Supporting Information for

Withaphysalins from medicinal and edible *Physalis minima* and their anti-inflammatory activities

Table of Content

Figure S1. Key HMBC correlations of typical compounds **1, 2, 3, 6, 10, 12, 15, 18 and 20** 7
Figure S2. Key NOESY/ROESY correlations of typical compounds **1, 2, 3, 6, 10, 12, 15, 18 and 20** ... 8
Figure S3. Calculated NMR data of Physaminim L (**12**) 9
Figure S4. Calculated NMR data of Physaminim M (**13**) 9
Figure S5. Calculated NMR data of Physaminim N (**14**) 9
Figure S6. HRESIMS Spectrum of Withaminilide A (**1**) 10
Figure S7. IR Spectrum of Withaminilide A (**1**) 10
Figure S8. ^{1}H NMR Spectrum of Withaminilide A (**1**) in CD_3OD, 600 MHz 11
Figure S9. ^{13}C NMR Spectrum of Withaminilide A (**1**) in CD_3OD, 150 MHz 11
Figure S10. ^{1}H-^{1}H COSY Spectrum of Withaminilide A (**1**) in CD_3OD 12
Figure S11. HSQC Spectrum of Withaminilide A (**1**) in CD_3OD 12
Figure S12. HMBC Spectrum of Withaminilide A (**1**) in CD_3OD 13
Figure S13. NOESY Spectrum of Withaminilide A (**1**) in CD_3OD 13
Figure S14. Experimental ECD Spectrum of Withaminilide A (**1**) 14
Figure S15. HRESIMS Spectrum of Withaminilide B (**2**) 14
Figure S16. IR Spectrum of Withaminilide B (**2**) 15
Figure S17. ^{1}H NMR Spectrum of Withaminilide B (**2**) in $CDCl_3$, 600 MHz 15
Figure S18. ^{13}C NMR Spectrum of Withaminilide B (**2**) in $CDCl_3$, 125 MHz 16
Figure S19. ^{1}H-^{1}H COSY Spectrum of Withaminilide B (**2**) in $CDCl_3$ 16
Figure S20. HSQC Spectrum of Withaminilide B (**2**) in $CDCl_3$ 17
Figure S21. HMBC Spectrum of Withaminilide B (**2**) in $CDCl_3$ 17
Figure S22. NOESY Spectrum of Withaminilide B (**2**) in $CDCl_3$ 18
Figure S23. Experimental ECD Spectrum of Withaminilide B (**2**) 18
Figure S24. HRESIMS Spectrum of Withaminilide C (**3**) 19
Figure S25. IR Spectrum of Withaminilide C (**3**) 19
Figure S26. ^{1}H NMR Spectrum of Withaminilide C (**3**) in $CDCl_3$, 600 MHz 20
Figure S27. ^{13}C NMR Spectrum of Withaminilide C (**3**) in $CDCl_3$, 150 MHz 20
Figure S28. ^{1}H-^{1}H COSY Spectrum of Withaminilide C (**3**) in $CDCl_3$ 21
Figure S29. HSQC Spectrum of Withaminilide C (**3**) in $CDCl_3$ 21
Figure S30. HMBC Spectrum of Withaminilide C (**3**) in $CDCl_3$ 22
Figure S31. NOESY Spectrum of Withaminilide C (**3**) in $CDCl_3$ 22
Figure S32. Experimental ECD Spectrum of Withaminilide C (**3**) 23
Figure S33. HRESIMS Spectrum of Withaminilide D (**4**) 23
Figure S34. IR Spectrum of Withaminilide D (**4**) 24
Figure S35. ^{1}H NMR Spectrum of Withaminilide D (**4**) in C_5D_5N, 600 MHz 24
Figure S36. ^{13}C NMR Spectrum of Withaminilide D (**4**) in C_5D_5N, 125 MHz 25
Figure S37. ^{1}H-^{1}H COSY Spectrum of Withaminilide D (**4**) in C_5D_5N 25
Figure S38. HSQC Spectrum of Withaminilide D (**4**) in C_5D_5N 26
Figure S39. HMBC Spectrum of Withaminilide D (**4**) in C_5D_5N 26
Figure S40. NOESY Spectrum of Withaminilide D (**4**) in C_5D_5N 27
Figure S41. Experimental ECD Spectrum of Withaminilide D (**4**) 27
Figure S42. HRESIMS Spectrum of Withaminilide E (**5**) 28

Figure S43. IR Spectrum of Withaminilide E (**5**) 28
Figure S44. ^{1}H NMR Spectrum of Withaminilide E (**5**) in $CDCl_3$, 600 MHz 29
Figure S45. ^{13}C NMR Spectrum of Withaminilide E (**5**) in $CDCl_3$, 150 MHz 29
Figure S46. ^{1}H-^{1}H COSY Spectrum of Withaminilide E (**5**) in $CDCl_3$ 30
Figure S47. HSQC Spectrum of Withaminilide E (**5**) in $CDCl_3$ 30
Figure S48. HMBC Spectrum of Withaminilide E (**5**) in $CDCl_3$ 31
Figure S49. NOESY Spectrum of Withaminilide E (**5**) in $CDCl_3$ 31
Figure S50. Experimental ECD Spectrum of Withaminilide E (**5**) 32
Figure S51. HRESIMS Spectrum of Withaminilide F (**6**) 32
Figure S52. IR Spectrum of Withaminilide F (**6**) 33
Figure S53. ^{1}H NMR Spectrum of Withaminilide F (**6**) in $CDCl_3$, 600 MHz 33
Figure S54. ^{13}C NMR Spectrum of Withaminilide F (**6**) in $CDCl_3$, 125 MHz 34
Figure S55. ^{1}H-^{1}H COSY Spectrum of Withaminilide F (**6**) in $CDCl_3$ 34
Figure S56. HSQC Spectrum of Withaminilide F (**6**) in $CDCl_3$ 35
Figure S57. HMBC Spectrum of Withaminilide F (**6**) in $CDCl_3$ 35
Figure S58. NOESY Spectrum of Withaminilide F (**6**) in $CDCl_3$ 36
Figure S59. Experimental ECD Spectrum of Withaminilide F (**6**) 36
Figure S60. HRESIMS Spectrum of Withaminilide G (**7**) 37
Figure S61. IR Spectrum of Withaminilide G (**7**) 37
Figure S62. ^{1}H NMR Spectrum of Withaminilide G (**7**) in $CDCl_3$, 600 MHz 38
Figure S63. ^{13}C NMR Spectrum of Withaminilide G (**7**) in $CDCl_3$, 125 MHz 38
Figure S64. ^{1}H-^{1}H COSY Spectrum of Withaminilide G (**7**) in $CDCl_3$ 39
Figure S65. HSQC Spectrum of Withaminilide G (**7**) in $CDCl_3$ 39
Figure S66. HMBC Spectrum of Withaminilide G (**7**) in $CDCl_3$ 40
Figure S67. NOESY Spectrum of Withaminilide G (**7**) in $CDCl_3$ 40
Figure S68. Experimental ECD Spectrum of Withaminilide G (**7**) 41
Figure S69. HRESIMS Spectrum of Withaminilide H (**8**) 41
Figure S70. IR Spectrum of Withaminilide H (**8**) 42
Figure S71. ^{1}H NMR Spectrum of Withaminilide H (**8**) in CD_3OD, 500 MHz 42
Figure S72. ^{13}C NMR Spectrum of Withaminilide H (**8**) in CD_3OD, 125 MHz 43
Figure S73. ^{1}H-^{1}H COSY Spectrum of Withaminilide H (**8**) in CD_3OD 43
Figure S74. HSQC Spectrum of Withaminilide H (**8**) in CD_3OD 44
Figure S75. HMBC Spectrum of Withaminilide H (**8**) in CD_3OD 44
Figure S76. NOESY Spectrum of Withaminilide H (**8**) in CD_3OD 45
Figure S77. Experimental ECD Spectrum of Withaminilide H (**8**) 45
Figure S78. HRESIMS Spectrum of Withaminilide I (**9**) 46
Figure S79. IR Spectrum of Withaminilide I (**9**) 46
Figure S80. ^{1}H NMR Spectrum of Withaminilide I (**9**) in C_5D_5N, 600 MHz 47
Figure S81. ^{13}C NMR Spectrum of Withaminilide I (**9**) in C_5D_5N, 125 MHz 47
Figure S82. ^{1}H-^{1}H COSY Spectrum of Withaminilide I (**9**) in C_5D_5N 48
Figure S83. HSQC Spectrum of Withaminilide I (**9**) in C_5D_5N 48
Figure S84.HMBC Spectrum of Withaminilide I (**9**) in C_5D_5N 49
Figure S85. NOESY Spectrum of Withaminilide I (**9**) in C_5D_5N 49
Figure S86. Experimental ECD Spectrum of Withaminilide I (**9**) 50

Figure S87. HRESIMS Spectrum of Withaminilide J (**10**) 50
Figure S88. IR Spectrum of Withaminilide J (**10**) 51
Figure S89. ^{1}H NMR Spectrum of Withaminilide J (**10**) in $CDCl_3$, 400 MHz 51
Figure S90. ^{13}C NMR Spectrum of Withaminilide J (**10**) in $CDCl_3$, 125 MHz 52
Figure S91. ^{1}H-^{1}H COSY Spectrum of Withaminilide J (**10**) in $CDCl_3$ 52
Figure S92. HSQC Spectrum of Withaminilide J (**10**) in $CDCl_3$ 53
Figure S93. HMBC Spectrum of Withaminilide J (**10**) in $CDCl_3$ 53
Figure S94. NOESY Spectrum of Withaminilide J (**10**) in $CDCl_3$ 54
Figure S95. Experimental ECD Spectrum of Withaminilide J (**10**) 54
Figure S96. HRESIMS Spectrum of Withaminilide K (**11**) 55
Figure S97. IR Spectrum of Withaminilide K (**11**) 55
Figure S98. ^{1}H NMR Spectrum of Withaminilide K (**11**) in $CDCl_3$, 500 MHz 56
Figure S99. ^{13}C NMR Spectrum of Withaminilide K (**11**) in $CDCl_3$, 125 MHz 56
Figure S100. ^{1}H-^{1}H COSY Spectrum of Withaminilide K (**11**) in $CDCl_3$ 57
Figure S101. HSQC Spectrum of Withaminilide K (**11**) in $CDCl_3$ 57
Figure S102. HMBC Spectrum of Withaminilide K (**11**) in $CDCl_3$ 58
Figure S103. NOESY Spectrum of Withaminilide K (**11**) in $CDCl_3$ 58
Figure S104. Experimental ECD Spectrum of Withaminilide K (**11**) 59
Figure S105. HRESIMS Spectrum of Withaminilide L (**12**) 59
Figure S106. IR Spectrum of Withaminilide L (**12**) 60
Figure S107. ^{1}H NMR Spectrum of Withaminilide L (**12**) in $CDCl_3$, 600 MHz 60
Figure S108. ^{13}C NMR Spectrum of Withaminilide L (**12**) in $CDCl_3$, 125 MHz 61
Figure S109. ^{1}H-^{1}H COSY Spectrum of Withaminilide L (**12**) in $CDCl_3$ 61
Figure S110. HSQC Spectrum of Withaminilide L (**12**) in $CDCl_3$ 62
Figure S111. HMBC Spectrum of Withaminilide L (**12**) in $CDCl_3$ 62
Figure S112. NOESY Spectrum of Withaminilide L (**12**) in $CDCl_3$ 63
Figure S113. Experimental ECD Spectrum of Withaminilide L (**12**) 63
Figure S114. HRESIMS Spectrum of Withaminilide M (**13**) 64
Figure S115. IR Spectrum of Withaminilide M (**13**) 64
Figure S116. ^{1}H NMR Spectrum of Withaminilide M (**13**) in CD_3OD, 500 MHz 65
Figure S117. ^{13}C NMR Spectrum of Withaminilide M (**13**) in CD_3OD, 125 MHz 65
Figure S118. ^{1}H-^{1}H COSY Spectrum of Withaminilide M (**13**) in CD_3OD 66
Figure S119. HSQC Spectrum of Withaminilide M (**13**) in CD_3OD 66
Figure S120. HMBC Spectrum of Withaminilide M (**13**) in CD_3OD 67
Figure S121. NOESY Spectrum of Withaminilide M (**13**) in CD_3OD 67
Figure S122. Experimental ECD Spectrum of Withaminilide M (**13**) 68
Figure S123. HRESIMS Spectrum of Withaminilide N (**14**) 68
Figure S124. IR Spectrum of Withaminilide N (**14**) 69
Figure S125. ^{1}H NMR Spectrum of Withaminilide N (**14**) in C_5D_5N, 600 MHz 69
Figure S126. ^{13}C NMR Spectrum of Withaminilide N (**14**) in C_5D_5N, 125 MHz 70
Figure S127. ^{1}H-^{1}H COSY Spectrum of Withaminilide N (**14**) in C_5D_5N 70
Figure S128. HSQC Spectrum of Withaminilide N (**14**) in C_5D_5N 71
Figure S129. HMBC Spectrum of Withaminilide N (**14**) in C_5D_5N 71
Figure S130. NOESY Spectrum of Withaminilide N (**14**) in C_5D_5N 72

Figure S131. Experimental ECD Spectrum of Withaminilide N (**14**)....72
Figure S132. HRESIMS Spectrum of Withaminilide O (**15**)....73
Figure S133. IR Spectrum of Withaminilide O (**15**)....73
Figure S134. ^{1}H NMR Spectrum of Withaminilide O (**15**) in $CDCl_3$, 600 MHz....74
Figure S135. ^{13}C NMR Spectrum of Withaminilide O (**15**) in $CDCl_3$, 150 MHz....74
Figure S136. ^{1}H-^{1}H COSY Spectrum of Withaminilide O (**15**) in $CDCl_3$....75
Figure S137. HSQC Spectrum of Withaminilide O (**15**) in $CDCl_3$....75
Figure S138. HMBC Spectrum of Withaminilide O (**15**) in $CDCl_3$....76
Figure S139. NOESY Spectrum of Withaminilide O (**15**) in $CDCl_3$....76
Figure S140. Experimental ECD Spectrum of Withaminilide O (**15**)....77
Figure S141. HRESIMS Spectrum of Withaminilide P (**16**)....77
Figure S142. IR Spectrum of Withaminilide P (**16**)....78
Figure S143. ^{1}H NMR Spectrum of Withaminilide P (**16**) in $CDCl_3$, 600 MHz....78
Figure S144. ^{13}C NMR Spectrum of Withaminilide P (**16**) in $CDCl_3$, 125 MHz....79
Figure S145. ^{1}H-^{1}H COSY Spectrum of Withaminilide P (**16**) in $CDCl_3$....79
Figure S146. HSQC Spectrum of Withaminilide P (**16**) in $CDCl_3$....80
Figure S147. HMBC Spectrum of Withaminilide P (**16**) in $CDCl_3$....80
Figure S148. NOESY Spectrum of Withaminilide P (**16**) in $CDCl_3$....81
Figure S149. Experimental ECD Spectrum of Withaminilide P (**16**)....81
Figure S150. HRESIMS Spectrum of Withaminilide Q (**17**)....82
Figure S151. IR Spectrum of Withaminilide Q (**17**)....82
Figure S152. ^{1}H NMR Spectrum of Withaminilide Q (**17**) in C_5D_5N, 600 MHz....83
Figure S153. ^{13}C NMR Spectrum of Withaminilide Q (**17**) in C_5D_5N, 125 MHz....83
Figure S154. ^{1}H-^{1}H COSY Spectrum of Withaminilide Q (**17**) in C_5D_5N....84
Figure S155. HSQC Spectrum of Withaminilide Q (**17**) in C_5D_5N....84
Figure S156. HMBC Spectrum of Withaminilide Q (**17**) in C_5D_5N....85
Figure S157. NOESY Spectrum of Withaminilide Q (**17**) in C_5D_5N....85
Figure S158. Experimental ECD Spectrum of Withaminilide Q (**17**)....86
Figure S159. HRESIMS Spectrum of Withaminilide R (**18**)....86
Figure S160. IR Spectrum of Withaminilide R (**18**)....87
Figure S161. ^{1}H NMR Spectrum of Withaminilide R (**18**) in $CDCl_3$, 600 MHz....87
Figure S162. ^{13}C NMR Spectrum of Withaminilide R (**18**) in $CDCl_3$, 125 MHz....88
Figure S163. ^{1}H-^{1}H COSY Spectrum of Withaminilide R (**18**) in $CDCl_3$....88
Figure S164. HSQC Spectrum of Withaminilide R (**18**) in $CDCl_3$....89
Figure S165. HMBC Spectrum of Withaminilide R (**18**) in $CDCl_3$....89
Figure S166. ROESY Spectrum of Withaminilide R (**18**) in $CDCl_3$....90
Figure S167. Experimental ECD Spectrum of Withaminilide R (**18**)....90
Figure S168. HRESIMS Spectrum of Withaminilide S (**19**)....91
Figure S169. IR Spectrum of Withaminilide S (**19**)....91
Figure S170. ^{1}H NMR Spectrum of Withaminilide S (**19**) in $CDCl_3$, 600 MHz....92
Figure S171. ^{13}C NMR Spectrum of Withaminilide S (**19**) in $CDCl_3$, 125 MHz....92
Figure S172. ^{1}H-^{1}H COSY Spectrum of Withaminilide S (**19**) in $CDCl_3$....93
Figure S173. HSQC Spectrum of Withaminilide S (**19**) in $CDCl_3$....93
Figure S174. HMBC Spectrum of Withaminilide S (**19**) in $CDCl_3$....94

Figure S175. NOESY Spectrum of Withaminilide S (**19**) in $CDCl_3$ 94
Figure S176. Experimental ECD Spectrum of Withaminilide S (**19**) 95
Figure S177. HRESIMS Spectrum of Withaminilide T (**20**) 95
Figure S178. IR Spectrum of Withaminilide T (**20**) 96
Figure S179. ^{1}H NMR Spectrum of Withaminilide T (**20**) in $CDCl_3$, 600 MHz 96
Figure S180. ^{13}C NMR Spectrum of Withaminilide T (**20**) in $CDCl_3$, 125 MHz 97
Figure S181. ^{1}H-^{1}H COSY Spectrum of Withaminilide T (**20**) in $CDCl_3$ 97
Figure S182. HSQC Spectrum of Withaminilide T (**20**) in $CDCl_3$ 98
Figure S183. HMBC Spectrum of Withaminilide T (**20**) in $CDCl_3$ 98
Figure S184. NOESY Spectrum of Withaminilide T (**20**) in $CDCl_3$ 99
Figure S185. Experimental ECD Spectrum of Withaminilide T (**20**) 99
Figure S186. HRESIMS Spectrum of Withaminilide U (**21**) 100
Figure S187. IR Spectrum of Withaminilide U (**21**) 100
Figure S188. ^{1}H NMR Spectrum of Withaminilide U (**21**) in $CDCl_3$, 600 MHz 101
Figure S189. ^{13}C NMR Spectrum of Withaminilide U (**21**) in $CDCl_3$, 125 MHz 101
Figure S190. ^{1}H-^{1}H COSY Spectrum of Withaminilide U (**21**) in $CDCl_3$ 102
Figure S191. HSQC Spectrum of Withaminilide U (**21**) in $CDCl_3$ 102
Figure S192. HMBC Spectrum of Withaminilide U (**21**) in $CDCl_3$ 103
Figure S193. NOESY Spectrum of Withaminilide U (**21**) in $CDCl_3$ 103
Figure S194. Experimental ECD Spectrum of Withaminilide U (**21**) 104
Figure S195. HRESIMS Spectrum of Withaminilide V (**22**) 104
Figure S196. IR Spectrum of Withaminilide V (**22**) 105
Figure S197. ^{1}H NMR Spectrum of Withaminilide V (**22**) in CD_3OD, 600 MHz 105
Figure S198. ^{13}C NMR Spectrum of Withaminilide V (**22**) in CD_3OD, 125 MHz 106
Figure S199. ^{1}H-^{1}H COSY Spectrum of Withaminilide V (**22**) in CD_3OD 106
Figure S200. HSQC Spectrum of Withaminilide V (**22**) in CD_3OD 107
Figure S201.HMBC Spectrum of Withaminilide V (**22**) in CD_3OD 107
Figure S202. NOESY Spectrum of Withaminilide V (**22**) in CD_3OD 108
Figure S203. Experimental ECD Spectrum of Withaminilide V (**22**) 108
Figure S204. ^{1}H NMR Spectrum of Withaminilide F (**6**) in CD_3OD, 400 MHz 109
Figure S205. ^{13}C NMR Spectrum of Withaminilide F (**6**) in CD_3OD, 150 MHz 109
Figure S206. ^{1}H NMR Spectrum of Withaminilide F (**6**) in C_5D_5N, 600 MHz 110
Figure S207. ^{13}C NMR Spectrum of Withaminilide F (**6**) in C_5D_5N, 150 MHz 110

^{1}H and ^{13}C NMR data of Withaminilide F (6) in CD_3OD 111
^{1}H and ^{13}C NMR data of Withaminilide F (6) in C_5D_5N 111

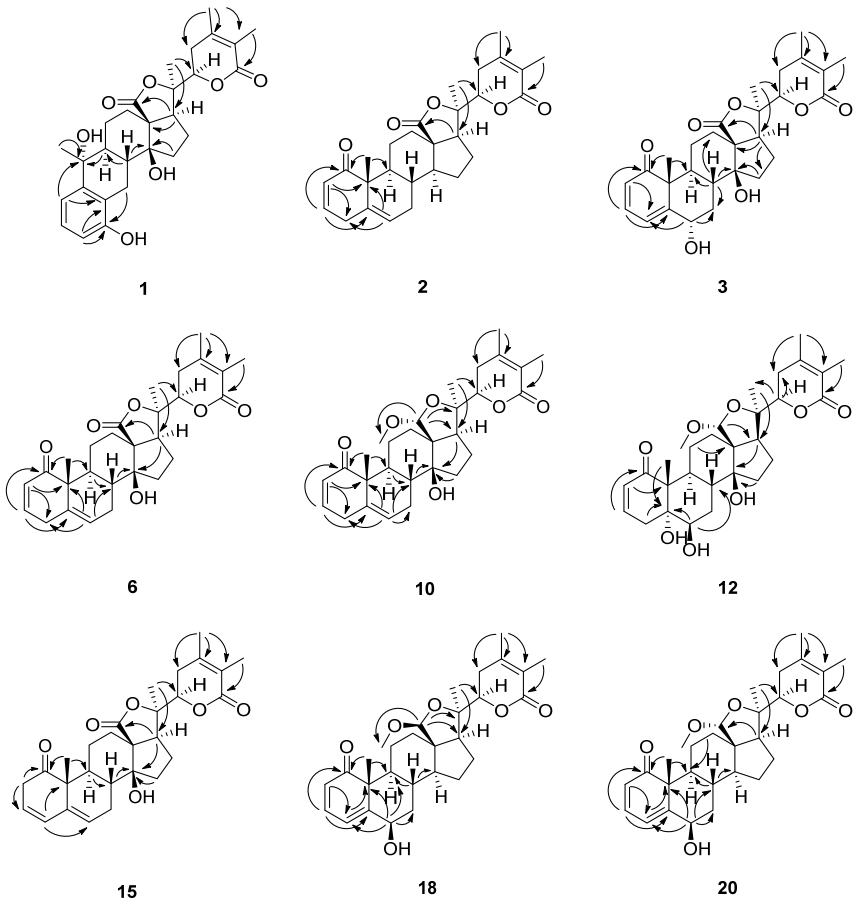


Figure S1. Key HMBC correlations of typical compounds **1, 2, 3, 6, 10, 12, 15, 18 and 20**

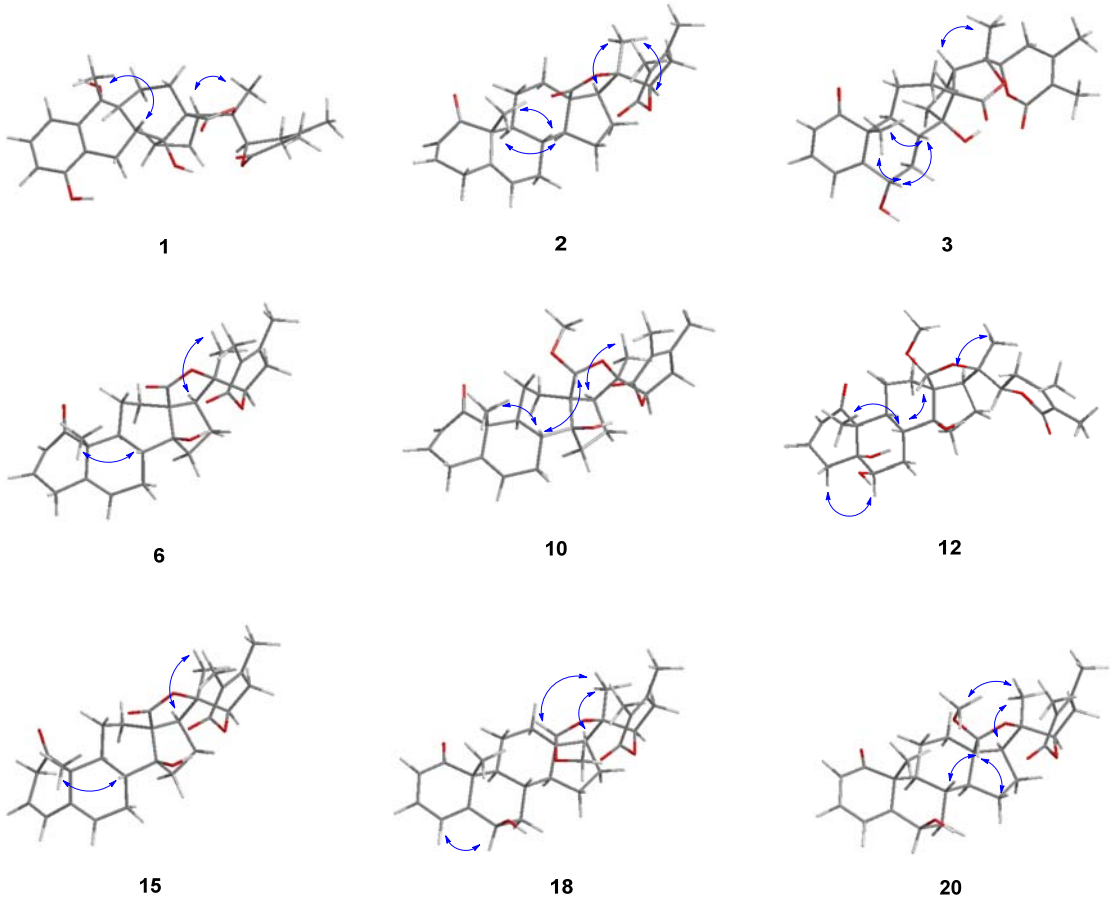


Figure S2. Key NOESY/ROESY correlations of typical compounds **1, 2, 3, 6, 10, 12, 15, 18 and 20**

12a 12b

Custom parameters	1	2
sDP4+ (H data)	0.00%	100.00%
sDP4+ (C data)	0.05%	99.95%
sDP4+ (all data)	0.00%	100.00%
uDP4+ (H data)	0.00%	100.00%
uDP4+ (C data)	0.00%	100.00%
uDP4+ (all data)	0.00%	100.00%
DP4+ (H data)	0.00%	100.00%
DP4+ (C data)	0.00%	100.00%
DP4+ (all data)	0.00%	100.00%

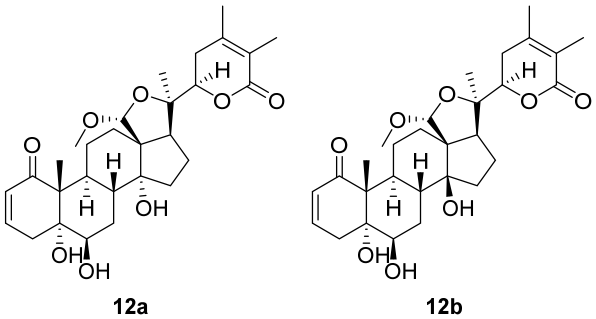


Figure S3. Calculated NMR data of Physaminim L (**12**)

13a 13b

Custom parameters	1	2
sDP4+ (H data)	0.00%	100.00%
sDP4+ (C data)	0.00%	100.00%
sDP4+ (all data)	0.00%	100.00%
uDP4+ (H data)	0.00%	100.00%
uDP4+ (C data)	0.00%	100.00%
uDP4+ (all data)	0.00%	100.00%
DP4+ (H data)	0.00%	100.00%
DP4+ (C data)	0.00%	100.00%
DP4+ (all data)	0.00%	100.00%

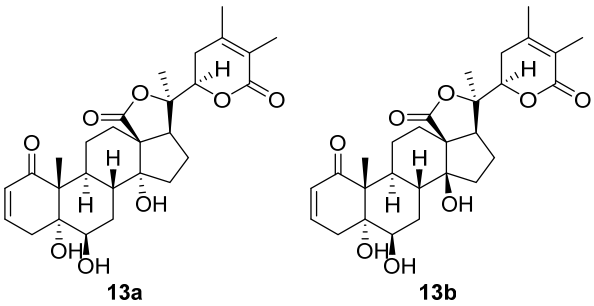


Figure S4. Calculated NMR data of Physaminim M (**13**)

14a 14b

Custom parameters	1	2
sDP4+ (H data)	91.79%	8.21%
sDP4+ (C data)	0.00%	100.00%
sDP4+ (all data)	0.03%	99.97%
uDP4+ (H data)	98.93%	1.07%
uDP4+ (C data)	0.00%	100.00%
uDP4+ (all data)	0.00%	100.00%
DP4+ (H data)	99.90%	0.10%
DP4+ (C data)	0.00%	100.00%
DP4+ (all data)	0.00%	100.00%

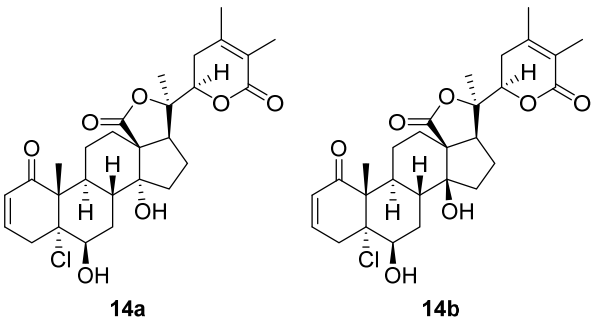


Figure S5. Calculated NMR data of Physaminim N (**14**)

Elemental Composition Report

Tolerance = 3.0 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

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

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Minimum:	80.00					-1.5		
Maximum:	100.00			3.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
527.2308	527.2281	2.7	5.1	12.5	623.4	n/a	n/a	C29H35O9

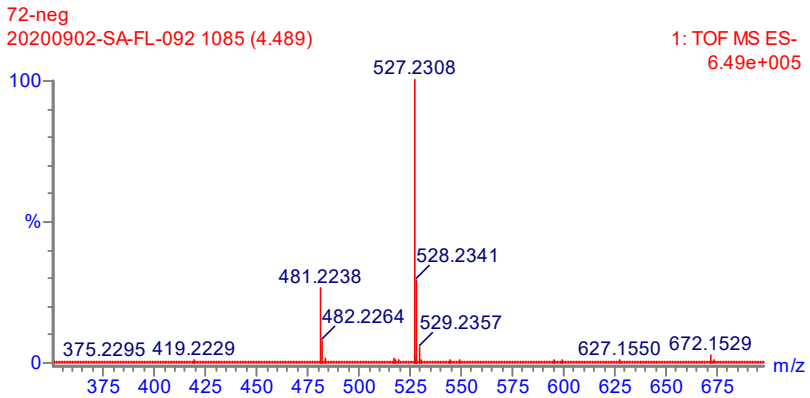


Figure S6. HRESIMS Spectrum of Withaminilide A (**1**)

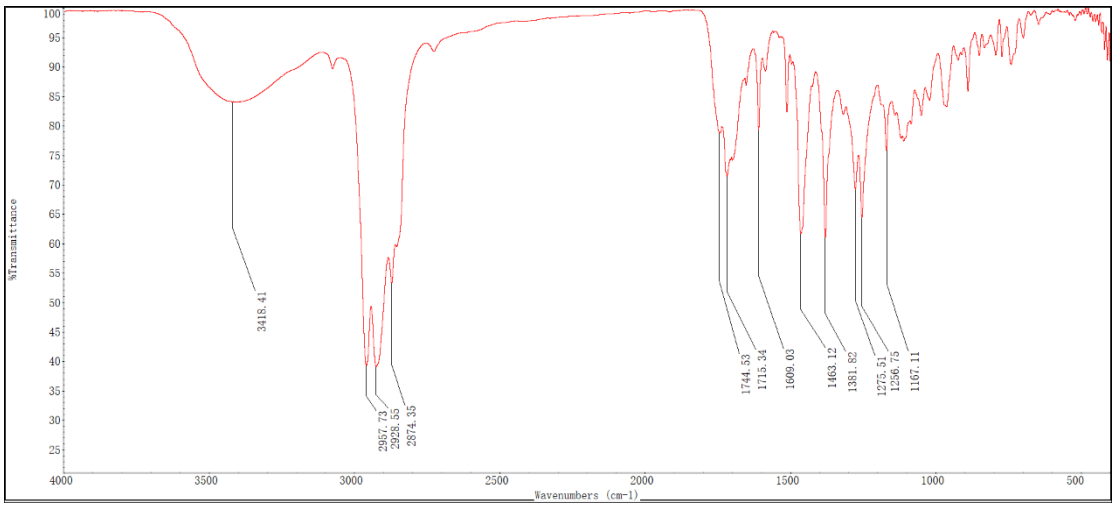


Figure S7. IR Spectrum of Withaminilide A (**1**)

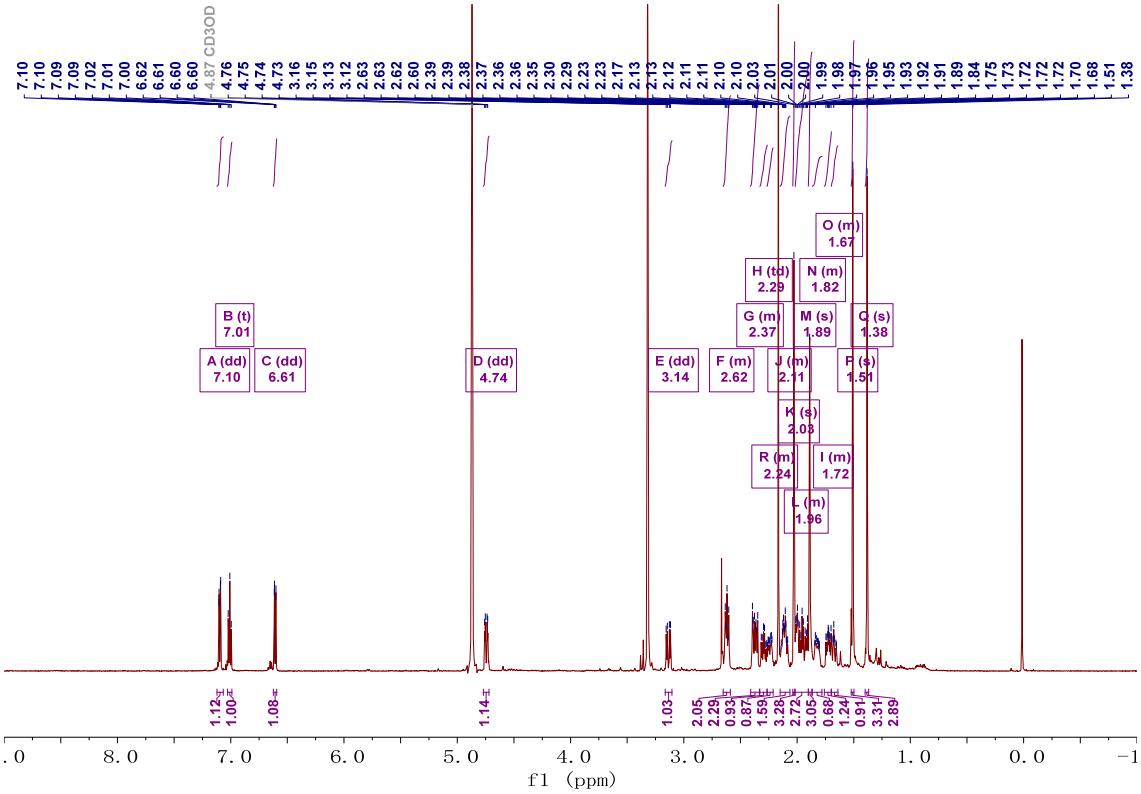


Figure S8. ^{1}H NMR Spectrum of Withaminilide A (**1**) in CD_3OD, 600 MHz

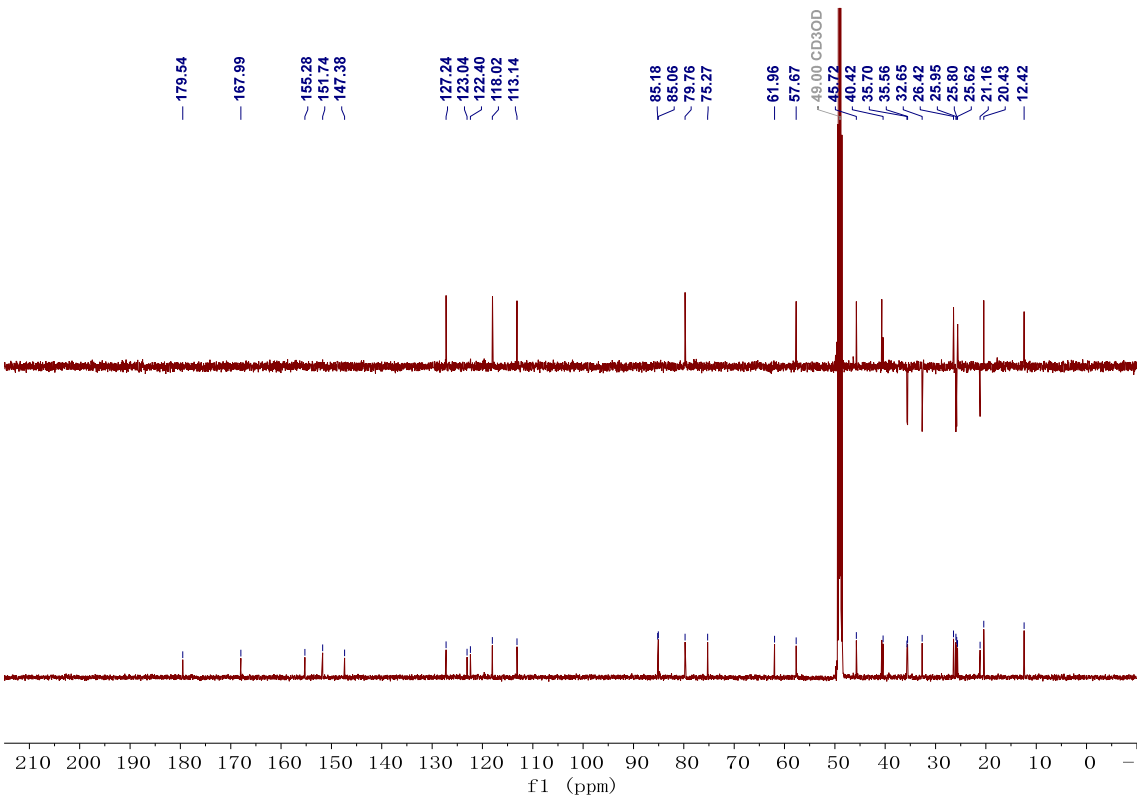


Figure S9. ^{13}C NMR Spectrum of Withaminilide A (**1**) in CD_3OD, 150 MHz

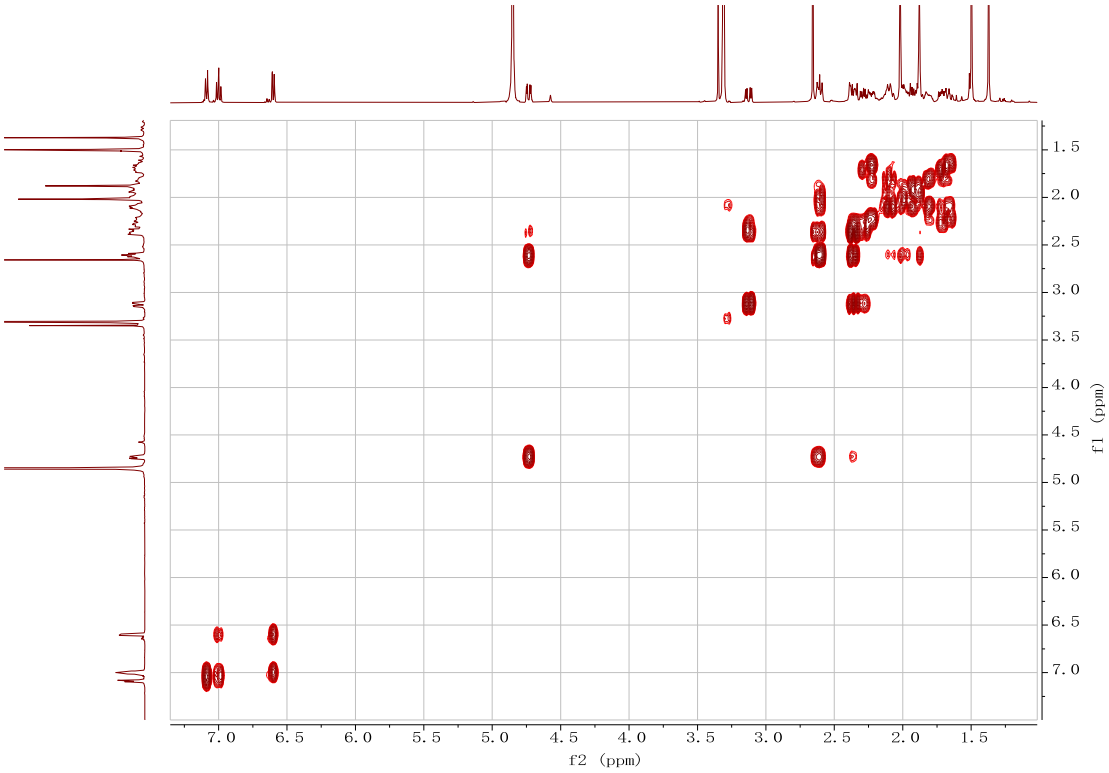


Figure S10. ^{1}H-^{1}H COSY Spectrum of Withaminilide A (**1**) in CD_3OD

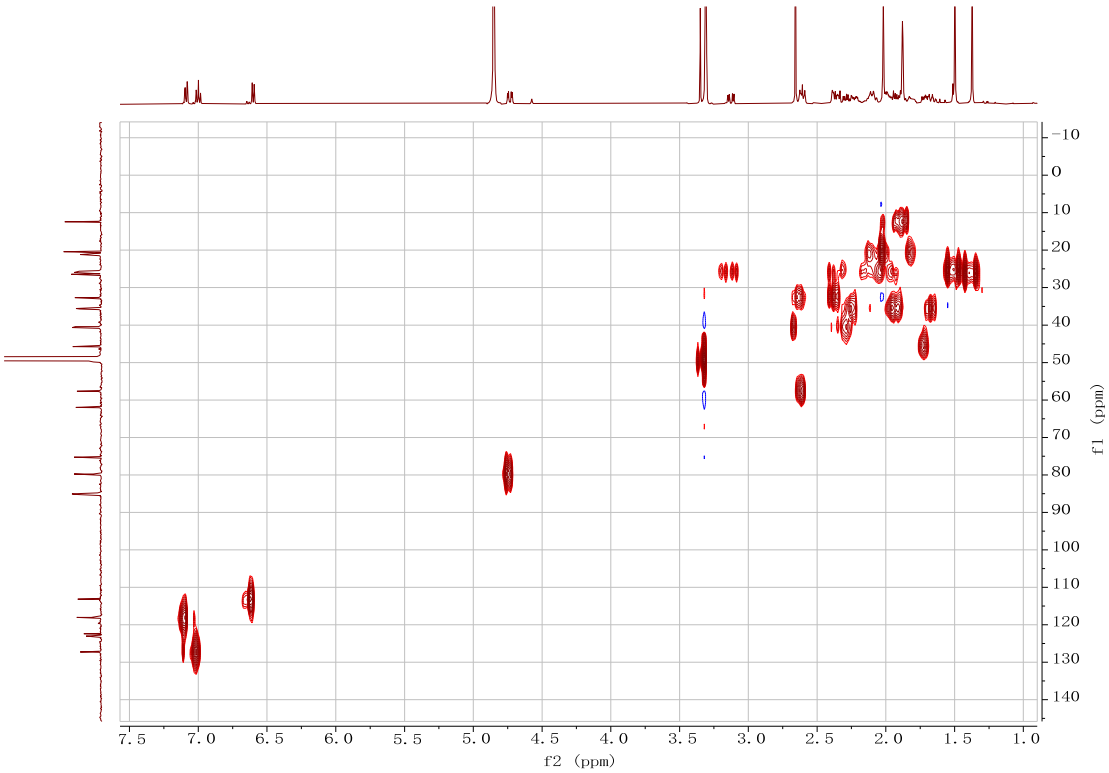


Figure S11. HSQC Spectrum of Withaminilide A (**1**) in CD_3OD

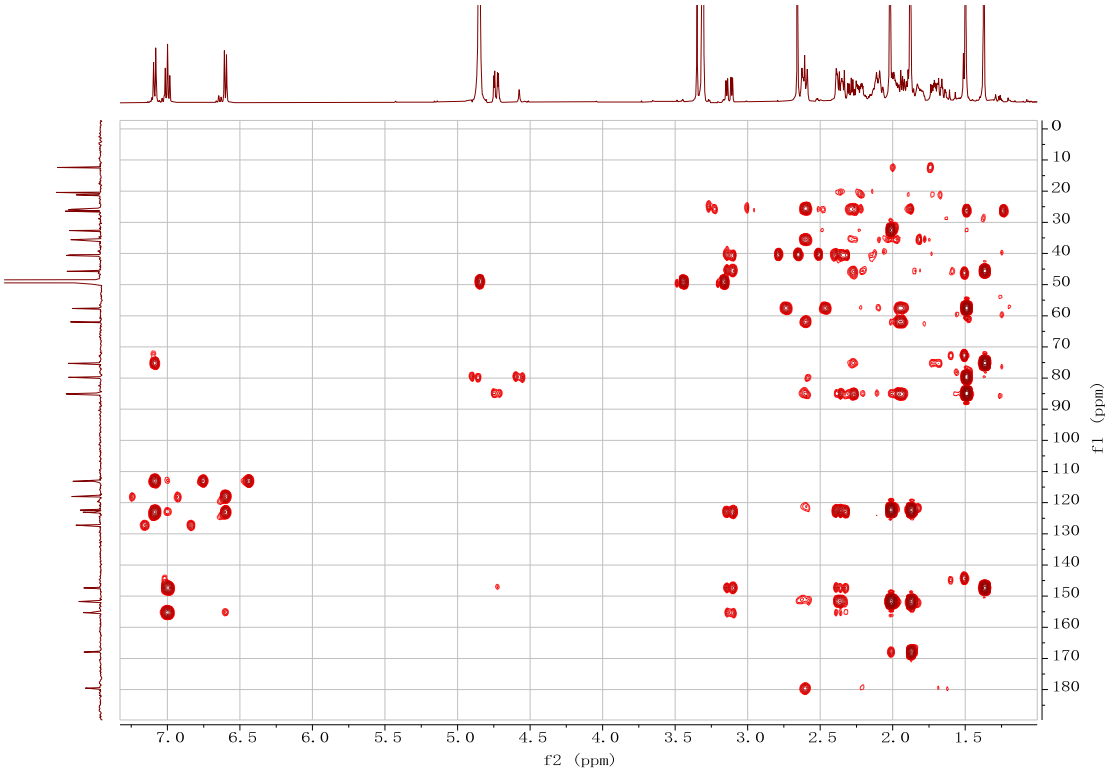


Figure S12. HMBC Spectrum of Withaminilide A (**1**) in CD_3OD

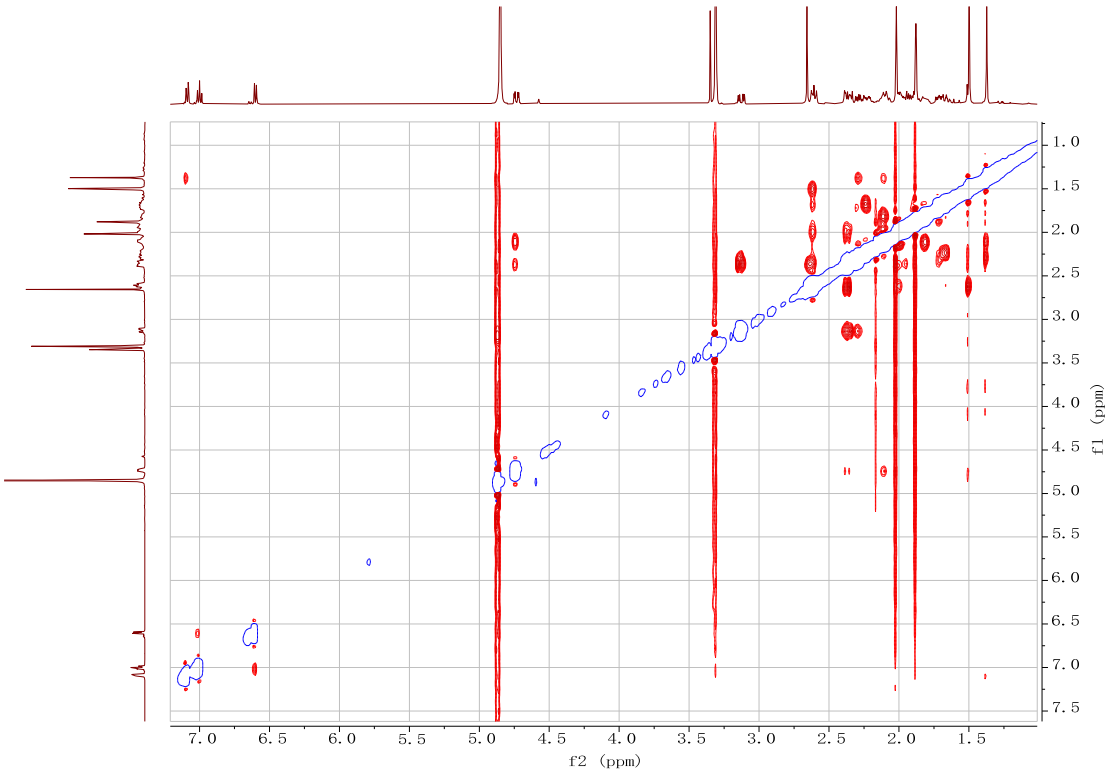


Figure S13. NOESY Spectrum of Withaminilide A (**1**) in CD_3OD

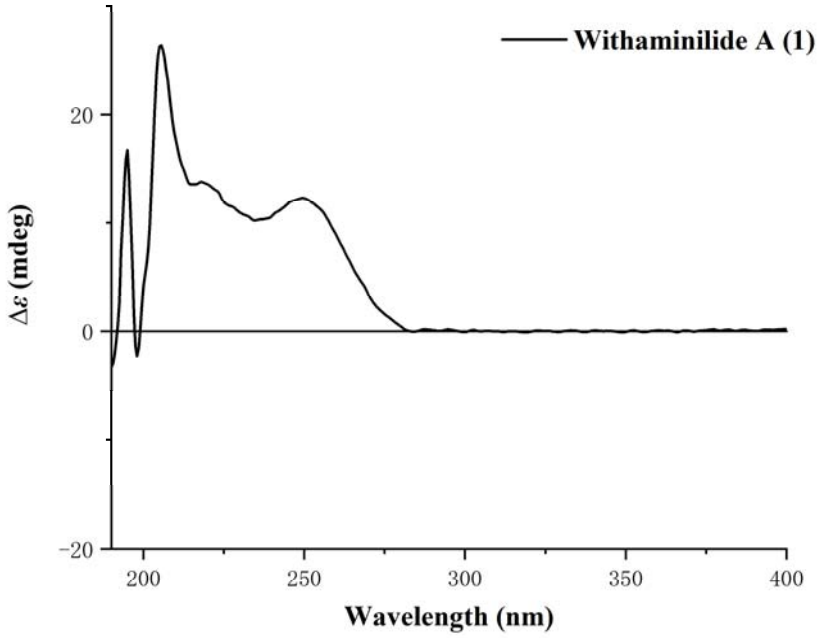


Figure S14. Experimental ECD Spectrum of Withaminilide A (**1**)

Elemental Composition Report
Single Mass Analysis
Tolerance = 1.0 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
206 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200 Na: 0-1

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
451.2483	451.2484	-0.1	-0.2	11.5	635.4	n/a	n/a	C28H35O5

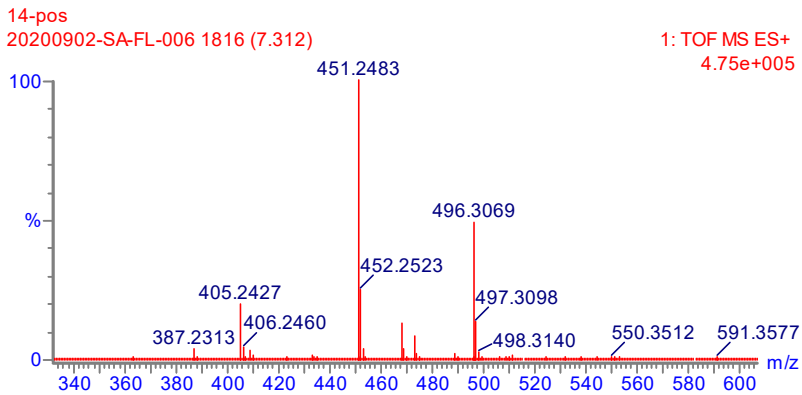


Figure S15. HRESIMS Spectrum of Withaminilide B (**2**)

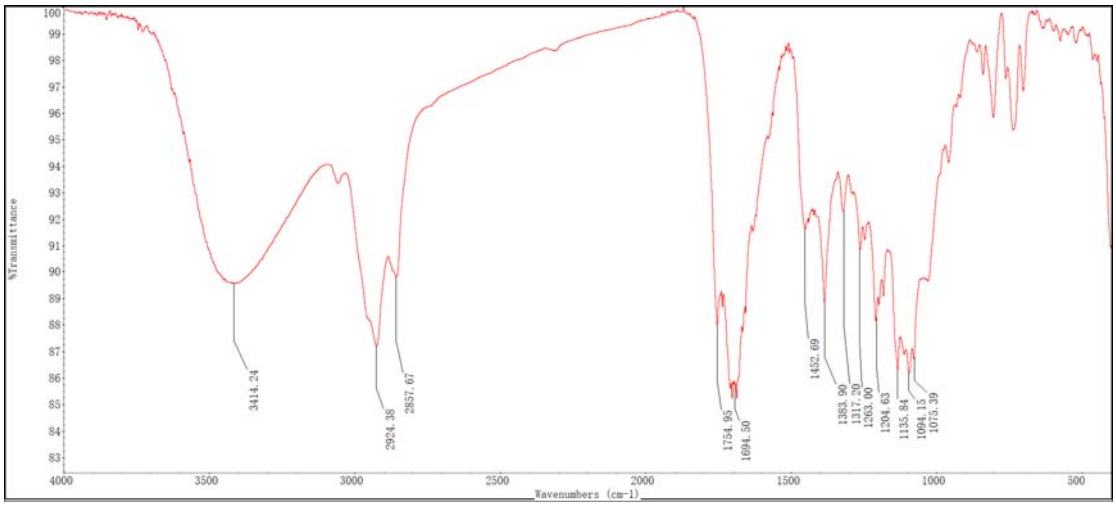


Figure S16. IR Spectrum of Withaminilide B (**2**)

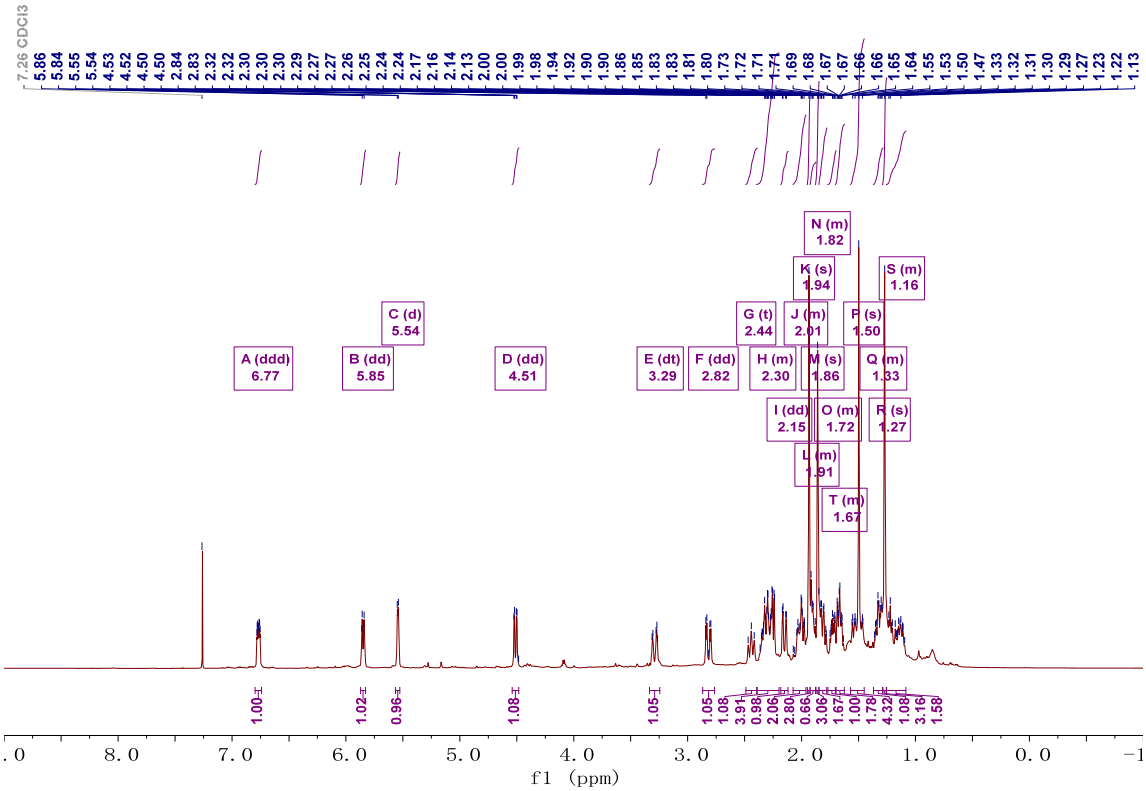


Figure S17. ^{1}H NMR Spectrum of Withaminilide B (**2**) in $CDCl_3$, 600 MHz

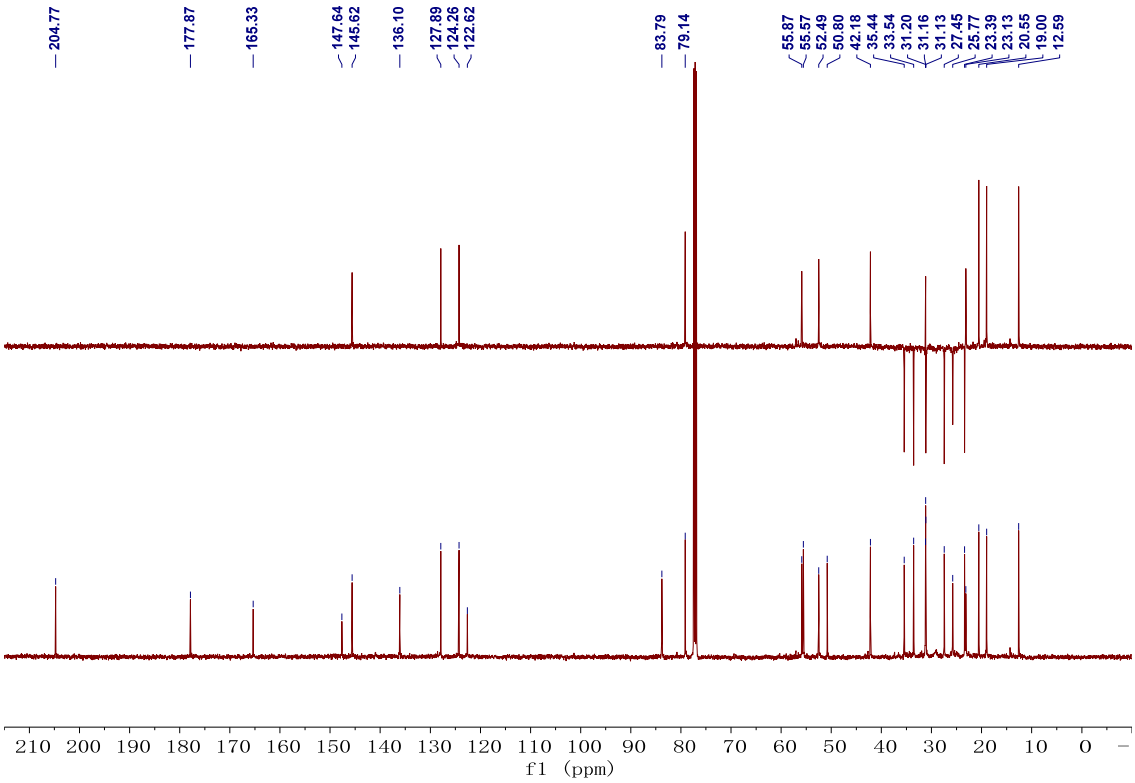


Figure S18. ^{13}C NMR Spectrum of Withaminilide B (**2**) in $CDCl_3$, 125 MHz

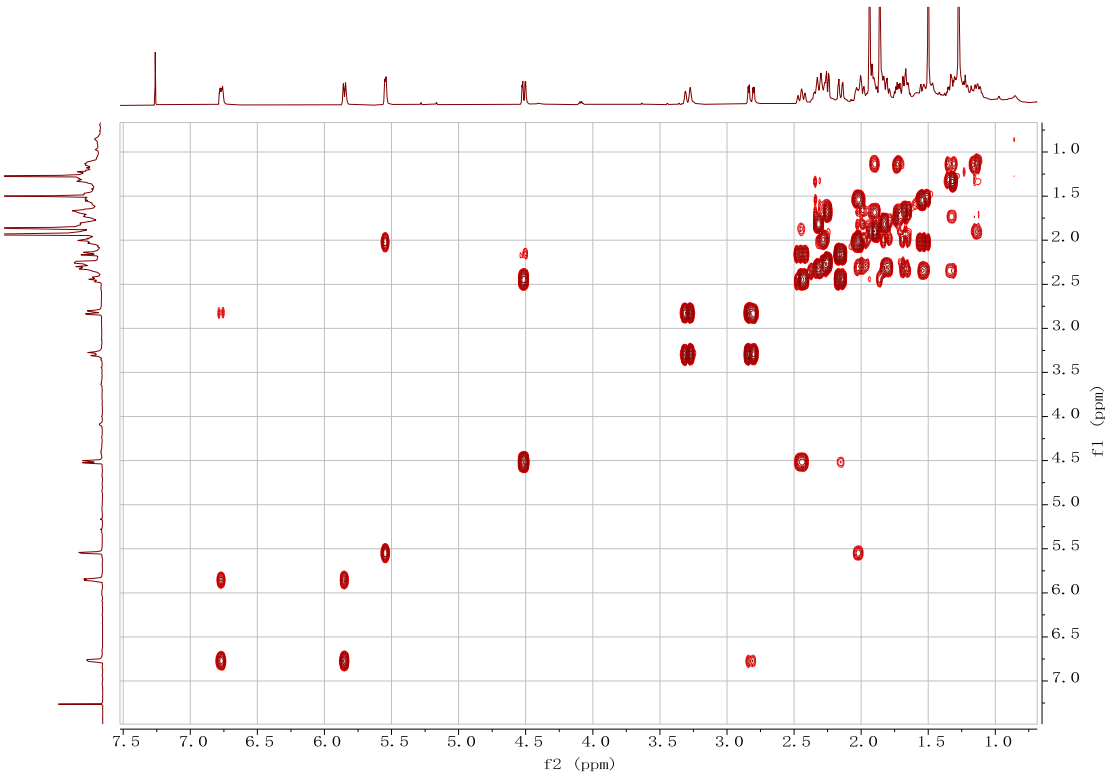


Figure S19. ^{1}H-^{1}H COSY Spectrum of Withaminilide B (**2**) in $CDCl_3$

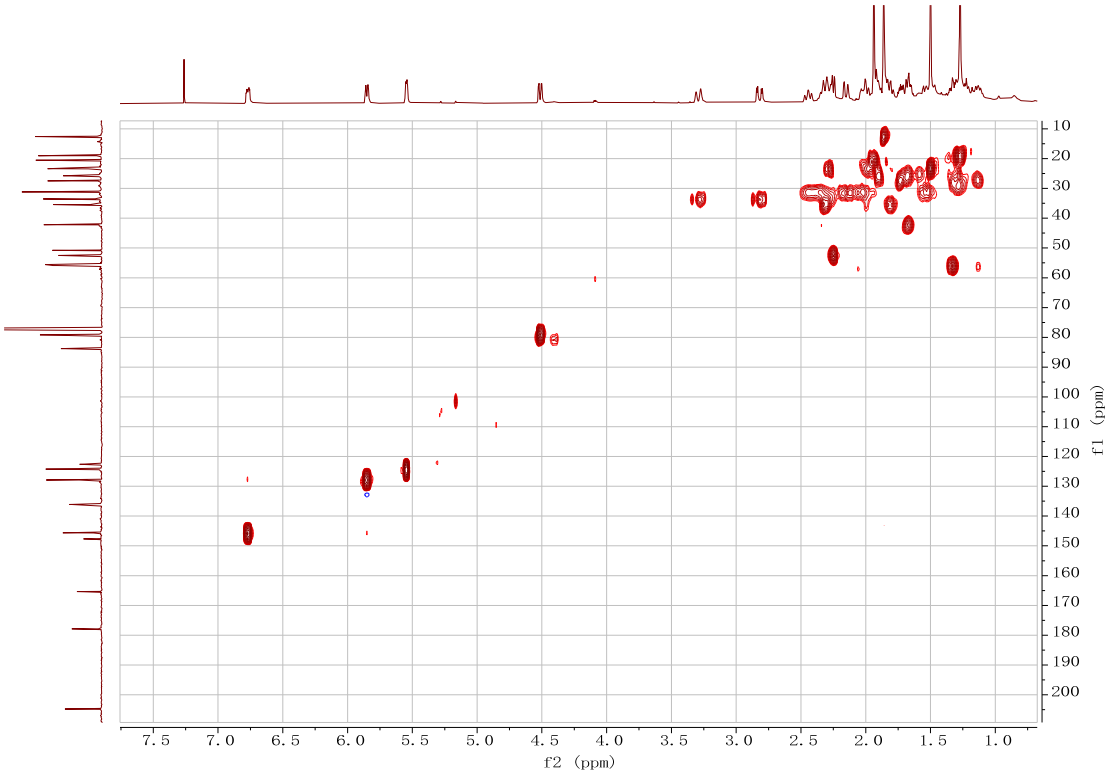


Figure S20. HSQC Spectrum of Withaminilide B (**2**) in $CDCl_3$

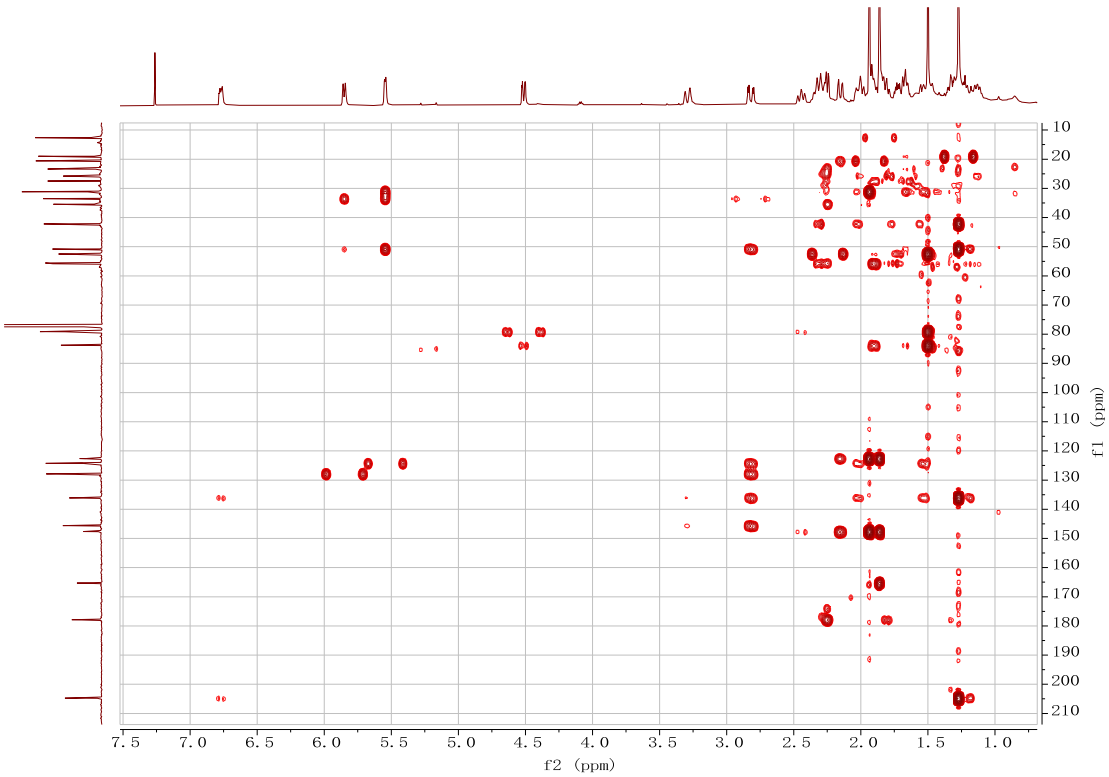


Figure S21. HMBC Spectrum of Withaminilide B (**2**) in $CDCl_3$

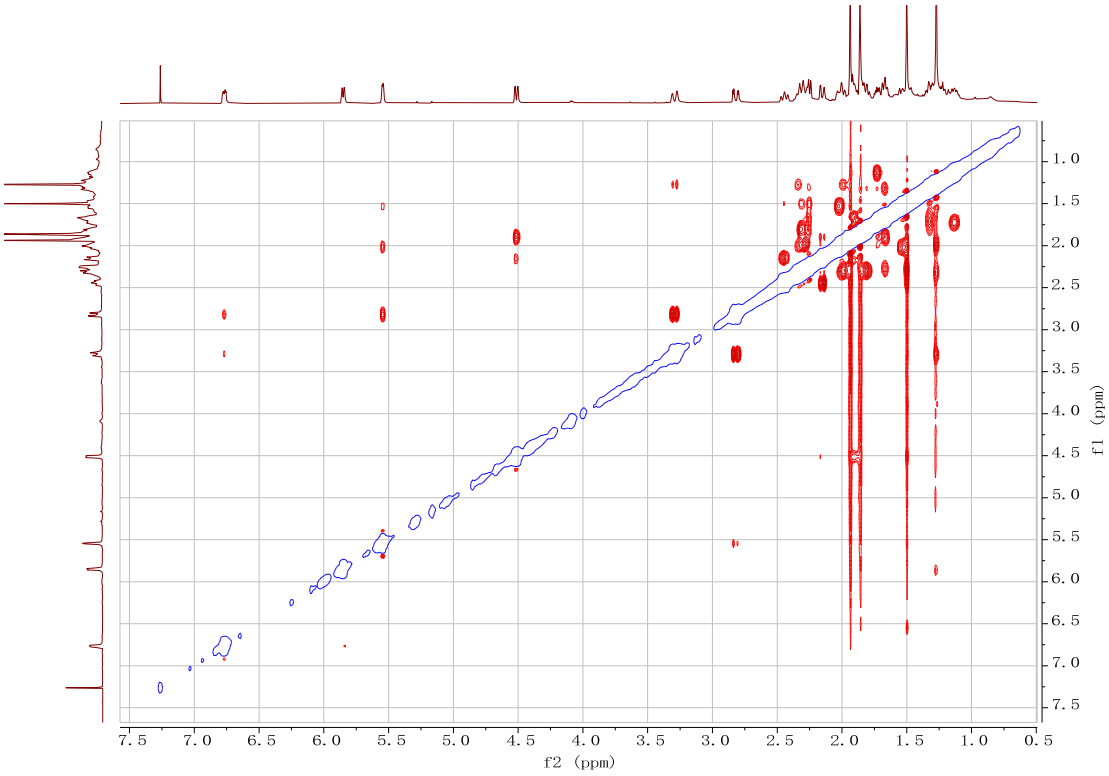


Figure S22. NOESY Spectrum of Withaminilide B (**2**) in $CDCl_3$

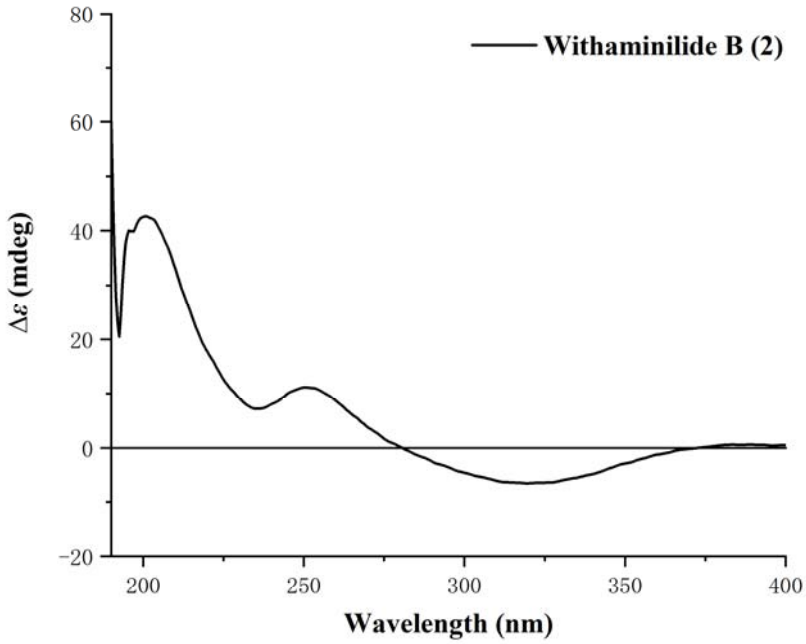


Figure S23. Experimental ECD Spectrum of Withaminilide B (**2**)

