

Supporting information for

Chantriolides F–P, Highly Oxidized Withanolides with Hepatoprotective

Activity from *Tacca chantrieri*

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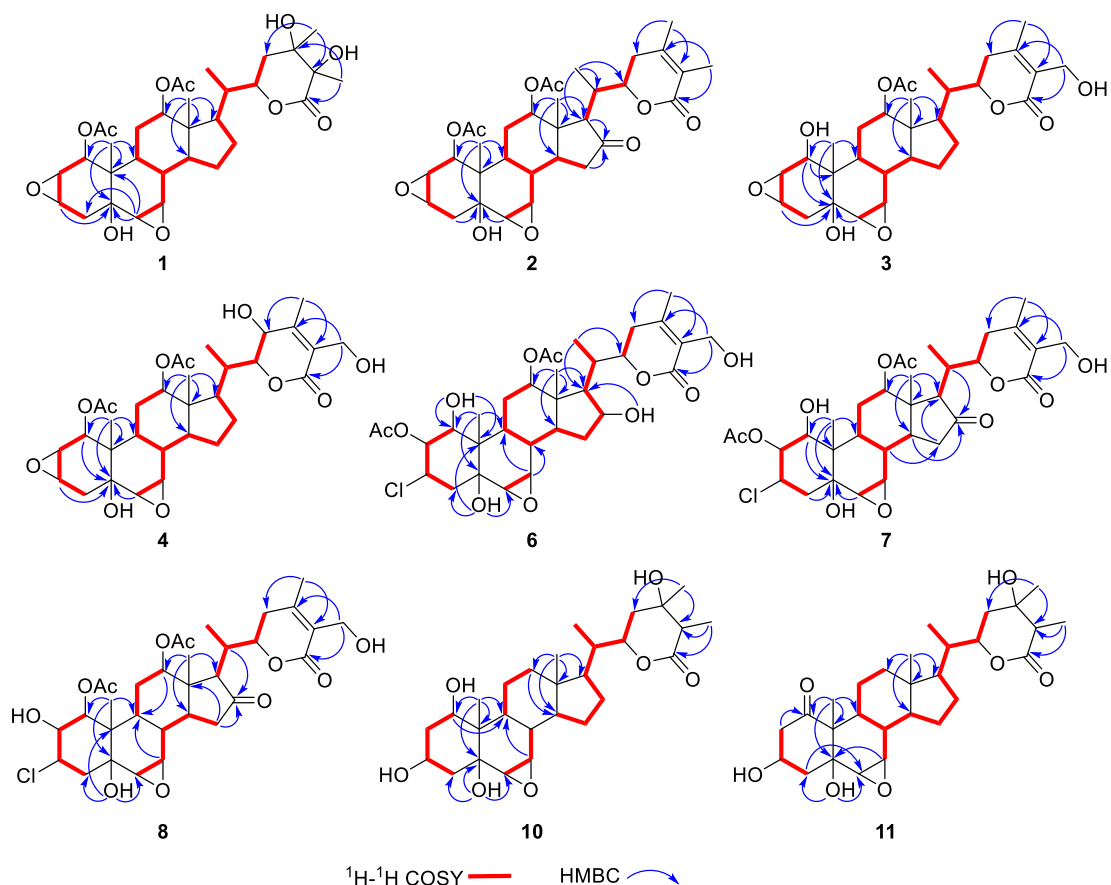


Figure S1. Key ^1H - ^1H COSY and HMBC correlations of compounds 1–4, 6–8, 10, and 11.

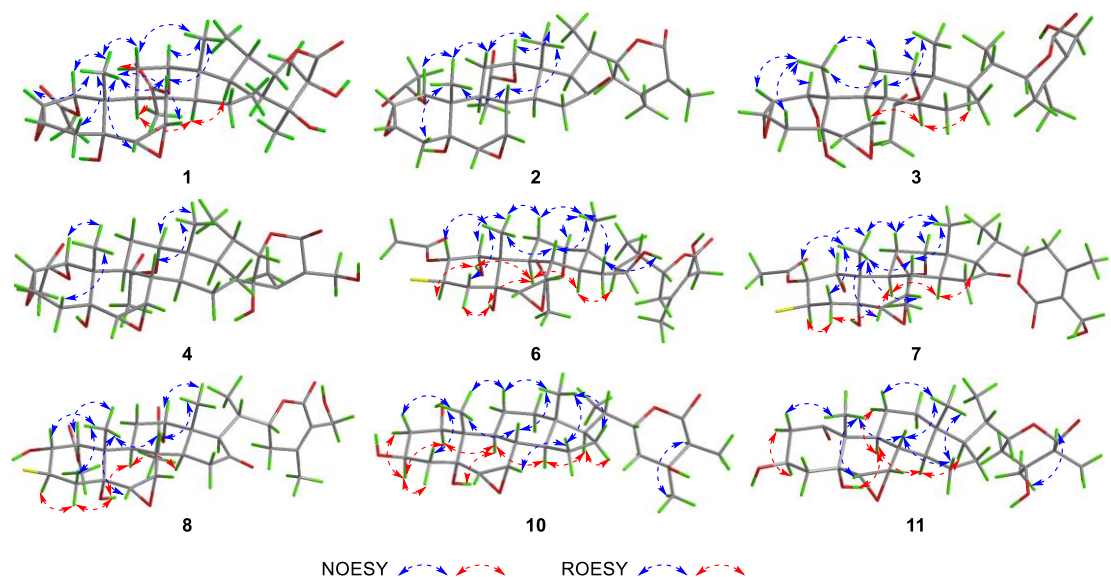


Figure S2. NOESY correlations of compounds 1–3 and ROESY correlations of compounds 4, 6–8, 10, and 11.

Elemental Composition Report

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

104 formula(e) evaluated with 3 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

C: 0-50 H: 0-60 O: 0-20

Minimum: -1.5

Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
651.3023	651.3017	0.6	0.9	10.5	592.1	0.232	79.31	C33 H47 O13

JGS-B2J1B2
20210123-YY-B2J1B2 1115 (4.600)

1: TOF MS ES-
5.42e+005

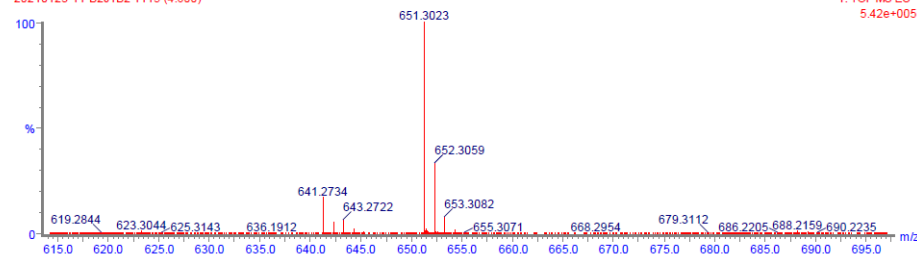


Figure S3. HRESIMS spectrum of chantriolide F (1)

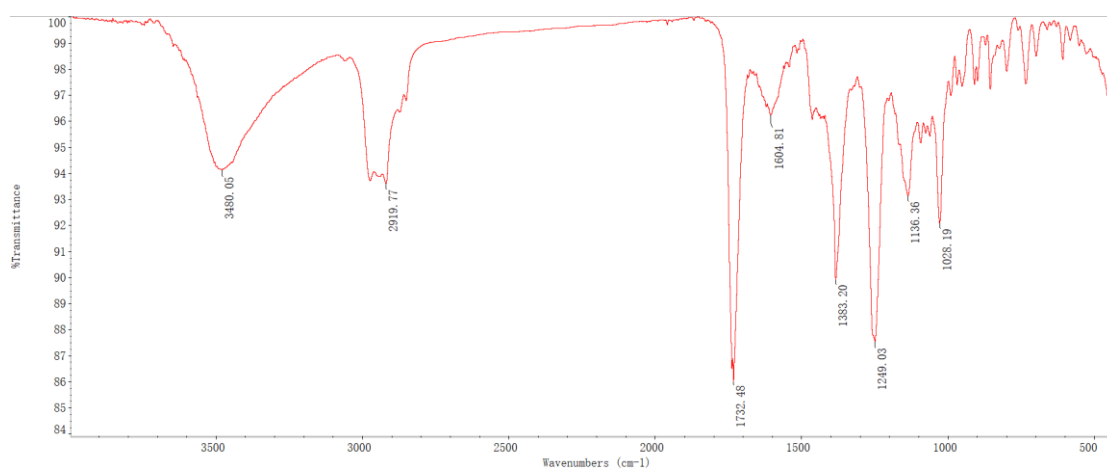


Figure S4. IR spectrum of chantriolide F (1)

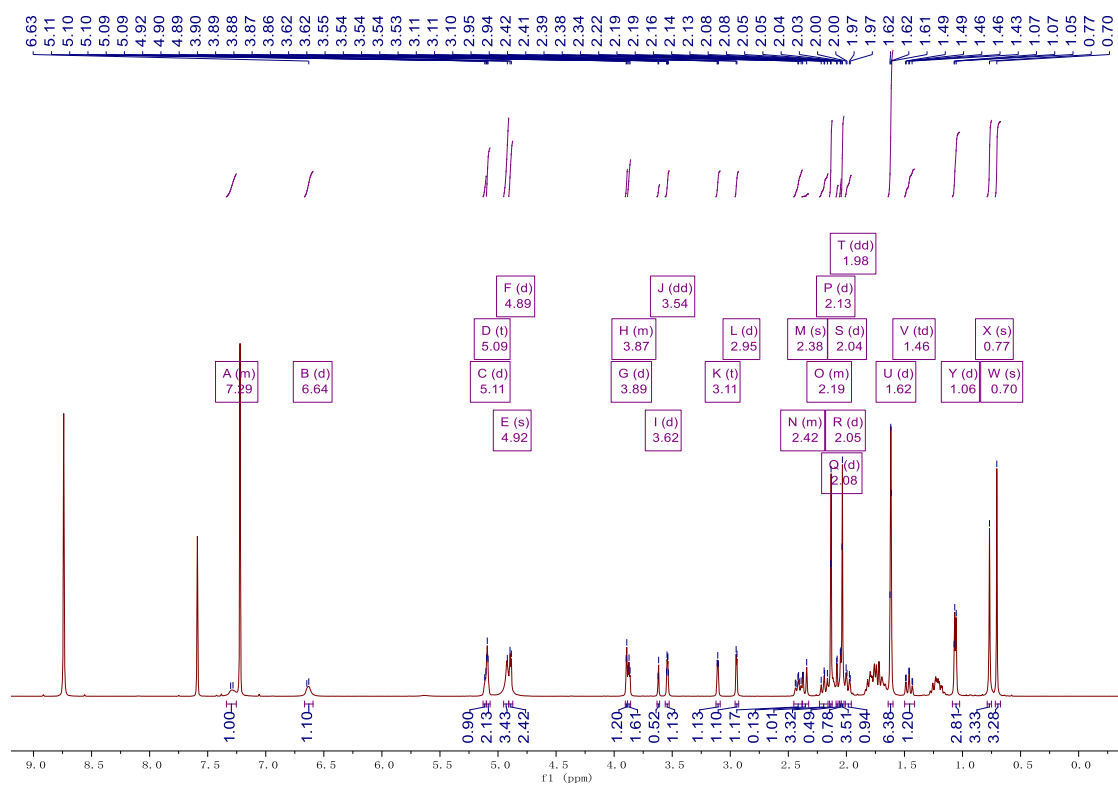


Figure S5. ^1H NMR (500 MHz) spectrum of chantriolide F (1) in $\text{C}_5\text{D}_5\text{N}$

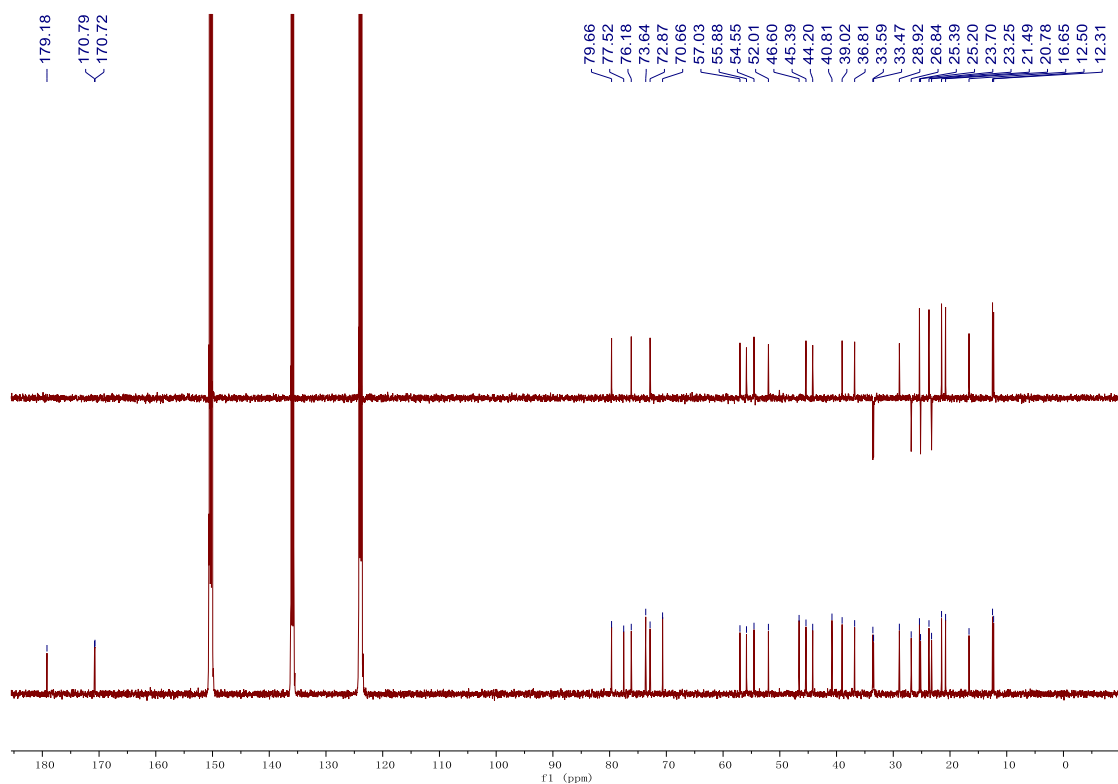


Figure S6. ^{13}C and DEPT-135 NMR (125 MHz) spectra of chantriolide F (1) in $\text{C}_5\text{D}_5\text{N}$

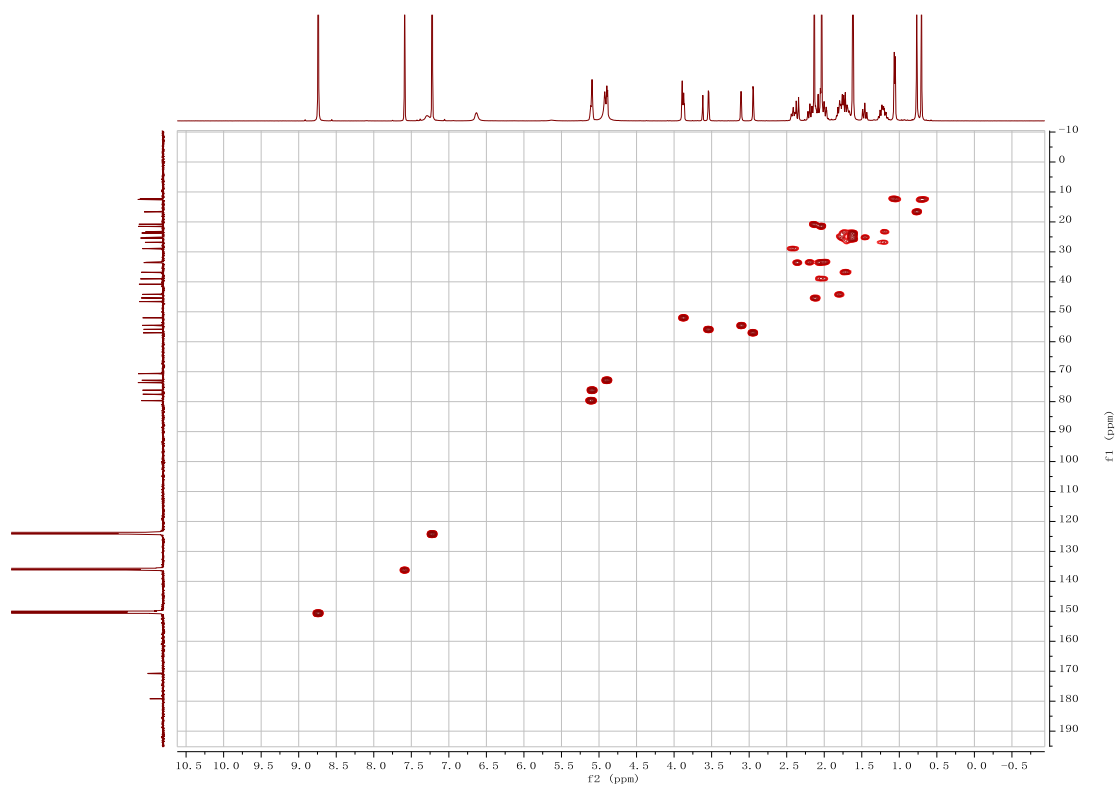


Figure S7. HSQC spectrum of chantriolide F (**1**) in C_5D_5N

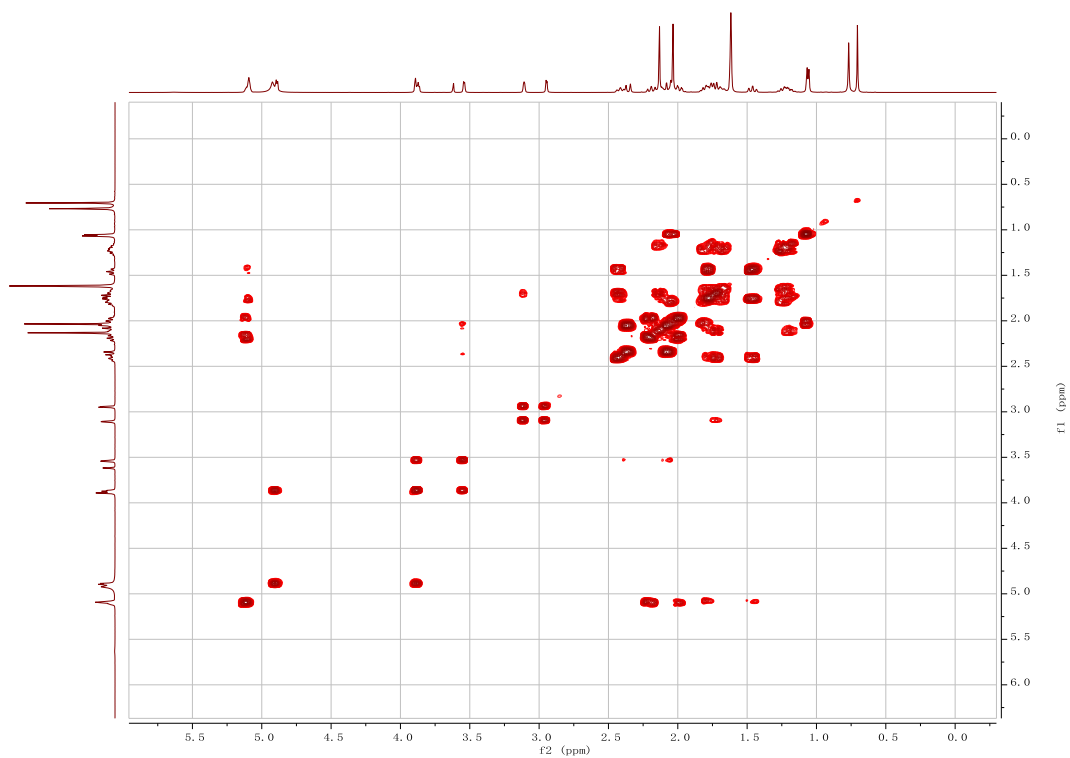


Figure S8. 1H - 1H COSY spectrum of chantriolide F (**1**) in C_5D_5N

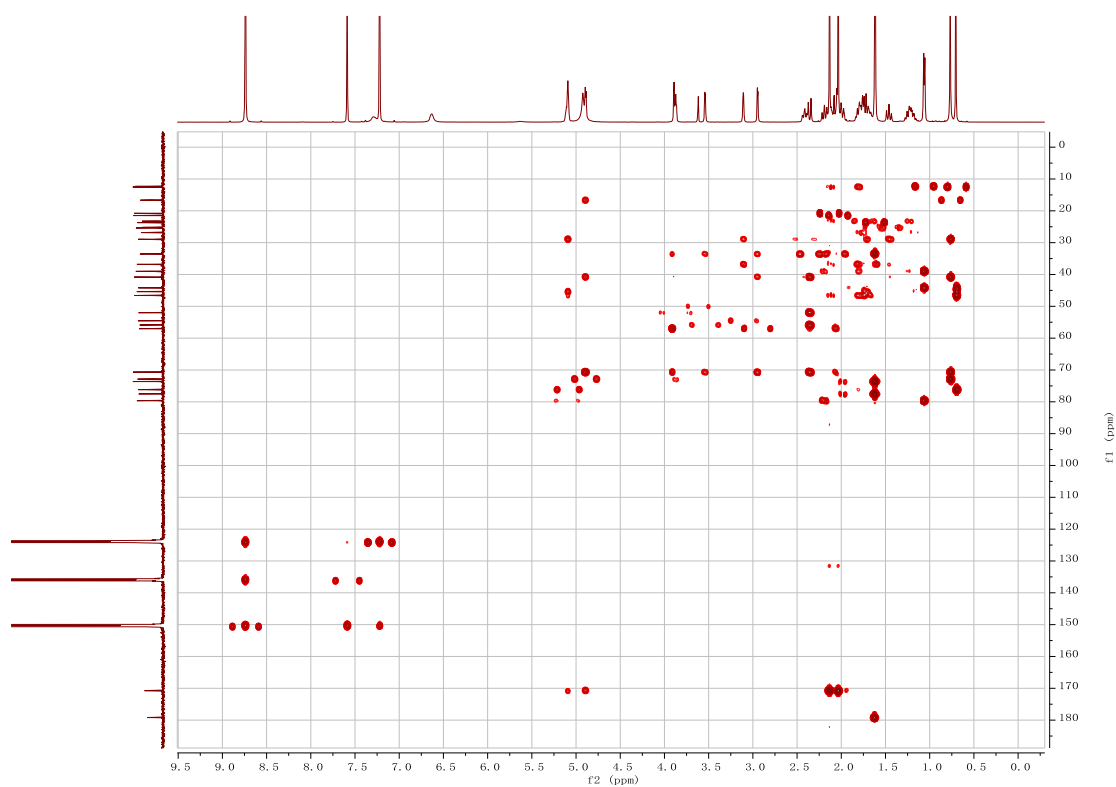


Figure S9. HMBC spectrum of chantriolide F (**1**) in C₅D₅N

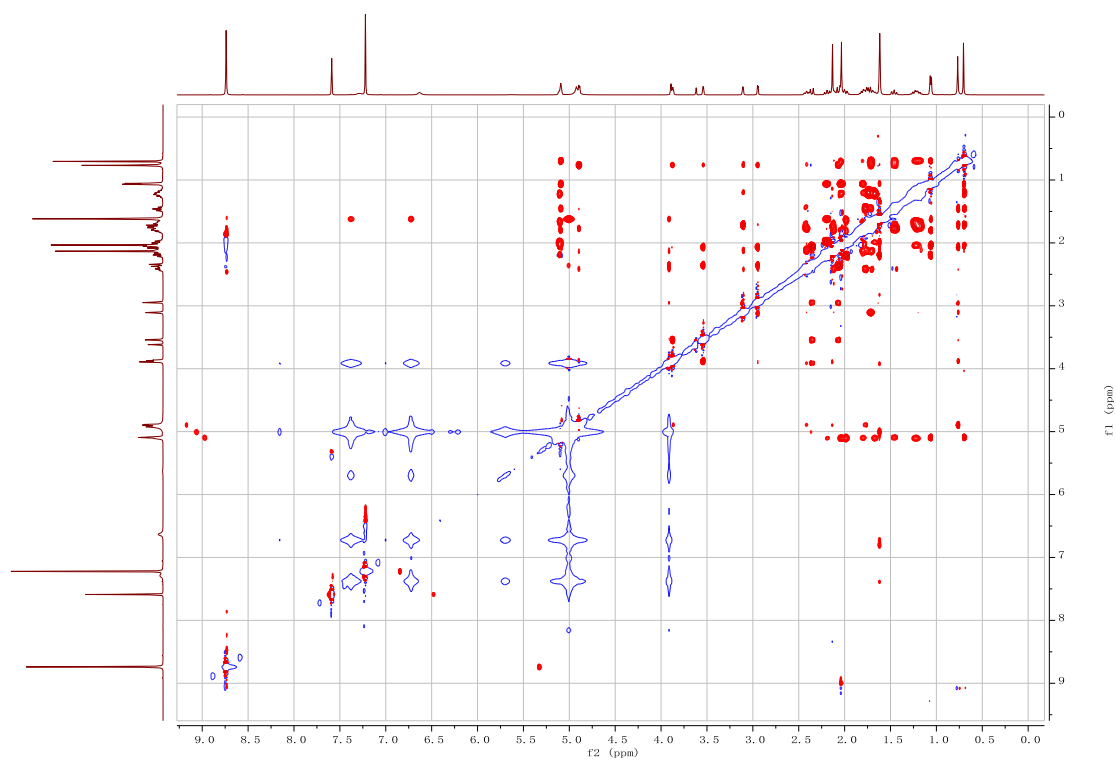


Figure S10. NOESY spectrum of chantriolide F (**1**) in C₅D₅N

Elemental Composition Report

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

104 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-34 H: 0-200 O: 0-30

Minimum:

Maximum:

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
587.2865	100.00	587.2856	0.9	1.5	11.5	518.4	n/a	n/a	C32 H43 O10

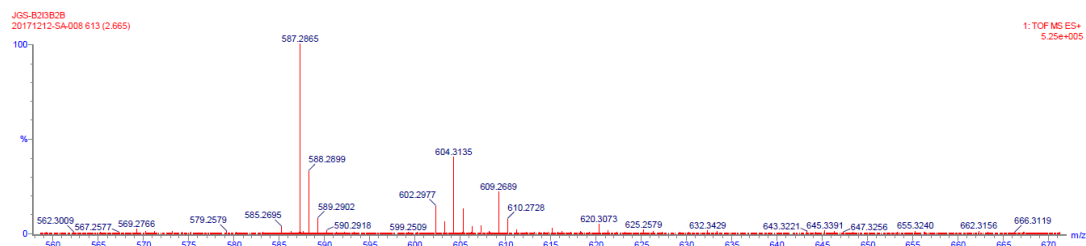


Figure S11. HRESIMS spectrum of chantriolide G (2)

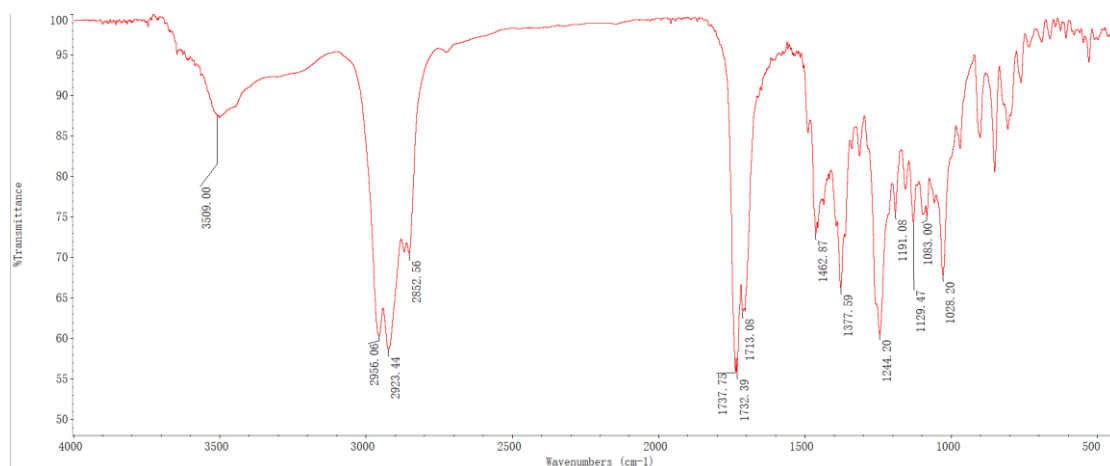


Figure S12. IR spectrum of chantriolide G (2)

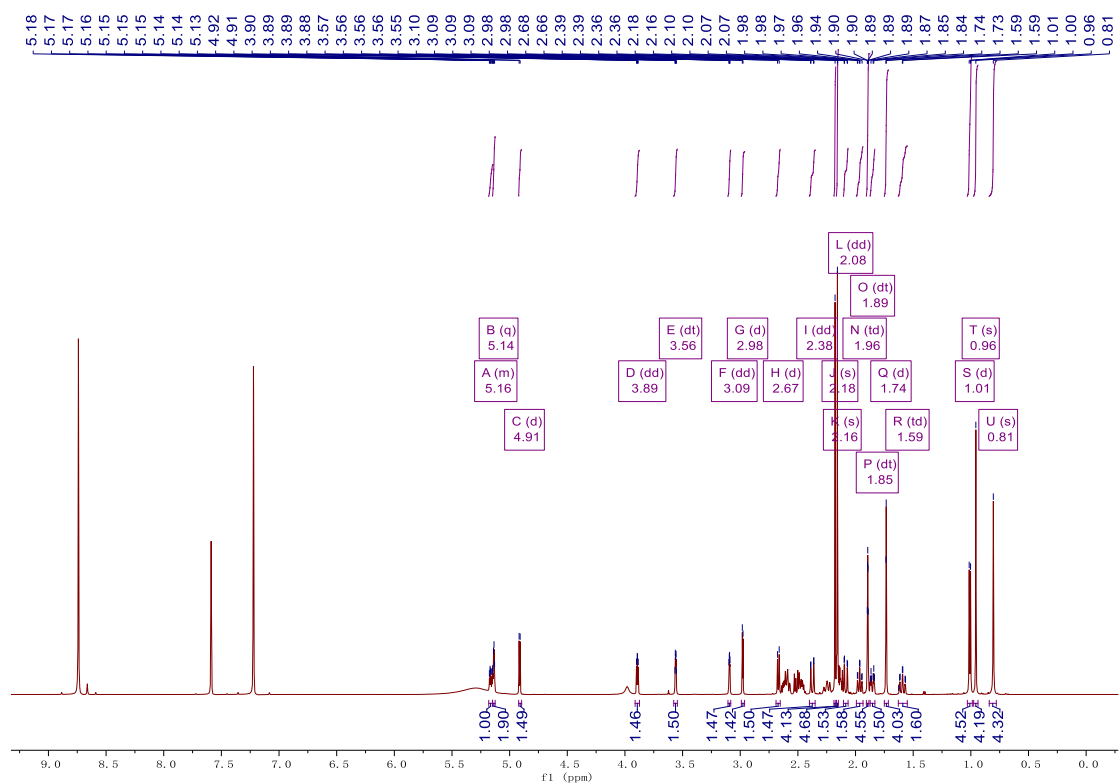


Figure S13. ^1H NMR (600 MHz) spectrum of chantriolide G (2) in $\text{C}_5\text{D}_5\text{N}$

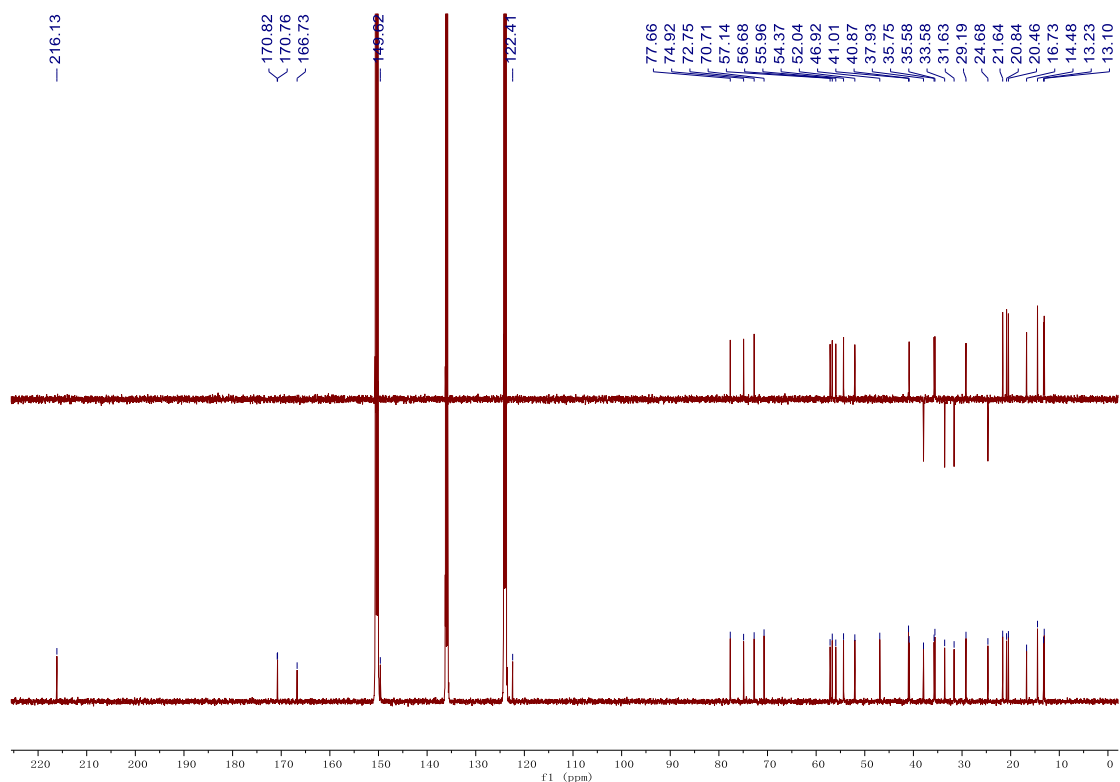


Figure S14. ^{13}C and DEPT-135 NMR (125 MHz) spectra of chantriolide G (2) in $\text{C}_5\text{D}_5\text{N}$

