

Supporting Information

Limonoids from *Aphanamixis polystachya* and Their Antifeedant Activity

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1. Key ROESY correlations of selected limonoids

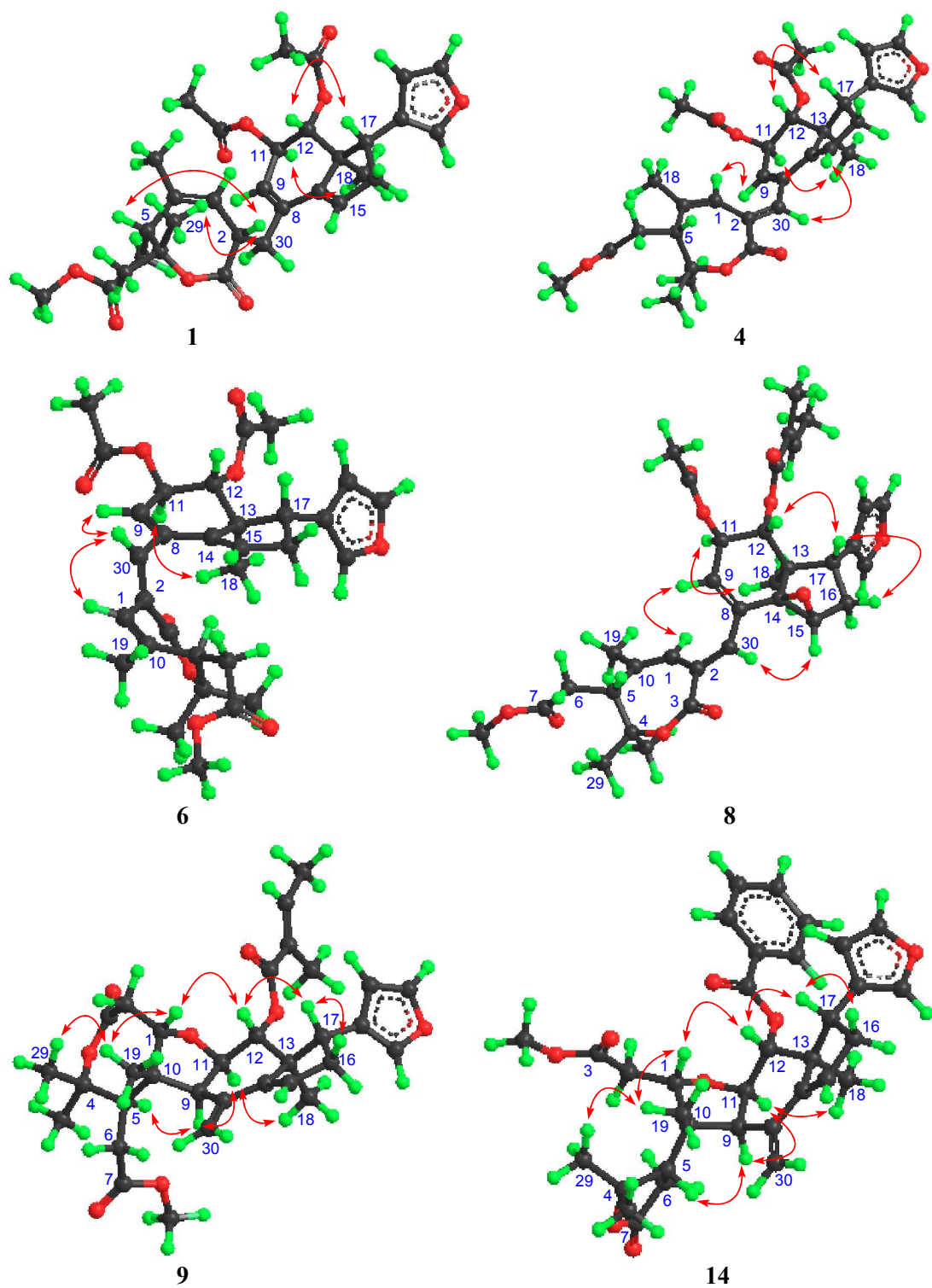


Figure S1. Key ROESY correlations ($\leftrightarrow$) of selected limonoids.

2. Antifeedant Activity Assay.

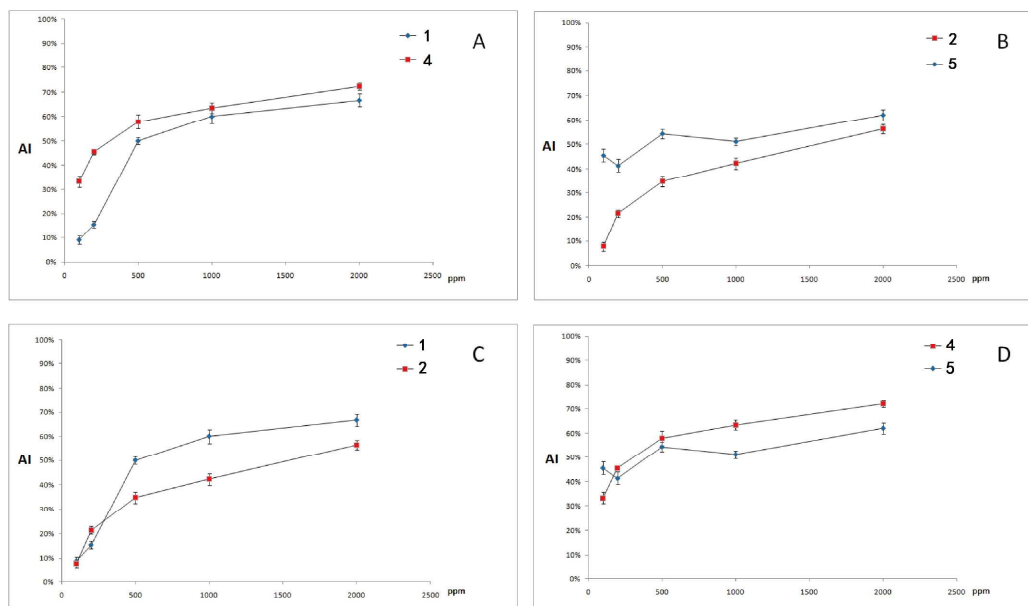


Figure S2. Comparison of antifeedant indices (AI) of selected compounds at concentrations of 100, 200, 500, 1000, and 2000 ppm.

Table S1. EC₅₀ (means ± SD) of Antifeedant Activity of 1, 2, 4, 5, 7, and neem oil against *Helicoverpa armigera*.

Compound	EC ₅₀ (μg/cm ²)	EC ₅₀ (μmol/cm ²)
aphanamixoid C (1)	9.27 ± 0.64	0.017 ± 0.0012
aphanamixoid D (2)	29.24 ± 2.25	0.049 ± 0.0038
aphanamixoid F (4)	4.28 ± 0.78	0.008 ± 0.0014
aphanamixoid G (5)	6.82 ± 0.49	0.012 ± 0.0008
aphanamixoid I (7)	16.94 ± 1.90	0.028 ± 0.0022
commercial neem oil	2.62 ± 0.10	

Table S2. Antifeedant Index (AI) of Selected Compounds against *Helicoverpa armigera*. at 2000 ppm.

Compounds	(AI $\pm$ SD) %
aphanamixoid E (3)	33.88 % $\pm$ 1.12 %
aphanamixoid J (8)	23.42 % $\pm$ 0.72 %
aphanamixoid K (9)	47.31 % $\pm$ 2.02%
aphanamixoid L (10)	23.39 % $\pm$ 5.07 %
aphanamixoid M (11)	34.02 % $\pm$ 1.25 %
aphanamixoid N (12)	11.11 % $\pm$ 3.37 %
aphanamixoid O (13)	42.80 % $\pm$ 1.98 %
aphanamixoid P (14)	28.62 % $\pm$ 4.11 %

3. NMR, MS and IR Spectra of aphanamixoids C-P (1-14)

Figure S3. ^1H NMR spectrum of aphanamixoid C (**1**) in CDCl_3

Figure S4. ^{13}C NMR spectrum of aphanamixoid C (**1**) in CDCl_3

Figure S5. HSQC spectrum of aphanamixoid C (**1**) in CDCl_3

Figure S6. HMBC spectrum of aphanamixoid C (**1**) in CDCl_3

Figure S7. ^1H - ^1H COSY spectrum of aphanamixoid C (**1**) in CDCl_3

Figure S8. ROESY spectrum of aphanamixoid C (**1**) in CDCl_3

Figure S9. ESI (+) MS of aphanamixoid C (**1**)

Figure S10. HR-EI (+) MS of aphanamixoid C (**1**)

Figure S11. IR spectrum of aphanamixoid C (**1**)

Figure S12. CD spectrum of aphanamixoid C (**1**)

Figure S13. ^1H NMR spectrum of aphanamixoid D (**2**) in CDCl_3

Figure S14. ^{13}C NMR spectrum of aphanamixoid D (**2**) in CDCl_3

Figure S15. HSQC spectrum of aphanamixoid D (**2**) in CDCl_3

Figure S16. HMBC spectrum of aphanamixoid D (**2**) in CDCl_3

Figure S17. ^1H - ^1H COSY spectrum of aphanamixoid D (**2**) in CDCl_3

Figure S18. ROESY spectrum of aphanamixoid D (**2**) in CDCl_3

Figure S19. ESI (+) MS of aphanamixoid D (**2**)

Figure S20. HR-EI (+) MS of aphanamixoid D (**2**)

Figure S21. IR spectrum of aphanamixoid D (**2**)

Figure S22. CD spectrum of aphanamixoid D (**2**)

Figure S23. ^1H NMR spectrum of aphanamixoid E (**3**) in CDCl_3

Figure S24. ^{13}C NMR spectrum of aphanamixoid E (**3**) in CDCl_3

Figure S25. HSQC spectrum of aphanamixoid E (**3**) in CDCl_3

Figure S26. HMBC spectrum of aphanamixoid E (**3**) in CDCl_3

Figure S27. ^1H - ^1H COSY spectrum of aphanamixoid E (**3**) in CDCl_3

Figure S28. ROESY spectrum of aphanamixoid E (**3**) in CDCl_3

Figure S29. ESI (+) MS of aphanamixoid E (**3**)

Figure S30. HR-EI (+) MS of aphanamixoid E (**3**)

Figure S31. IR spectrum of aphanamixoid E (**3**)

Figure S32. CD spectrum of aphanamixoid E (**3**)

Figure S33. ^1H NMR spectrum of aphanamixoid F (**4**) in CDCl_3

Figure S34. ^{13}C NMR spectrum of aphanamixoid F (**4**) in CDCl_3

Figure S35. HSQC spectrum of aphanamixoid F (**4**) in CDCl_3

Figure S36. HMBC spectrum of aphanamixoid F (**4**) in CDCl_3

Figure S37. ^1H - ^1H COSY spectrum of aphanamixoid F (**4**) in CDCl_3

Figure S38. ROESY spectrum of aphanamixoid F (**4**) in CDCl_3

Figure S39. ESI (+) MS of aphanamixoid F (**4**)

Figure S40. HR-EI (+) MS of aphanamixoid F (**4**)

Figure S41. IR spectrum of aphanamixoid F (**4**)

Figure S42. CD spectrum of aphanamixoid F (**4**)

Figure S43. ^1H NMR spectrum of aphanamixoid G (**5**) in CDCl_3

Figure S44. ^{13}C NMR spectrum of aphanamixoid G (**5**) in CDCl_3

Figure S45. HSQC spectrum of aphanamixoid G (**5**) in CDCl_3

Figure S46. HMBC spectrum of aphanamixoid G (**5**) in CDCl_3

Figure S47. ^1H - ^1H COSY spectrum of aphanamixoid G (**5**) in CDCl_3

Figure S48. ROESY spectrum of aphanamixoid G (**5**) in CDCl_3

Figure S49. ESI (+) MS of aphanamixoid G (**5**)

Figure S50. HR-EI (+) MS of aphanamixoid G (**5**)

Figure S51. IR spectrum of aphanamixoid G (**5**)

Figure S52. CD spectrum of aphanamixoid G (**5**)

Figure S53. ^1H NMR spectrum of aphanamixoid H (**6**) in CDCl_3

Figure S54. ^{13}C NMR spectrum of aphanamixoid H (**6**) in CDCl_3

Figure S55. HSQC spectrum of aphanamixoid H (**6**) in CDCl_3

Figure S56. HMBC spectrum of aphanamixoid H (**6**) in CDCl_3

Figure S57. ^1H - ^1H COSY spectrum of aphanamixoid H (**6**) in CDCl_3

Figure S58. ROESY spectrum of aphanamixoid H (**6**) in CDCl_3

Figure S59. ESI (+) MS of aphanamixoid H (**6**)

Figure S60. HR-EI (+) MS of aphanamixoid H (**6**)

Figure S61. IR spectrum of aphanamixoid H (**6**)

Figure S62. CD spectrum of aphanamixoid H (**6**)