Elemental Composition Report

Tolerance = 3.0 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

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

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Minimum:	80.00					-1.5		
Maximum:	100.00			3.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
527.2289	527.2281	0.8	1.5	12.5	653.3	n/a	n/a	C29H35O9

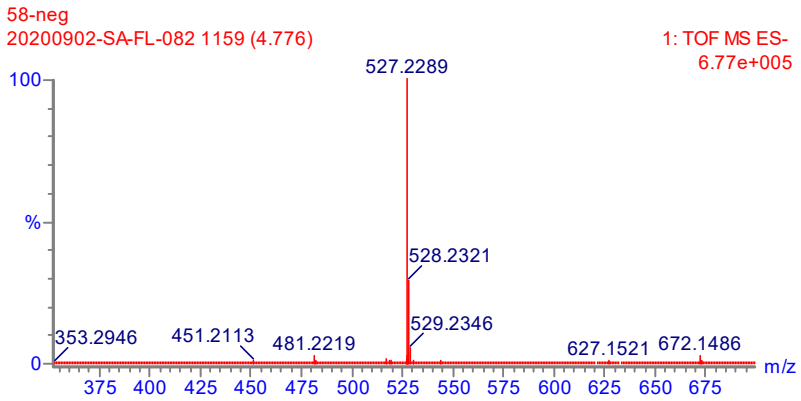


Figure S24. HRESIMS Spectrum of Withaminilide C (**3**)

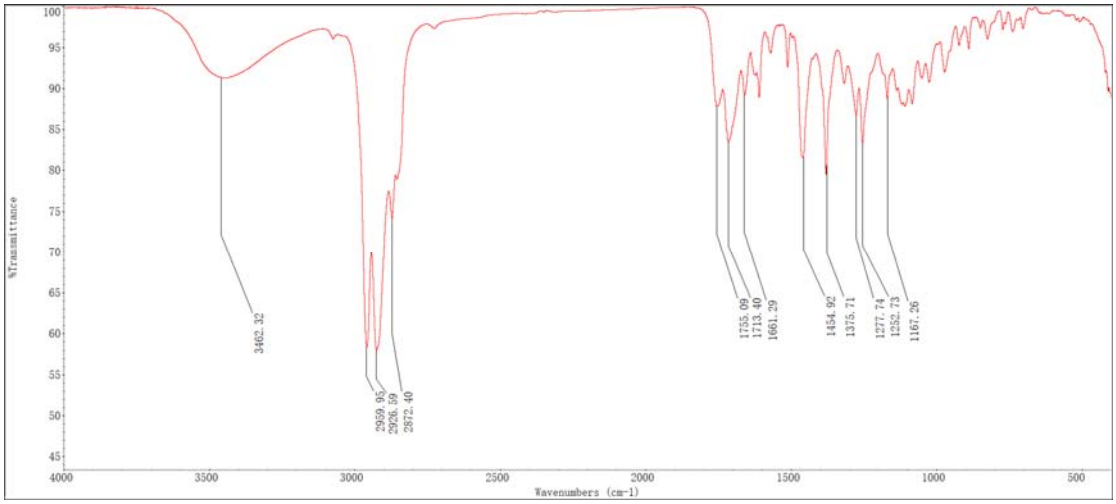


Figure S25. IR Spectrum of Withaminilide C (**3**)

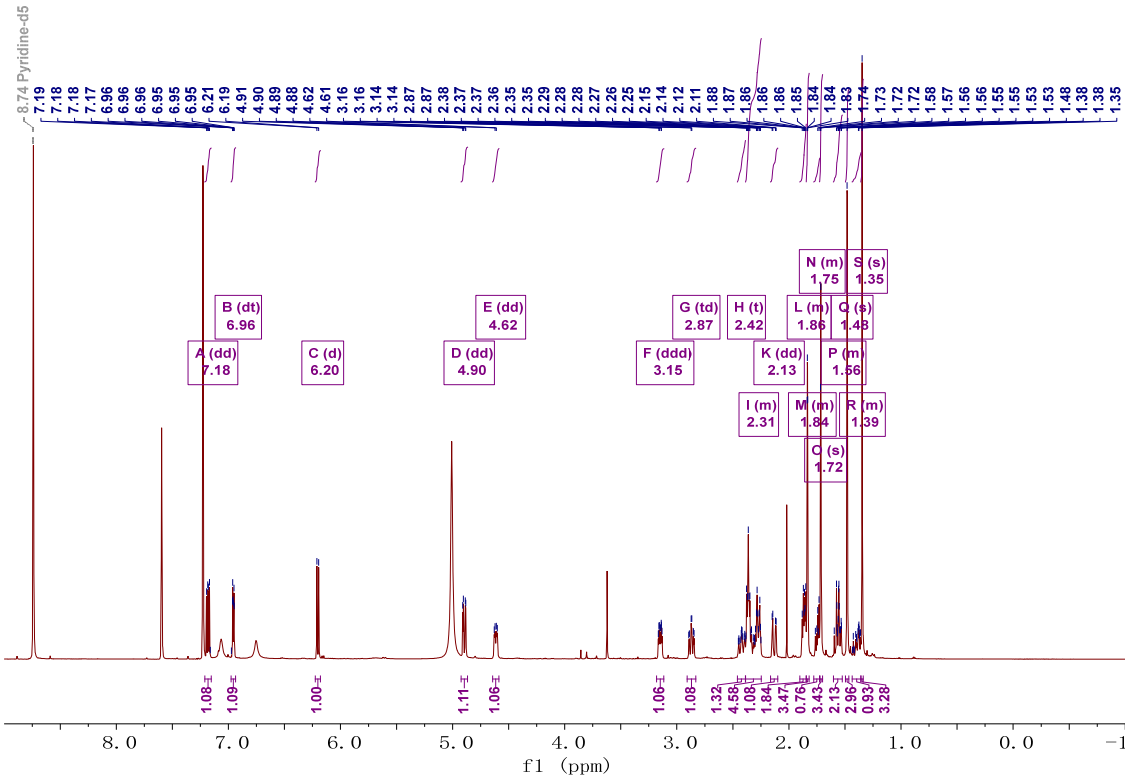


Figure S26. ^{1}H NMR Spectrum of Withaminilide C (**3**) in $CDCl_3$, 600 MHz

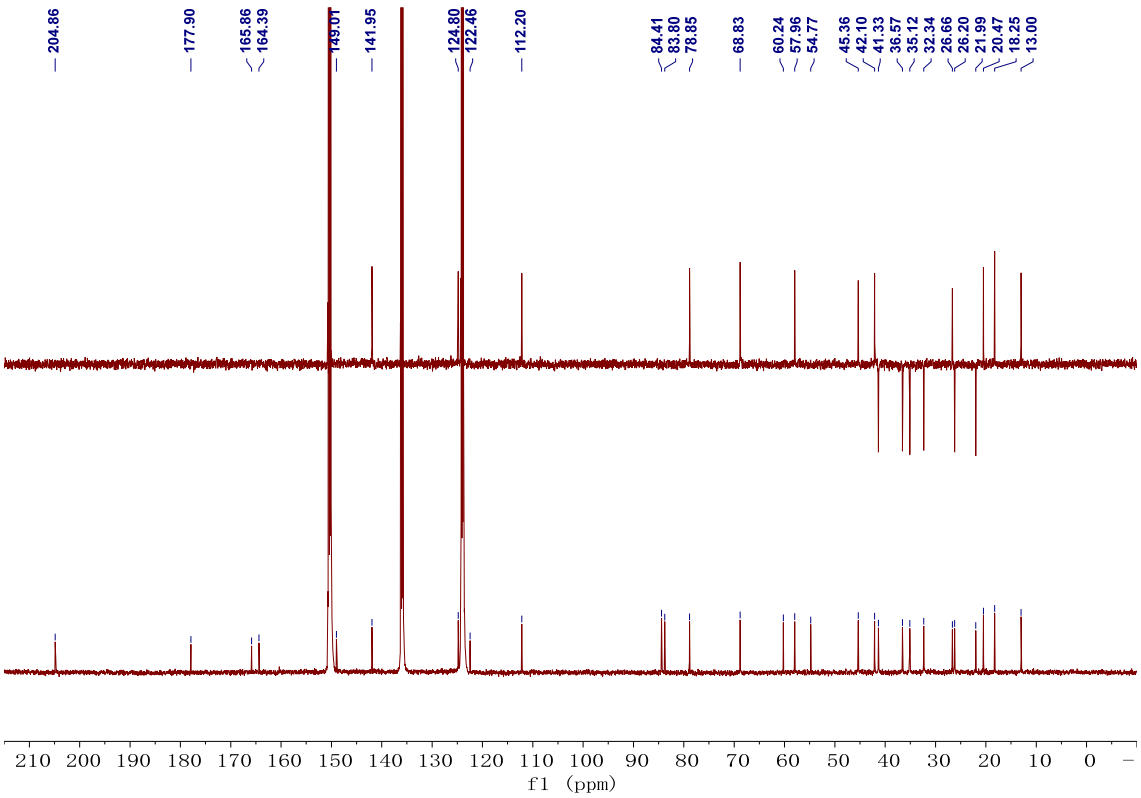


Figure S27. ^{13}C NMR Spectrum of Withaminilide C (**3**) in $CDCl_3$, 150 MHz

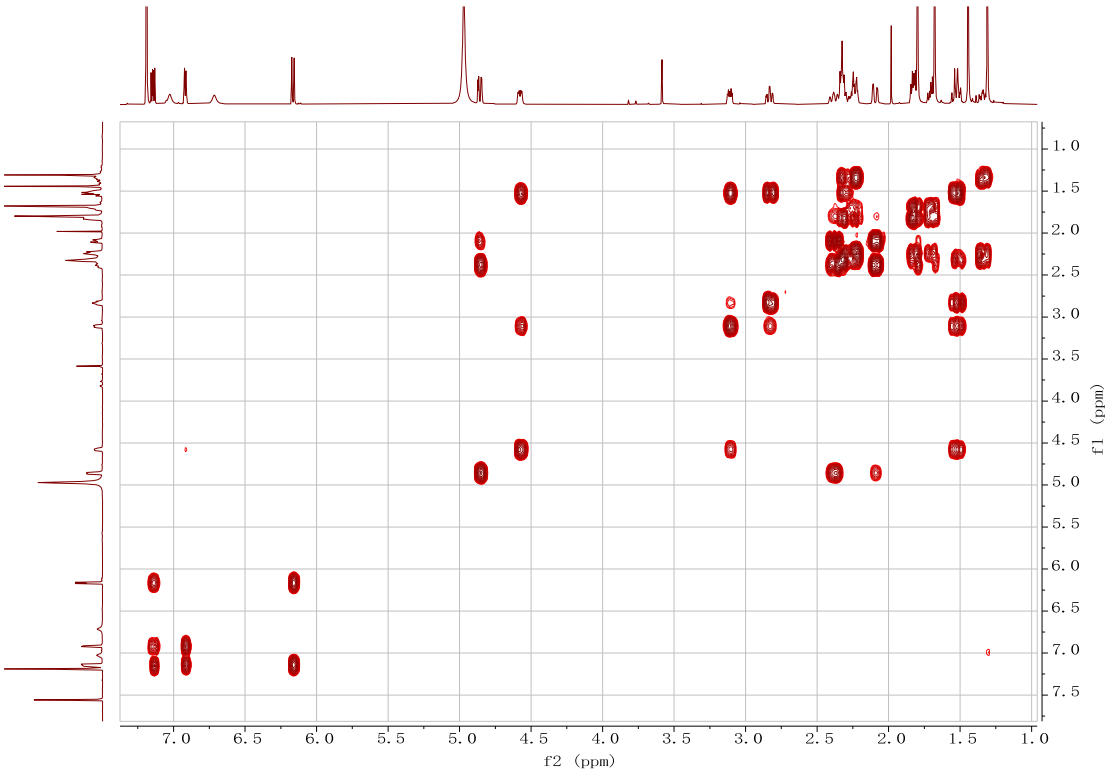


Figure S28. ^{1}H-^{1}H COSY Spectrum of Withaminilide C (**3**) in $CDCl_3$

Figure S29. HSQC Spectrum of Withaminilide C (**3**) in $CDCl_3$

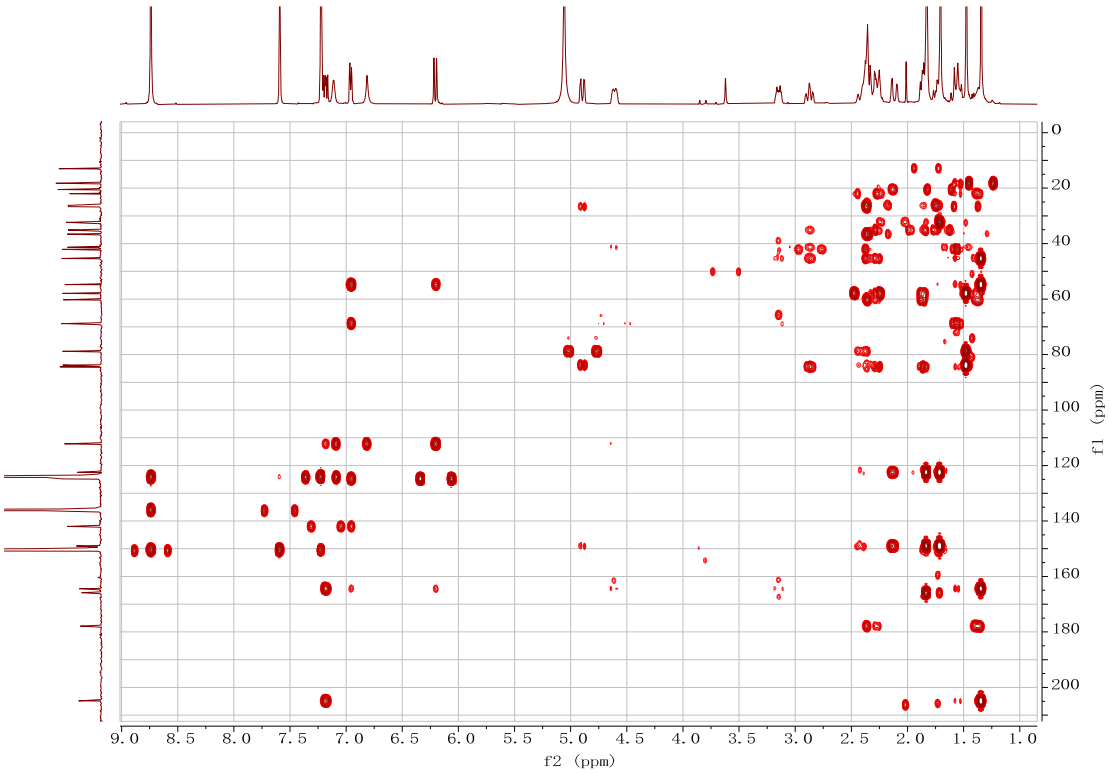


Figure S30. HMBC Spectrum of Withaminilide C (**3**) in $CDCl_3$

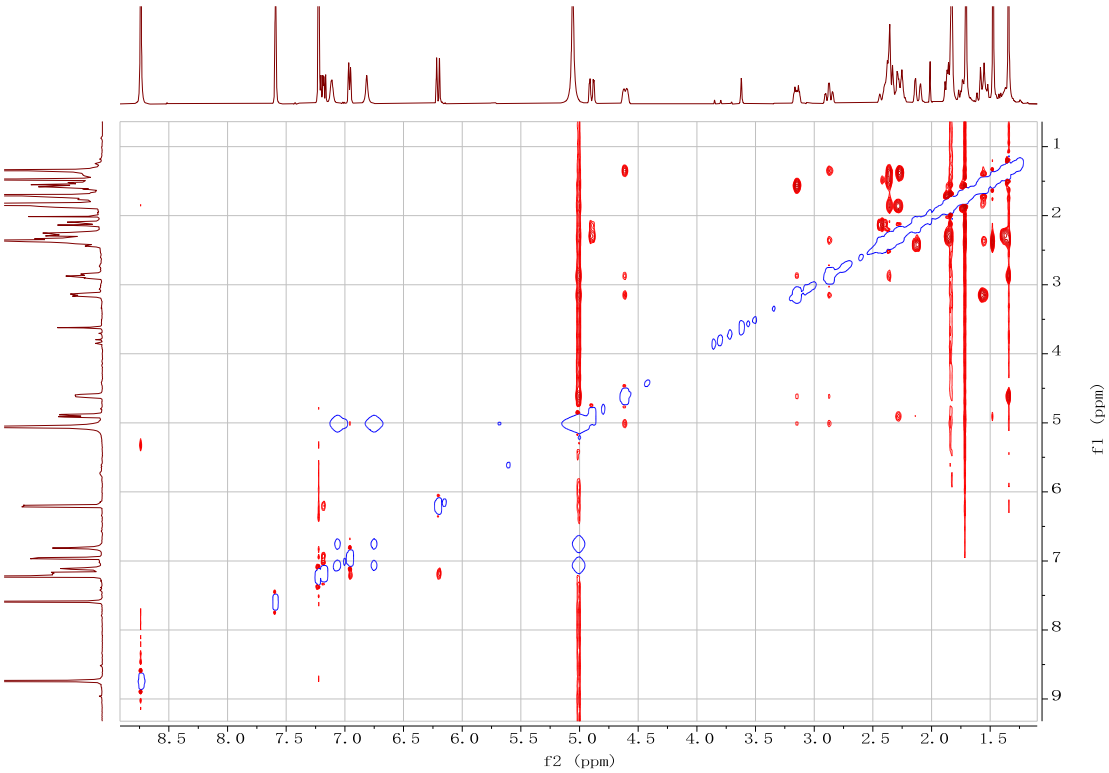


Figure S31. NOESY Spectrum of Withaminilide C (**3**) in $CDCl_3$

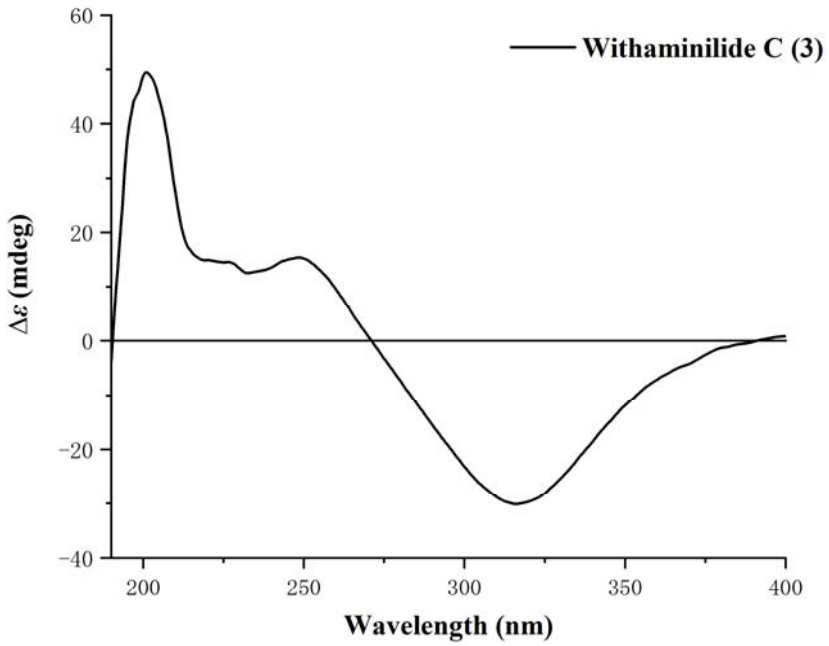


Figure S32. Experimental ECD Spectrum of Withaminilide C (**3**)

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
1063 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200

Minimum:	80.00					-1.5		
Maximum:	100.00			3.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
527.2296	527.2281	1.5	2.8	12.5	650.6	n/a	n/a	C29H35O9

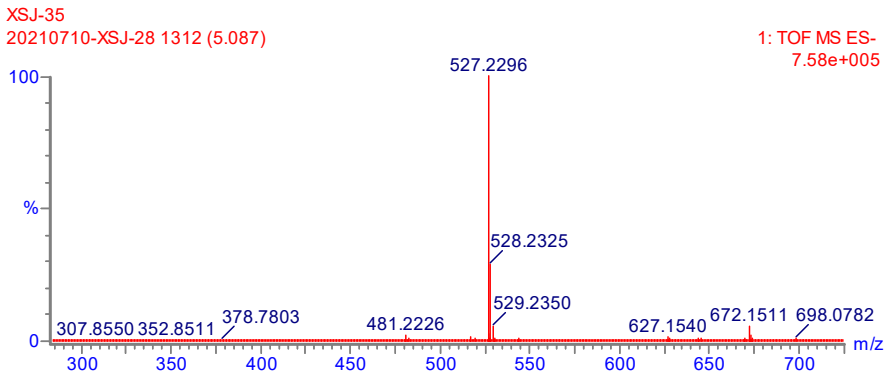


Figure S33. HRESIMS Spectrum of Withaminilide D (**4**)

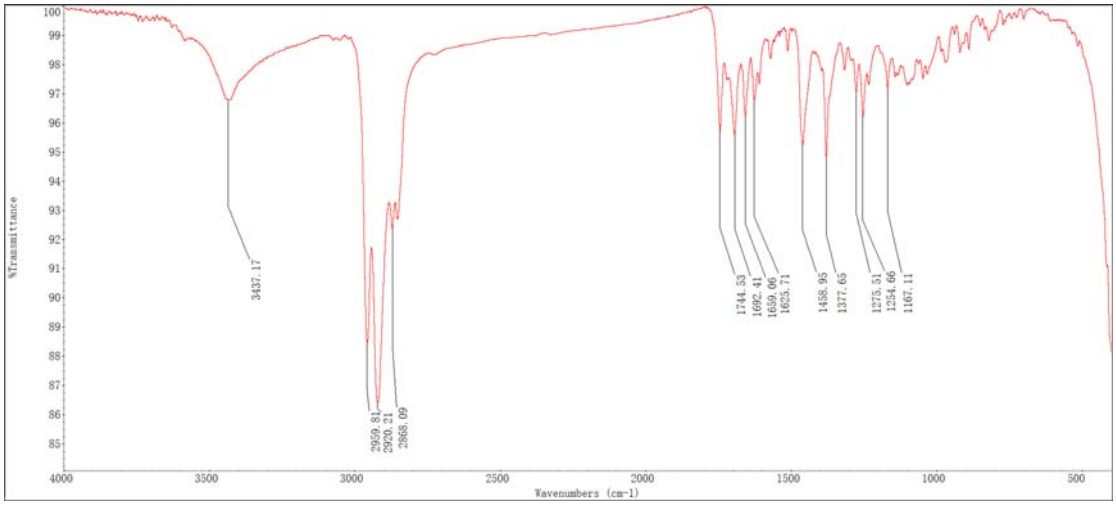


Figure S34. IR Spectrum of Withaminilide D (**4**)

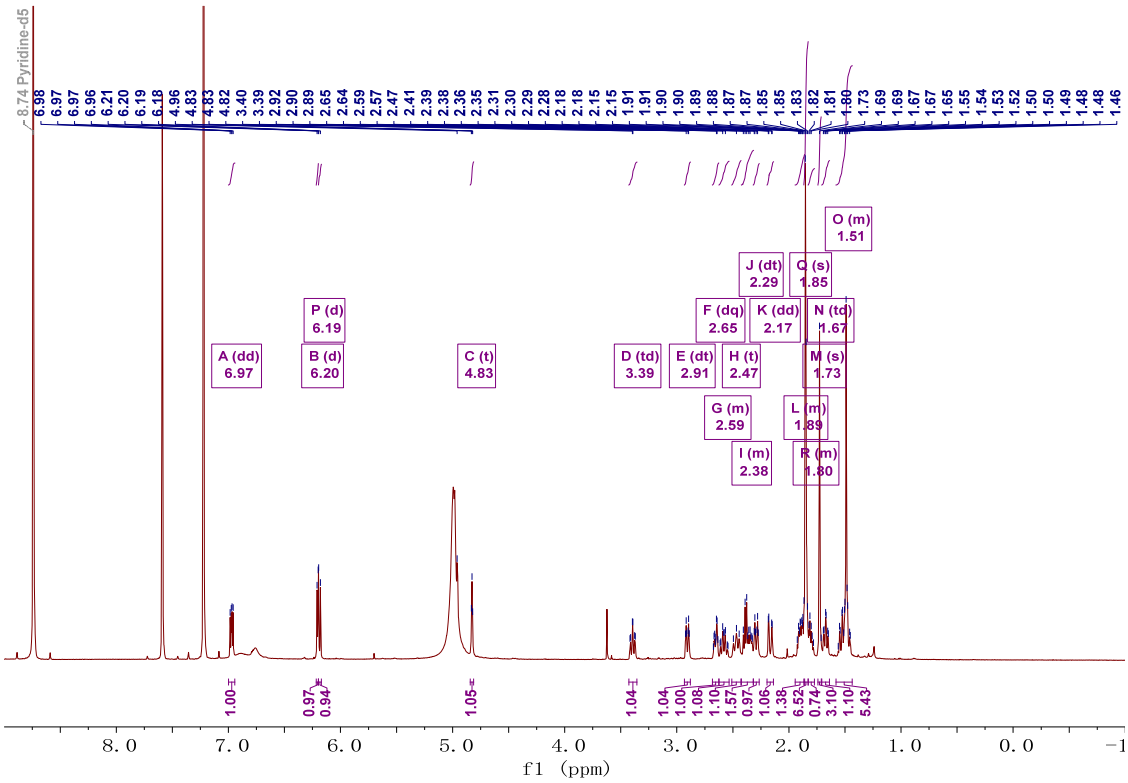


Figure S35. ^{1}H NMR Spectrum of Withaminilide D (**4**) in C_5D_5N, 600 MHz

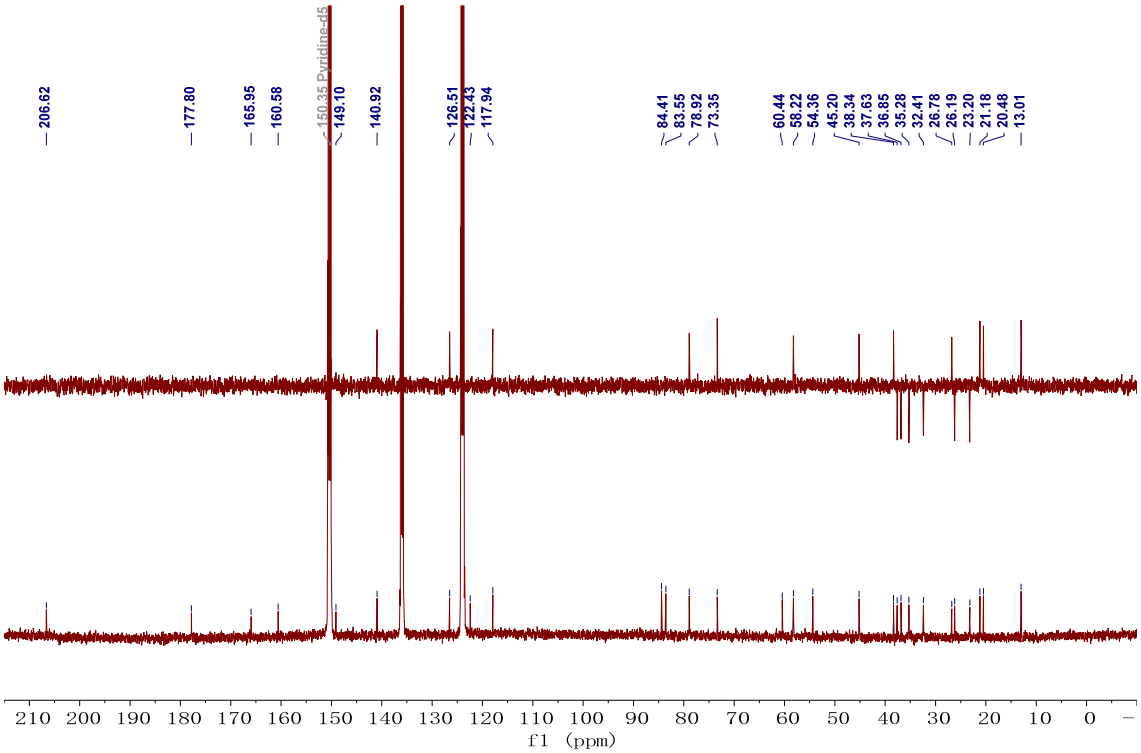


Figure S36. ^{13}C NMR Spectrum of Withaminilide D (**4**) in C_5D_5N, 125 MHz

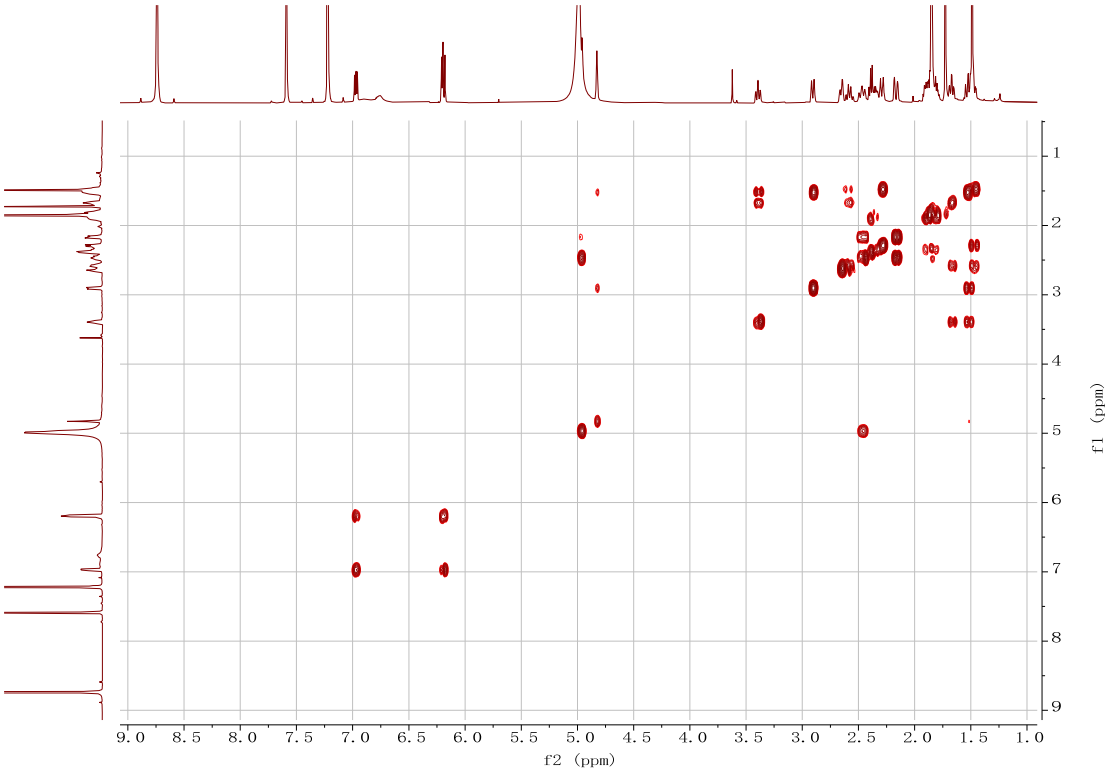


Figure S37. ^{1}H-^{1}H COSY Spectrum of Withaminilide D (**4**) in C_5D_5N

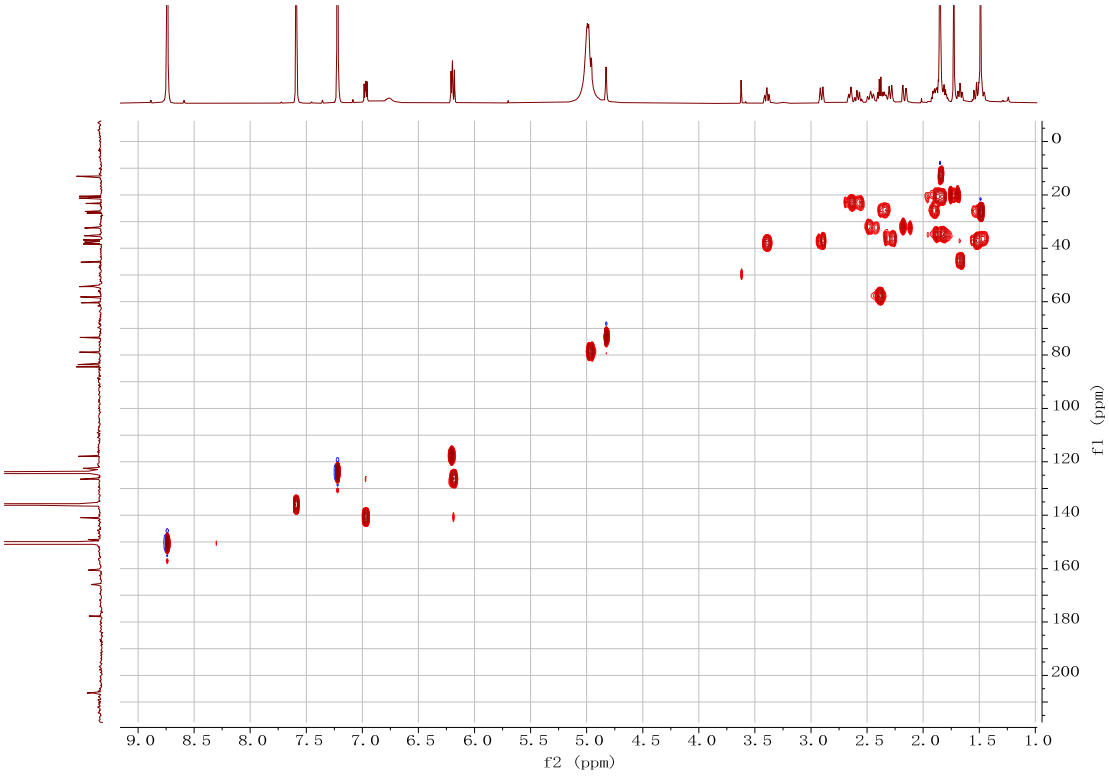


Figure S38. HSQC Spectrum of Withaminilide D (**4**) in C_5D_5N

Figure S39. HMBC Spectrum of Withaminilide D (**4**) in C_5D_5N

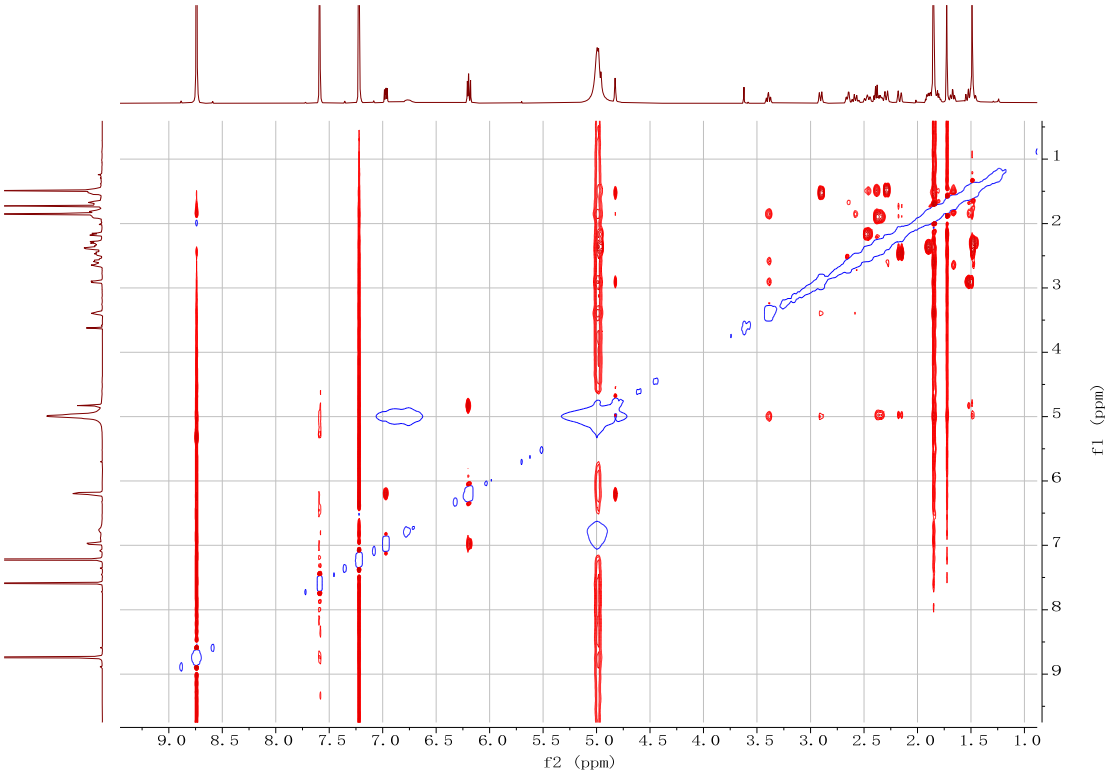


Figure S40. NOESY Spectrum of Withaminilide D (**4**) in C_5D_5N

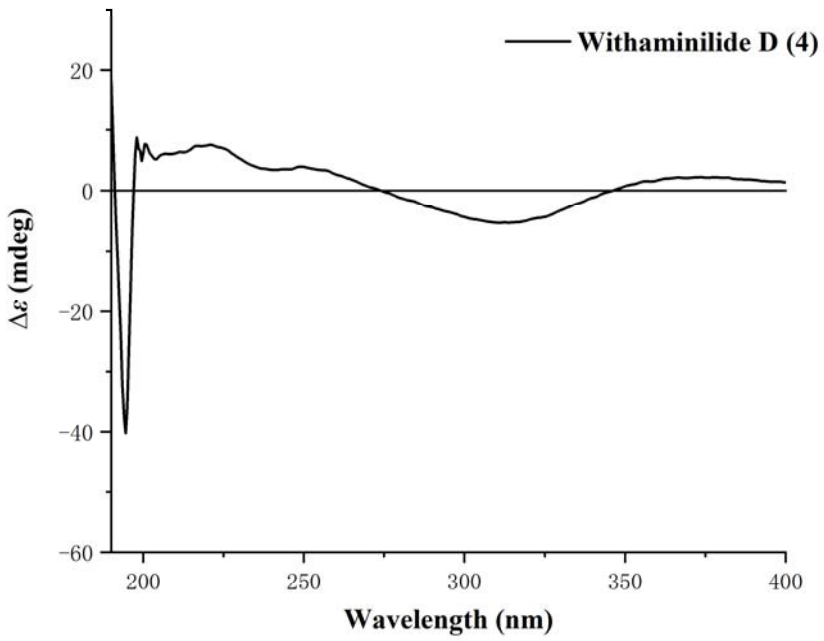


Figure S41. Experimental ECD Spectrum of Withaminilide D (**4**)

Elemental Composition Report

Single Mass Analysis

Tolerance = 3.0 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

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

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Minimum:					-1.5			
Maximum:			3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
467.2437	467.2434	0.3	0.6	11.5	737.8	n/a	n/a	C28H35O6

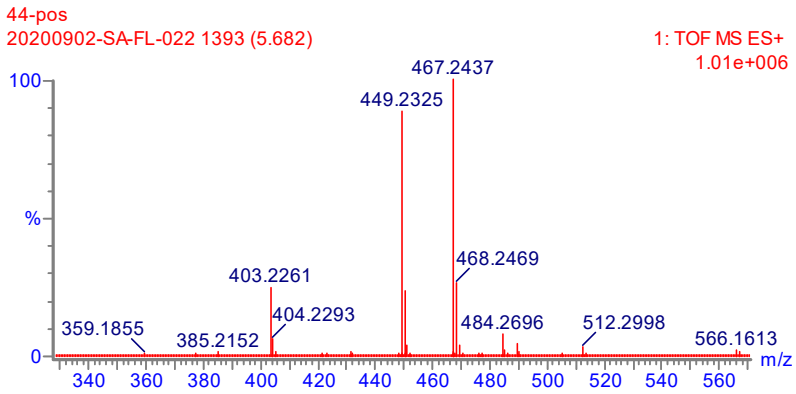


Figure S42. HRESIMS Spectrum of Withaminilide E (**5**)

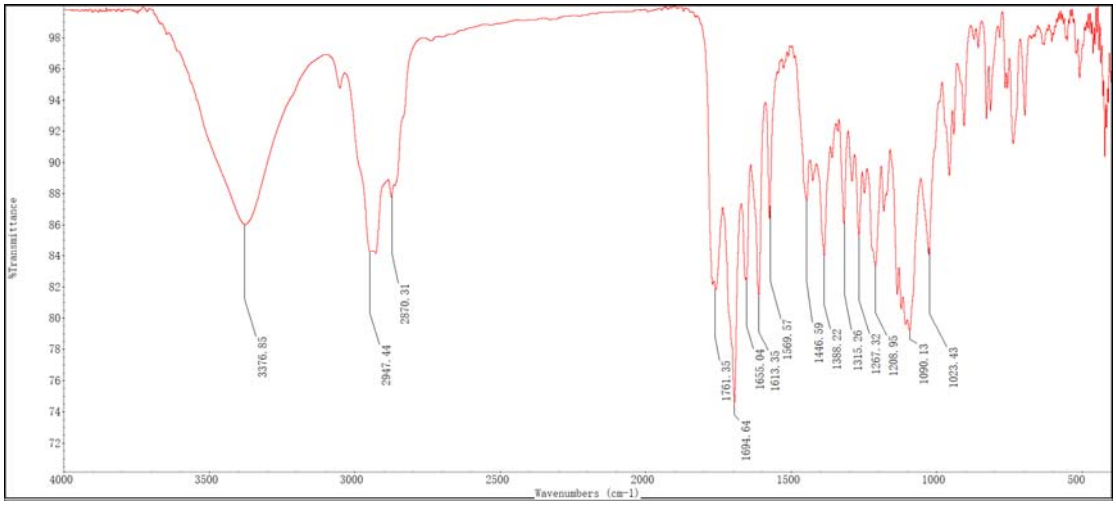


Figure S43. IR Spectrum of Withaminilide E (**5**)

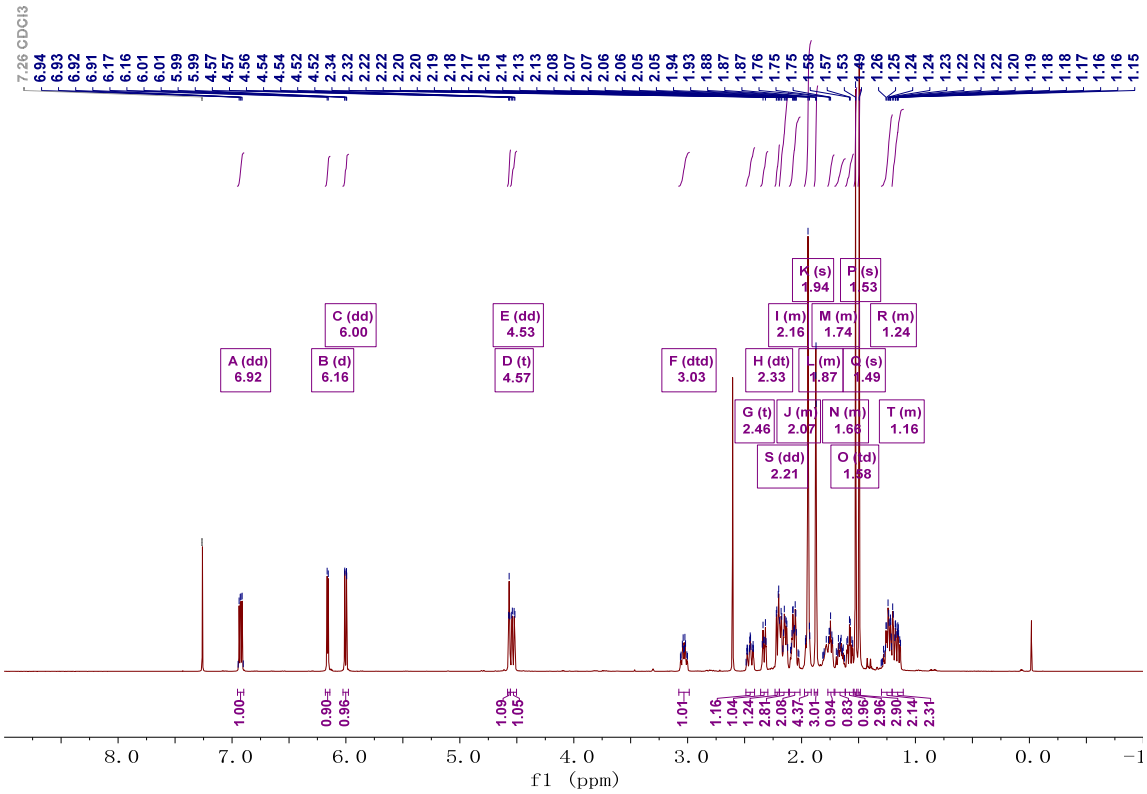


Figure S44. ^{1}H NMR Spectrum of Withaminilide E (**5**) in $CDCl_3$, 600 MHz

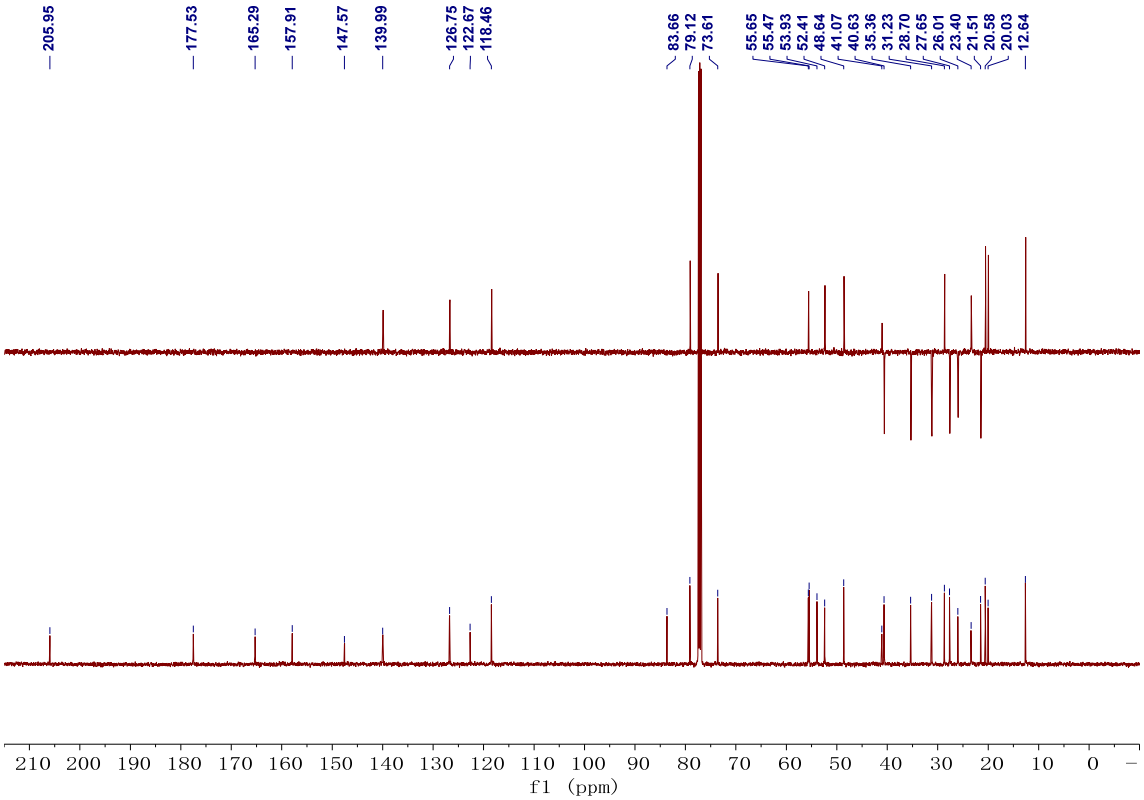


Figure S45. ^{13}C NMR Spectrum of Withaminilide E (**5**) in $CDCl_3$, 150 MHz

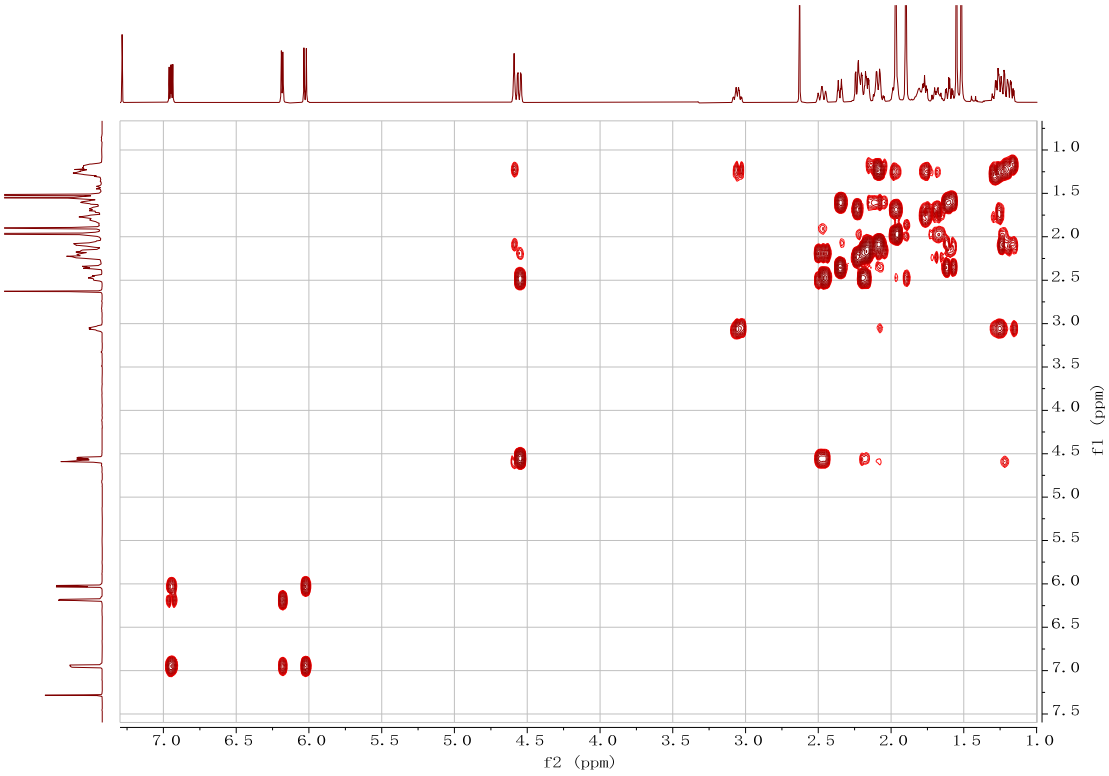


Figure S46. ^{1}H-^{1}H COSY Spectrum of Withaminilide E (**5**) in $CDCl_3$

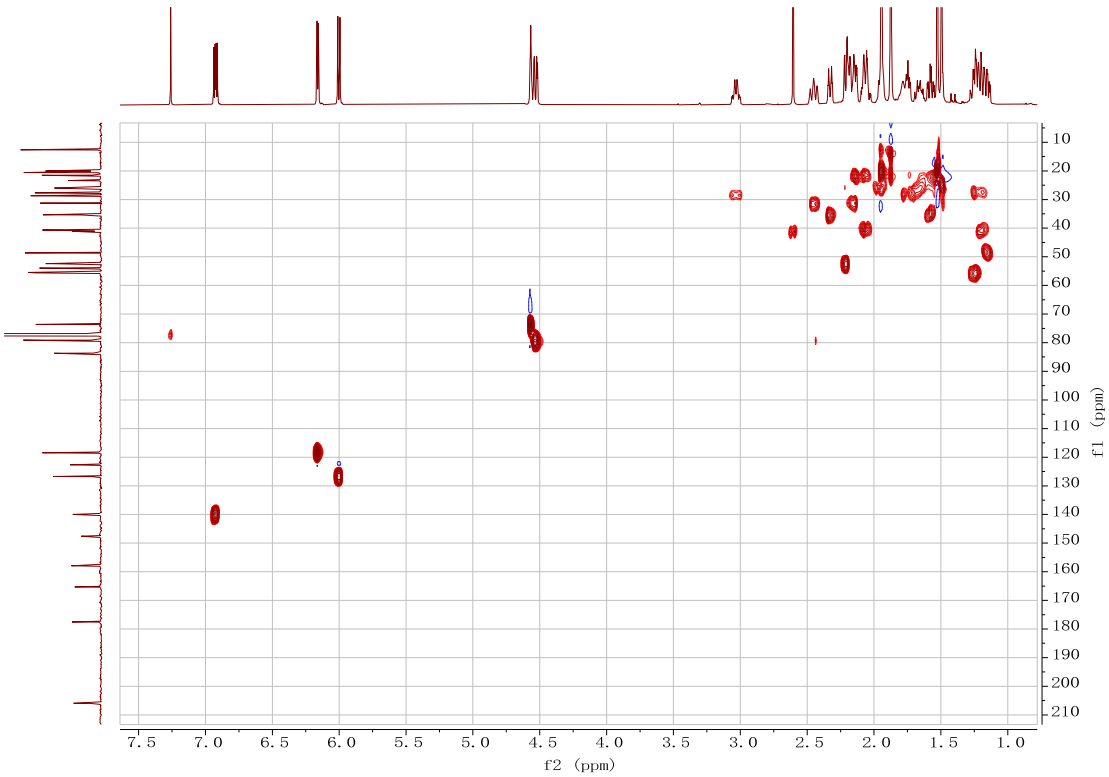


Figure S47. HSQC Spectrum of Withaminilide E (**5**) in $CDCl_3$

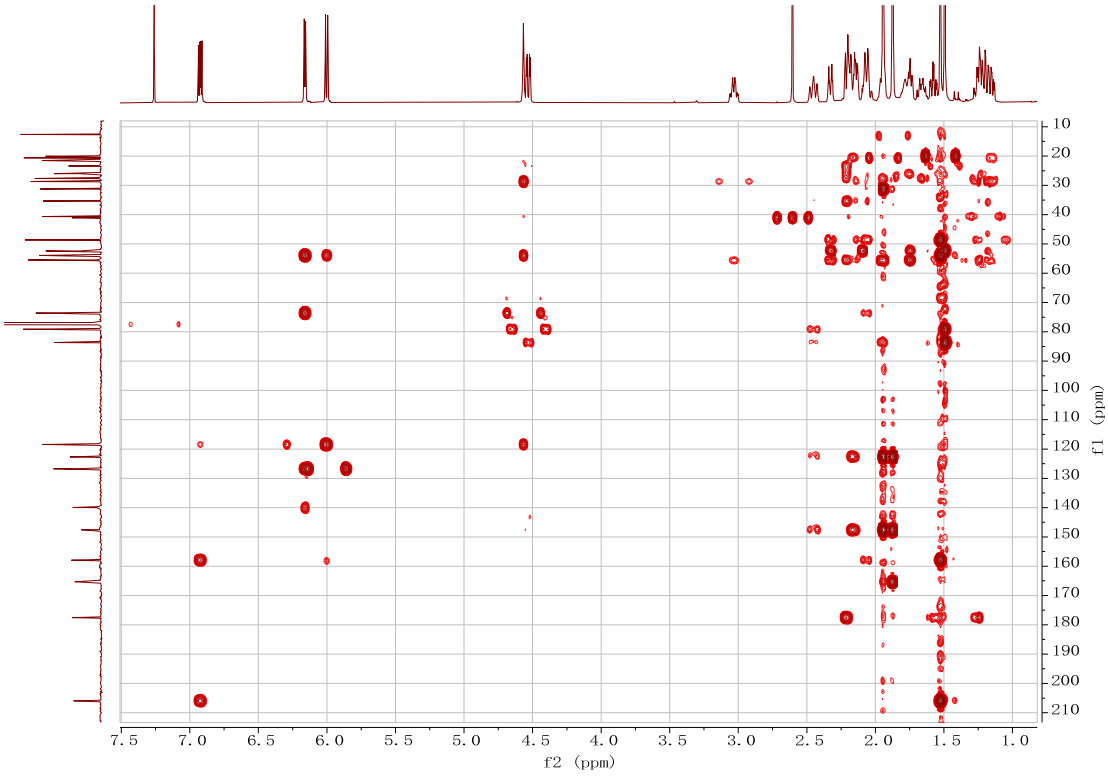


Figure S48. HMBC Spectrum of Withaminilide E (**5**) in $CDCl_3$

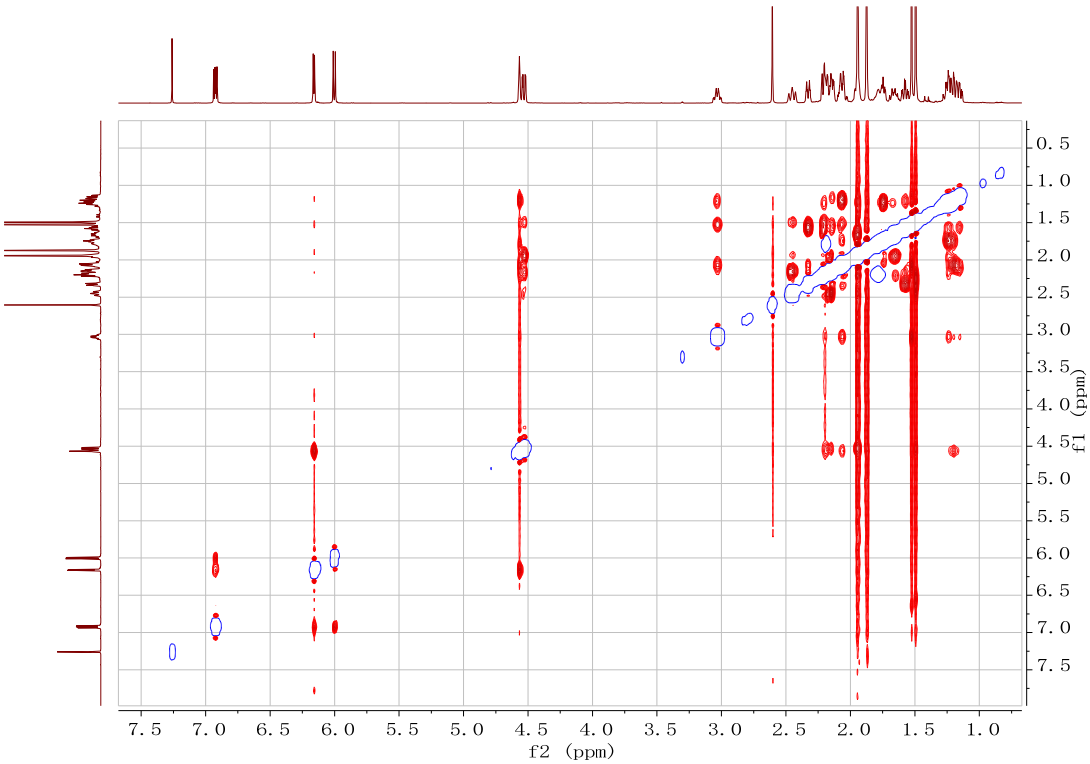


Figure S49. NOESY Spectrum of Withaminilide E (**5**) in $CDCl_3$

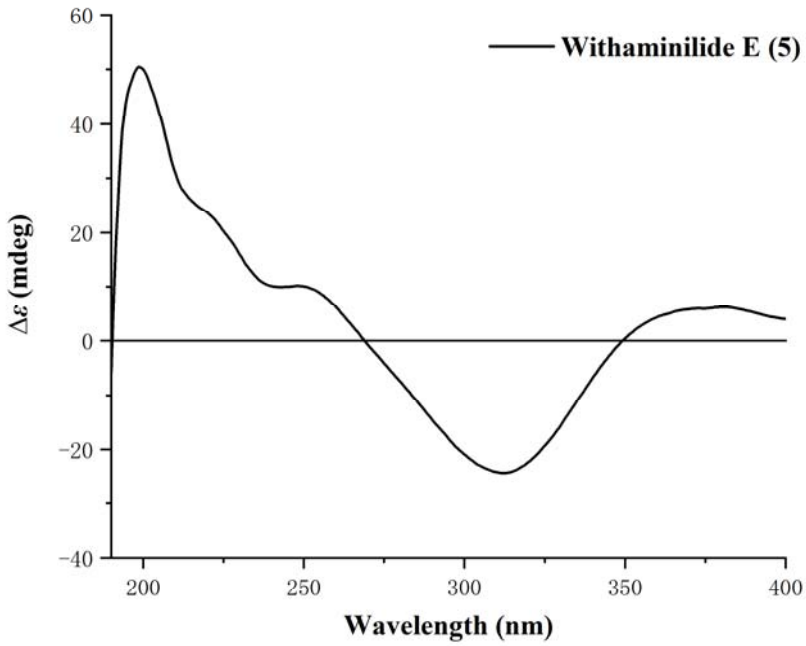


Figure S50. Experimental ECD Spectrum of Withaminilide E (**5**)

