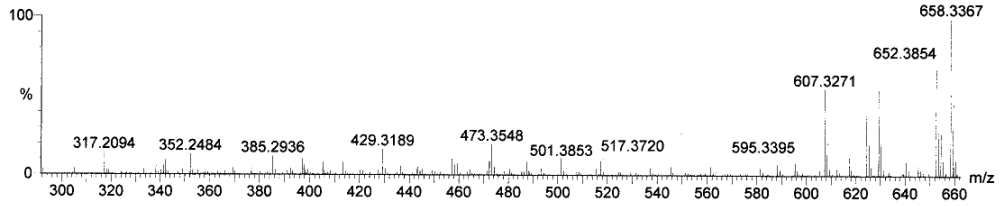
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 2.0 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
313 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-70 H: 0-80 O: 0-30 Na: 0-1

WAL-22 LCT PXE KE324 28-Dec-2011 14:25:43

WAL-22_1228 11 (0.229) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (11:30) 1: TOF MS ES+ 1.81e+004



Minimum:				-1.5			
Maximum:		5.0	2.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
607.3271	607.3271	0.0	0.0	13.5	66.1	0.0	C36 H47 O8

Figure S134. IR spectrum of walsucochinoid R (**16**)