Figure S63. ^1H NMR spectrum of aphanamixoid I (**7**) in CDCl_3

Figure S64. ^{13}C NMR spectrum of aphanamixoid I (**7**) in CDCl_3

Figure S65. HSQC spectrum of aphanamixoid I (**7**) in CDCl_3

Figure S66. HMBC spectrum of aphanamixoid I (**7**) in CDCl_3

Figure S67. ^1H - ^1H COSY spectrum of aphanamixoid I (**7**) in CDCl_3

Figure S68. ROESY spectrum of aphanamixoid I (**7**) in CDCl_3

Figure S69. ESI (+) MS of aphanamixoid I (**7**)

Figure S70. HR-EI (+) MS of aphanamixoid I (**7**)

Figure S71. IR spectrum of aphanamixoid I (**7**)

Figure S72. CD spectrum of aphanamixoid I (**7**)

Figure S73. ^1H NMR spectrum of aphanamixoid J (**8**) in CDCl_3

Figure S74. ^{13}C NMR spectrum of aphanamixoid J (**8**) in CDCl_3

Figure S75. HSQC spectrum of aphanamixoid J (**8**) in CDCl_3

Figure S76. HMBC spectrum of aphanamixoid J (**8**) in CDCl_3

Figure S77. ^1H - ^1H COSY spectrum of aphanamixoid J (**8**) in CDCl_3

Figure S78. ROESY spectrum of aphanamixoid J (**8**) in CDCl_3

Figure S79. ESI (+) MS of aphanamixoid J (**8**)

Figure S80. HR-EI (+) MS of aphanamixoid J (**8**)

Figure S81. IR spectrum of aphanamixoid J (**8**)

Figure S82. CD spectrum of aphanamixoid J (**8**)

Figure S83. ^1H NMR spectrum of aphanamixoid K (**9**) in CDCl_3

Figure S84. ^{13}C NMR spectrum of aphanamixoid K (**9**) in CDCl_3

Figure S85. HSQC spectrum of aphanamixoid K (**9**) in CDCl_3

Figure S86. HMBC spectrum of aphanamixoid K (**9**) in CDCl_3

Figure S87. ^1H - ^1H COSY spectrum of aphanamixoid K (**9**) in CDCl_3

Figure S88. ROESY spectrum of aphanamixoid K (**9**) in CDCl_3

Figure S89. ESI (+) MS of aphanamixoid K (**9**)

Figure S90. HR-EI (+) MS of aphanamixoid K (**9**)

Figure S91. IR spectrum of aphanamixoid K (**9**)

Figure S92. CD spectrum of aphanamixoid K (**9**)

Figure S93. ^1H NMR spectrum of aphanamixoid L (**10**) in CDCl_3

Figure S94. ^{13}C NMR spectrum of aphanamixoid L (**10**) in CDCl_3

Figure S95. HSQC spectrum of aphanamixoid L (**10**) in CDCl_3

Figure S96. HMBC spectrum of aphanamixoid L (**10**) in CDCl_3

Figure S97. ^1H - ^1H COSY spectrum of aphanamixoid L (**10**) in CDCl_3

Figure S98. ROESY spectrum of aphanamixoid L (**10**) in CDCl_3

Figure S99. ESI (+) MS of aphanamixoid L (**10**)

Figure S100. HR-EI (+) MS of aphanamixoid L (**10**)

Figure S101. IR spectrum of aphanamixoid L (**10**)

Figure S102. CD spectrum of aphanamixoid L (**10**)

Figure S103. ^1H NMR spectrum of aphanamixoid M (**11**) in CDCl_3

Figure S104. ^{13}C NMR spectrum of aphanamixoid M (**11**) in CDCl_3

Figure S105. HSQC spectrum of aphanamixoid M (**11**) in CDCl_3

Figure S106. HMBC spectrum of aphanamixoid M (**11**) in CDCl_3

Figure S107. ^1H - ^1H COSY spectrum of aphanamixoid M (**11**) in CDCl_3

Figure S108. ROESY spectrum of aphanamixoid M (**11**) in CDCl_3

Figure S109. ESI (+) MS of aphanamixoid M (**11**)

Figure S110. HR-EI (+) MS of aphanamixoid M (**11**)

Figure S111. IR spectrum of aphanamixoid M (**11**)

Figure S112. CD spectrum of aphanamixoid M (**11**)

Figure S113. ^1H NMR spectrum of aphanamixoid N (**12**) in CDCl_3

Figure S114. ^{13}C NMR spectrum of aphanamixoid N (**12**) in CDCl_3

Figure S115. HSQC spectrum of aphanamixoid N (**12**) in CDCl_3

Figure S116. HMBC spectrum of aphanamixoid N (**12**) in CDCl_3

Figure S117. ^1H - ^1H COSY spectrum of aphanamixoid N (**12**) in CDCl_3

Figure S118. ROESY spectrum of aphanamixoid N (**12**) in CDCl_3

Figure S119. ESI (+) MS of aphanamixoid N (**12**)

Figure S120. HR-ESI (+) MS of aphanamixoid N (**12**)

Figure S121. IR spectrum of aphanamixoid N (**12**)

Figure S122. CD spectrum of aphanamixoid N (**12**)

Figure S123. ^1H NMR spectrum of aphanamixoid O (**13**) in CDCl_3

Figure S124. ^{13}C NMR spectrum of aphanamixoid O (**13**) in CDCl_3

Figure S125. HSQC spectrum of aphanamixoid O (**13**) in CDCl_3

Figure S126. HMBC spectrum of aphanamixoid O (**13**) in CDCl_3

Figure S127. ^1H - ^1H COSY spectrum of aphanamixoid O (**13**) in CDCl_3

Figure S128. ROESY spectrum of aphanamixoid O (**13**) in CDCl_3

Figure S129. ESI (+) MS of aphanamixoid O (**13**)

Figure S130. HR-EI (+) MS of aphanamixoid O (**13**)

Figure S131. IR spectrum of aphanamixoid O (**13**)

Figure S132. CD spectrum of aphanamixoid O (**13**)

Figure S133. ^1H NMR spectrum of aphanamixoid P (**14**) in CDCl_3

Figure S134. ^{13}C NMR spectrum of aphanamixoid P (**14**) in CDCl_3

Figure S135. HSQC spectrum of aphanamixoid P (**14**) in CDCl_3

Figure S136. HMBC spectrum of aphanamixoid P (**14**) in CDCl_3

Figure S137. ^1H - ^1H COSY spectrum of aphanamixoid P (**14**) in CDCl_3

Figure S138. ROESY spectrum of aphanamixoid P (**14**) in CDCl_3

Figure S139. ESI (+) MS of aphanamixoid P (**14**)

Figure S140. HR-ESI (+) MS of aphanamixoid P (**14**)

Figure S141. IR spectrum of aphanamixoid P (**14**)

Figure S142. CD spectrum of aphanamixoid P (**14**)

Chemical structure of compound 10 is shown above the ¹H NMR spectrum. The spectrum displays peaks corresponding to the structure, with chemical shifts (ppm) listed on the x-axis and integration values on the y-axis.

¹H NMR peaks (ppm): 7.3477, 7.2626, 7.2094, 6.2995, 5.8001, 5.5797, 5.5594, 5.3795, 5.2933, 5.2715, 5.1619, 3.7045, 3.2759, 3.2533, 2.9863, 2.9798, 2.8305, 2.7888, 2.7663, 2.6168, 2.5884, 2.5576, 2.4029, 2.3800, 2.2568, 2.2478, 2.2145, 2.2058, 2.0405, 1.8355, 1.7837, 1.6188, 1.3658, 1.0196.

Integration values: 1.02, 1.06, 1.08, 1.00, 1.05, 1.00, 0.98, 3.30, 1.04, 1.04, 1.04, 1.02, 1.04, 3.27, 2.99, 3.17, 3.02, 3.04, 2.98.

Chemical structure of compound 10 is shown above the spectra. The ^1H NMR spectrum (top) and ^{13}C NMR spectrum (bottom) are displayed, with peak assignments in ppm.

^1H NMR (400 MHz, CDCl_3) peaks (ppm): 8.163, 7.852, 7.731, 7.667, 7.256, 5.212, 5.112, 4.777, 4.548, 4.377, 3.833, 3.439, 3.391, 2.870, 2.580, 2.550, 2.108, 2.098, 1.432.

^{13}C NMR (100 MHz, CDCl_3) peaks (ppm): 173.35, 172.39, 170.90, 170.88, 146.39, 142.34, 139.98, 138.24, 133.38, 124.20, 124.16, 123.80, 119.74, 111.15.