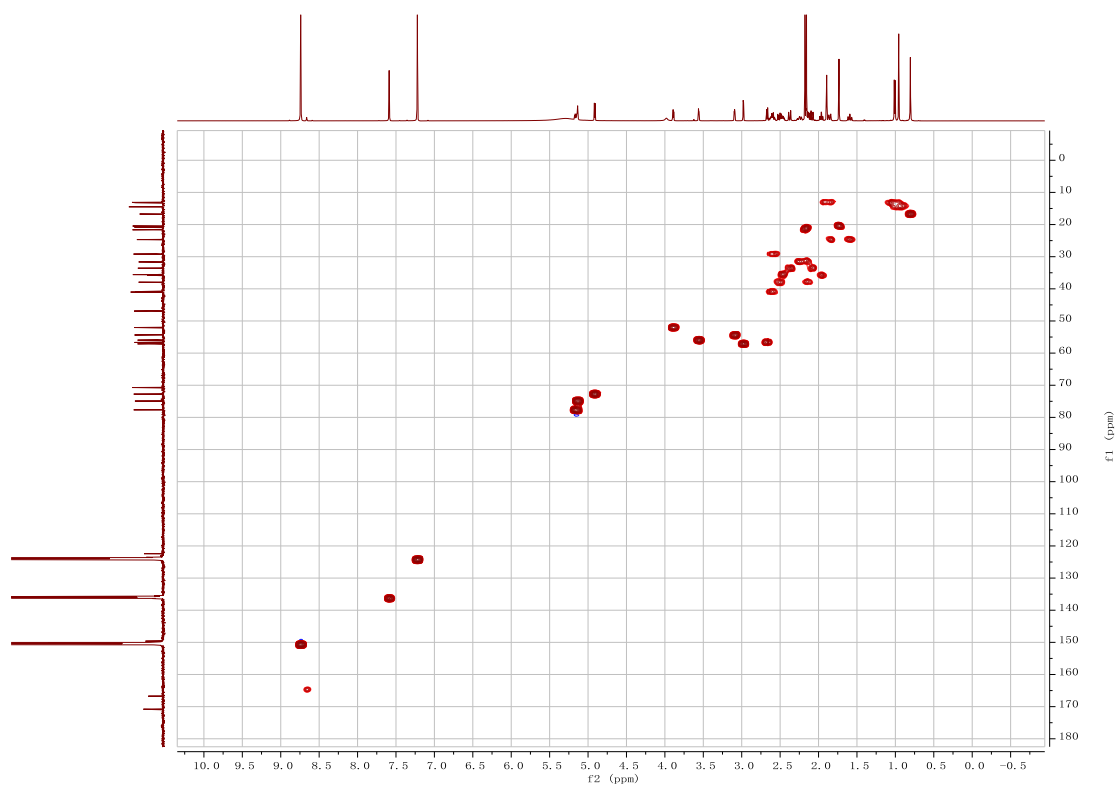


Figure S15. HSQC spectrum of chantriolide G (**2**) in C_5D_5N

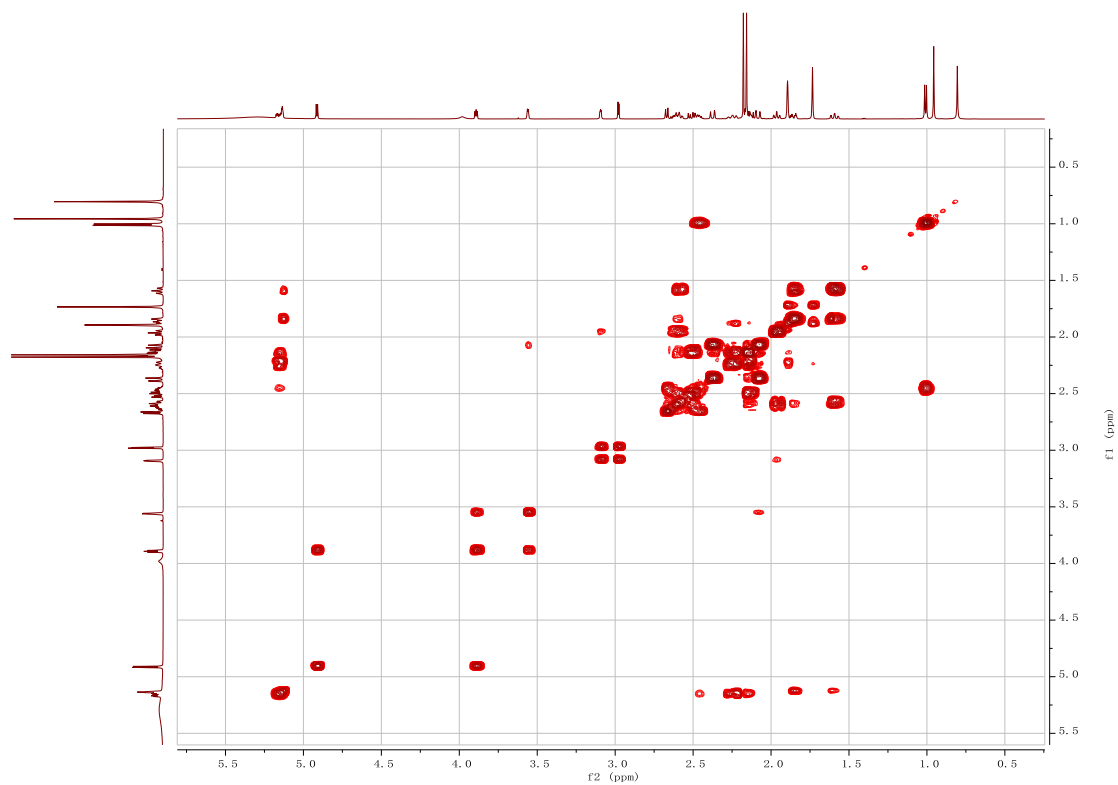


Figure S16. 1H - 1H COSY spectrum of chantriolide G (**2**) in C_5D_5N

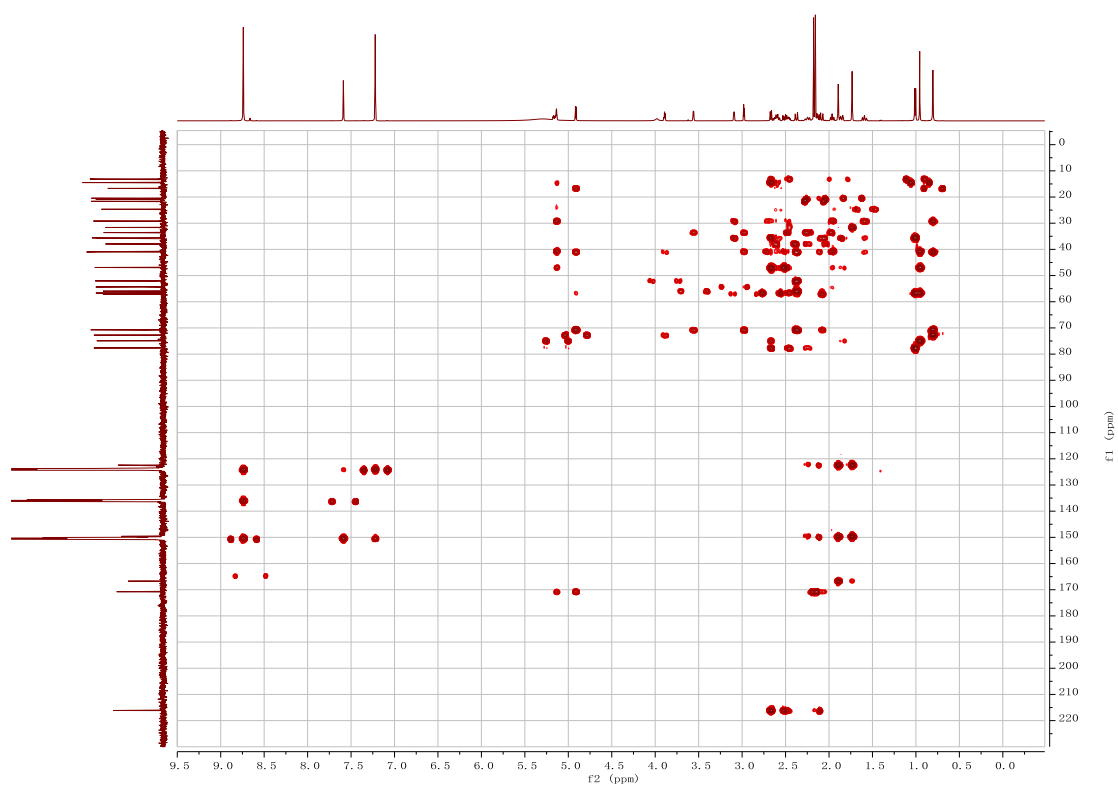


Figure S17. HMBC spectrum of chantriolide G (**2**) in C₅D₅N

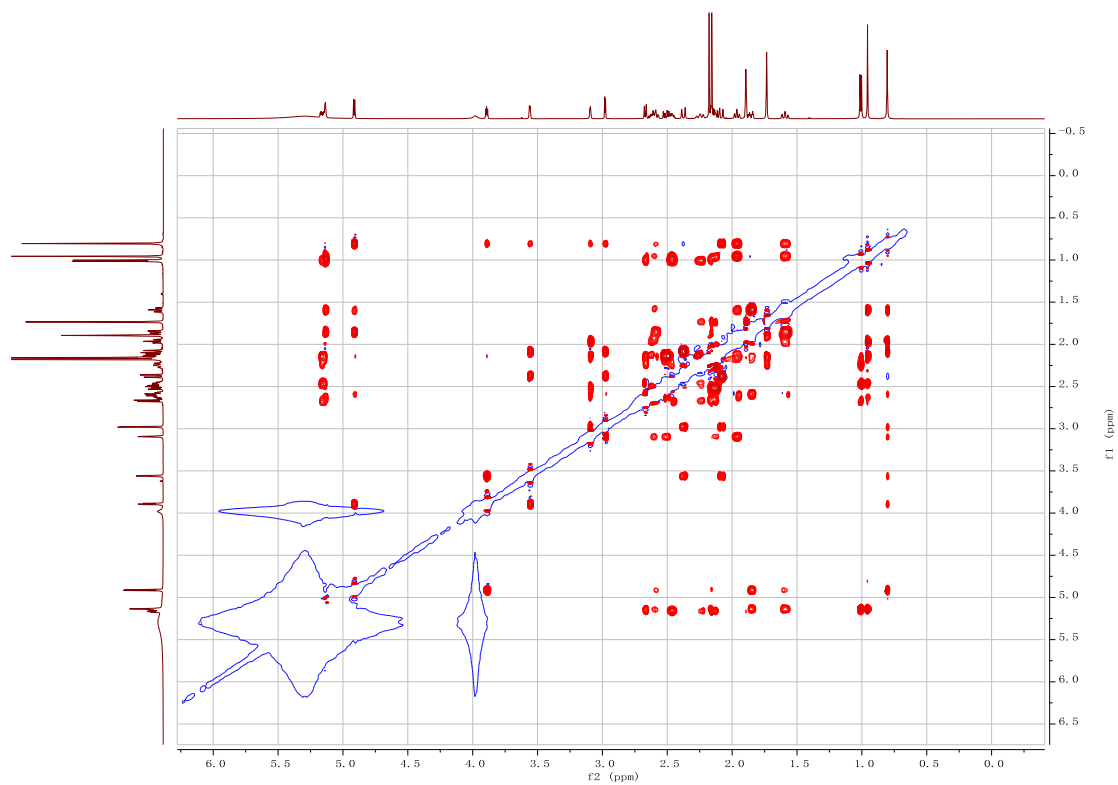


Figure S18. NOESY spectrum of chantriolide G (**2**) in C₅D₅N

Elemental Composition Report

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

105 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-34 H: 0-200 O: 0-30

Minimum: 80.00 -1.5

Maximum: 100.00 5.0 5.0 50.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
547.2914	100.00	547.2907	0.7	1.3	9.5	525.0	n/a	n/a	C30 H43 O9

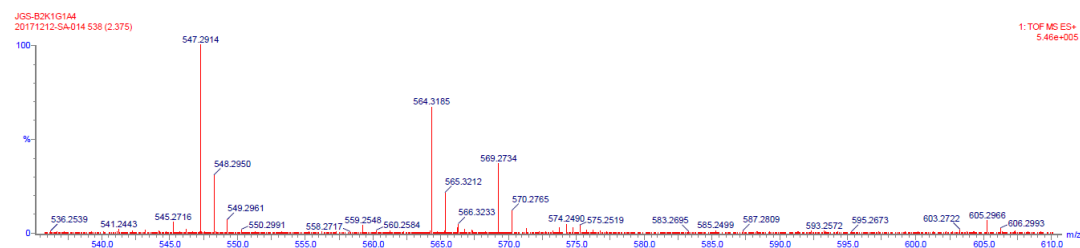


Figure S19. HRESIMS spectrum of chantriolide H (3)

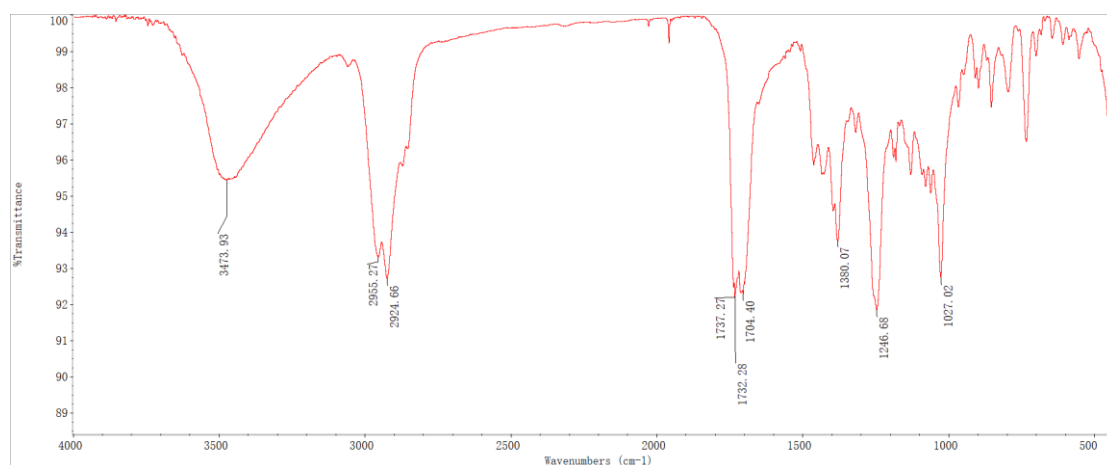


Figure S20. IR spectrum of chantriolide H (3)

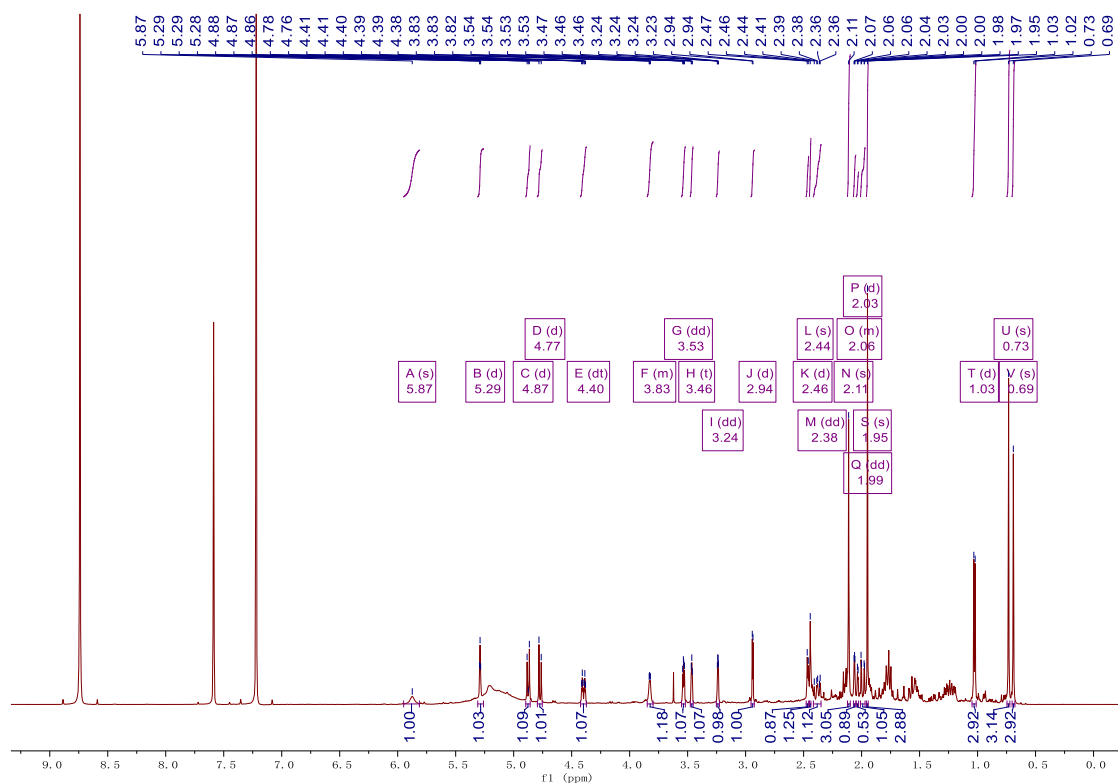


Figure S21. ^1H NMR (600 MHz) spectrum of chantrolide H (**3**) in $\text{C}_5\text{D}_5\text{N}$

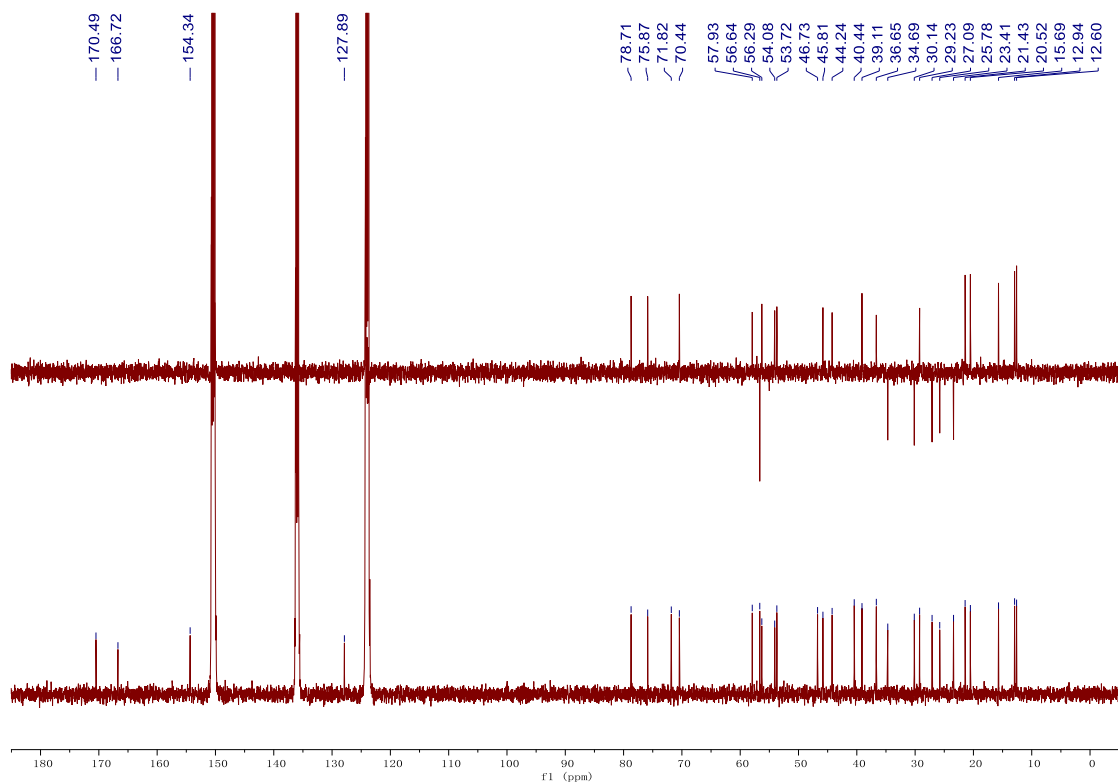


Figure S22. ^{13}C and DEPT-135 NMR (125 MHz) spectra of chantrolide H (**3**) in $\text{C}_5\text{D}_5\text{N}$

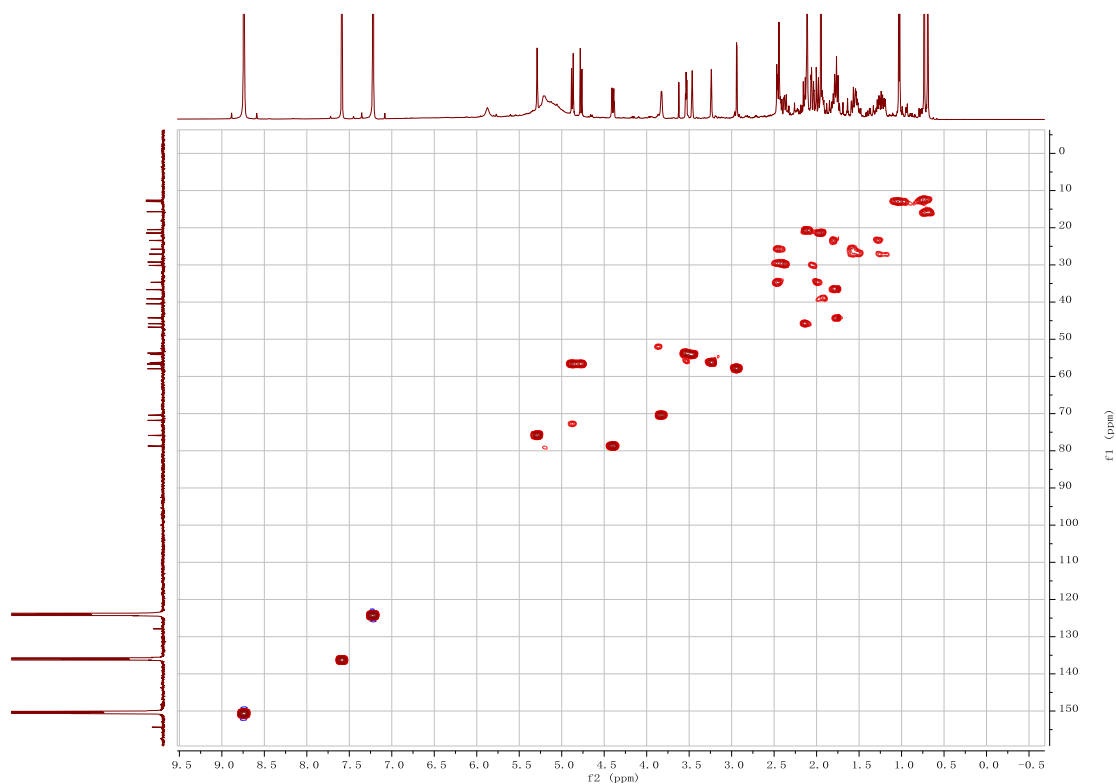


Figure S23. HSQC spectrum of chantriolide H (**3**) in C_5D_5N

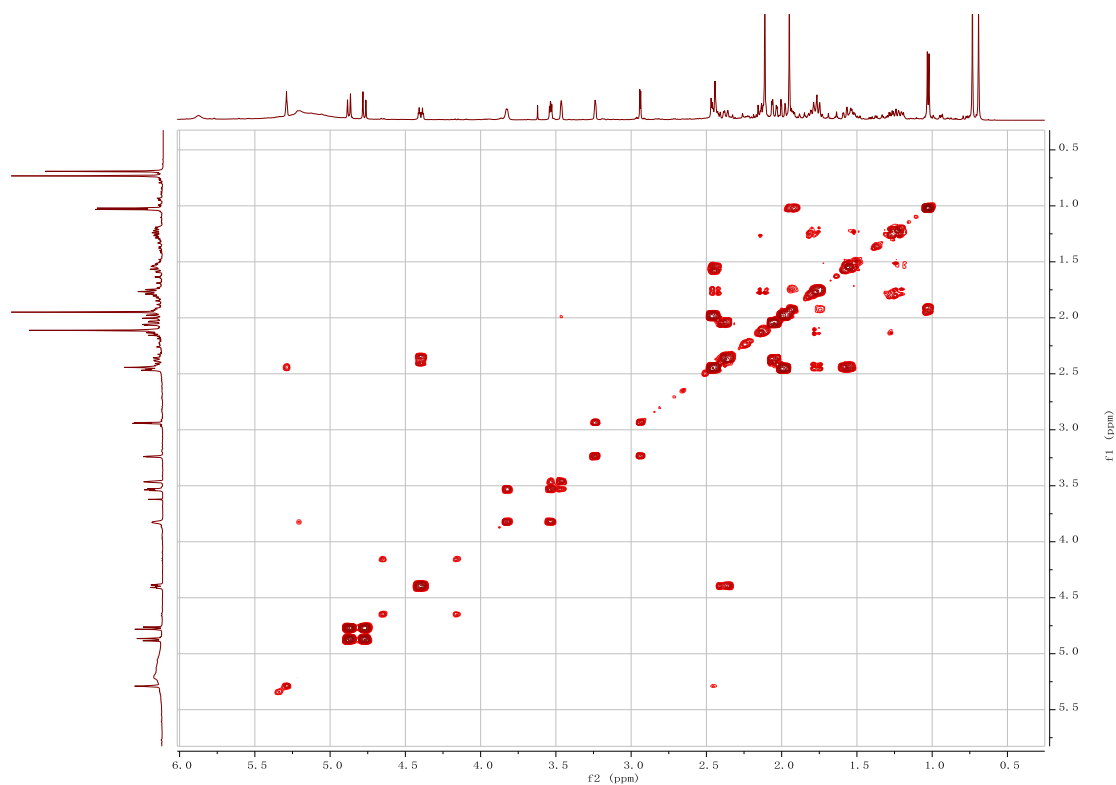


Figure S24. 1H - 1H COSY spectrum of chantriolide H (**3**) in C_5D_5N

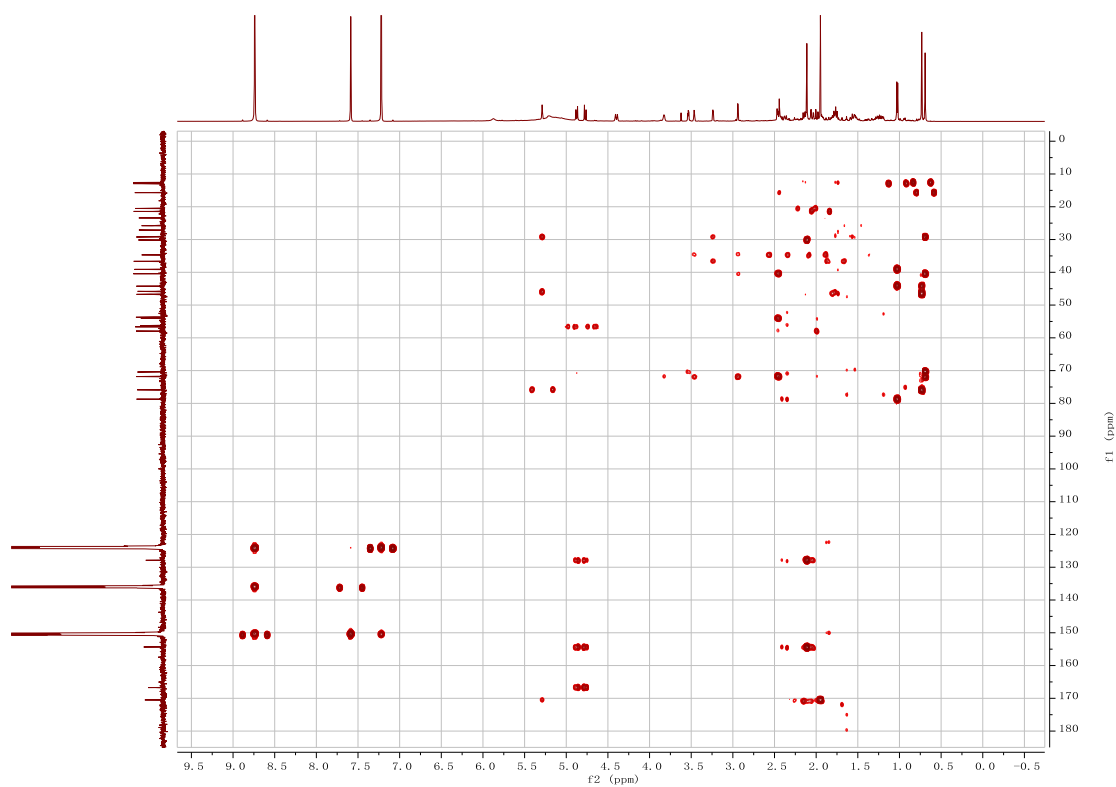


Figure S25. HMBC spectrum of chantriolide H (**3**) in C_5D_5N

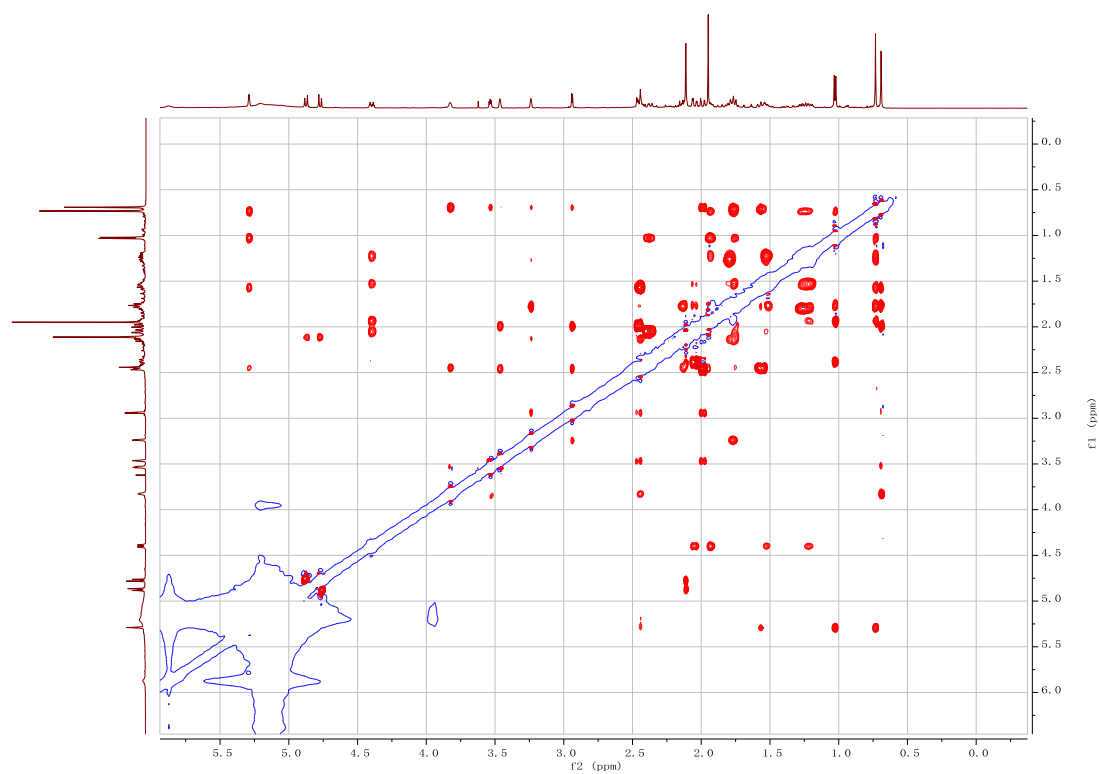


Figure S26. NOESY spectrum of chantriolide H (**3**) in C_5D_5N

Elemental Composition Report

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

196 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-34 H: 0-200 N: 0-1 O: 0-30