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

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

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Minimum:	80.00					-1.5		
Maximum:	100.00			3.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
511.2332	511.2332	0.0	0.0	12.5	517.3	n/a	n/a	C29H35O8

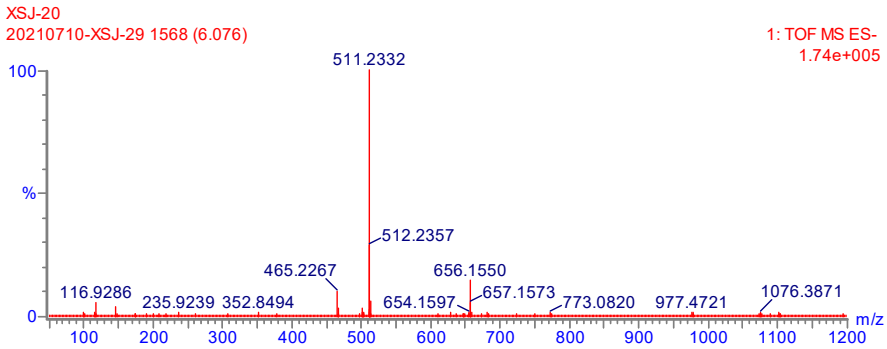


Figure S51. HRESIMS Spectrum of Withaminilide F (**6**)

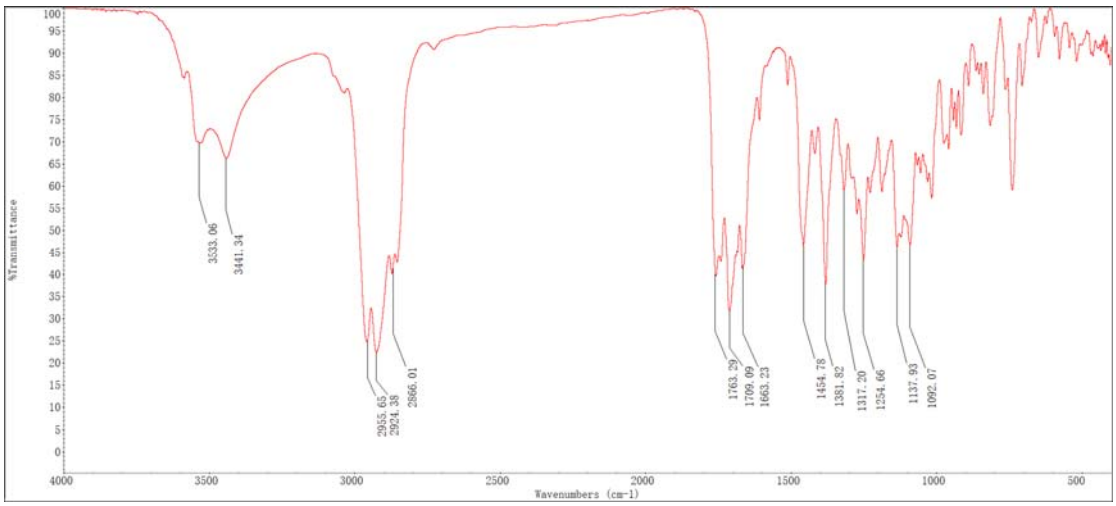


Figure S52. IR Spectrum of Withaminilide F (**6**)

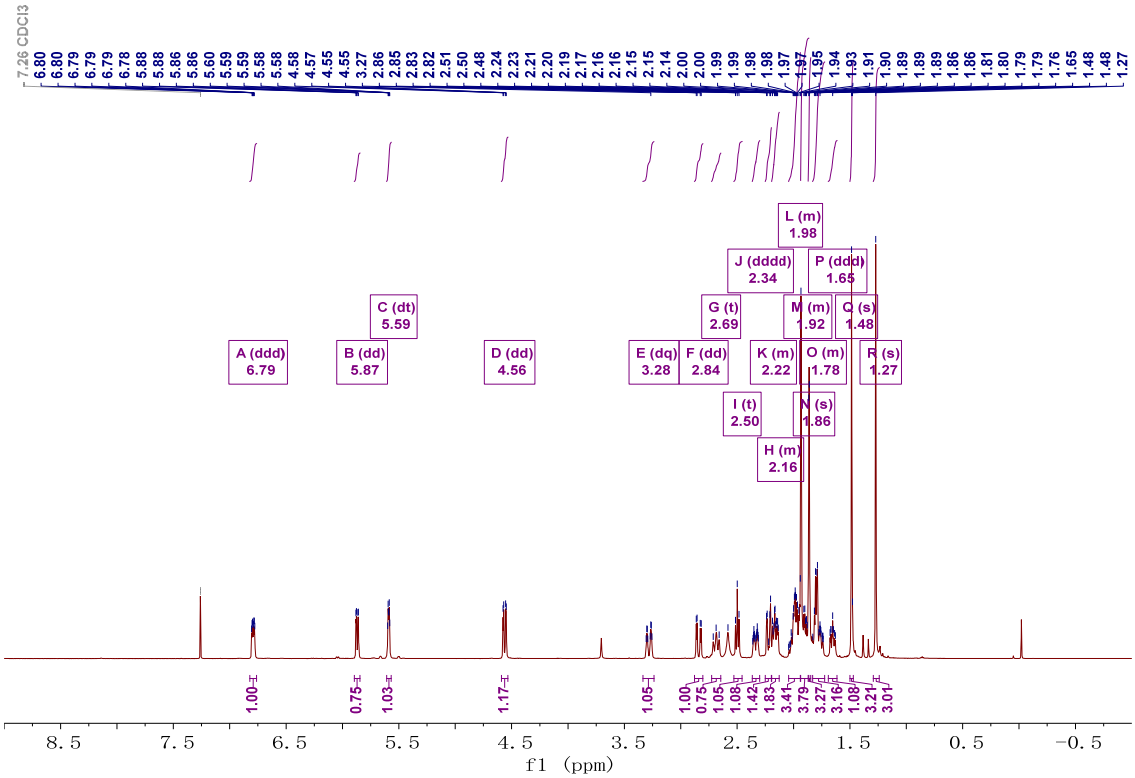


Figure S53. ^{1}H NMR Spectrum of Withaminilide F (**6**) in $CDCl_3$, 600 MHz

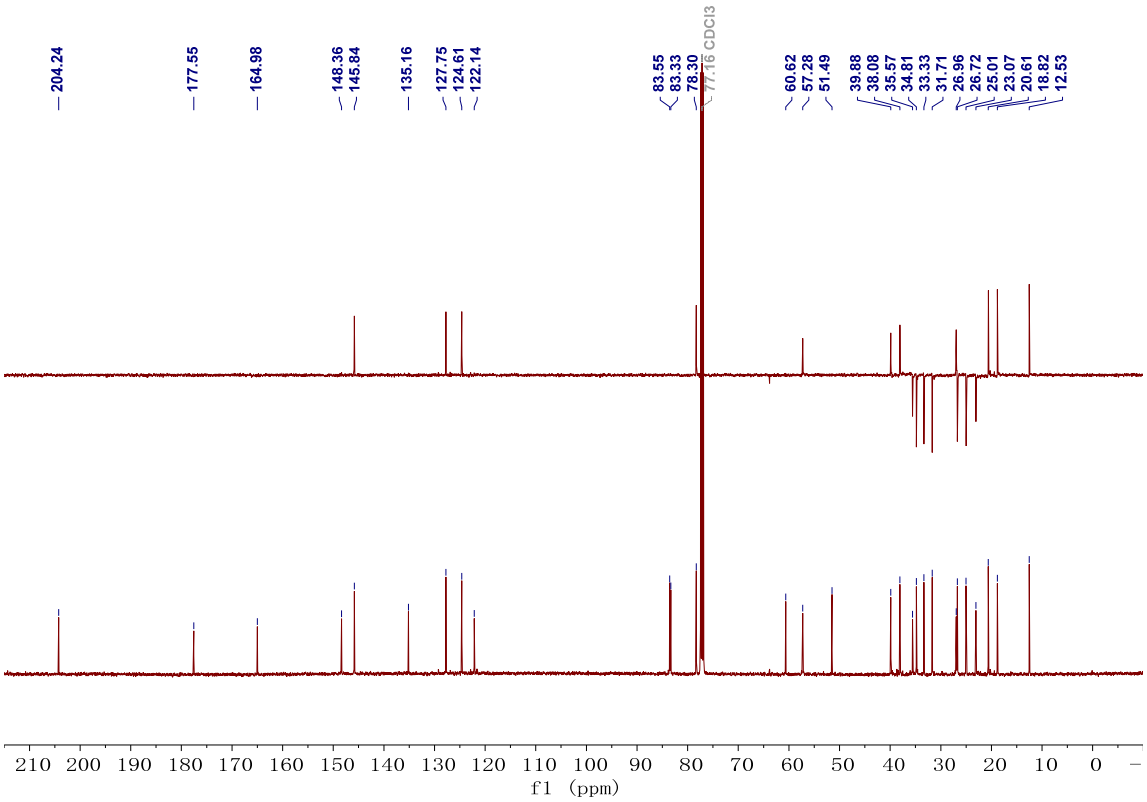


Figure S54. ^{13}C NMR Spectrum of Withaminilide F (**6**) in $CDCl_3$, 125 MHz

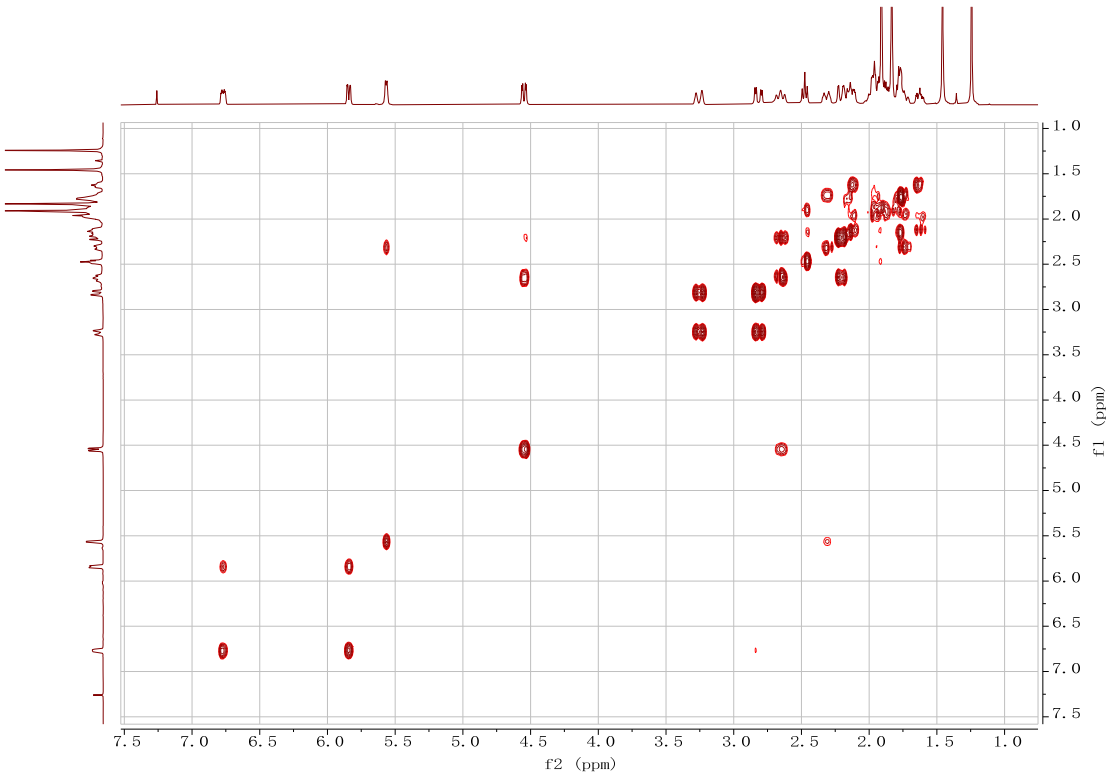


Figure S55. ^{1}H-^{1}H COSY Spectrum of Withaminilide F (**6**) in $CDCl_3$

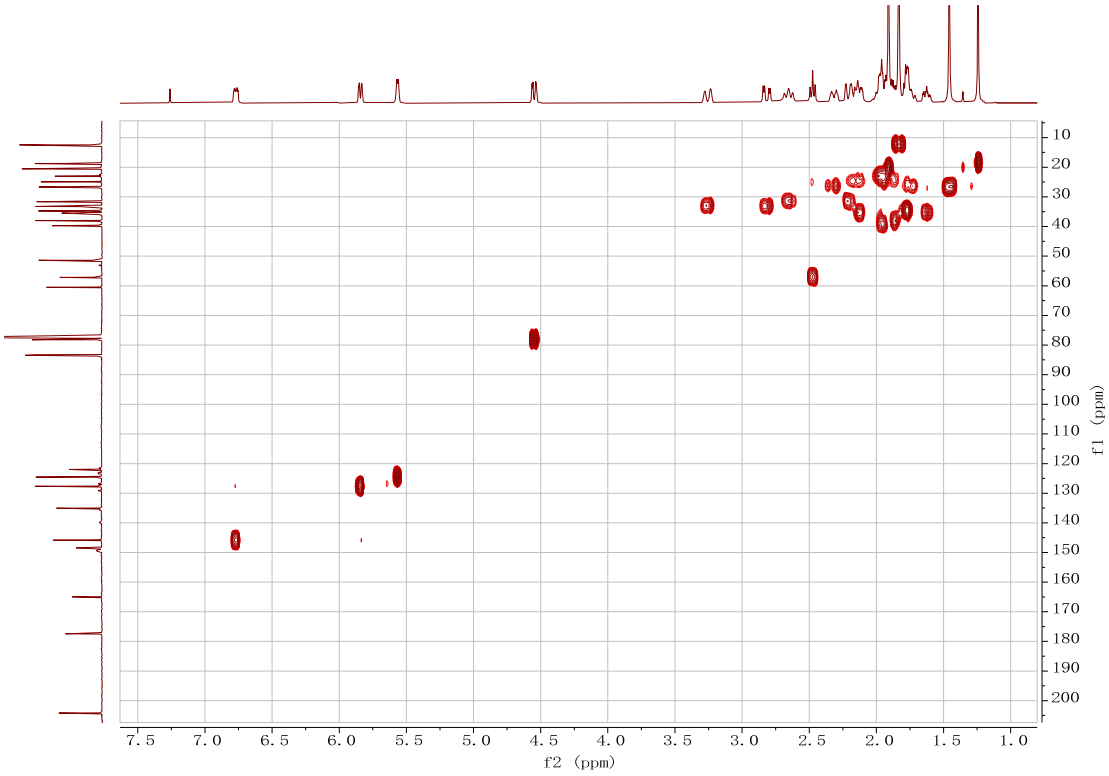


Figure S56. HSQC Spectrum of Withaminilide F (**6**) in $CDCl_3$

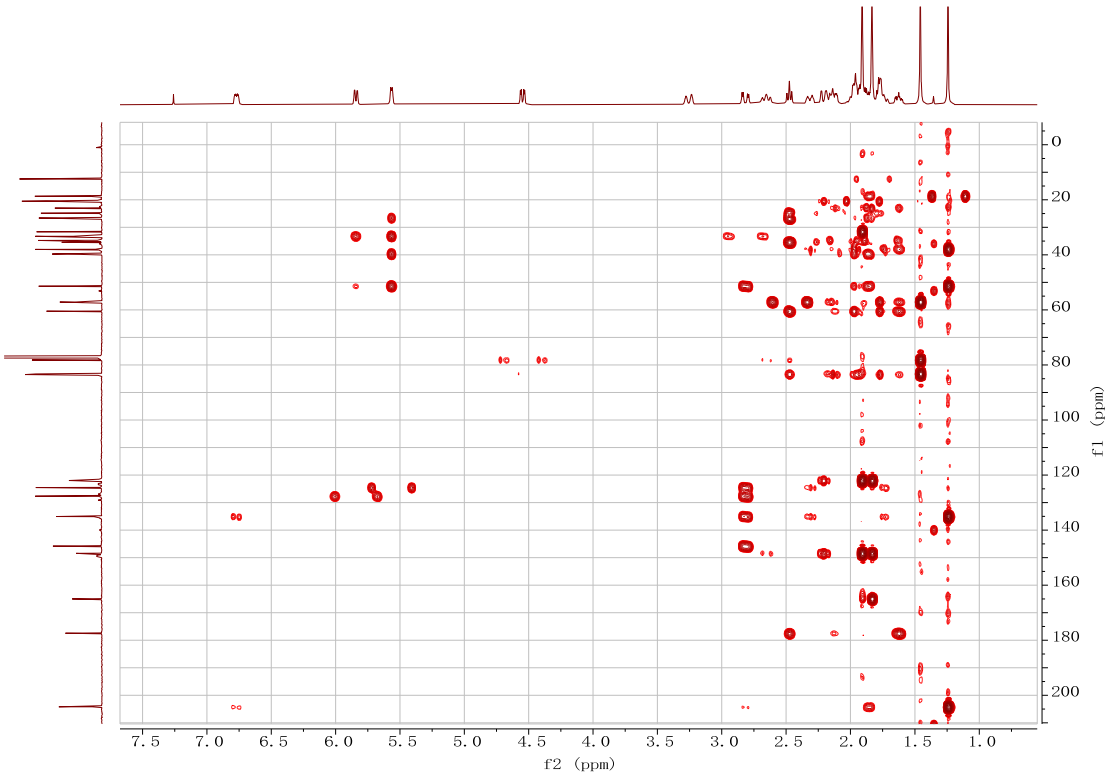


Figure S57. HMBC Spectrum of Withaminilide F (**6**) in $CDCl_3$

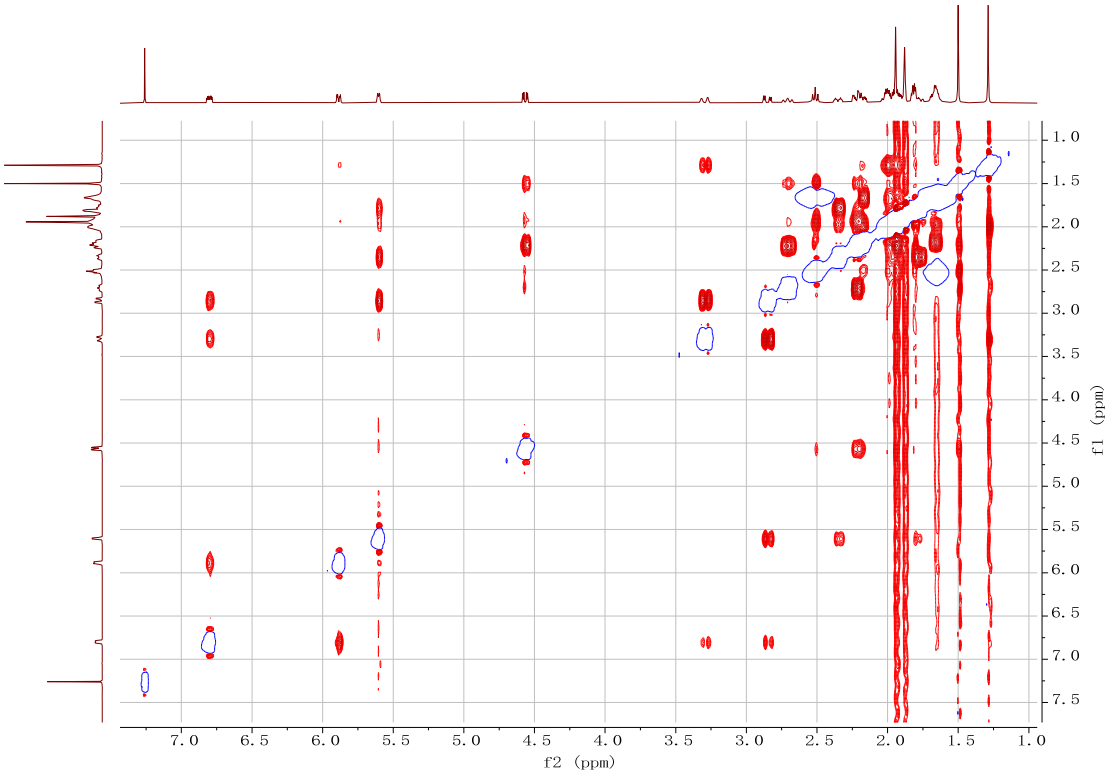


Figure S58. NOESY Spectrum of Withaminilide F (**6**) in $CDCl_3$

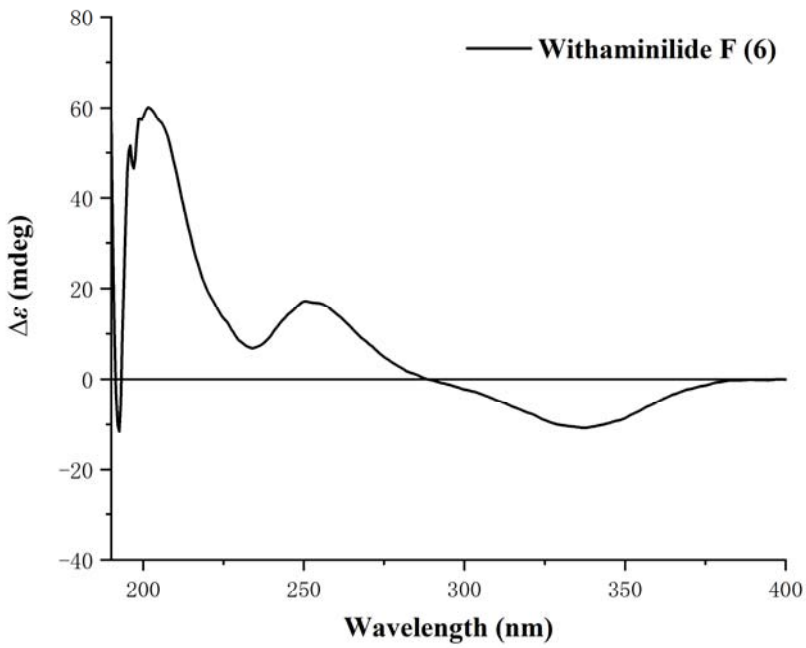


Figure S59. Experimental ECD Spectrum of Withaminilide F (**6**)

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

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

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Minimum:		80.00				-1.5		
Maximum:		100.00		3.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
527.2300	527.2281	1.9	3.6	12.5	645.6	n/a	n/a	C29H35O9

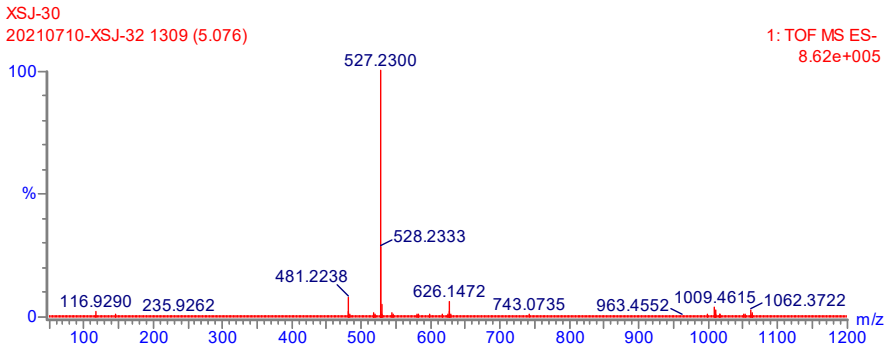


Figure S60. HRESIMS Spectrum of Withaminilide G (**7**)

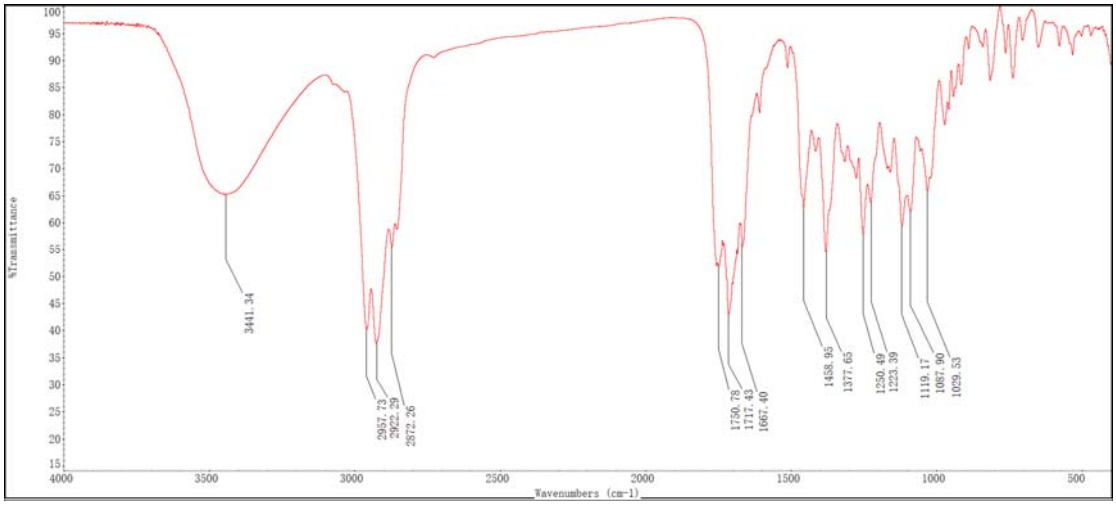


Figure S61. IR Spectrum of Withaminilide G (**7**)

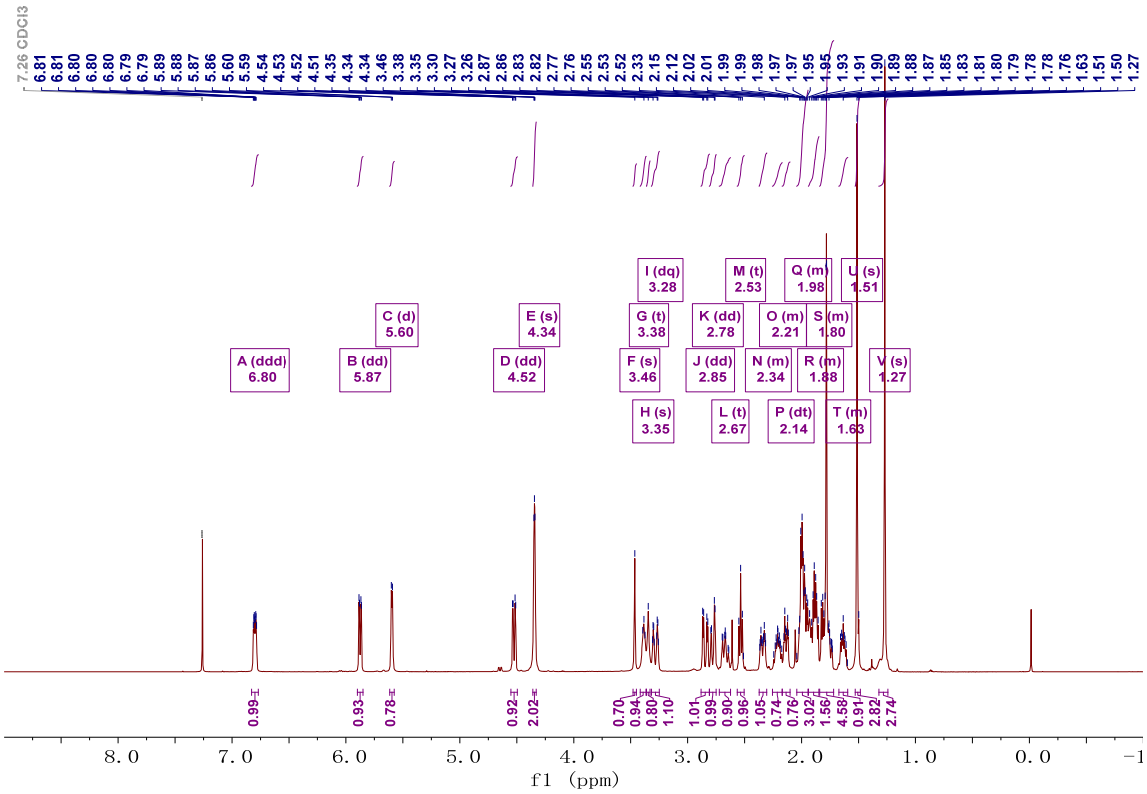


Figure S62. ^{1}H NMR Spectrum of Withaminilide G (**7**) in $CDCl_3$, 600 MHz

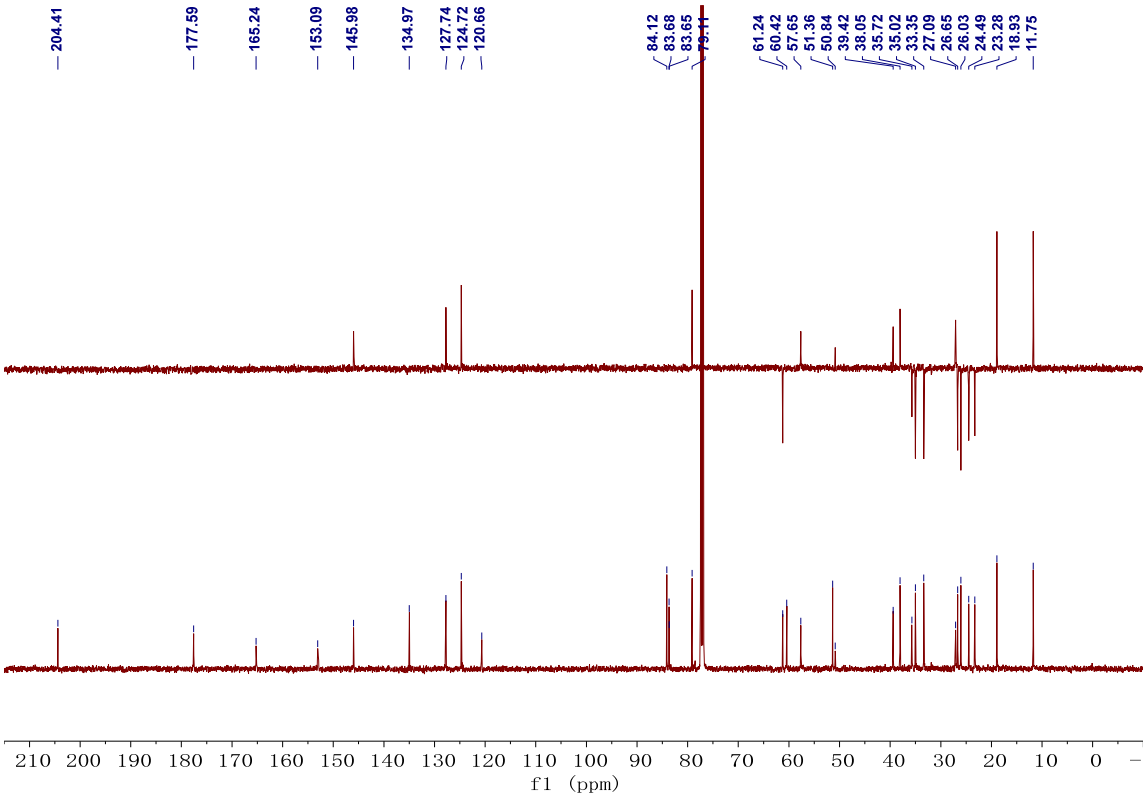


Figure S63. ^{13}C NMR Spectrum of Withaminilide G (**7**) in $CDCl_3$, 125 MHz

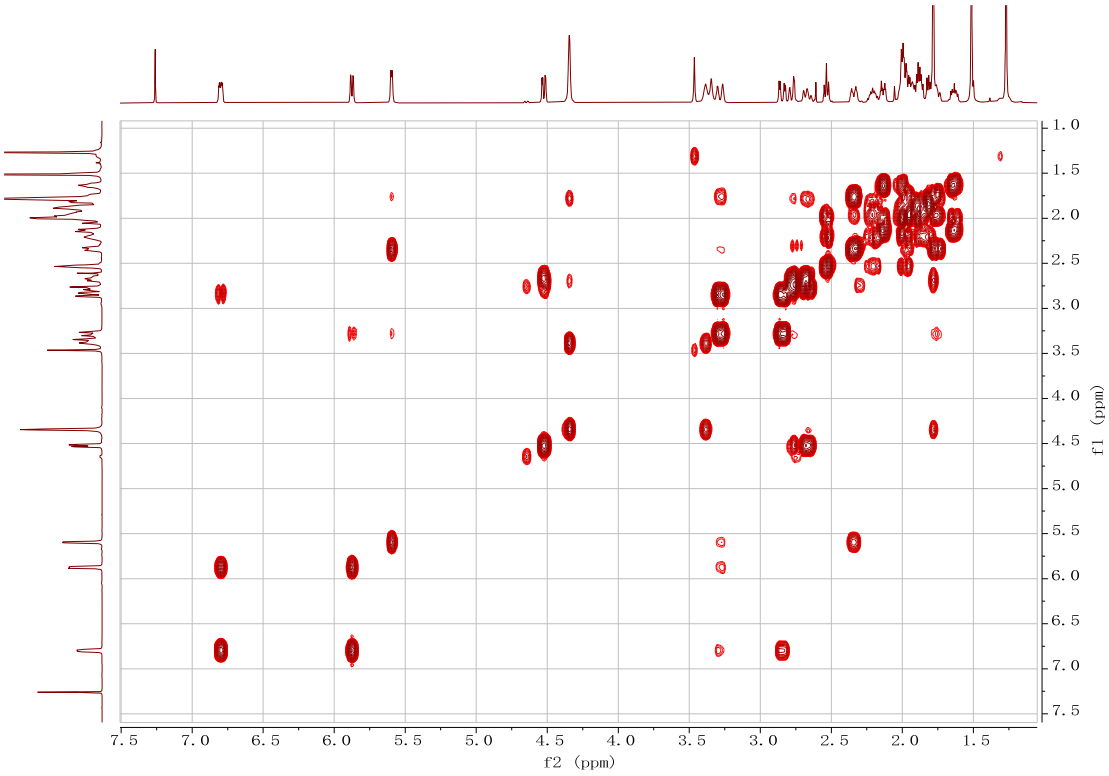


Figure S64. ^{1}H-^{1}H COSY Spectrum of Withaminilide G (**7**) in $CDCl_3$

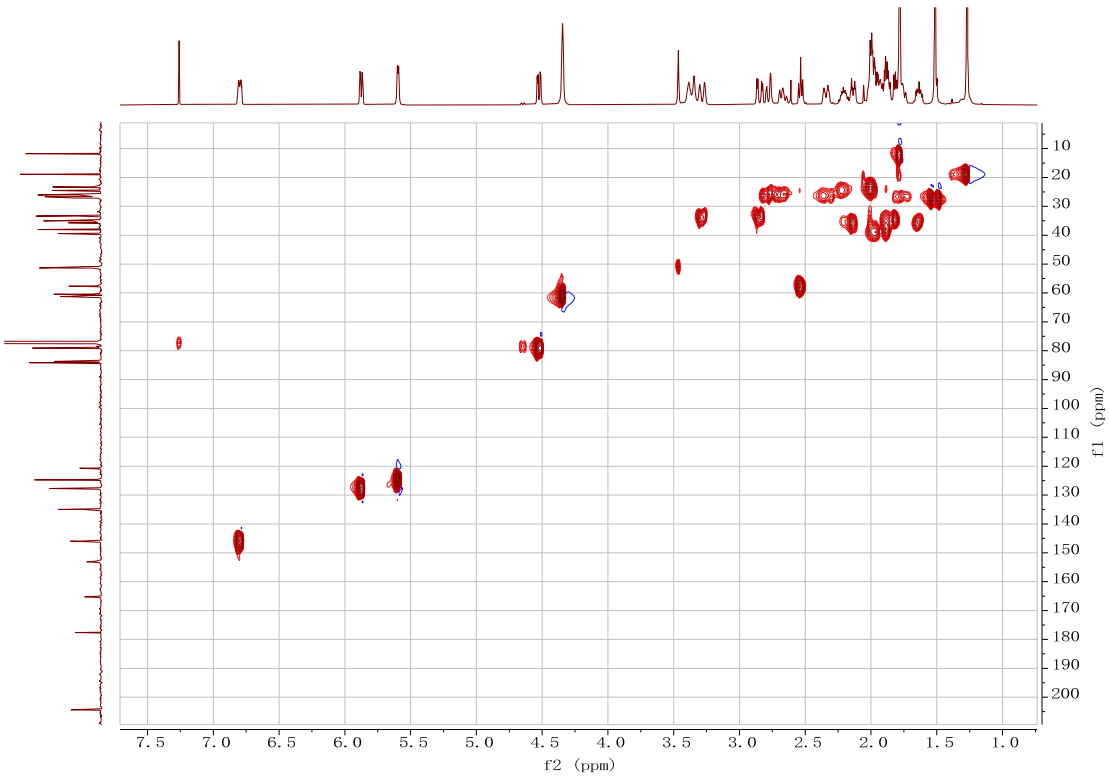


Figure S65. HSQC Spectrum of Withaminilide G (**7**) in $CDCl_3$

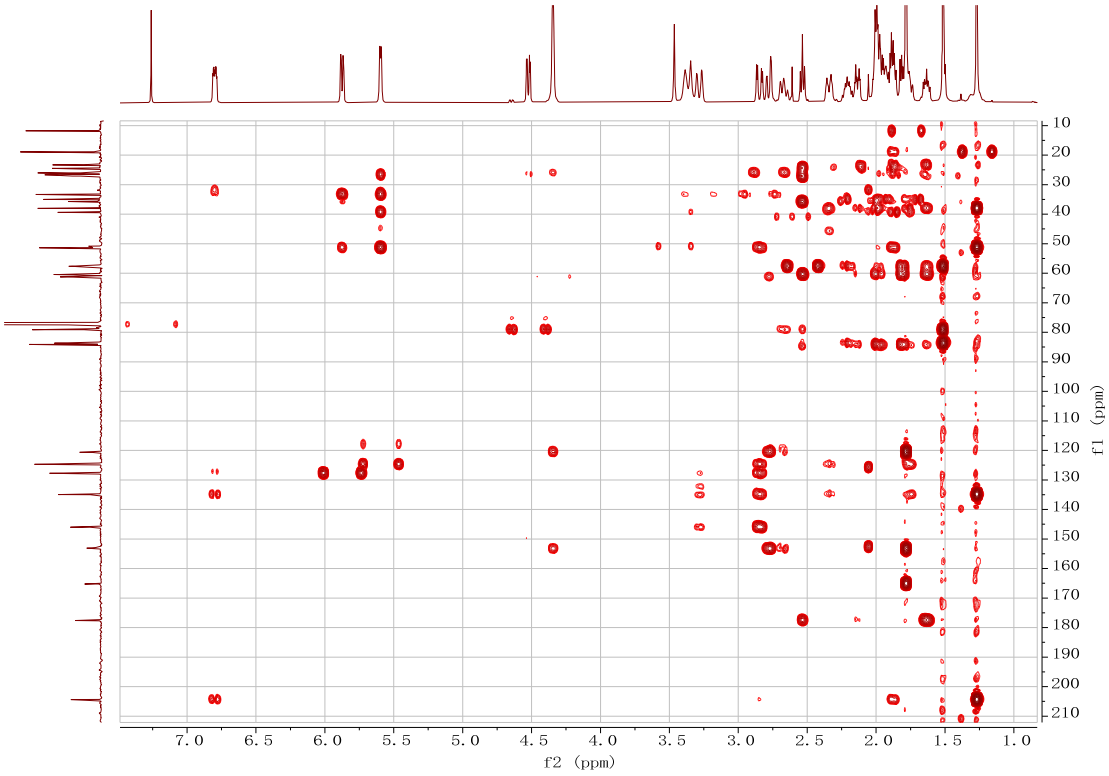


Figure S66. HMBC Spectrum of Withaminilide G (**7**) in $CDCl_3$

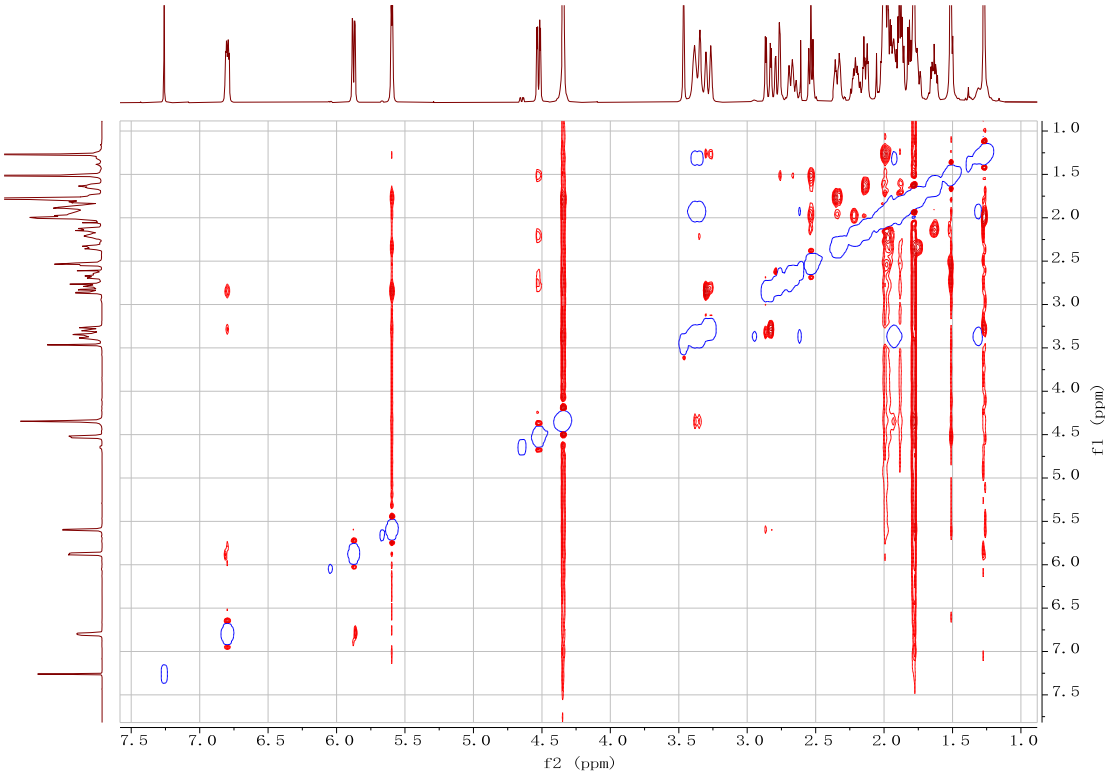


Figure S67. NOESY Spectrum of Withaminilide G (**7**) in $CDCl_3$

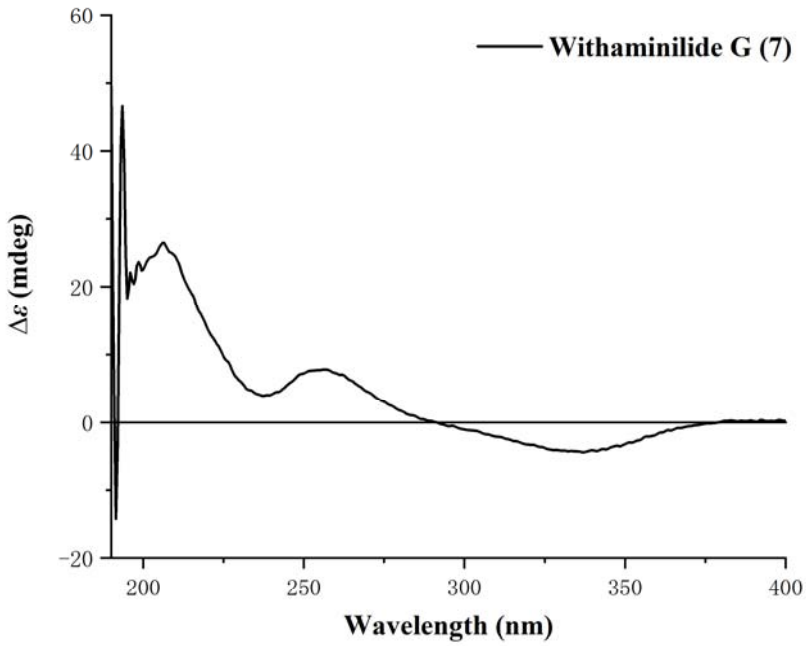


Figure S68. Experimental ECD Spectrum of Withaminilide G (**7**)

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
143 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200

Minimum:	80.00					-1.5		
Maximum:	100.00			3.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
527.2298	527.2281	1.7	3.2	12.5	547.0	n/a	n/a	C29H35O9

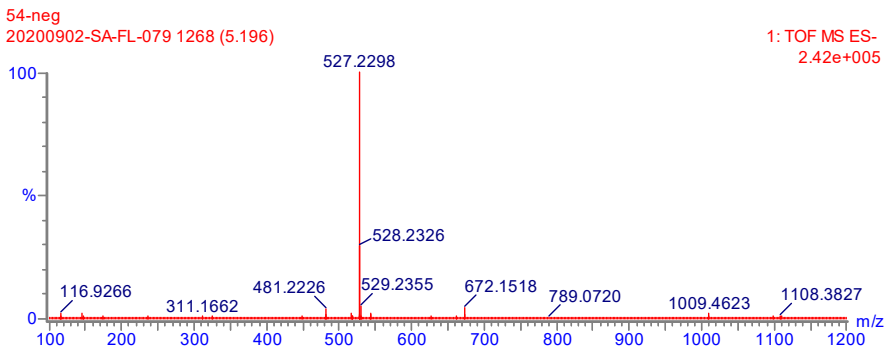


Figure S69. HRESIMS Spectrum of Withaminilide H (**8**)

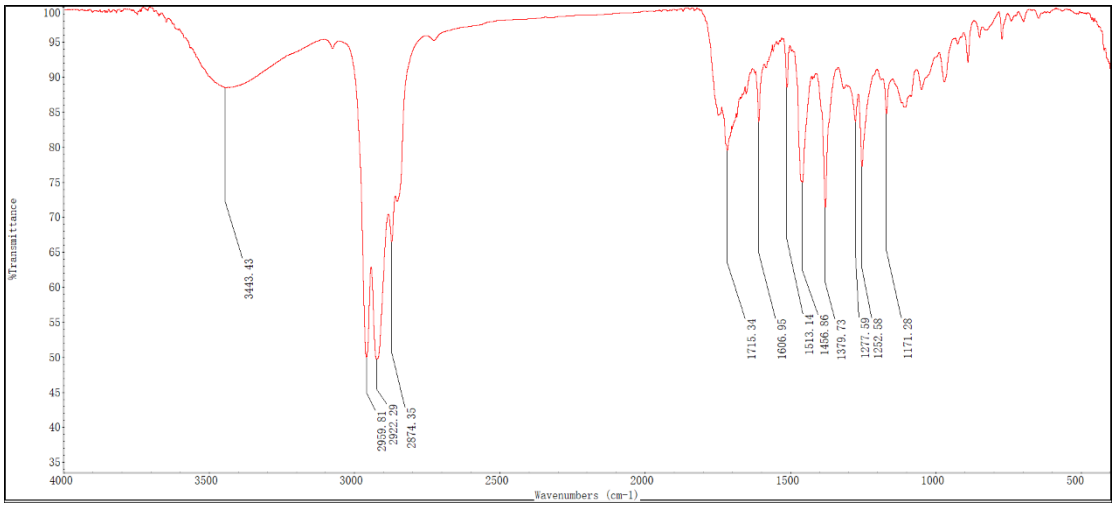


Figure S70. IR Spectrum of Withaminilide H (**8**)

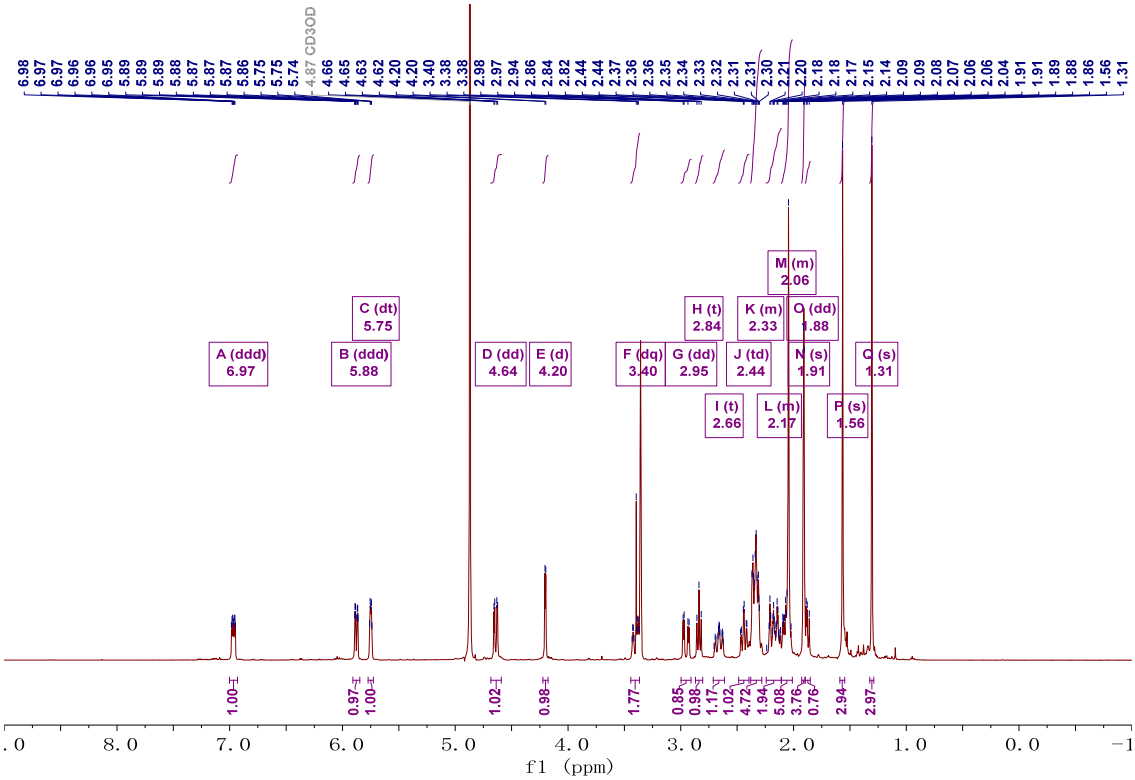


Figure S71. ^{1}H NMR Spectrum of Withaminilide H (**8**) in CD_3OD, 500 MHz

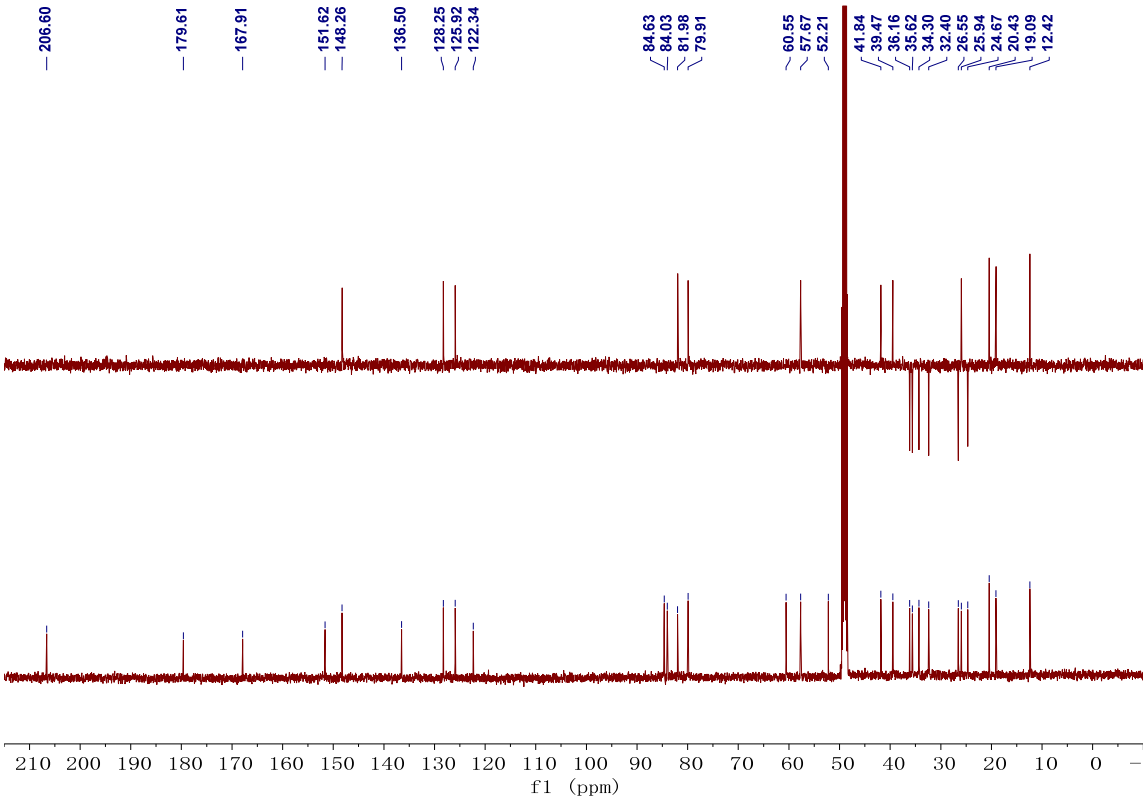


Figure S72. ^{13}C NMR Spectrum of Withaminilide H (**8**) in CD_3OD, 125 MHz

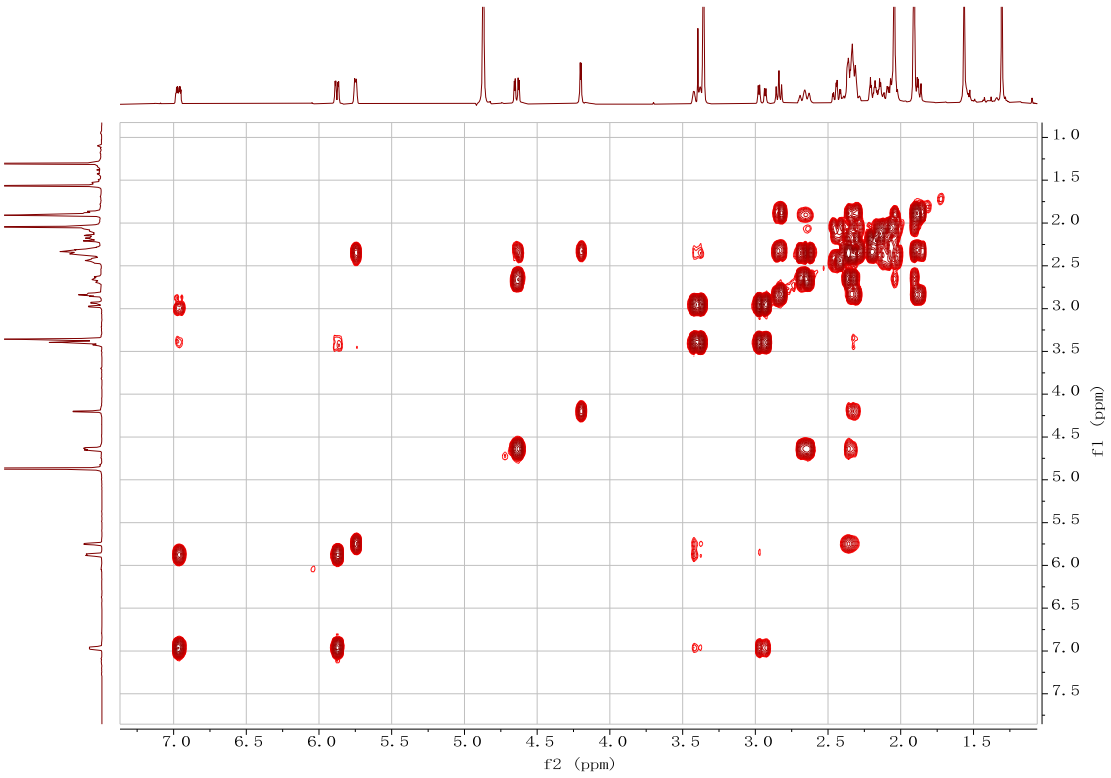


Figure S73. ^{1}H-^{1}H COSY Spectrum of Withaminilide H (**8**) in CD_3OD

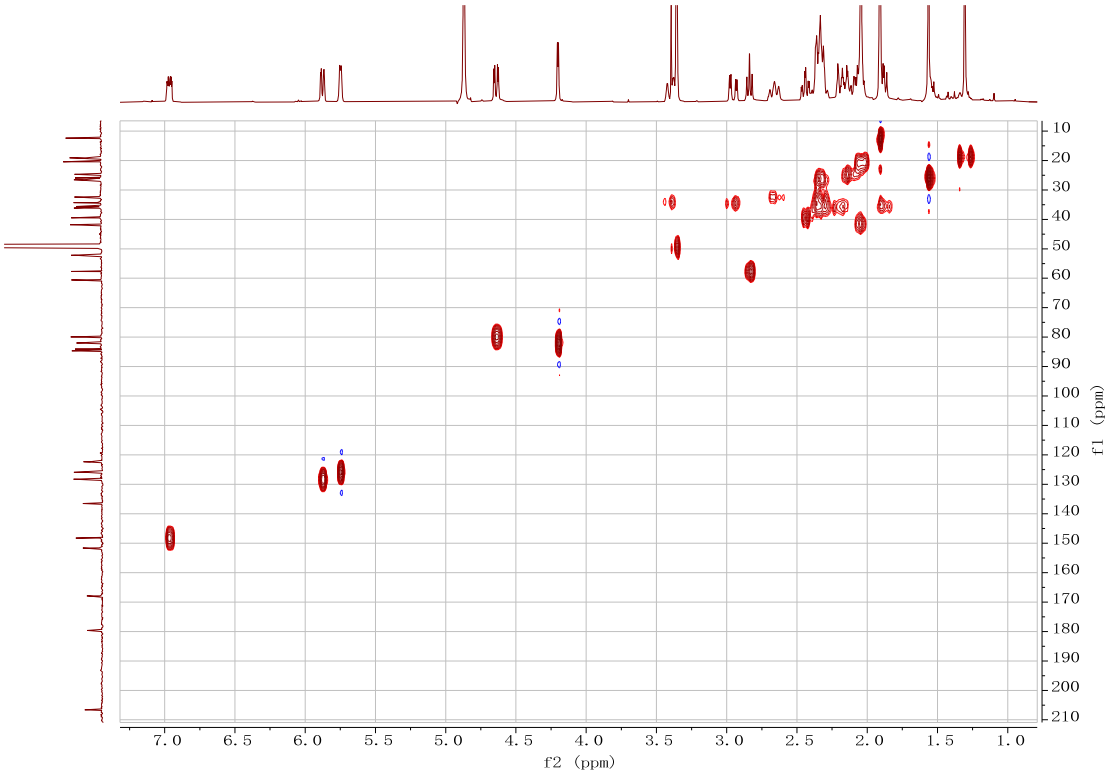


Figure S74. HSQC Spectrum of Withaminilide H (**8**) in CD_3OD

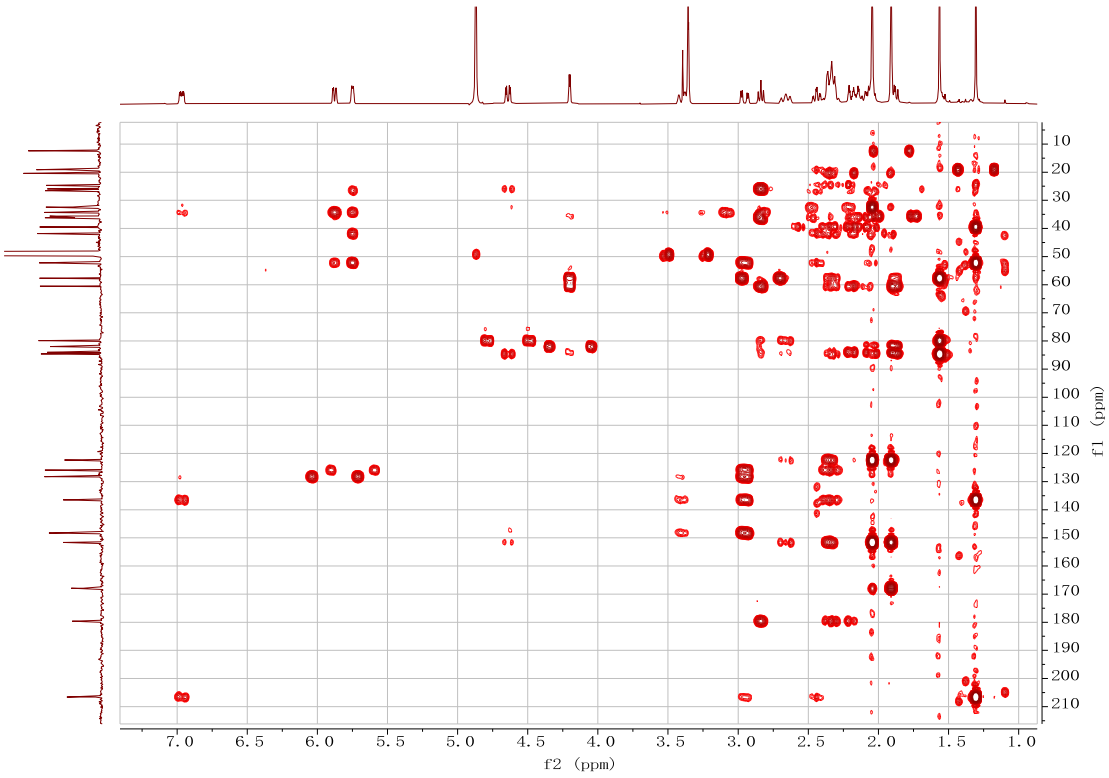


Figure S75. HMBC Spectrum of Withaminilide H (**8**) in CD_3OD

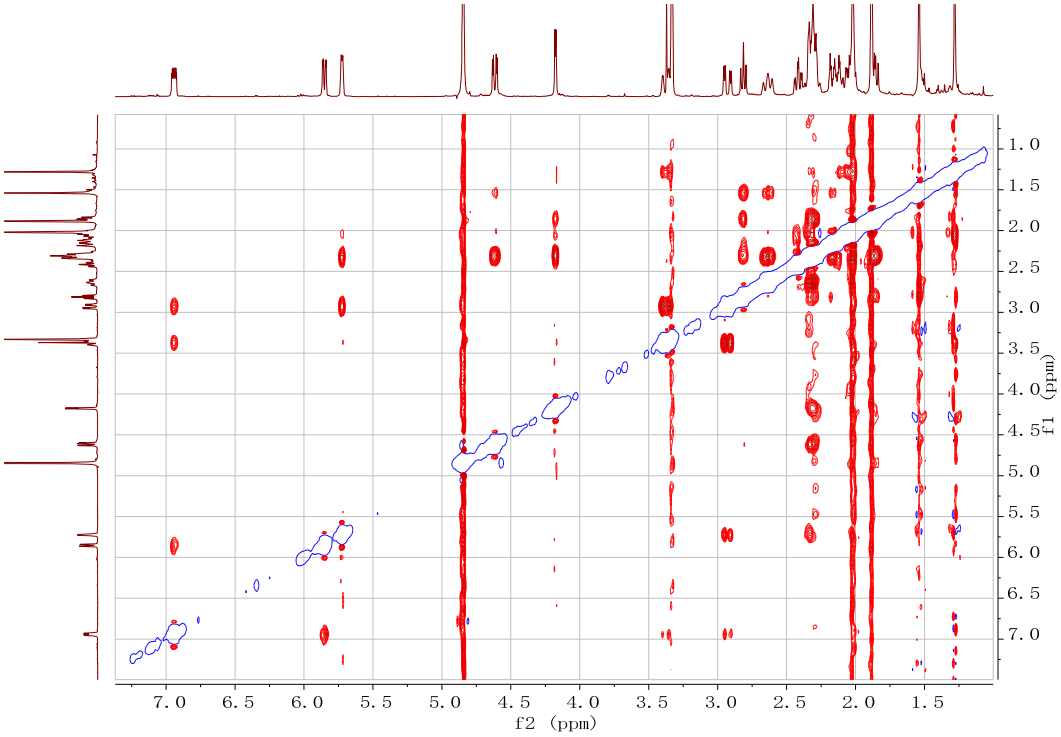


Figure S76. NOESY Spectrum of Withaminilide H (**8**) in CD_3OD

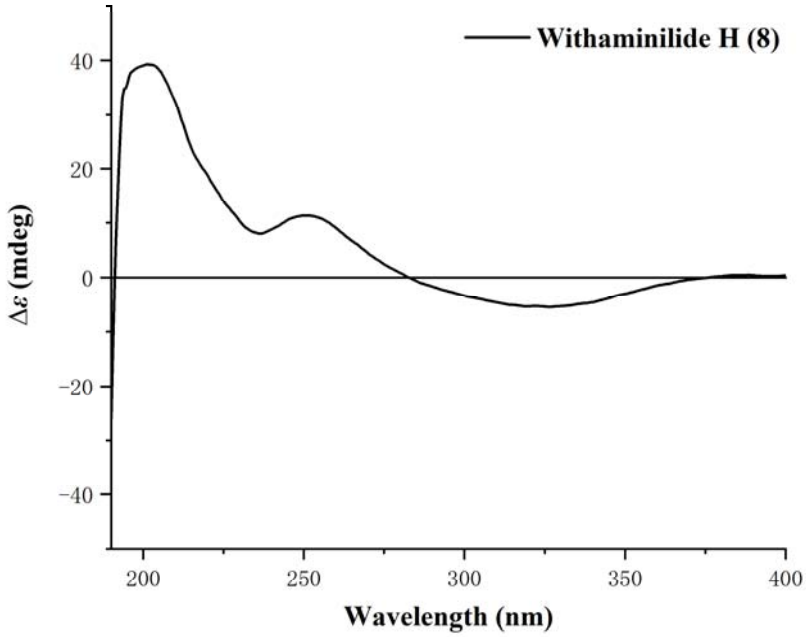


Figure S77. Experimental ECD Spectrum of Withaminilide H (**8**)