Figure S5. HSQC spectrum of aphanamixoid C (**1**) in CDCl₃

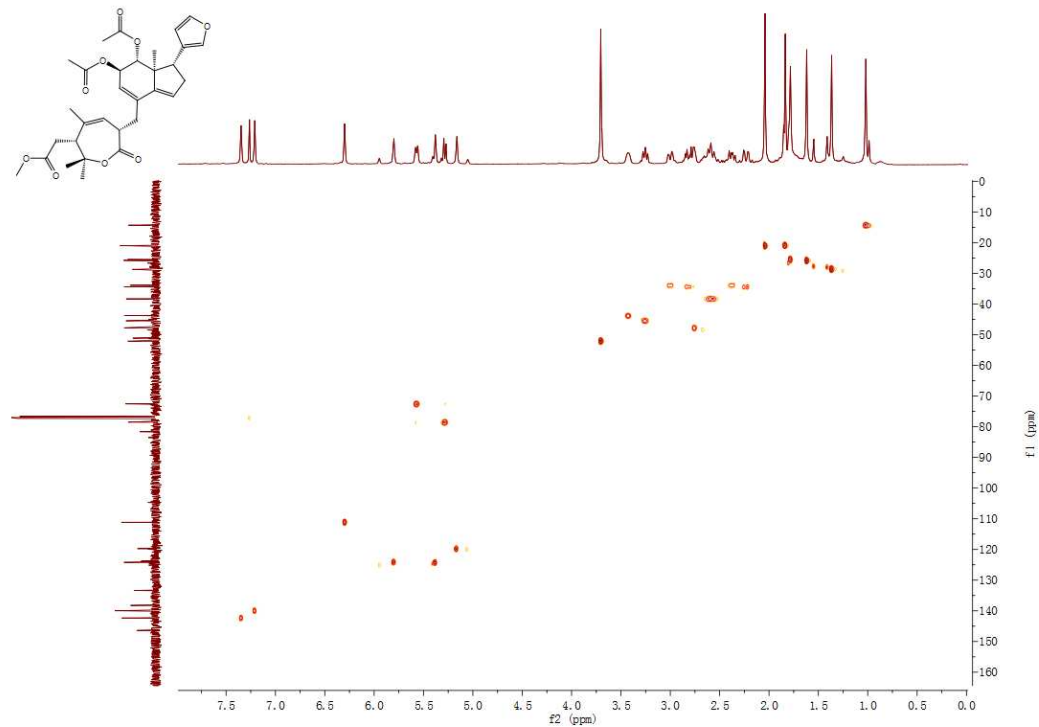


Figure S6. HMBC spectrum of aphanamixoid C (**1**) in CDCl₃

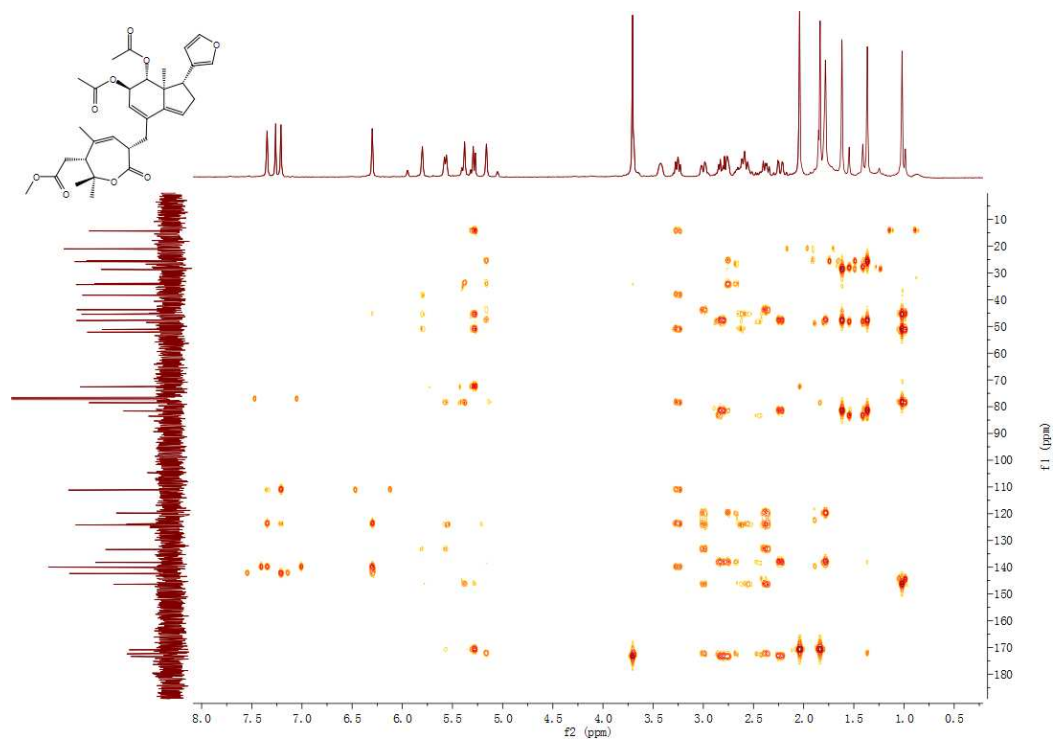


Figure S7. ^1H - ^1H COSY spectrum of aphanamixoid C (**1**) in CDCl_3

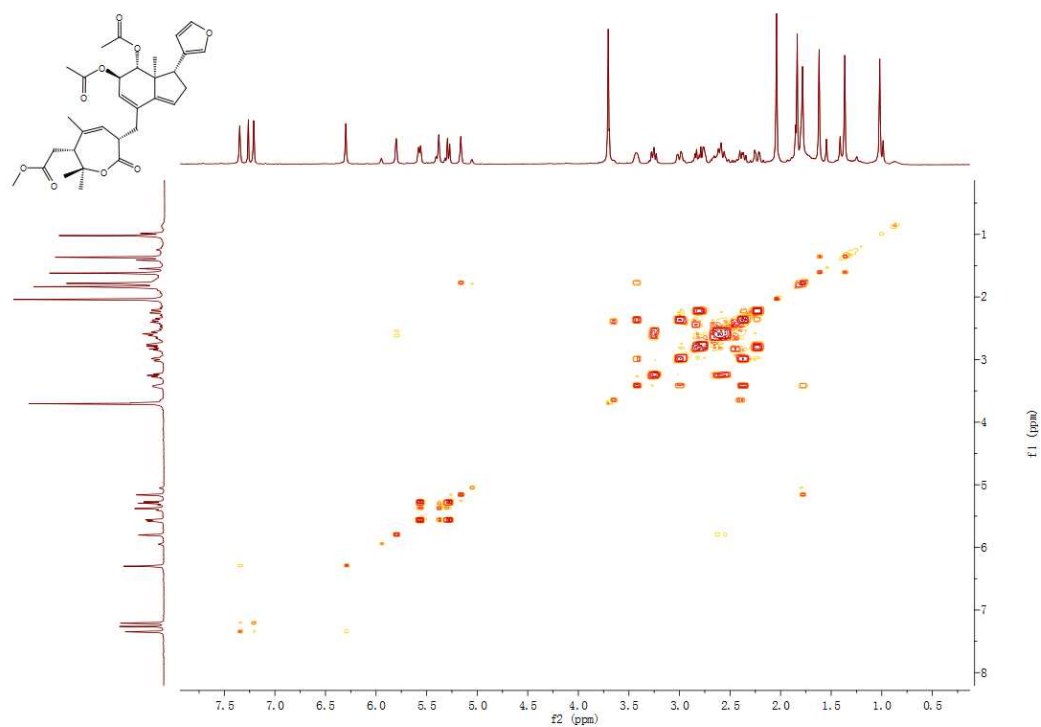


Figure S8. ROESY spectrum of aphanamixoid C (**1**) in CDCl_3

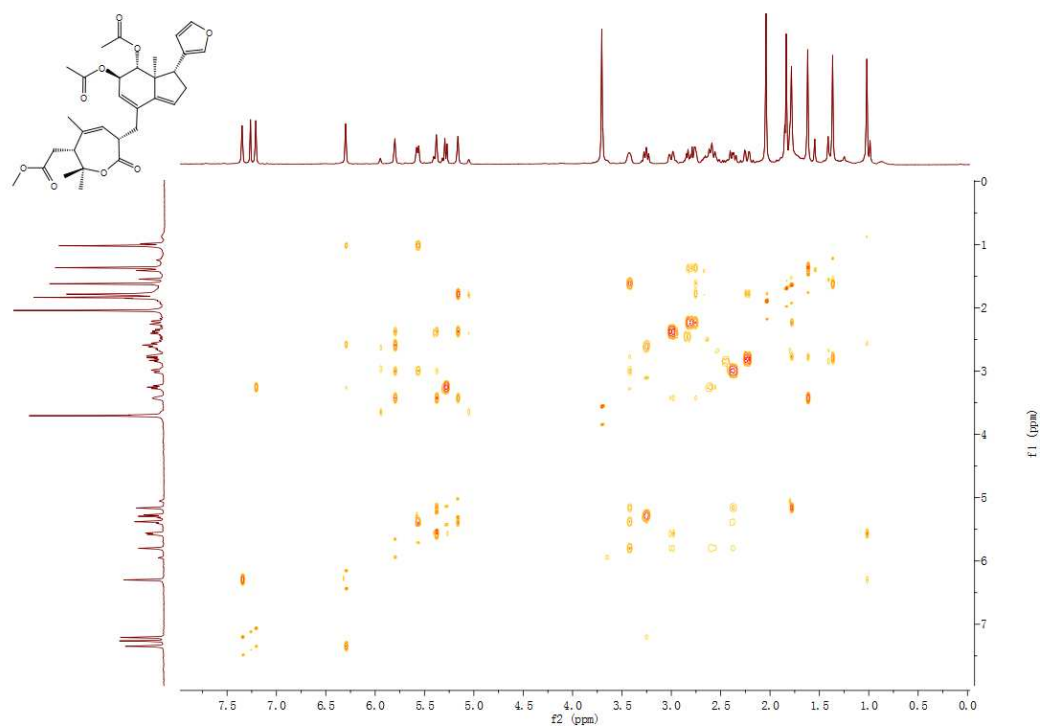


Figure S9. ESI (+) MS of aphanamixoid C (1)

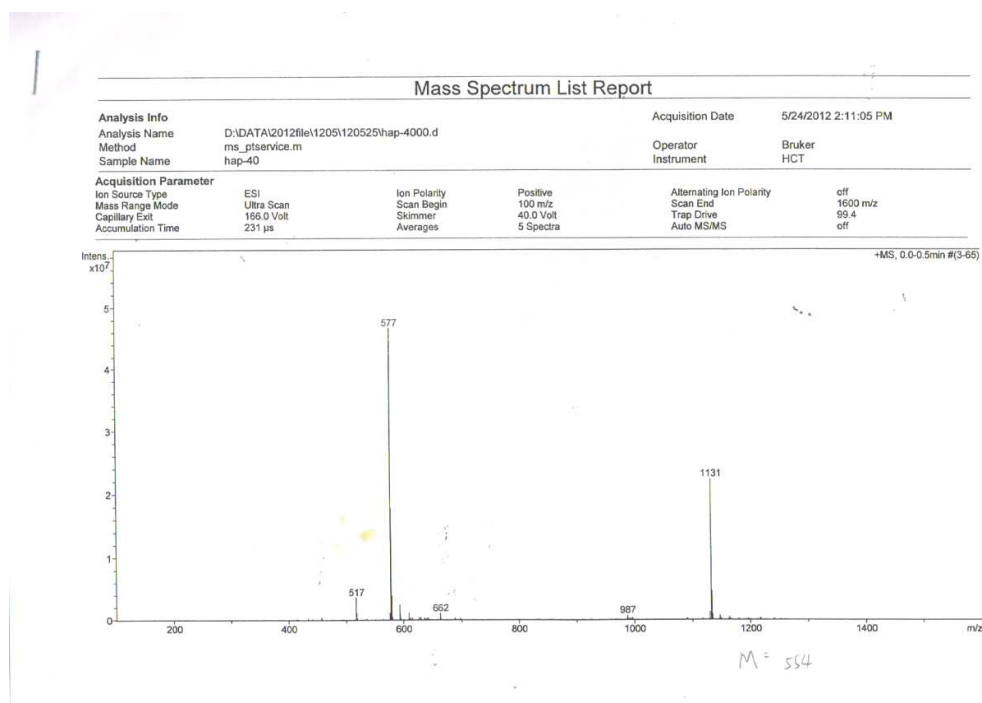


Figure S10. HR-EI (+) MS of aphanamixoid C (1)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

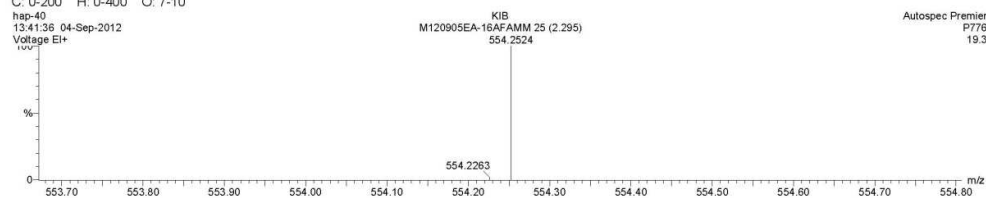
Monoisotopic Mass, Odd and Even Electron Ions
27 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 7-10

hap-40
13.4136 04-Sep-2012

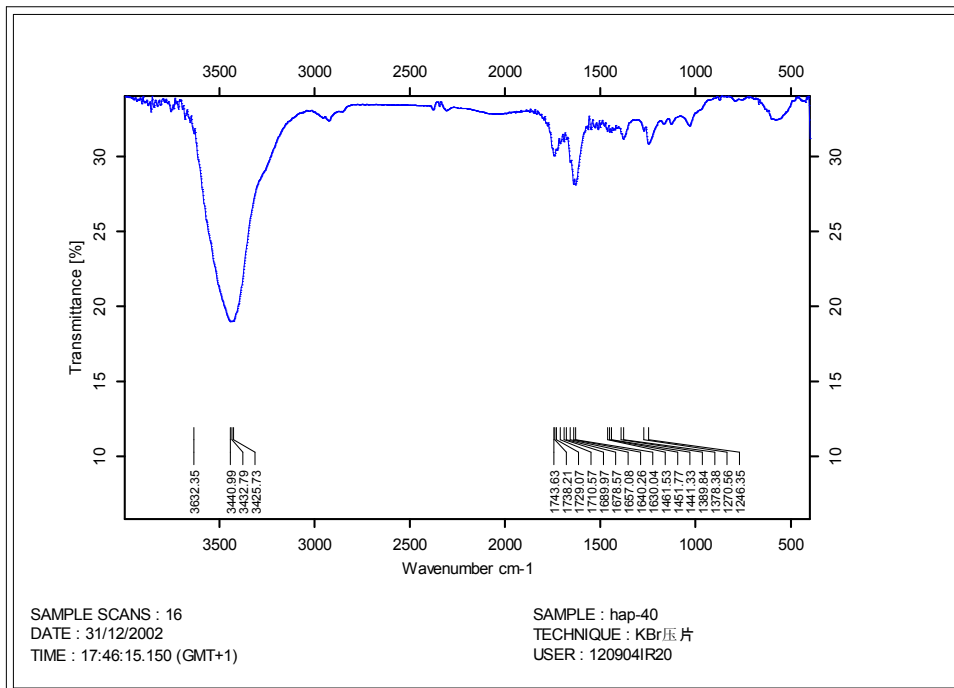
Voltage EI+



Autospec Premier
P776
19.3

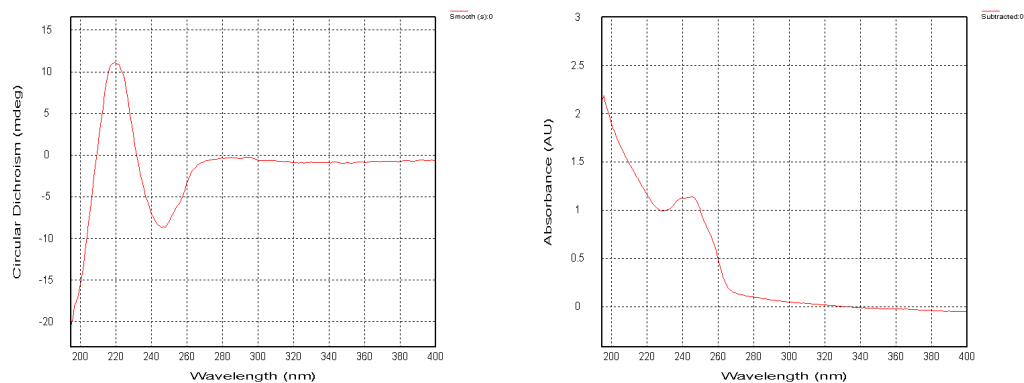
Minimum:						
Maximum:	100.0	10.0	-10.0			
			120.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
554.2524	554.2516	0.8	1.4	13.0	5546030.0	C31 H38 O9