Minimum: 80.00 -1.5

Maximum: 100.00 5.0 5.0 50.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
622.3237	100.00	622.3227	1.0	1.6	9.5	475.6	n/a	n/a	C32 H48 N O11

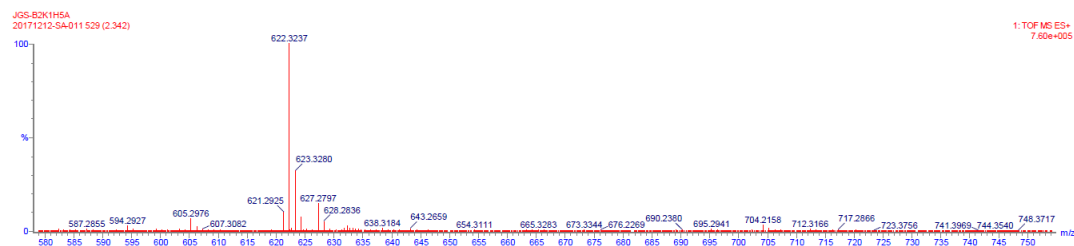


Figure S27. HRESIMS spectrum of chantriolide I (4)

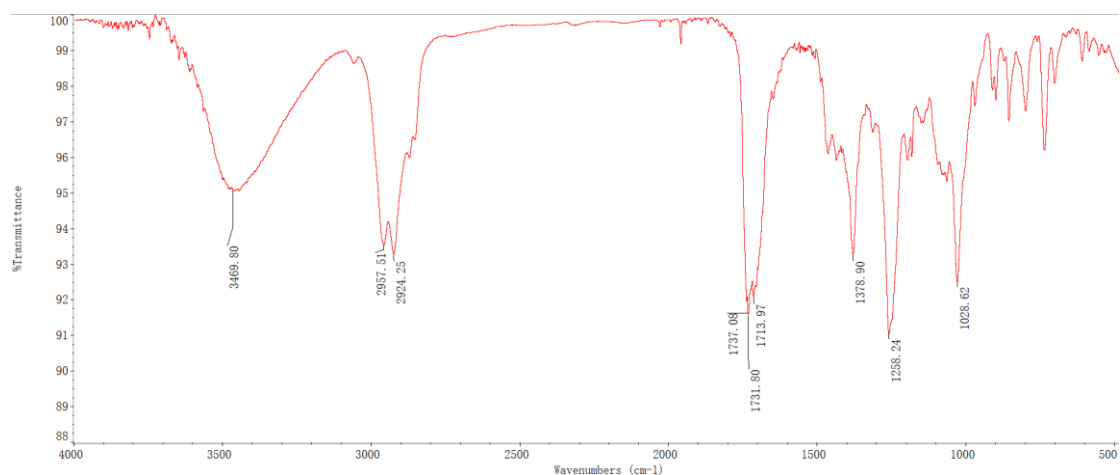


Figure S28. IR spectrum of chantriolide I (4)

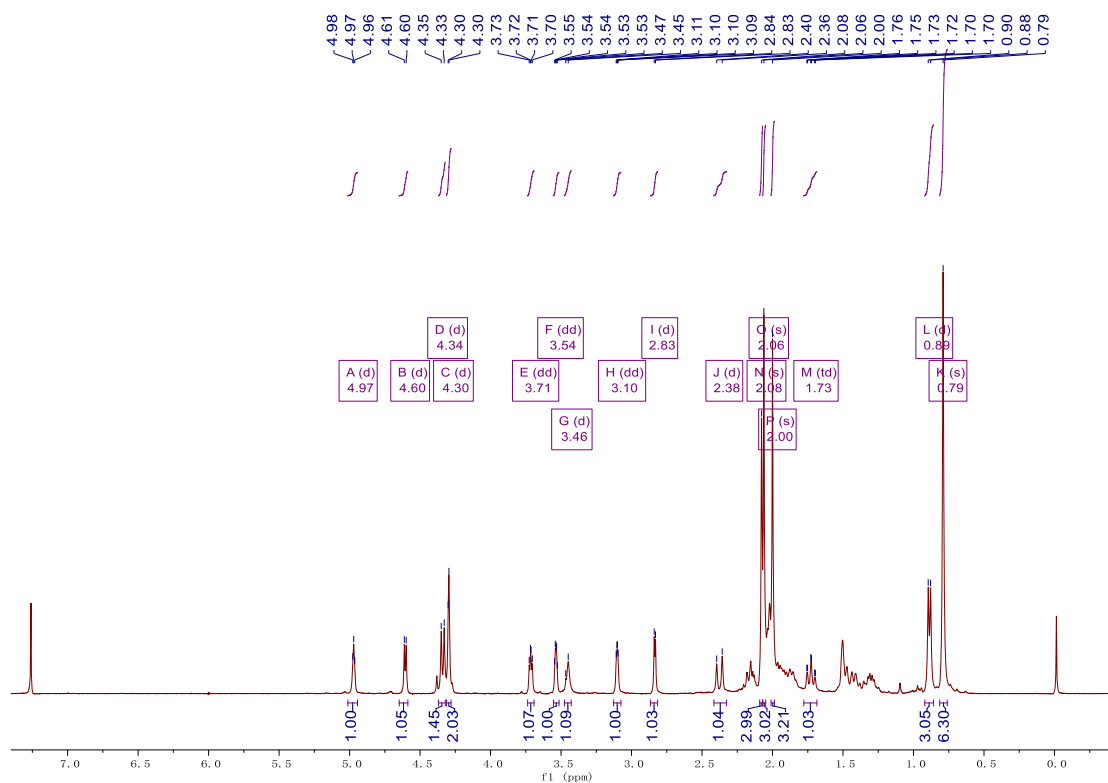


Figure S29. ¹H NMR (400 MHz) spectrum of chantriolide I (**4**) in CDCl₃

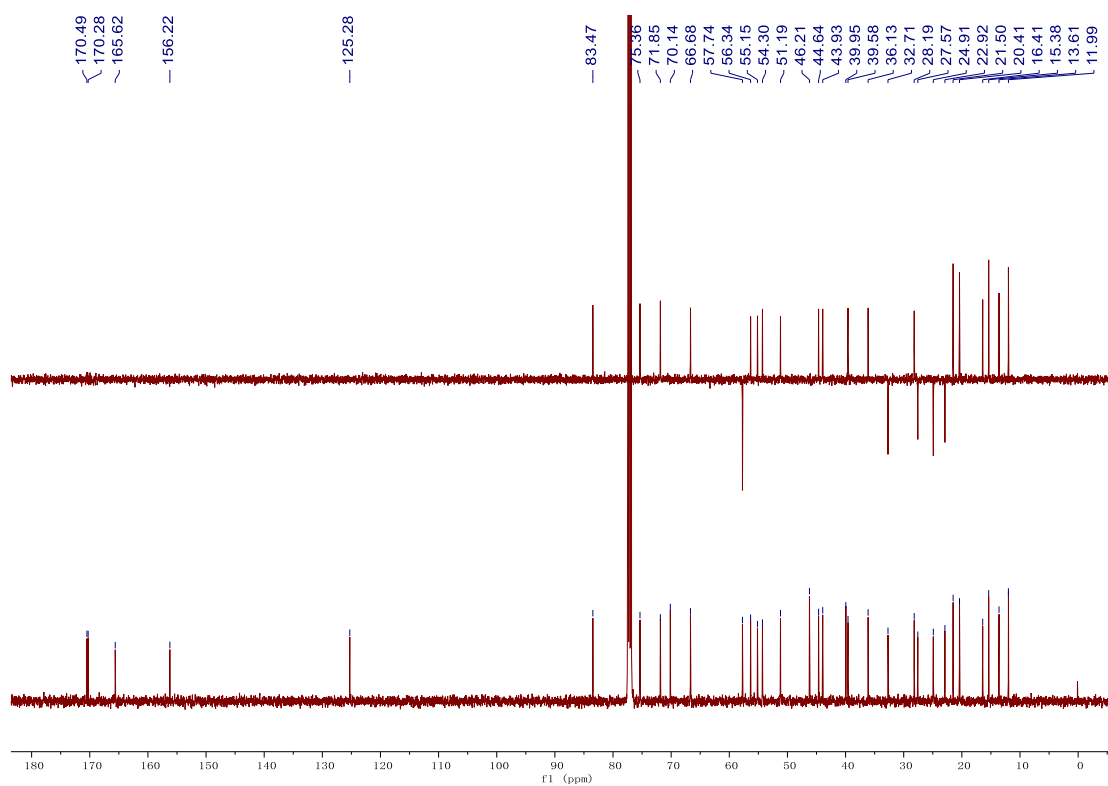


Figure S30. ¹³C and DEPT-135 NMR (125 MHz) spectra of chantriolide I (**4**) in CDCl₃

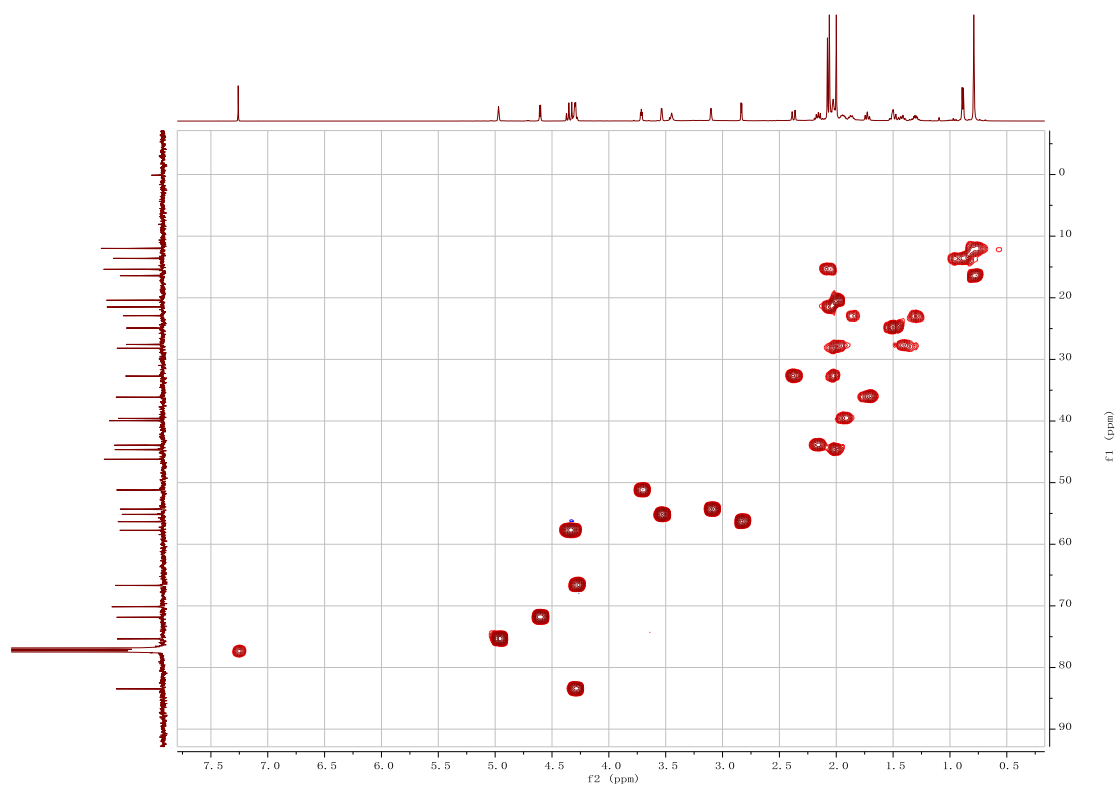


Figure S31. HSQC spectrum of chantriolide I (**4**) in CDCl_3

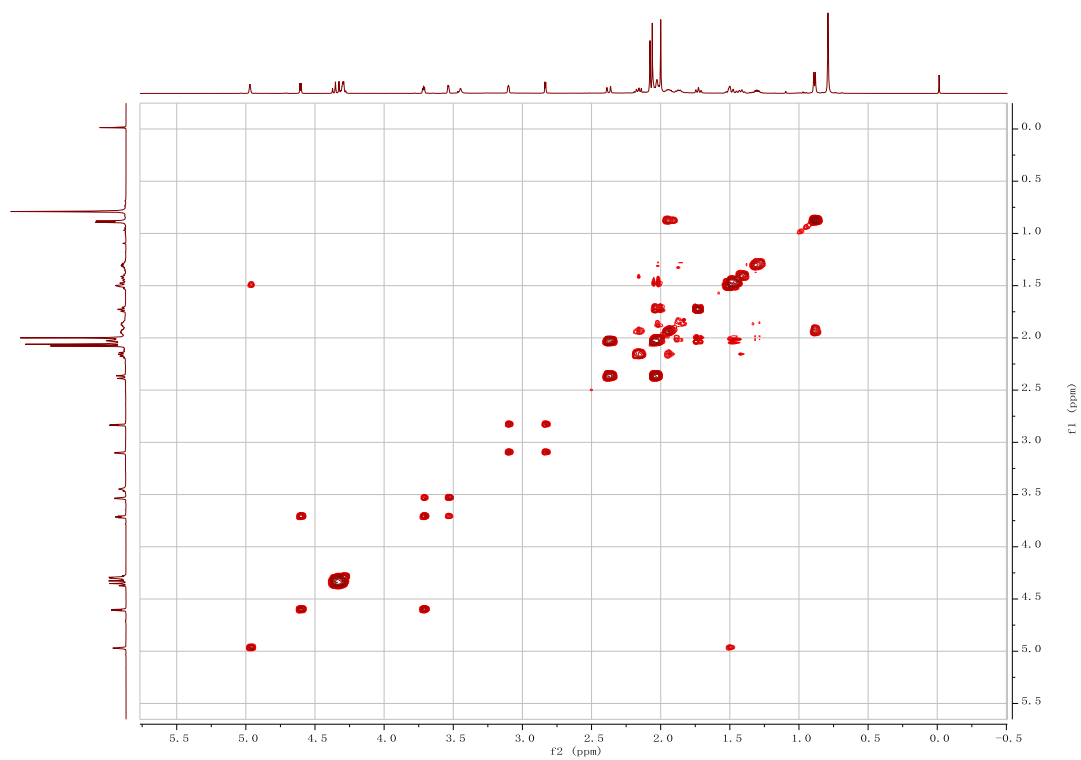


Figure S32. ^1H - ^1H COSY spectrum of chantriolide I (**4**) in CDCl_3

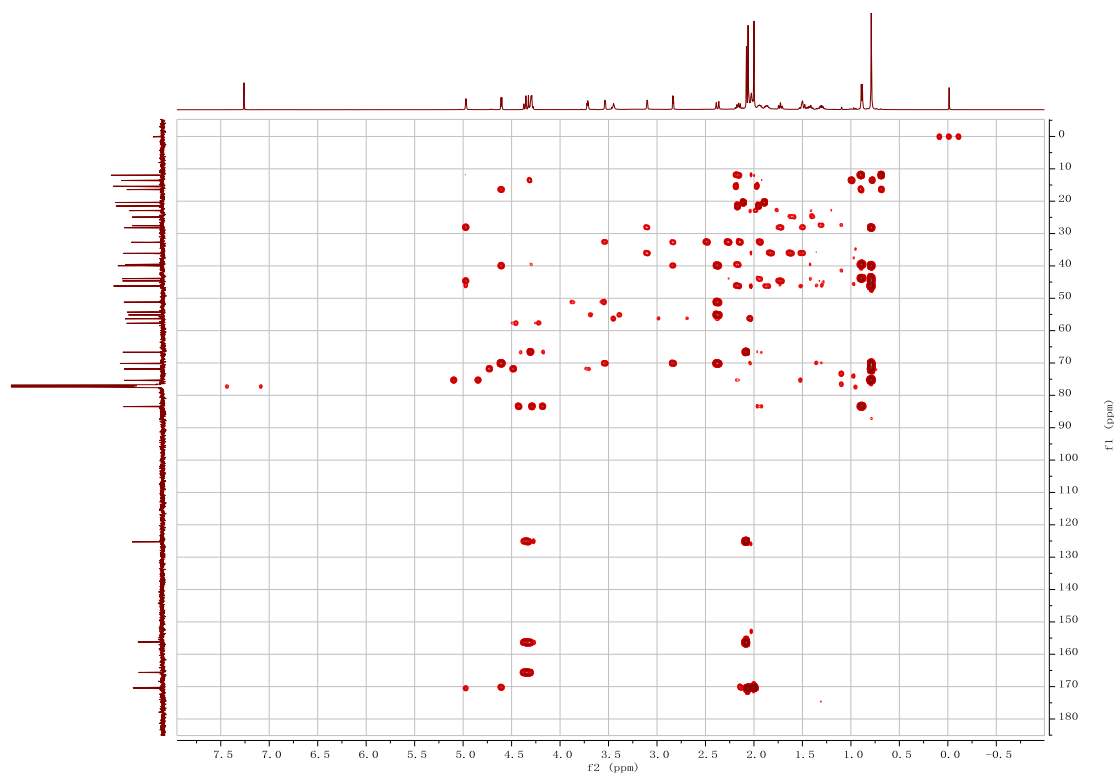


Figure S33. HMBC spectrum of chantriolide I (**4**) in CDCl_3

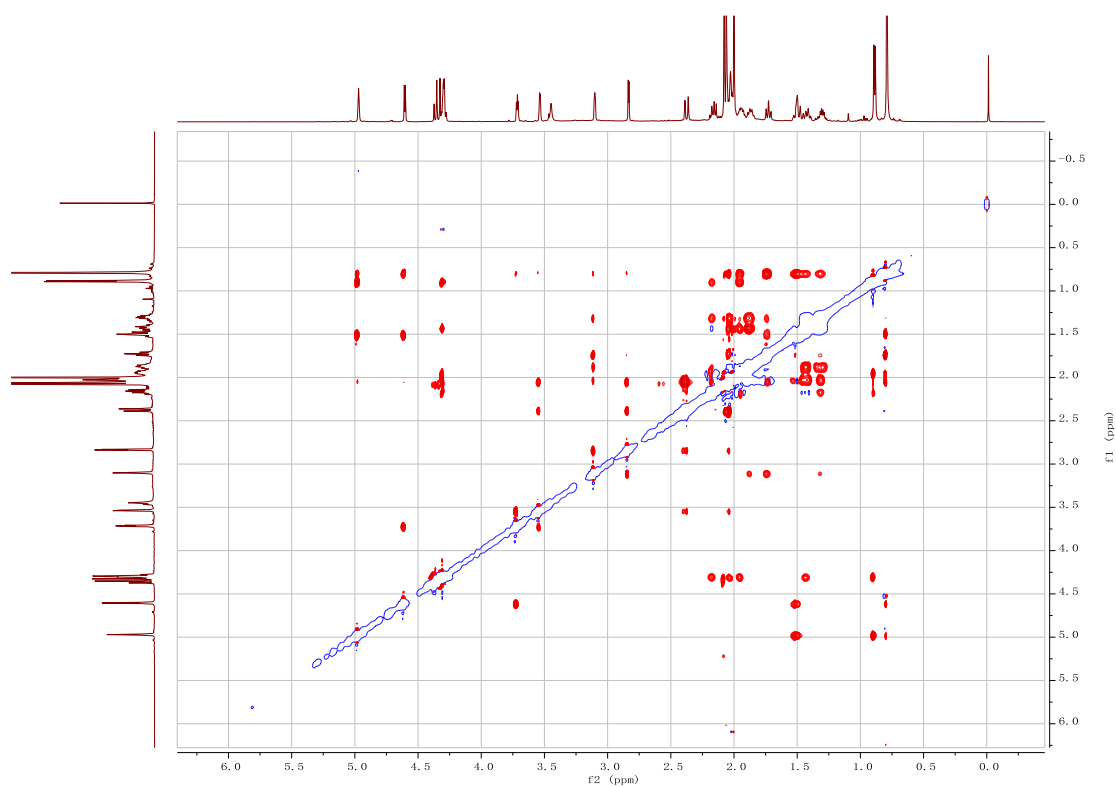


Figure S34. ROESY spectrum of chantriolide I (**4**) in CDCl_3

Elemental Composition Report

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

161 formula(e) evaluated with 3 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

C: 30-50 H: 0-60 O: 0-20 Cl: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
669.2689	669.2678	1.1	1.6	10.5	625.5	0.000	100.00	C33 H46 O12 Cl

JGS-B3B5E1

20210123-YY-B3B5E1 1414 (5.759)

1: TOF MS ES-
4.92e+005

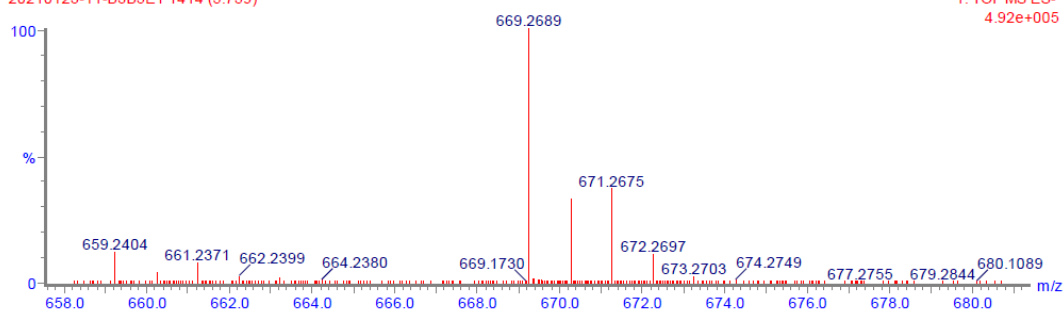


Figure S35. HRESIMS spectrum of chantriolide J (5)

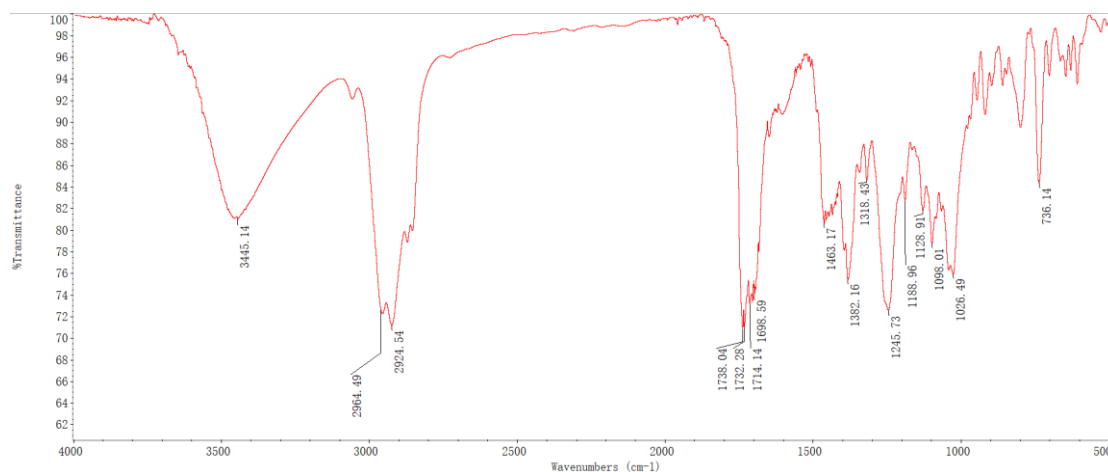


Figure S36. IR spectrum of chantriolide J (5)

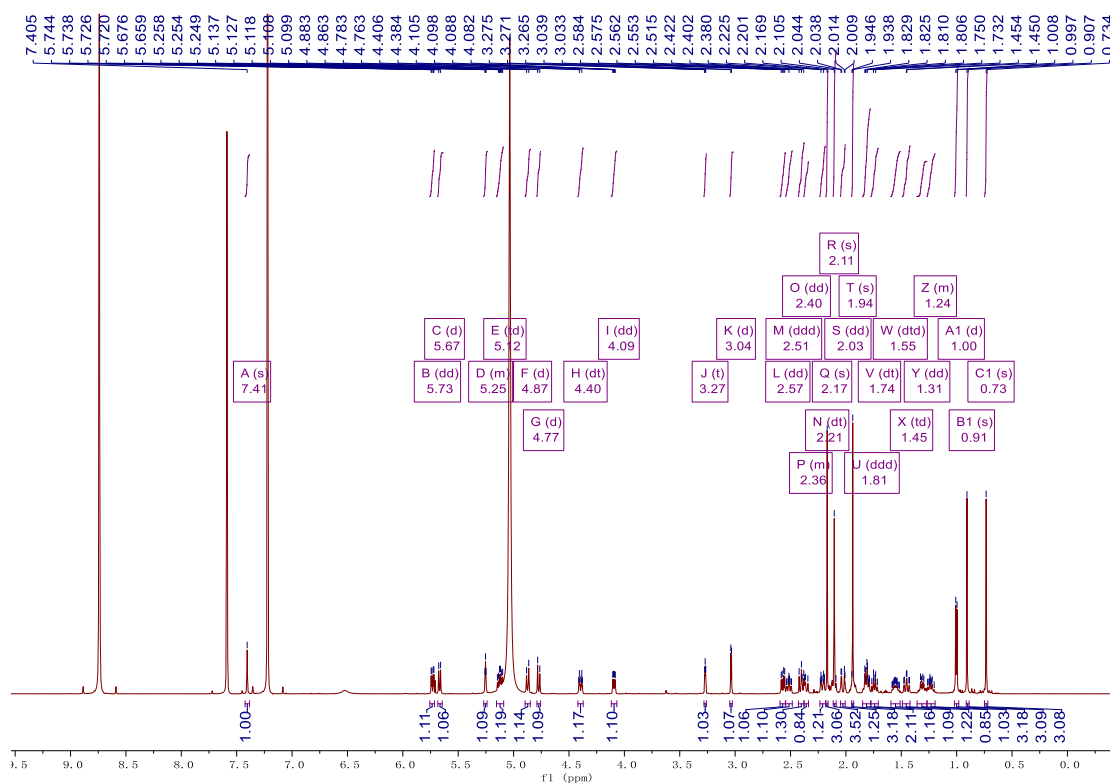


Figure S37. ¹H NMR (600 MHz) spectrum of chantriolide J (**5**) in C₅D₅N

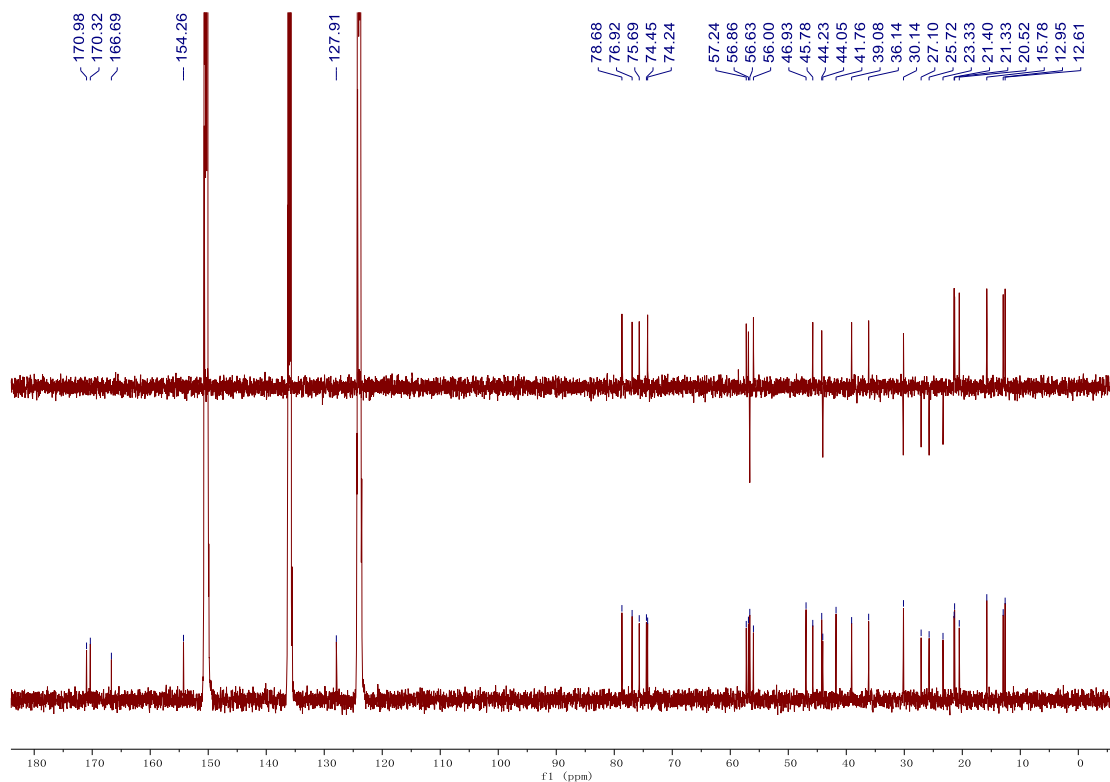


Figure S38. ¹³C and DEPT-135 NMR (125 MHz) spectra of chantriolide J (**5**) in C₅D₅N