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

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

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Minimum:	80.00					-1.5		
Maximum:	100.00		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
527.2283	527.2281	0.2	0.4	12.5	587.4	n/a	n/a	$C_{29}H_{35}O_9$

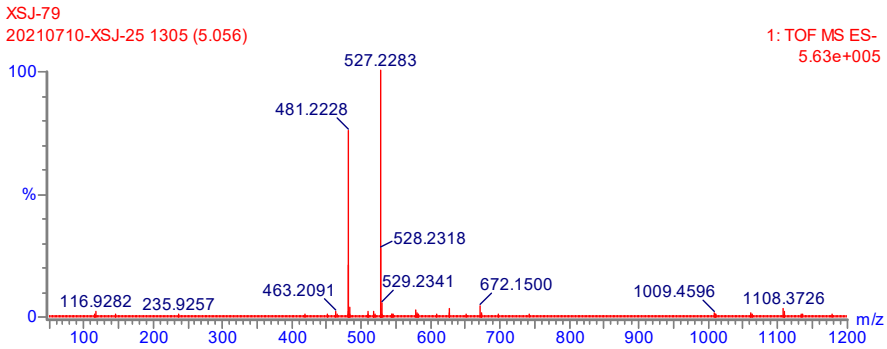


Figure S78. HRESIMS Spectrum of Withaminilide I (**9**)

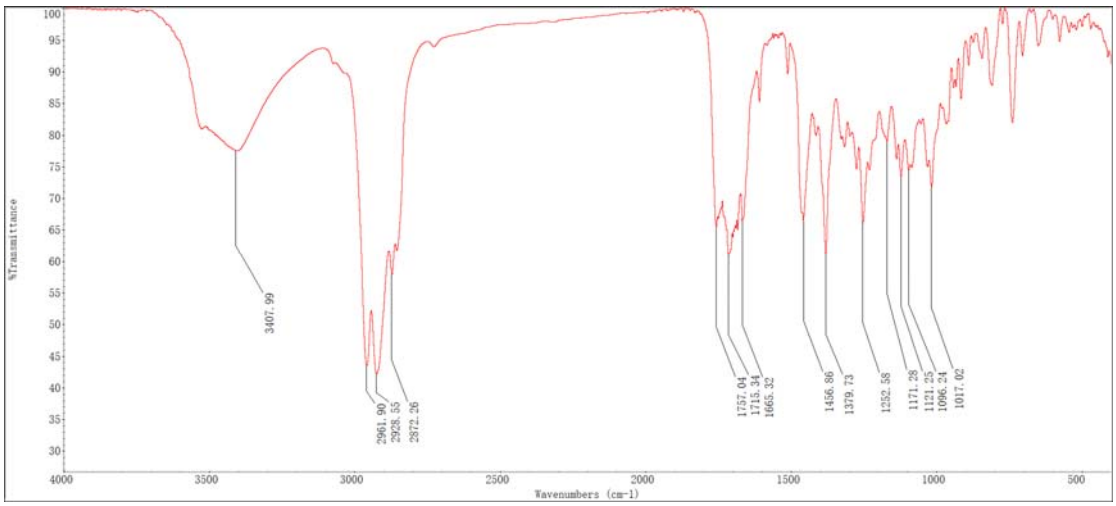


Figure S79. IR Spectrum of Withaminilide I (**9**)

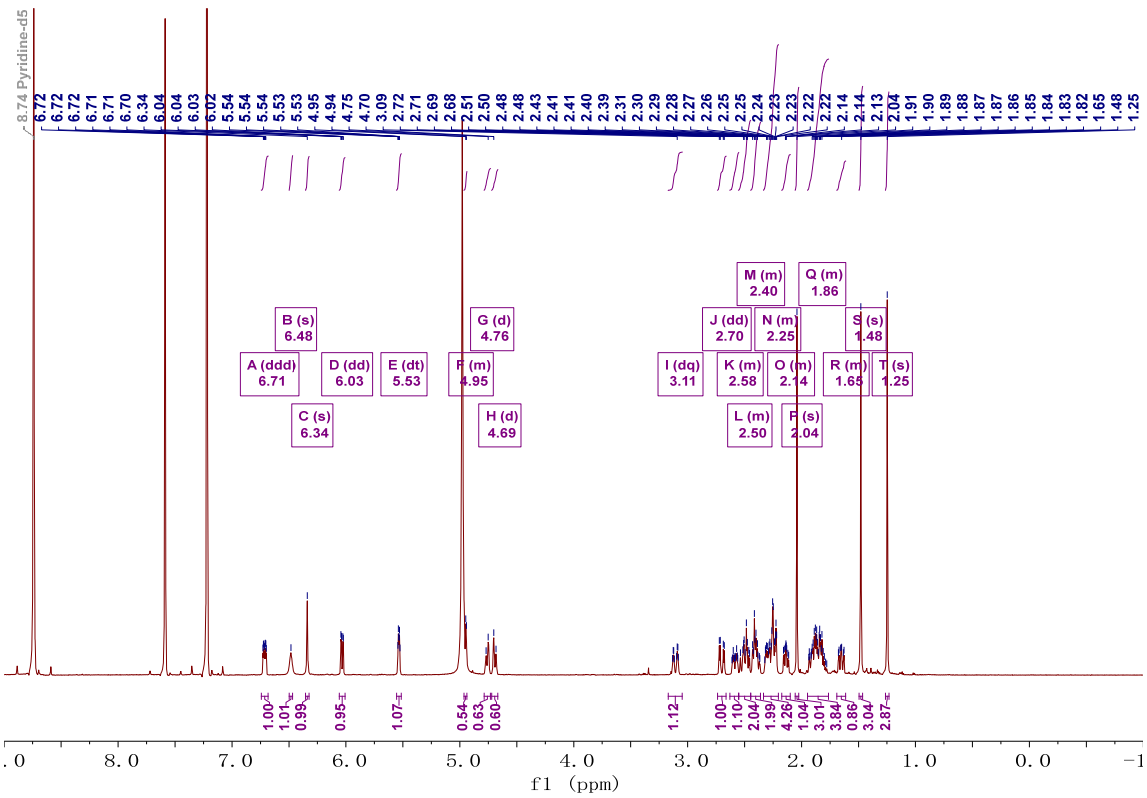


Figure S80. ^{1}H NMR Spectrum of Withaminilide I (**9**) in C_5D_5N, 600 MHz

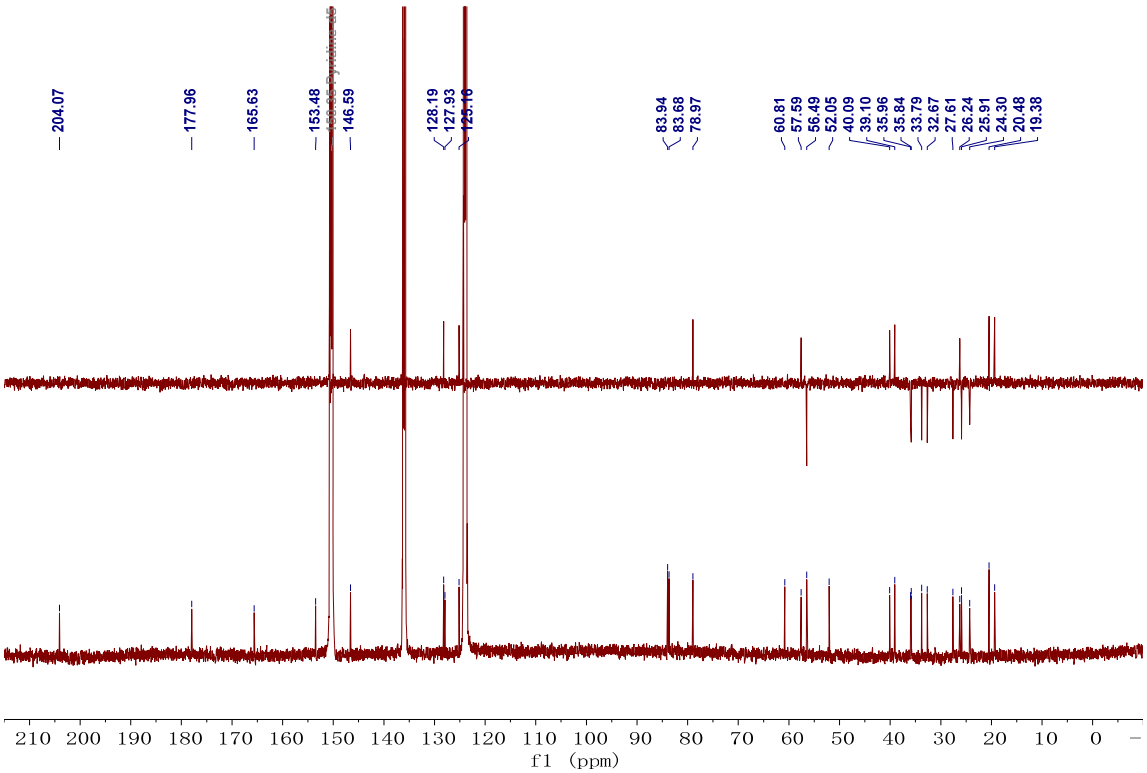


Figure S81. ^{13}C NMR Spectrum of Withaminilide I (**9**) in C_5D_5N, 125 MHz

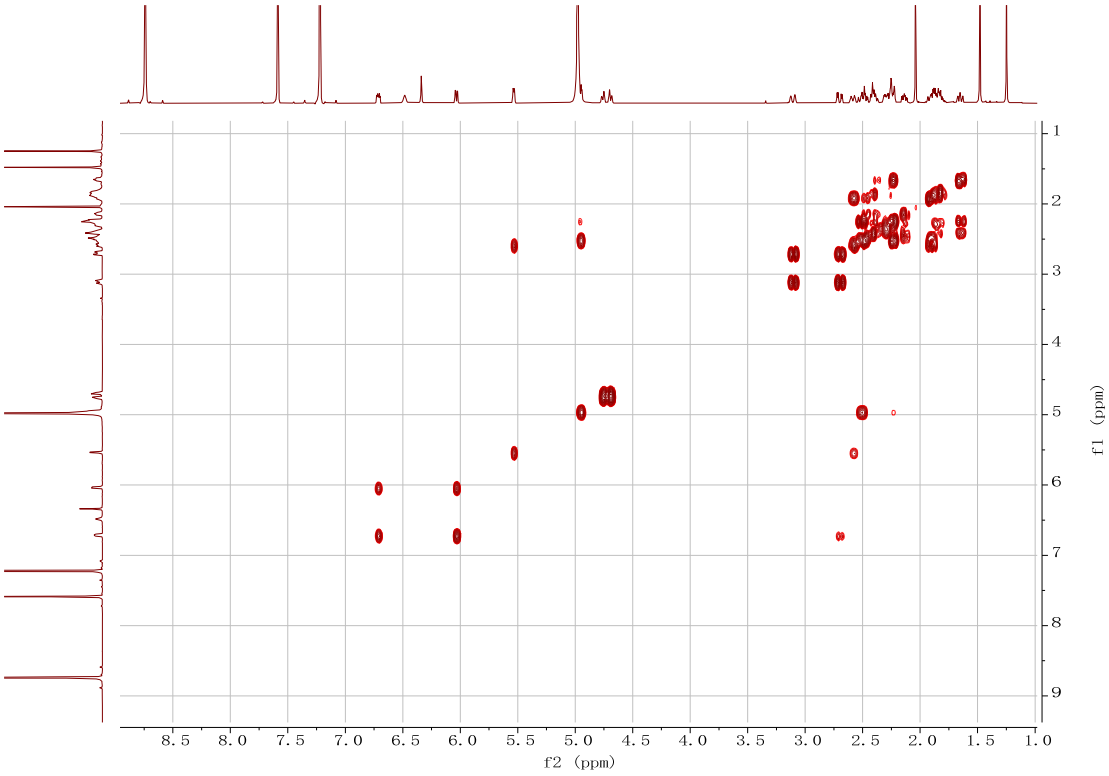


Figure S82. ^{1}H-^{1}H COSY Spectrum of Withaminilide I (**9**) in C_5D_5N

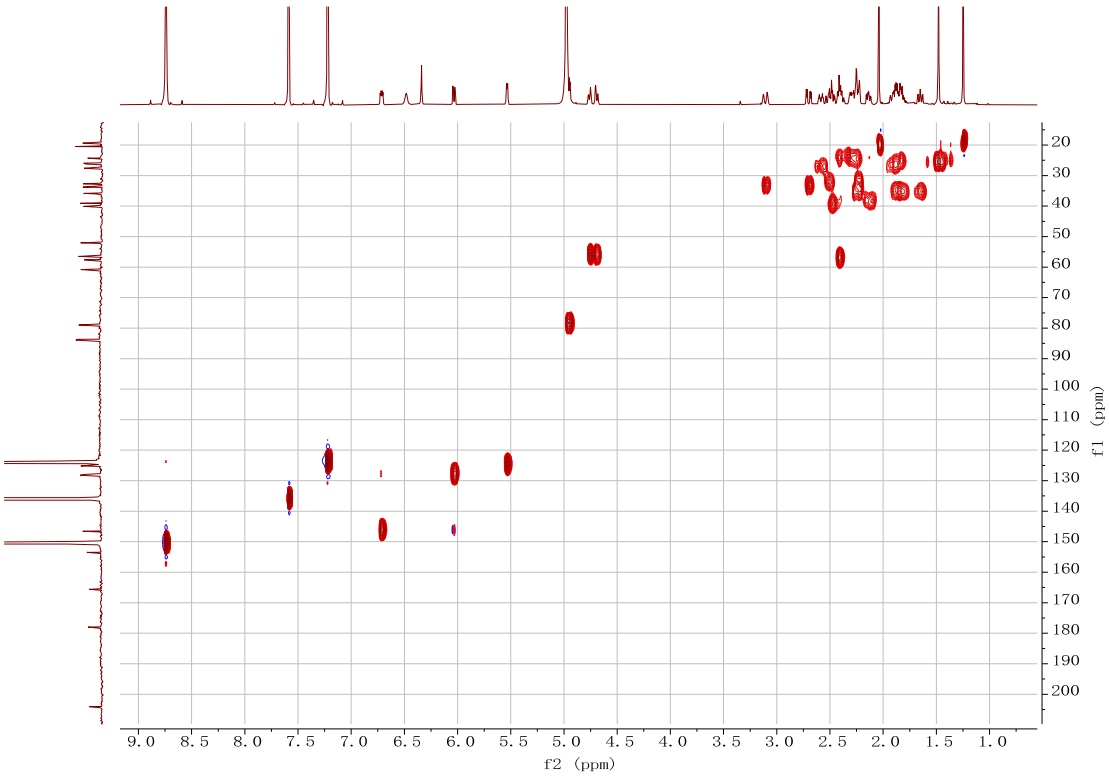


Figure S83. HSQC Spectrum of Withaminilide I (**9**) in C_5D_5N

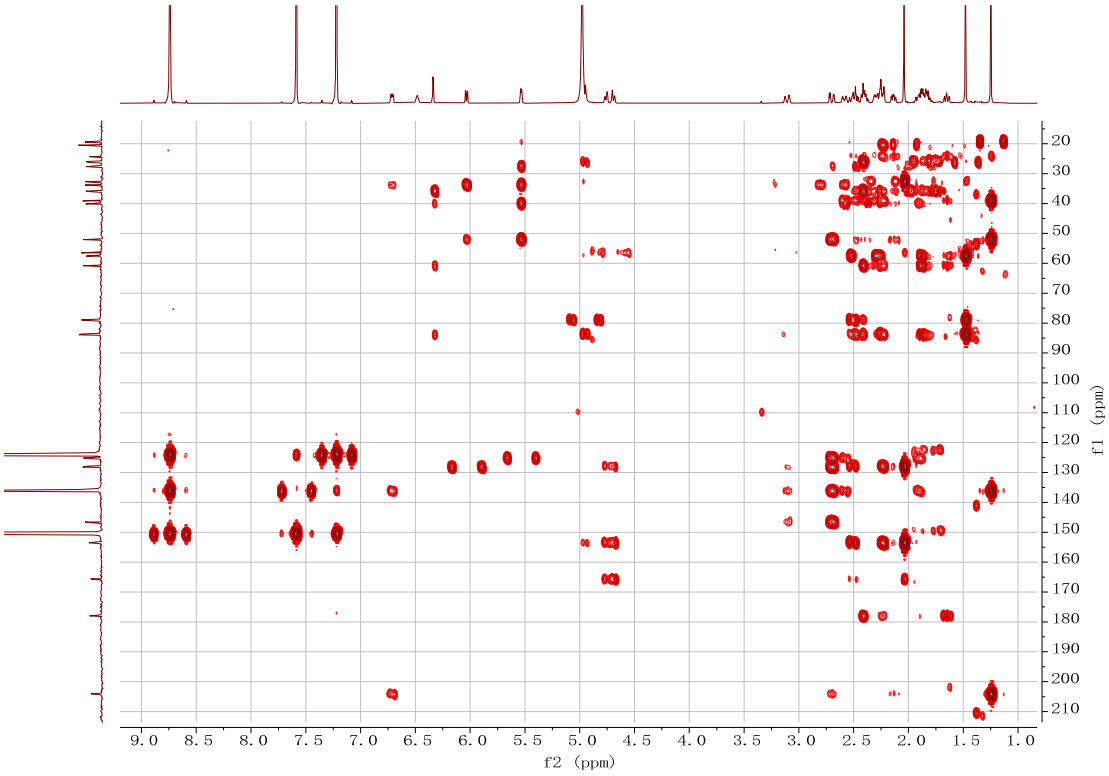


Figure S84.HMBC Spectrum of Withaminilide I (**9**) in C_5D_5N

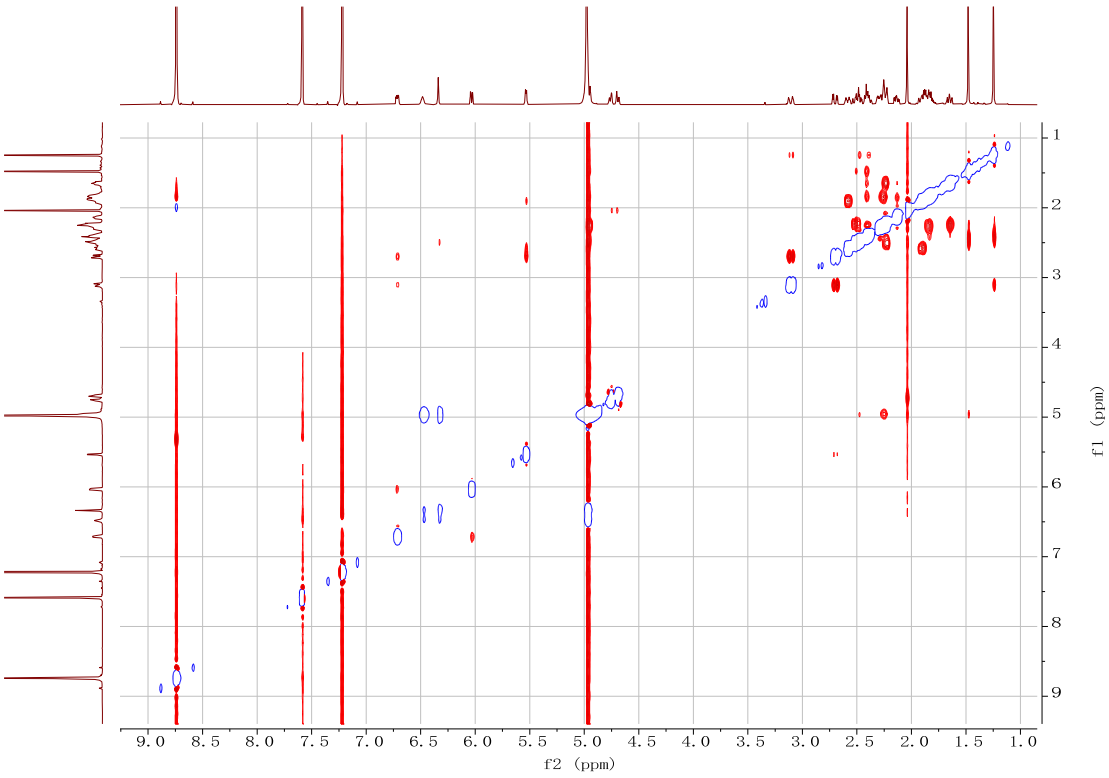


Figure S85. NOESY Spectrum of Withaminilide I (**9**) in C_5D_5N

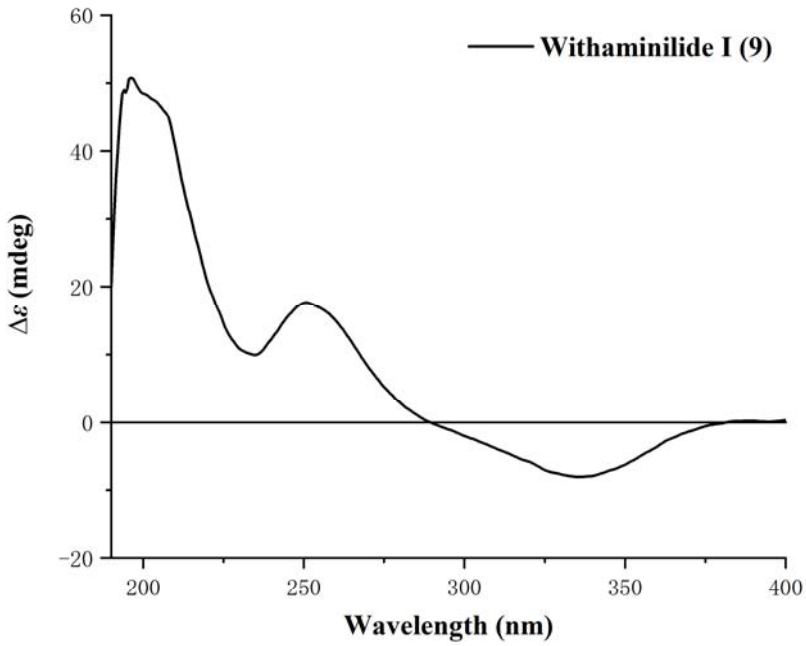


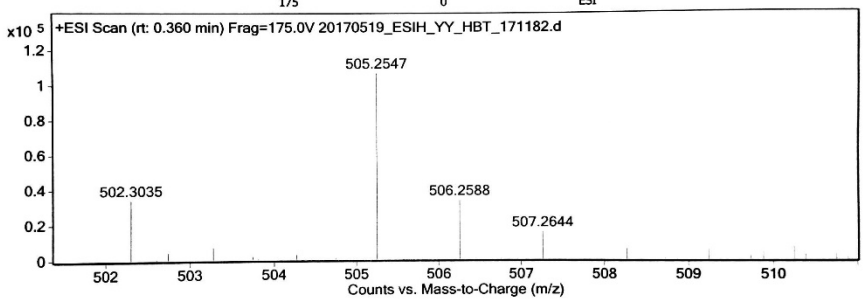
Figure S86. Experimental ECD Spectrum of Withaminilide I (**9**)

Qualitative Analysis Report

Data Filename	20170519_ESIH_YY_HBT_171182.d	**Sample Name**	XSJB804324-2
Sample Type	Sample	**Position**	P1-A6
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/19/2017 11:13:21 AM	**IRM Calibration Status**	[redacted]
DA Method	small molecular data analysis method.m	**Comment**	ESIH

User Spectra

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
	175	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
505.2547	505.2561	1.36	2.69	C29 H38 Na O6	(M+Na)+

--- End Of Report ---

Agilent Technologies Page 1 of 1 Printed at: 11:46 AM on: 5/19/2017

Figure S87. HRESIMS Spectrum of Withaminilide J (**10**)

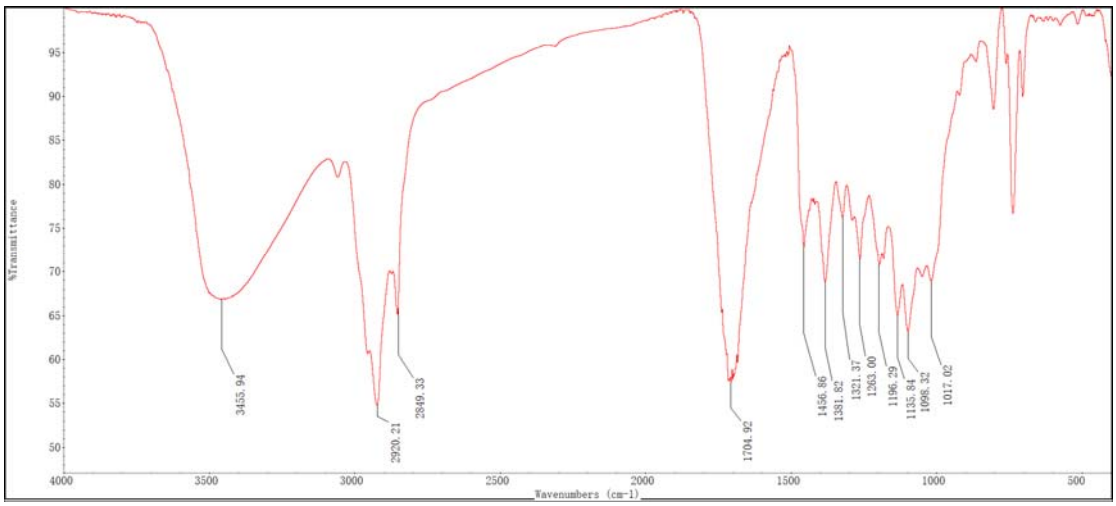


Figure S88. IR Spectrum of Withaminilide J (**10**)

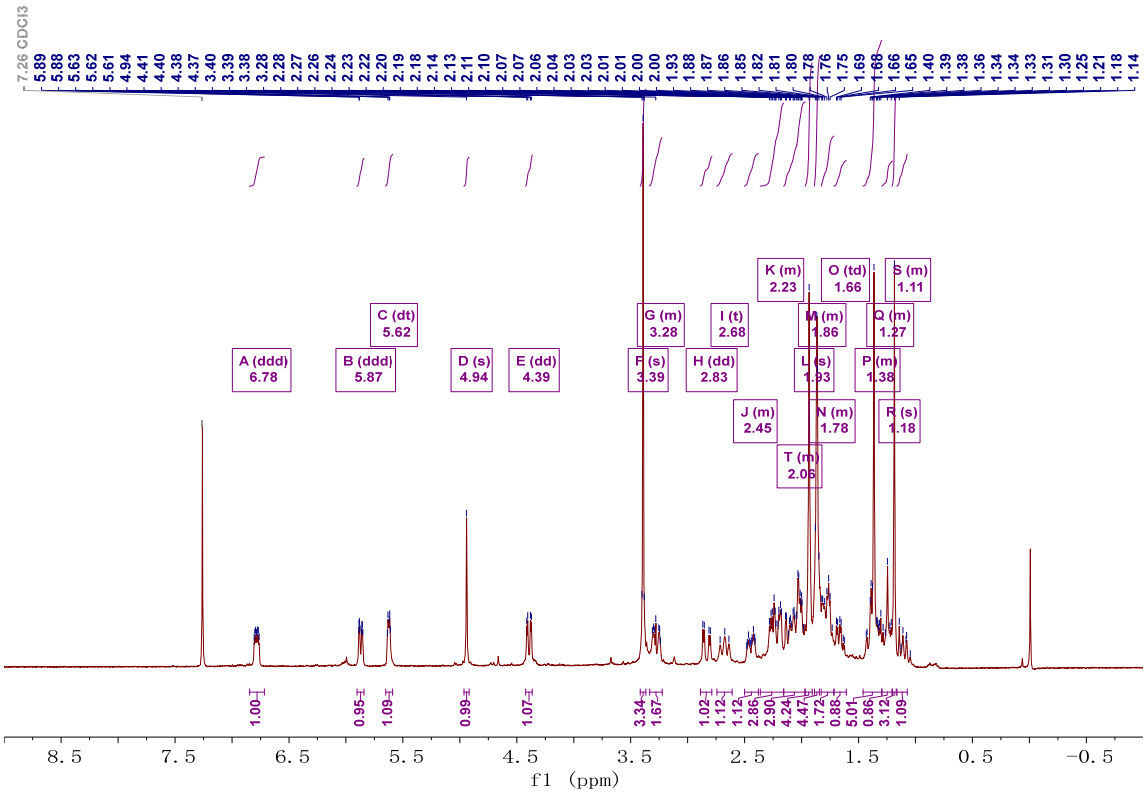


Figure S89. ^{1}H NMR Spectrum of Withaminilide J (**10**) in $CDCl_3$, 400 MHz

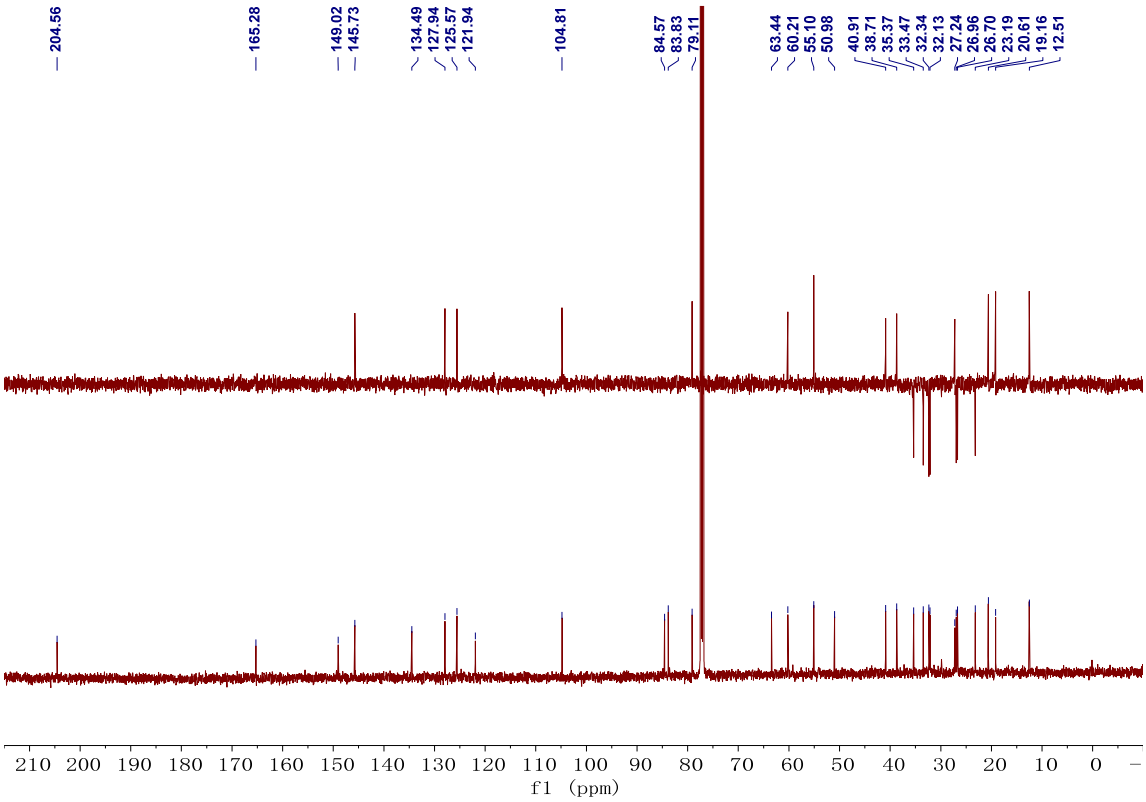


Figure S90. ^{13}C NMR Spectrum of Withaminilide J (**10**) in $CDCl_3$, 125 MHz

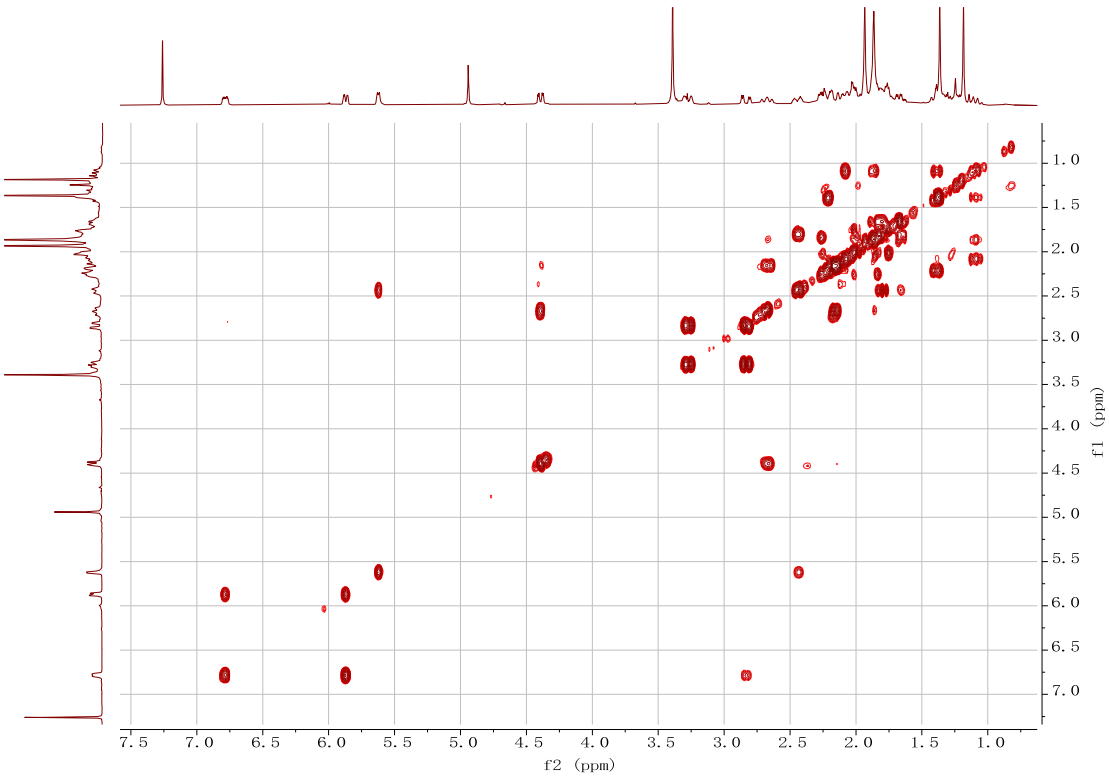


Figure S91. ^{1}H-^{1}H COSY Spectrum of Withaminilide J (**10**) in $CDCl_3$

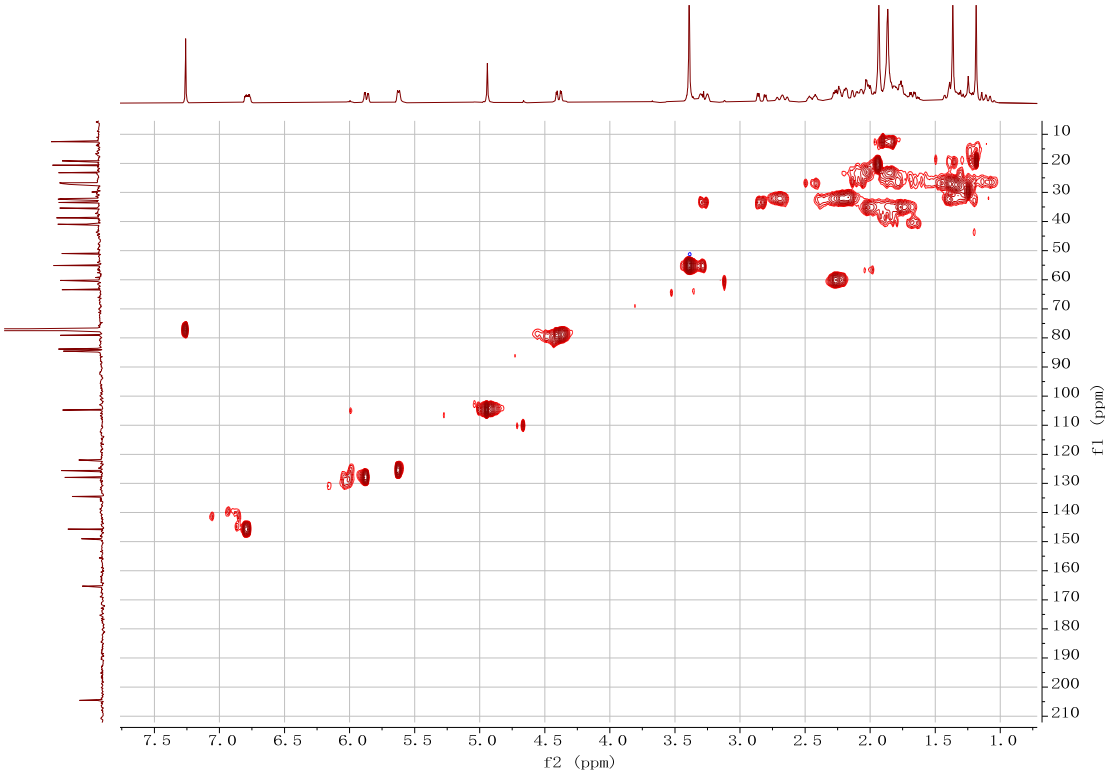


Figure S92. HSQC Spectrum of Withaminilide J (**10**) in $CDCl_3$

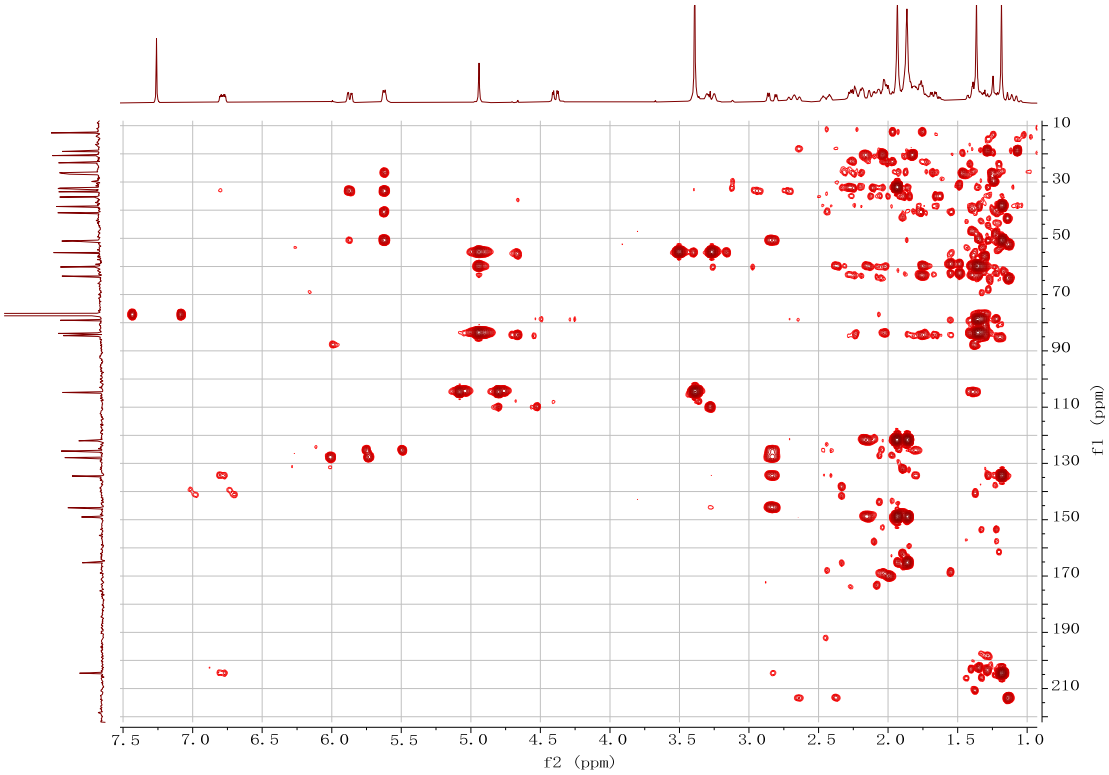


Figure S93. HMBC Spectrum of Withaminilide J (**10**) in $CDCl_3$

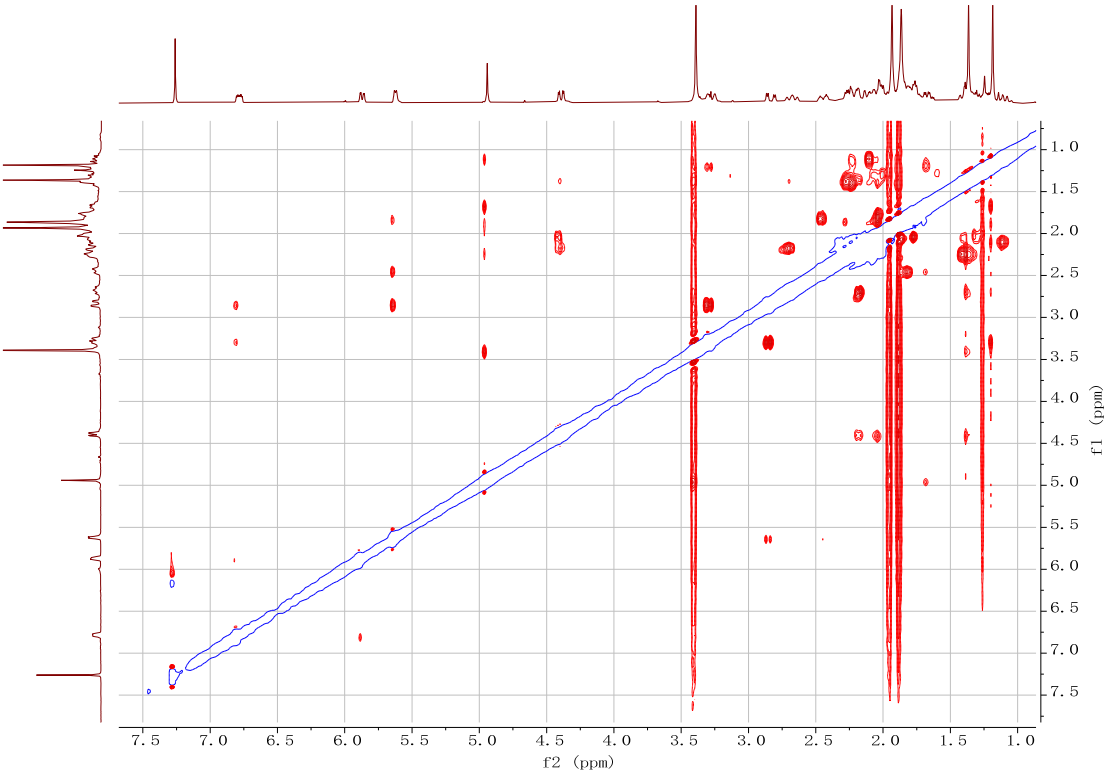


Figure S94. NOESY Spectrum of Withaminilide J (**10**) in $CDCl_3$

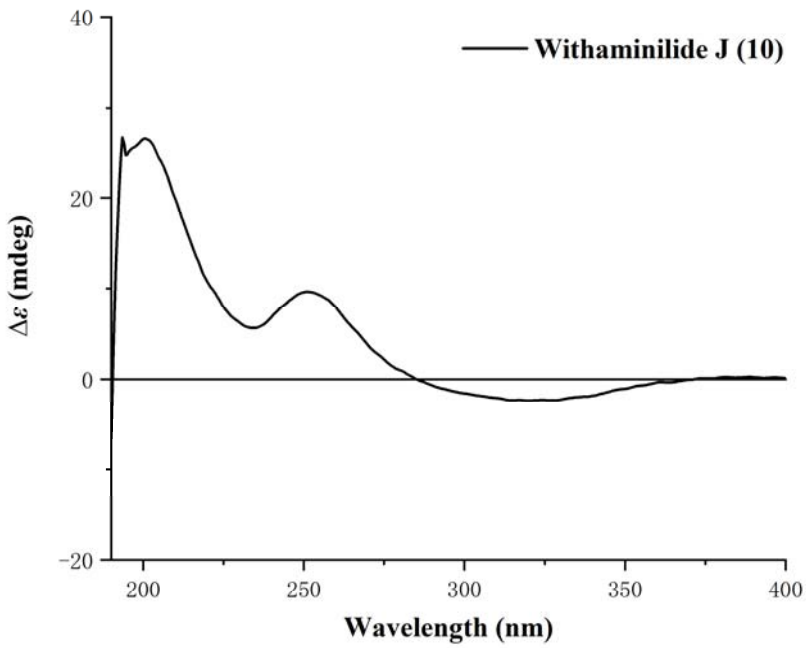
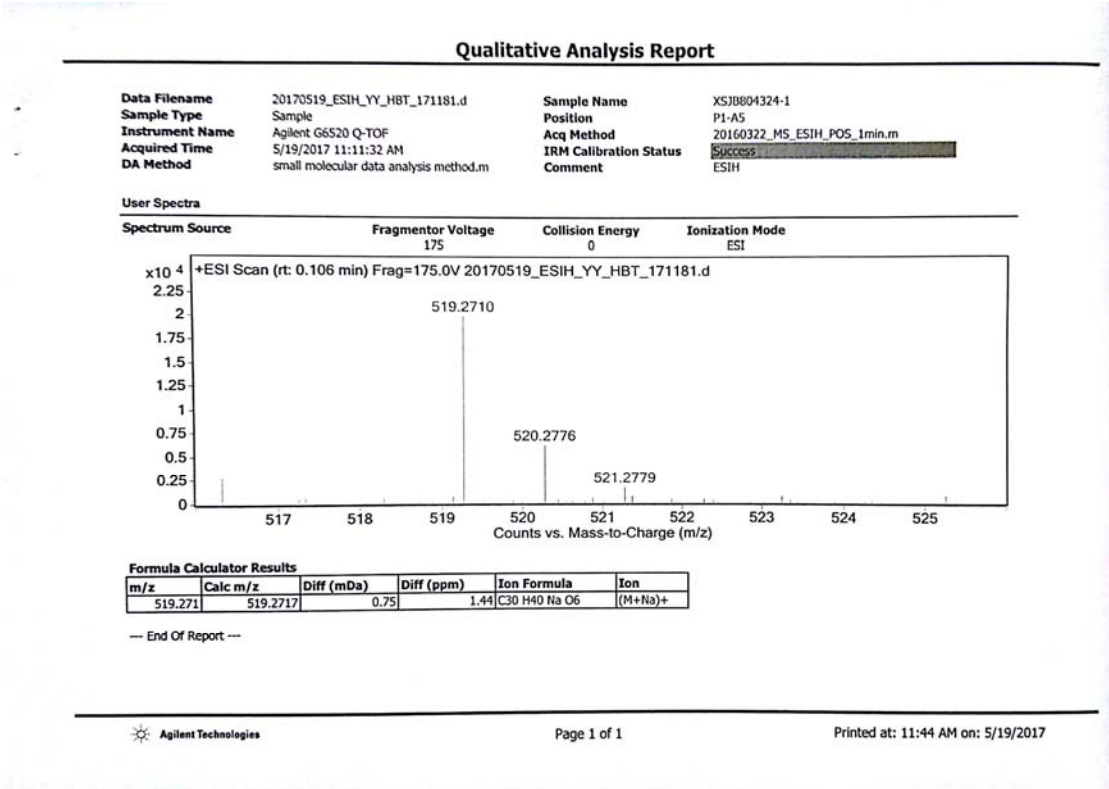


Figure S95. Experimental ECD Spectrum of Withaminilide J (**10**)



Qualitative Analysis Report

Data Filename	20170519_ESIH_YY_HBT_171181.d	**Sample Name**	XSJB804324-1
Sample Type	Sample	**Position**	P1-A5
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/19/2017 11:11:32 AM	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH

User Spectra

Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
	175	0	ESI

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
519.271	519.2717	0.75	1.44	C30 H40 Na O6	(M+Na)+

--- End Of Report ---

Agilent Technologies Page 1 of 1 Printed at: 11:44 AM on: 5/19/2017

Figure S96. HRESIMS Spectrum of Withaminilide K (**11**)

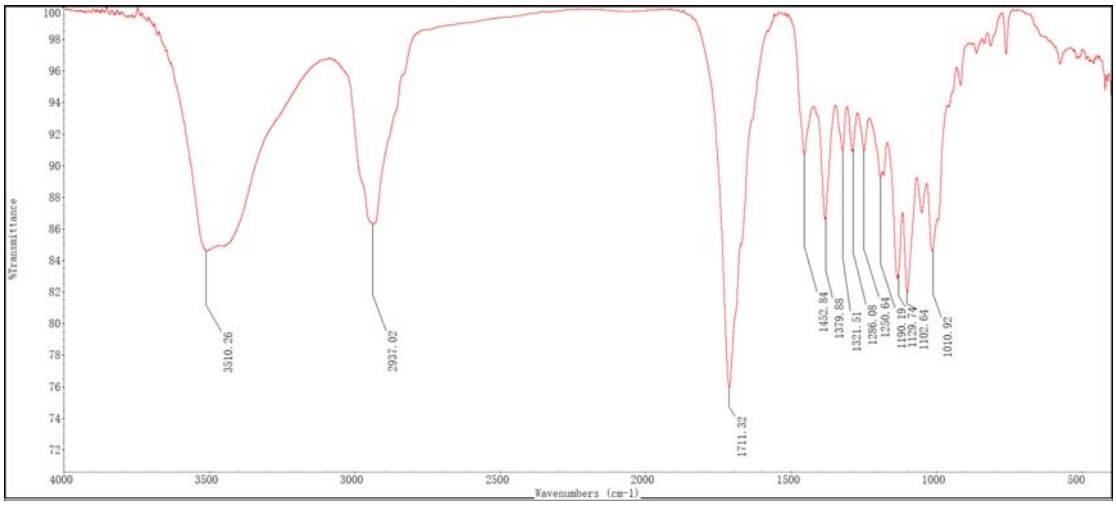


Figure S97. IR Spectrum of Withaminilide K (**11**)

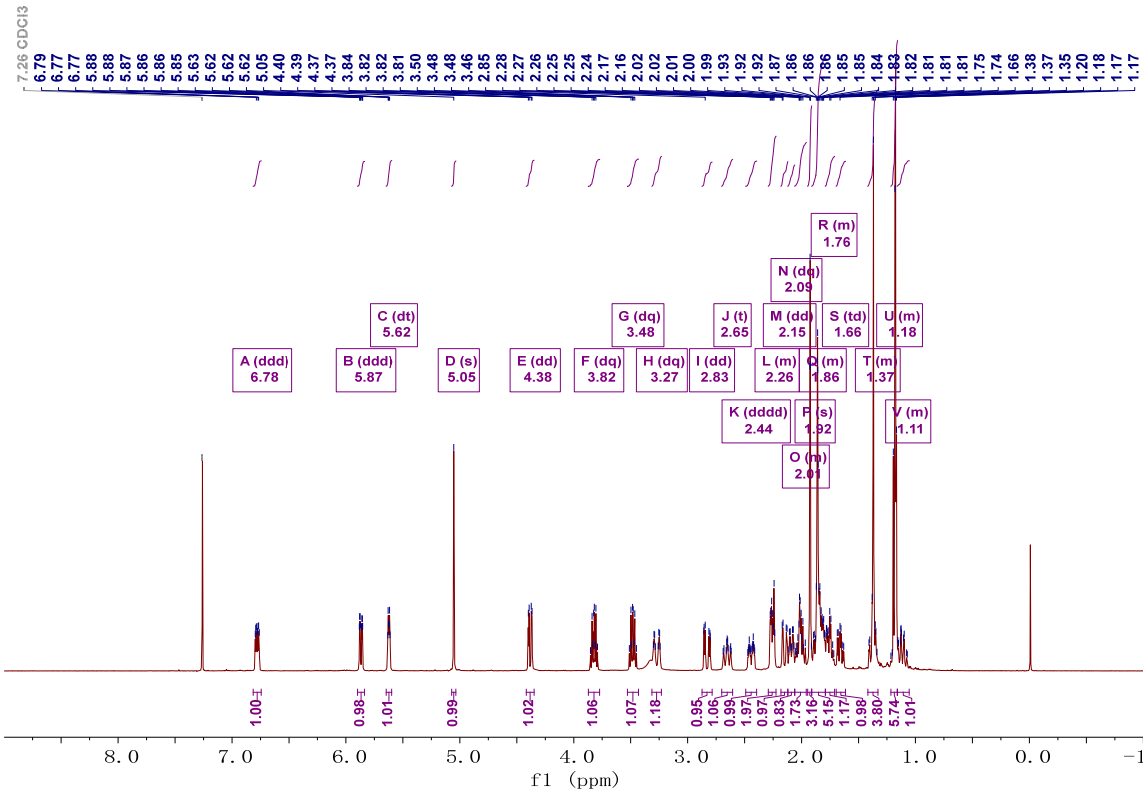


Figure S98. ^{1}H NMR Spectrum of Withaminilide K (**11**) in $CDCl_3$, 500 MHz

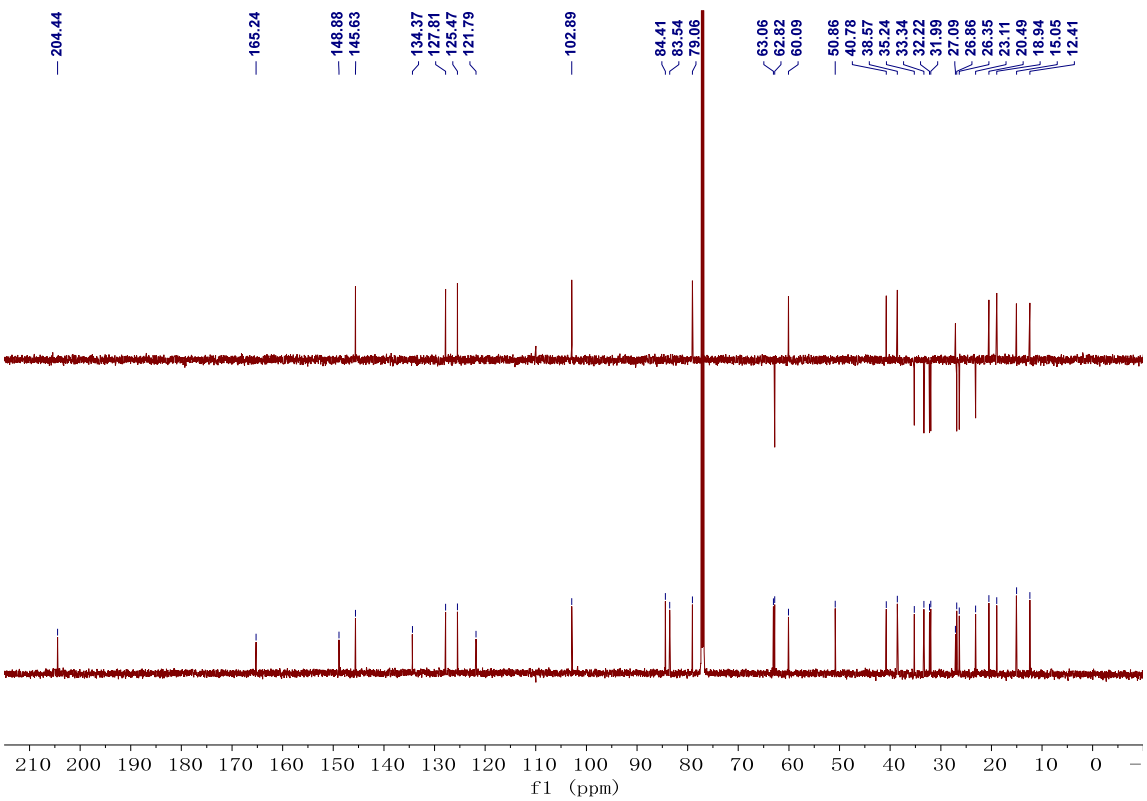


Figure S99. ^{13}C NMR Spectrum of Withaminilide K (**11**) in $CDCl_3$, 125 MHz

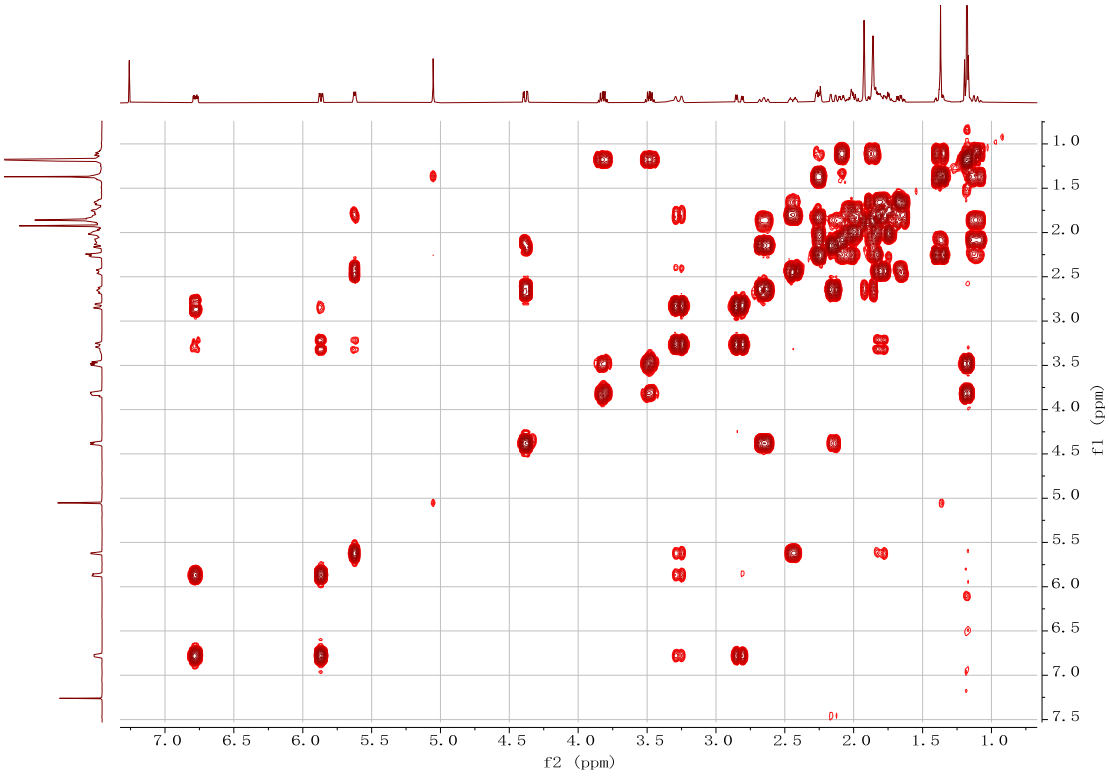


Figure S100. ^{1}H-^{1}H COSY Spectrum of Withaminilide K (**11**) in $CDCl_3$

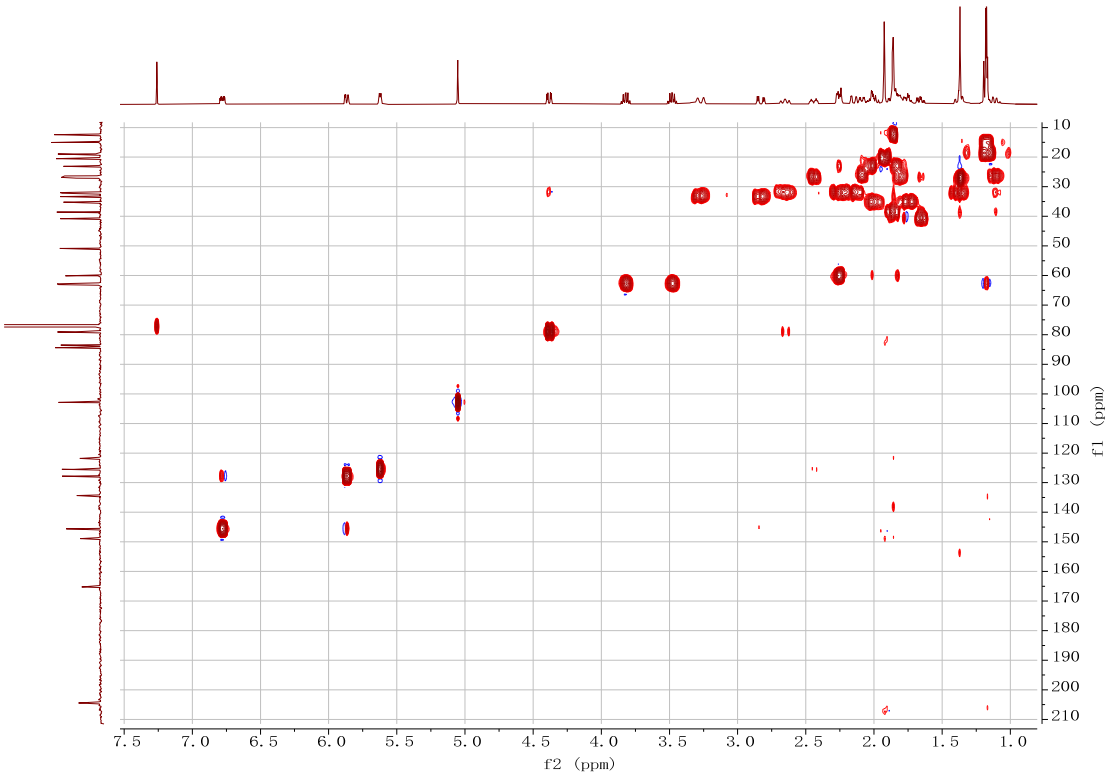


Figure S101. HSQC Spectrum of Withaminilide K (**11**) in $CDCl_3$

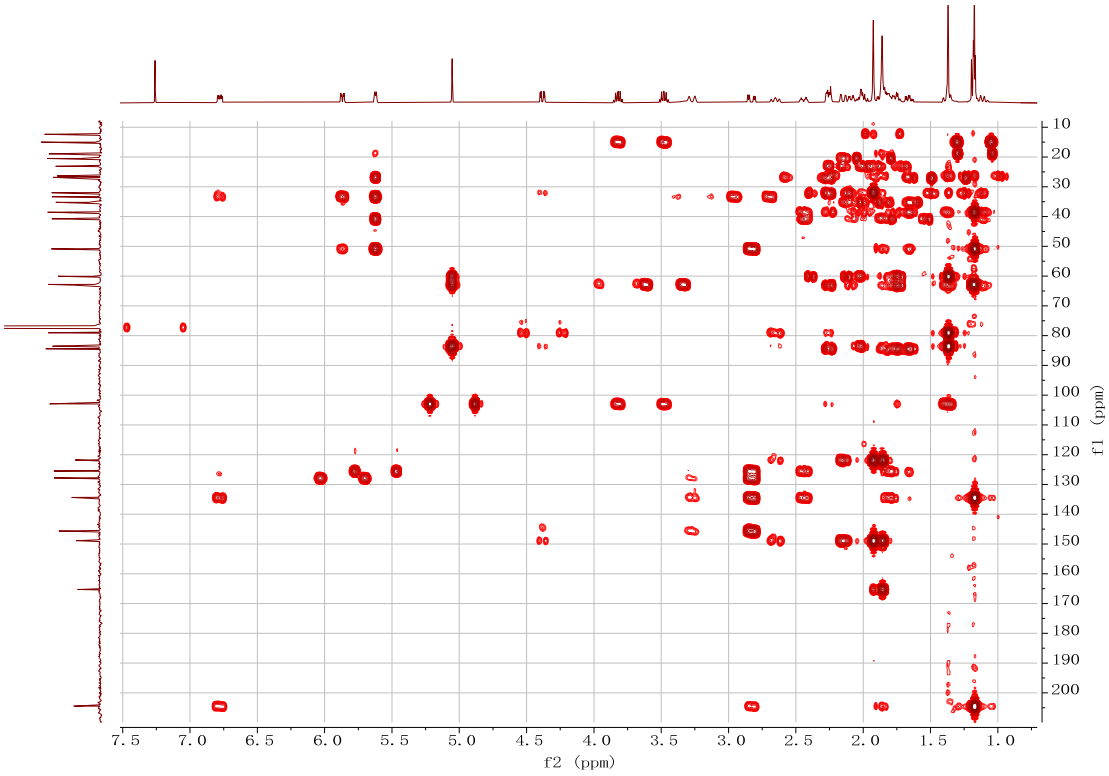


Figure S102. HMBC Spectrum of Withaminilide K (**11**) in $CDCl_3$

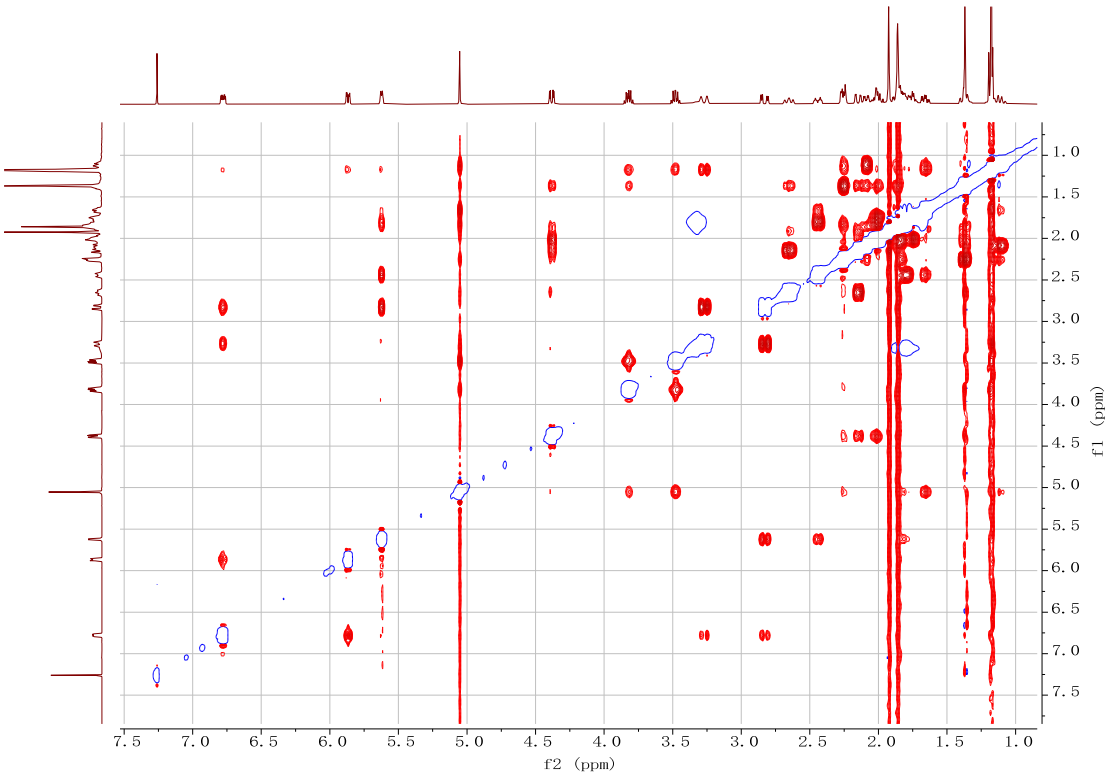


Figure S103. NOESY Spectrum of Withaminilide K (**11**) in $CDCl_3$

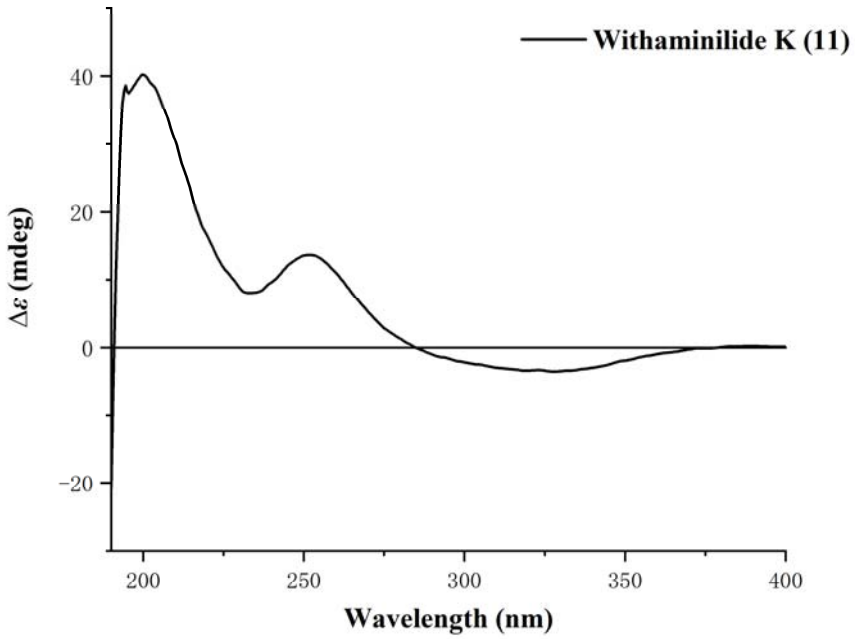


Figure S104. Experimental ECD Spectrum of Withaminilide K (**11**)