Figure S11. IR spectrum of aphanamixoid C (1)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
571.308	0.325	0.000	10.890	0.055561	0
582.080	0.324	0.016	6.882	10.600125	0
595.647	0.325	0.000	2.866	0.027225	0
601.144	0.325	0.000	14.658	0.025282	0
1031.659	0.320	0.010	37.227	4.514119	0
1127.776	0.321	0.004	19.036	2.534488	0
1166.800	0.322	0.003	21.051	1.442146	0
1246.353	0.308	0.025	34.417	12.514580	0
1270.561	0.317	0.004	12.342	1.859111	0
1378.383	0.311	0.014	21.712	8.717895	0
1389.836	0.315	0.000	2.536	0.120045	0
1401.204	0.319	0.000	3.386	0.047054	0
1413.770	0.319	0.002	7.823	0.783524	0
1424.193	0.318	0.002	5.896	0.440601	0
1432.492	0.317	0.002	3.686	1.388746	0
1441.330	0.316	0.006	5.589	3.138639	0
1451.768	0.316	0.003	5.085	1.425767	0
1461.529	0.317	0.005	4.249	2.898410	0
1548.192	0.318	0.008	11.522	4.483424	0
1564.482	0.318	0.005	5.809	1.600342	0
1572.714	0.319	0.001	3.414	0.374828	0
1630.044	0.281	0.057	22.022	36.895111	0
1640.264	0.281	0.004	8.456	2.383668	0
1657.075	0.296	0.002	5.580	1.329953	0
1678.567	0.311	0.003	4.812	1.095019	0
1689.965	0.310	0.006	7.349	3.259378	0
1710.566	0.308	0.004	11.229	2.273934	0
1729.066	0.304	0.002	11.876	0.512838	0
1738.213	0.300	0.017	3.915	10.312168	0
1743.628	0.300	0.001	16.029	0.303920	0
1776.453	0.320	0.002	4.619	1.523663	0
3425.729	0.190	0.000	36.987	0.057266	0
3432.794	0.190	0.000	3.793	0.086663	0
3440.992	0.190	0.150	187.054	99.969803	0
3632.350	0.315	0.004	13.624	2.356106	0

Figure S12. CD spectrum of aphanamixoid C (**1**)



File: CD HAP-40-1mm(195-400)12090421.dsx

ProBinaryX

Attributes :

- Time Stamp :Tue Sep 04 16:43:04 2012

- File ID : {45850A3C-989D-4e80-8895-AF70D51BAFCF}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.6000mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Figure S13. ^1H NMR spectrum of aphanamixoid D (**2**) in CDCl_3