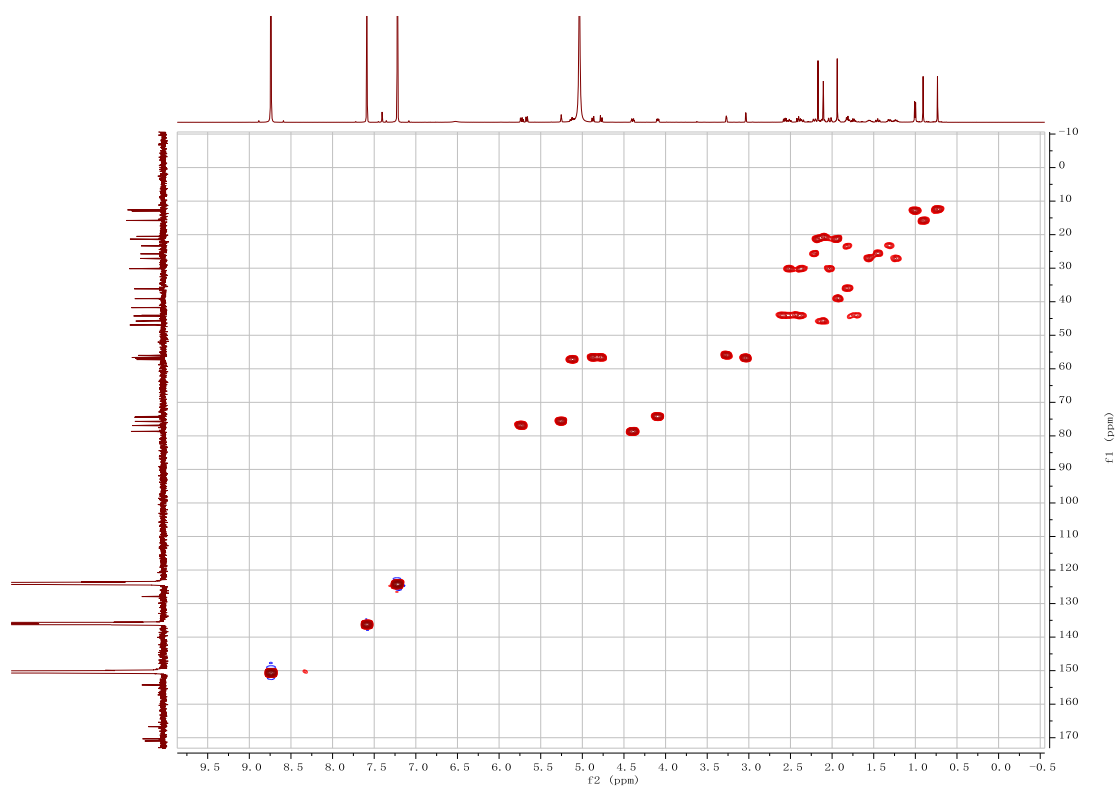


Figure S39. HSQC spectrum of chantriolide J (**5**) in C_5D_5N

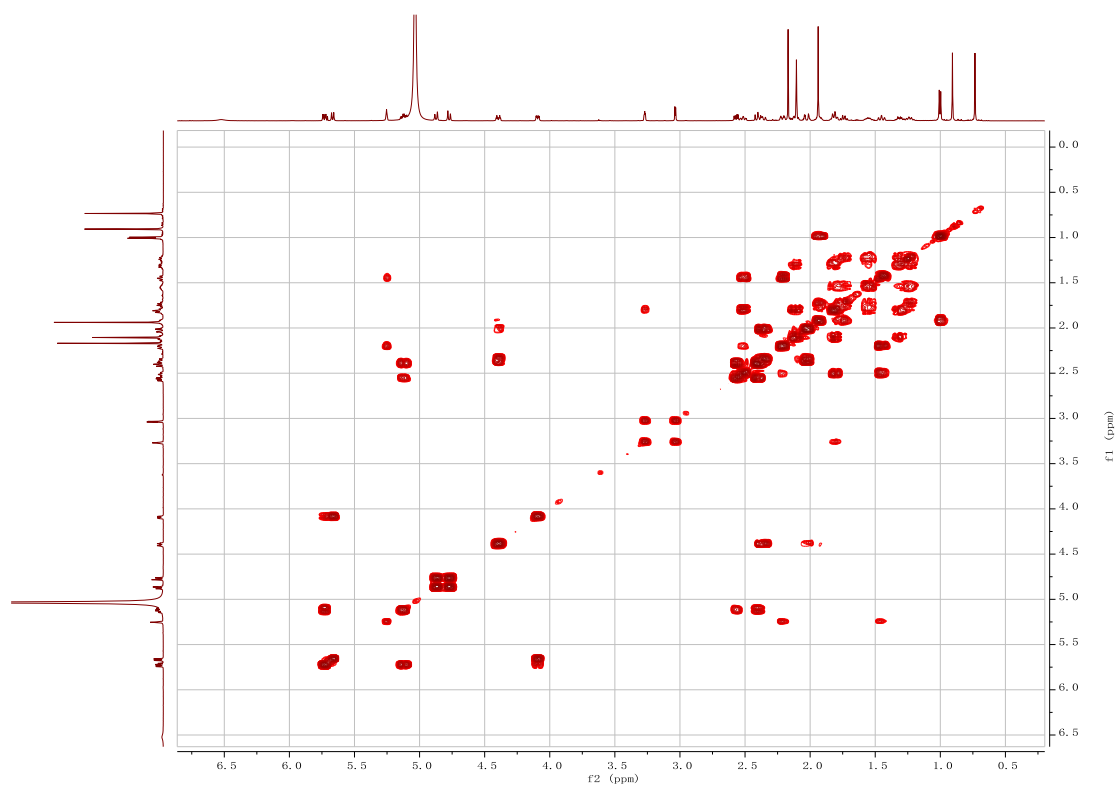


Figure S40. 1H - 1H COSY spectrum of chantriolide J (**5**) in C_5D_5N

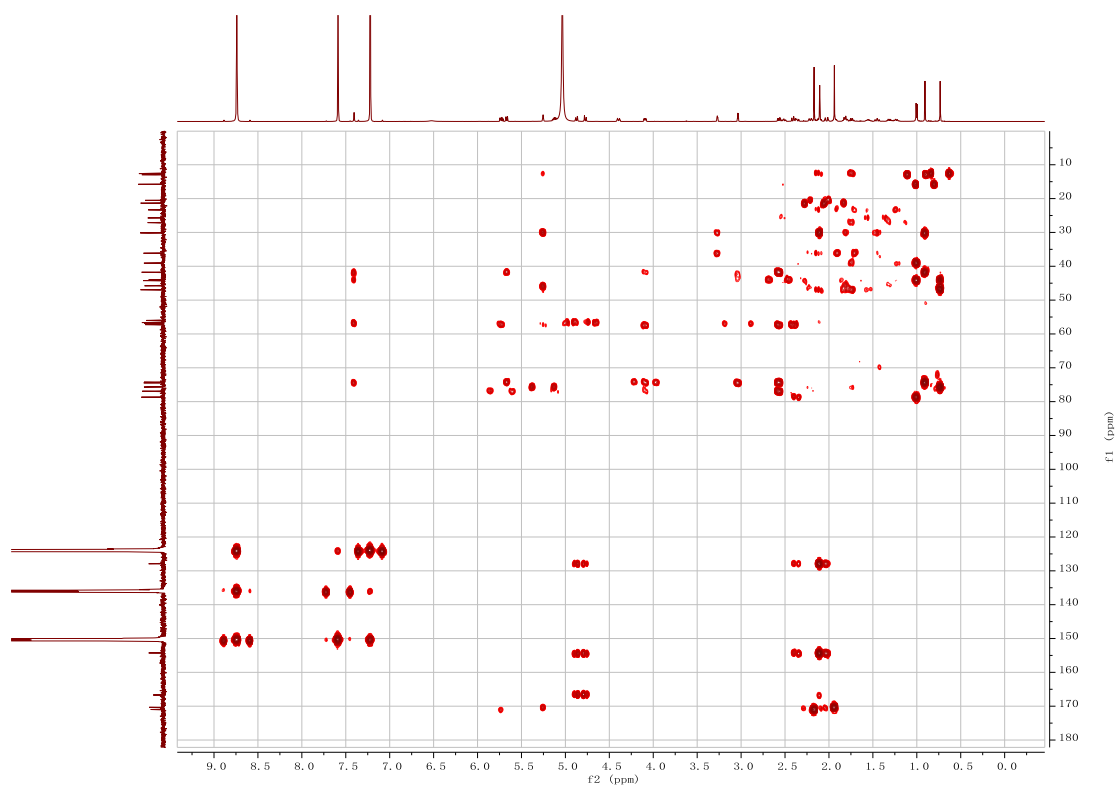


Figure S41. HMBC spectrum of chantriolide J (**5**) in C_5D_5N

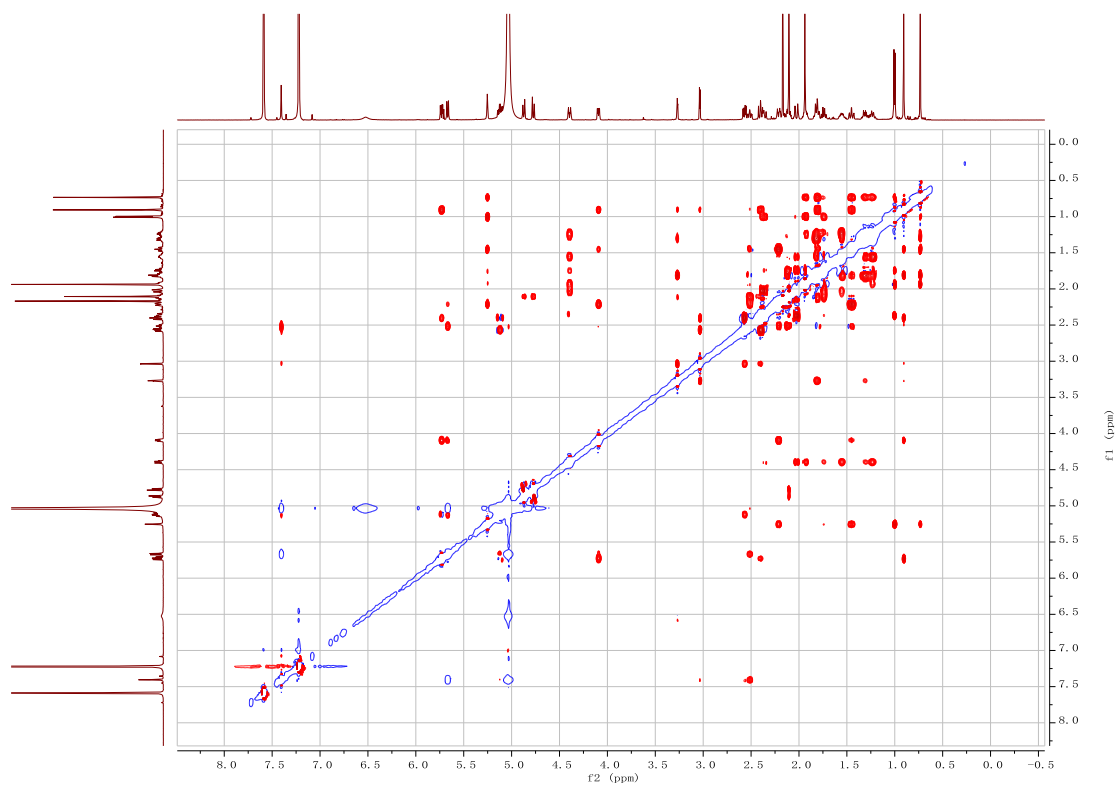


Figure S42. ROESY spectrum of chantriolide J (**5**) in C_5D_5N

Elemental Composition Report

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

1102 formula(e) evaluated with 7 results within limits (up to 10 closest results for each mass)

Elements Used:

C: 20-50 H: 0-70 N: 0-1 O: 0-15 Na: 0-1 Cl: 0-2

Minimum: -1.5

Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
641.2735	641.2729	0.6	0.9	9.5	506.2	0.471	62.42	C32 H46 O11 Cl

JGS-B2K1G1B5A

20180205-SA-TOF-026 690 (2.959)

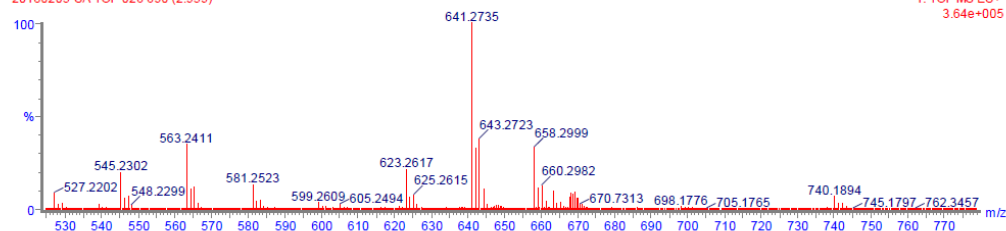


Figure S43. HRESIMS spectrum of chantriolide K (6)

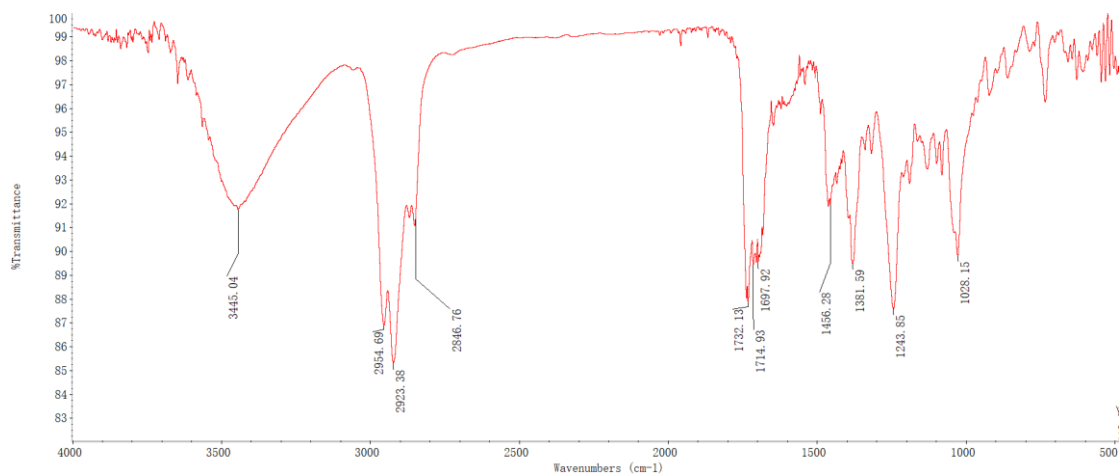


Figure S44. IR spectrum of chantriolide K (6)

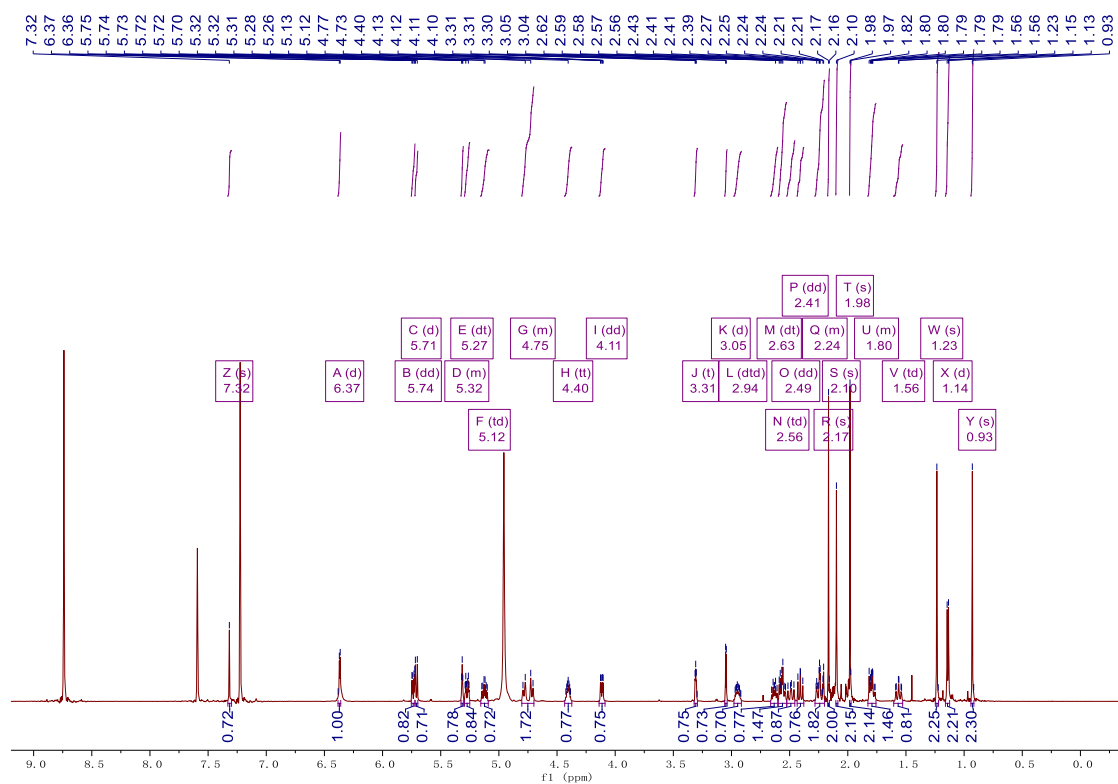


Figure S45. ^1H NMR (600 MHz) spectrum of chantriolide K (6) in $\text{C}_5\text{D}_5\text{N}$

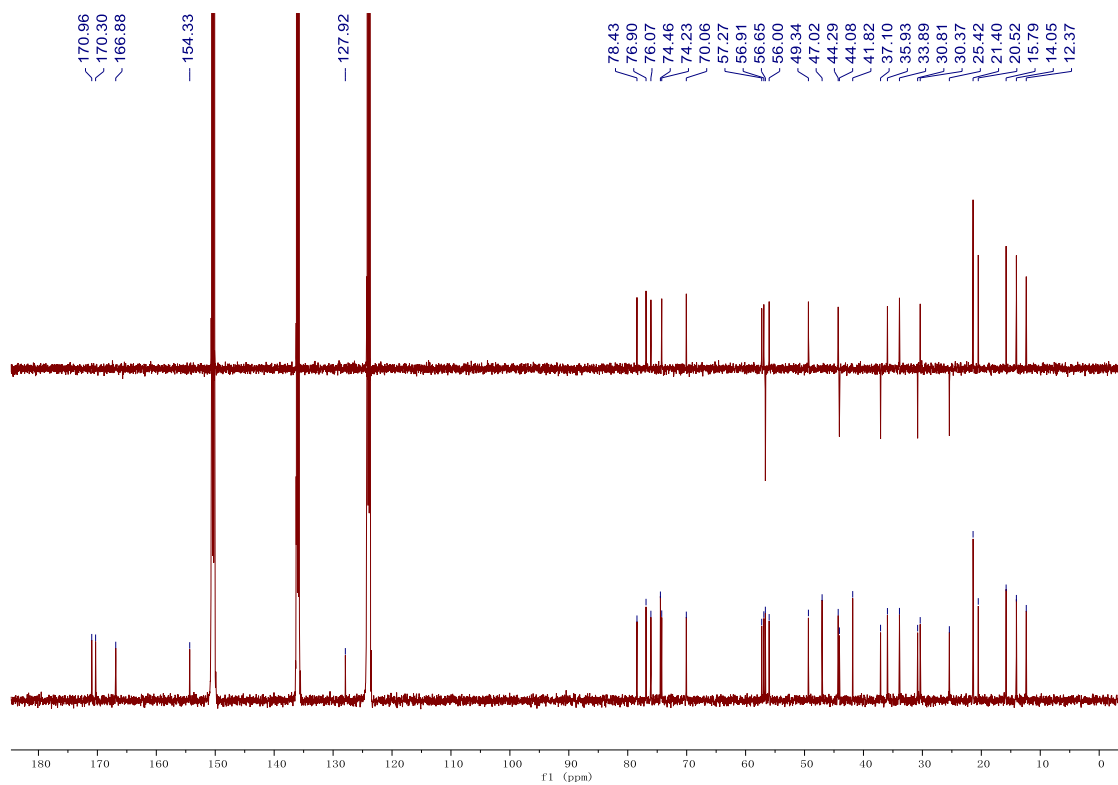


Figure S46. ^{13}C and DEPT-135 NMR (125 MHz) spectra of chantriolide K (6) in $\text{C}_5\text{D}_5\text{N}$

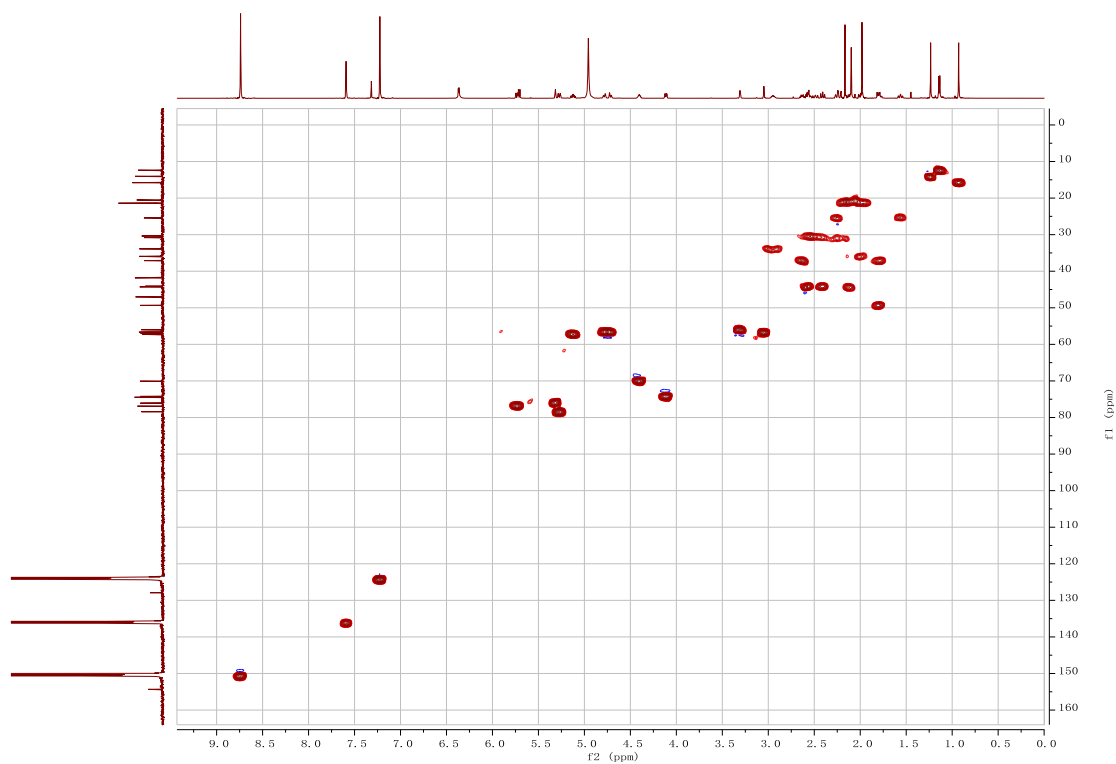


Figure S47. HSQC spectrum of chantriolide K (**6**) in C_5D_5N

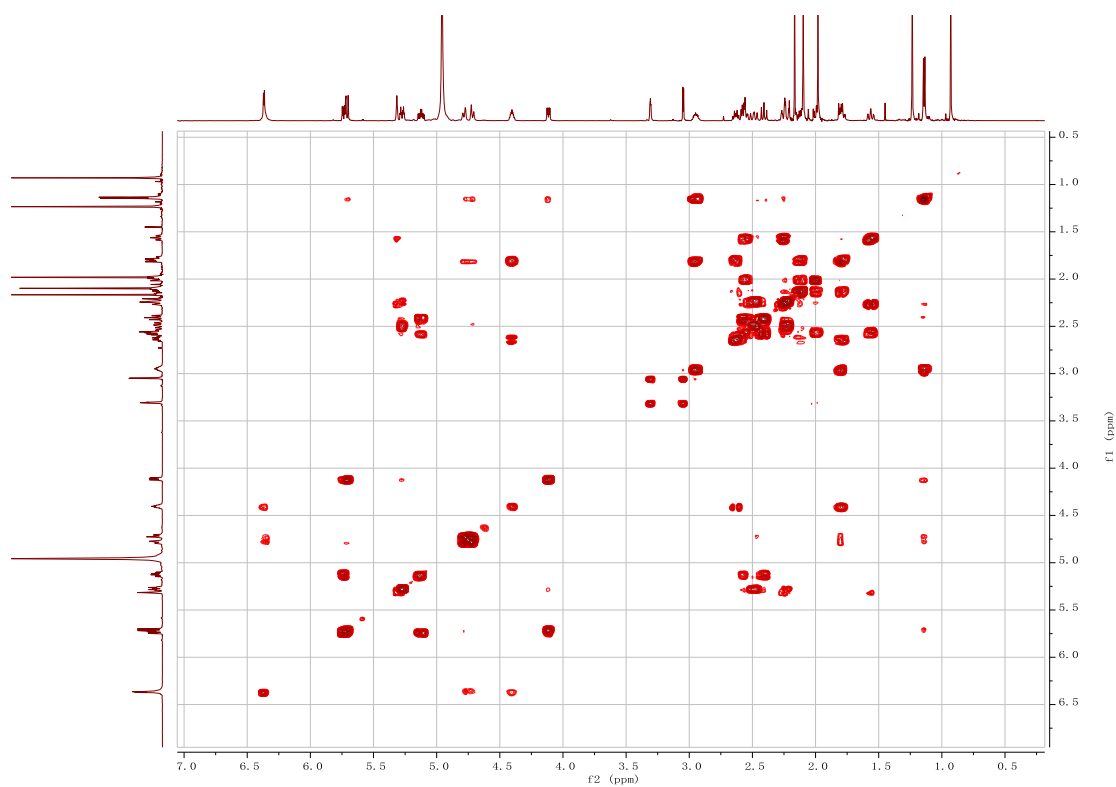


Figure S48. 1H - 1H COSY spectrum of chantriolide K (**6**) in C_5D_5N

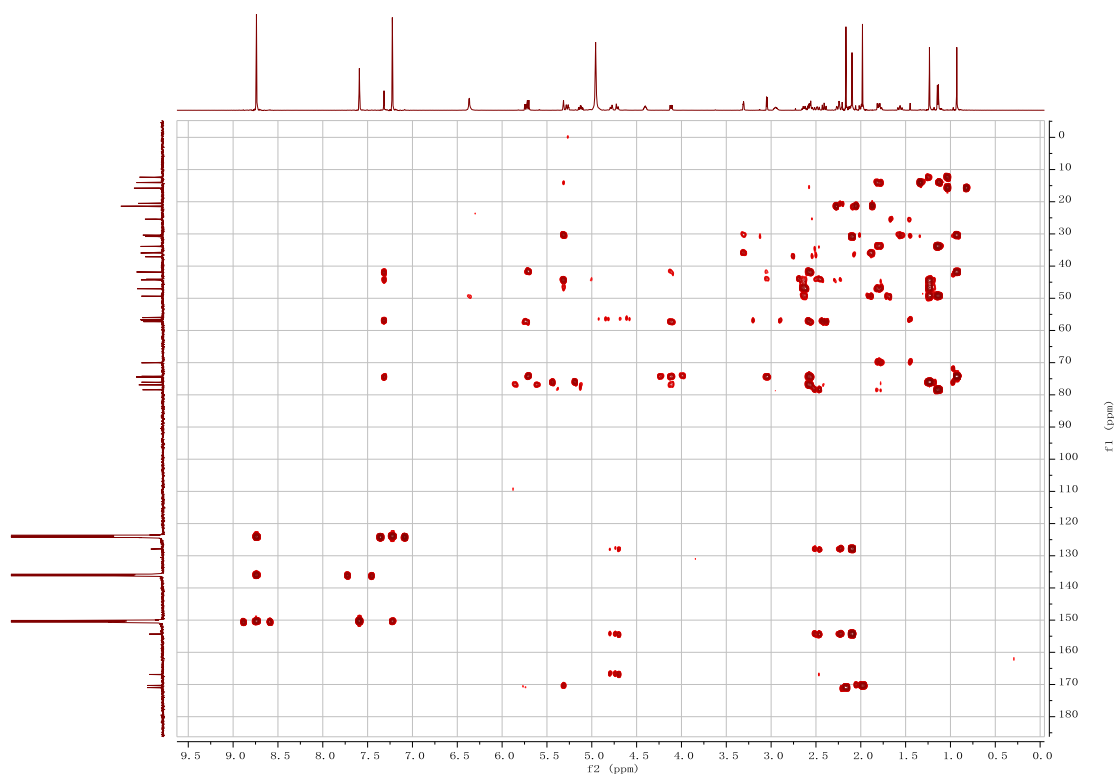


Figure S49. HMBC spectrum of chantriolide K (**6**) in C_5D_5N

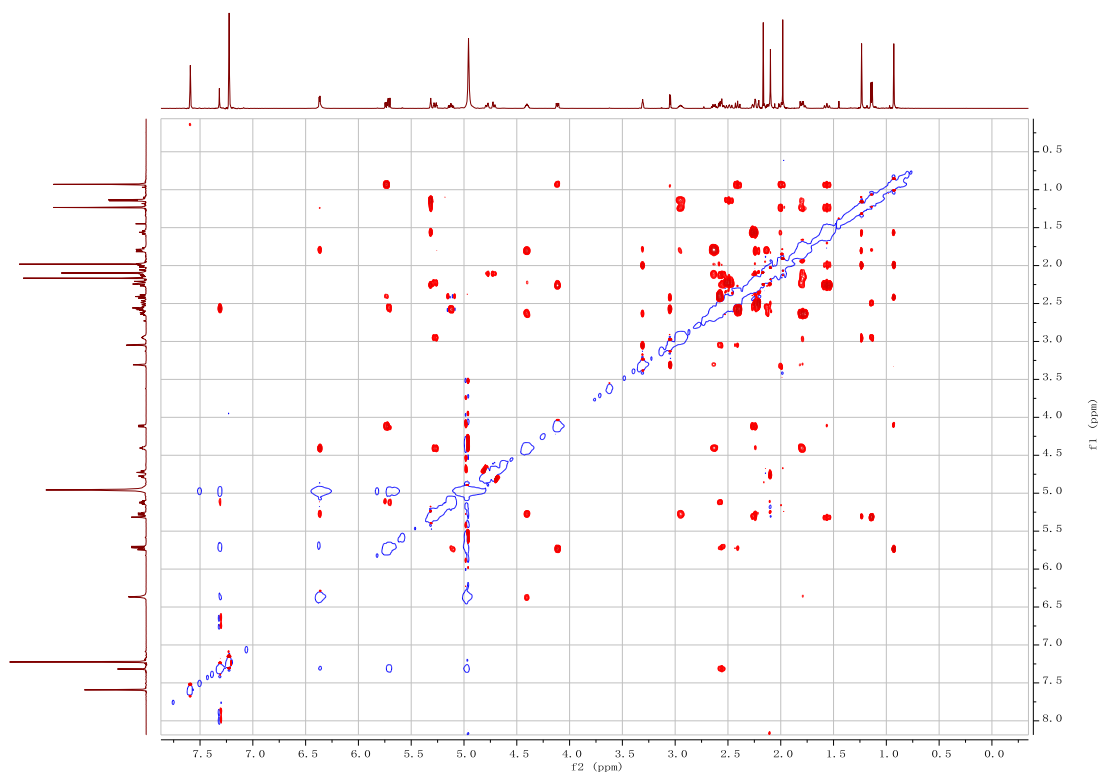
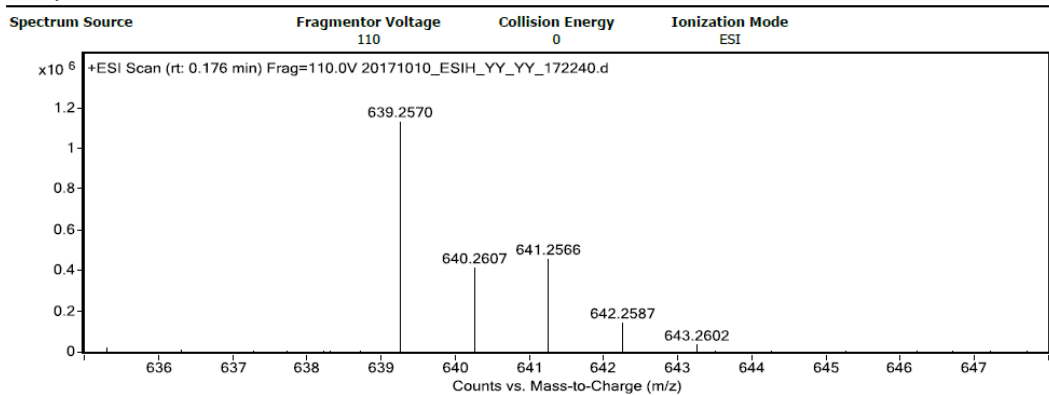


Figure S50. ROESY spectrum of chantriolide K (**6**) in C_5D_5N

Data Filename 20171010_ESIH_YY_YY_172240.d
Sample Type Sample
Instrument Name Agilent G6520 Q-TOF
Acquired Time 10/10/2017 10:34:22 AM
DA Method small molecular data analysis method.m

Sample Name D3-JGS-B2K1ESC
Position P2-A3
Acq Method 20160322_MS_ESIH_POS_1min.m
IRM Calibration Status Success
Comment ESIH by ZZY

User Spectra



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
639.257	639.2567	-0.29	-0.45	C32 H44 Cl O11	(M+H)+

Figure S51. HRESIMS spectrum of chantriolide L (7)

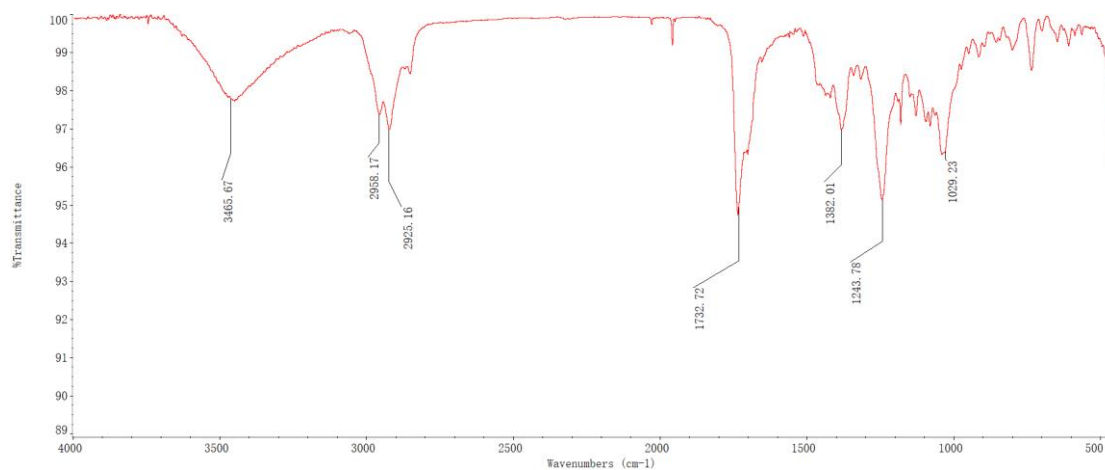


Figure S52. IR spectrum of chantriolide L (7)