Elemental Composition Report
Tolerance = 4.0 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
154 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200

Minimum:	80.00					-1.5		
Maximum:	100.00			4.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
561.2706	561.2700	0.6	1.1	10.5	639.4	n/a	n/a	C30H41O10

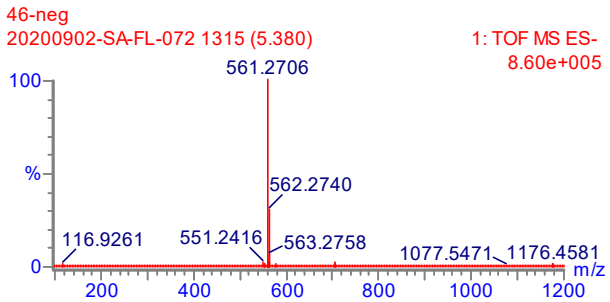


Figure S105. HRESIMS Spectrum of Withaminilide L (**12**)

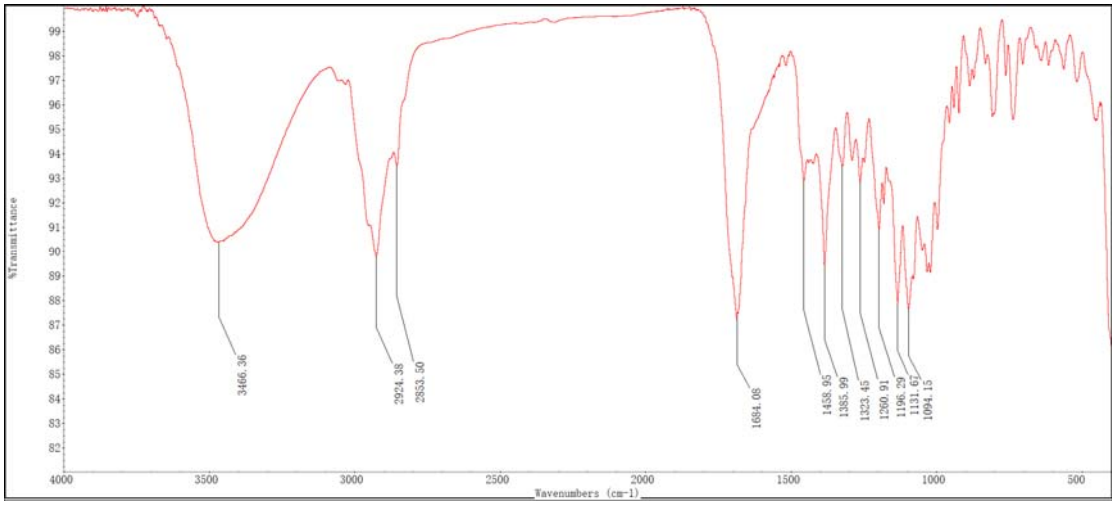


Figure S106. IR Spectrum of Withaminilide L (**12**)

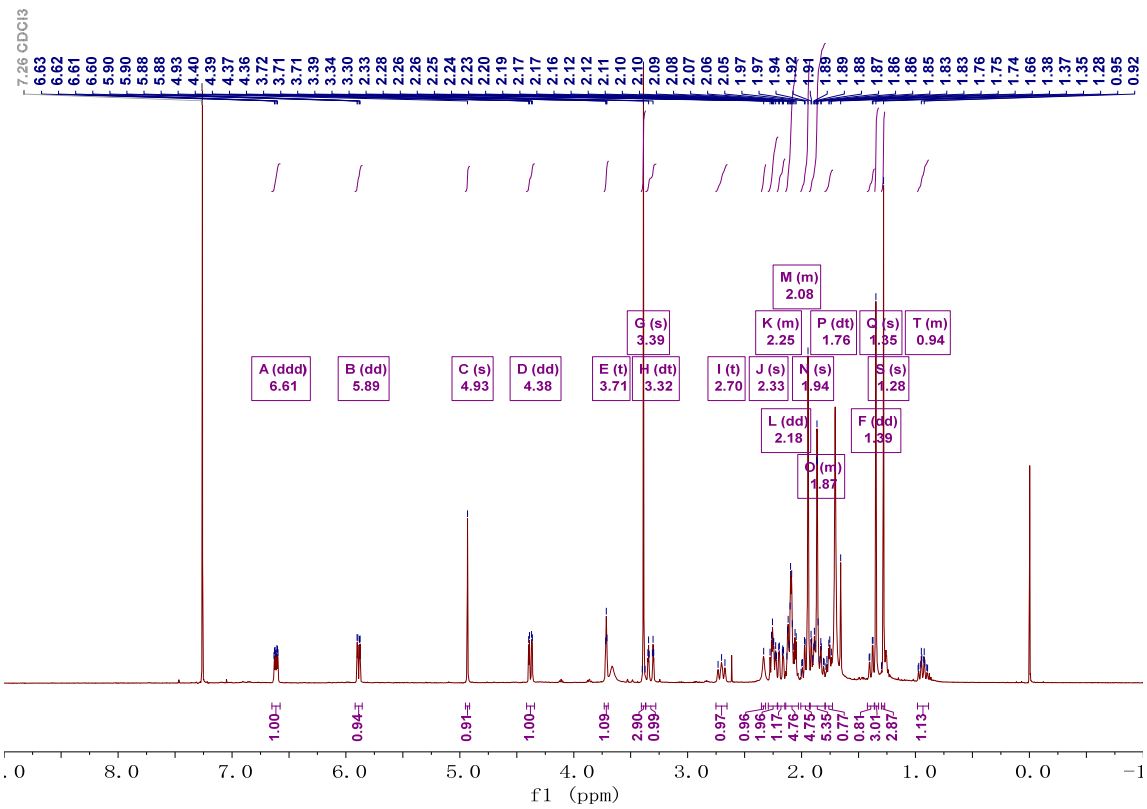


Figure S107. ^{1}H NMR Spectrum of Withaminilide L (**12**) in $CDCl_3$, 600 MHz

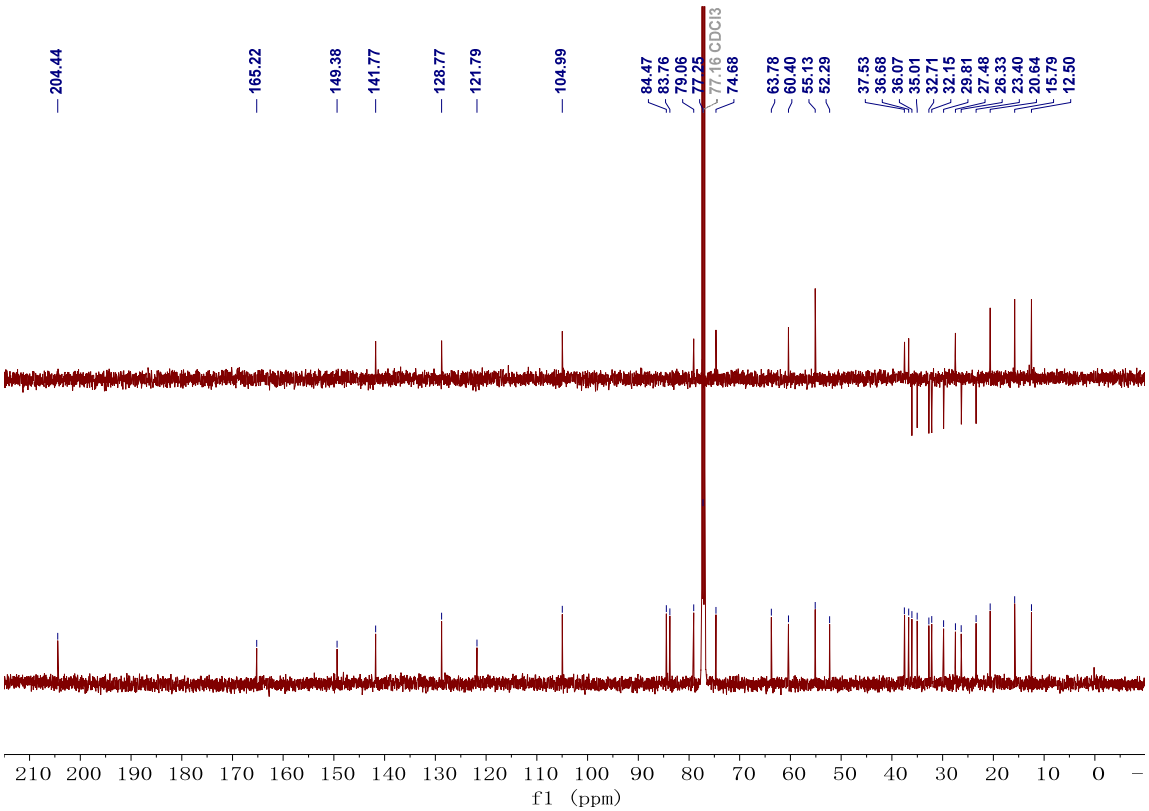


Figure S108. ^{13}C NMR Spectrum of Withaminilide L (**12**) in $CDCl_3$, 125 MHz

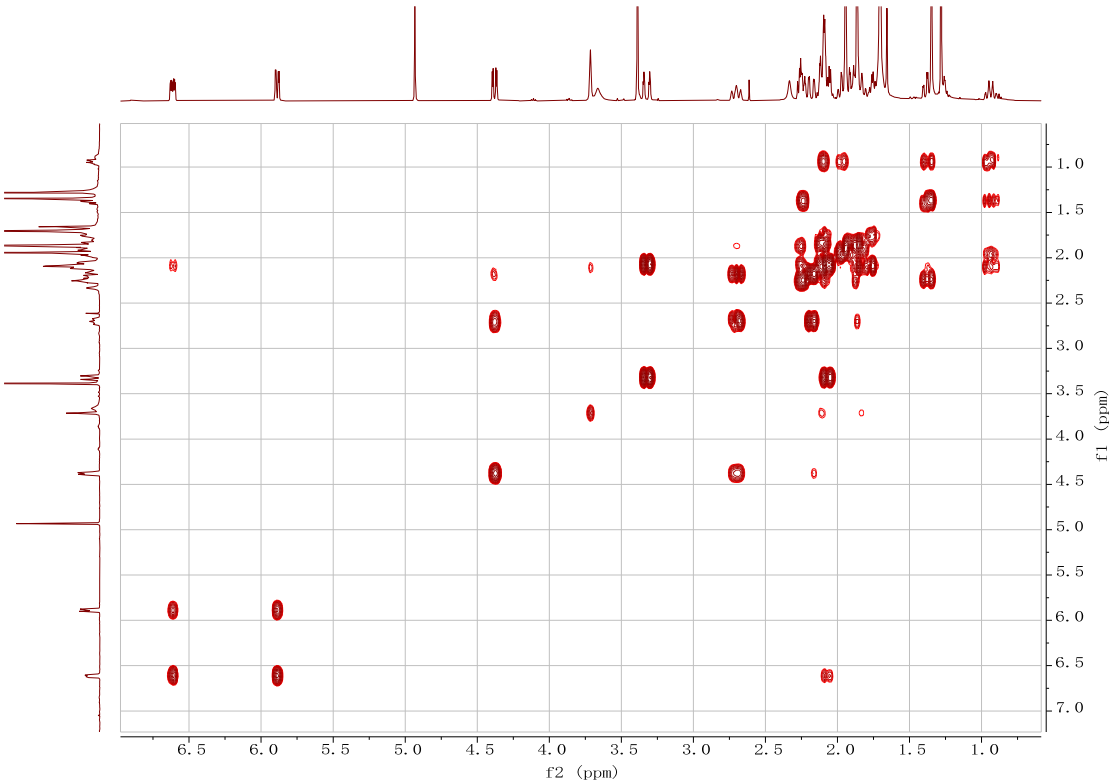


Figure S109. ^{1}H-^{1}H COSY Spectrum of Withaminilide L (**12**) in $CDCl_3$

Figure S110. HSQC Spectrum of Withaminilide L (**12**) in $CDCl_3$

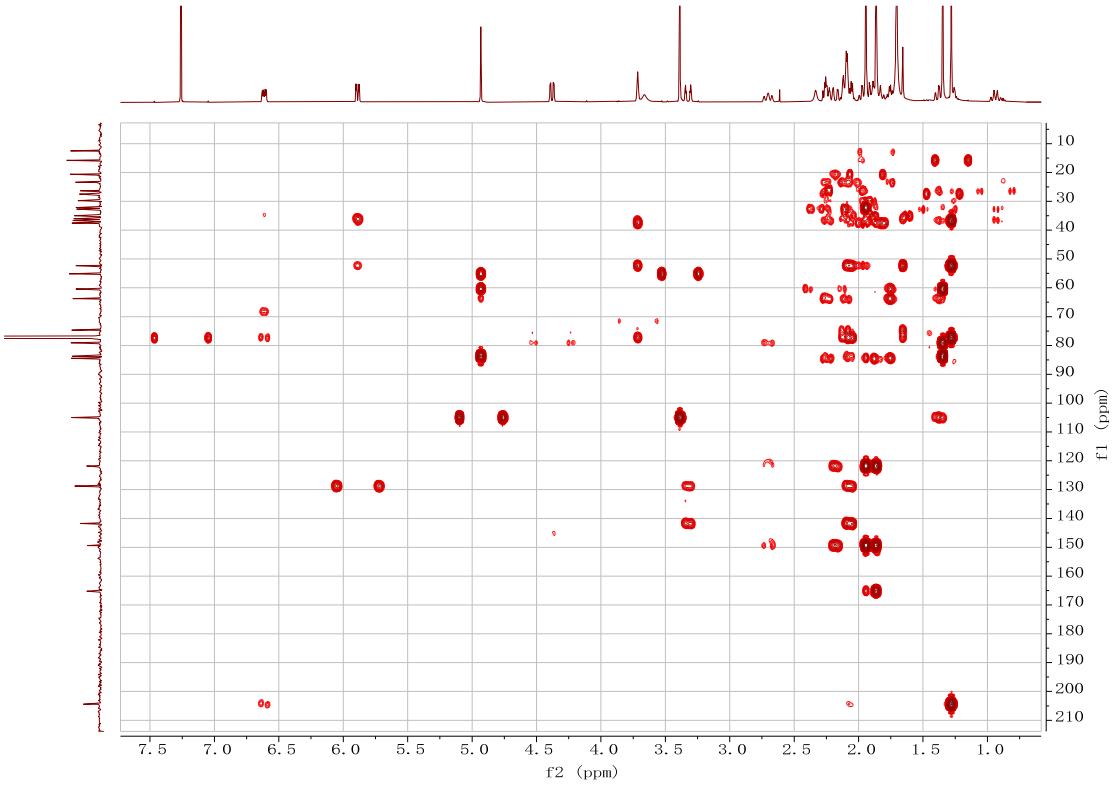


Figure S111. HMBC Spectrum of Withaminilide L (**12**) in $CDCl_3$

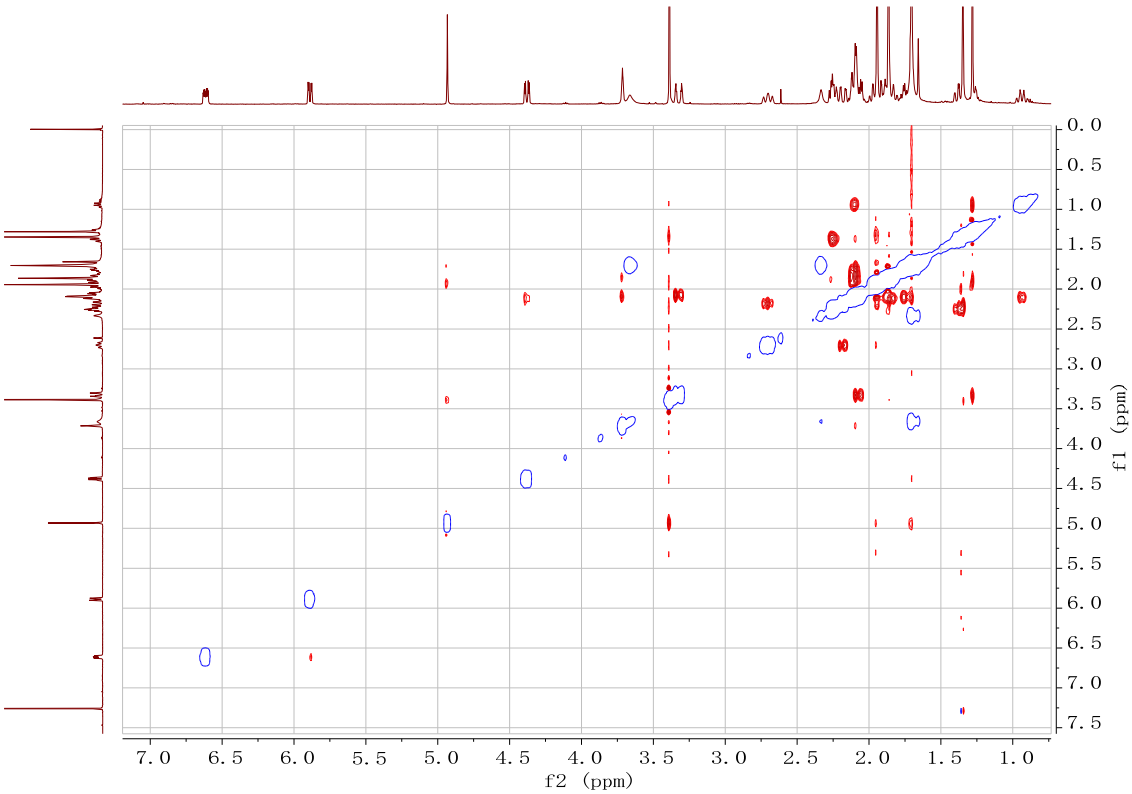


Figure S112. NOESY Spectrum of Withaminilide L (**12**) in $CDCl_3$

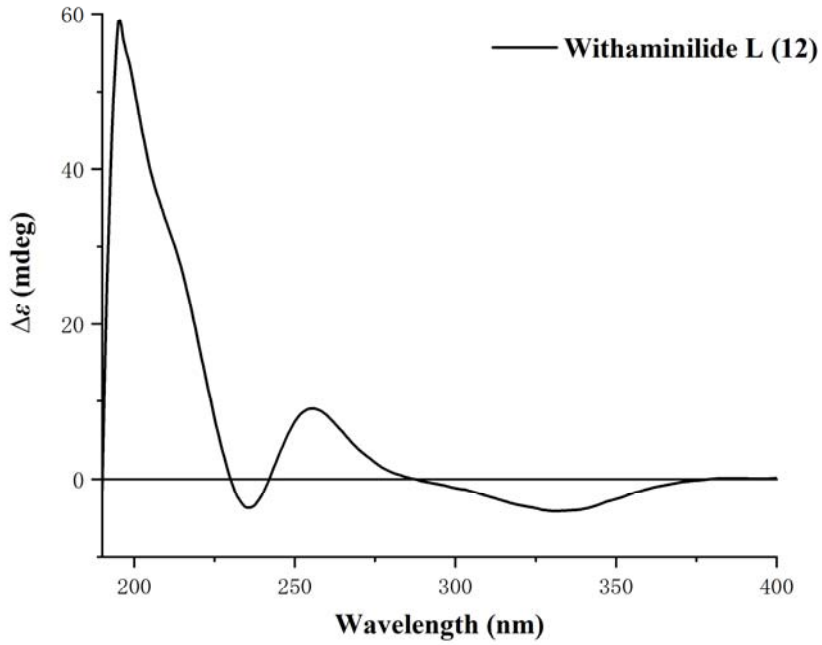


Figure S113. Experimental ECD Spectrum of Withaminilide L (**12**)

Elemental Composition Report

Tolerance = 3.0 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

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

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Minimum:	80.00					-1.5		
Maximum:	100.00			3.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
545.2412	545.2387	2.5	4.6	11.5	625.0	n/a	n/a	C29H37O10

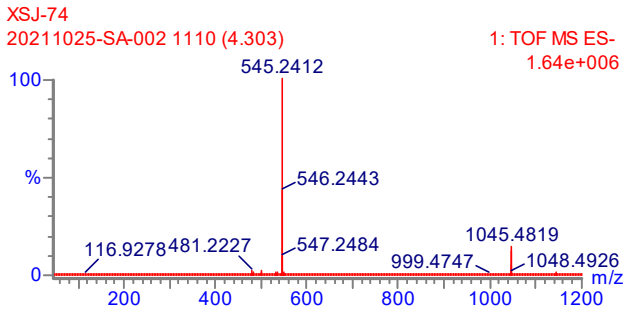


Figure S114. HRESIMS Spectrum of Withaminilide M (**13**)

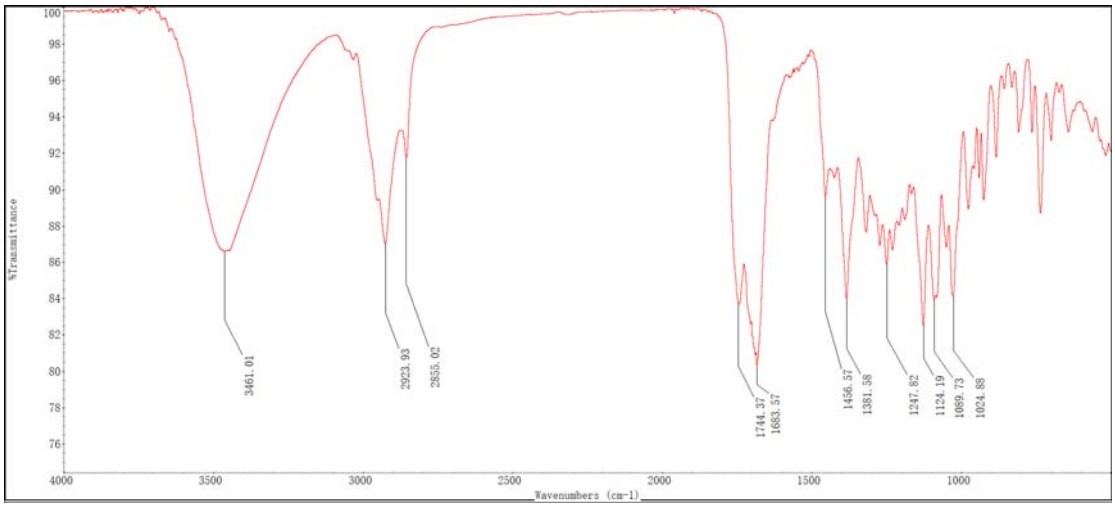


Figure S115. IR Spectrum of Withaminilide M (**13**)

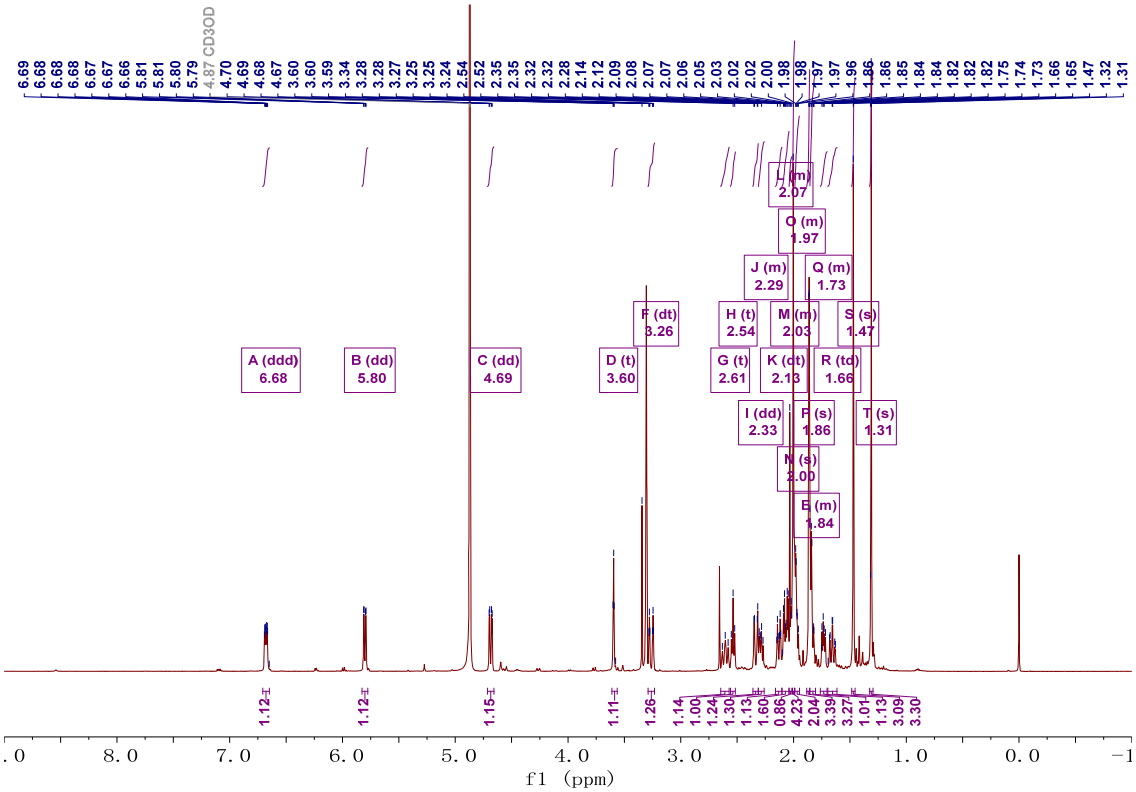


Figure S116. ^{1}H NMR Spectrum of Withaminilide M (**13**) in CD_3OD, 500 MHz

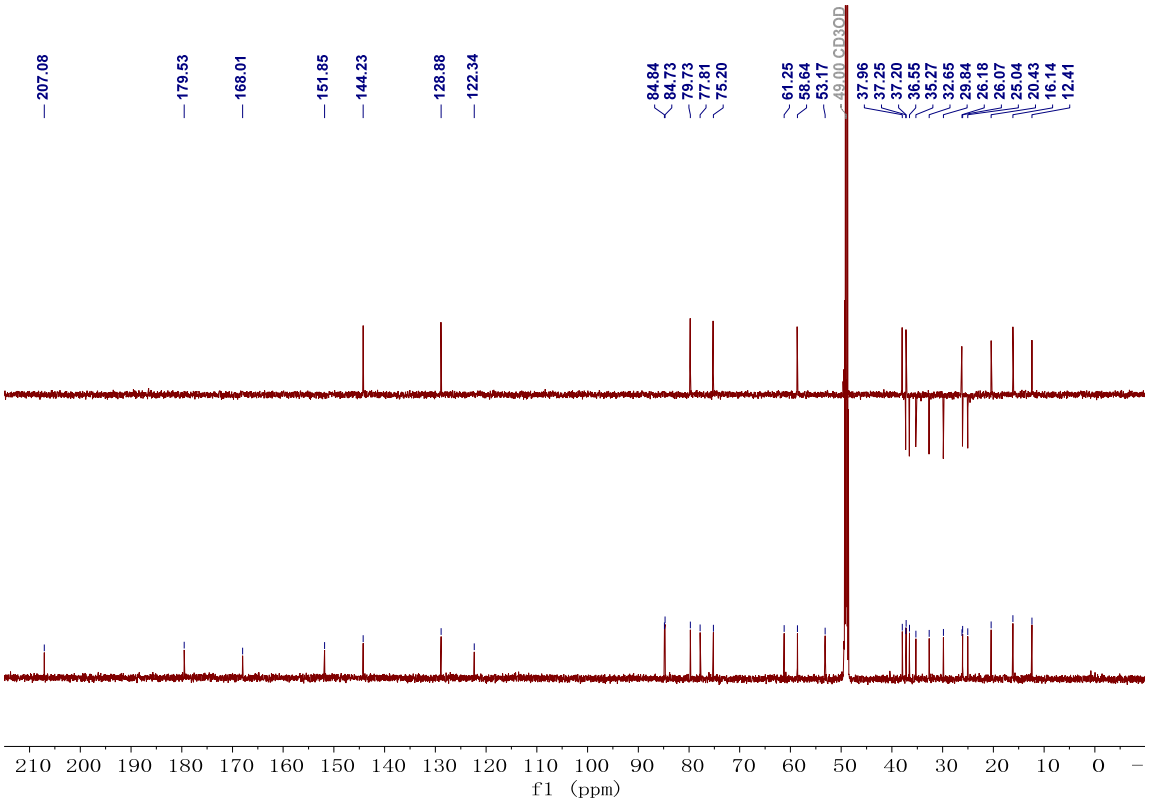


Figure S117. ^{13}C NMR Spectrum of Withaminilide M (**13**) in CD_3OD, 125 MHz

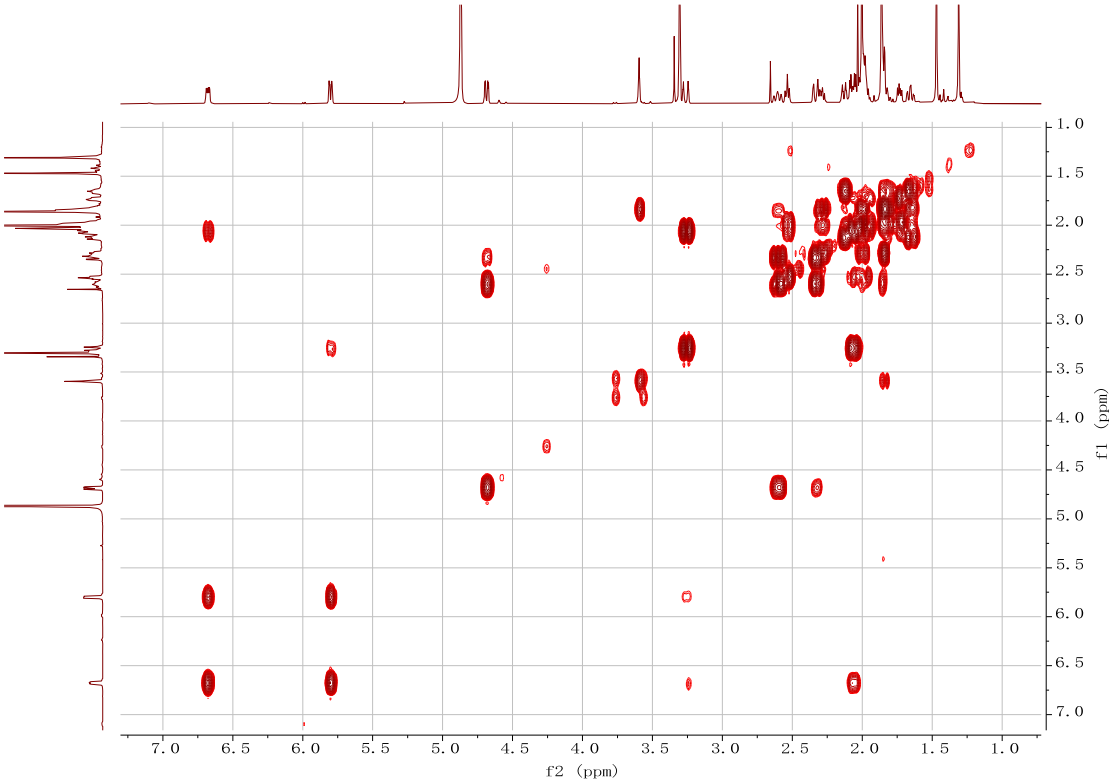


Figure S118. ^{1}H-^{1}H COSY Spectrum of Withaminilide M (**13**) in CD_3OD

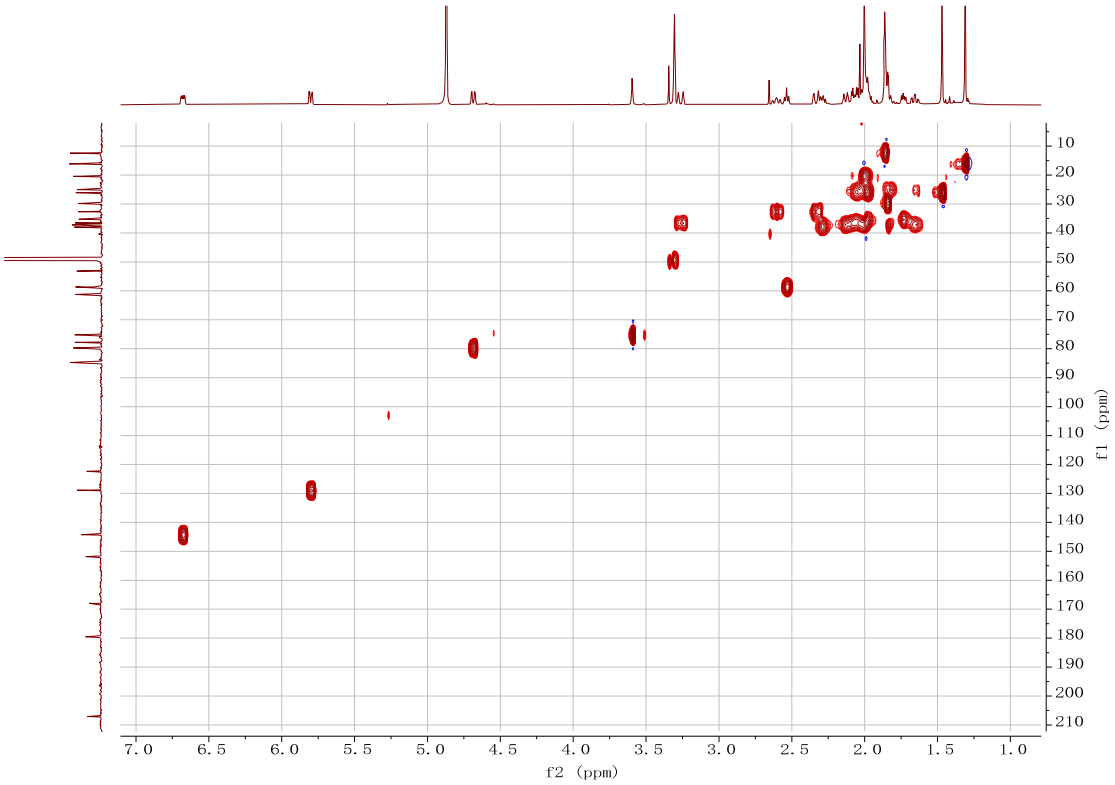


Figure S119. HSQC Spectrum of Withaminilide M (**13**) in CD_3OD

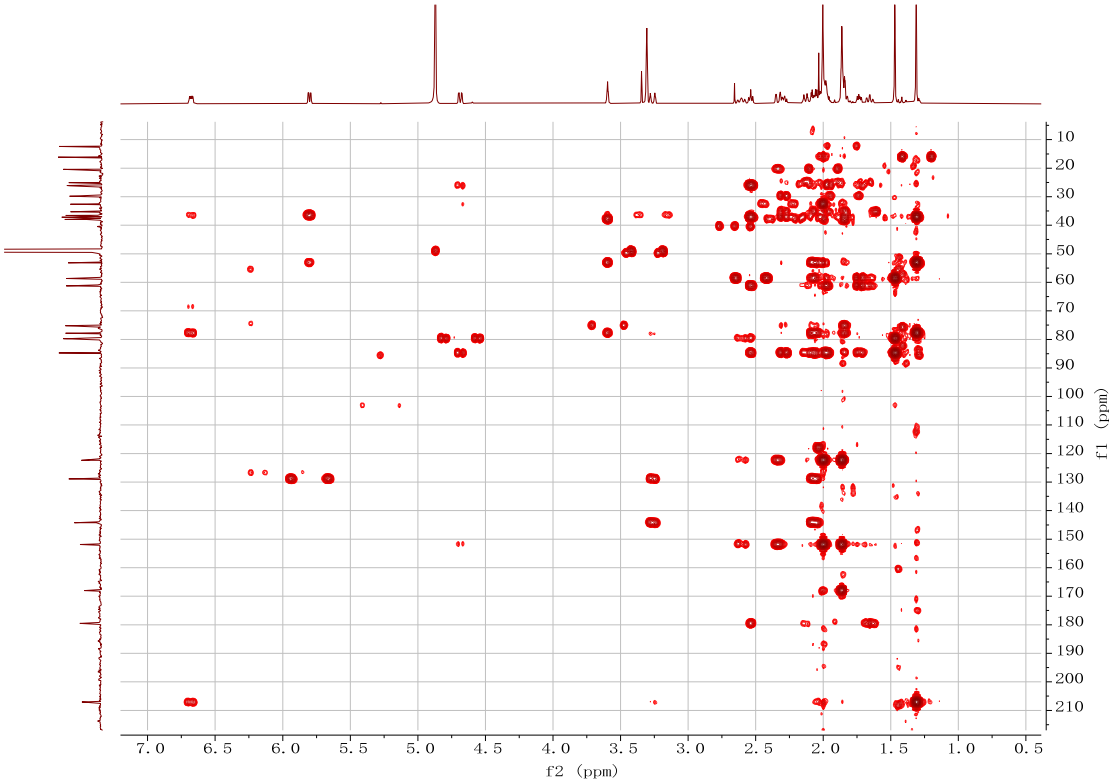


Figure S120. HMBC Spectrum of Withaminilide M (**13**) in CD_3OD

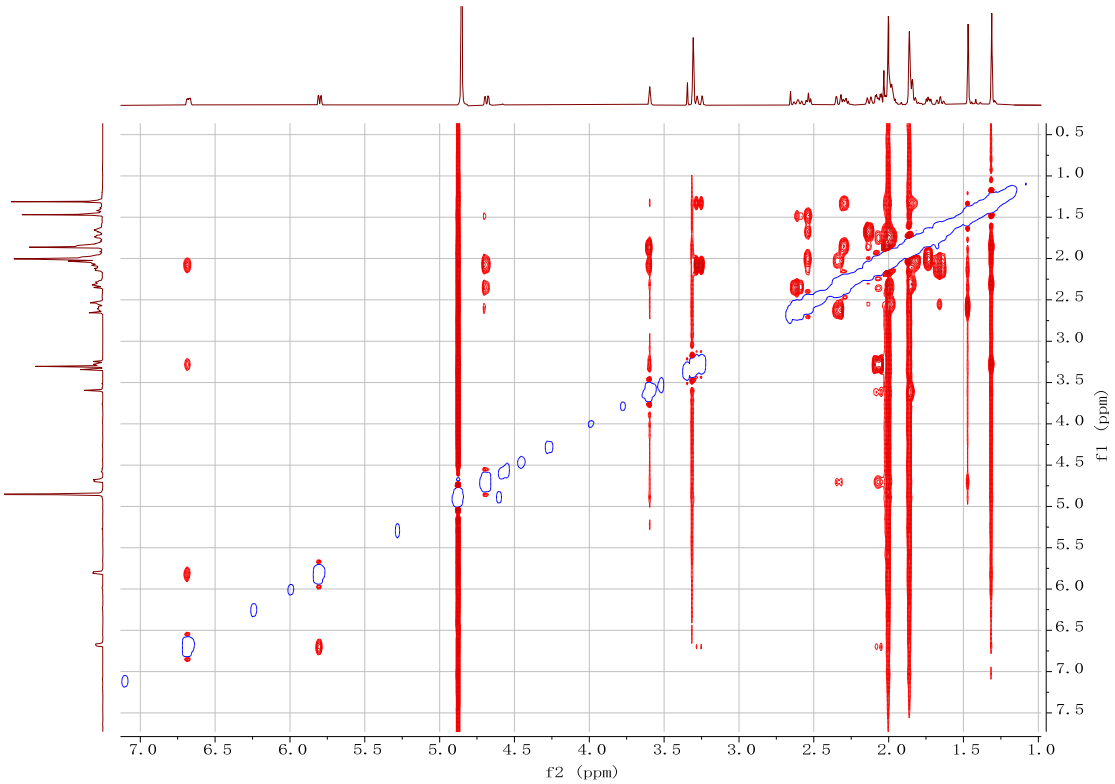


Figure S121. NOESY Spectrum of Withaminilide M (**13**) in CD_3OD

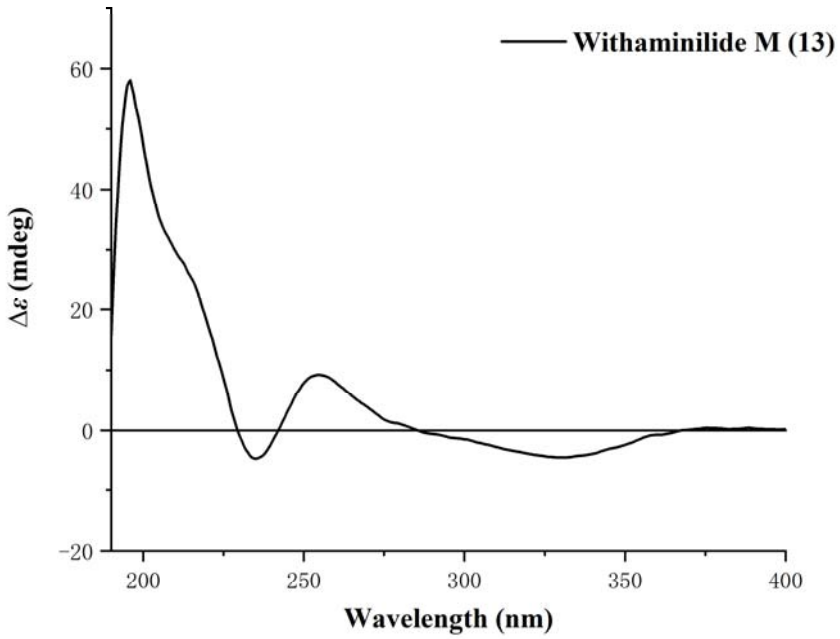


Figure S122. Experimental ECD Spectrum of Withaminilide M (**13**)

Elemental Composition Report
Single Mass Analysis
Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
114 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-500 H: 0-1000 O: 0-200 Cl: 1-1

Minimum:				-1.5	
Maximum:		3.0	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
517.1972	517.1993	-2.1	-4.1	11.5	C28H34O7Cl

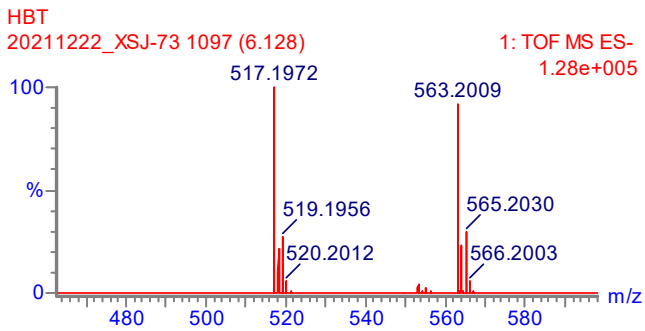


Figure S123. HRESIMS Spectrum of Withaminilide N (**14**)

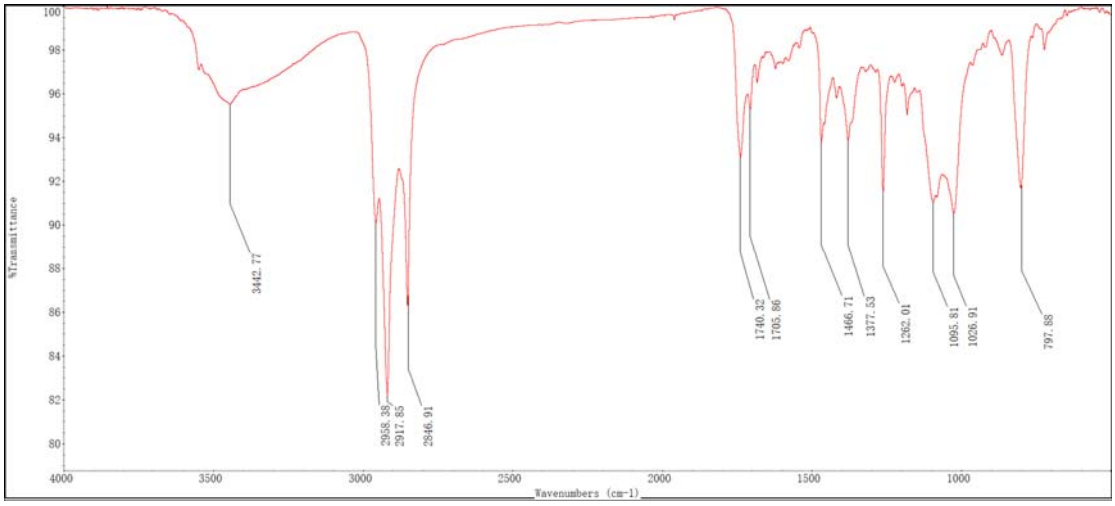


Figure S124. IR Spectrum of Withaminilide N (**14**)

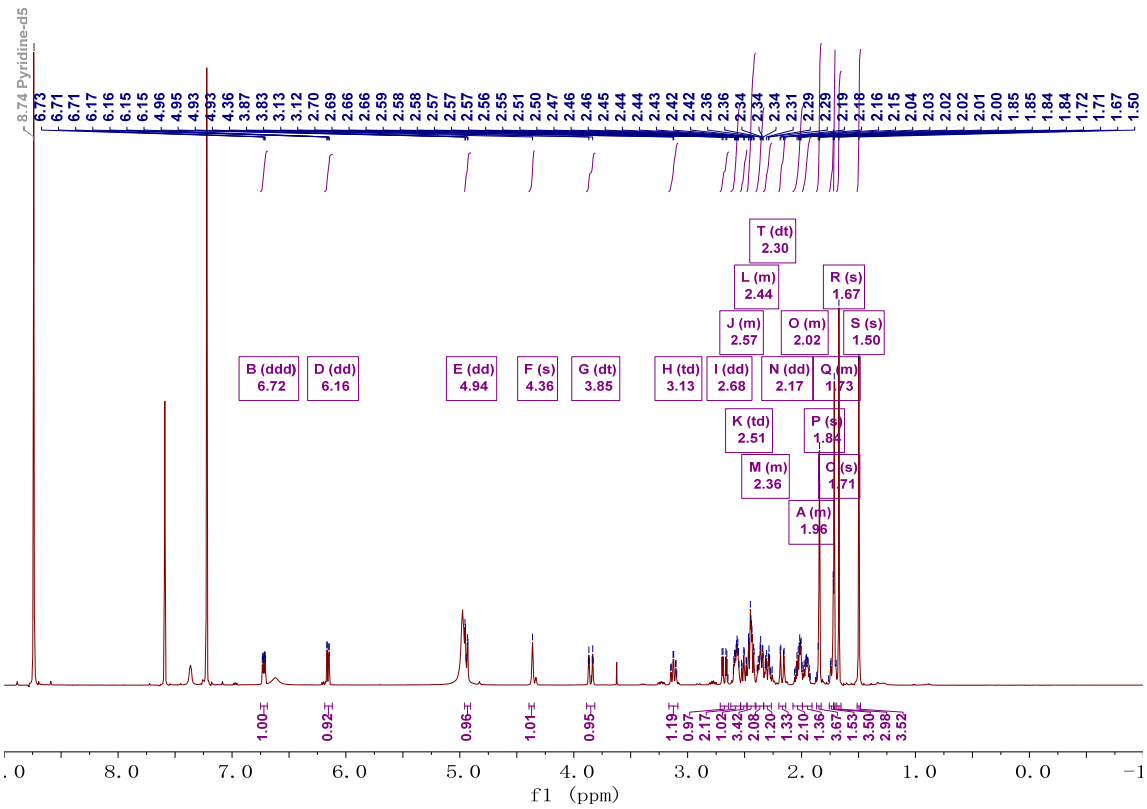


Figure S125. ^{1}H NMR Spectrum of Withaminilide N (**14**) in C_5D_5N, 600 MHz

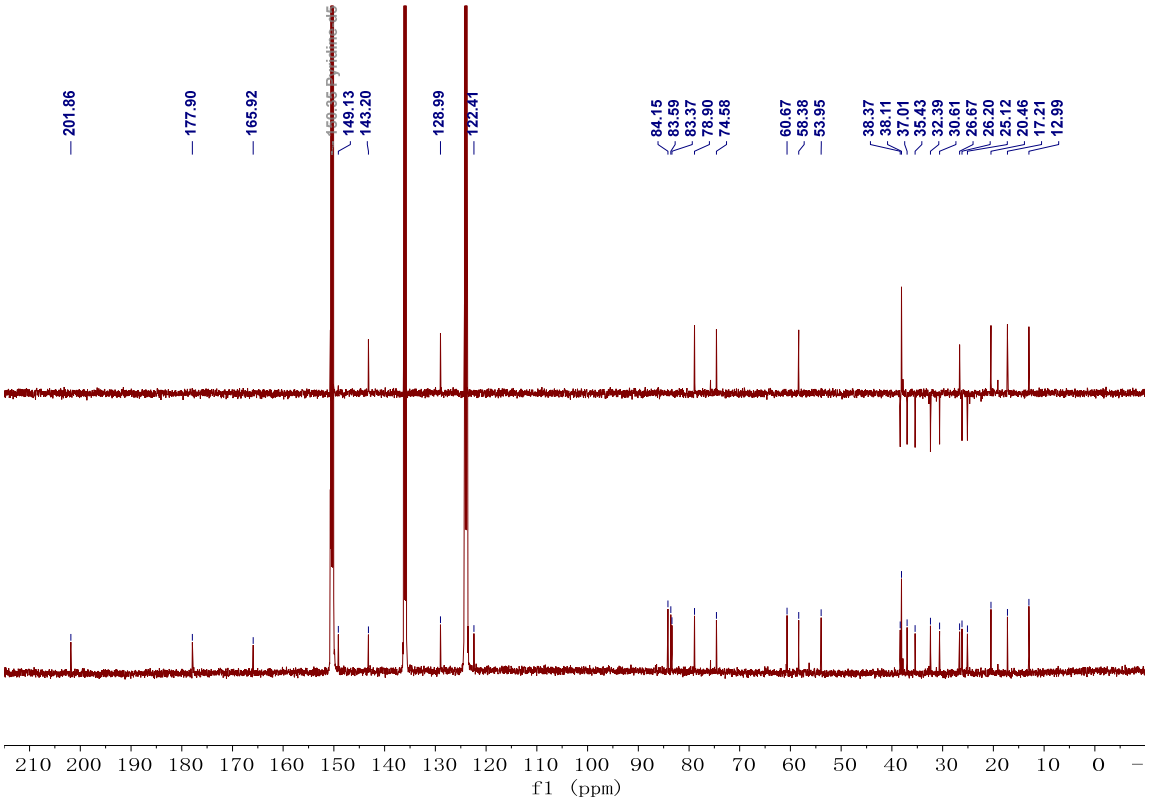


Figure S126. ^{13}C NMR Spectrum of Withaminilide N (**14**) in C_5D_5N, 125 MHz

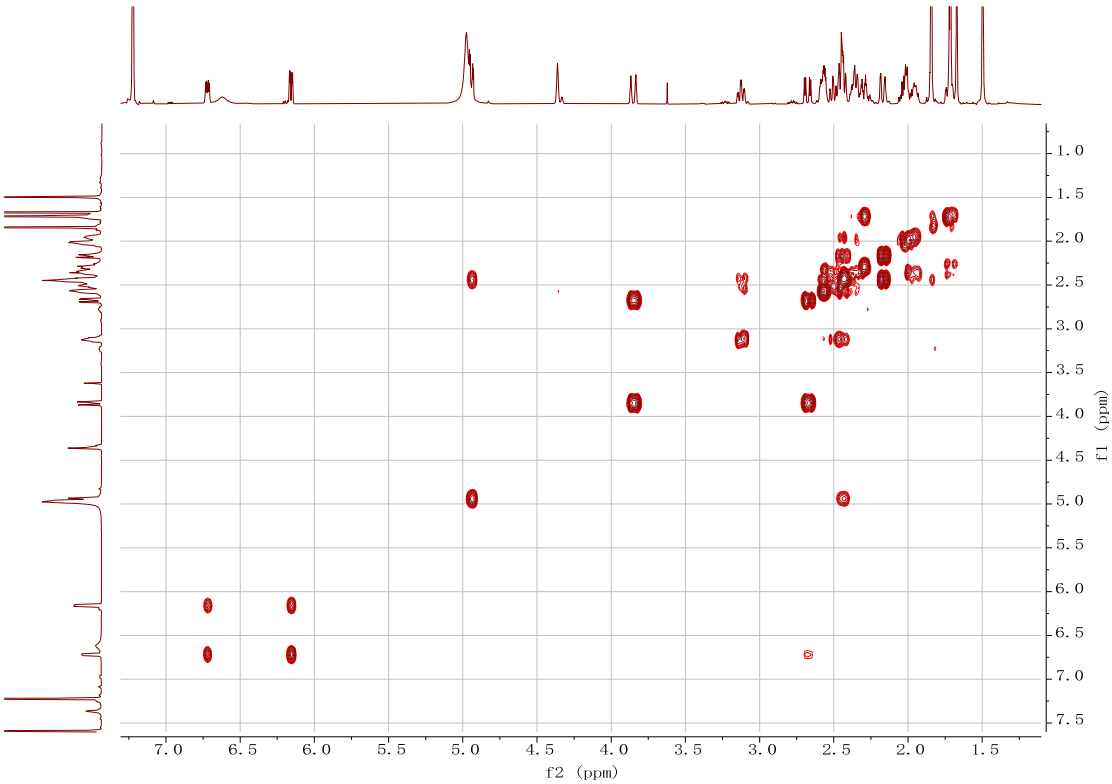


Figure S127. ^{1}H-^{1}H COSY Spectrum of Withaminilide N (**14**) in C_5D_5N

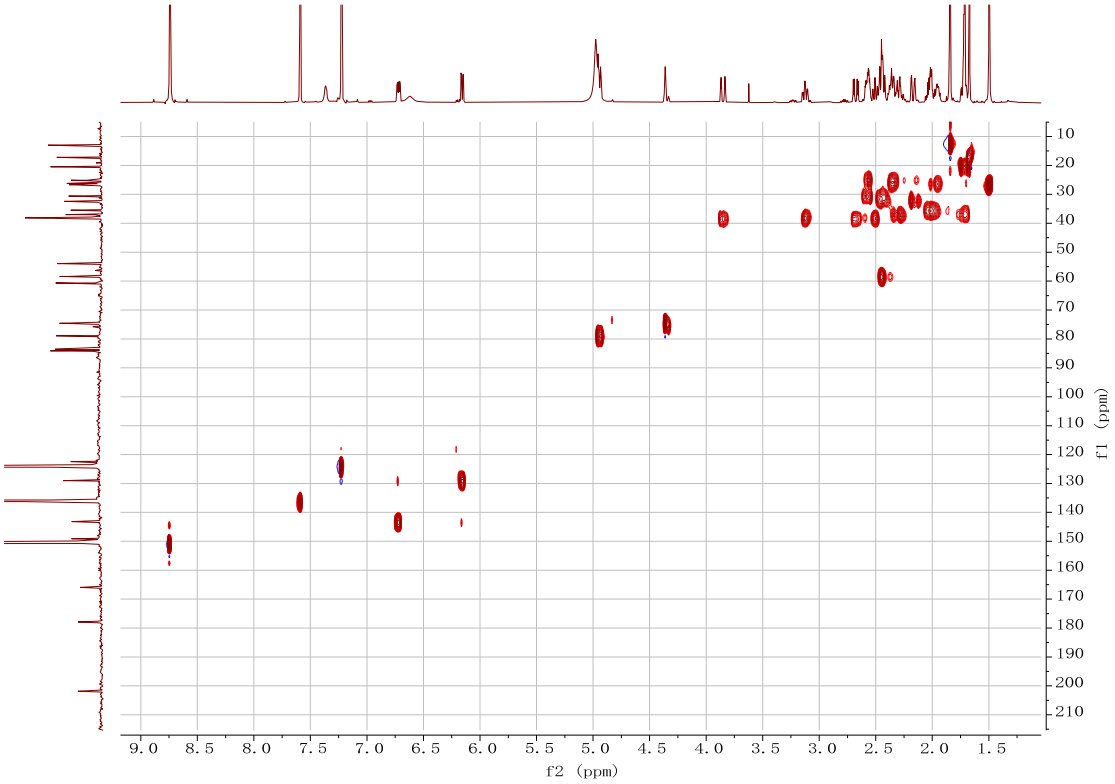


Figure S128. HSQC Spectrum of Withaminilide N (**14**) in C_5D_5N

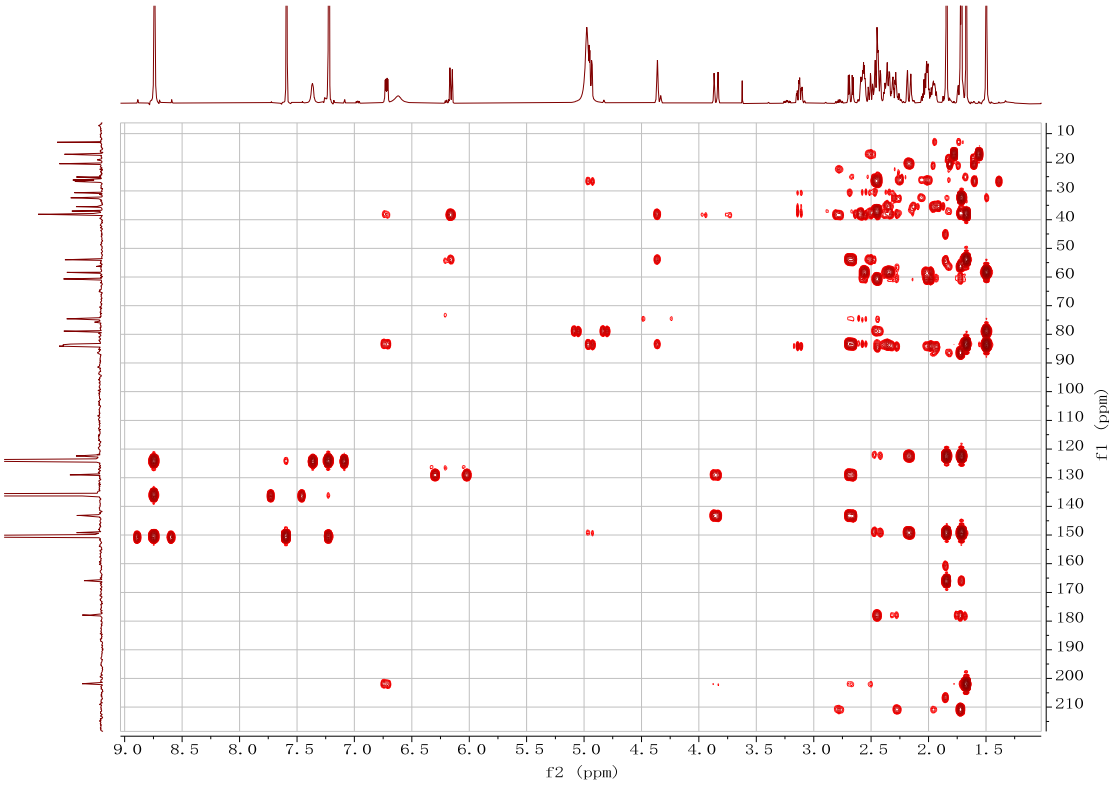


Figure S129. HMBC Spectrum of Withaminilide N (**14**) in C_5D_5N

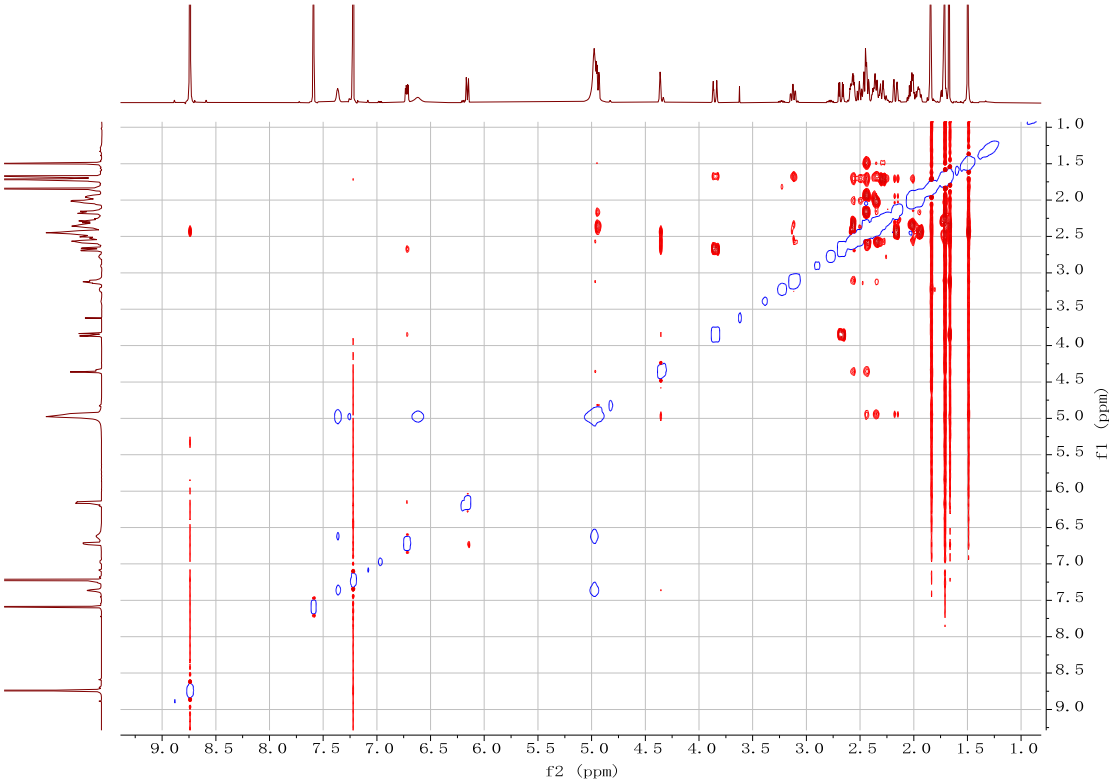


Figure S130. NOESY Spectrum of Withaminilide N (**14**) in C_5D_5N

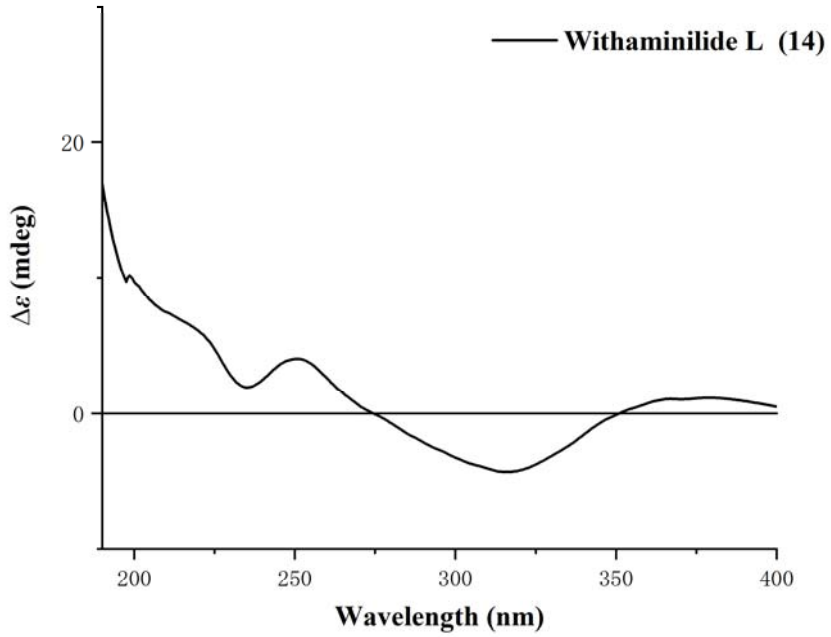


Figure S131. Experimental ECD Spectrum of Withaminilide N (**14**)