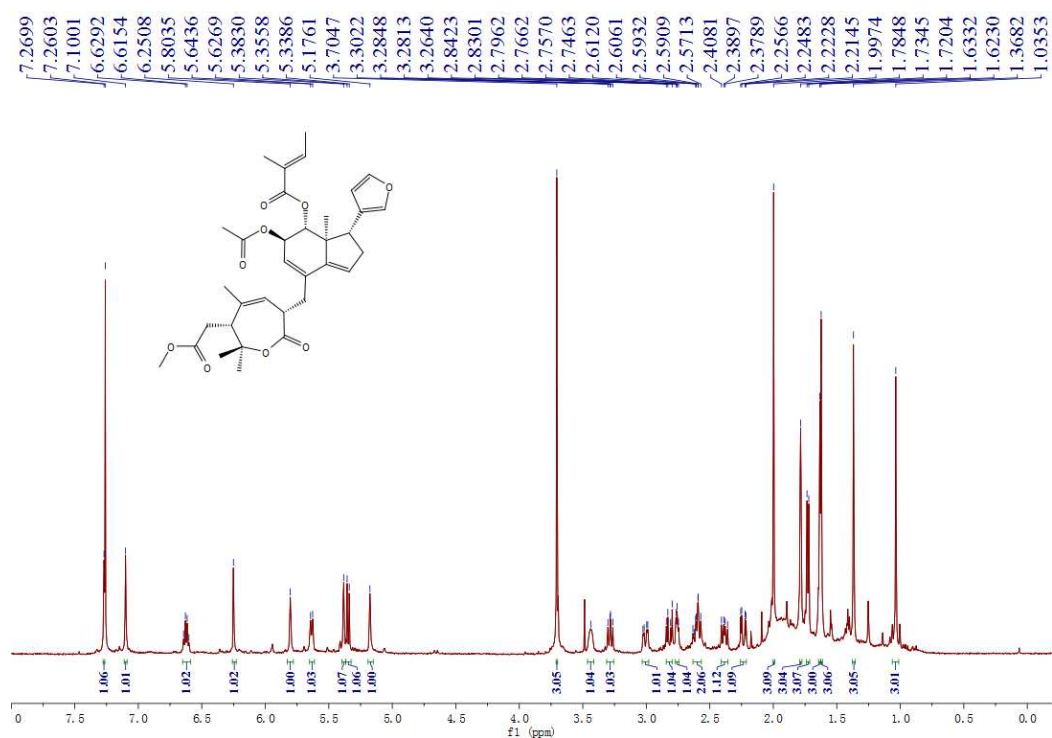


Figure S14. ^{13}C NMR spectrum of aphanamixoid D (**2**) in CDCl_3

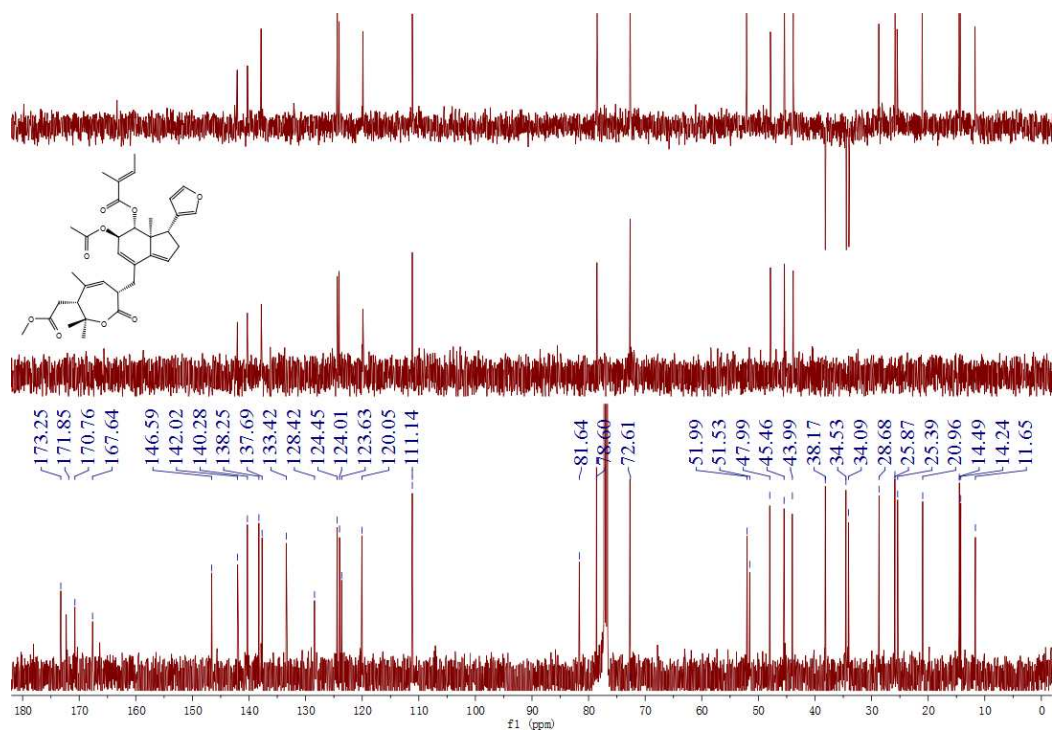


Figure S15. HSQC spectrum of aphanamixoid D (**2**) in CDCl₃

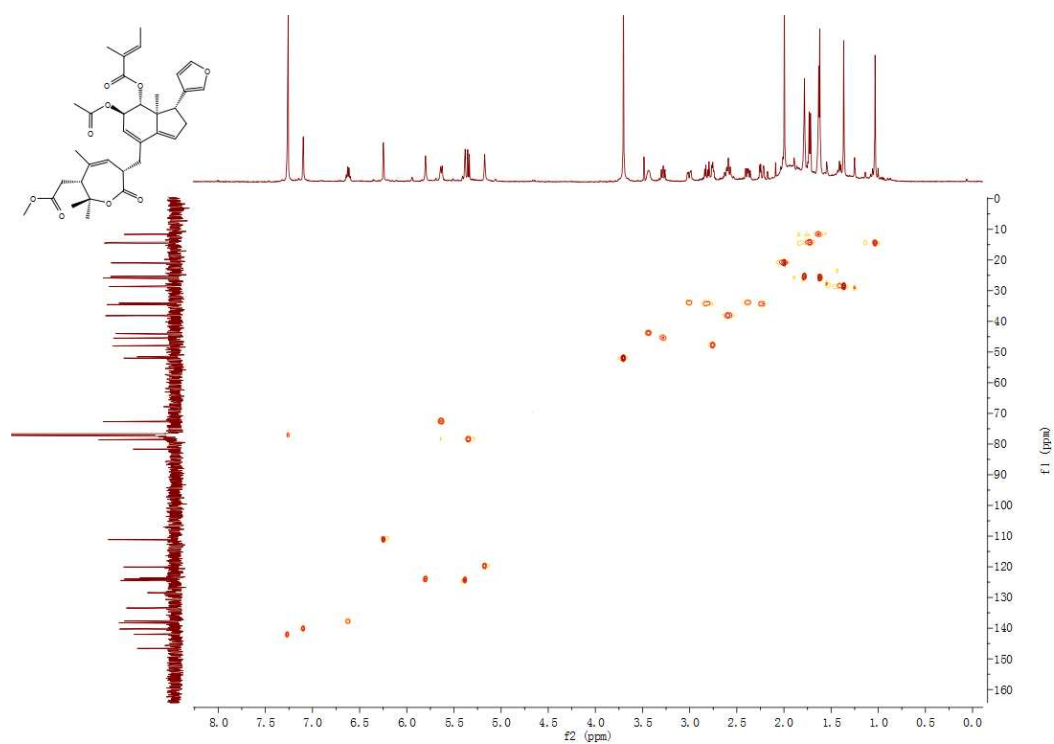


Figure S16. HMBC spectrum of aphanamixoid D (**2**) in CDCl₃

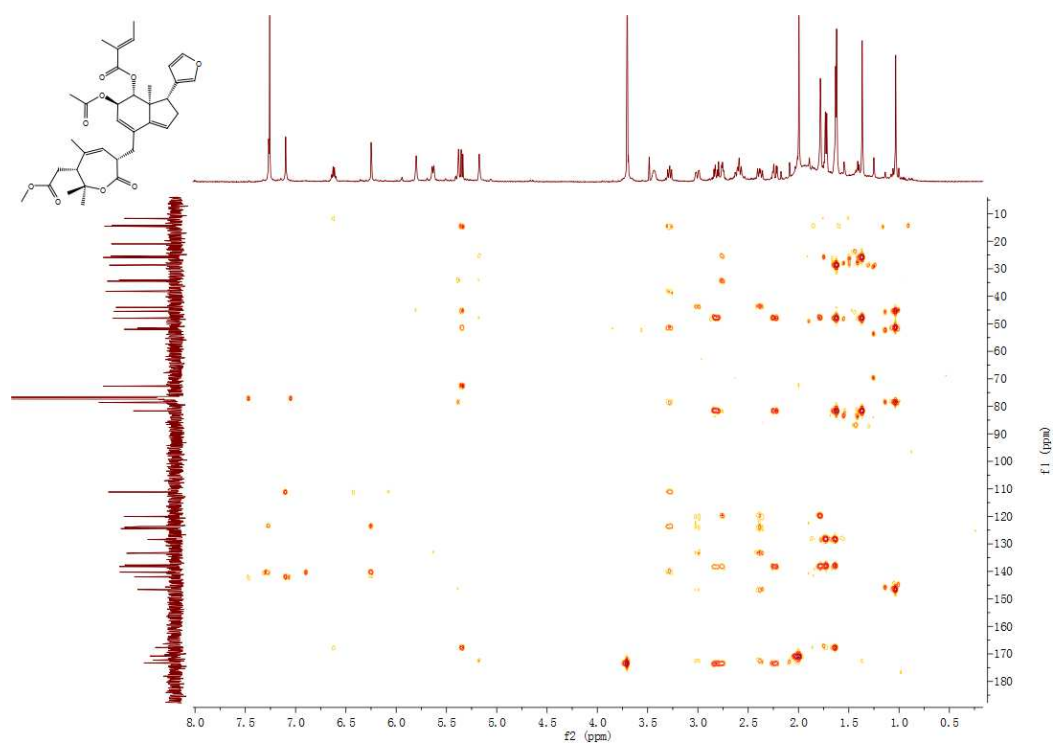


Figure S17. ^1H - ^1H COSY spectrum of aphanamixoid D (**2**) in CDCl_3

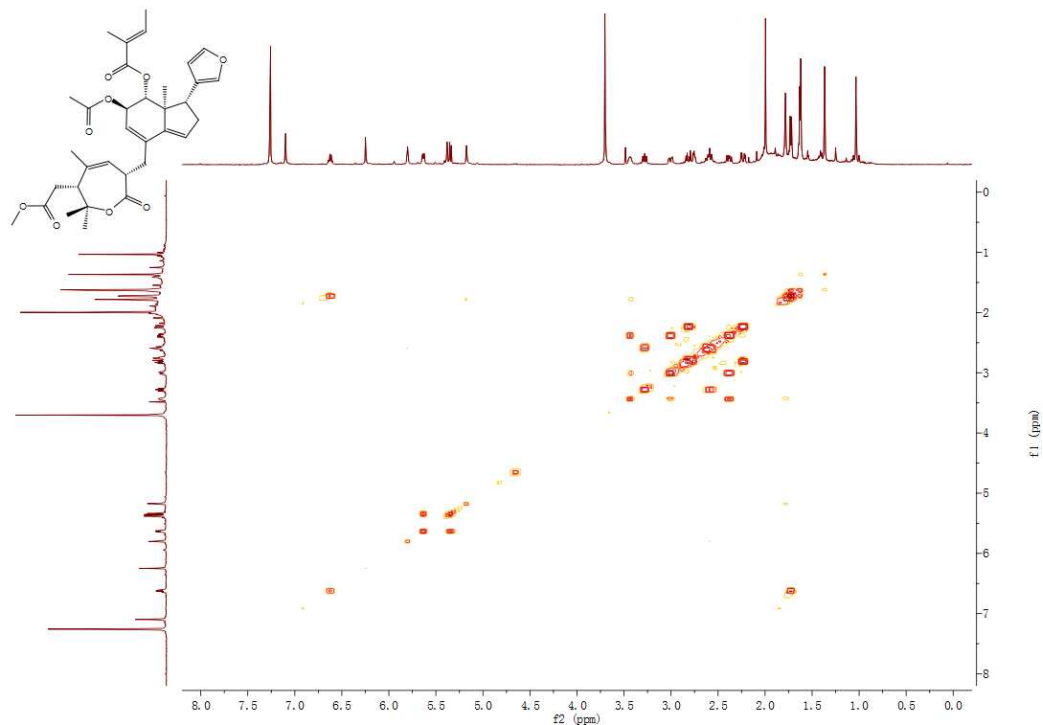


Figure S18. ROESY spectrum of aphanamixoid D (**2**) in CDCl_3

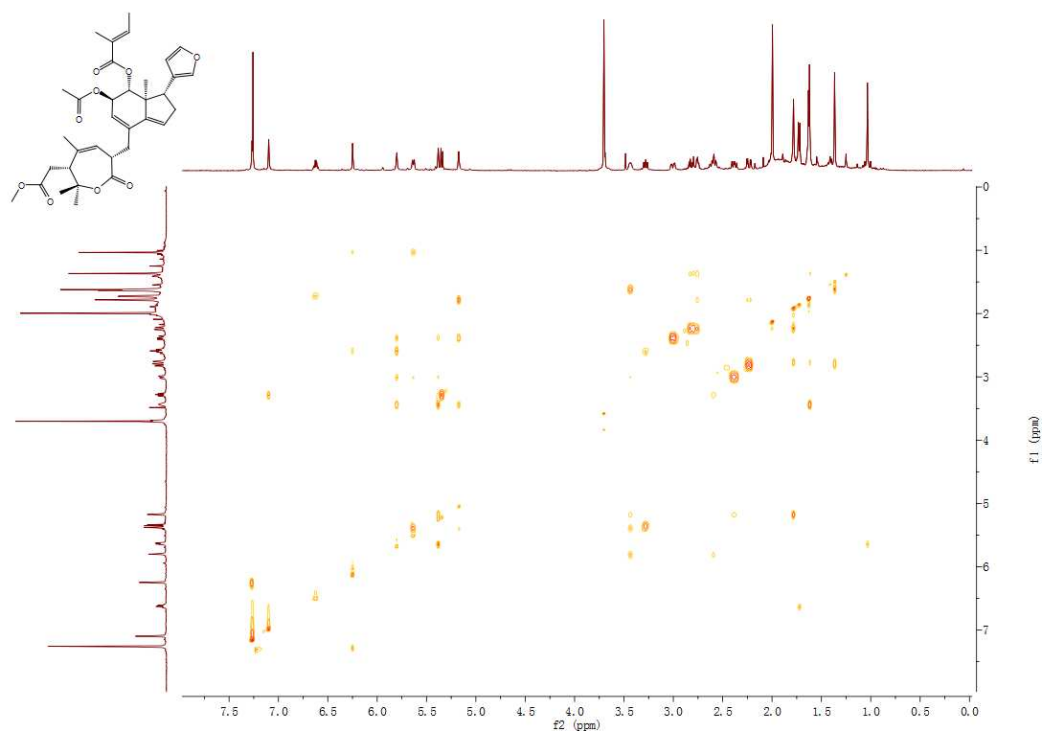


Figure S19. ESI (+) MS of aphanamixoid D (2)

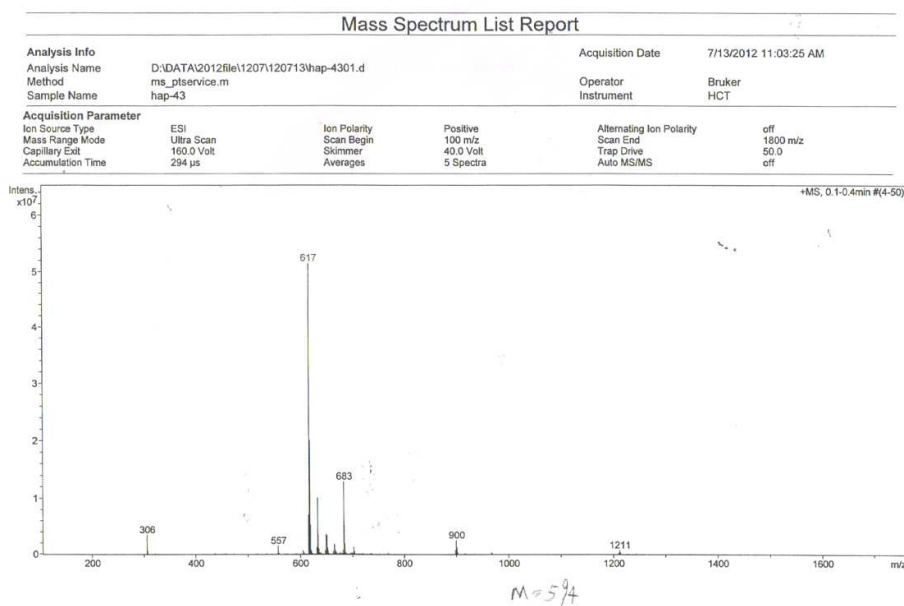


Figure S20. HR-EI (+) MS of aphanamixoid D (2)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
30 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 7-10

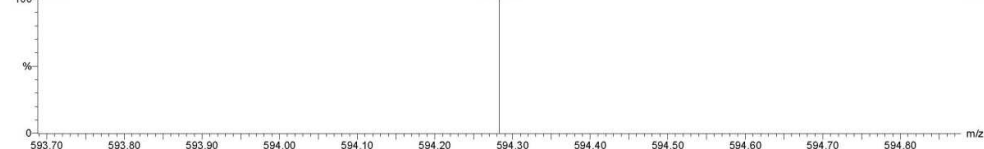
hap-43

13:47:09 04-Sep-2012

Voltage EI+

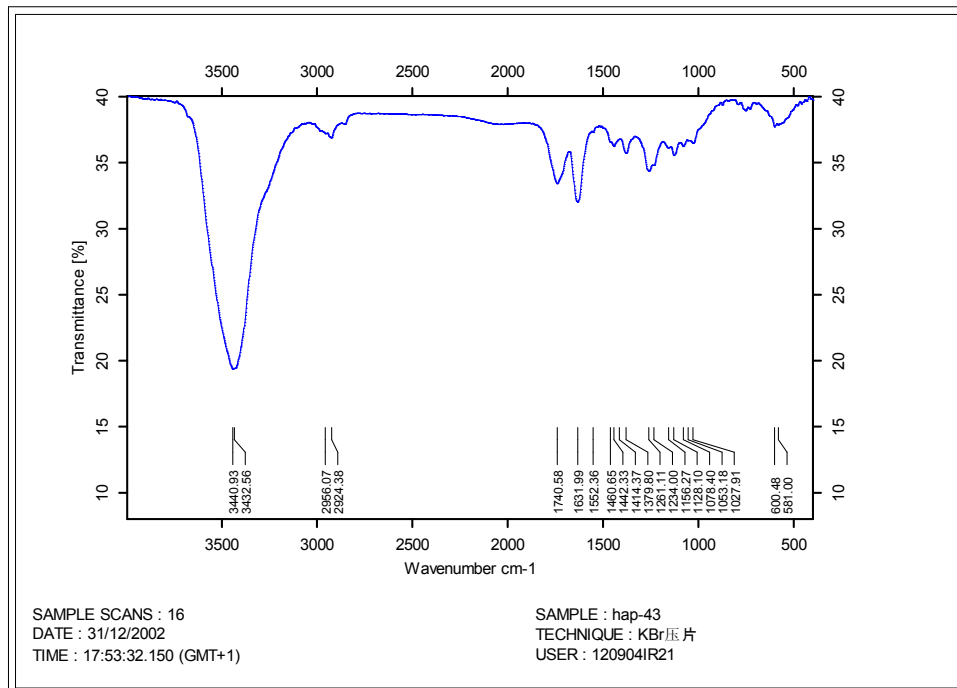
KIB
M120905EA-17AFAMM 24 (2.203)
594.2830

Autospec Premier
P776
51.8



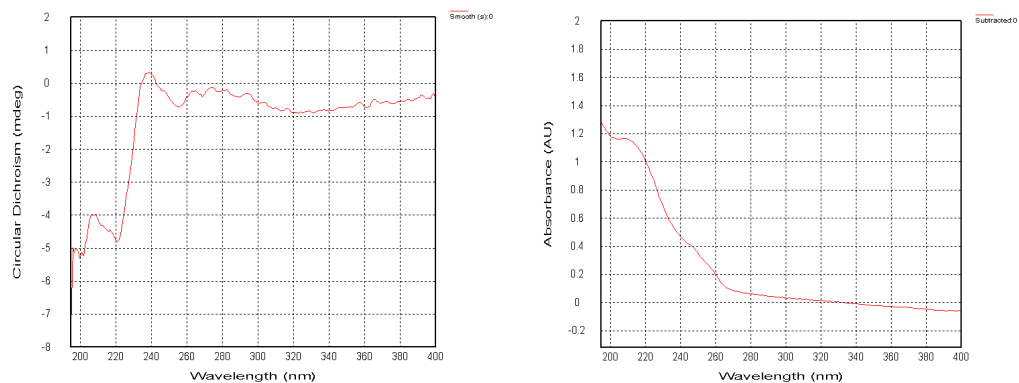
Minimum:						
Maximum:	100.0	10.0	-10.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
594.2830	594.2829	0.1	0.2	14.0	5546045.5	C34 H42 O9

Figure S21. IR spectrum of aphanamixoid D (2)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
555.820	0.380	0.001	39.310	0.129447	0
570.255	0.379	0.000	7.951	0.011008	0
580.998	0.378	0.002	9.107	0.659917	0
600.475	0.377	0.022	12.637	10.032131	0
1027.912	0.364	0.004	23.601	1.280008	0
1053.183	0.367	0.000	7.539	0.057577	0
1078.400	0.362	0.004	18.852	1.405190	0
1128.102	0.355	0.013	21.805	5.196657	0
1156.271	0.361	0.002	22.241	0.389019	0
1234.003	0.348	0.001	16.404	0.122877	0
1261.105	0.343	0.040	26.707	16.562296	0
1379.795	0.357	0.015	29.744	6.347952	0
1414.368	0.368	0.000	4.490	0.002089	0
1442.328	0.362	0.008	18.457	2.635344	0
1460.651	0.366	0.000	12.380	0.017679	0
1552.355	0.373	0.002	10.422	0.502862	0
1631.989	0.320	0.074	48.789	32.599537	0
1740.584	0.334	0.026	73.265	11.712383	0
2924.375	0.369	0.015	23.197	5.791806	0
2956.068	0.372	0.001	12.784	0.280767	0
3432.564	0.194	0.000	51.679	0.045776	0
3440.925	0.193	0.207	148.523	99.895714	0

Figure S22. CD spectrum of aphanamixoid D (2)



File: CD HAP-43-1mm(195-400)12090423.dsx

ProBinaryX

Attributes :

- Time Stamp :Tue Sep 04 17:07:50 2012

- File ID : {3F536135-81BE-4427-AE93-E79D7E2DF005}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.2400mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Figure S23. ^1H NMR spectrum of aphanamixoid E (**3**) in CDCl_3