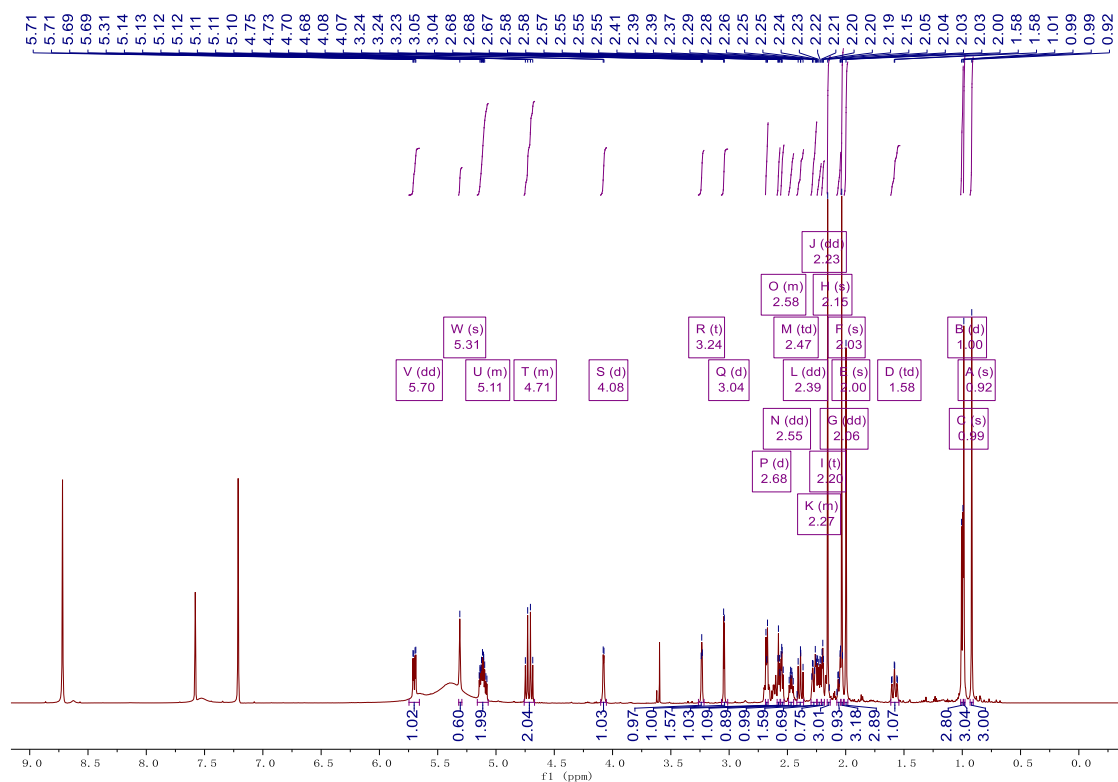


Figure S53. ^1H NMR (600 MHz) spectrum of chantriolide L (**7**) in $\text{C}_5\text{D}_5\text{N}$

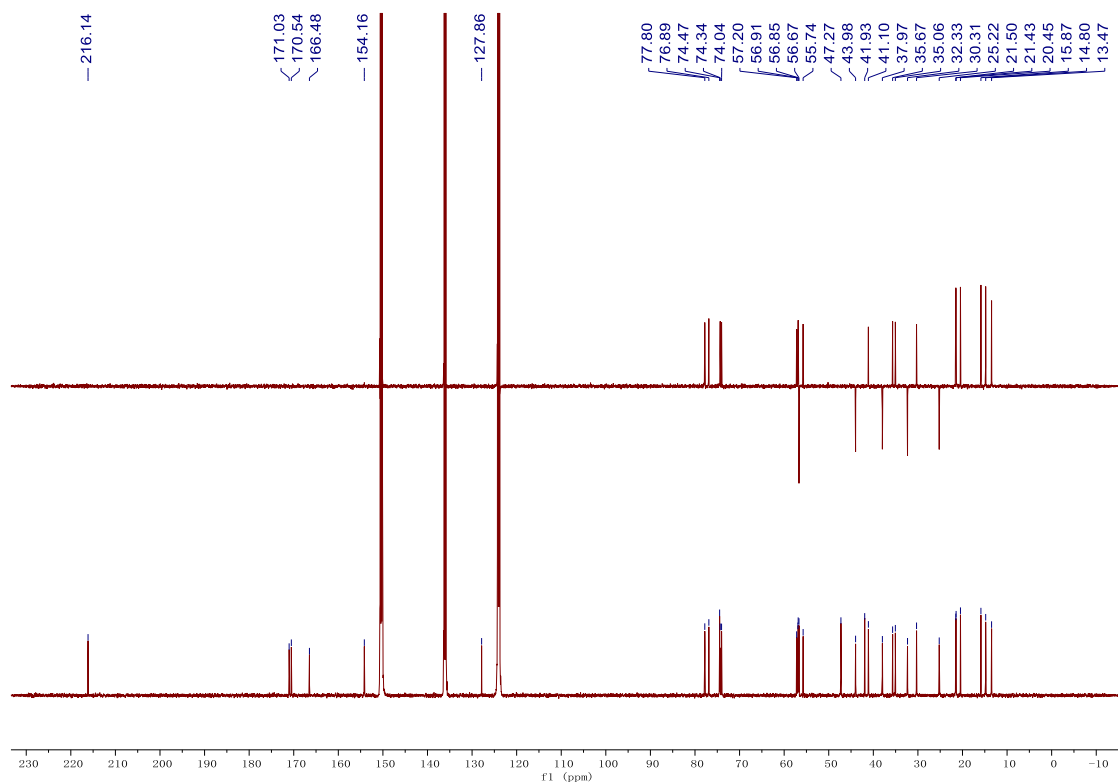


Figure S54. ^{13}C and DEPT-135 NMR (125 MHz) spectra of chantriolide L (**7**) in $\text{C}_5\text{D}_5\text{N}$

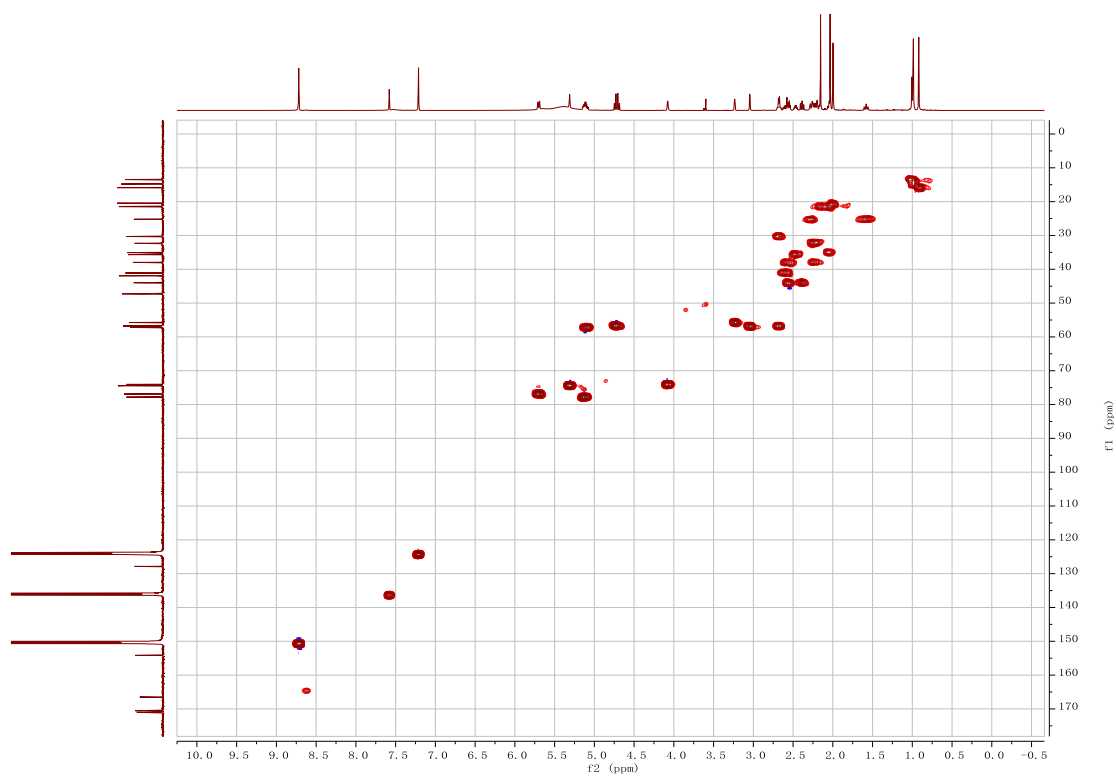


Figure S55. HSQC spectrum of chantriolide L (7) in C₅D₅N

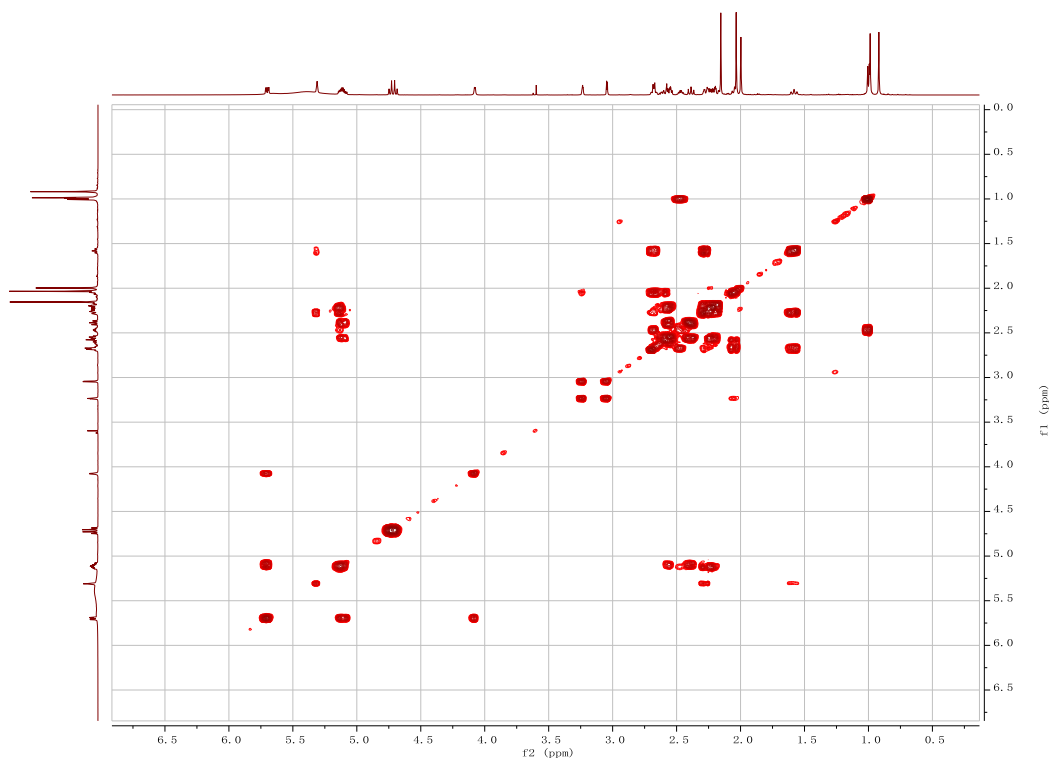


Figure S56. ¹H-¹H COSY spectrum of chantriolide L (7) in C₅D₅N

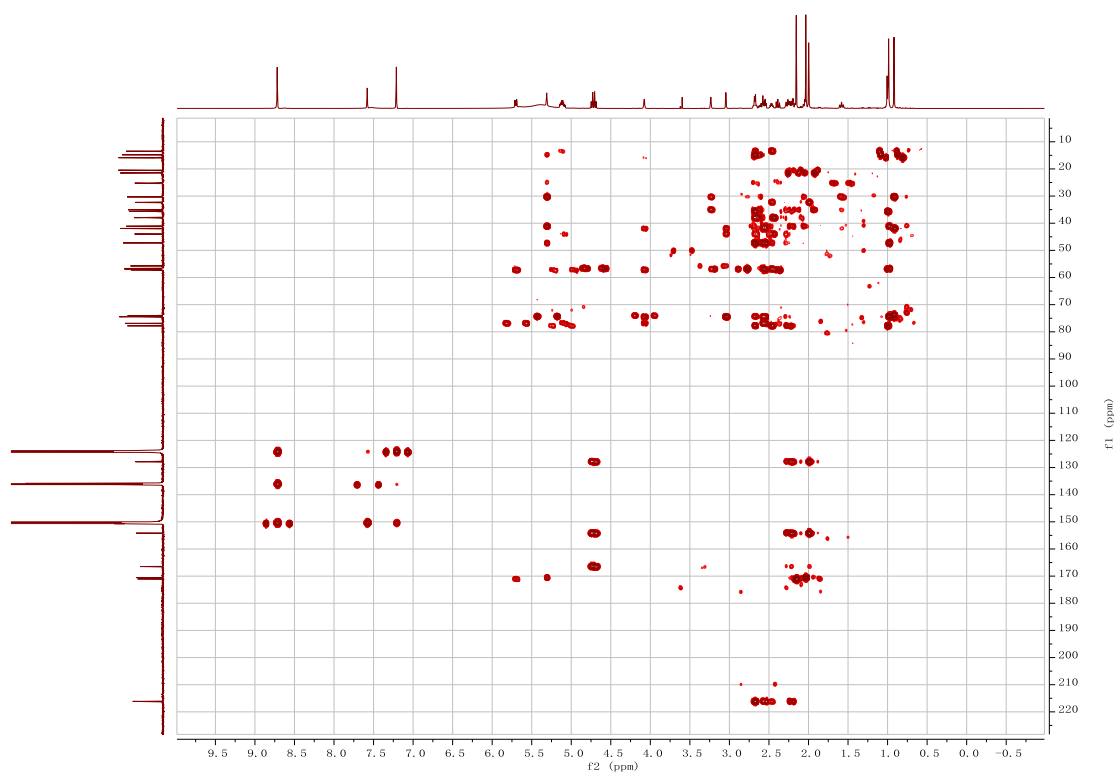


Figure S57. HMBC spectrum of chantriolide L (**7**) in C₅D₅N

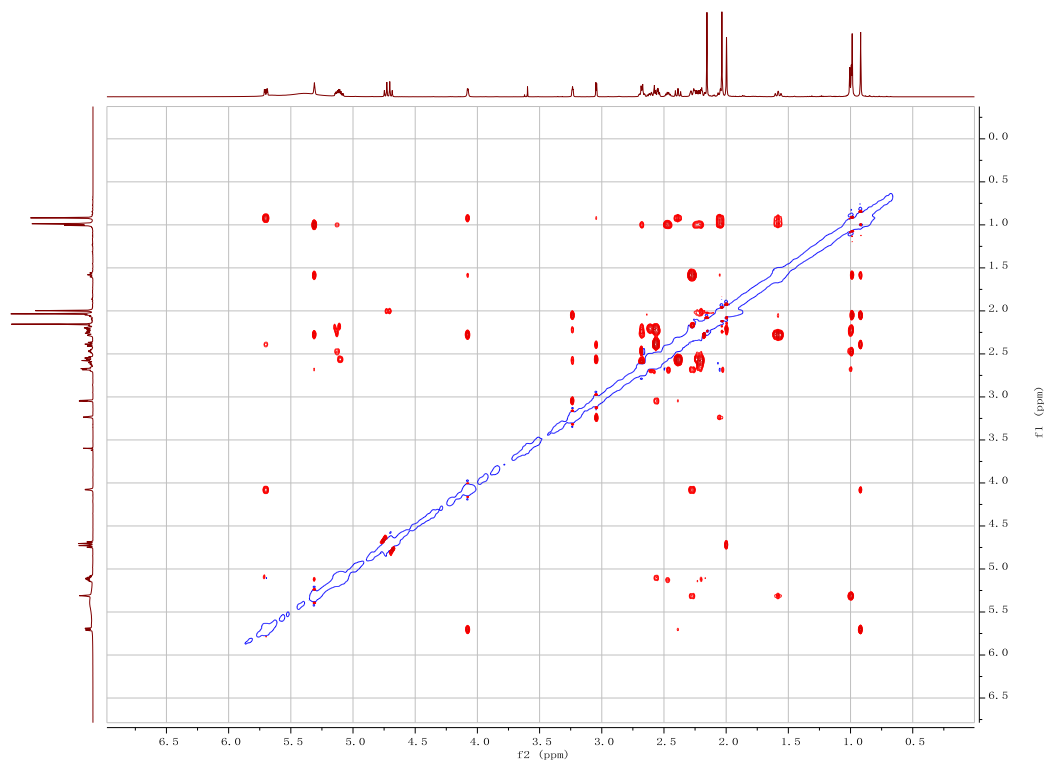
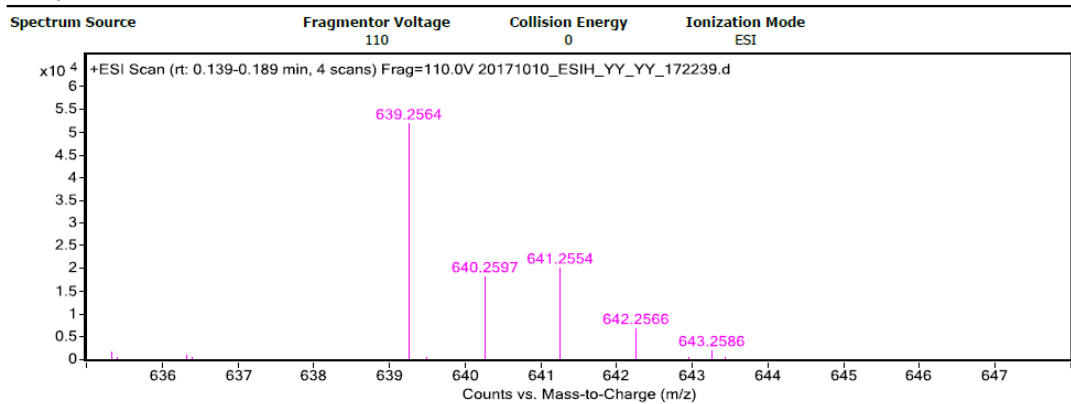


Figure S58. ROESY spectrum of chantriolide L (**7**) in C₅D₅N

Data Filename	20171010_ESIH_YY_YY_172239.d	Sample Name	D3-JGS-B2K1E5A
Sample Type	Sample	Position	P2-A2
Instrument Name	Agilent G6520 Q-TOF	Acq Method	20160322_MS_ESIH_POS_1min.m
Acquired Time	10/10/2017 10:32:29 AM	IRM Calibration Status	Success
DA Method	small molecular data analysis method.m	Comment	ESI/ by ZZY

User Spectra



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
639.2564	639.2567	0.22	0.35	C32 H44 Cl O11	(M+H)+

Figure S59. HRESIMS spectrum of chantriolide M (**8**)

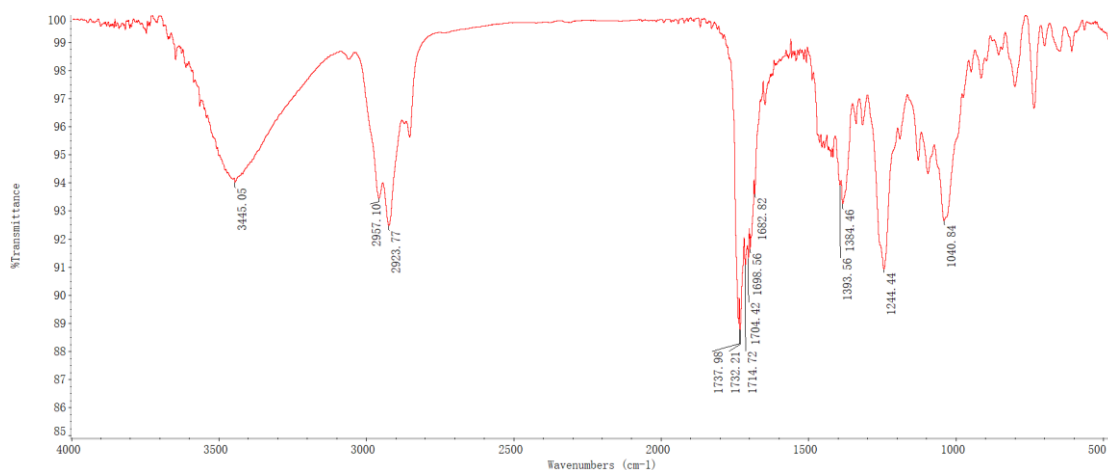
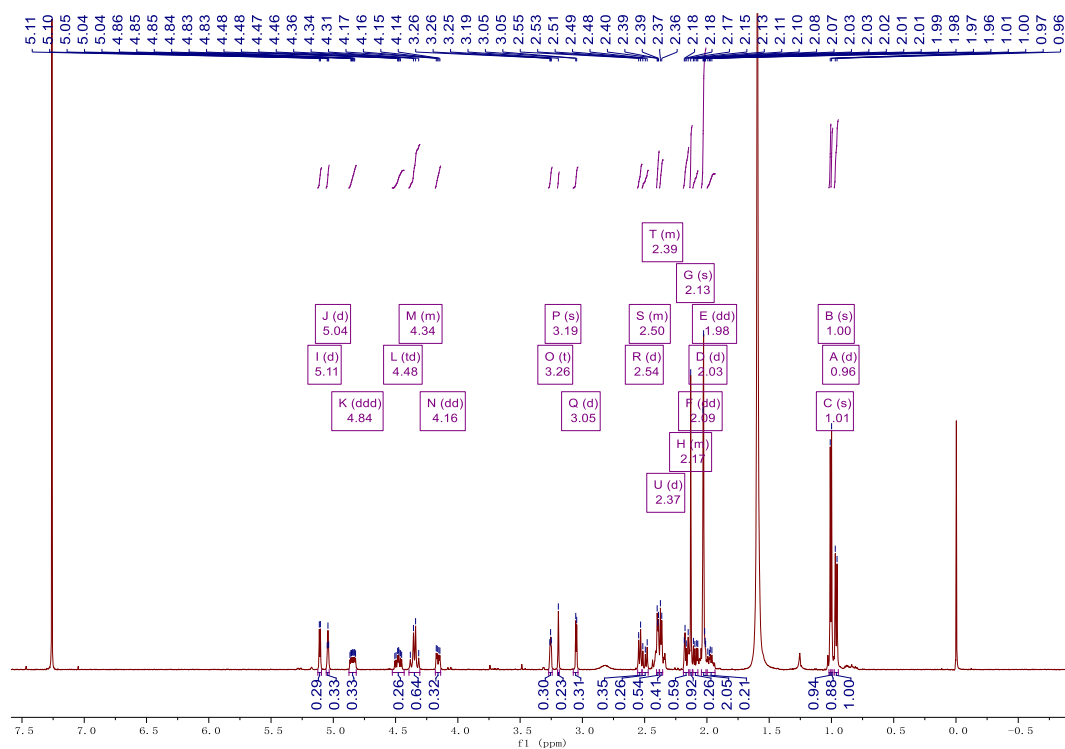


Figure S60. IR spectrum of chantriolide M (**8**)



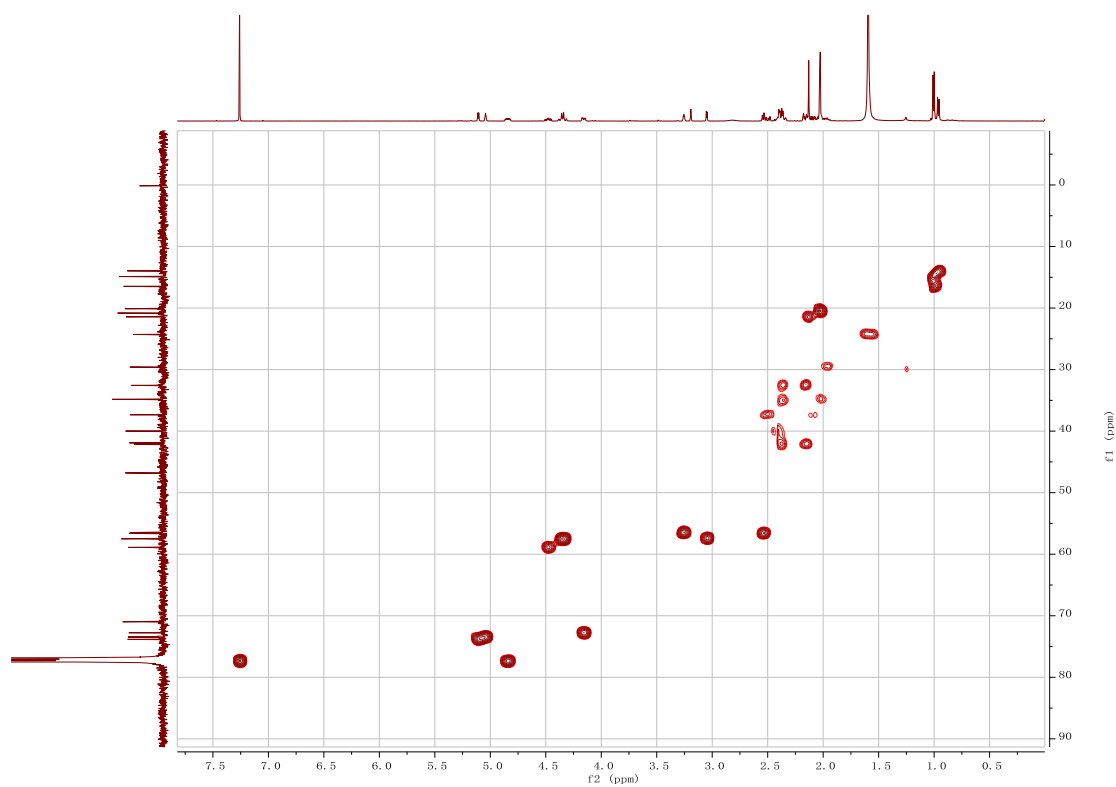


Figure S63. HSQC spectrum of chantriolide M (8) in CDCl₃

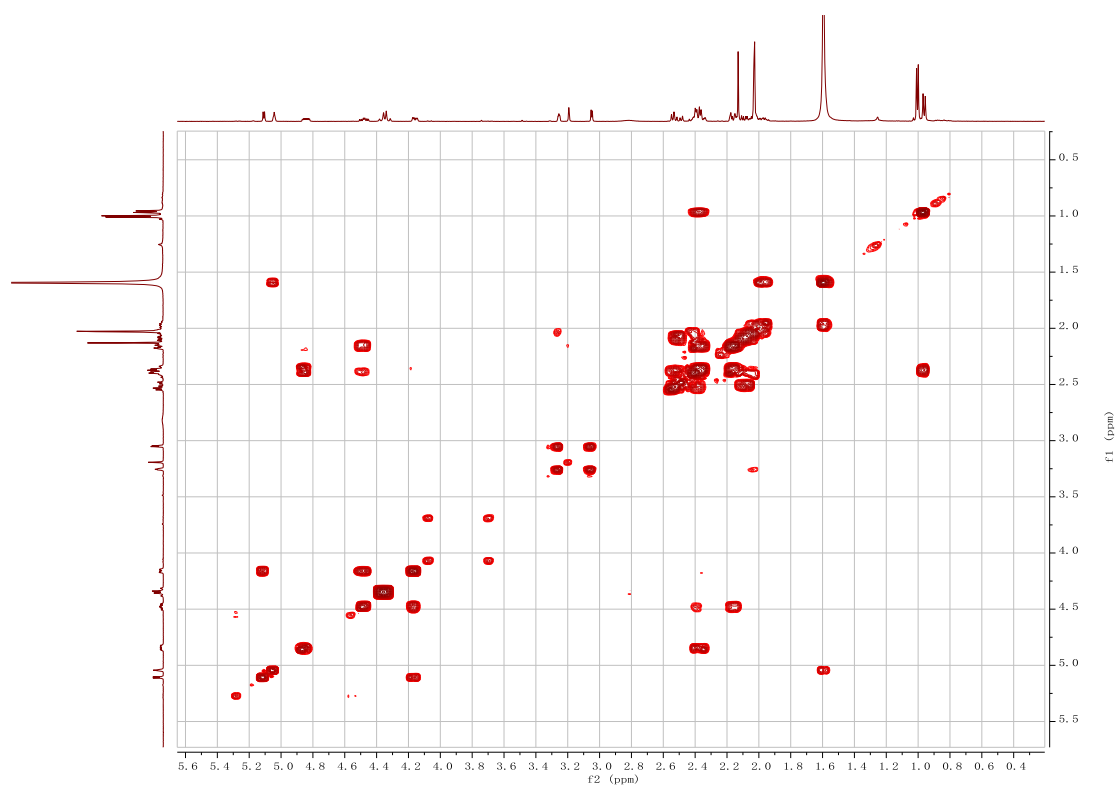


Figure S64. ¹H-¹H COSY spectrum of chantriolide M (8) in CDCl₃

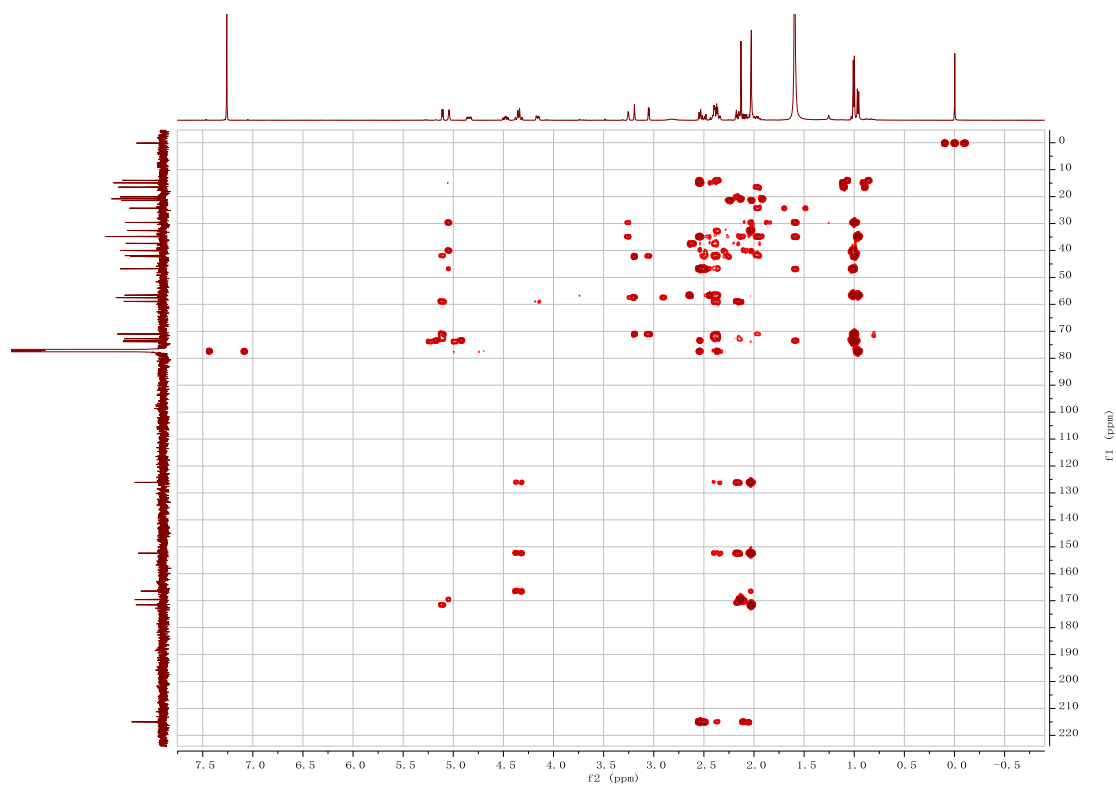


Figure S65. HMBC spectrum of chantriolide M (**8**) in CDCl_3

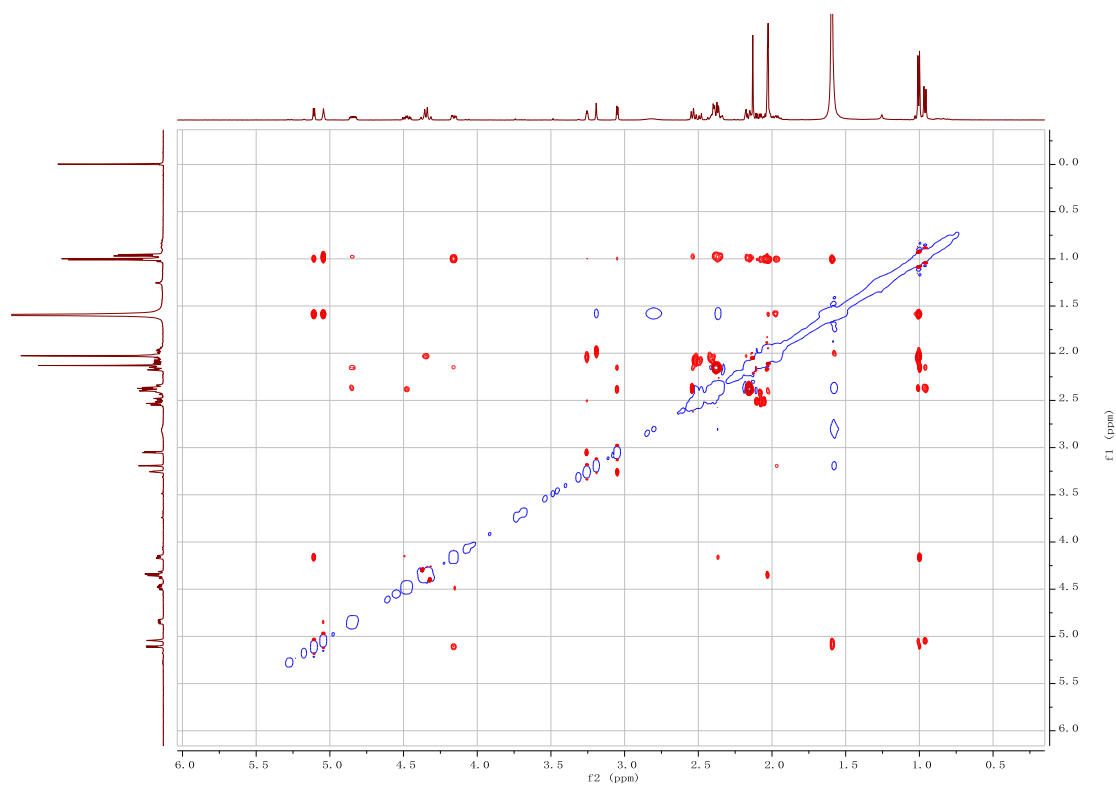


Figure S66. ROESY spectrum of chantriolide M (**8**) in CDCl_3

Elemental Composition Report

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

102 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-34 H: 0-200 O: 0-30 Na: 1-1