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

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

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Minimum:	80.00					-1.5		
Maximum:	100.00			3.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
511.2350	511.2332	1.8	3.5	12.5	531.0	n/a	n/a	C29H35O8

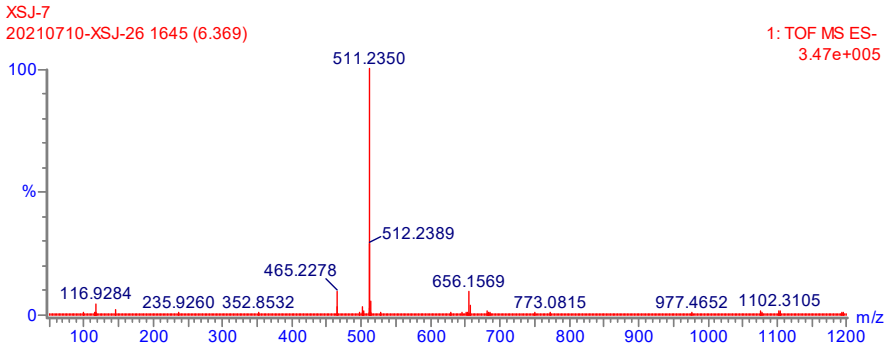


Figure S132. HRESIMS Spectrum of Withaminilide O (**15**)

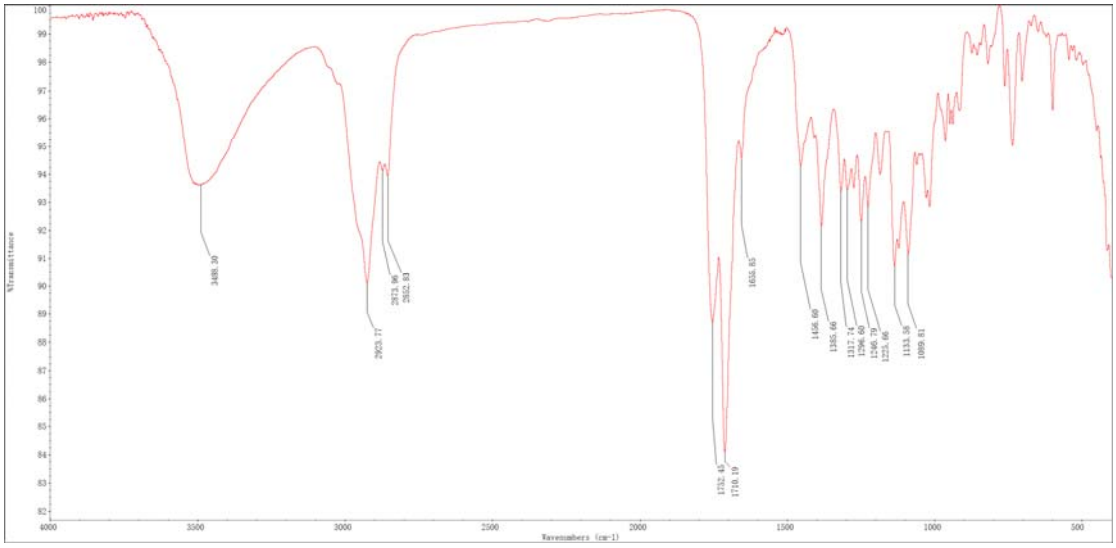


Figure S133. IR Spectrum of Withaminilide O (**15**)

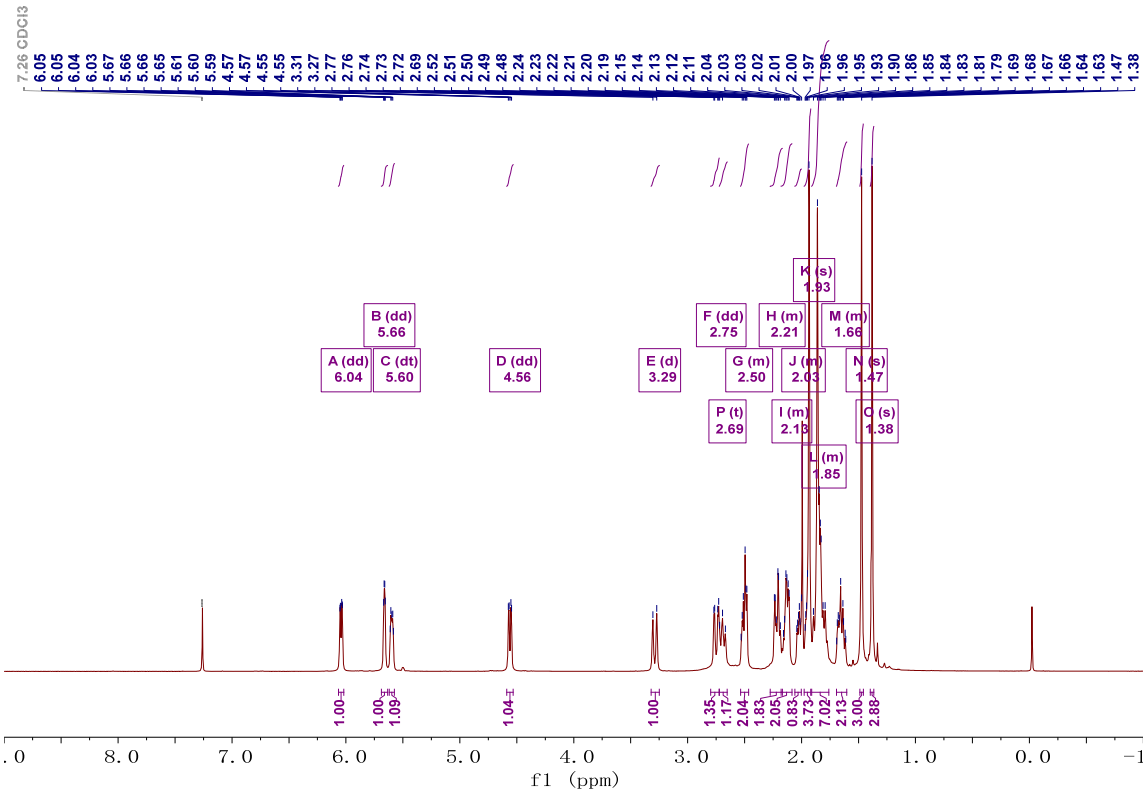


Figure S134. ^{1}H NMR Spectrum of Withaminilide O (**15**) in $CDCl_3$, 600 MHz

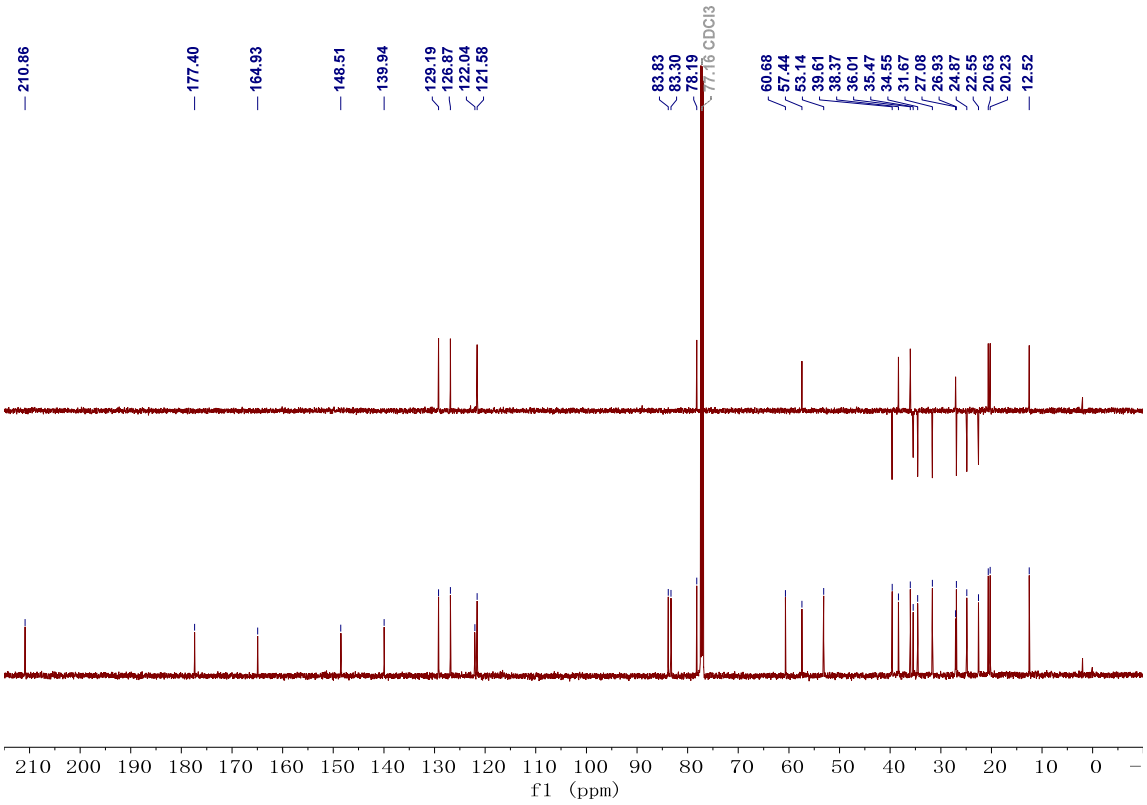


Figure S135. ^{13}C NMR Spectrum of Withaminilide O (**15**) in $CDCl_3$, 150 MHz

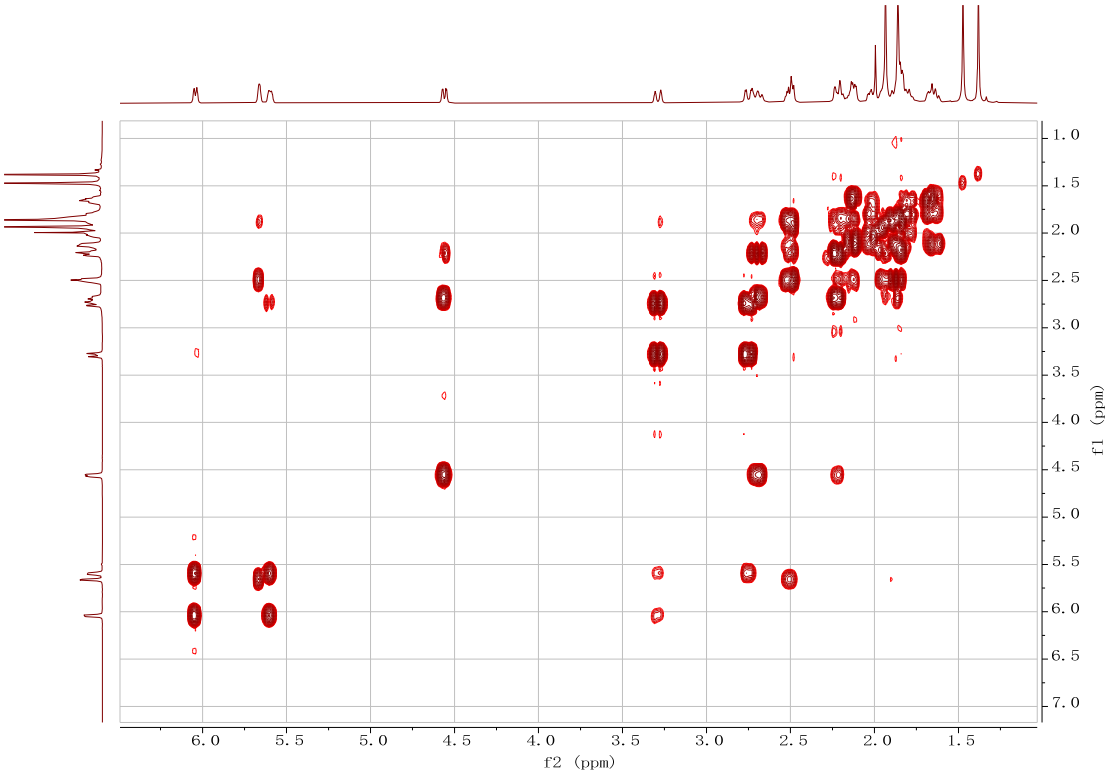


Figure S136. ^{1}H-^{1}H COSY Spectrum of Withaminilide O (**15**) in $CDCl_3$

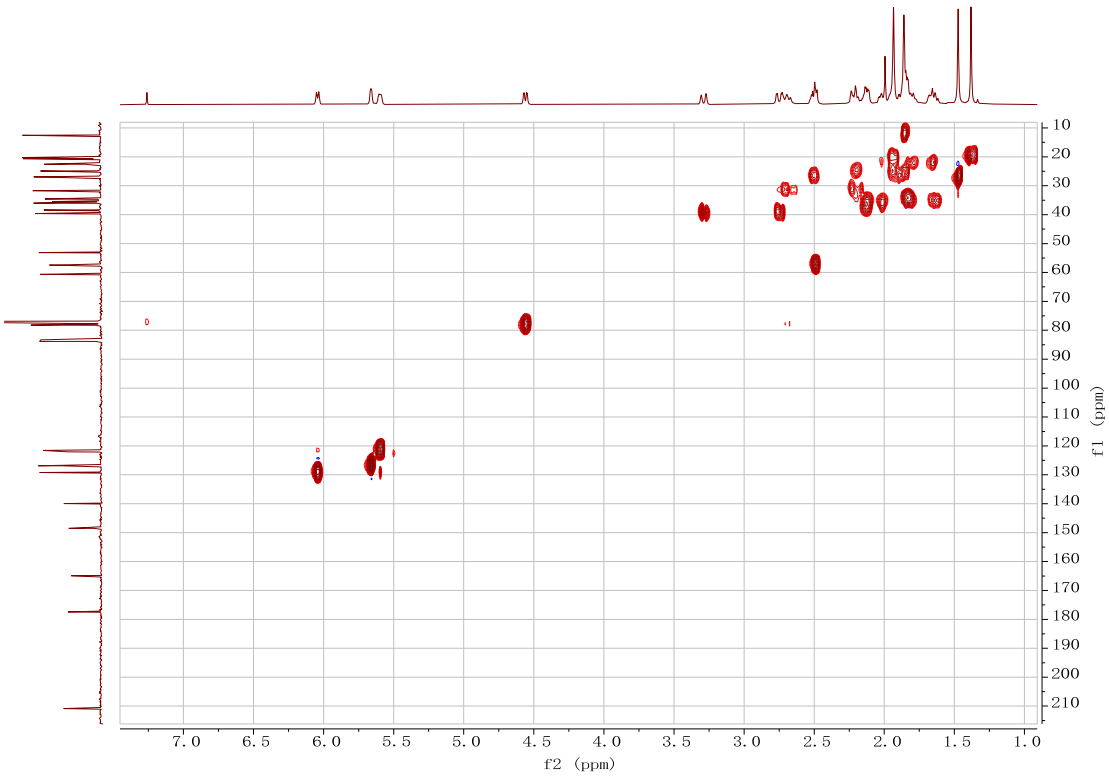


Figure S137. HSQC Spectrum of Withaminilide O (**15**) in $CDCl_3$

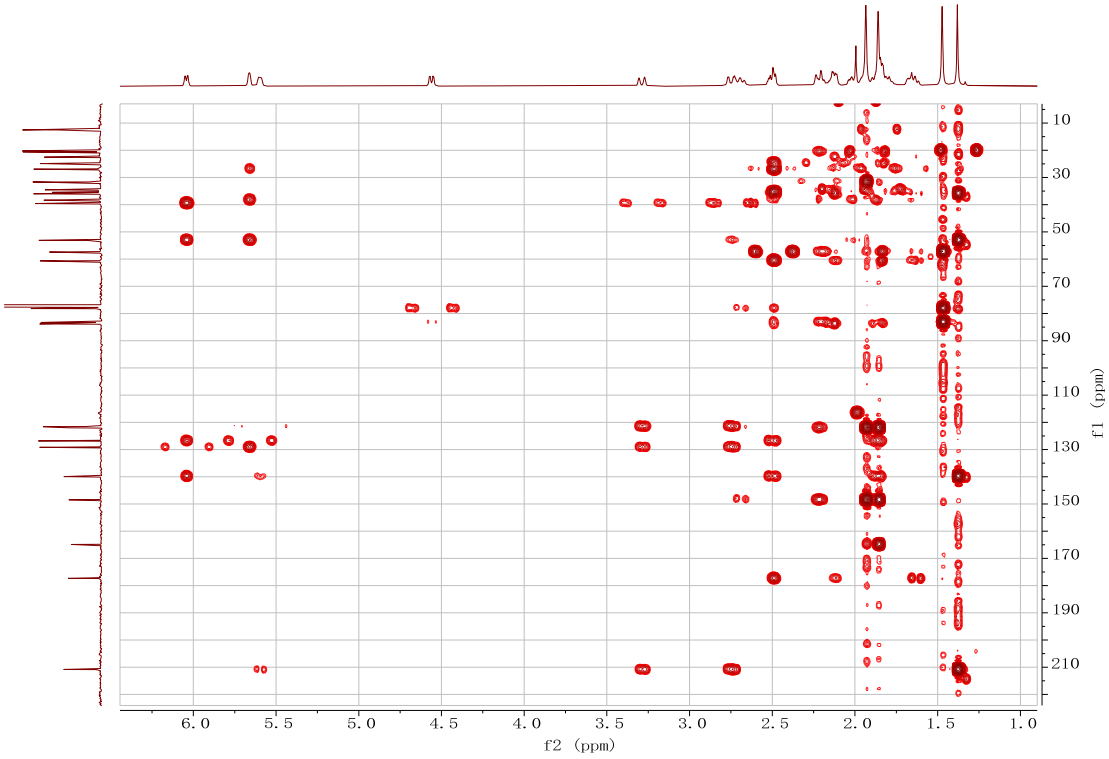


Figure S138. HMBC Spectrum of Withaminilide O (**15**) in $CDCl_3$

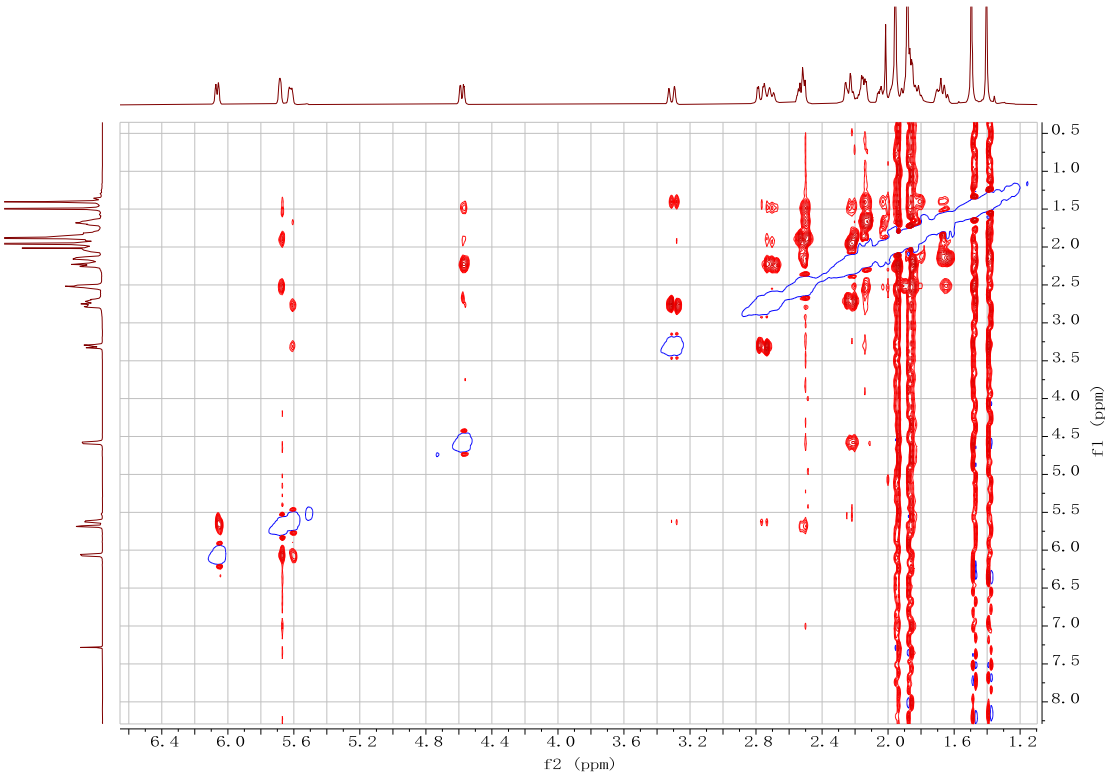


Figure S139. NOESY Spectrum of Withaminilide O (**15**) in $CDCl_3$

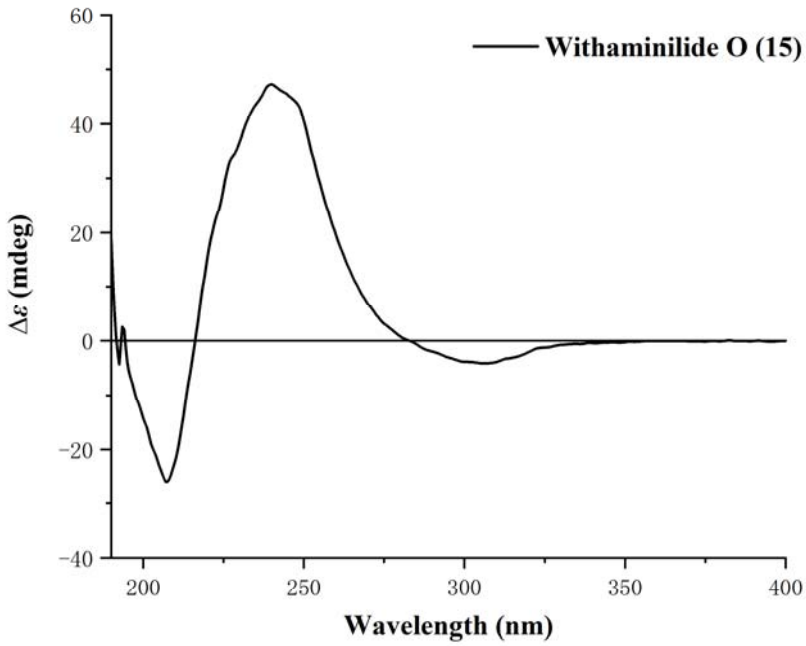


Figure S140. Experimental ECD Spectrum of Withaminilide O (**15**)

Elemental Composition Report

Single Mass Analysis

Tolerance = 3.0 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

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

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Minimum:					-1.5			
Maximum:			3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
481.2209	481.2226	-1.7	-3.5	12.5	436.4	n/a	n/a	C28H33O7

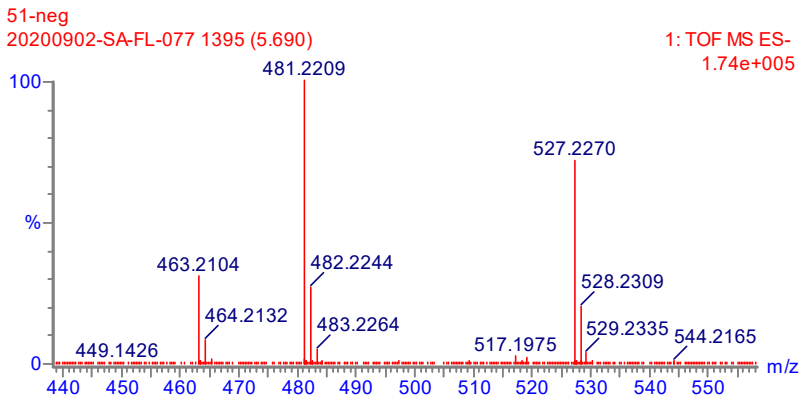


Figure S141. HRESIMS Spectrum of Withaminilide P (**16**)

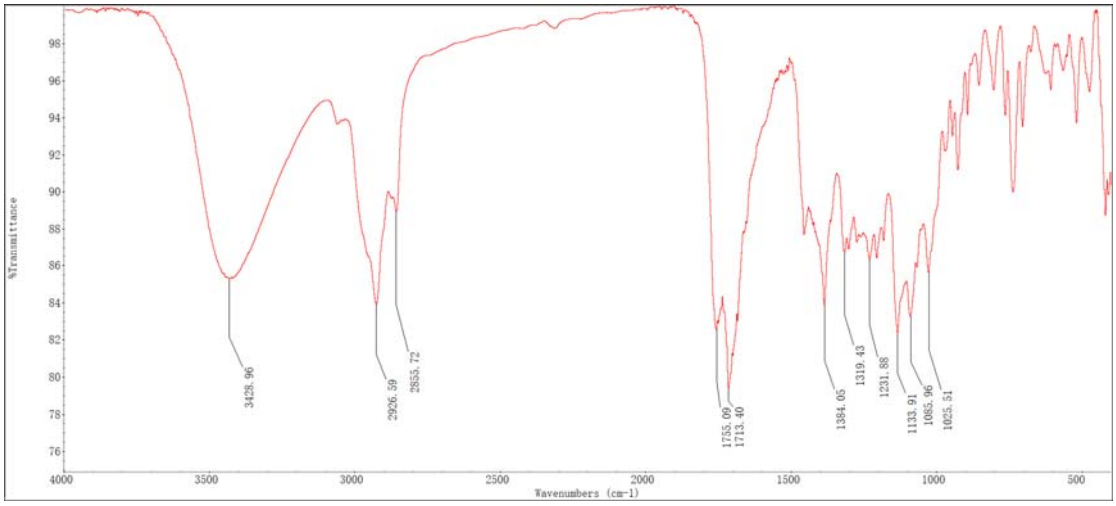


Figure S142. IR Spectrum of Withaminilide P (**16**)

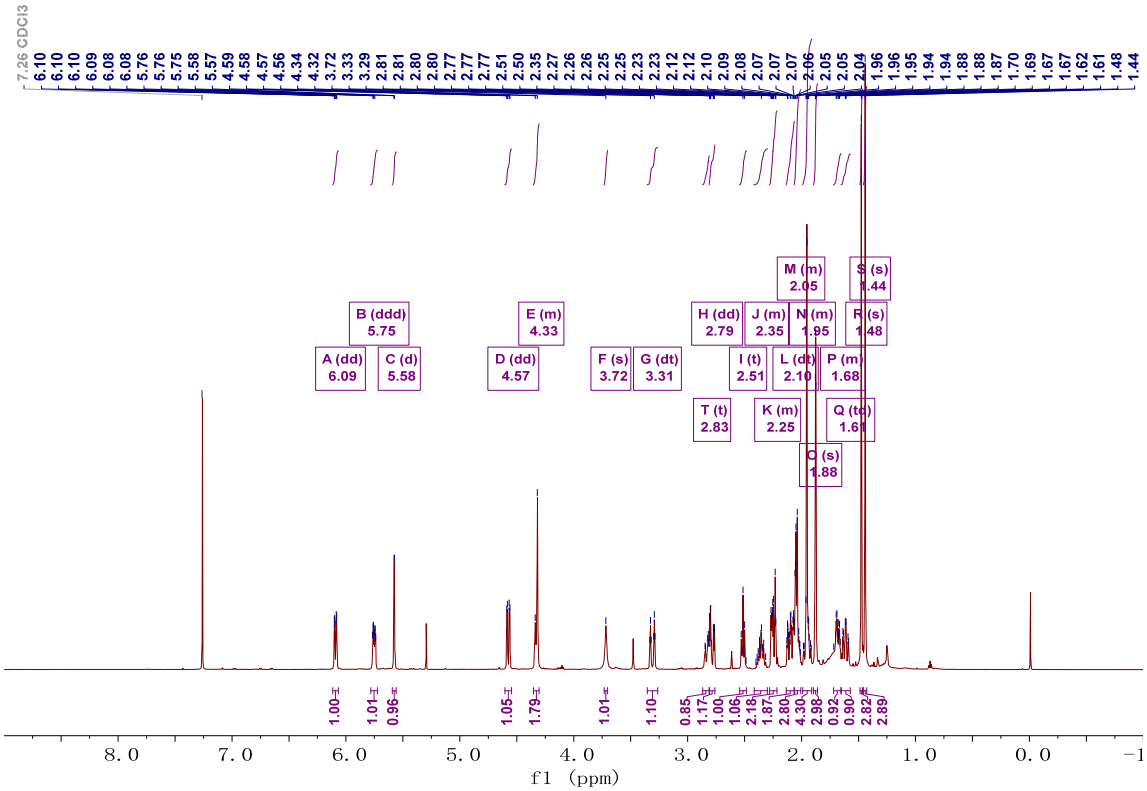


Figure S143. ^{1}H NMR Spectrum of Withaminilide P (**16**) in $CDCl_3$, 600 MHz

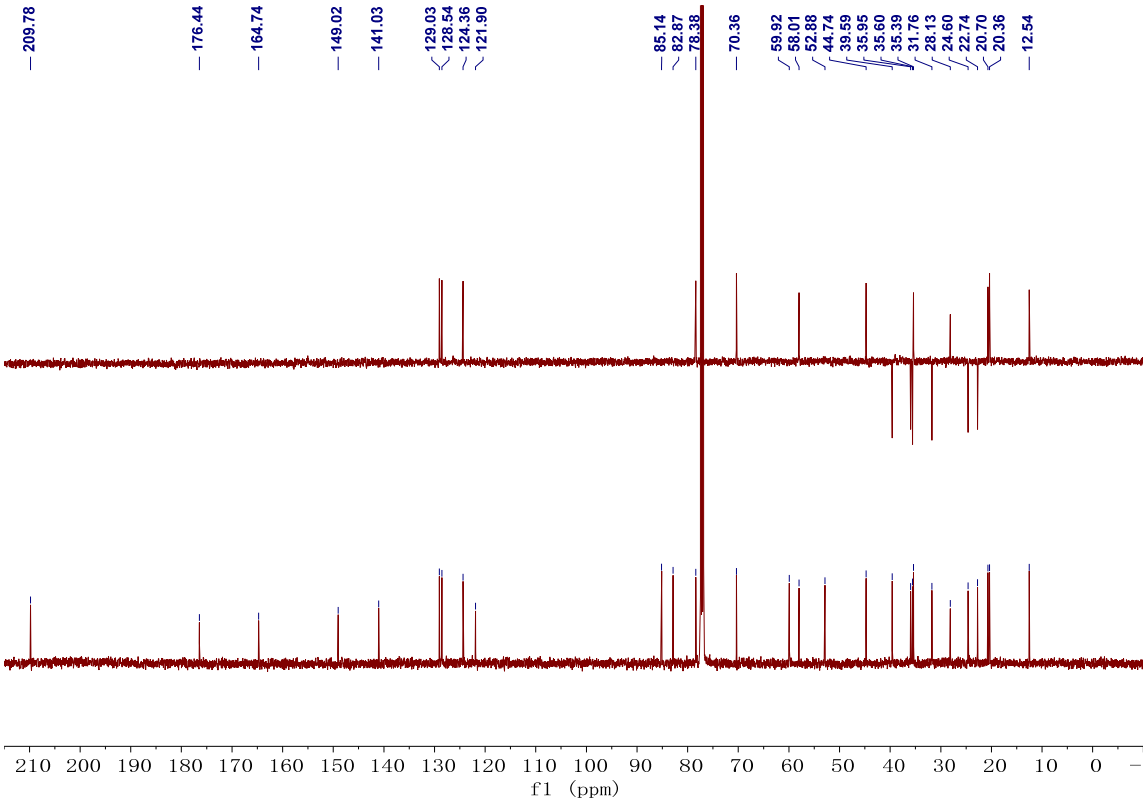


Figure S144. ^{13}C NMR Spectrum of Withaminilide P (**16**) in $CDCl_3$, 125 MHz

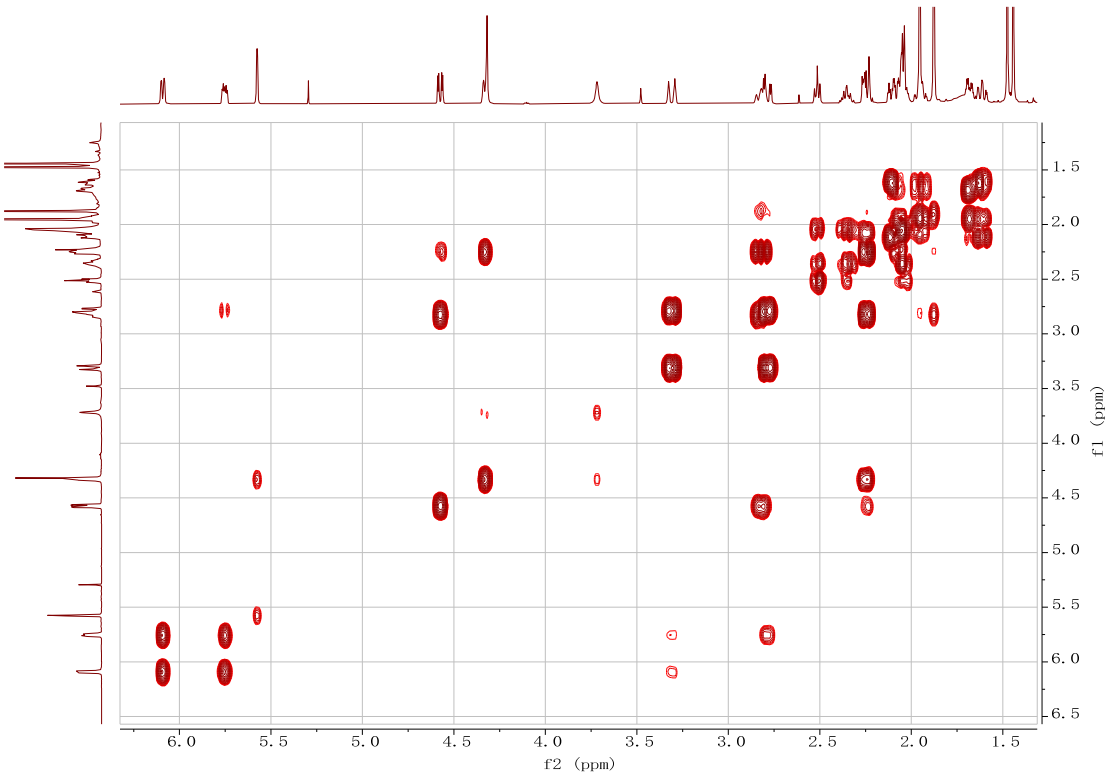


Figure S145. ^{1}H-^{1}H COSY Spectrum of Withaminilide P (**16**) in $CDCl_3$

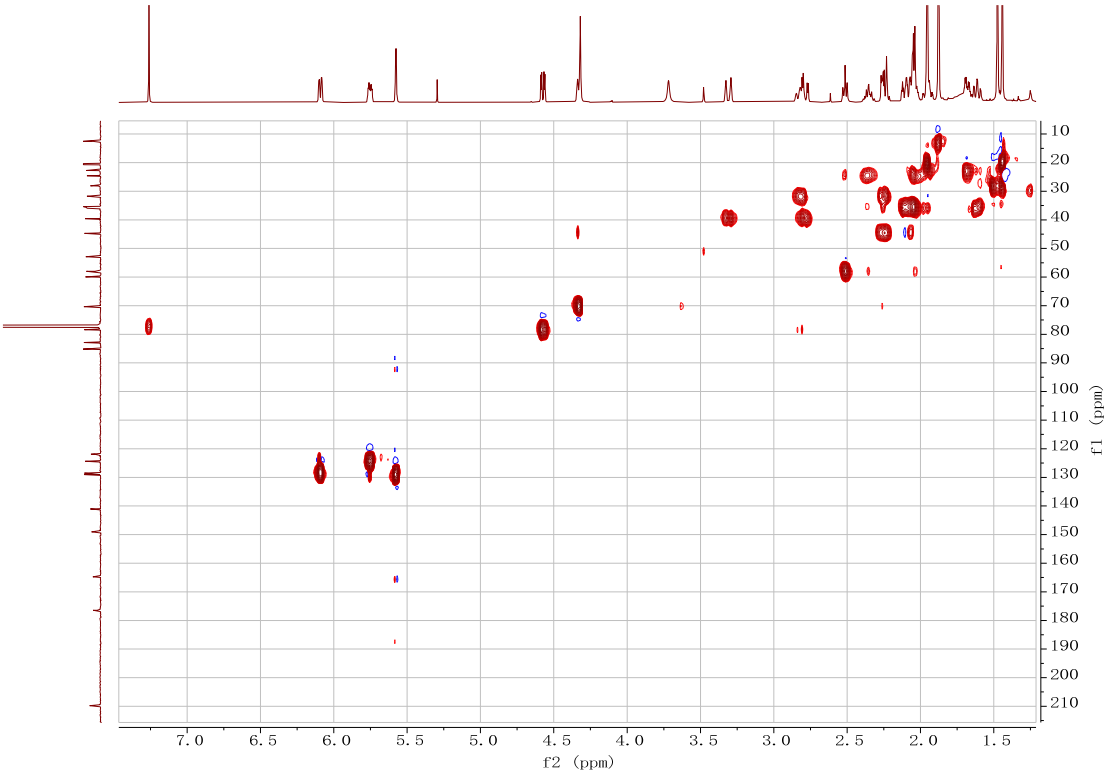


Figure S146. HSQC Spectrum of Withaminilide P (**16**) in $CDCl_3$

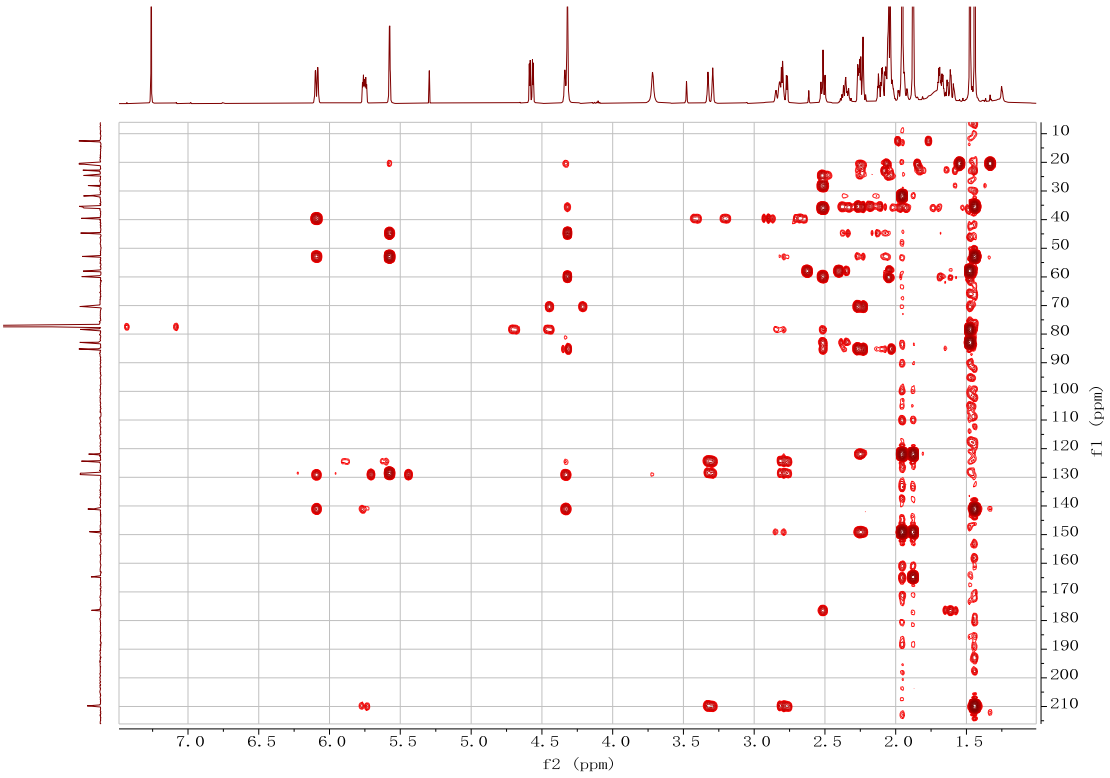


Figure S147. HMBC Spectrum of Withaminilide P (**16**) in $CDCl_3$

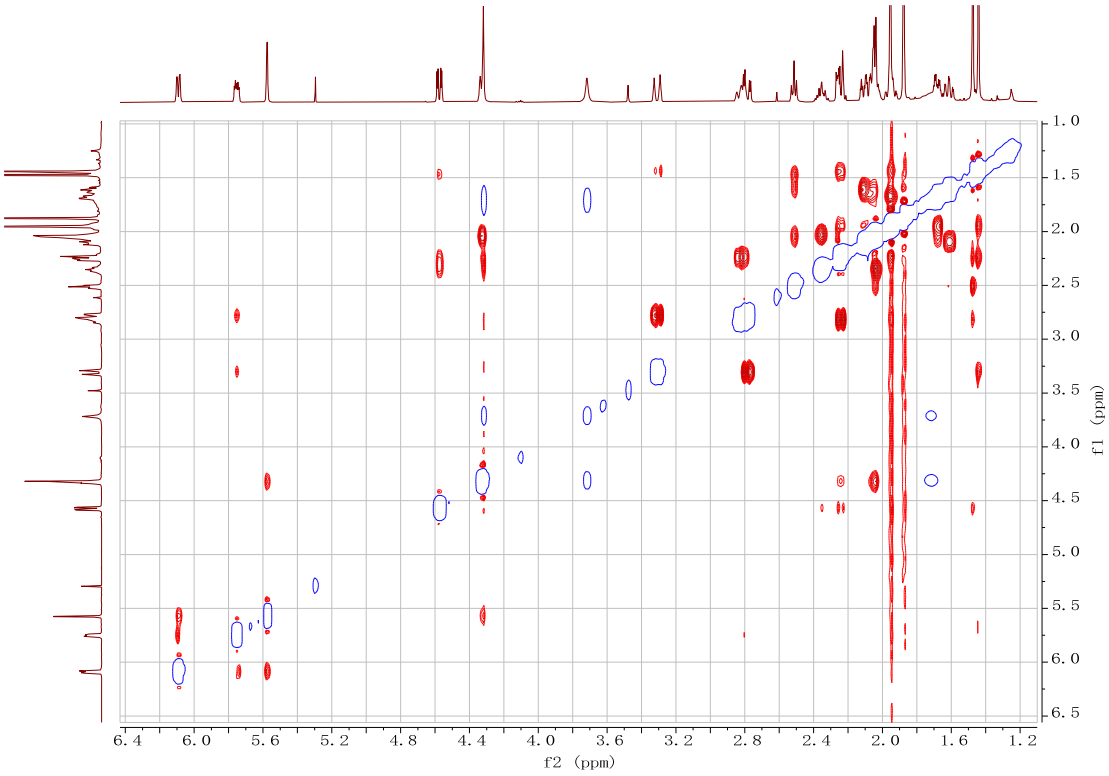


Figure S148. NOESY Spectrum of Withaminilide P (**16**) in $CDCl_3$

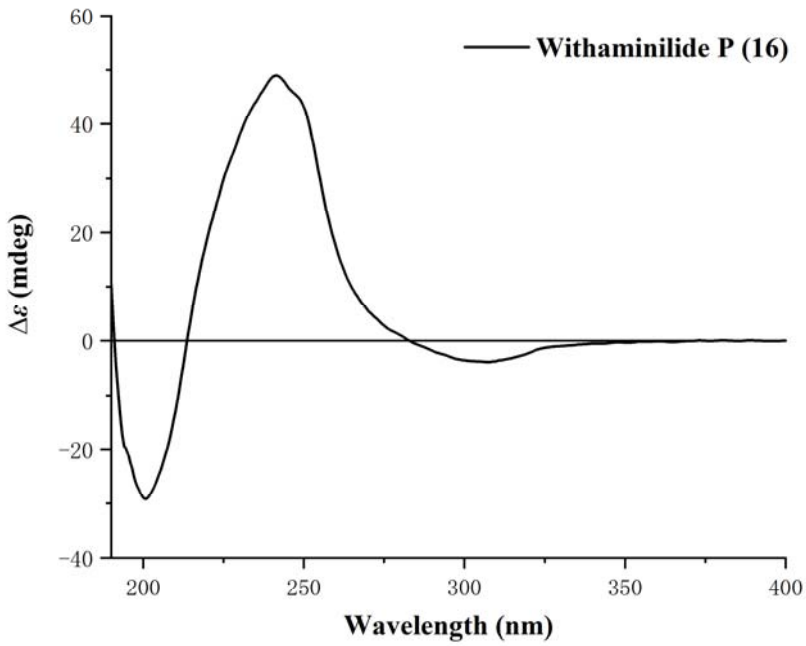


Figure S149. Experimental ECD Spectrum of Withaminilide P (**16**)

Elemental Composition Report

Single Mass Analysis

Tolerance = 3.0 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

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

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Minimum:					-1.5			
Maximum:			3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
527.2268	527.2281	-1.3	-2.5	12.5	527.0	n/a	n/a	C29H35O9

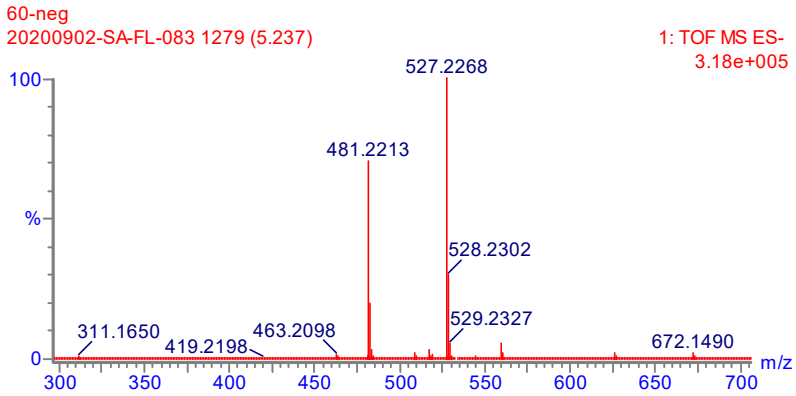


Figure S150. HRESIMS Spectrum of Withaminilide Q (**17**)

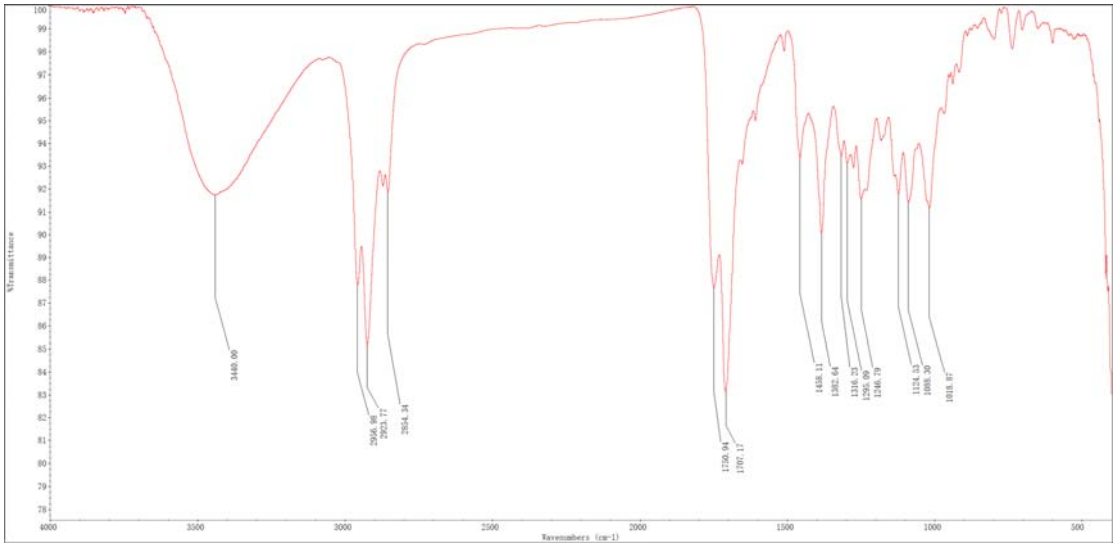


Figure S151. IR Spectrum of Withaminilide Q (**17**)

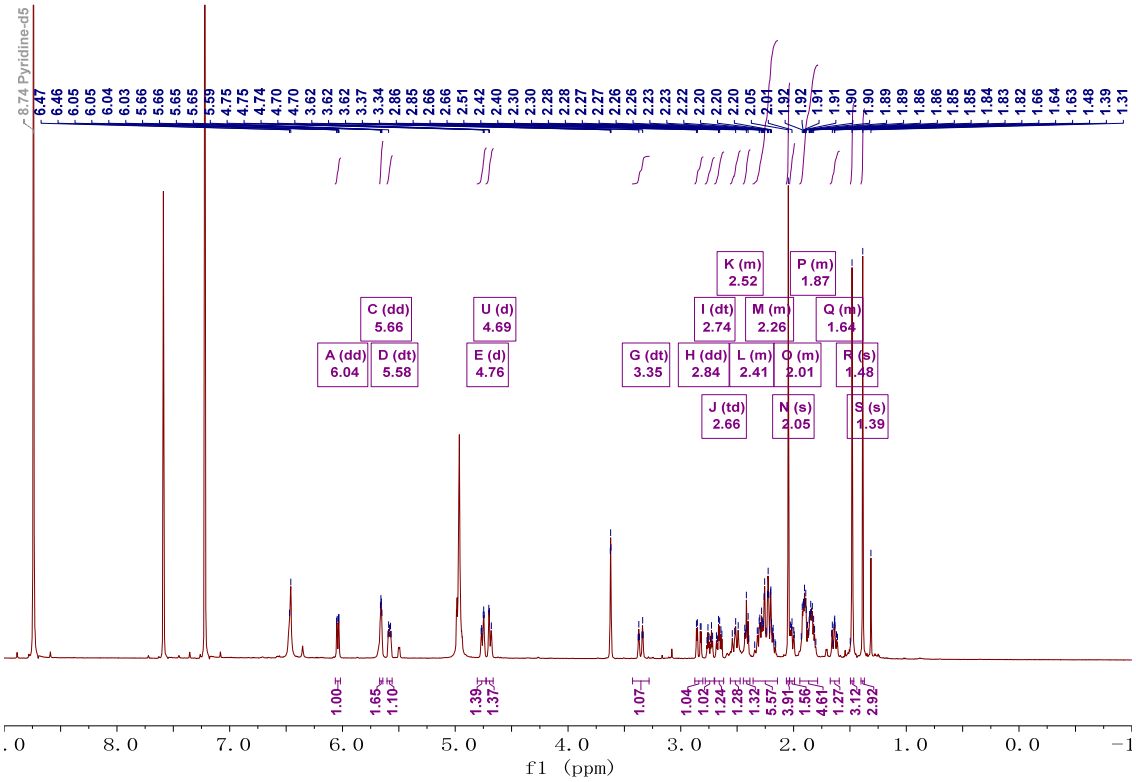


Figure S152. ^{1}H NMR Spectrum of Withaminilide Q (**17**) in C_5D_5N, 600 MHz

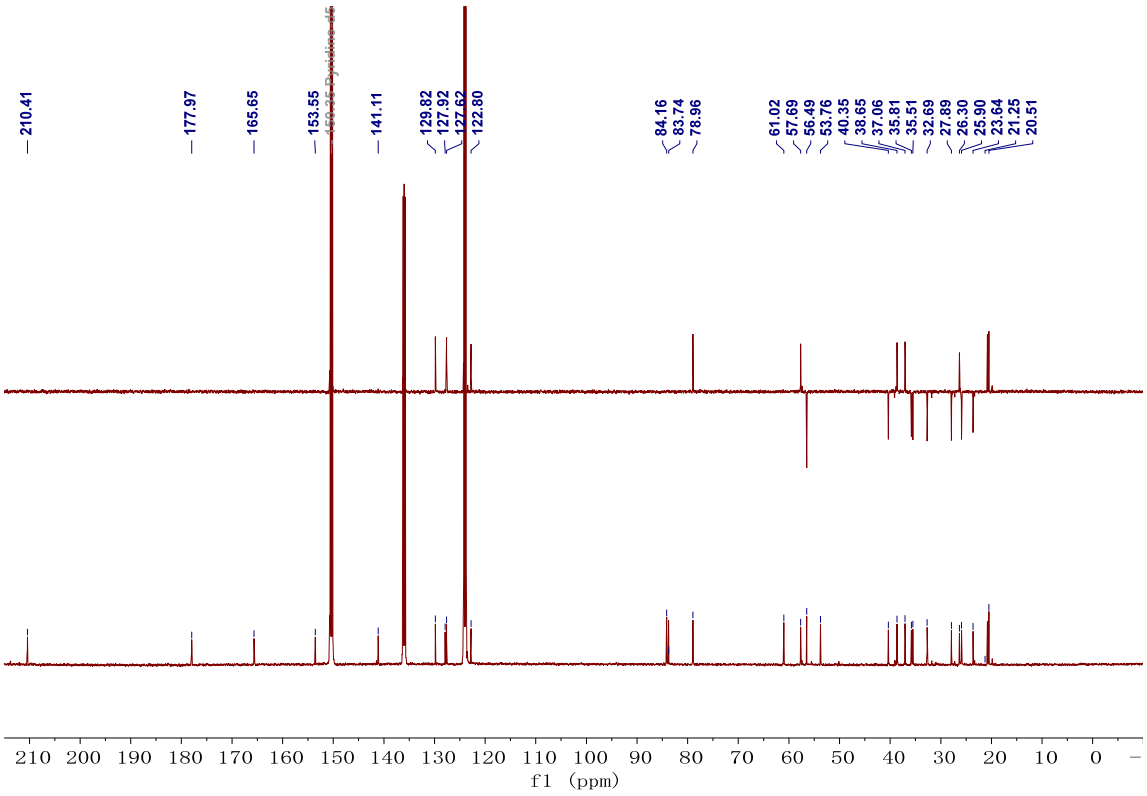


Figure S153. ^{13}C NMR Spectrum of Withaminilide Q (**17**) in C_5D_5N, 125 MHz

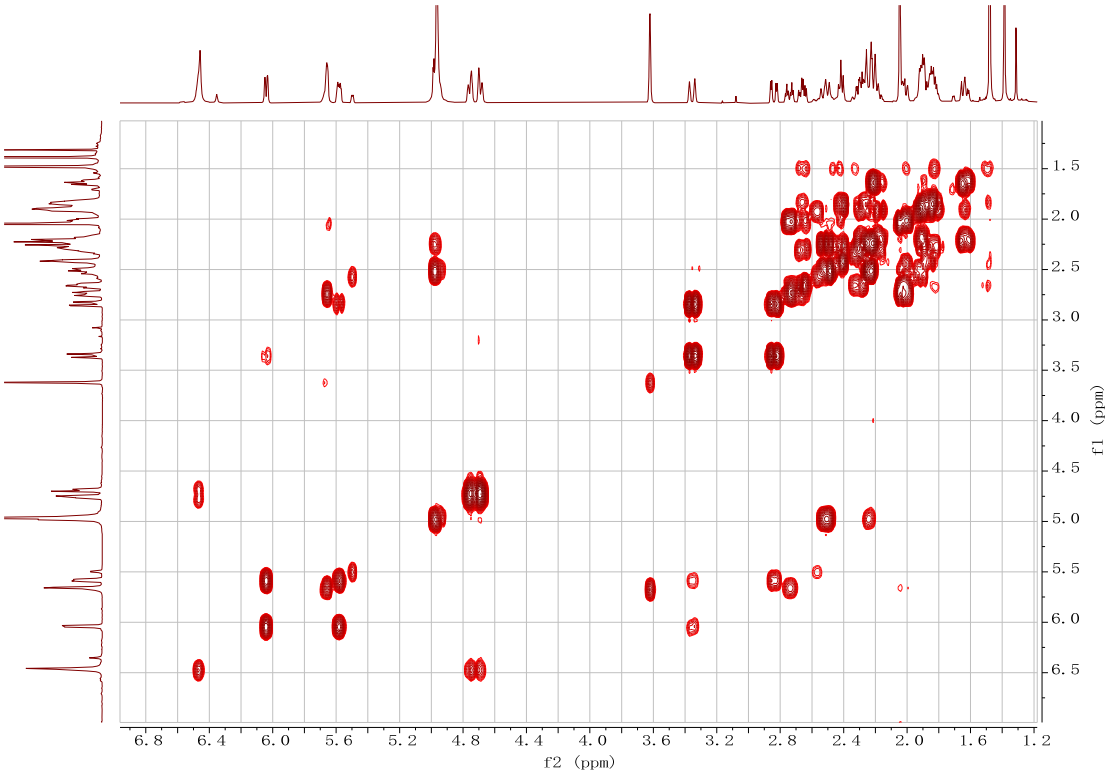


Figure S154. ^{1}H-^{1}H COSY Spectrum of Withaminilide Q (**17**) in C_5D_5N

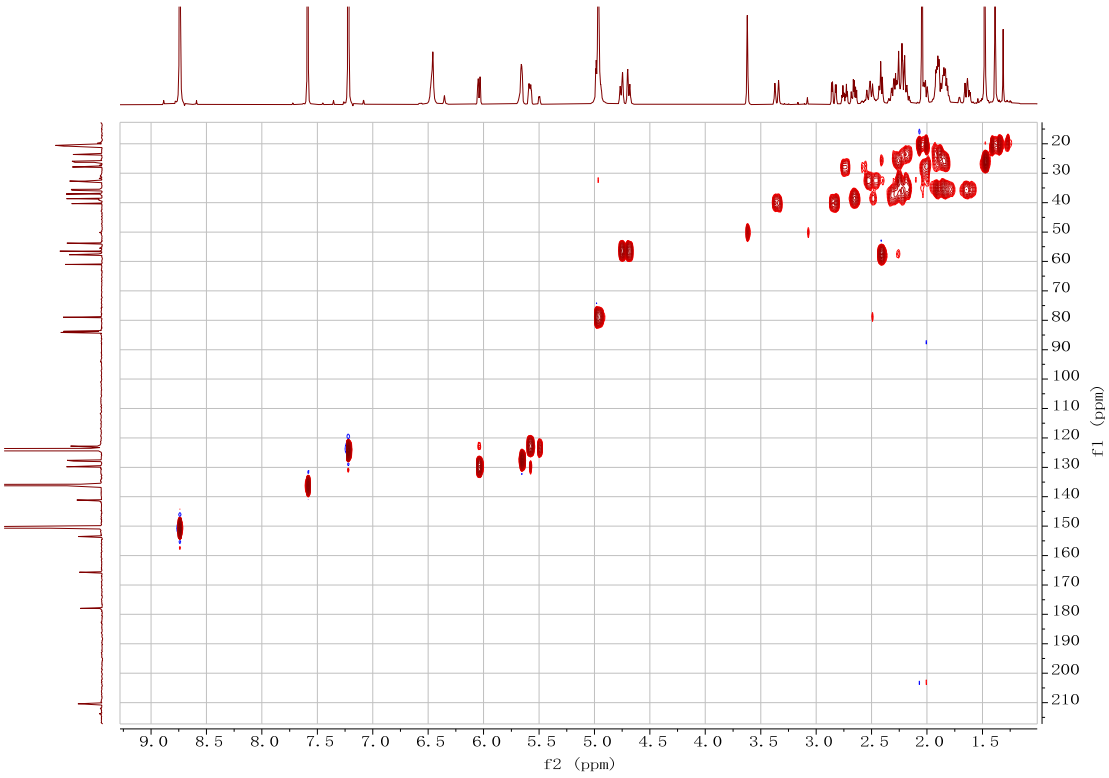


Figure S155. HSQC Spectrum of Withaminilide Q (**17**) in C_5D_5N

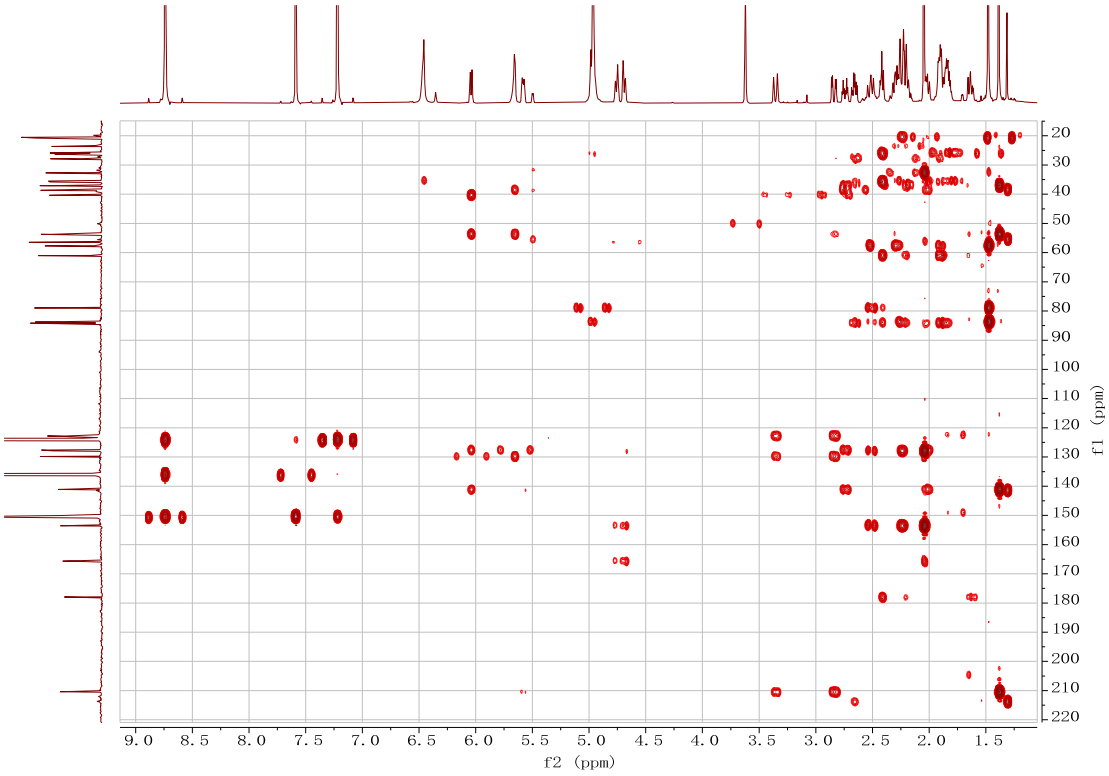


Figure S156. HMBC Spectrum of Withaminilide Q (**17**) in C_5D_5N

Figure S157. NOESY Spectrum of Withaminilide Q (**17**) in C_5D_5N

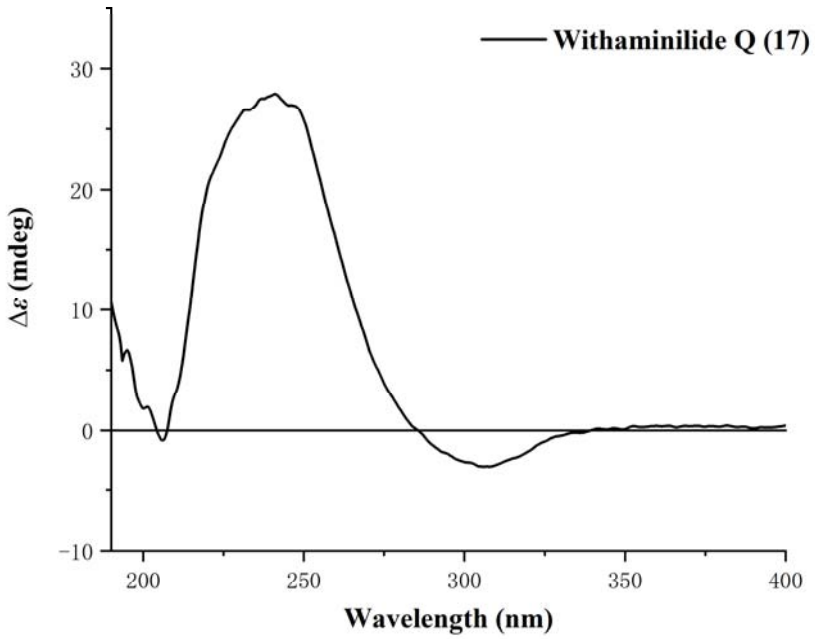


Figure S158. Experimental ECD Spectrum of Withaminilide Q (**17**)