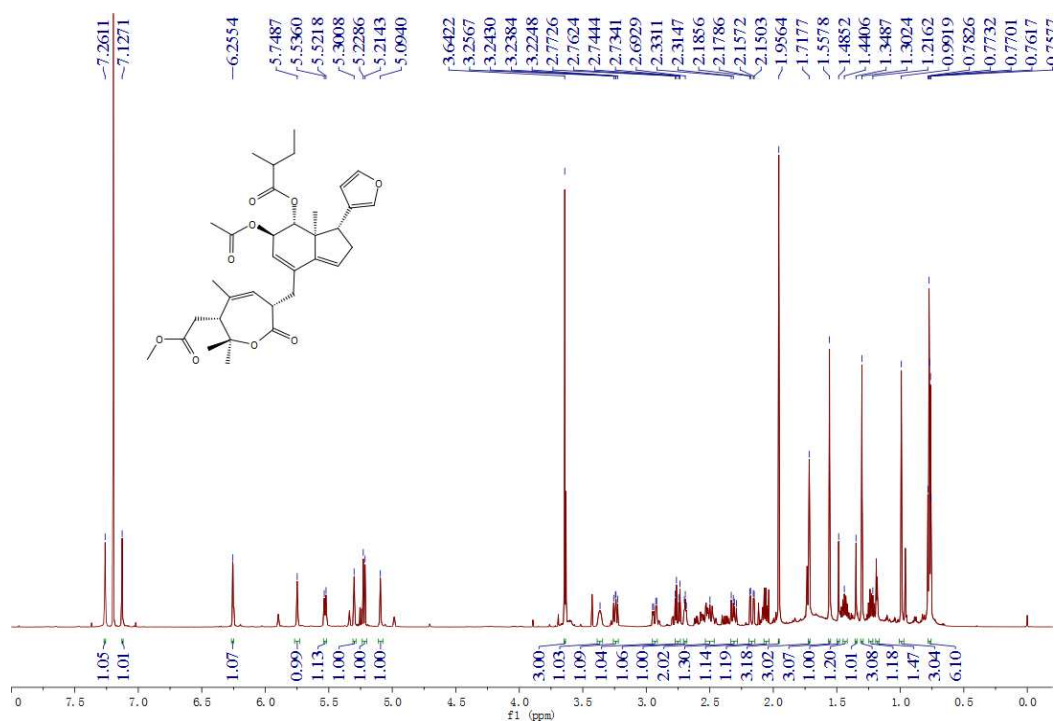


Figure S24. ^{13}C NMR spectrum of aphanamixoid E (**3**) in CDCl_3

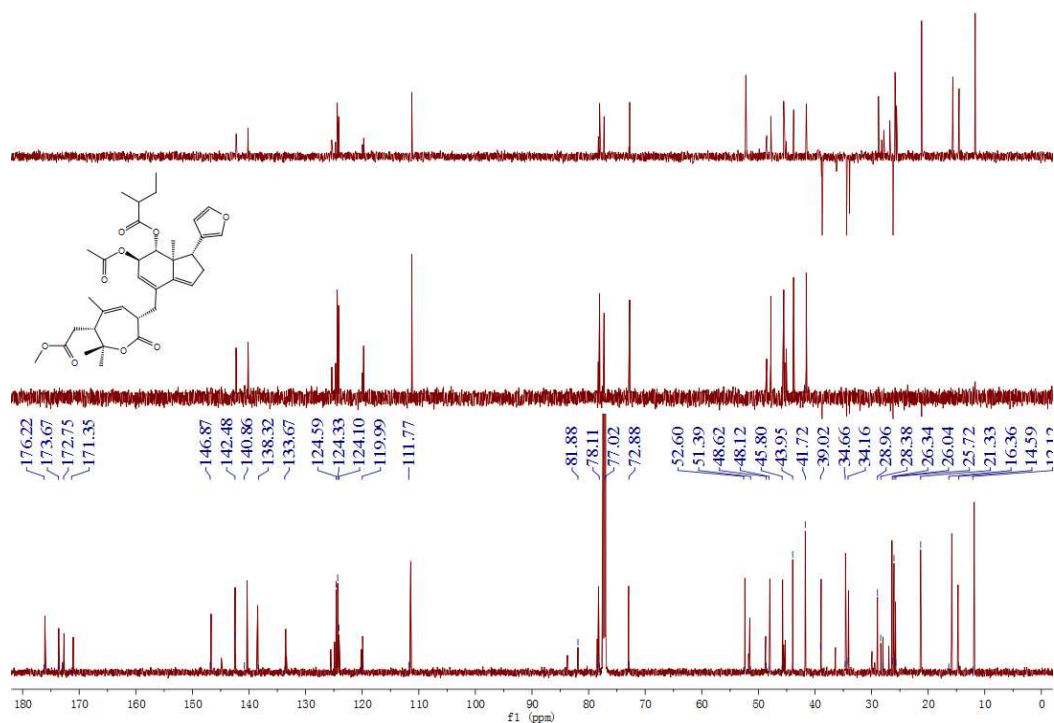


Figure S25. HSQC spectrum of aphanamixoid E (**3**) in CDCl₃

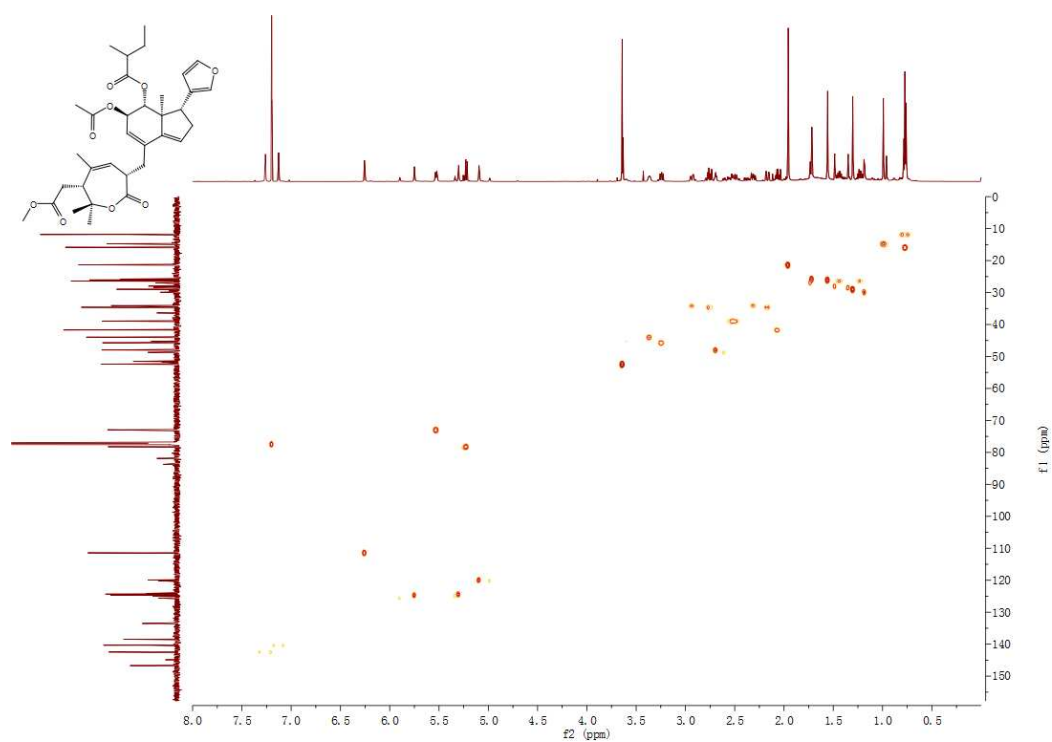


Figure S26. HMBC spectrum of aphanamixoid E (**3**) in CDCl₃

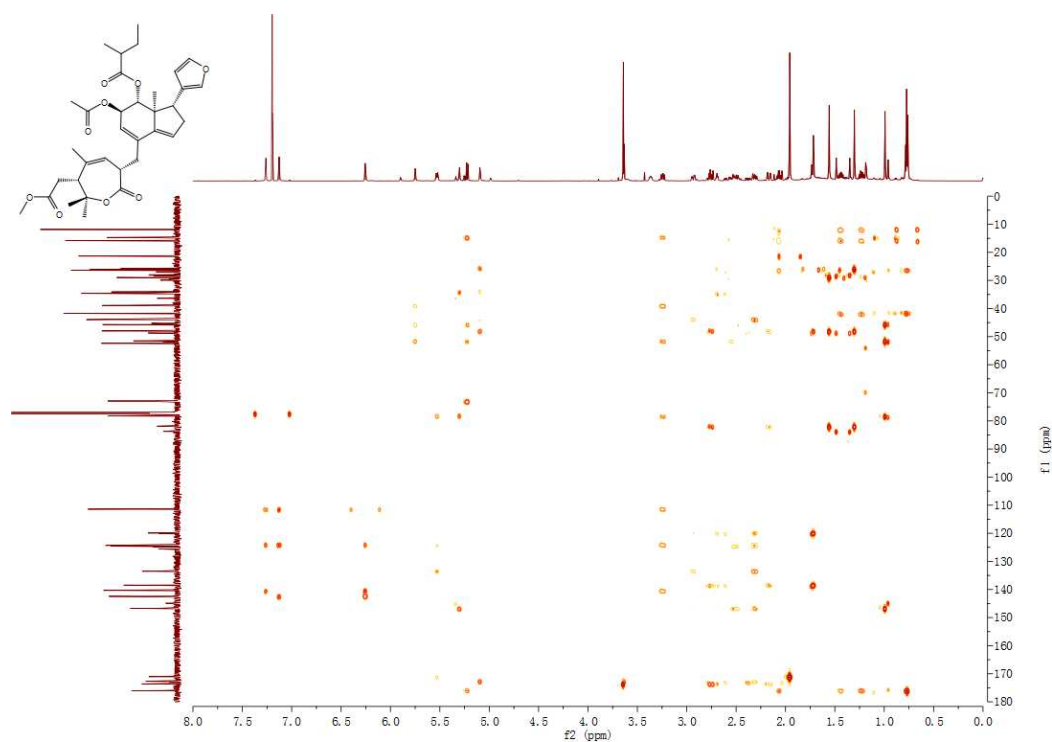


Figure S27. ^1H - ^1H COSY spectrum of aphanamixoid E (**3**) in CDCl_3

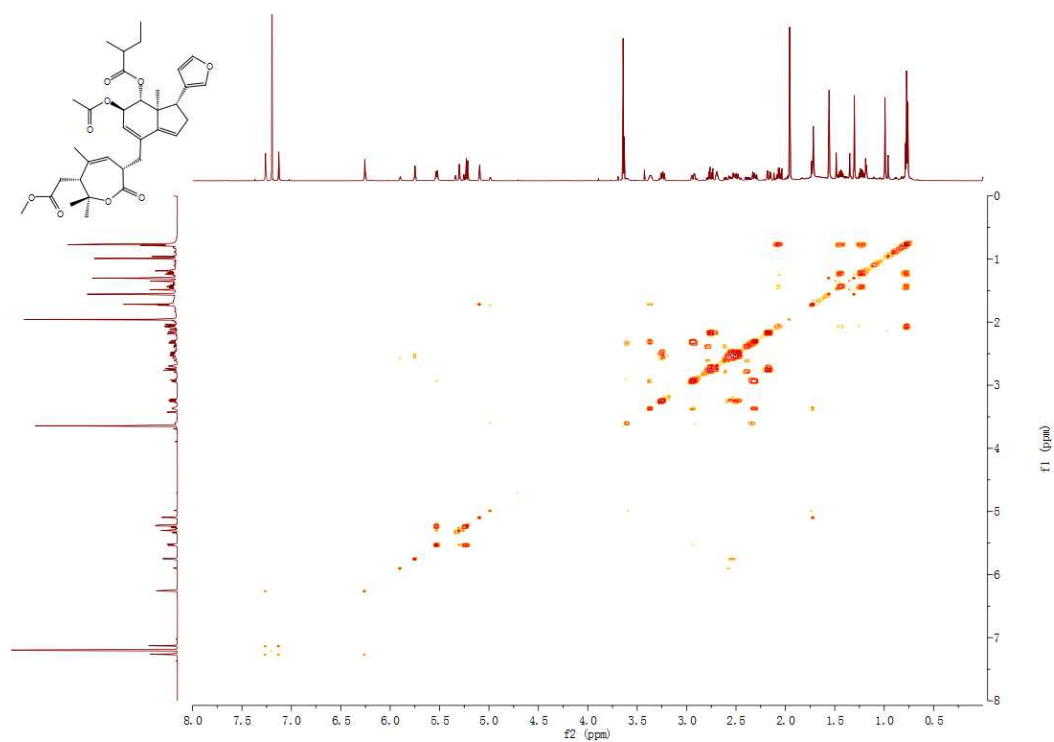


Figure S28. ROESY spectrum of aphanamixoid E (**3**) in CDCl_3

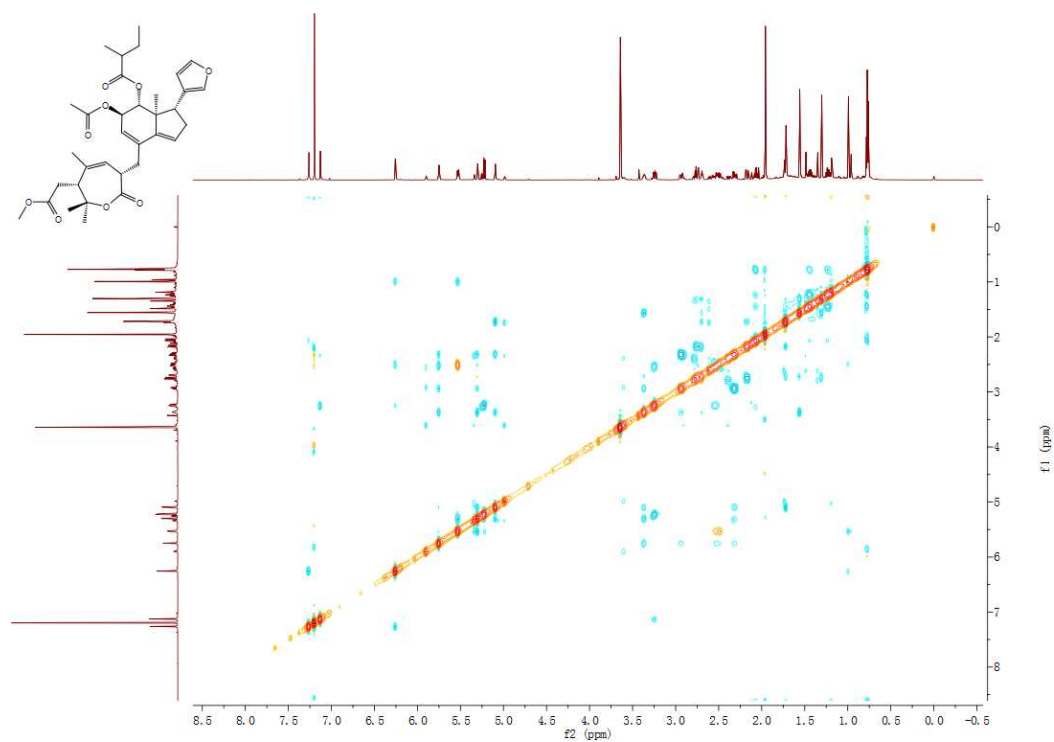


Figure S29. ESI (+) MS of aphanamixoid E (3)

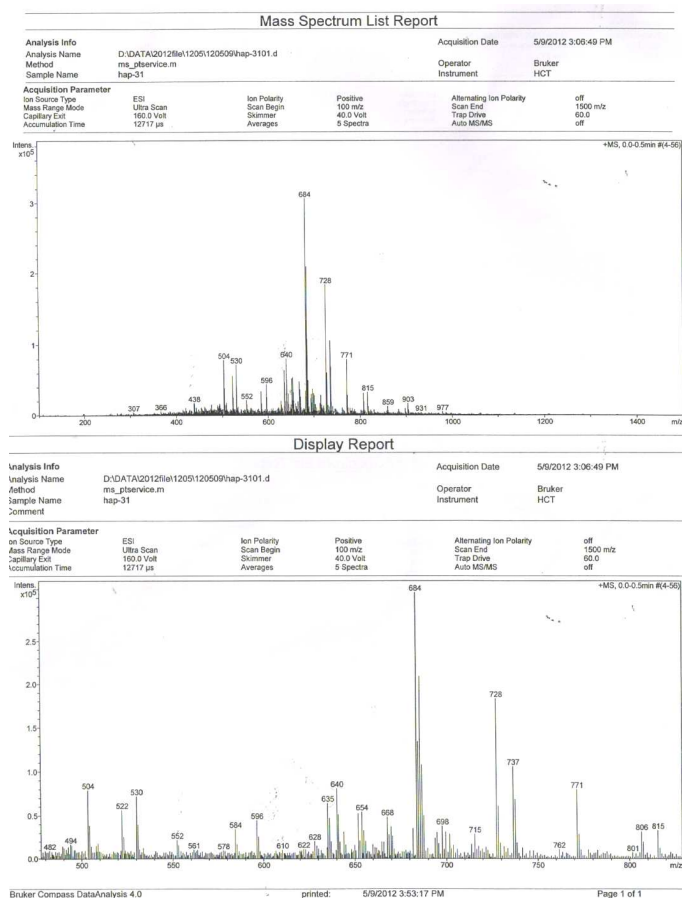


Figure S30. HR-EI (+) MS of aphanamixoid E (3)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

30 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 7-10

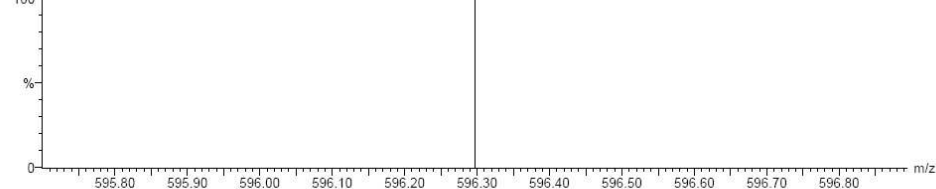
hap-31

11:32:13 29-Sep-2012

Voltage EI+

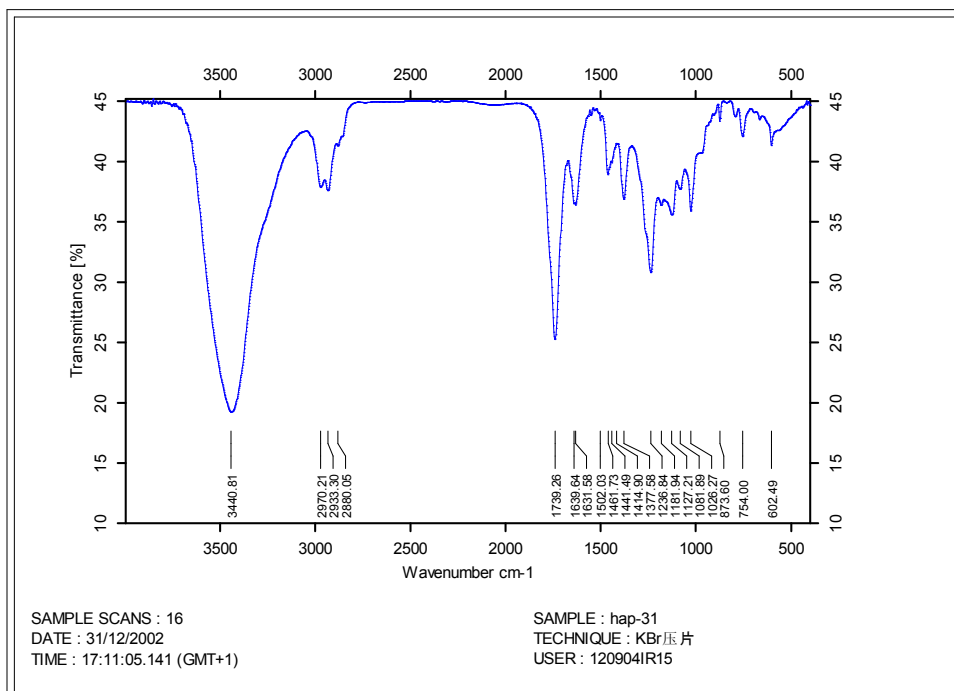
KIB
M120929EA-01AFAMM 14 (1.285)
596.2966

Autospec Premier
P776
1.11



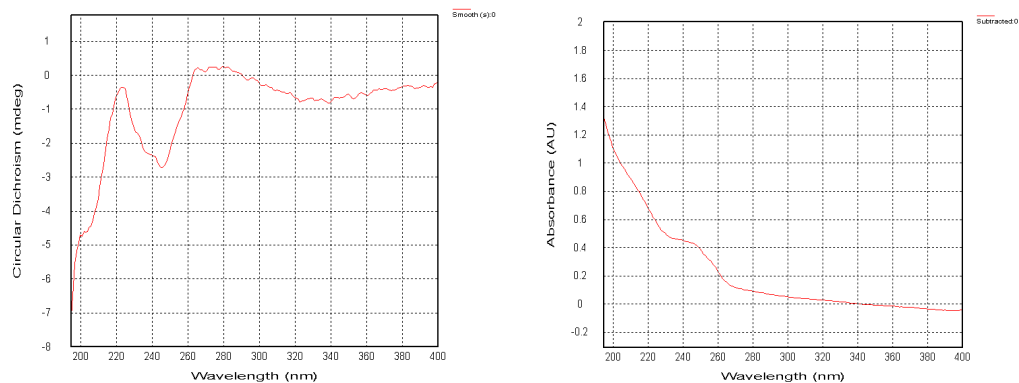
Minimum:						
Maximum:	100.0	10.0	-10.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
596.2966	596.2985	-1.9	-3.2	13.0	5546025.5	C34 H44 O9

Figure S31. IR spectrum of aphanamixoid E (**3**)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