Minimum:	80.00										-1.5
Maximum:	100.00		5.0	5.0							50.0
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula		
499.3026	100.00	499.3036	-1.0	-2.0	6.5	379.1	n/a	n/a	C28 H44 O6 Na		

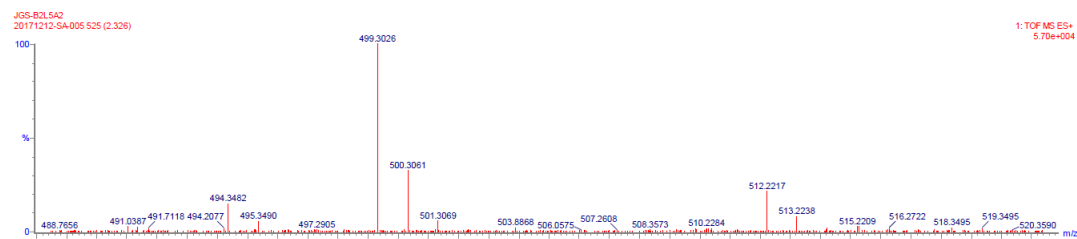


Figure S67. HRESIMS spectrum of chantriolide N (9)

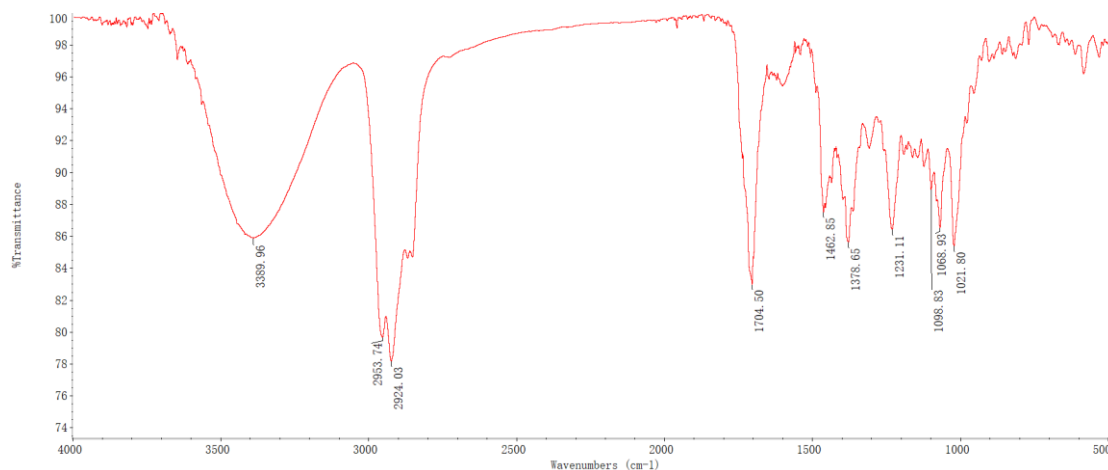


Figure S68. IR spectrum of chantriolide N (9)

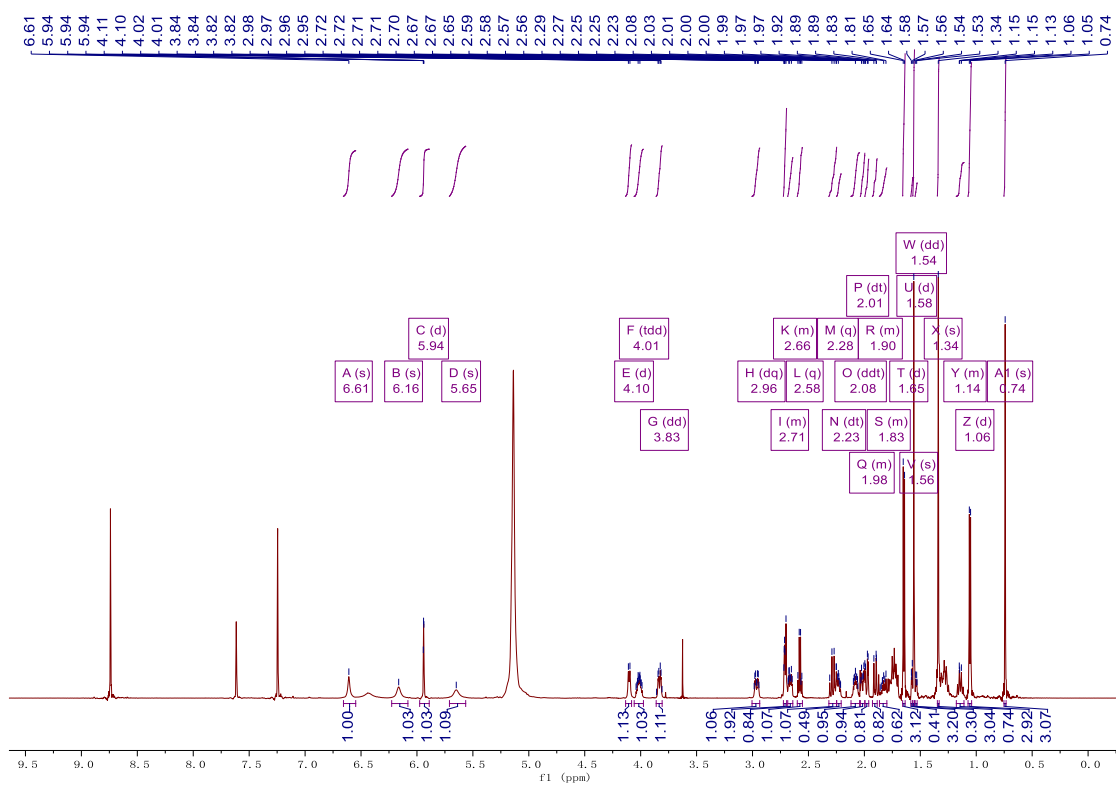


Figure S69. ¹H NMR (600 MHz) spectrum of chantriolide N (9) in C₅D₅N

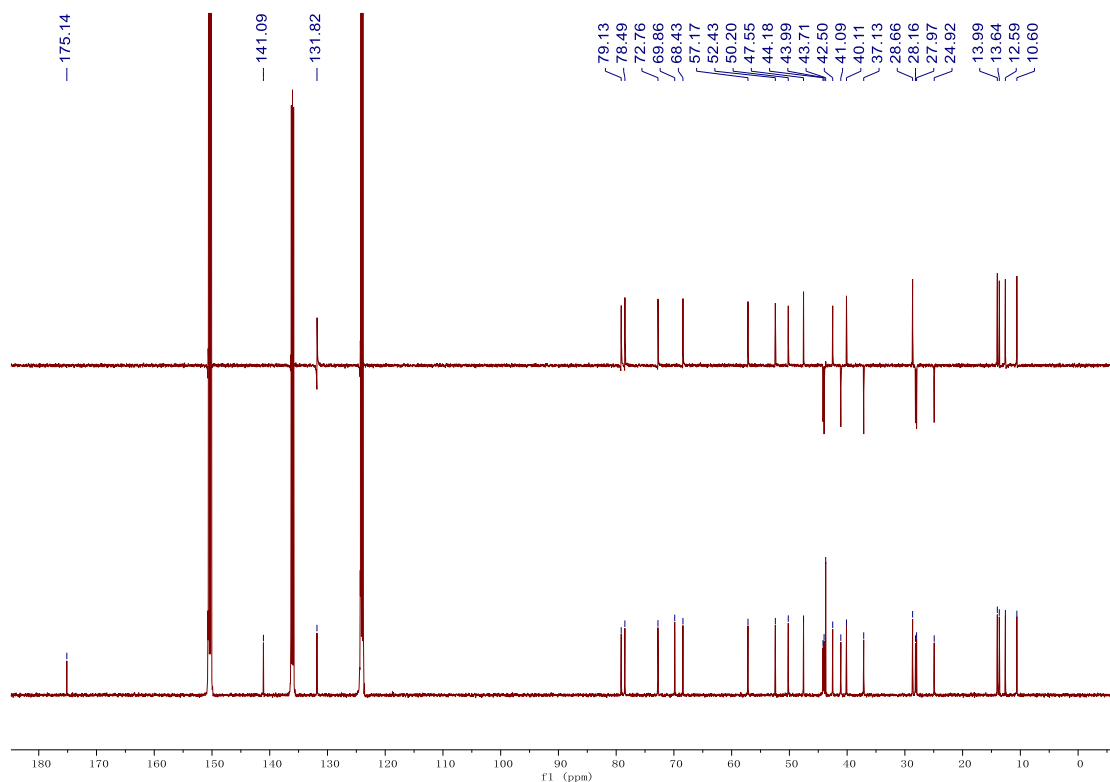


Figure S70. ¹³C and DEPT-135 NMR (125 MHz) spectra of chantriolide N (9) in C₅D₅N

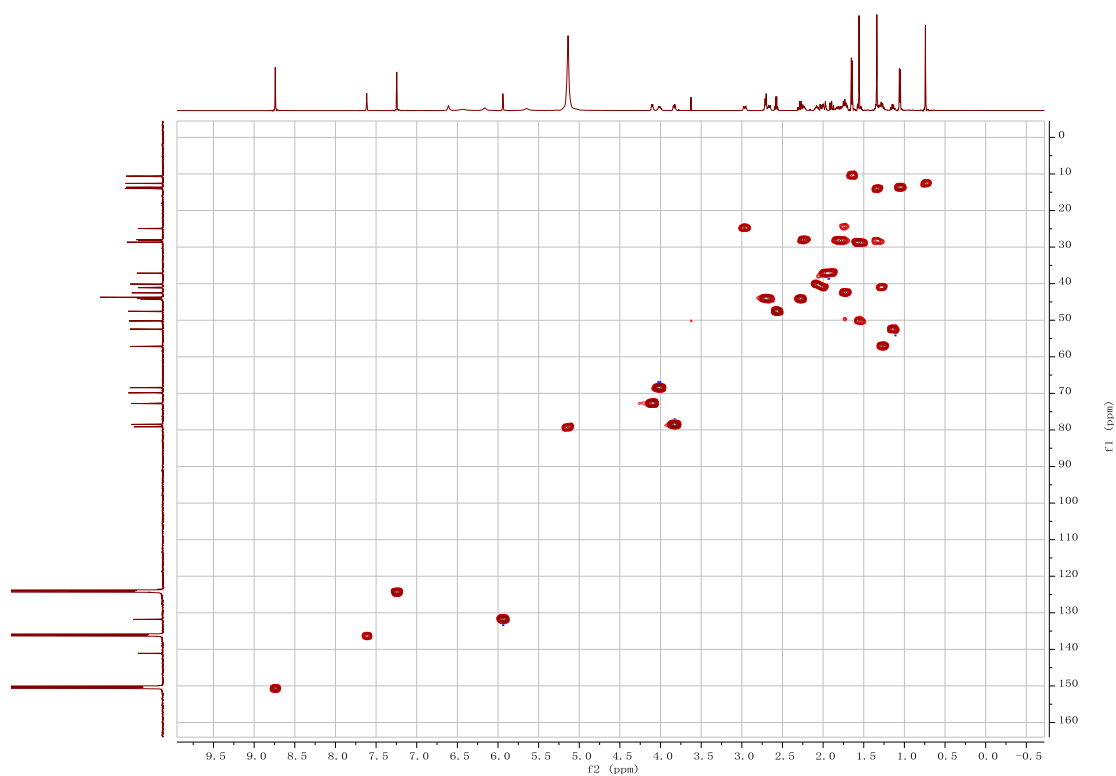


Figure S71. HSQC spectrum of chantriolide N (**9**) in C_5D_5N

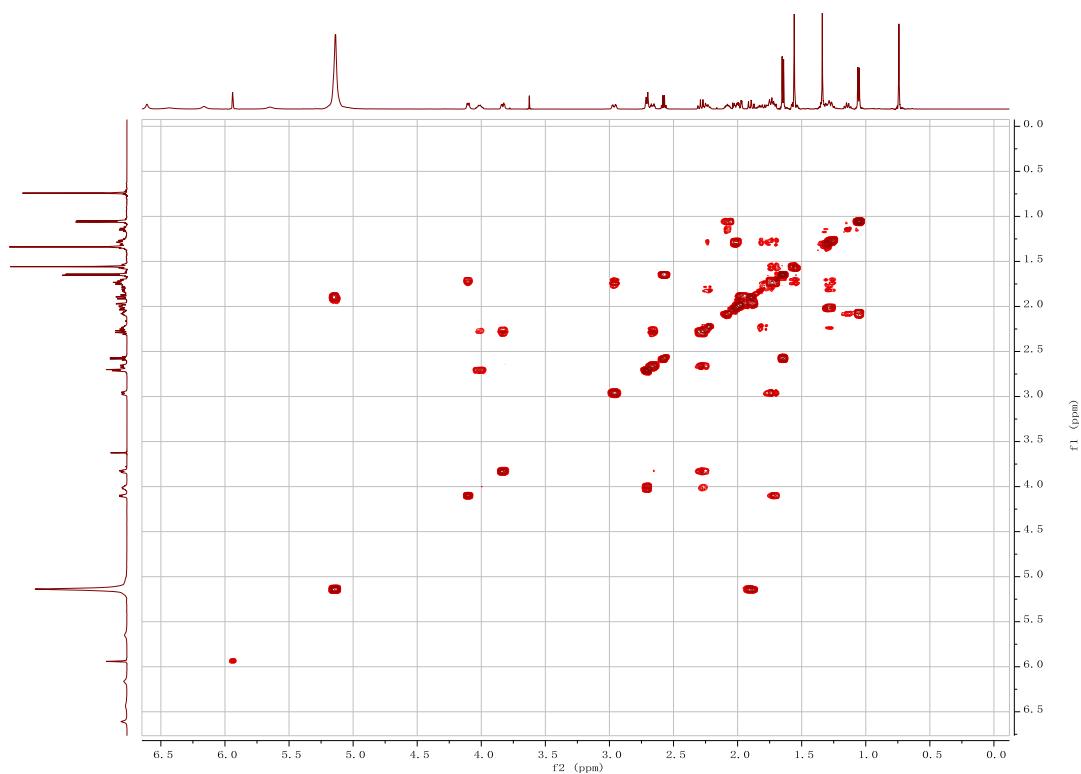


Figure S72. 1H - 1H COSY spectrum of chantriolide N (**9**) in C_5D_5N

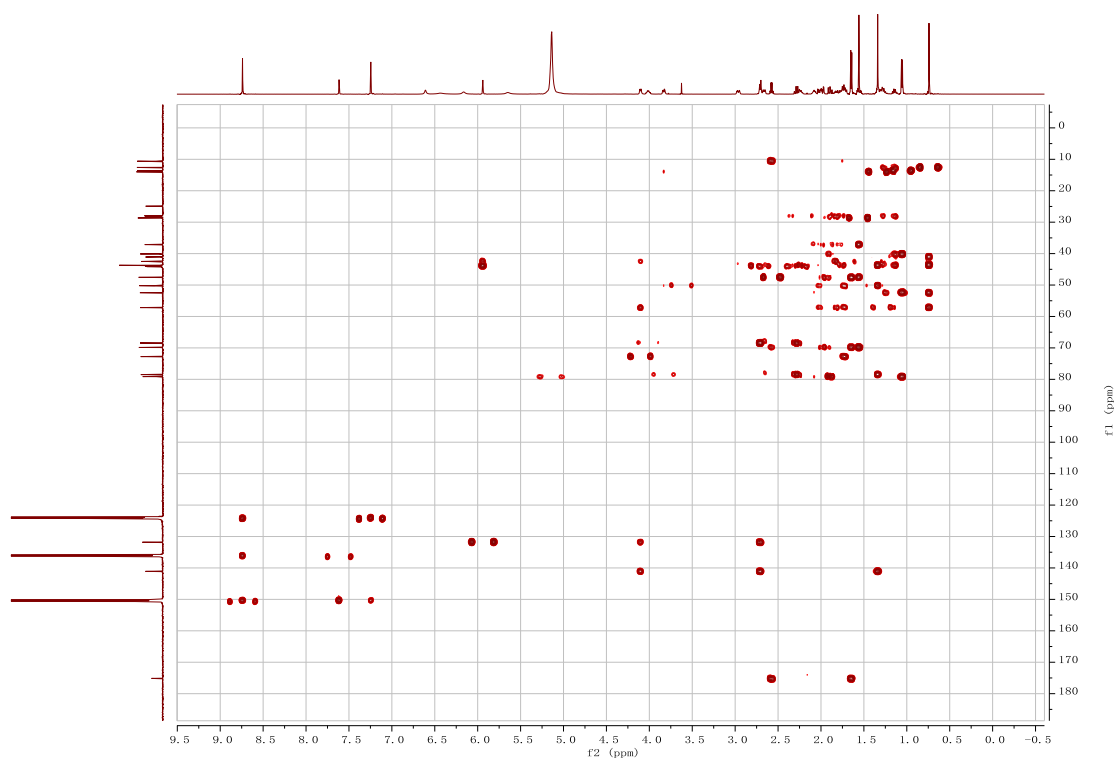


Figure S73. HMBC spectrum of chantriolide N (**9**) in C₅D₅N

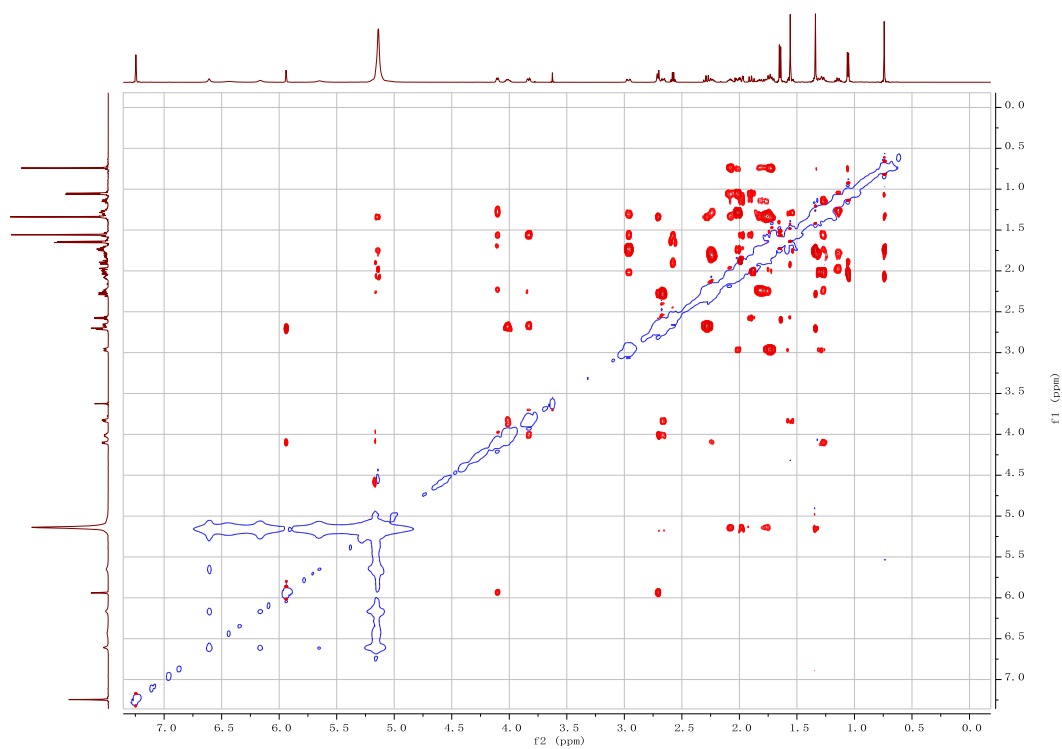


Figure S74. ROESY spectrum of chantriolide N (**9**) in C₅D₅N

Elemental Composition Report

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

22 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 20-30 H: 20-46 O: 0-15

Minimum: -1.5

Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
493.3180	493.3165	1.5	3.0	6.5	354.6	n/a	n/a	C ₂₈ H ₄₅ O ₇

JGS-B2K1G1B1

20171221-SA-009 637 (2.757)

1: TOF MS ES+
8.44e+004

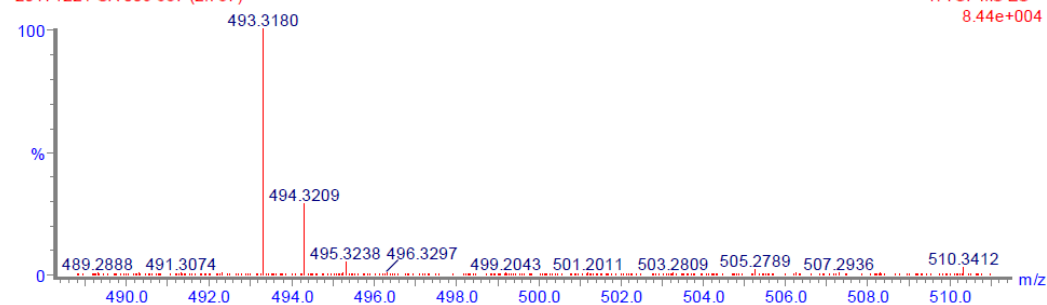


Figure S75. HRESIMS spectrum of chantriolide O (10)

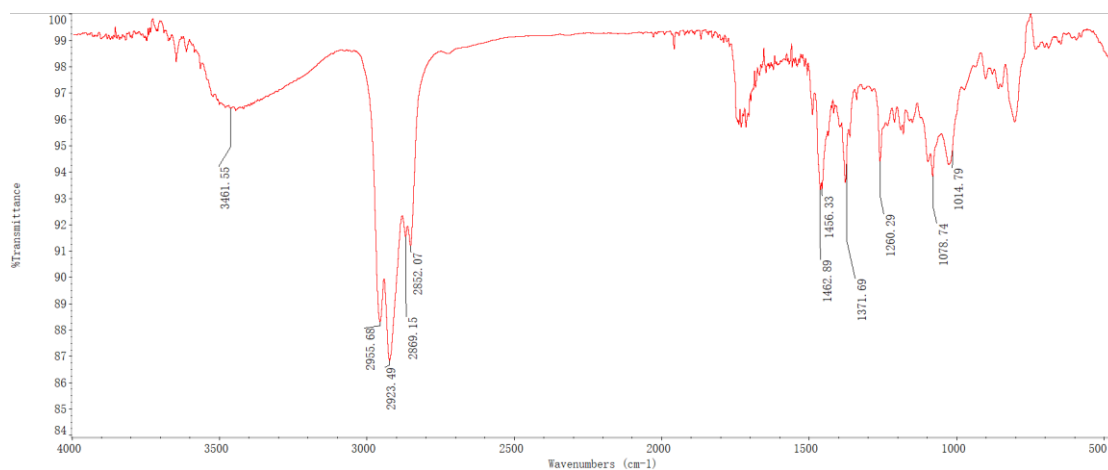


Figure S76. IR spectrum of chantriolide O (10)

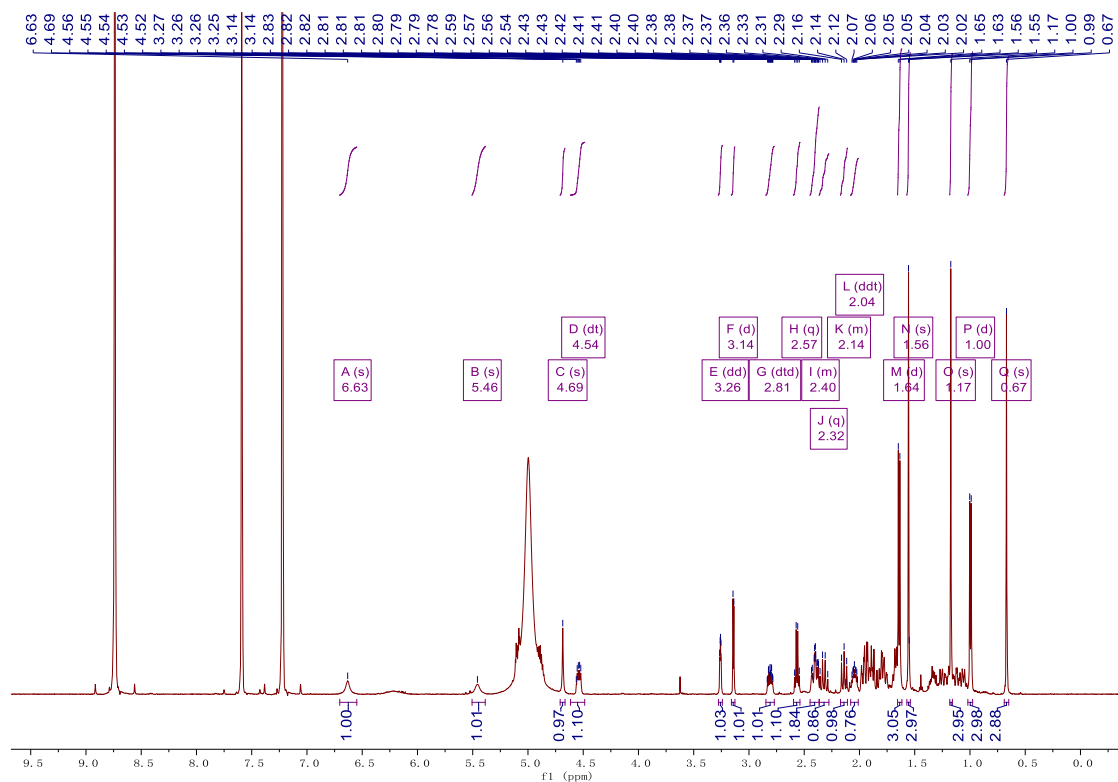


Figure S77. ¹H NMR (500 MHz) spectrum of chantriolide O (**10**) in C₅D₅N

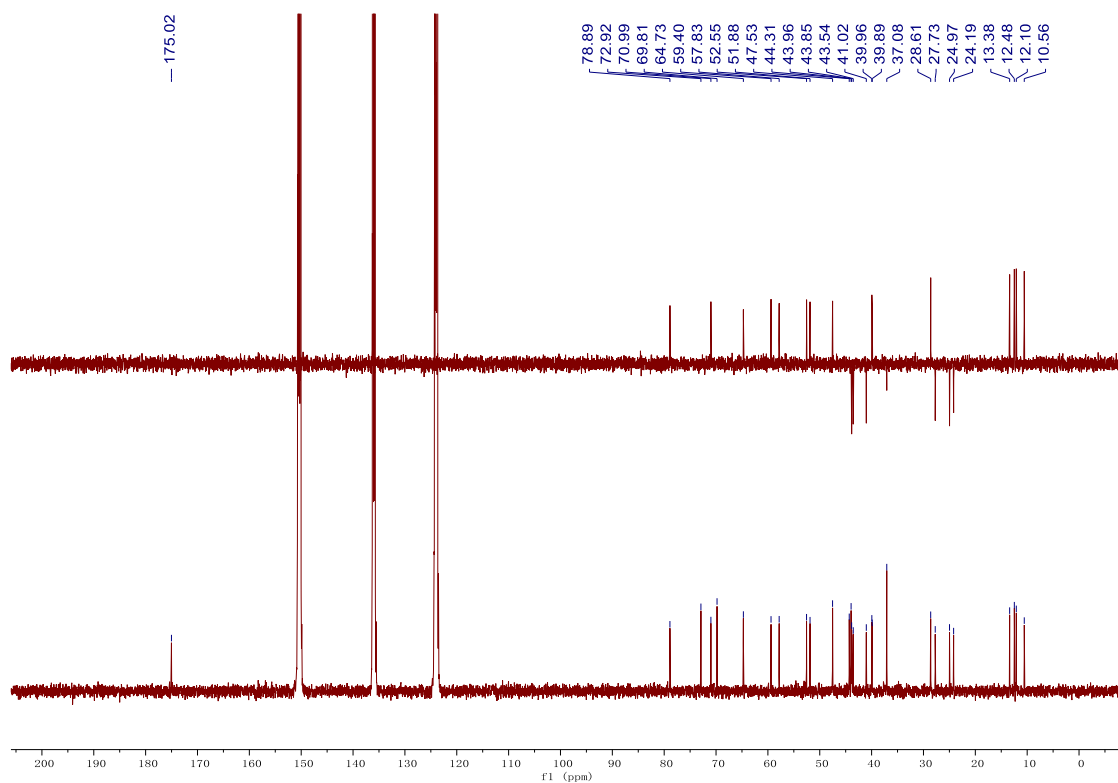


Figure S78. ¹³C and DEPT-135 NMR (125 MHz) spectra of chantriolide O (**10**) in C₅D₅N