Elemental Composition Report

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 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Na: 0-1

Minimum:					-1.5			
Maximum:			2.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
505.2559	505.2566	-0.7	-1.4	10.5	356.4	n/a	n/a	C29H38O6Na

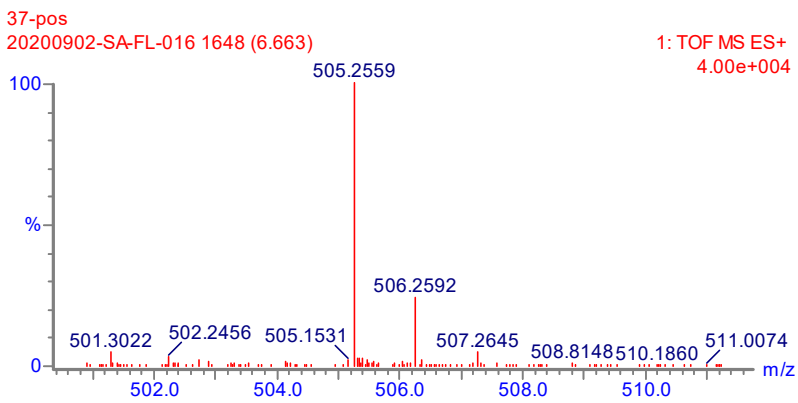


Figure S159. HRESIMS Spectrum of Withaminilide R (**18**)

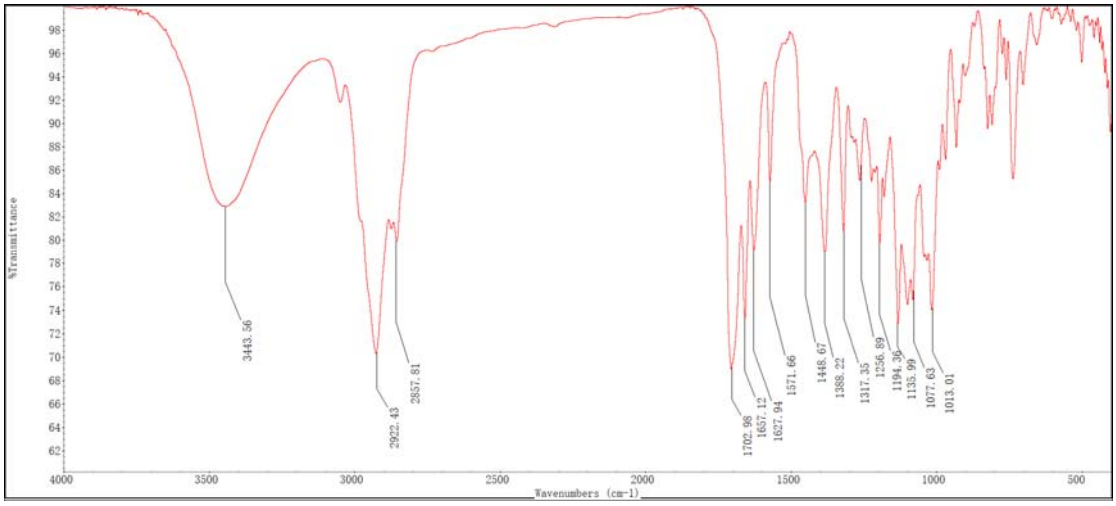


Figure S160. IR Spectrum of Withaminilide R (**18**)

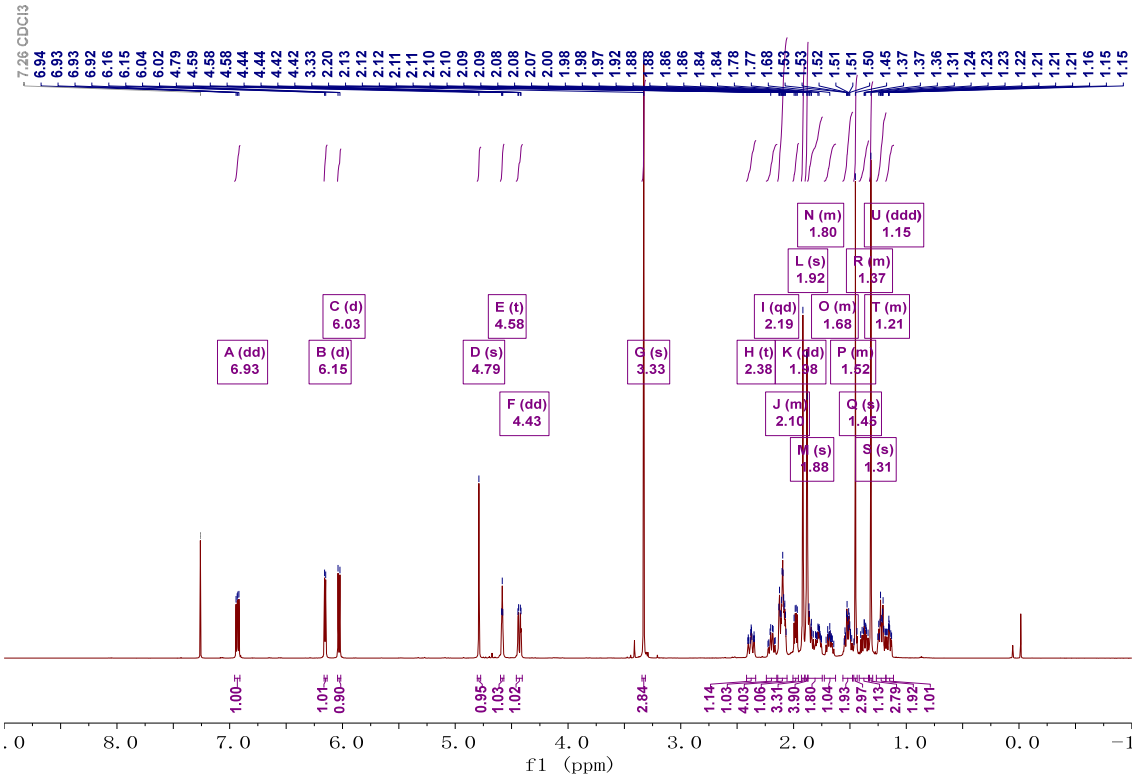


Figure S161. ^{1}H NMR Spectrum of Withaminilide R (**18**) in $CDCl_3$, 600 MHz

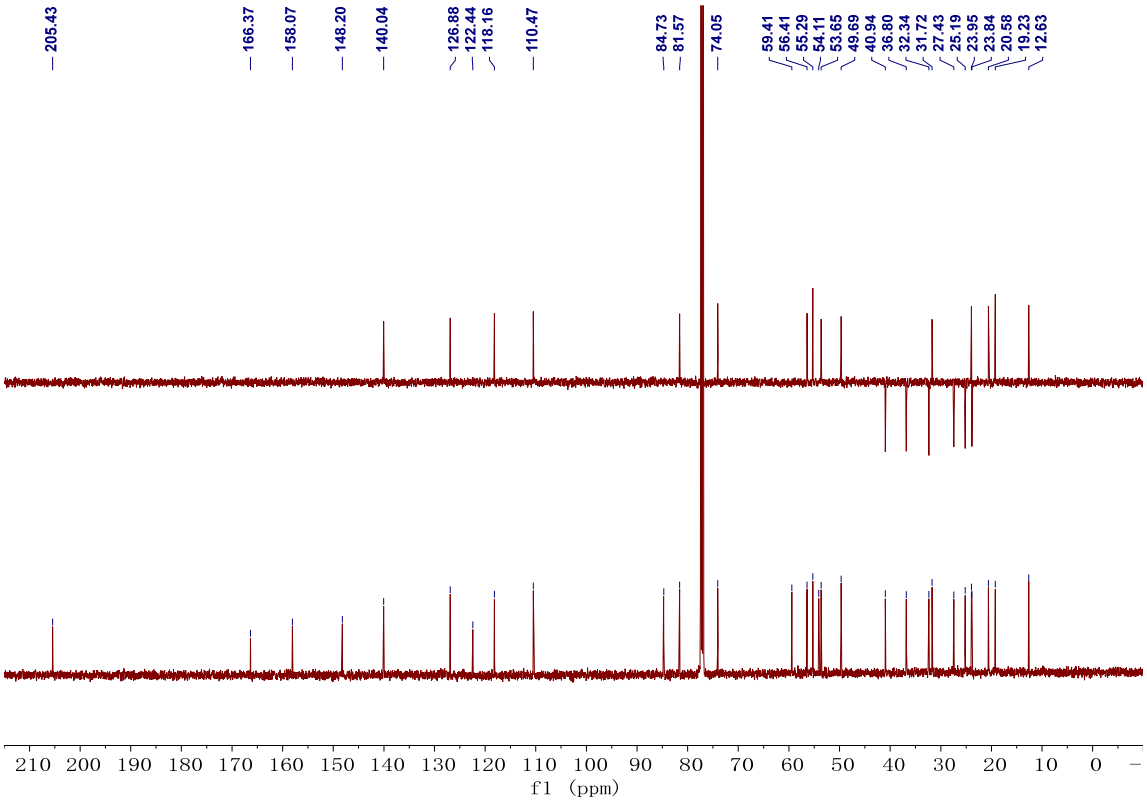


Figure S162. ^{13}C NMR Spectrum of Withaminilide R (**18**) in $CDCl_3$, 125 MHz

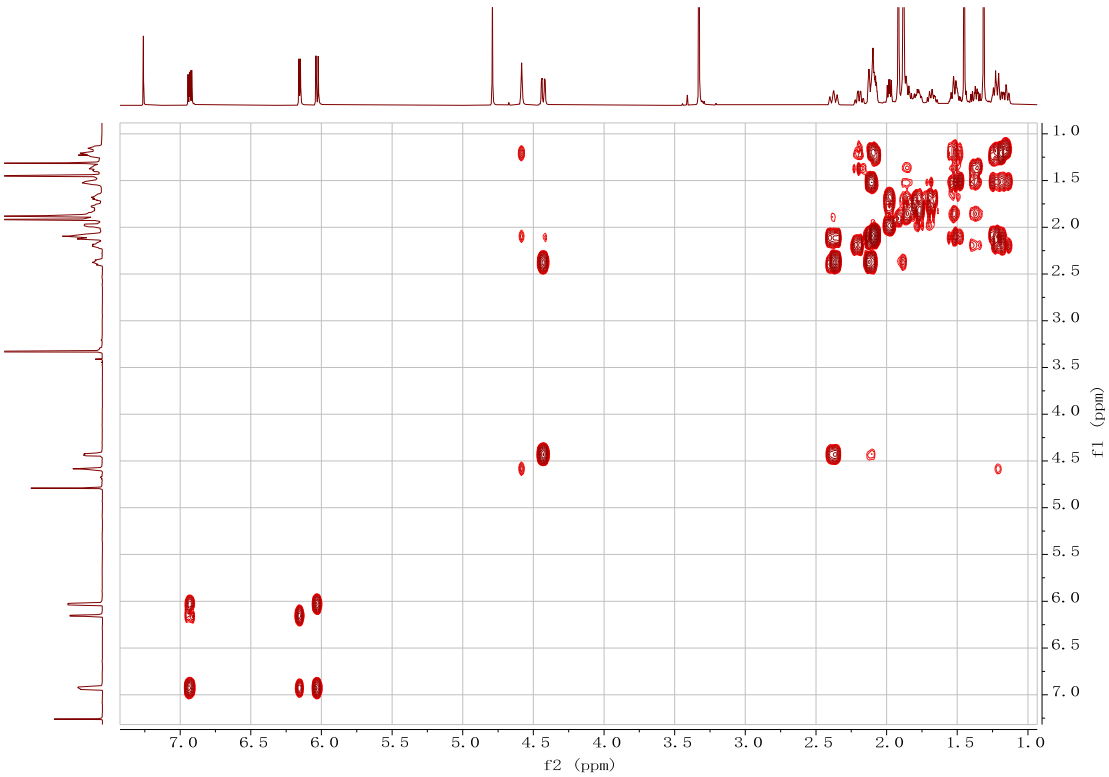


Figure S163. ^{1}H-^{1}H COSY Spectrum of Withaminilide R (**18**) in $CDCl_3$

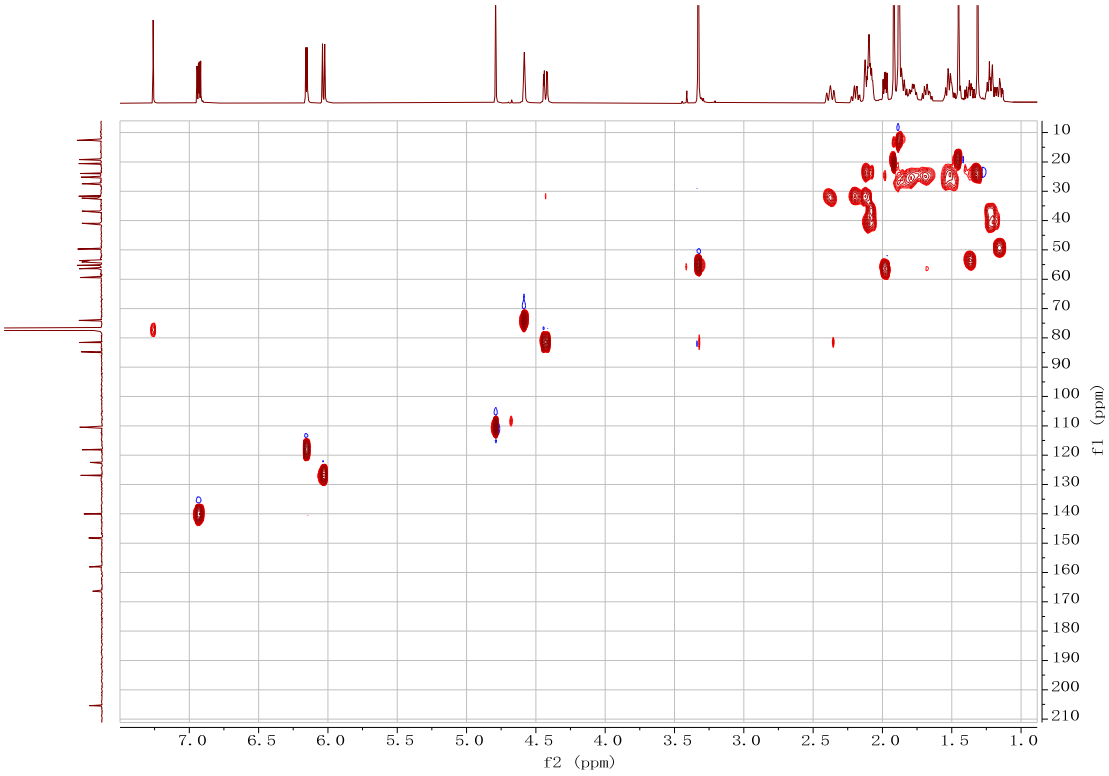


Figure S164. HSQC Spectrum of Withaminilide R (**18**) in $CDCl_3$

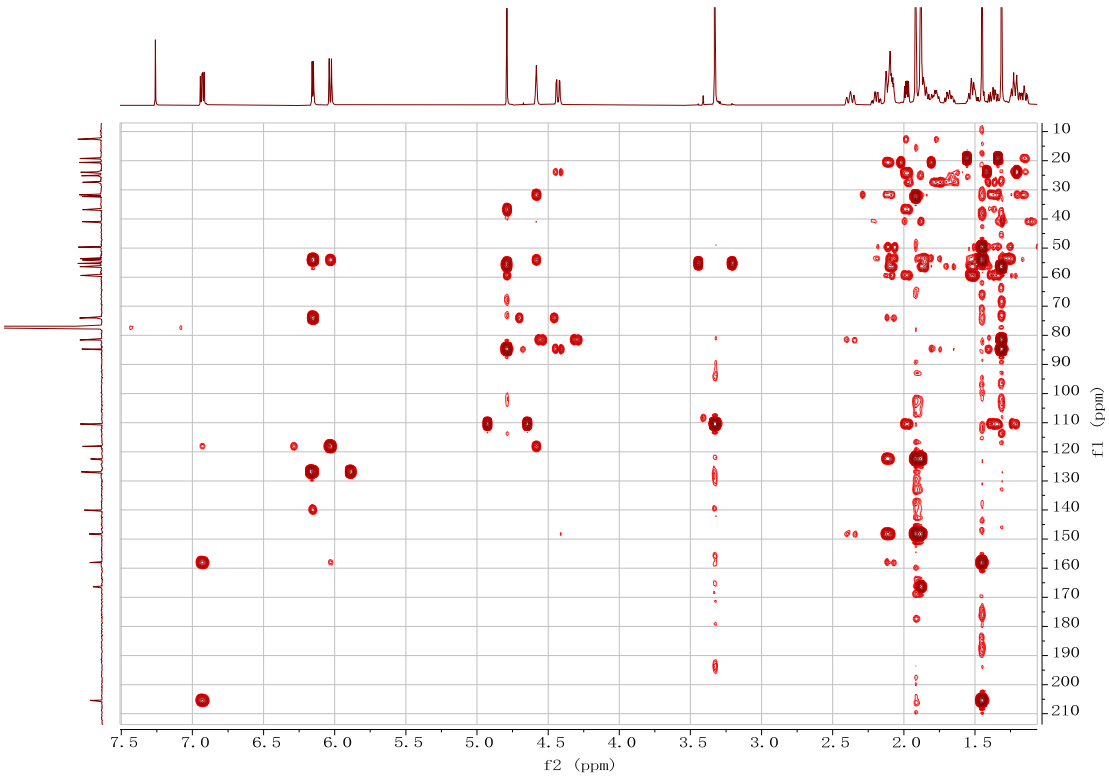


Figure S165. HMBC Spectrum of Withaminilide R (**18**) in $CDCl_3$

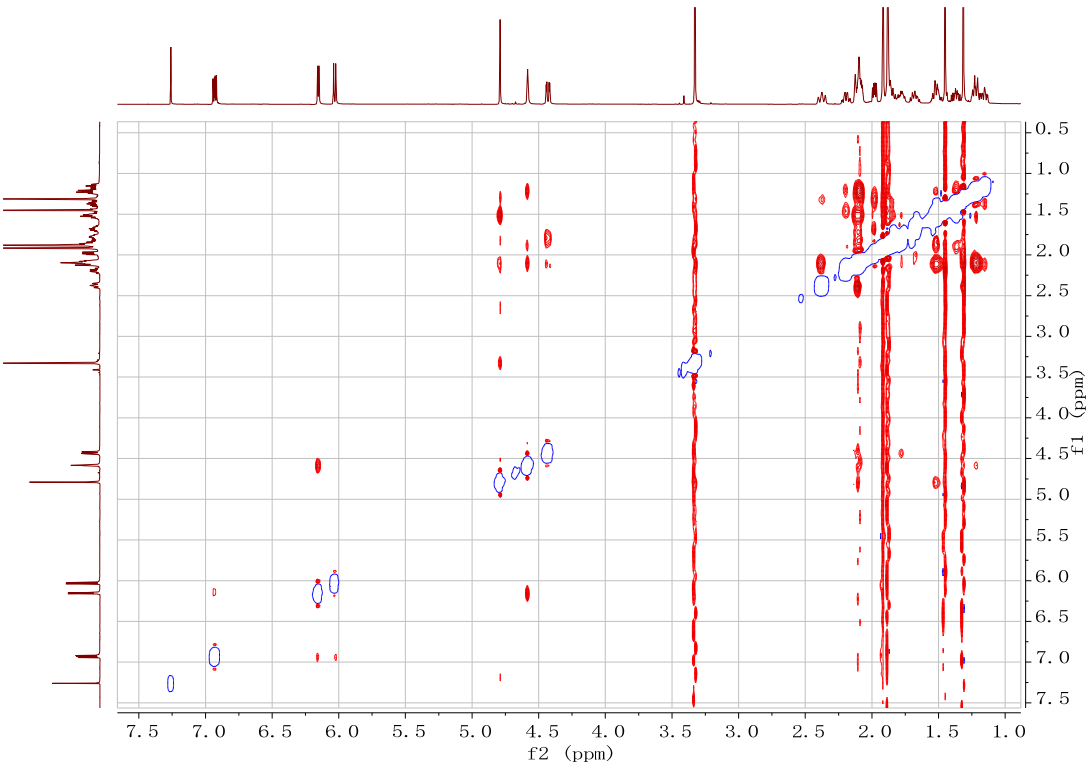


Figure S166. ROESY Spectrum of Withaminilide R (**18**) in $CDCl_3$

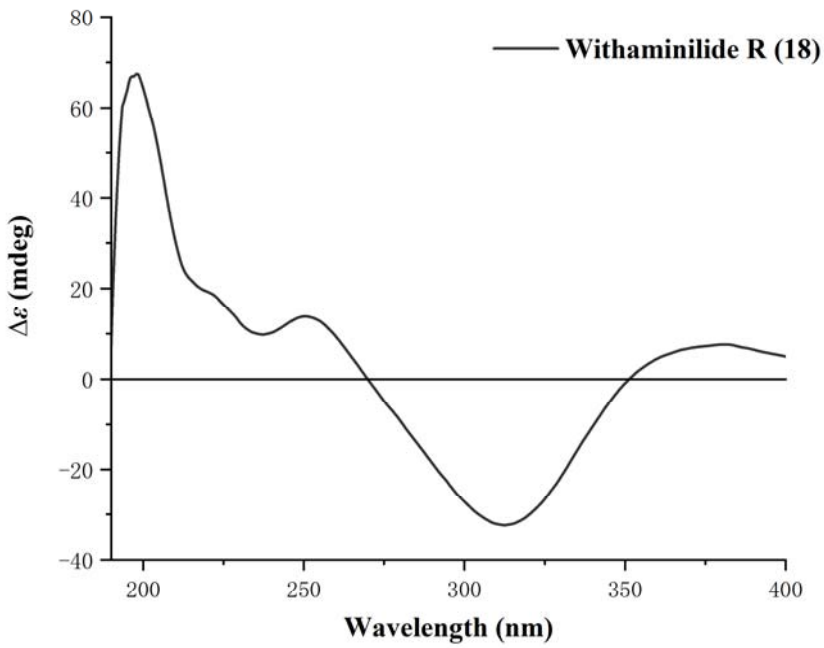


Figure S167. Experimental ECD Spectrum of Withaminilide R (**18**)

Elemental Composition Report

Single Mass Analysis

Tolerance = 1.0 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

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

Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Na: 0-1

Minimum:					-1.5			
Maximum:			1.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
521.2522	521.2515	0.7	1.3	10.5	349.2	n/a	n/a	C29H38O7Na

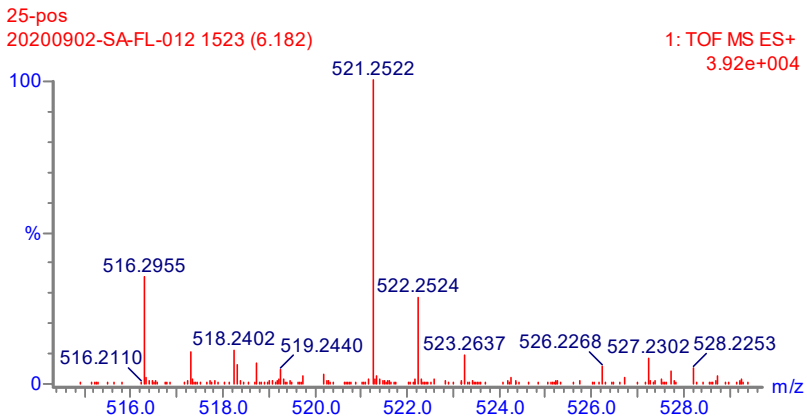


Figure S168. HRESIMS Spectrum of Withaminilide S (**19**)

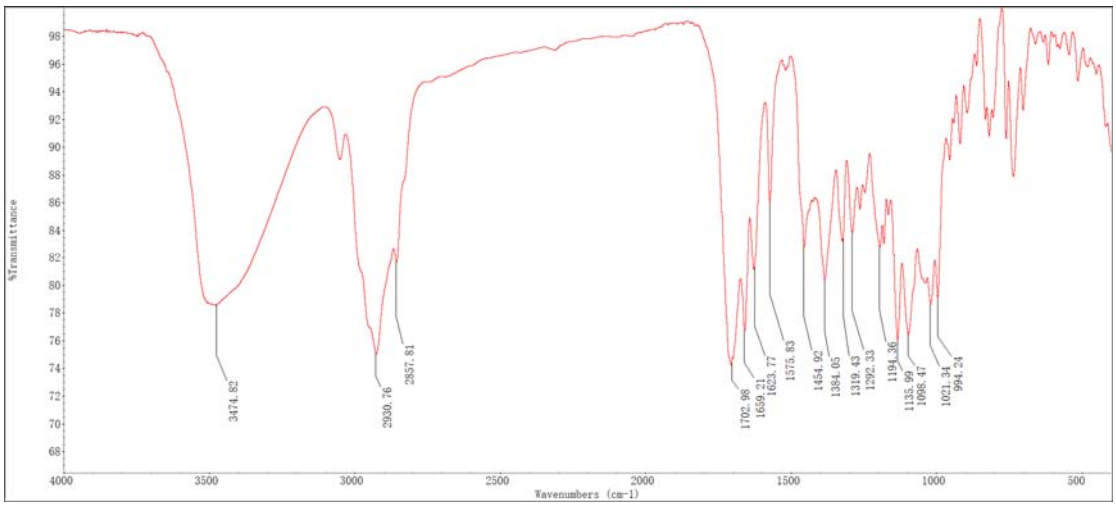


Figure S169. IR Spectrum of Withaminilide S (**19**)

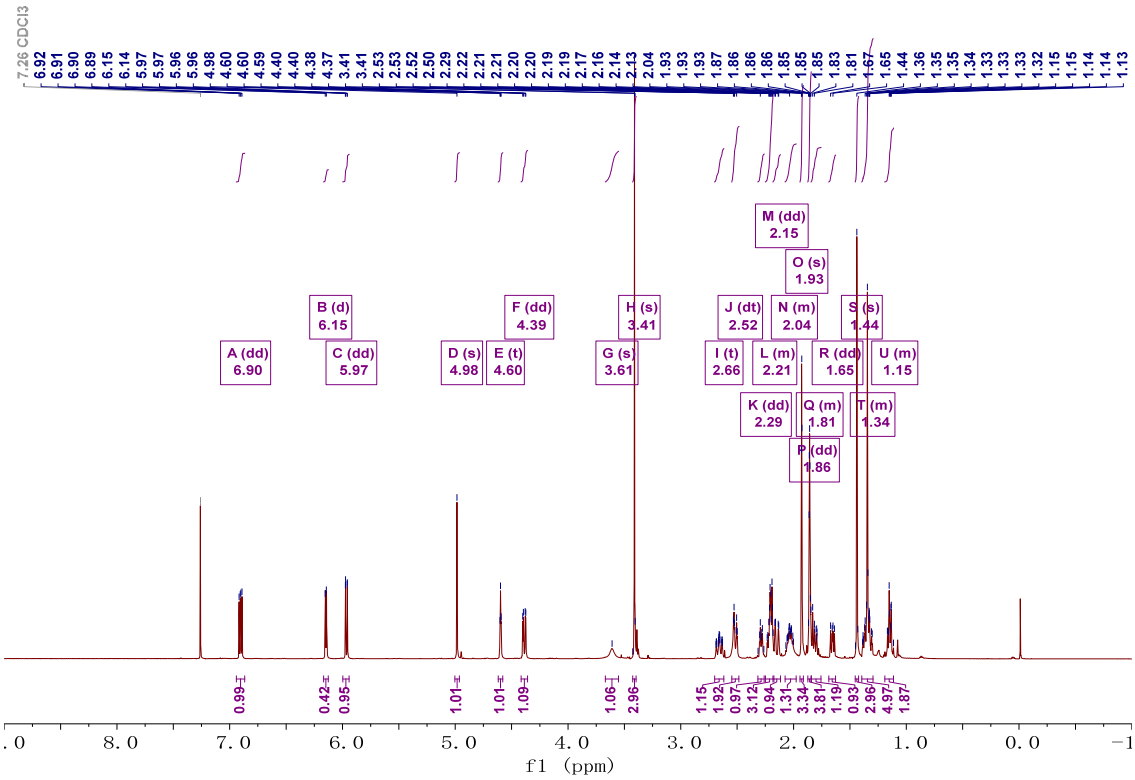


Figure S170. ^{1}H NMR Spectrum of Withaminilide S (**19**) in $CDCl_3$, 600 MHz

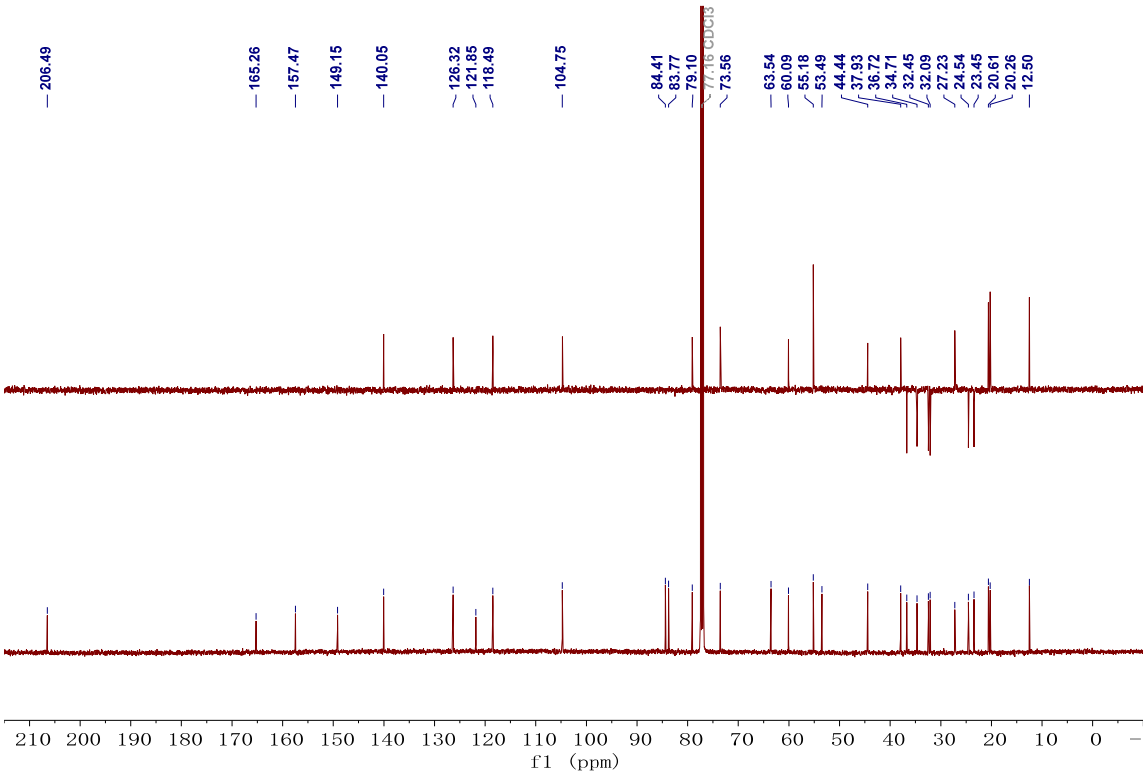


Figure S171. ^{13}C NMR Spectrum of Withaminilide S (**19**) in $CDCl_3$, 125 MHz

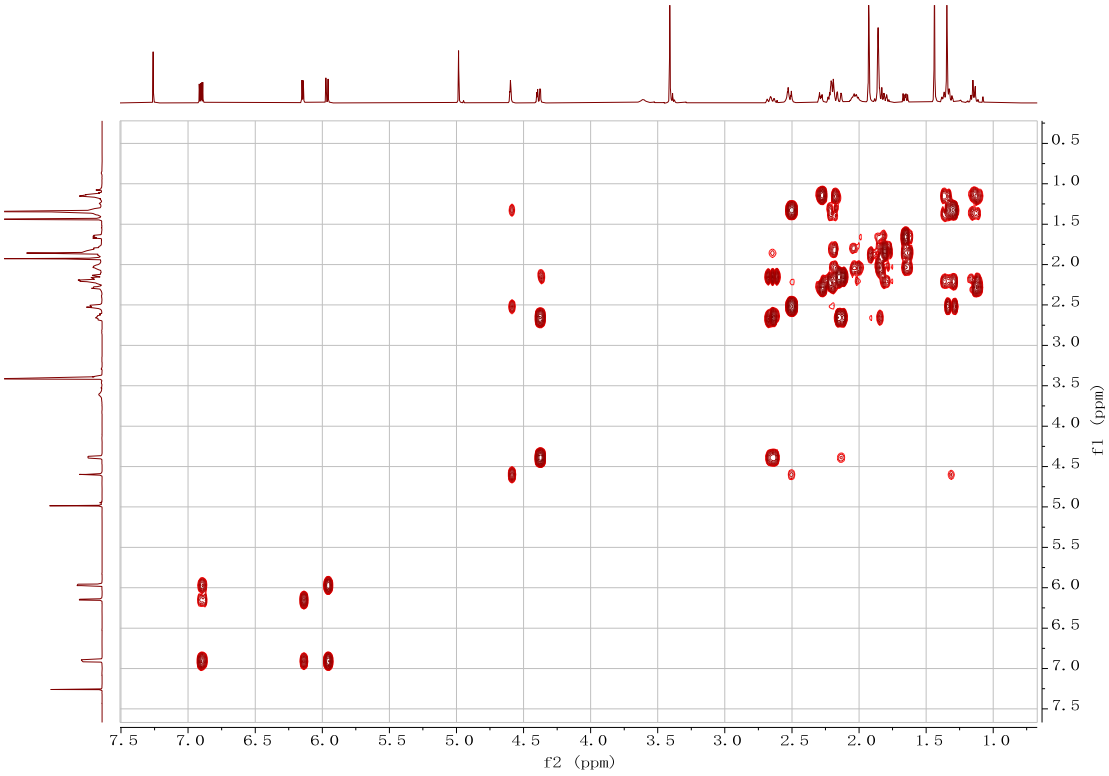


Figure S172. ^{1}H-^{1}H COSY Spectrum of Withaminilide S (**19**) in $CDCl_3$

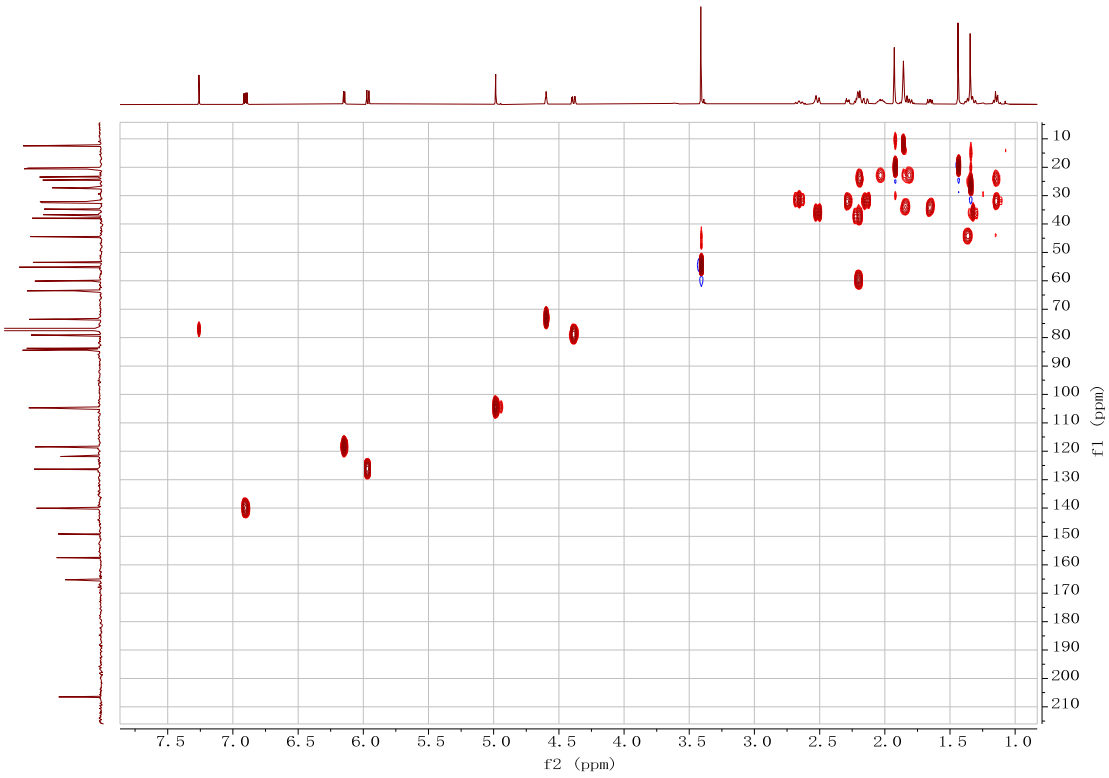


Figure S173. HSQC Spectrum of Withaminilide S (**19**) in $CDCl_3$

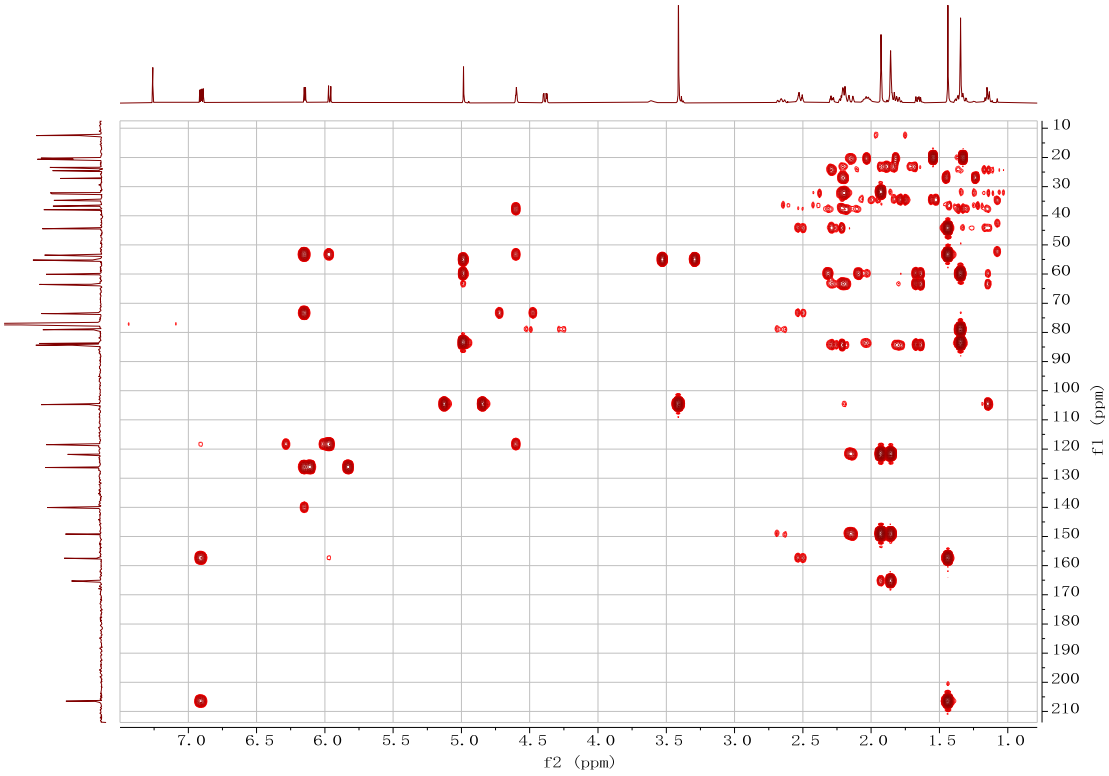


Figure S174. HMBC Spectrum of Withaminilide S (**19**) in $CDCl_3$

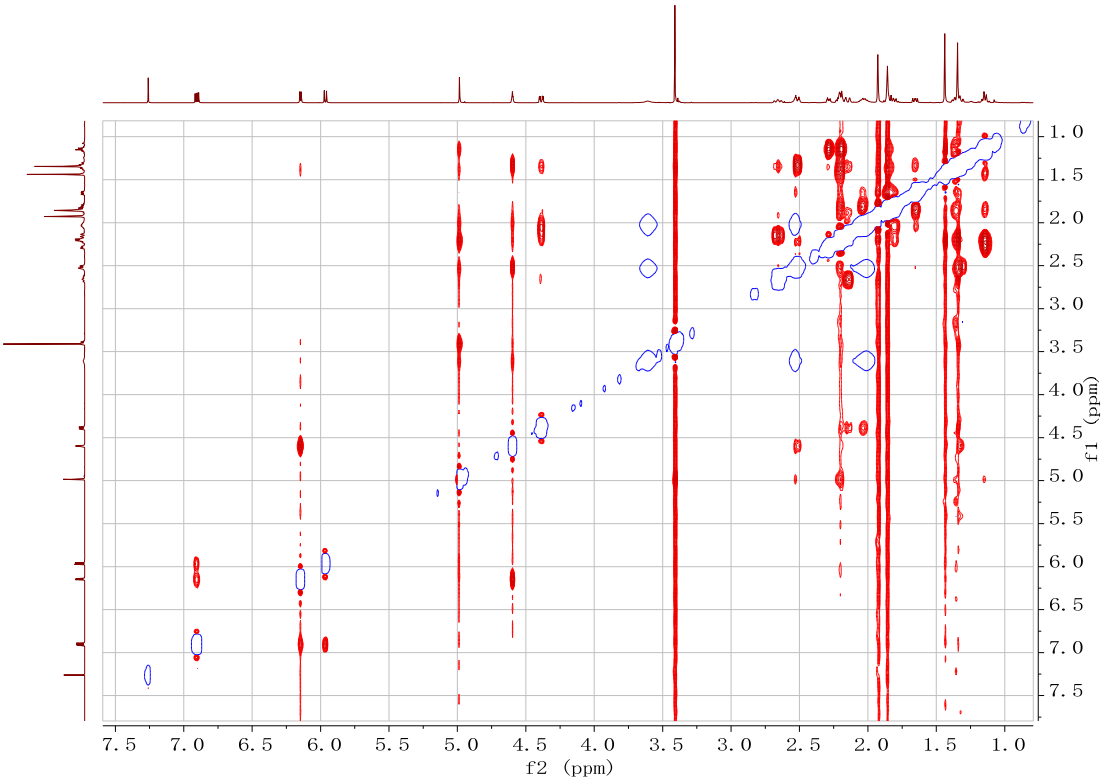


Figure S175. NOESY Spectrum of Withaminilide S (**19**) in $CDCl_3$

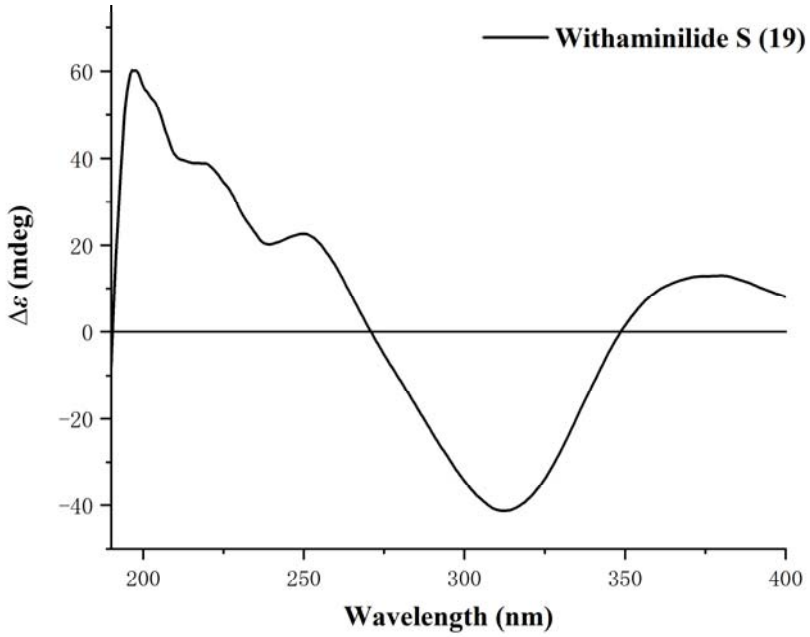


Figure S176. Experimental ECD Spectrum of Withaminilide S (**19**)

Elemental Composition Report

Single Mass Analysis

Tolerance = 1.9 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 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Na: 0-1

Minimum:					-1.5			
Maximum:			1.9	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
505.2551	505.2566	-1.5	-3.0	10.5	353.5	n/a	n/a	C29H38O6Na

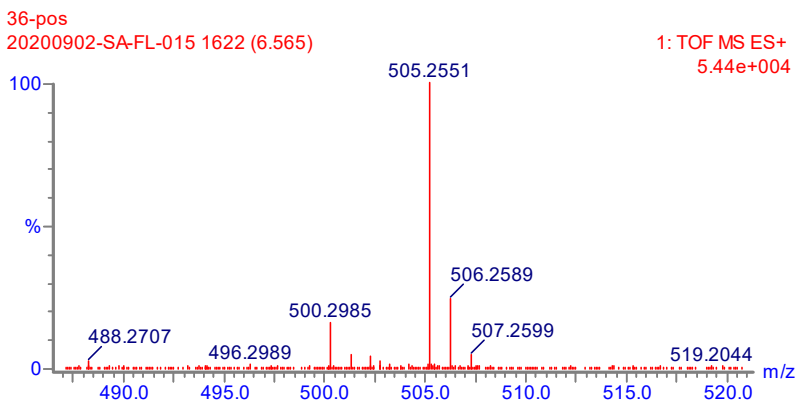


Figure S177. HRESIMS Spectrum of Withaminilide T (**20**)

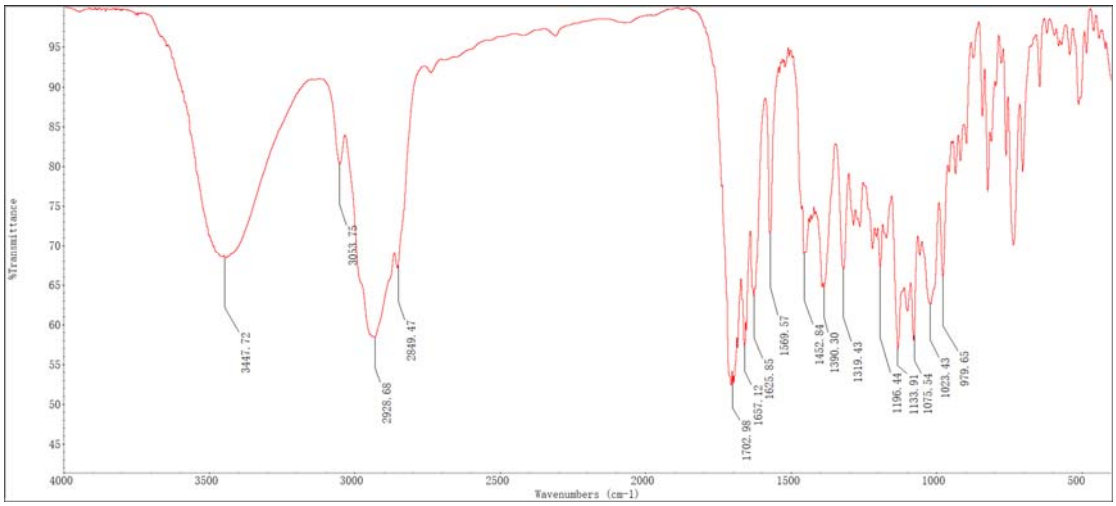


Figure S178. IR Spectrum of Withaminilide T (**20**)

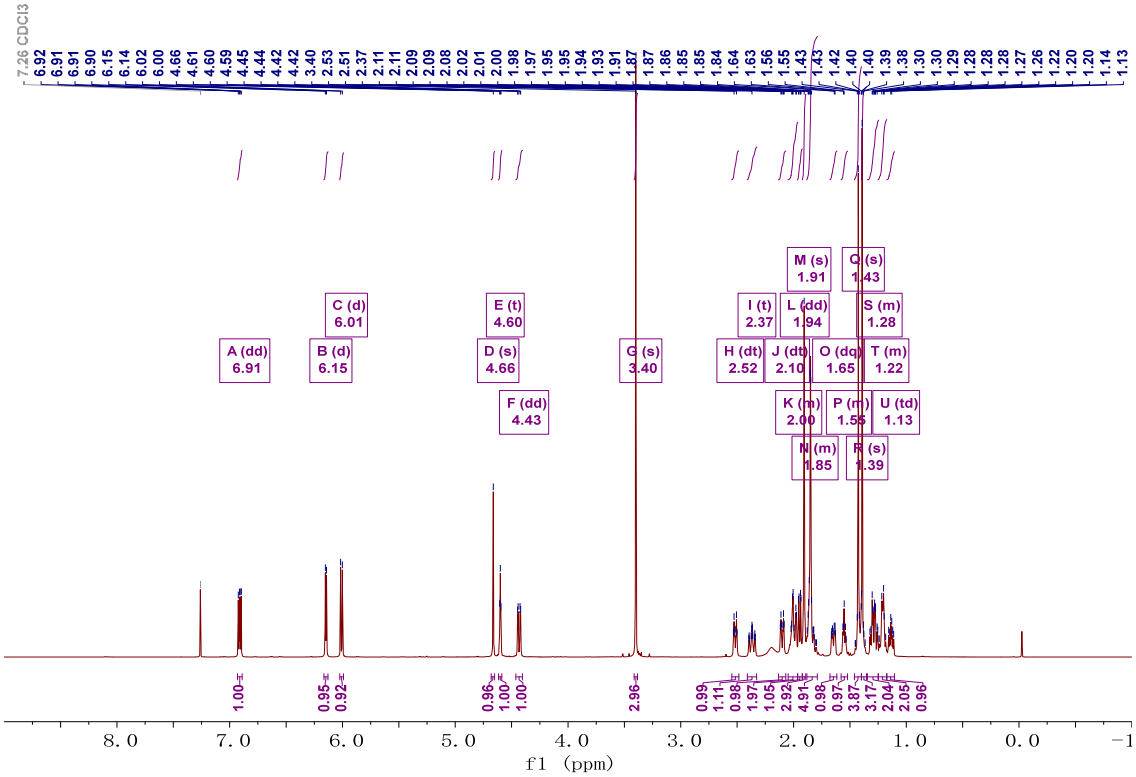


Figure S179. ^{1}H NMR Spectrum of Withaminilide T (**20**) in $CDCl_3$, 600 MHz

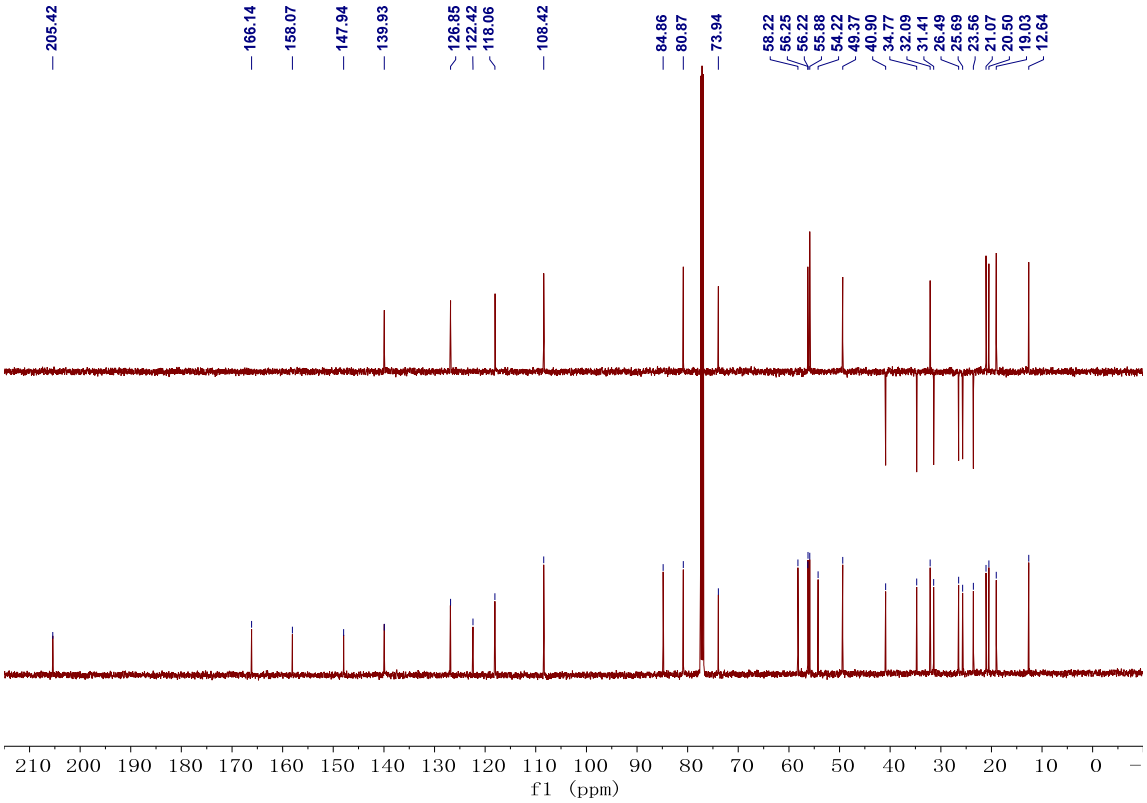


Figure S180. ^{13}C NMR Spectrum of Withaminilide T (**20**) in $CDCl_3$, 125 MHz