602.486	0.413	0.037	11.375	14.218742	0
666.405	0.435	0.005	11.353	1.206165	0
754.003	0.420	0.025	23.459	8.994852	0
792.697	0.437	0.008	19.063	2.511778	0
873.600	0.433	0.015	7.449	5.494808	0
905.787	0.439	0.003	16.076	0.334087	0
1026.265	0.359	0.038	23.539	13.466860	0
1081.889	0.377	0.012	23.720	2.690619	0
1127.207	0.356	0.022	31.674	5.450434	0
1181.936	0.364	0.006	13.789	1.889563	0
1236.841	0.308	0.138	51.570	52.713100	0
1377.582	0.368	0.051	29.407	17.232460	0
1414.898	0.414	0.001	3.642	0.290436	0
1441.485	0.399	0.004	10.307	0.516004	0
1461.734	0.389	0.037	12.239	10.089800	0
1502.028	0.434	0.005	5.638	1.653914	0
1631.578	0.364	0.050	17.895	14.181130	0
1639.641	0.365	0.005	11.915	0.392330	0
1739.256	0.253	0.198	63.207	76.080849	0
2880.046	0.413	0.003	11.315	0.838048	0
2933.297	0.376	0.053	26.303	19.130117	0
2970.206	0.379	0.015	27.382	2.320803	0
3440.808	0.192	0.260	244.324	99.387856	0

Figure S32. CD spectrum of aphanamixoid E (3)



File: CD HAP-31-1mm(195-400)12090414.dsx

ProBinaryX

Attributes :

- Time Stamp :Tue Sep 04 15:43:00 2012

- File ID : {BBE3BD59-833F-419d-89B0-5E206634C365}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.6000mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Figure S33. ^1H NMR spectrum of aphanamixoid F (**4**) in CDCl_3