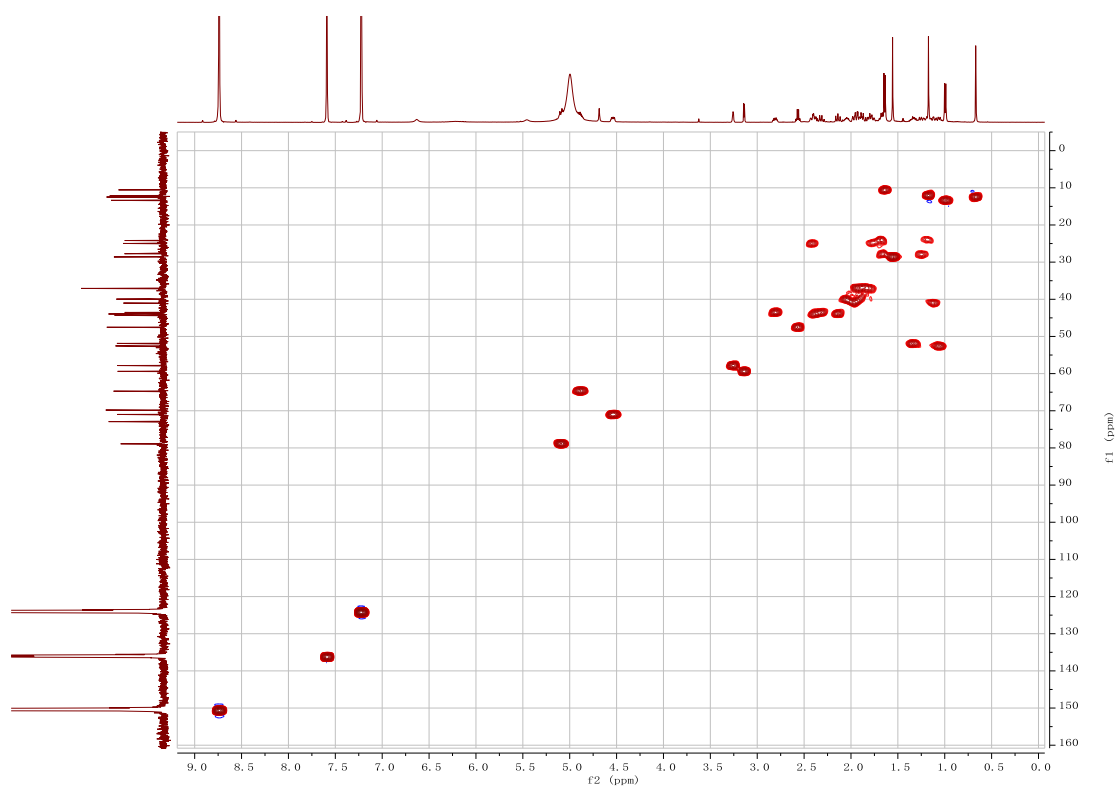


Figure S79. HSQC spectrum of chantriolide O (**10**) in C₅D₅N

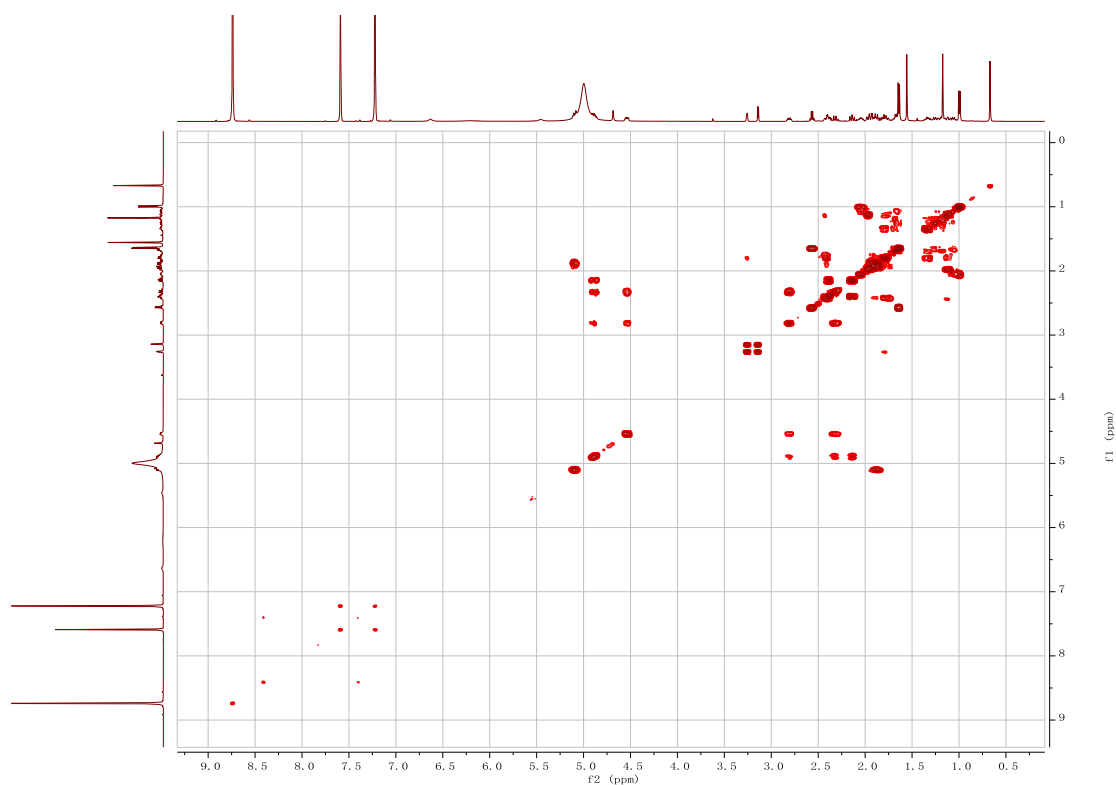


Figure S80. ¹H-¹H COSY spectrum of chantriolide O (**10**) in C₅D₅N

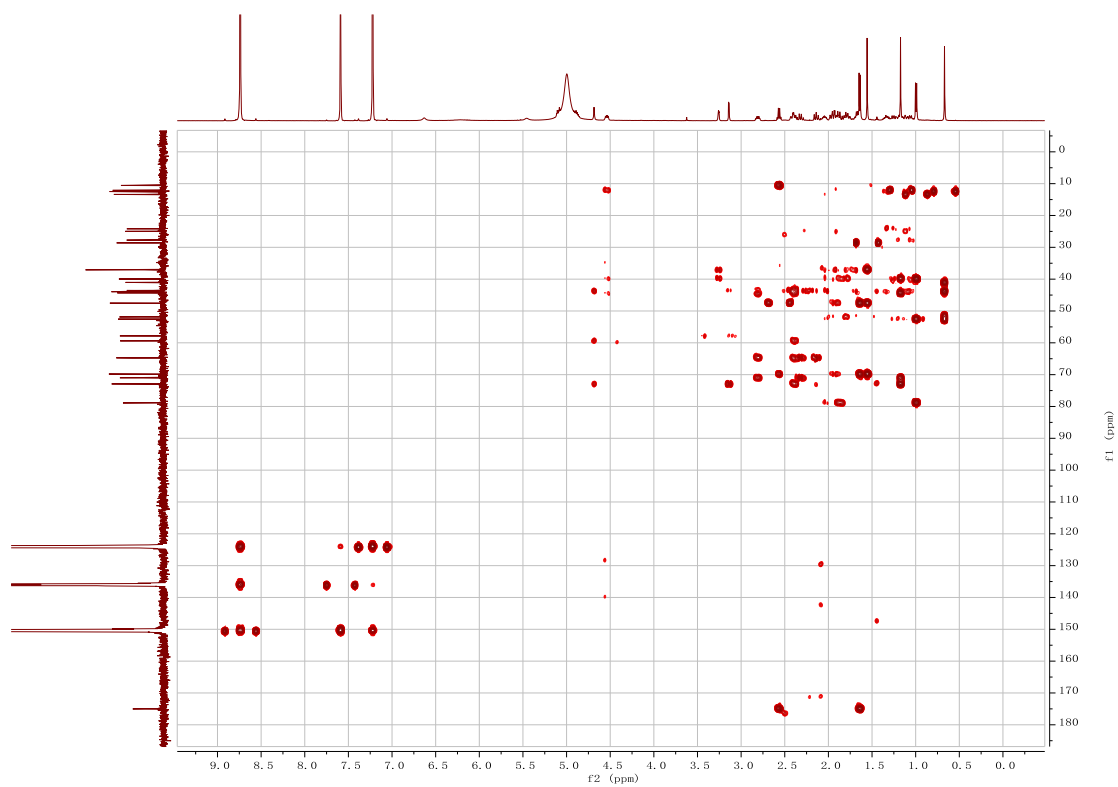


Figure S81. HMBC spectrum of chantriolide O (**10**) in C₅D₅N

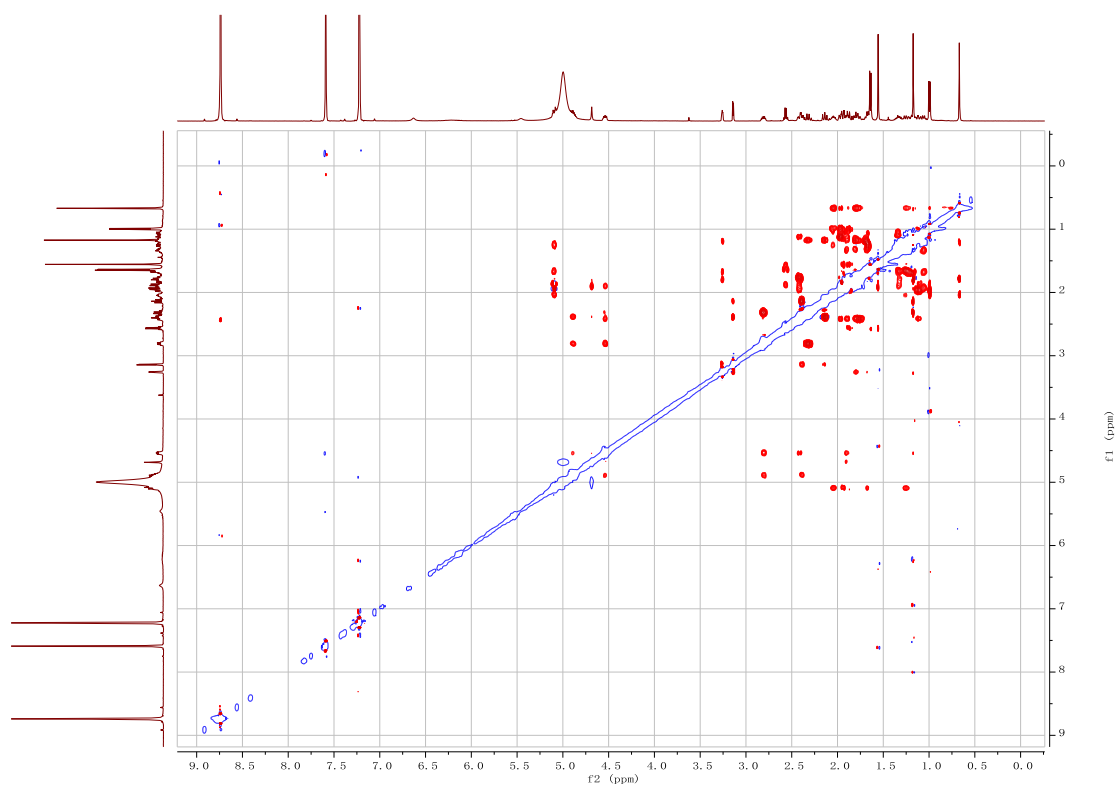


Figure S82. ROESY spectrum of chantriolide O (**10**) in C₅D₅N

Elemental Composition Report

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

208 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-34 H: 0-200 N: 0-1 O: 0-30

Minimum: 80.00 -1.5

Maximum: 100.00 5.0 5.0 50.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
508.3284	100.00	508.3274	1.0	2.0	6.5	583.2	n/a	n/a	C28 H46 N O7

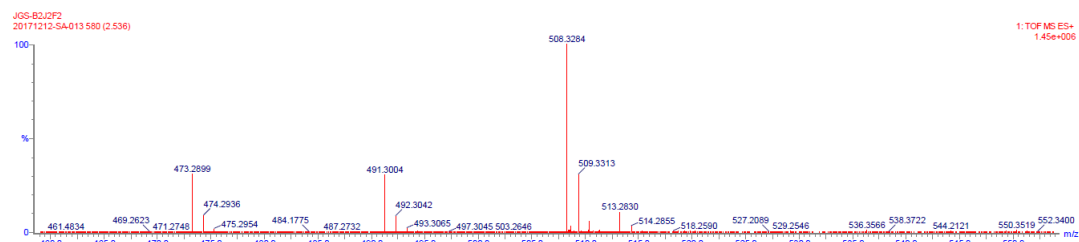


Figure S83. HRESIMS spectrum of chantriolide P (11)

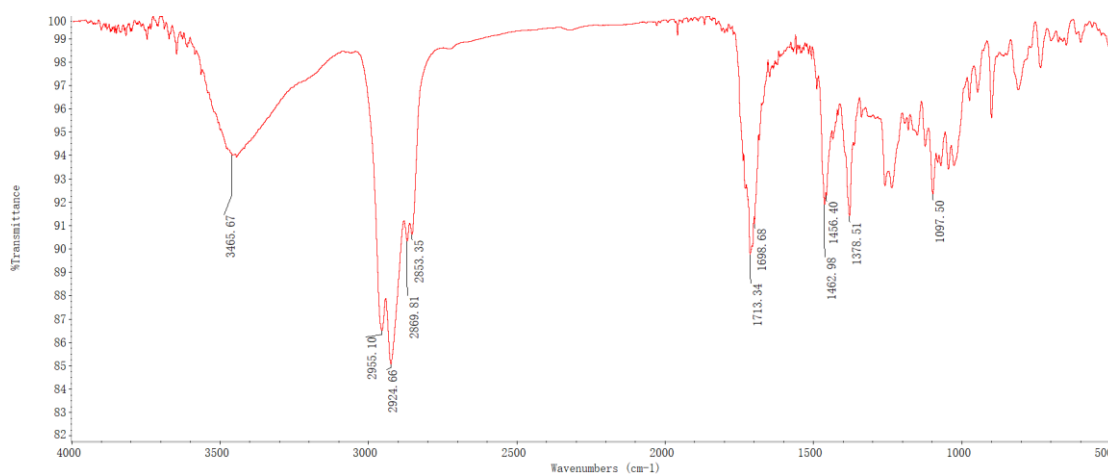


Figure S84. IR spectrum of chantriolide P (11)

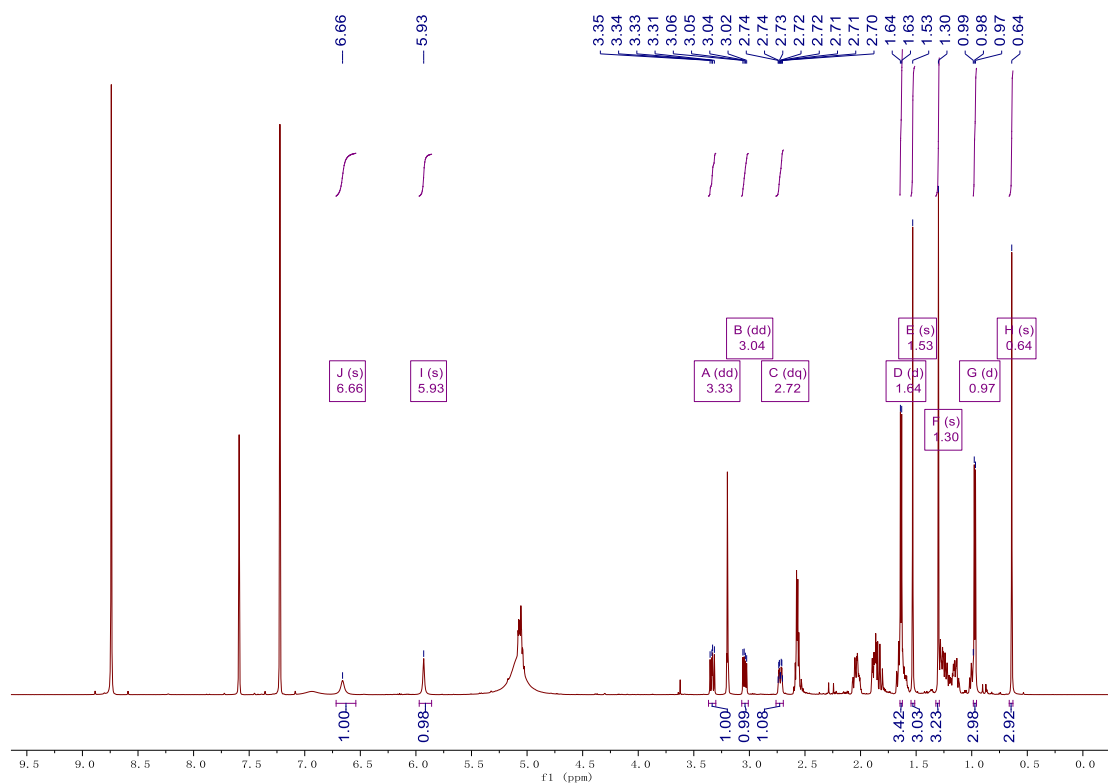


Figure S85. ¹H NMR (600 MHz) spectrum of chantriolide P (**11**) in C₅D₅N

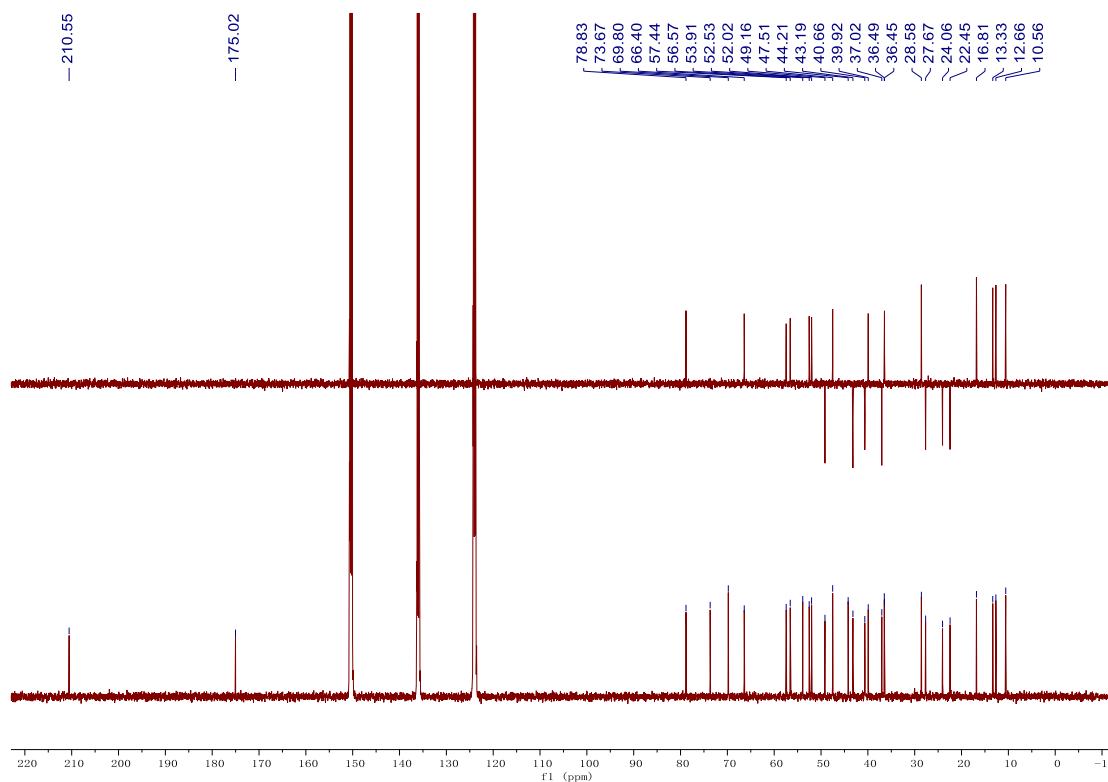


Figure S86. ¹³C and DEPT-135 NMR (125 MHz) spectra of chantriolide P (**11**) in C₅D₅N

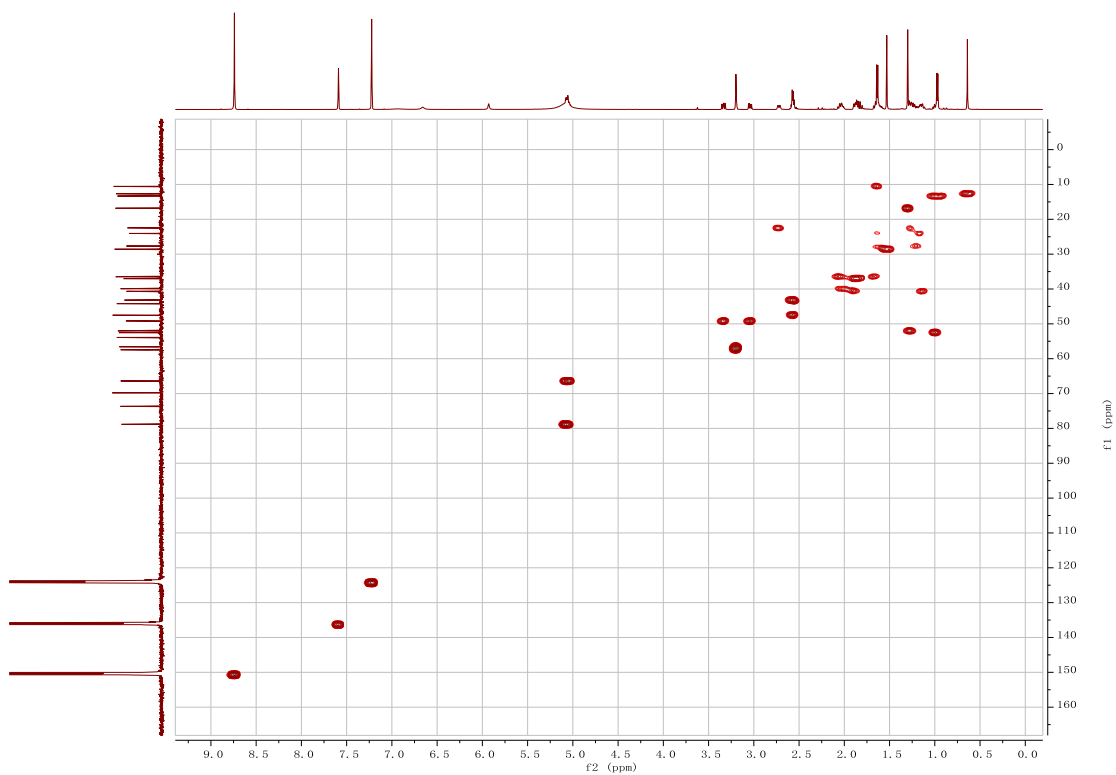


Figure S87. HSQC spectrum of chantriolide P (**11**) in C₅D₅N

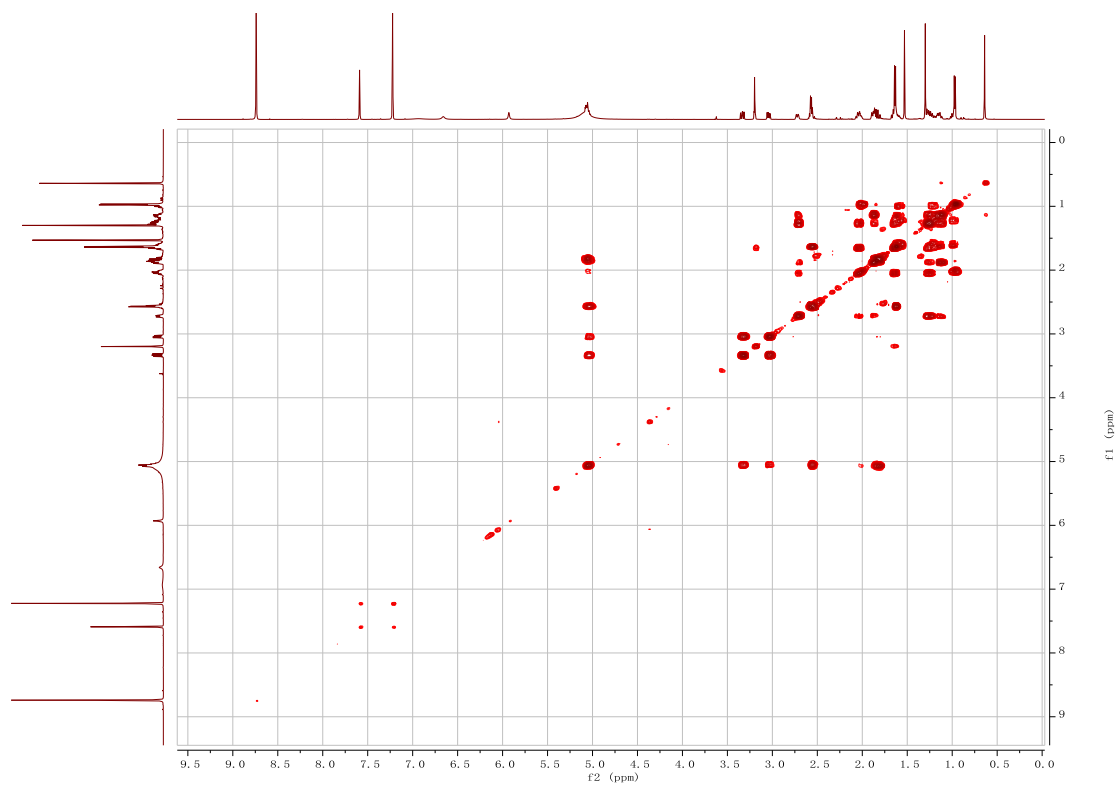


Figure S88. ¹H-¹H COSY spectrum of chantriolide P (**11**) in C₅D₅N

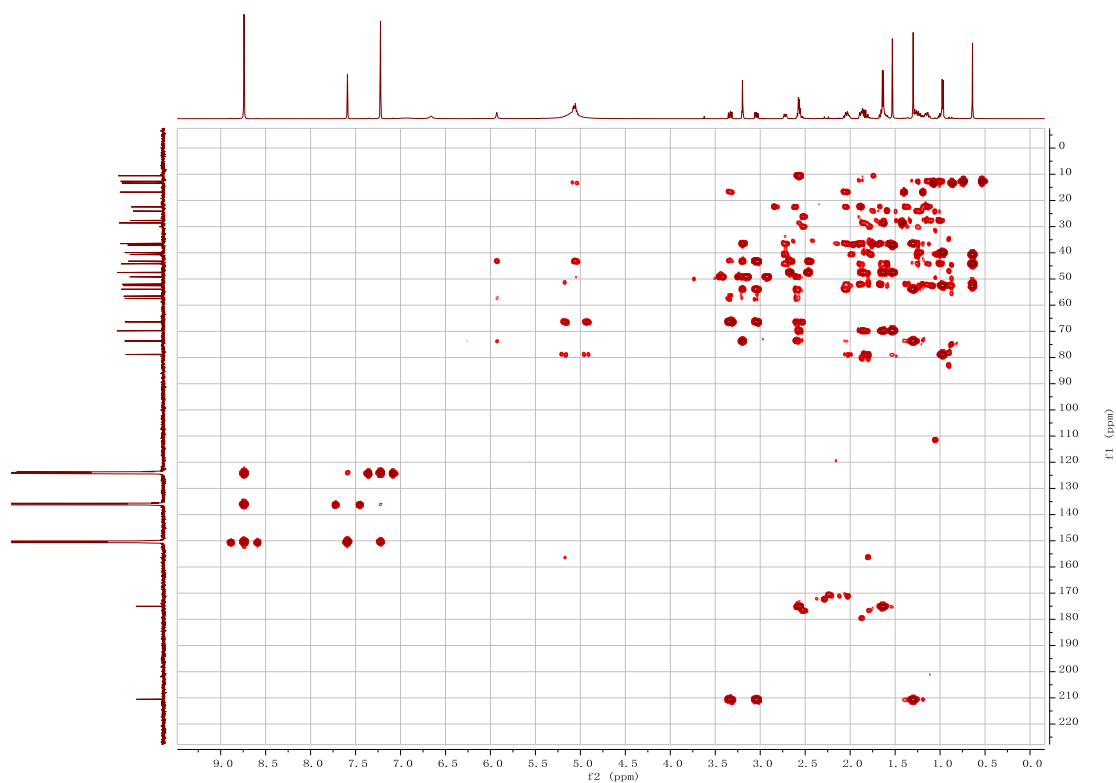


Figure S89. HMBC spectrum of chantriolide P (**11**) in C₅D₅N

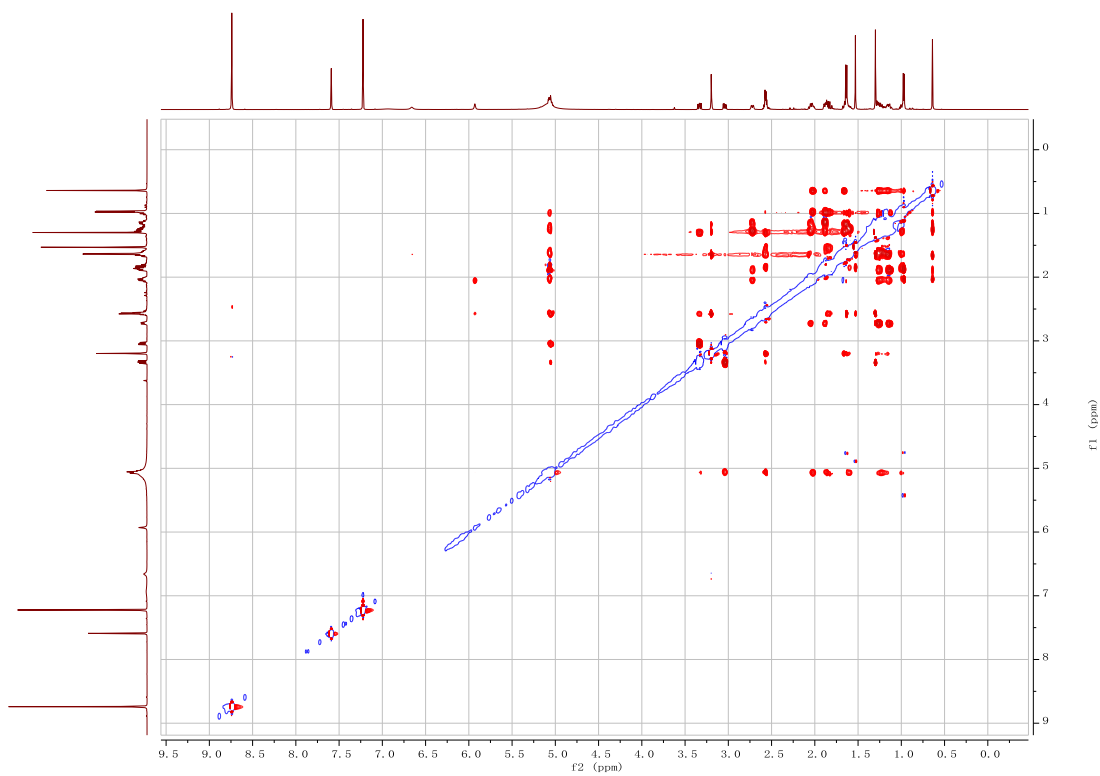


Figure S90. ROESY spectrum of chantriolide P (**11**) in C₅D₅N

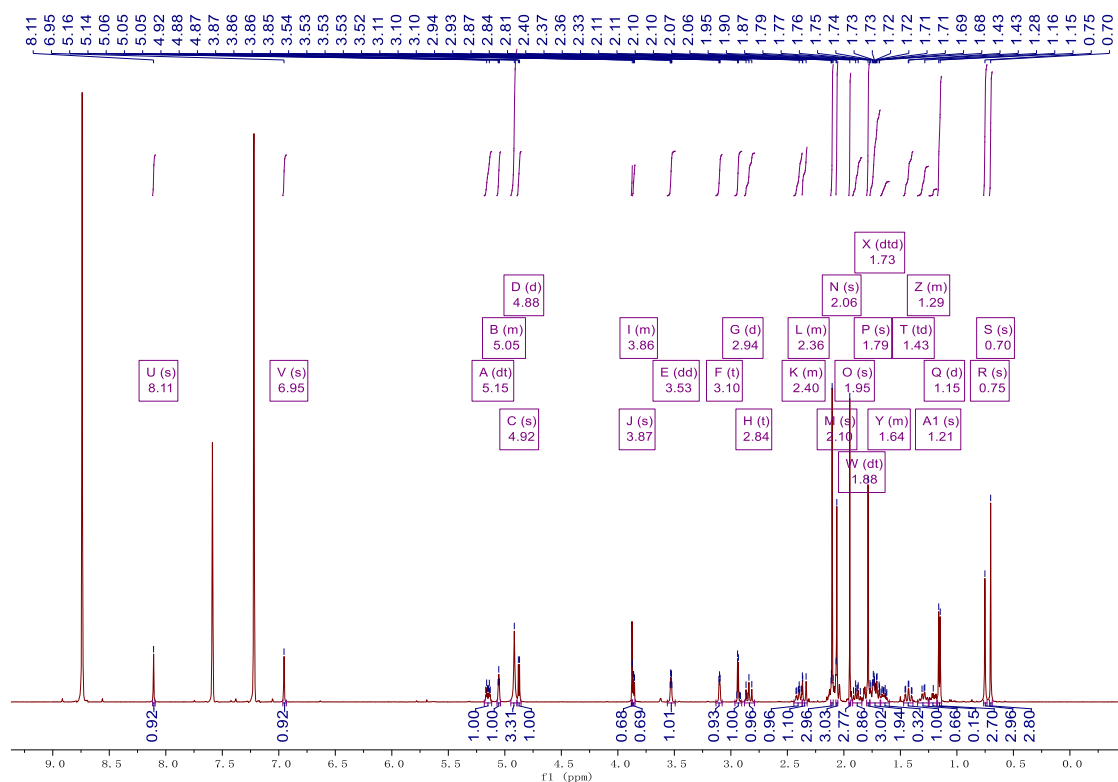


Figure S91. ^1H NMR (500 MHz) spectrum of plantagiolide E (12**) in $\text{C}_5\text{D}_5\text{N}$**

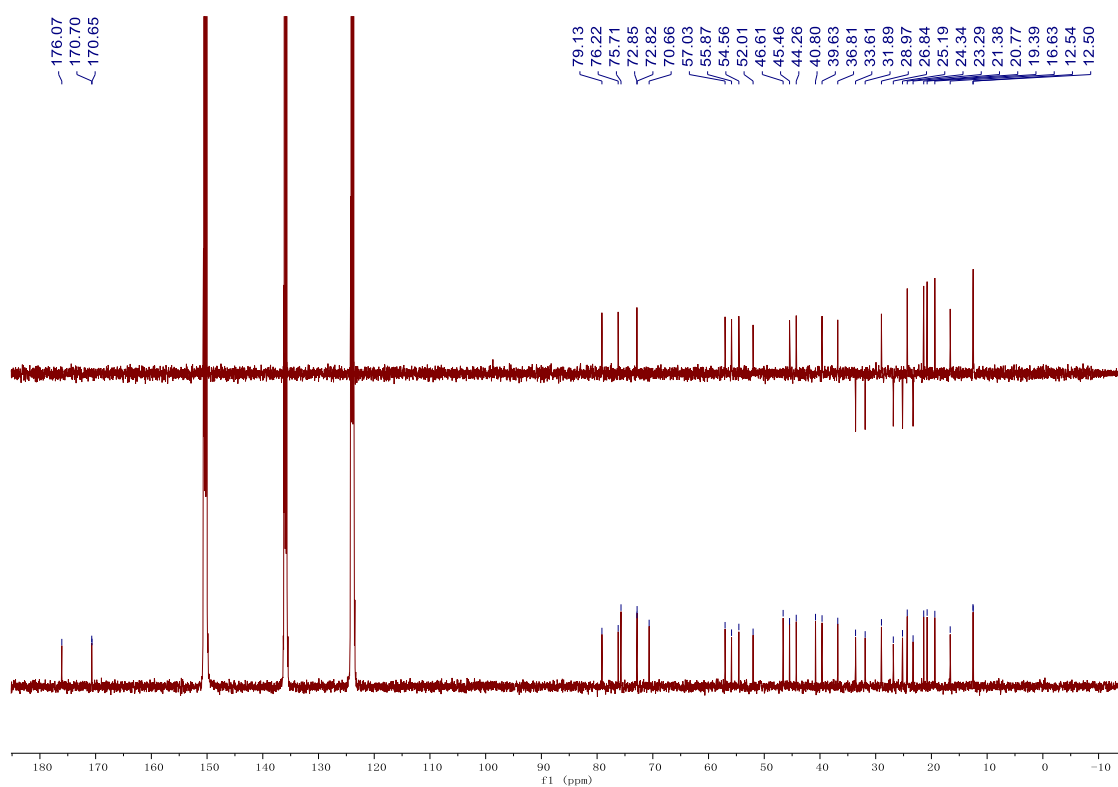


Figure S92. ^{13}C and DEPT-135 NMR (125 MHz) spectra of plantagiolide E (12**) in $\text{C}_5\text{D}_5\text{N}$**