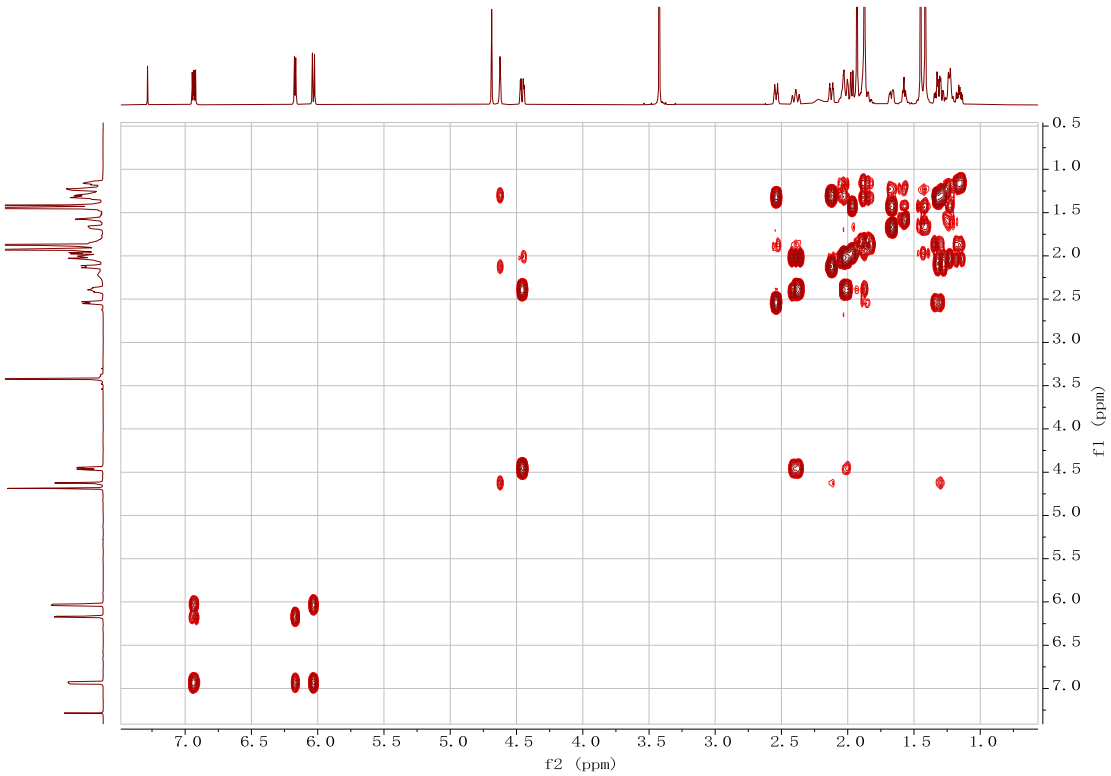


Figure S181. ^{1}H-^{1}H COSY Spectrum of Withaminilide T (**20**) in $CDCl_3$

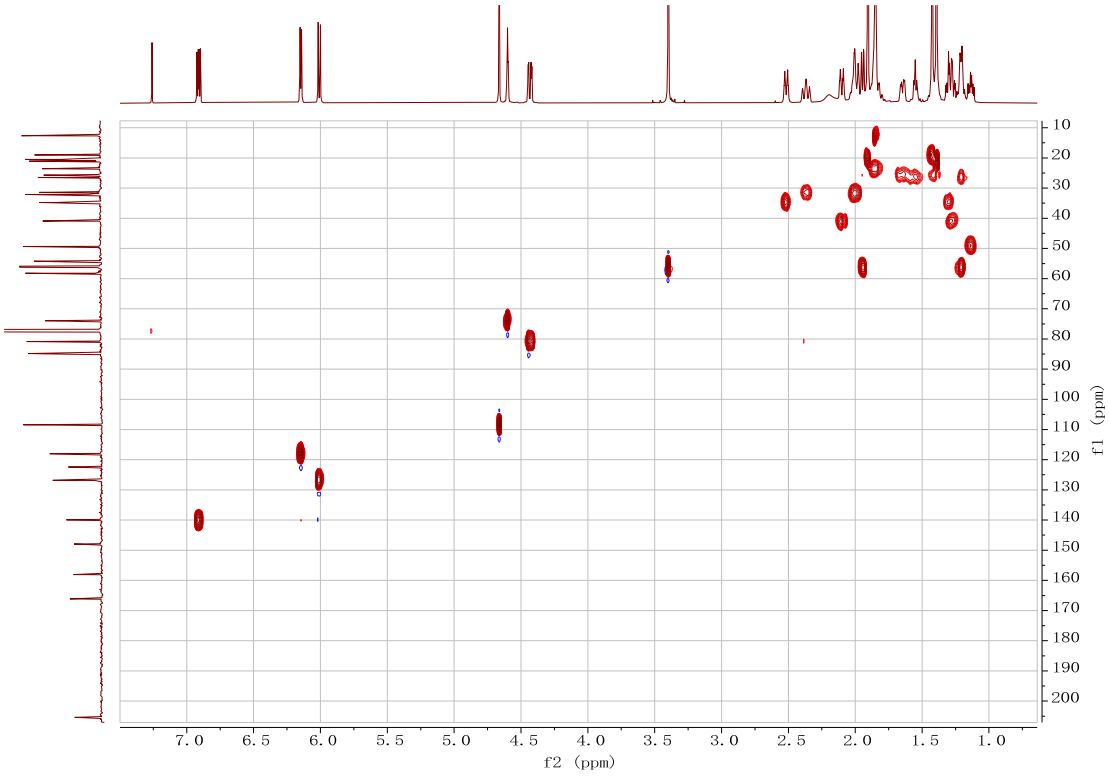


Figure S182. HSQC Spectrum of Withaminilide T (**20**) in $CDCl_3$

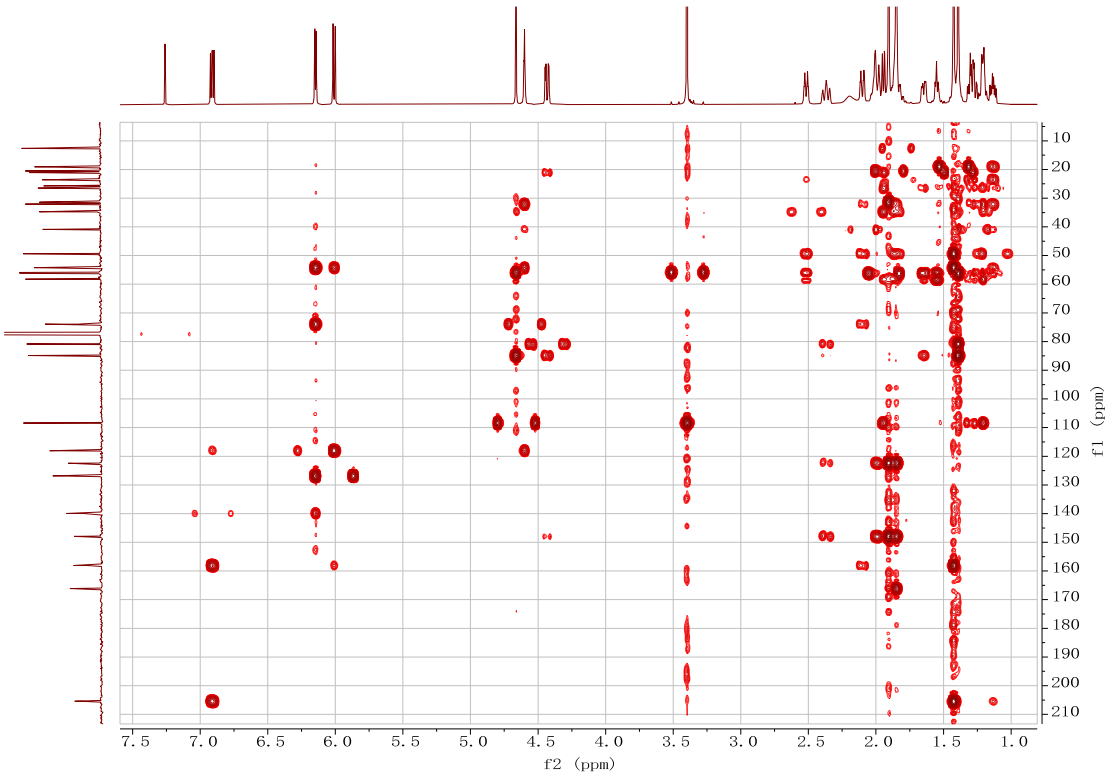


Figure S183. HMBC Spectrum of Withaminilide T (**20**) in $CDCl_3$

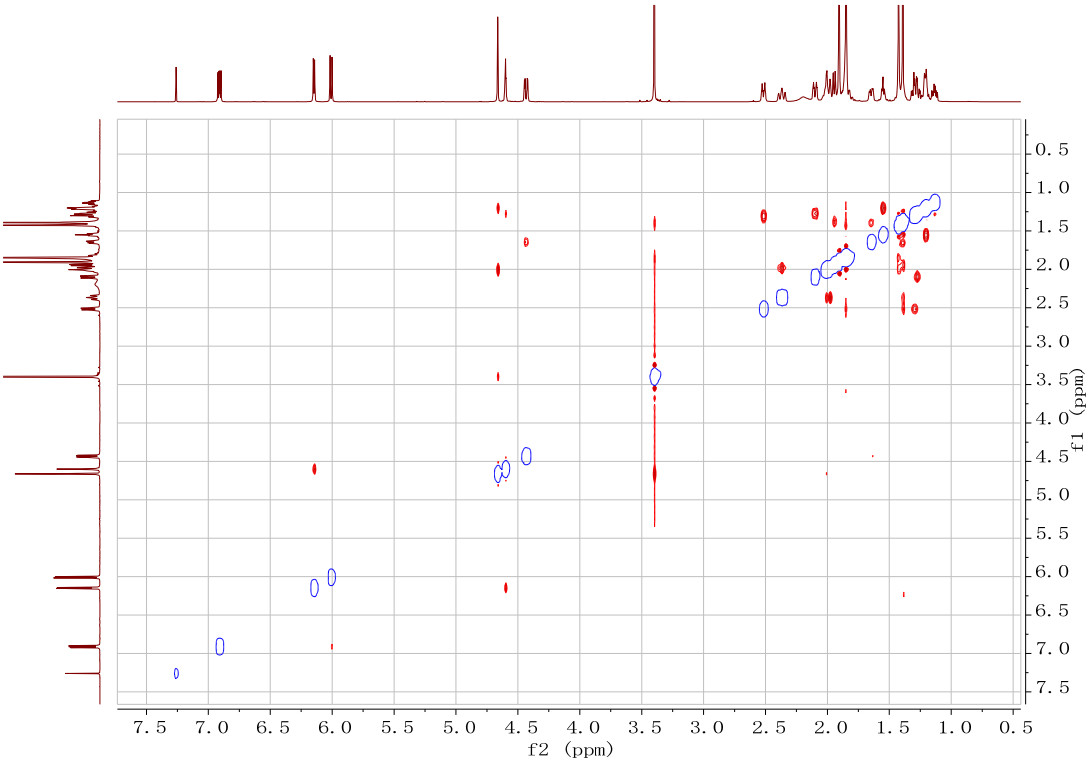


Figure S184. NOESY Spectrum of Withaminilide T (**20**) in $CDCl_3$

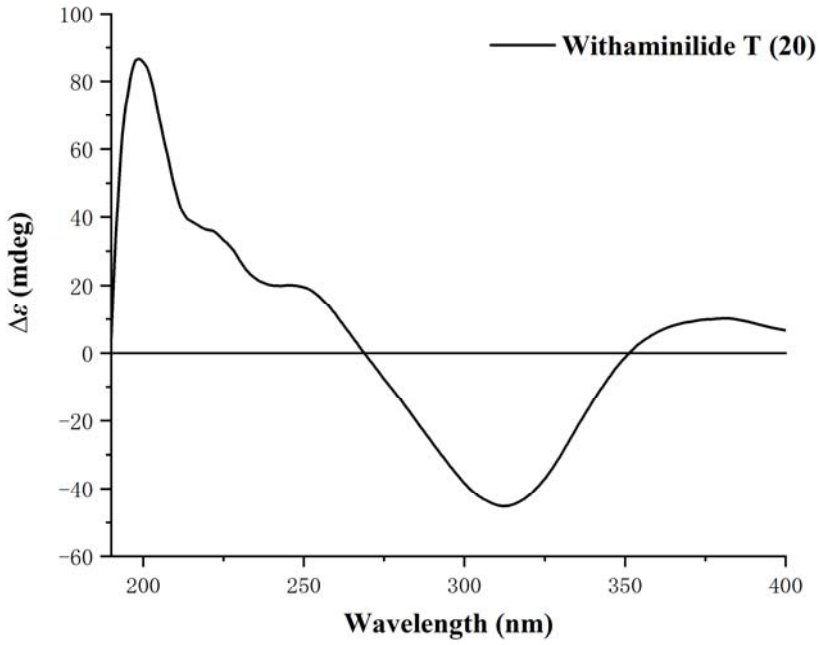


Figure S185. Experimental ECD Spectrum of Withaminilide T (**20**)

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

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

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Minimum:	80.00					-1.5		
Maximum:	100.00			3.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
513.2512	513.2488	2.4	4.7	11.5	555.2	n/a	n/a	C29H37O8

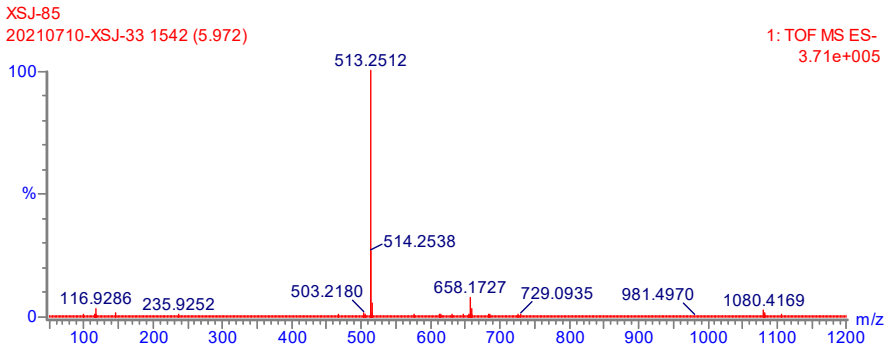


Figure S186. HRESIMS Spectrum of Withaminilide U (**21**)

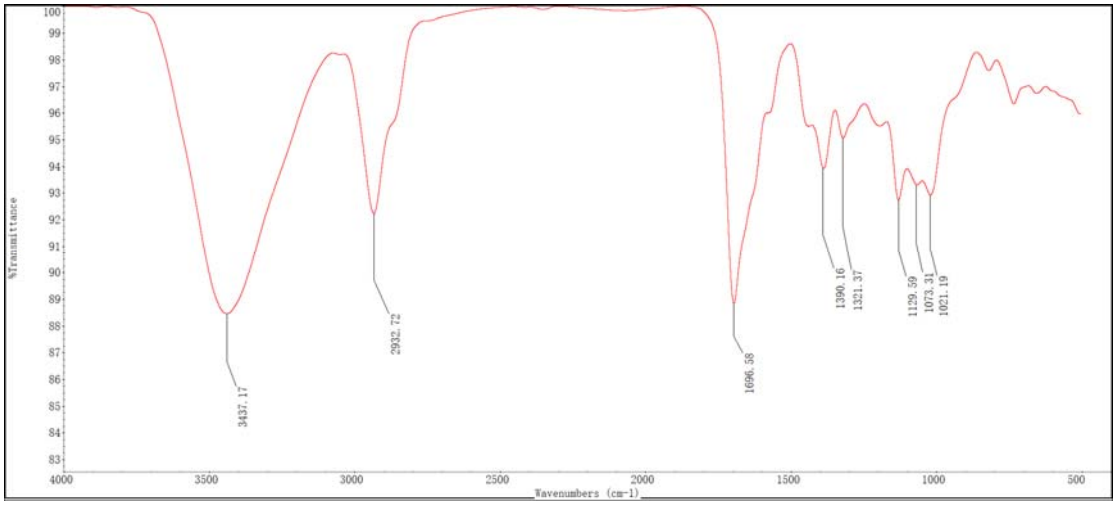


Figure S187. IR Spectrum of Withaminilide U (**21**)

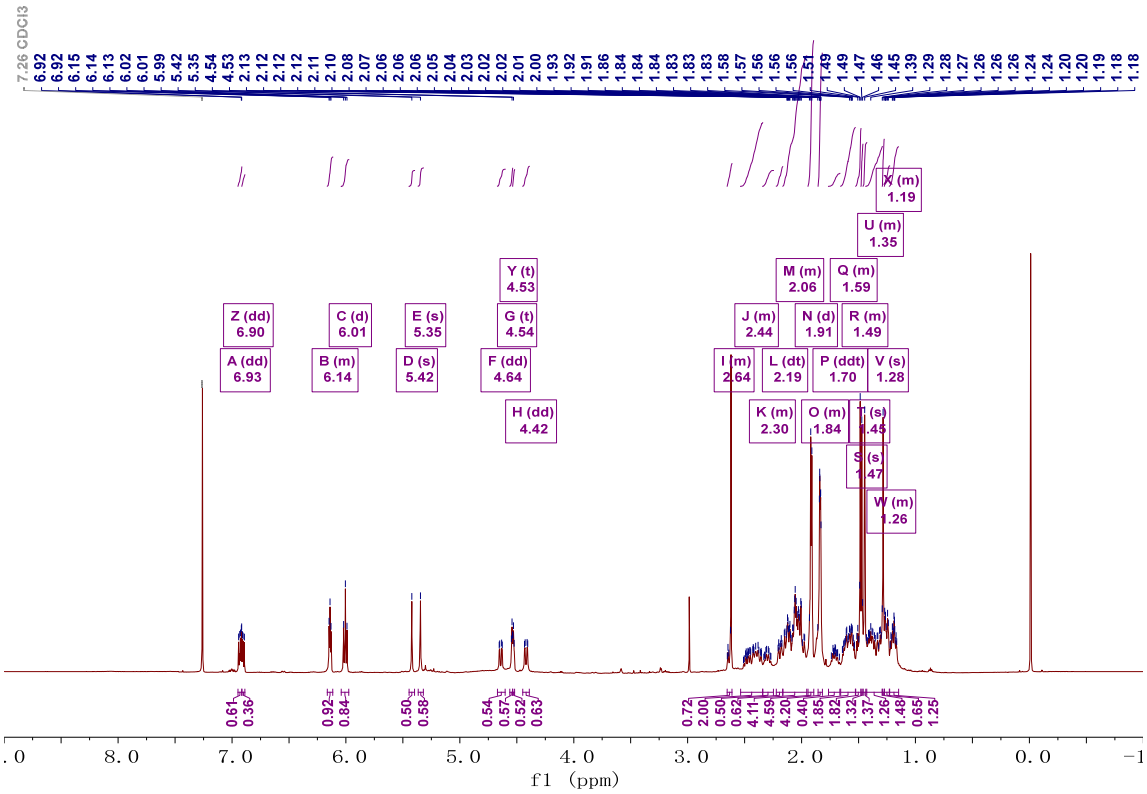


Figure S188. ^{1}H NMR Spectrum of Withaminilide U (**21**) in $CDCl_3$, 600 MHz

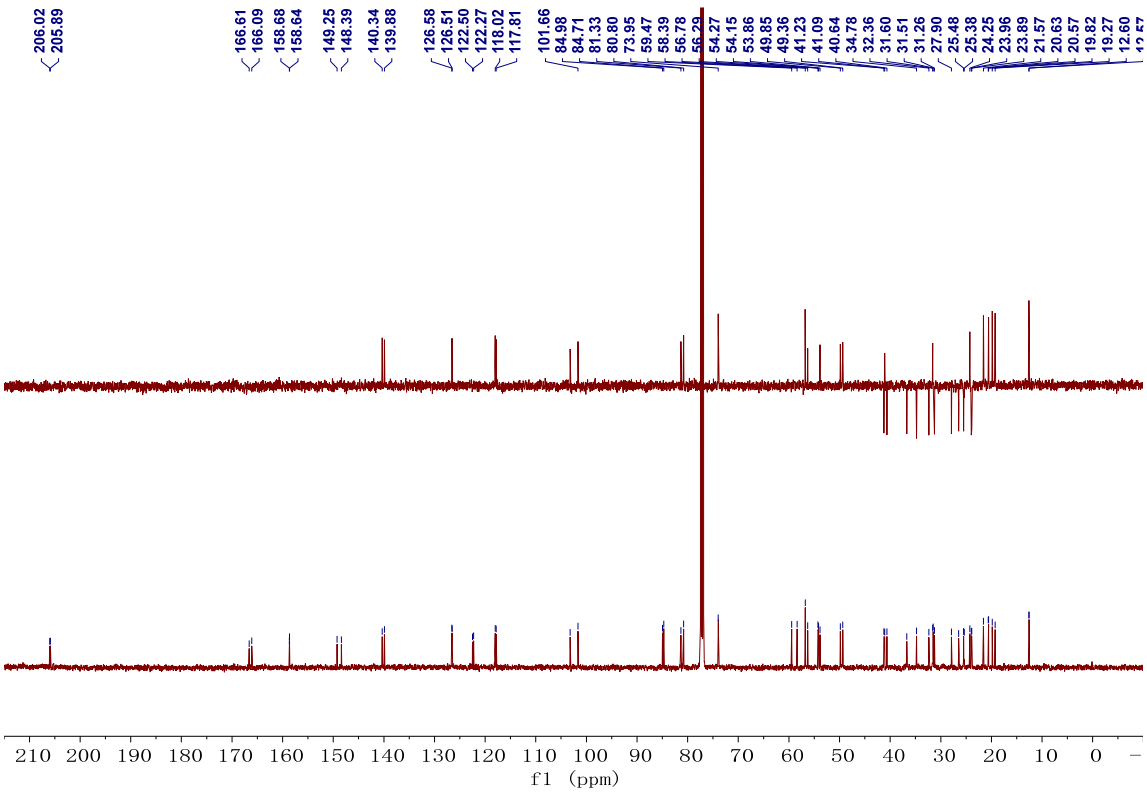


Figure S189. ^{13}C NMR Spectrum of Withaminilide U (**21**) in $CDCl_3$, 125 MHz

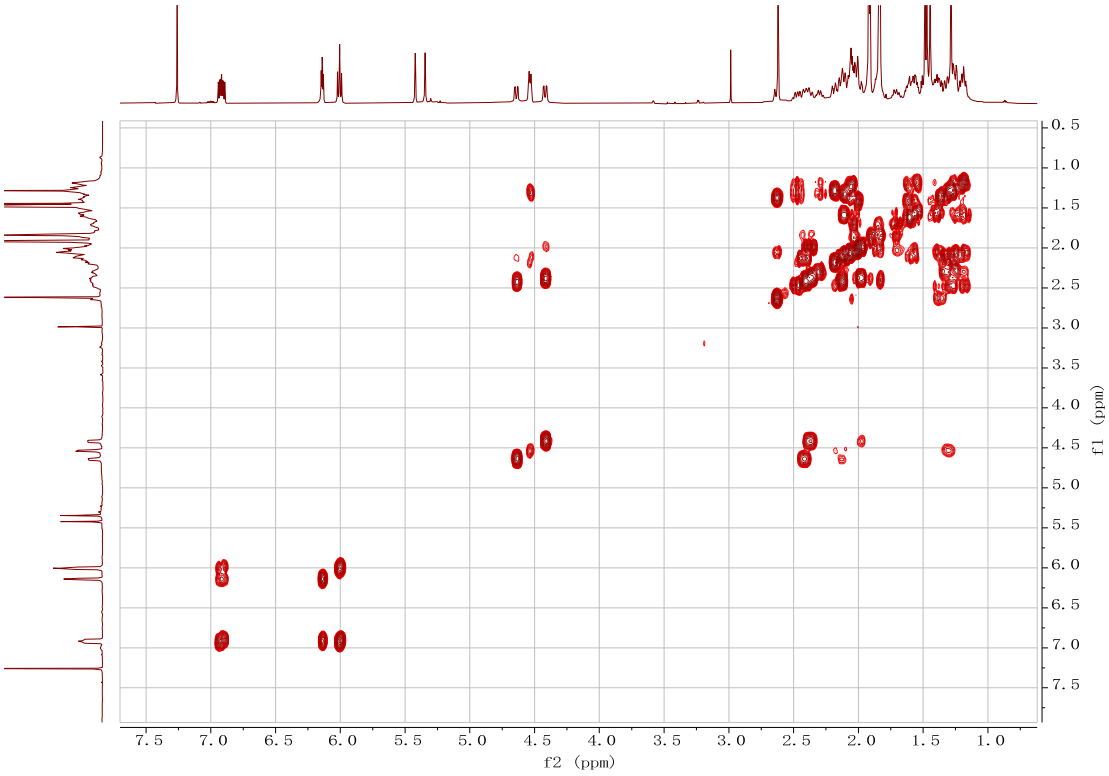


Figure S190. ^{1}H-^{1}H COSY Spectrum of Withaminilide U (**21**) in $CDCl_3$

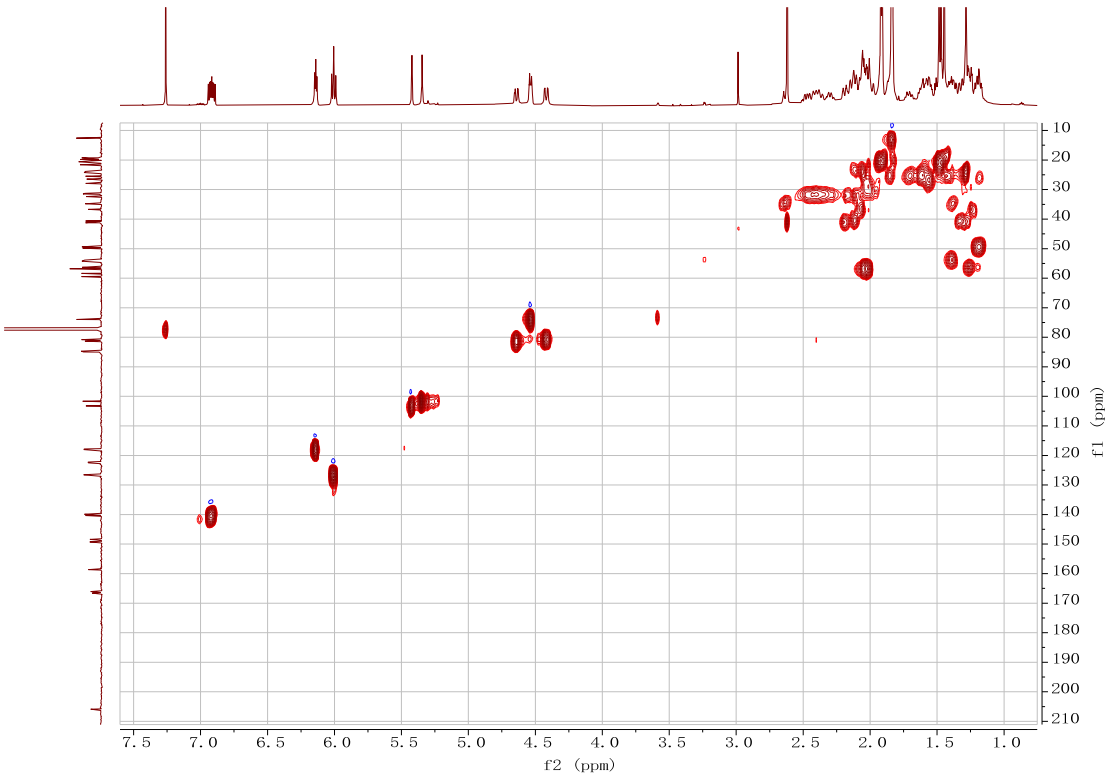


Figure S191. HSQC Spectrum of Withaminilide U (**21**) in $CDCl_3$

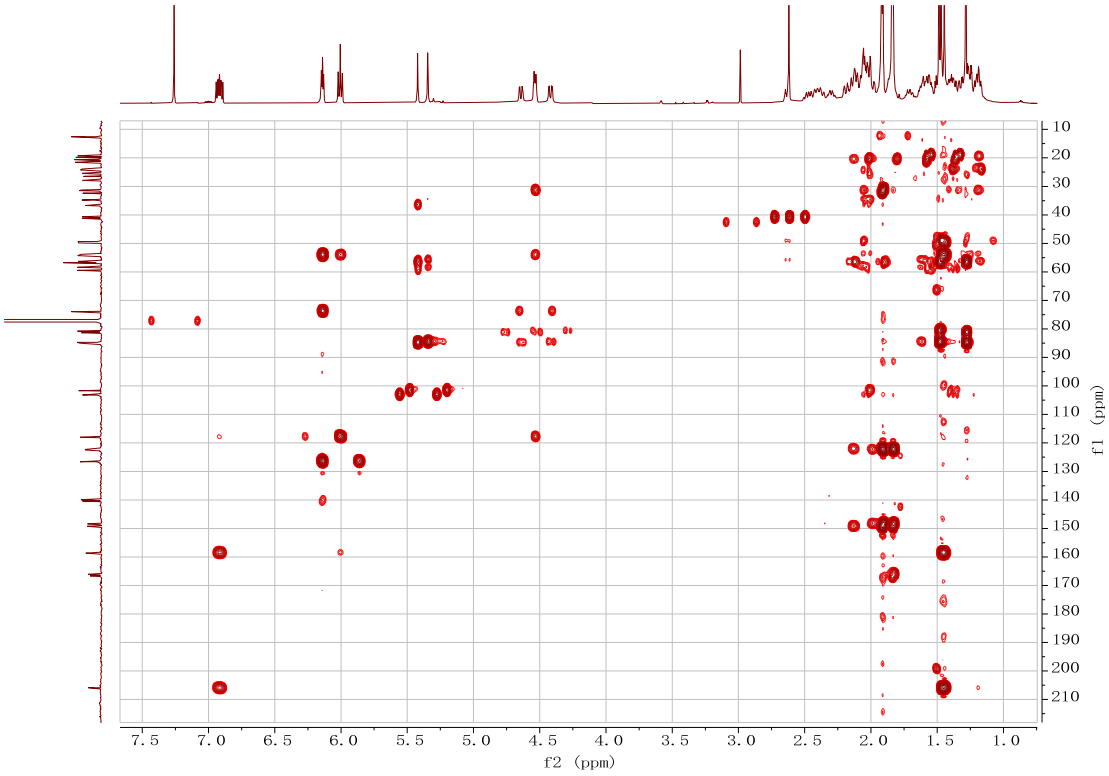


Figure S192. HMBC Spectrum of Withaminilide U (**21**) in $CDCl_3$

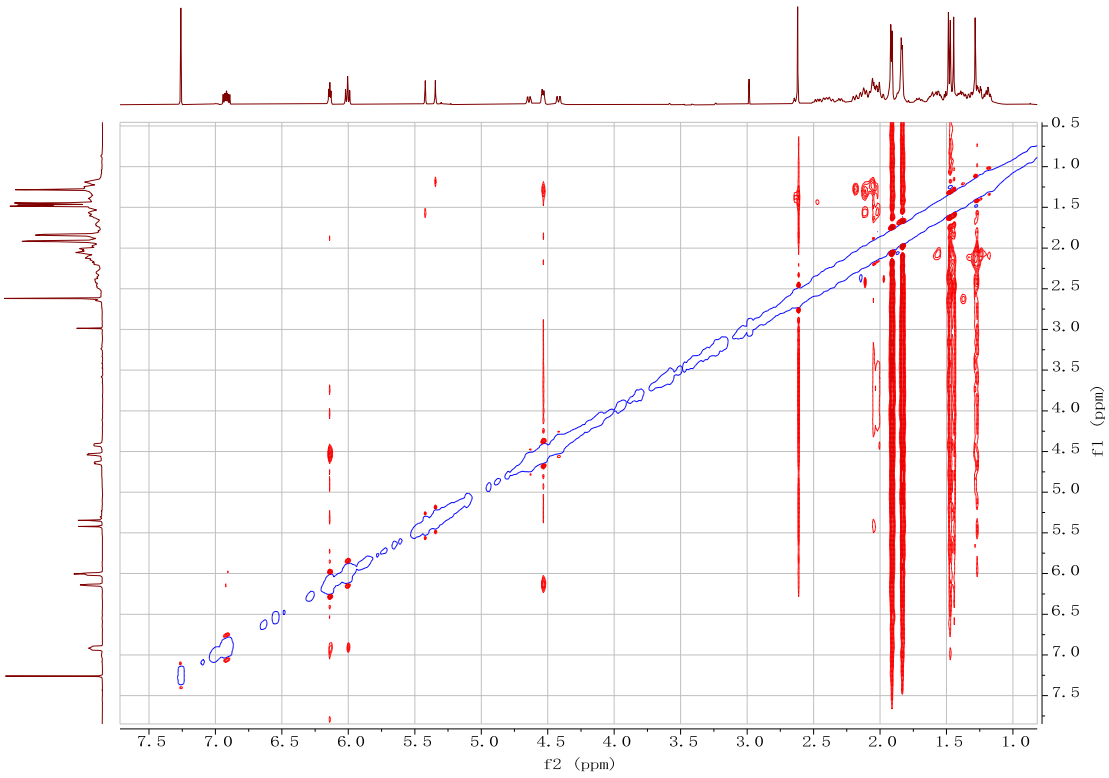


Figure S193. NOESY Spectrum of Withaminilide U (**21**) in $CDCl_3$

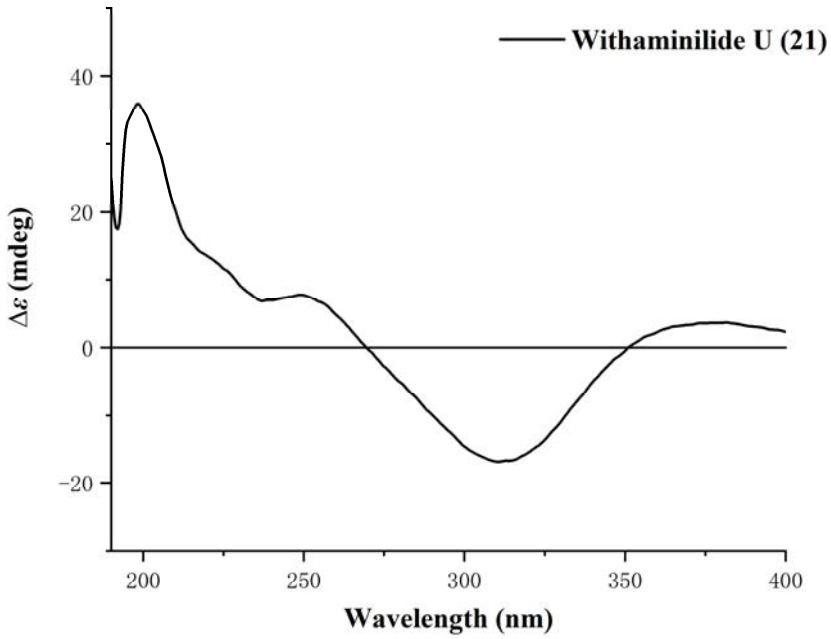


Figure S194. Experimental ECD Spectrum of Withaminilide U (**21**)

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

1080 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

Minimum:	80.00					-1.5		
Maximum:	100.00			3.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
529.2455	529.2438	1.7	3.2	11.5	709.3	n/a	n/a	C29H37O9

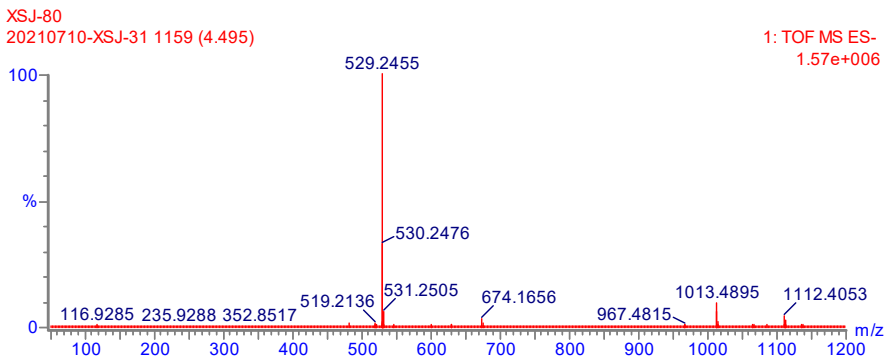


Figure S195. HRESIMS Spectrum of Withaminilide V (**22**)

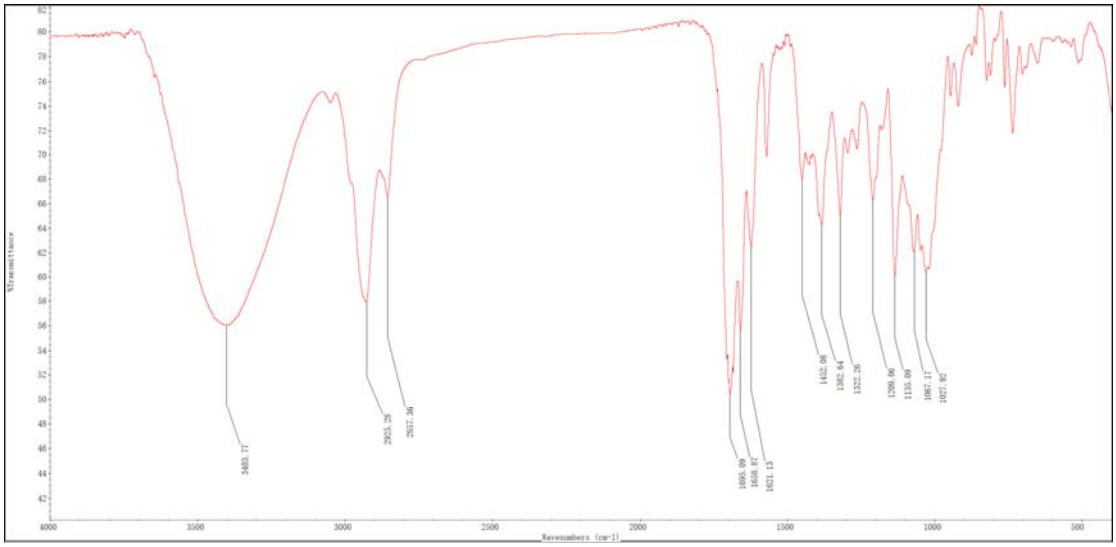


Figure S196. IR Spectrum of Withaminilide V (**22**)

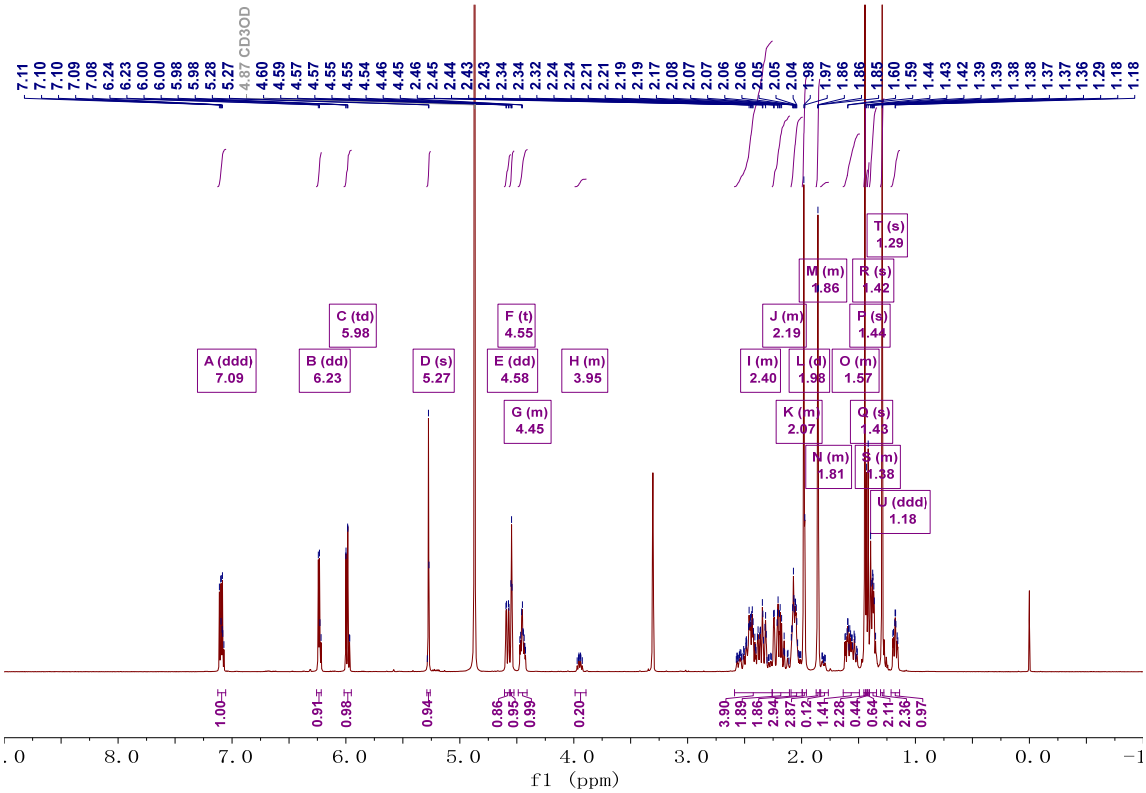


Figure S197. ^{1}H NMR Spectrum of Withaminilide V (**22**) in CD_3OD, 600 MHz

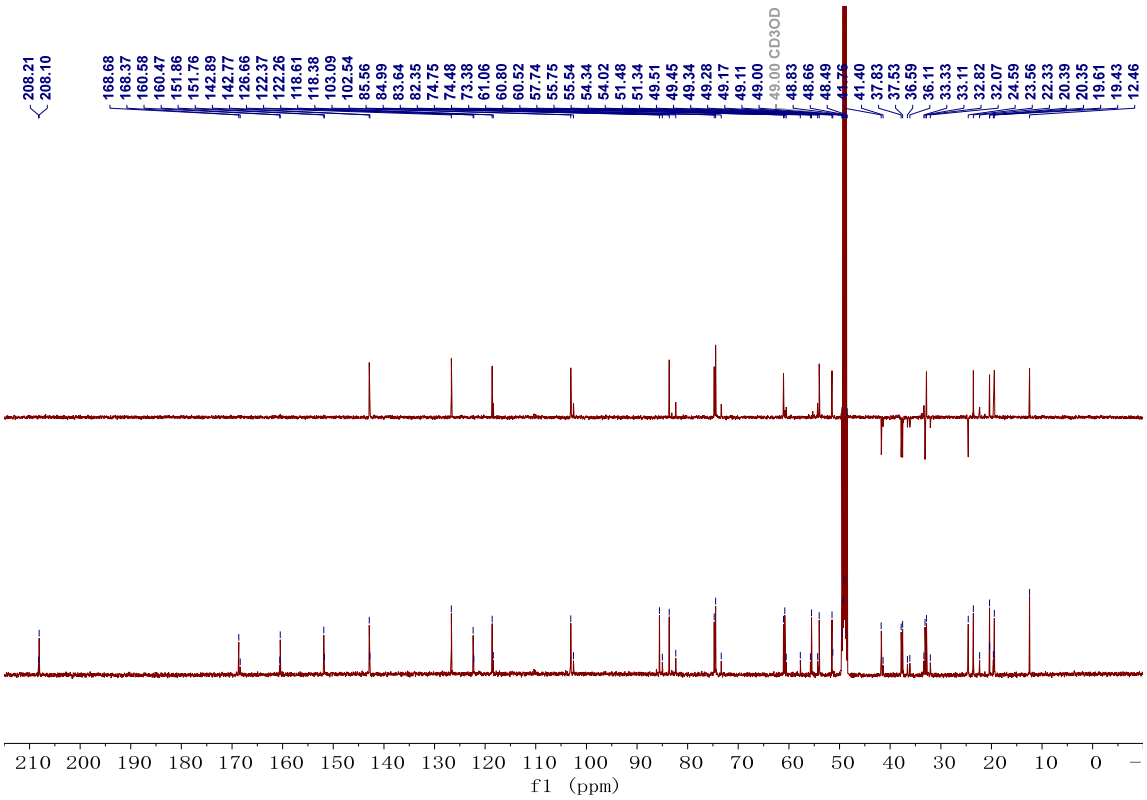


Figure S198. ^{13}C NMR Spectrum of Withaminilide V (**22**) in CD_3OD, 125 MHz

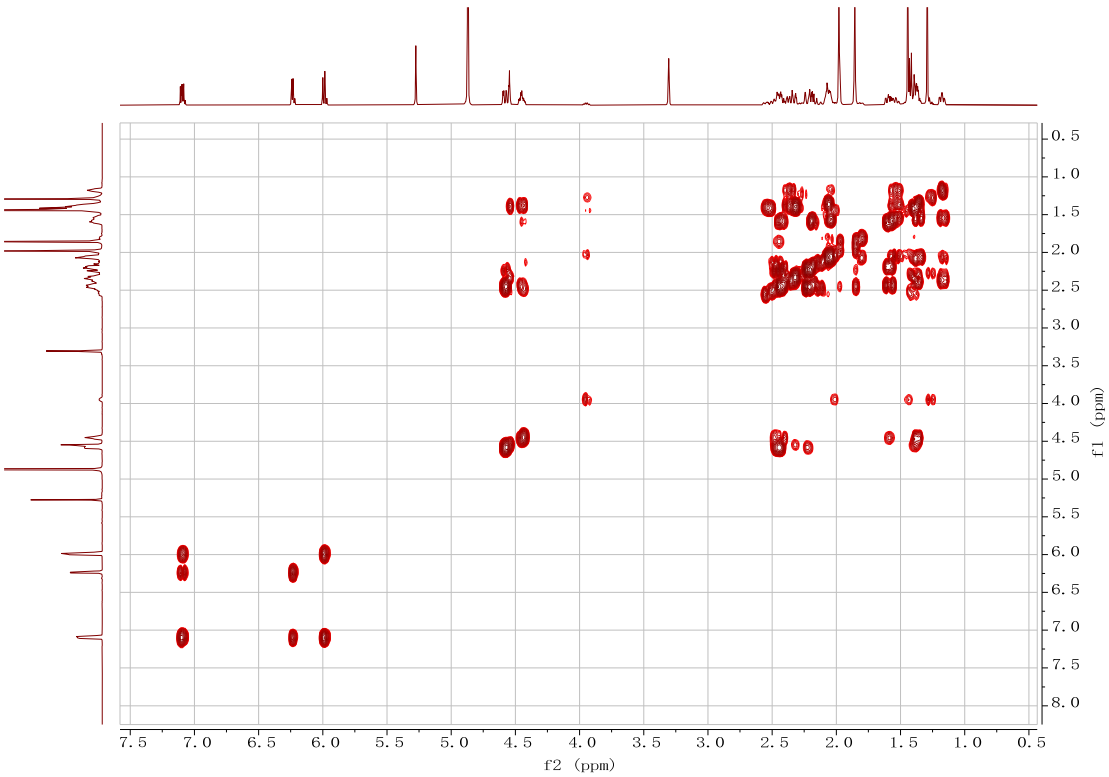


Figure S199. ^{1}H-^{1}H COSY Spectrum of Withaminilide V (**22**) in CD_3OD

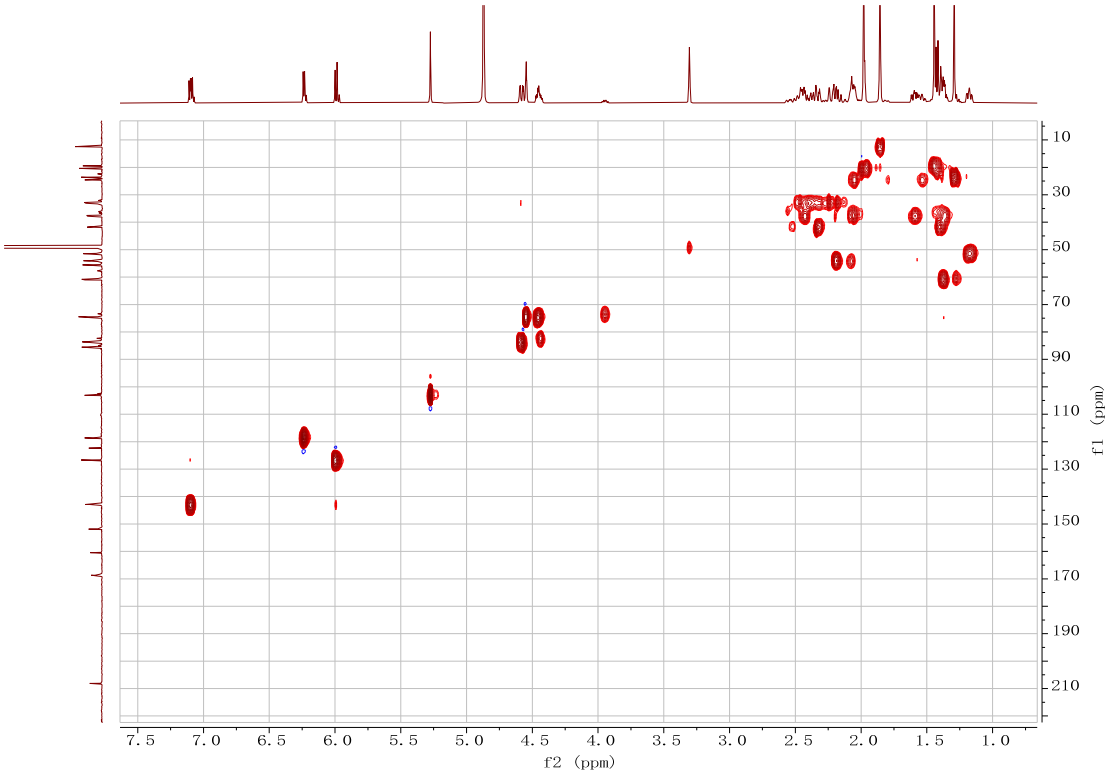


Figure S200. HSQC Spectrum of Withaminilide V (**22**) in CD_3OD

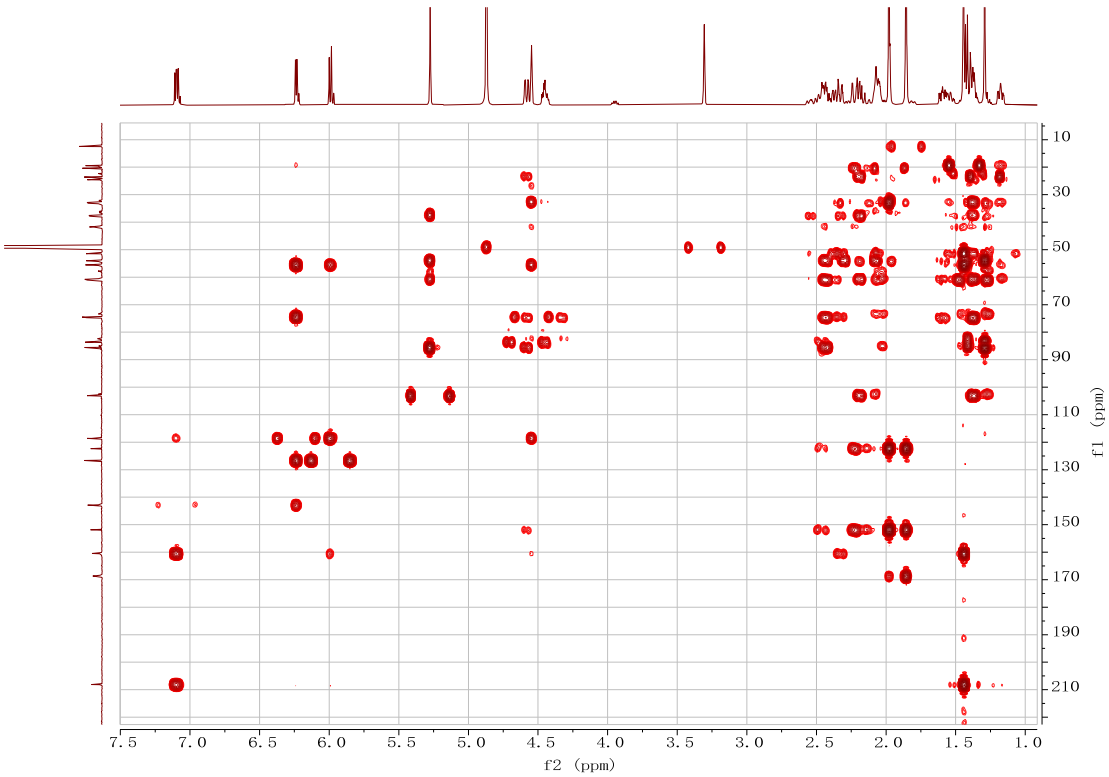


Figure S201.HMBC Spectrum of Withaminilide V (**22**) in CD_3OD

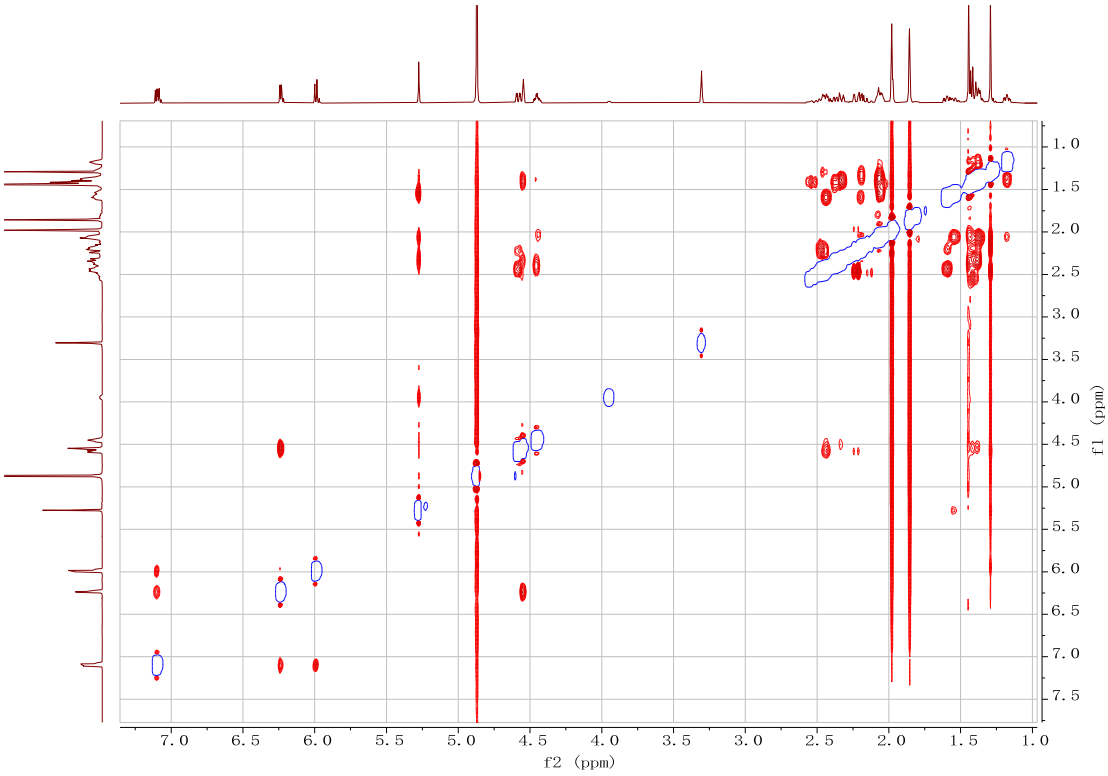


Figure S202. NOESY Spectrum of Withaminilide V (**22**) in CD_3OD

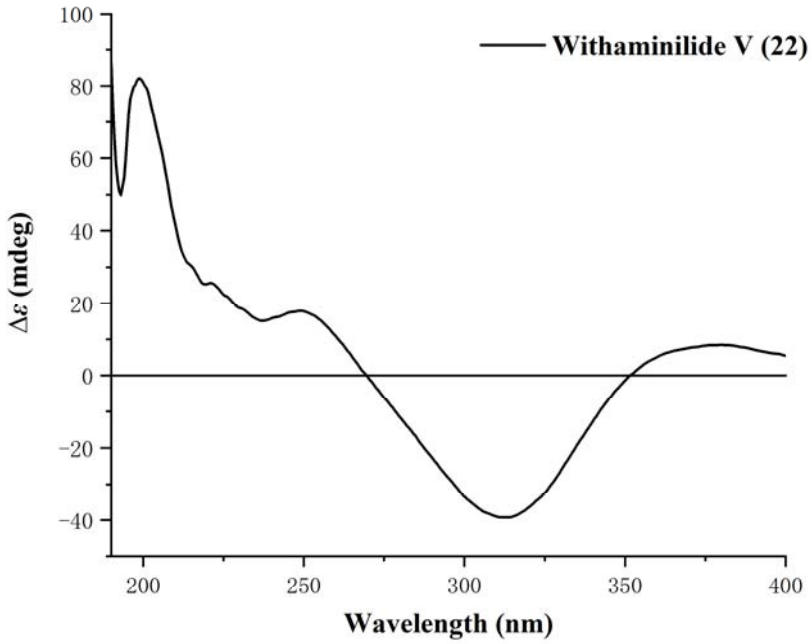


Figure S203. Experimental ECD Spectrum of Withaminilide V (**22**)

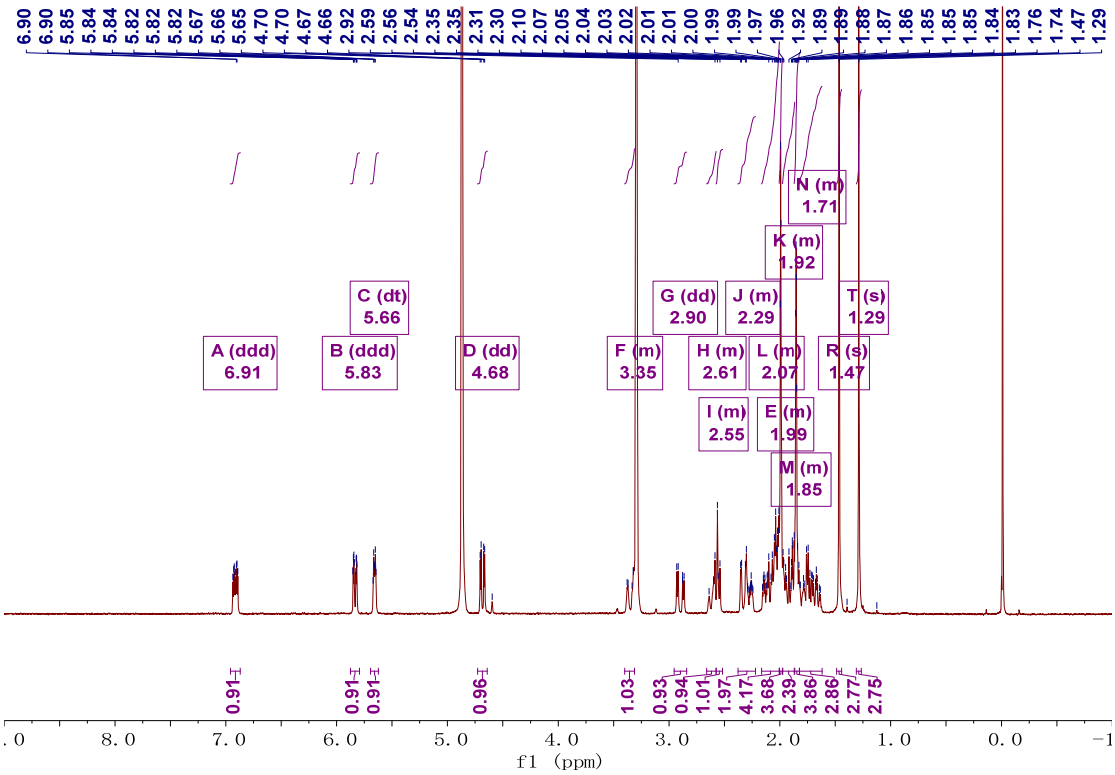


Figure S204. ^{1}H NMR Spectrum of Withaminilide F (**6**) in CD_3OD, 400 MHz

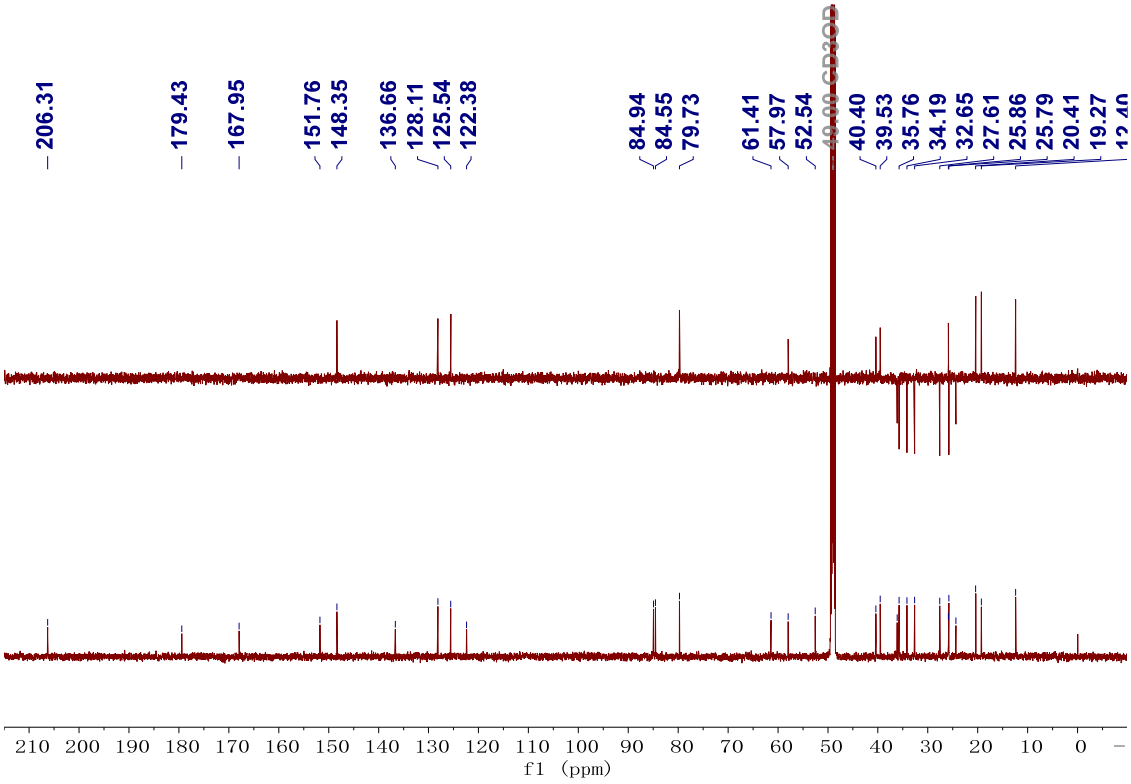


Figure S205. ^{13}C NMR Spectrum of Withaminilide F (**6**) in CD_3OD, 150 MHz

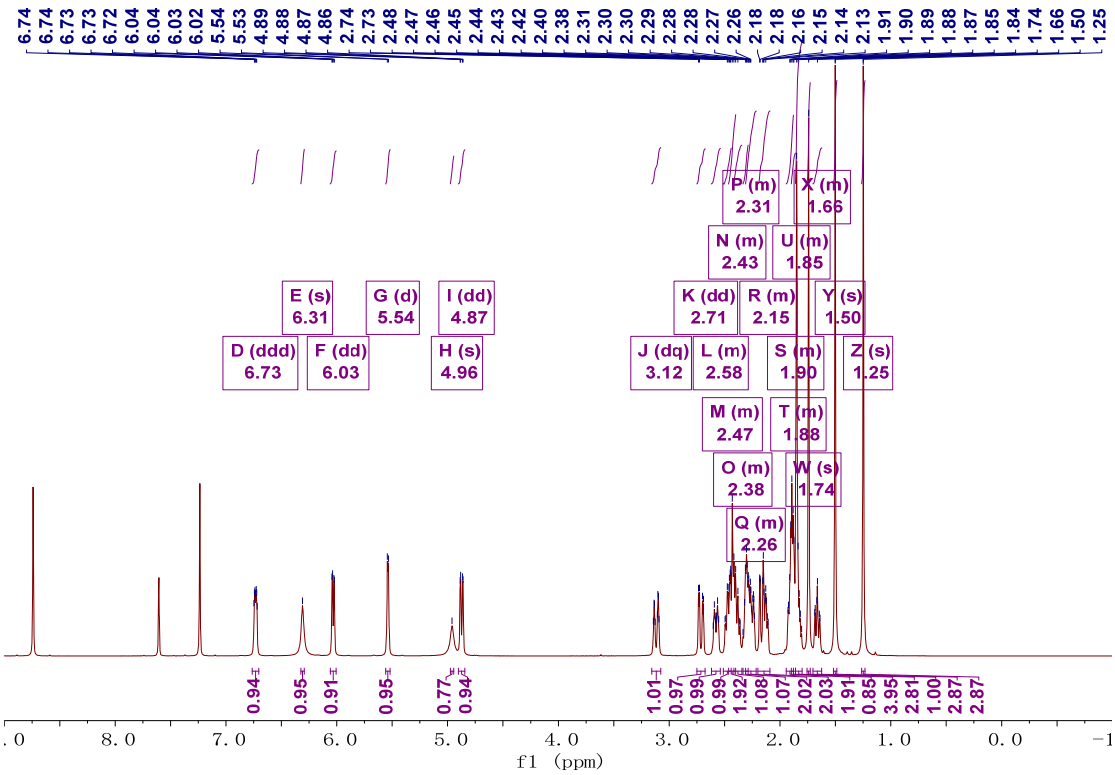


Figure S206. ^{1}H NMR Spectrum of Withaminilide F (**6**) in C_5D_5N, 600 MHz

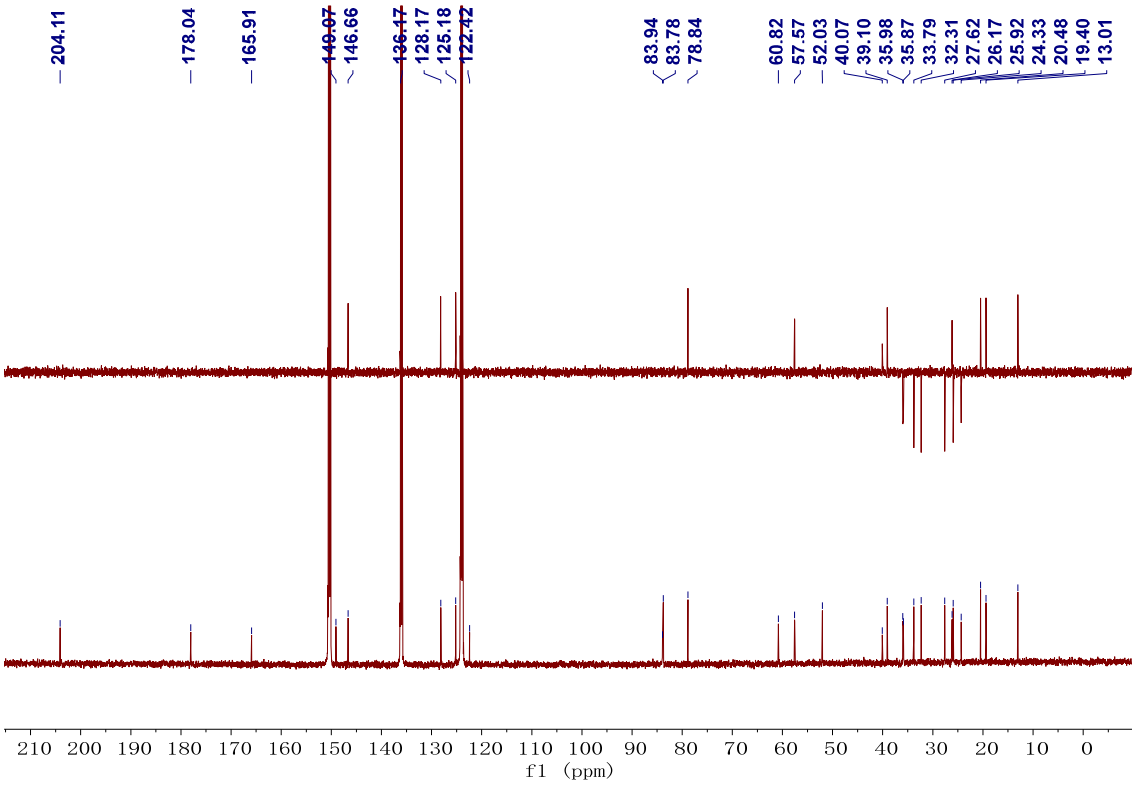


Figure S207. ^{13}C NMR Spectrum of Withaminilide F (**6**) in C_5D_5N, 150 MHz

^{1}H and ^{13}C NMR data of Withaminilide F (6) in CD_3OD

^{1}H NMR (400 MHz, CD_3OD) δ 6.91 (ddd, J = 10.0, 5.0, 2.8 Hz, 1H), 5.83 (ddd, J = 10.0, 2.8, 1.3 Hz, 1H), 5.66 (dt, J = 6.3, 2.1 Hz, 1H), 4.68 (dd, J = 12.9, 3.4 Hz, 1H), 3.40 – 3.31 (m, 1H), 2.90 (dd, J = 21.8, 5.0 Hz, 1H), 2.66 – 2.57 (m, 1H), 2.57 – 2.52 (m, 1H), 2.38 – 2.22 (m, 2H), 2.17 – 2.00 (m, 4H), 1.99 (s, 3H), 1.99 – 1.97 (m, 1H), 1.98 – 1.86 (m, 2H), 1.85 (s, 3H), 1.85 – 1.82 (m, 1H), 1.82 – 1.62 (m, 3H), 1.47 (s, 3H), 1.29 (s, 3H).

^{13}C NMR (150 MHz, CD_3OD) δ 206.3, 179.4, 167.9, 151.8, 148.3, 136.7, 128.1, 125.5, 122.4, 84.9, 84.6, 79.7, 61.4, 58.0, 52.5, 40.4, 39.5, 36.1, 35.8, 34.2, 32.7, 27.6, 25.9, 25.8, 24.4, 20.4, 19.3, 12.4.

^{1}H and ^{13}C NMR data of Withaminilide F (6) in C_5D_5N

^{1}H NMR (600 MHz, C_5D_5N) δ 6.73 (ddd, J = 10.0, 5.0, 2.7 Hz, 1H), 6.03 (dd, J = 10.0, 2.7 Hz, 1H), 5.54 (d, J = 6.0 Hz, 1H), 4.87 (dd, J = 13.0, 3.2 Hz, 1H), 3.12 (dq, J = 21.5, 2.7 Hz, 1H), 2.71 (dd, J = 21.5, 5.0 Hz, 1H), 2.62 – 2.54 (m, 1H), 2.51 – 2.44 (m, 1H), 2.46 – 2.40 (m, 2H), 2.42 – 2.34 (m, 1H), 2.33 – 2.29 (m, 1H), 2.31 – 2.22 (m, 2H), 2.20 – 2.09 (m, 2H), 1.94 – 1.88 (m, 2H), 1.90 – 1.86 (m, 1H), 1.85 (s, 3H), 1.85 – 1.80 (m, 1H), 1.74 (s, 3H), 1.70 – 1.62 (m, 1H), 1.50 (s, 3H), 1.25 (s, 3H).

^{13}C NMR (150 MHz, C_5D_5N) δ 204.1, 178.0, 165.9, 149.1, 146.7, 136.2, 128.2, 125.2, 122.4, 83.9, 83.8, 78.8, 60.8, 57.6, 52.0, 40.1, 39.1, 36.0, 35.9, 33.8, 32.3, 27.6, 26.2, 25.9, 24.3, 20.5, 19.4, 13.0.