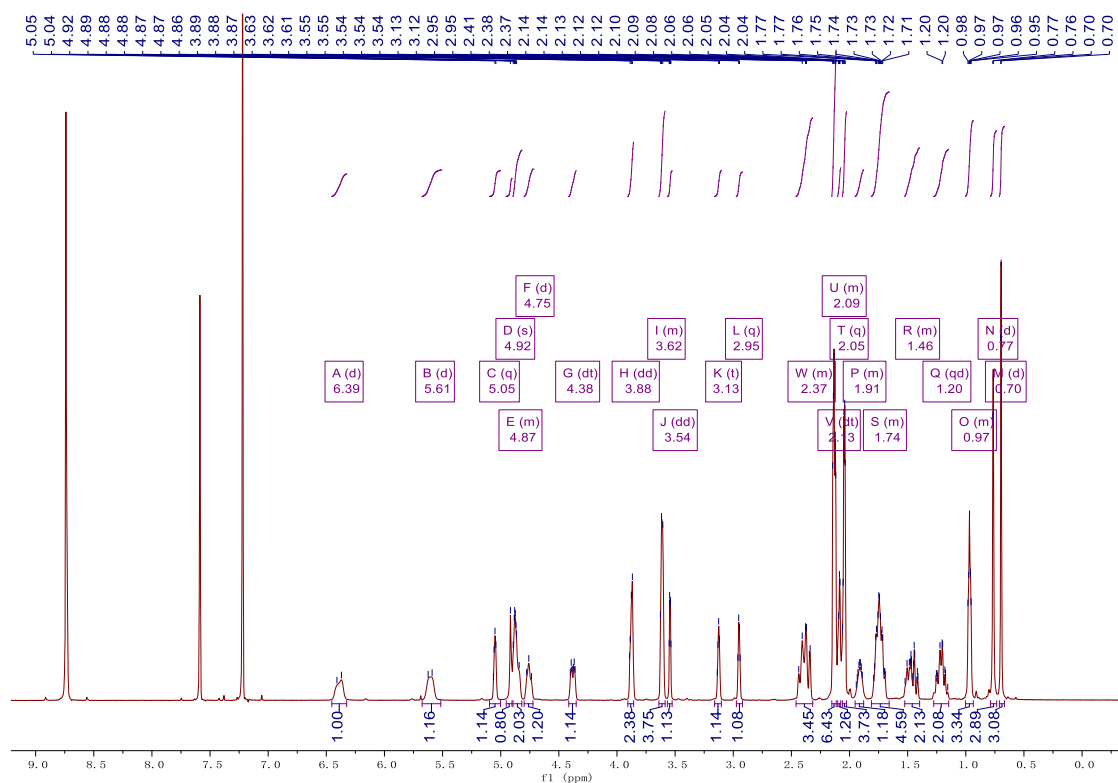


Figure S93. ^1H NMR (500 MHz) spectrum of plantagiolide C (13**) in $\text{C}_5\text{D}_5\text{N}$**

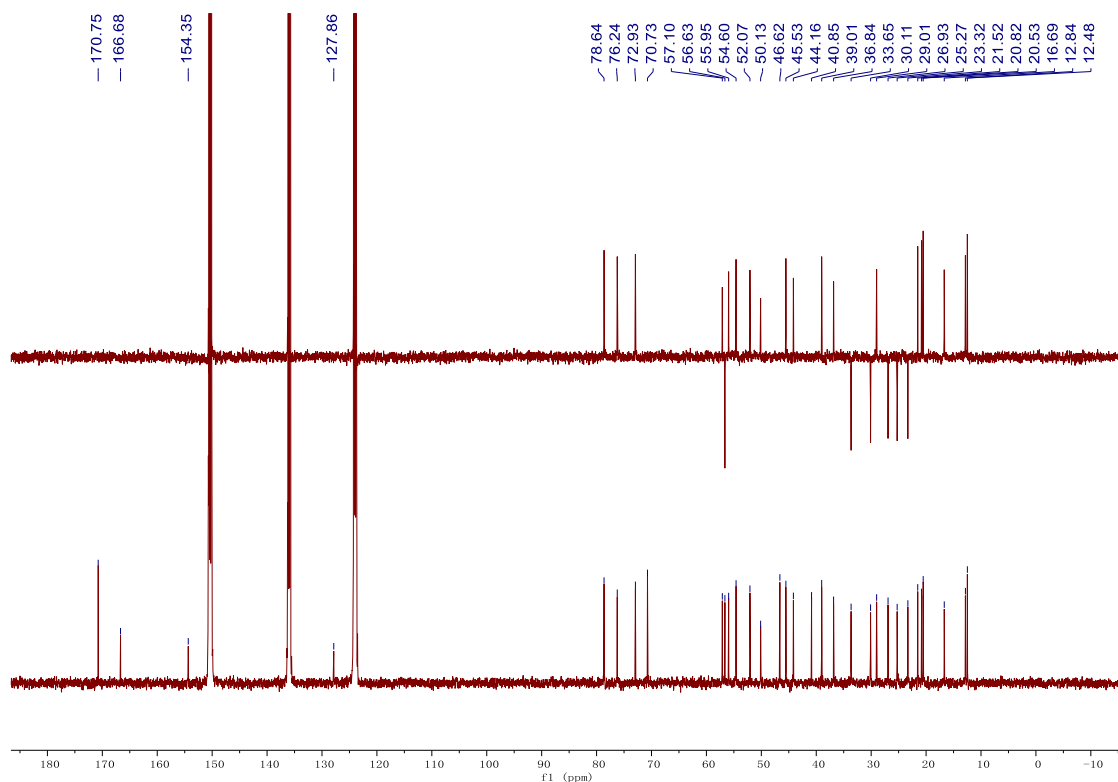


Figure S94. ^{13}C and DEPT-135 NMR (125 MHz) spectra of plantagiolide C (13**) in $\text{C}_5\text{D}_5\text{N}$**

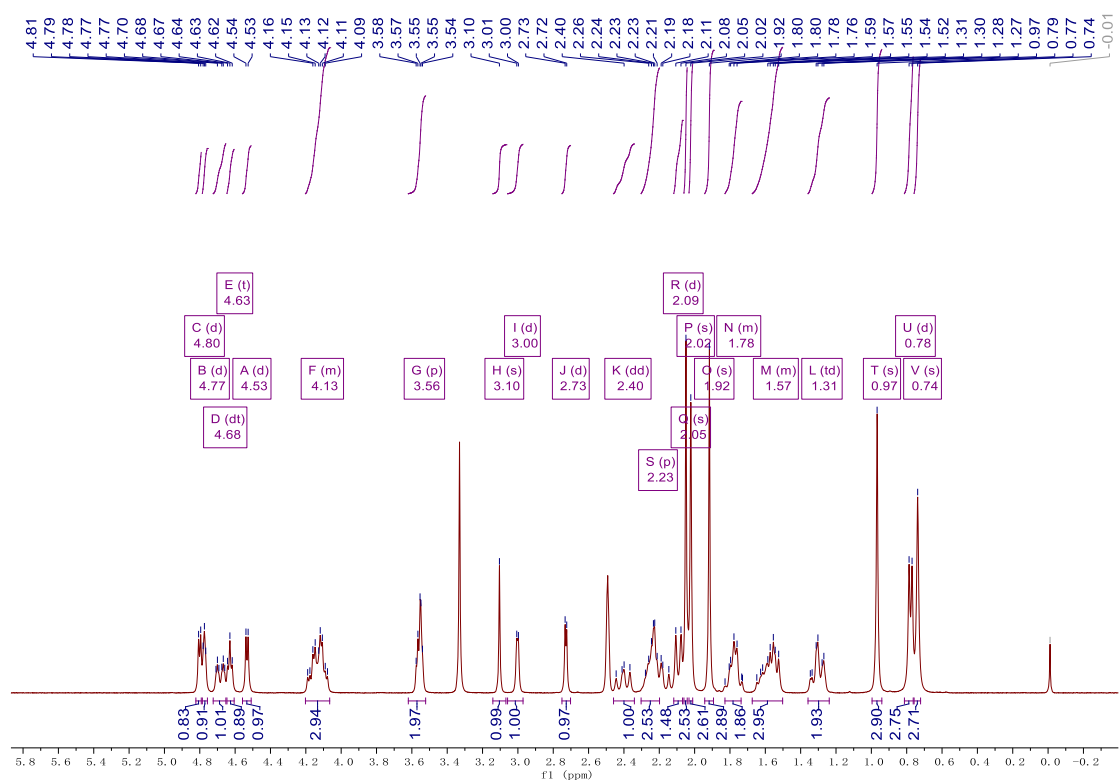


Figure S95. ^1H NMR (400 MHz) spectrum of plantagiolide B (**14**) in $\text{DMSO}-d_6$

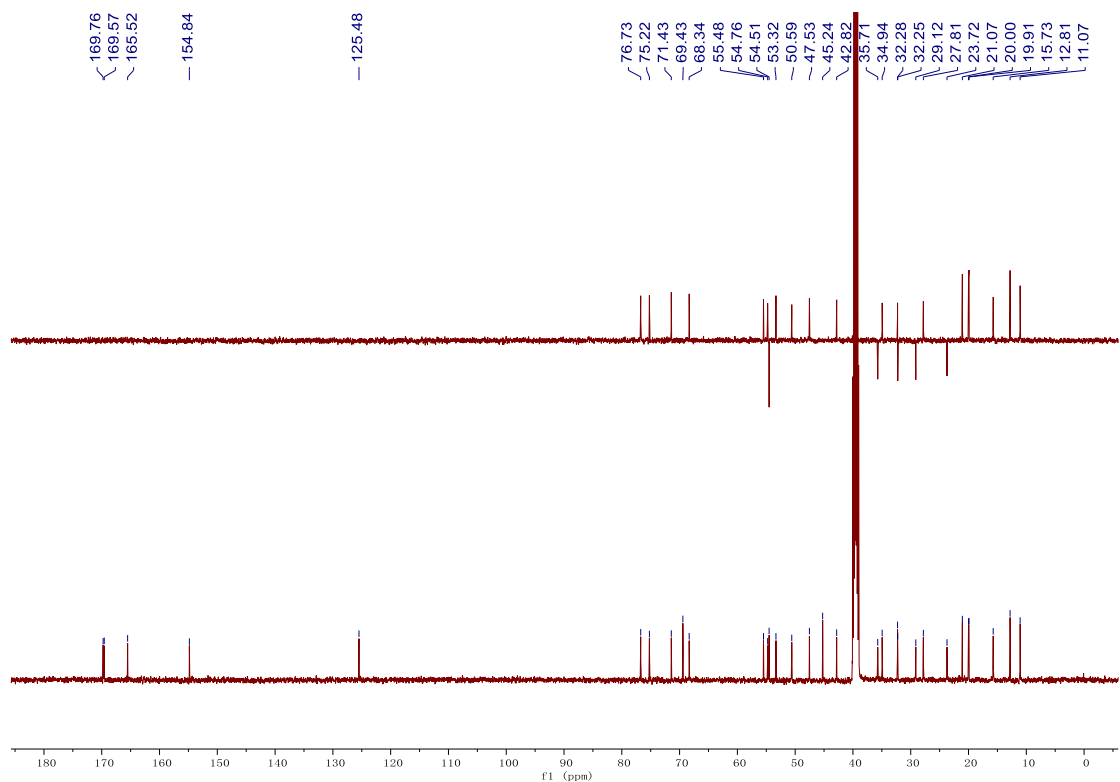


Figure S96. ^{13}C and DEPT-135 NMR (125 MHz) spectra of plantagiolide B (**14**) in $\text{DMSO}-d_6$

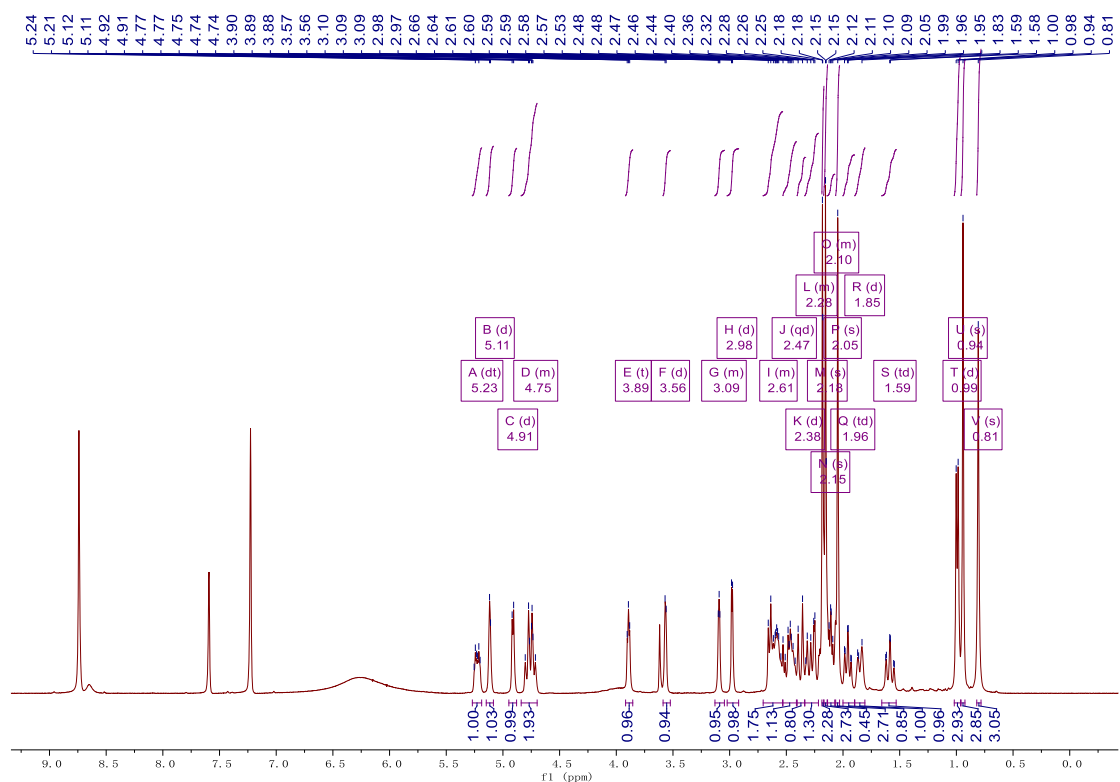


Figure S97. ^1H NMR (400 MHz) spectrum of plantagiolide A (15**) in $\text{C}_5\text{D}_5\text{N}$**

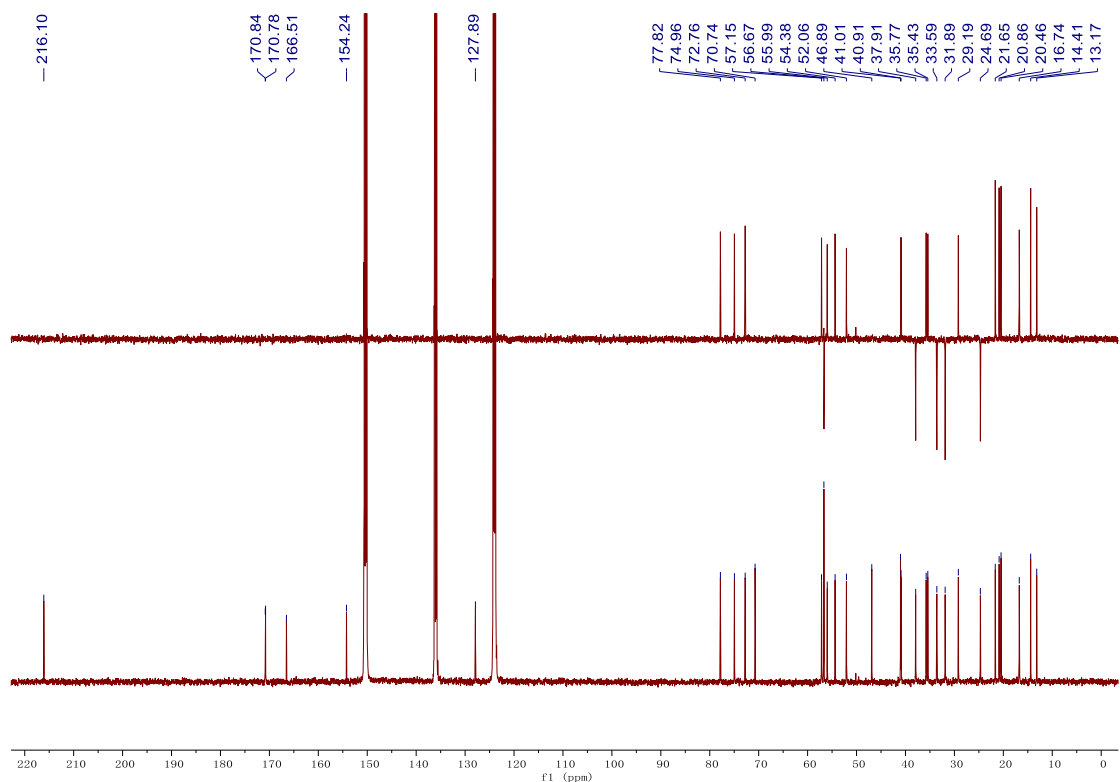


Figure S98. ^{13}C and DEPT-135 NMR (125 MHz) spectra of plantagiolide A (15**) in $\text{C}_5\text{D}_5\text{N}$**

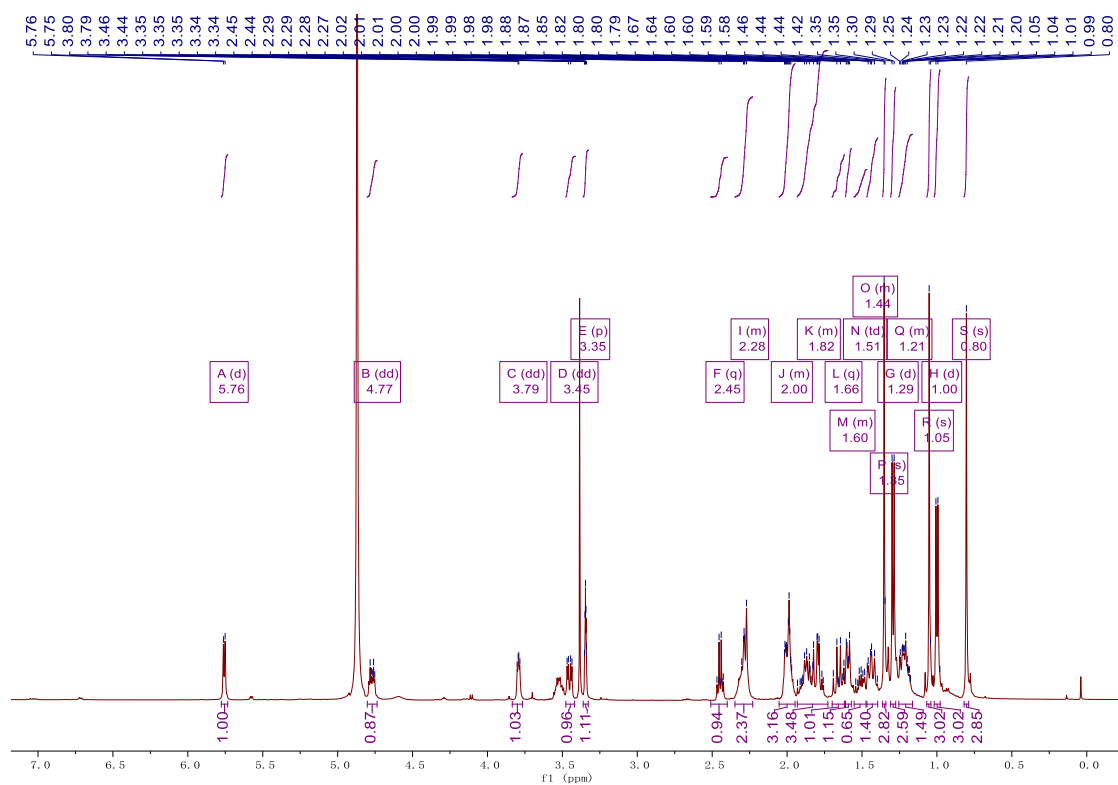


Figure S99. ^1H NMR (500 MHz) spectrum of plantagiolide M (**16**) in CD_3OD

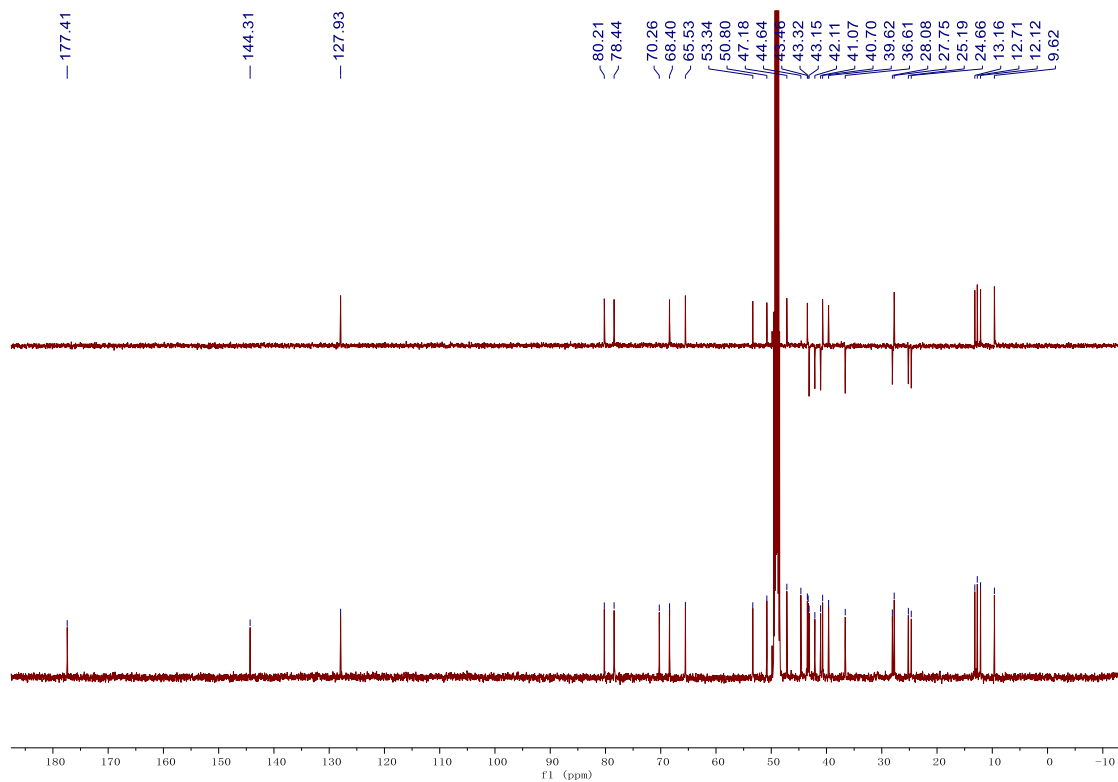


Figure S100. ^{13}C and DEPT-135 NMR (125 MHz) spectra of plantagiolide M (**16**) in CD_3OD

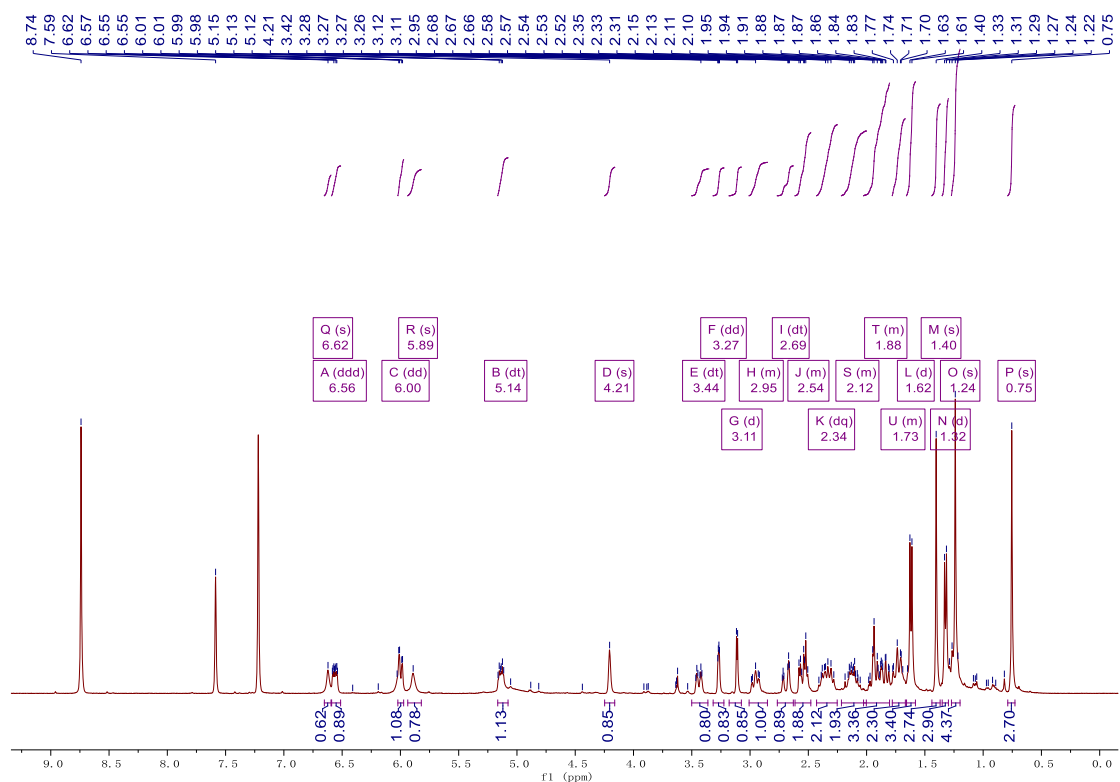


Figure S101. ^1H NMR (400 MHz) spectrum of chantriolide D (**17**) in $\text{C}_5\text{D}_5\text{N}$

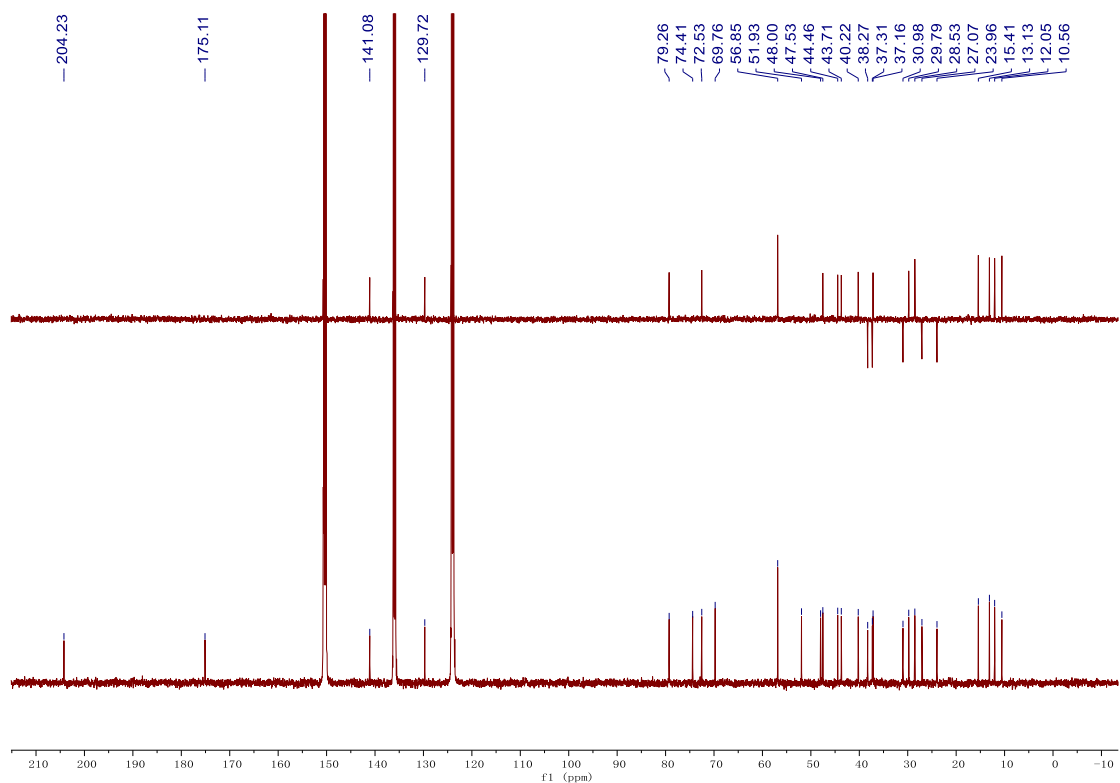


Figure S102. ^{13}C and DEPT-135 NMR (125 MHz) spectra of chantriolide D (**17**) in $\text{C}_5\text{D}_5\text{N}$

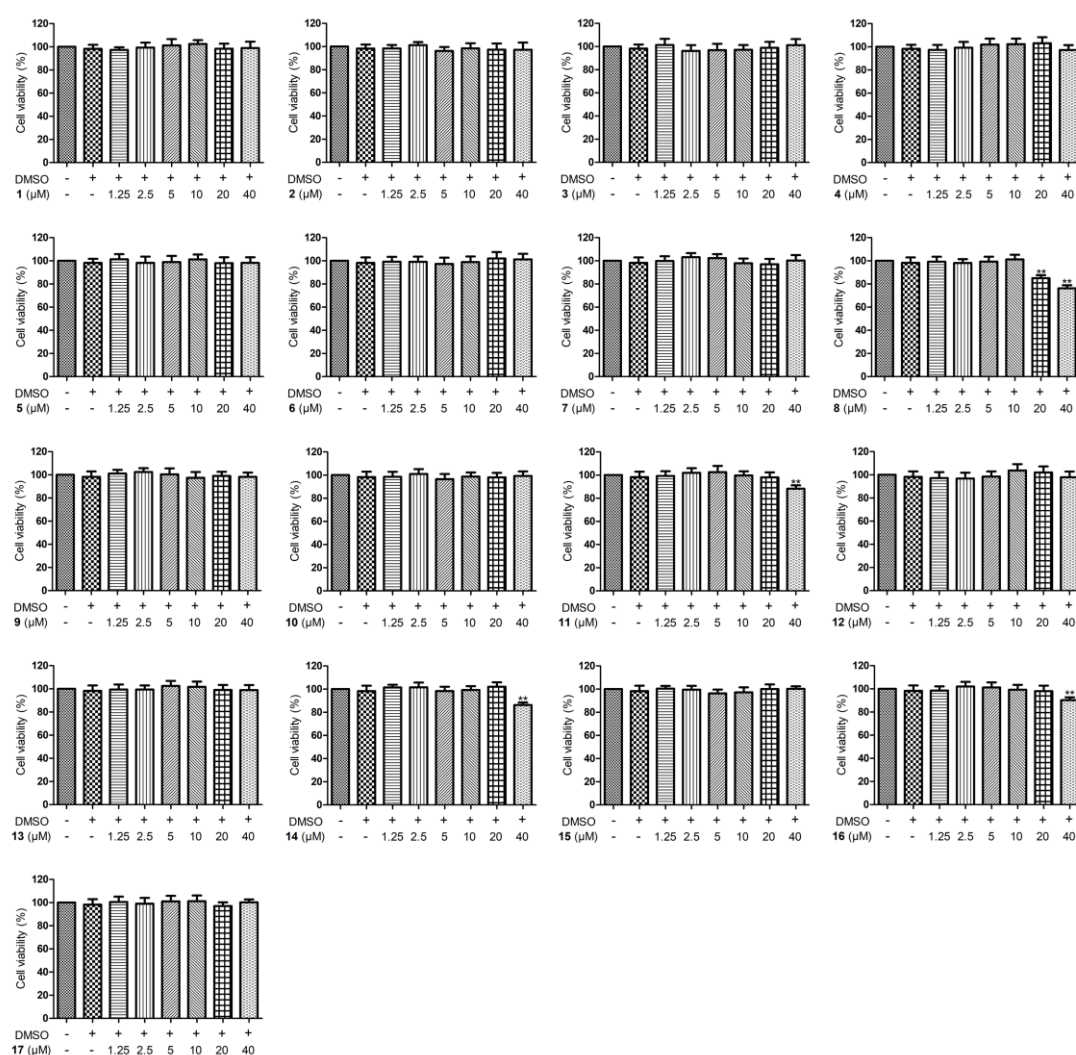


Figure S103. Cytotoxicity of compounds 1–17 on AML-12 hepatocytes. AML-12 cells were treated with different compounds at indicated concentrations for 24 hours. Data are shown as mean \pm S.D., $n = 3$. * $P < 0.05$ and ** $P < 0.01$ vs. DMSO.