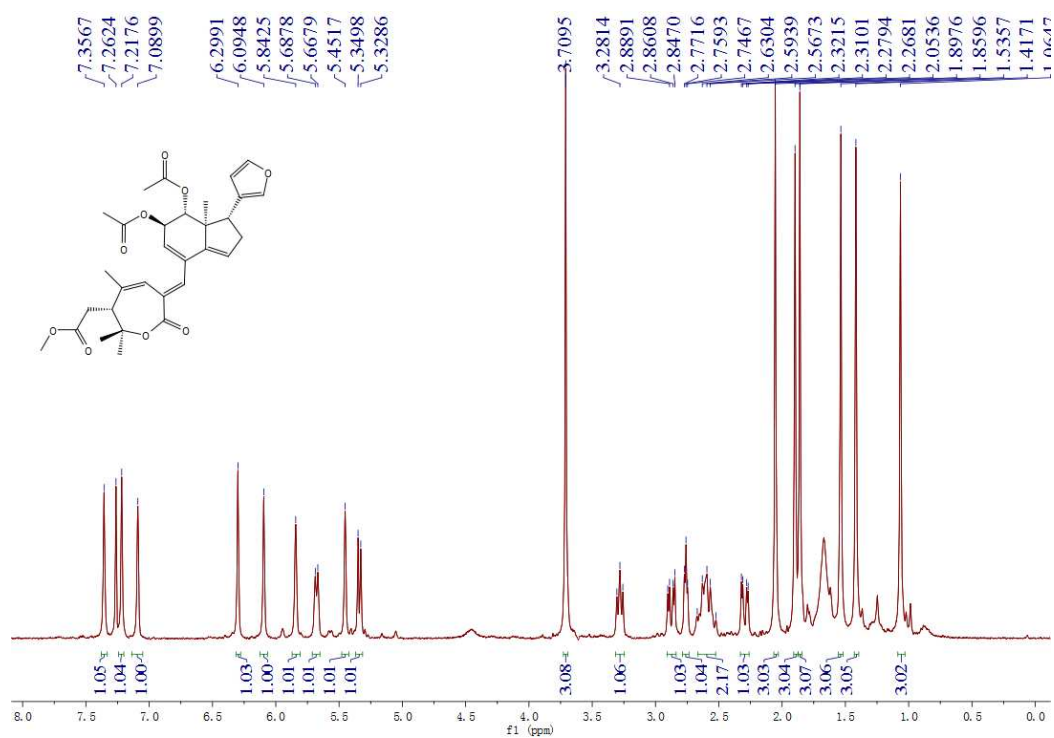


Figure S34. ^{13}C NMR spectrum of aphanamixoid F (**4**) in CDCl_3

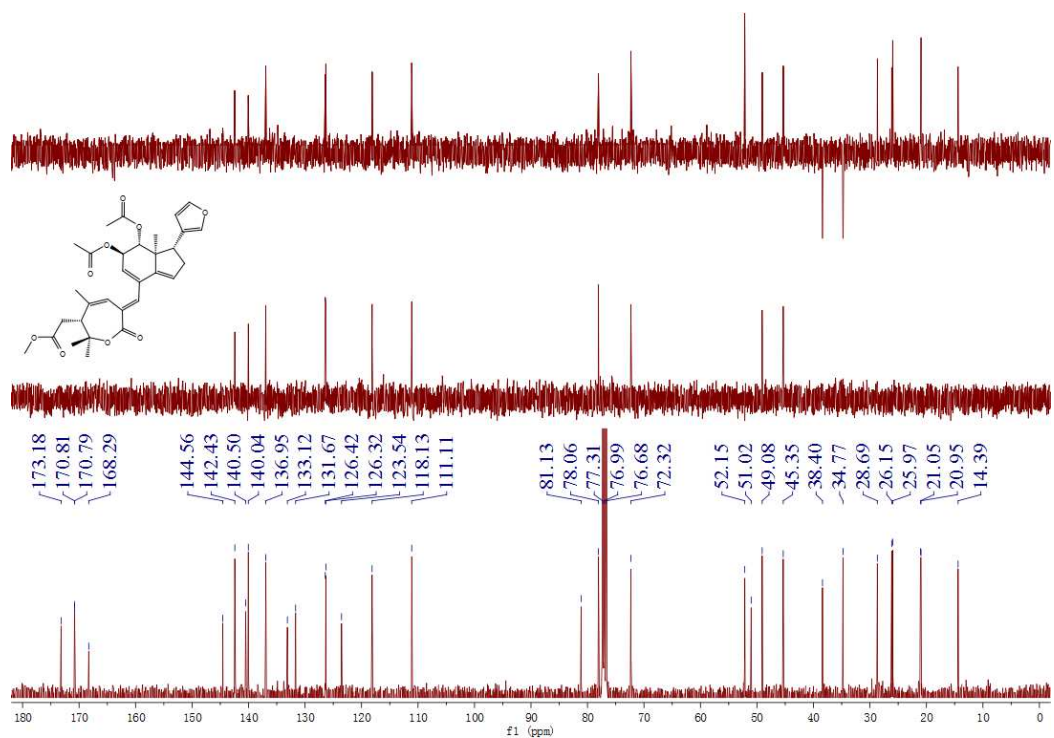


Figure S35. HSQC spectrum of aphanamixoid F (**4**) in CDCl₃

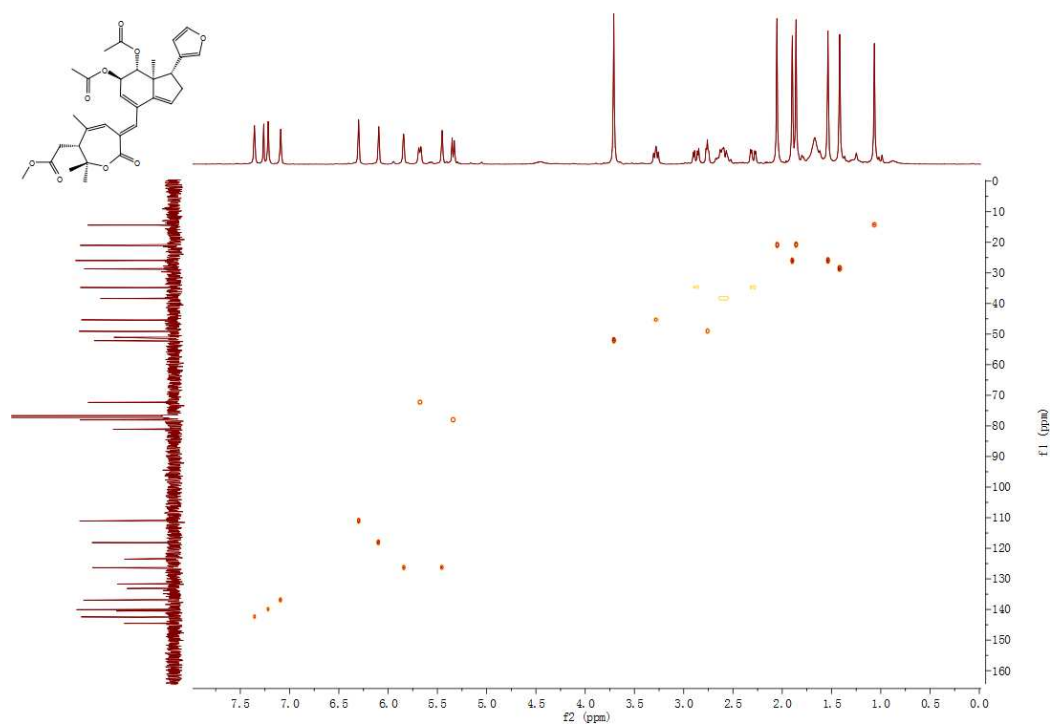


Figure S36. HMBC spectrum of aphanamixoid F (**4**) in CDCl₃

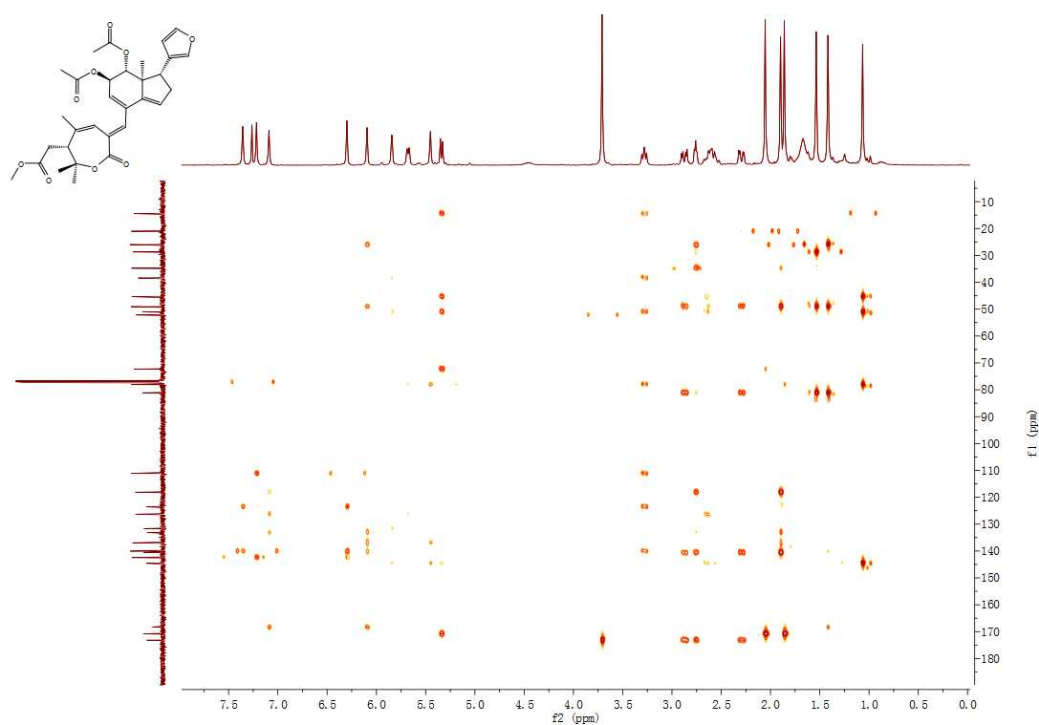


Figure S37. ^1H - ^1H COSY spectrum of aphanamixoid F (**4**) in CDCl_3

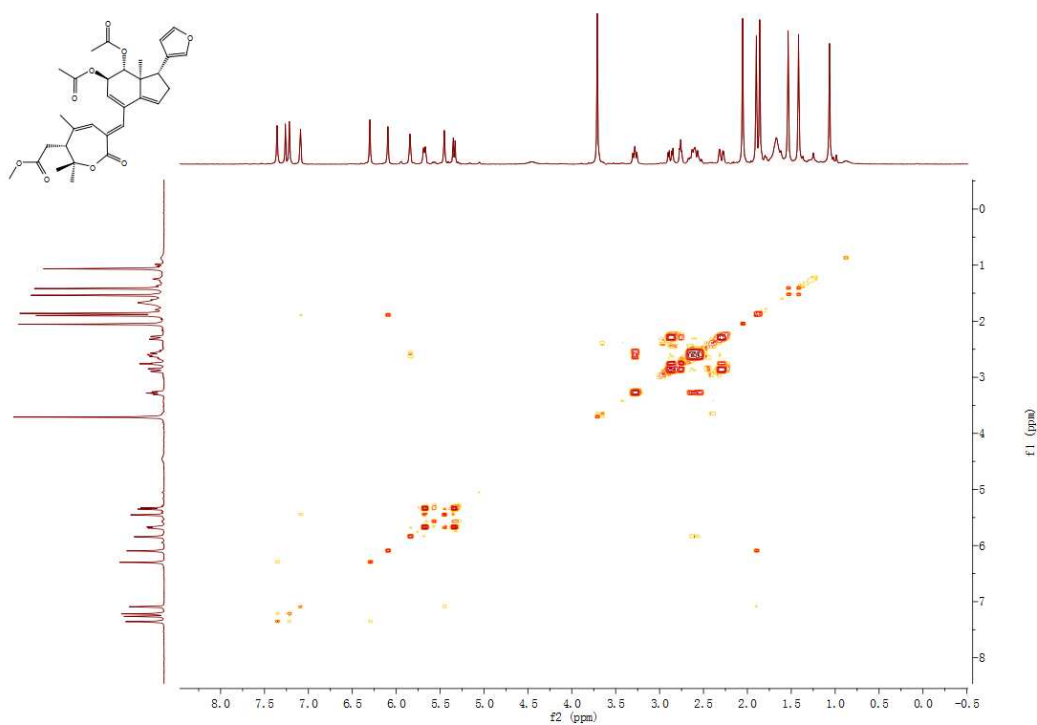


Figure S38. ROESY spectrum of aphanamixoid F (**4**) in CDCl_3

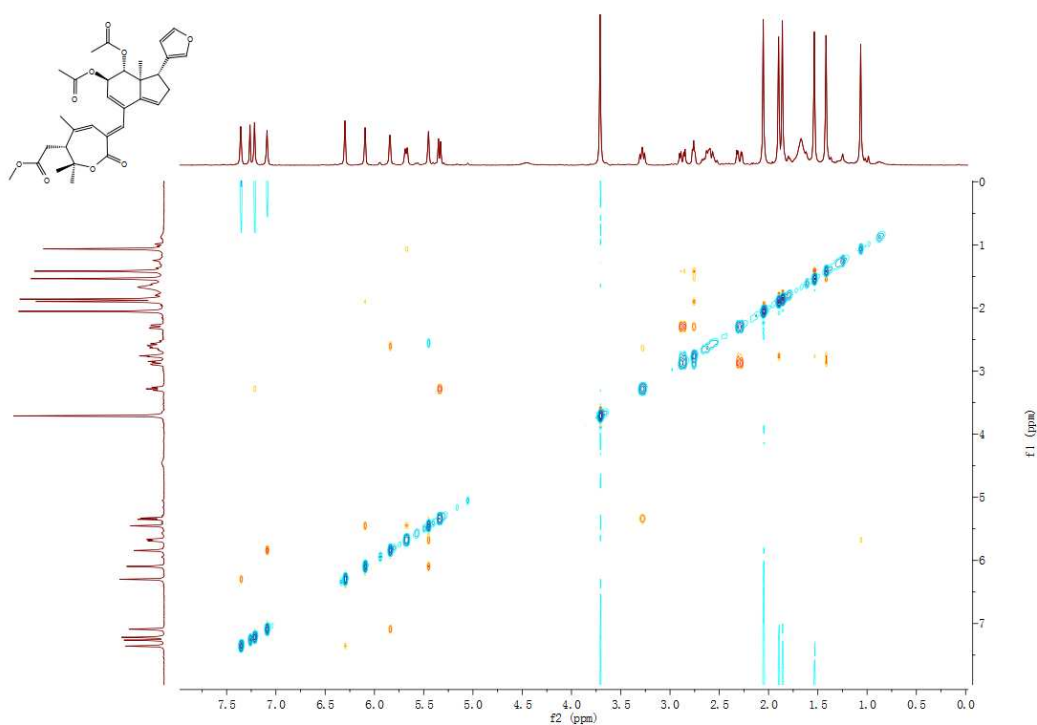


Figure S39. ESI (+) MS of aphanamixoid F (4)

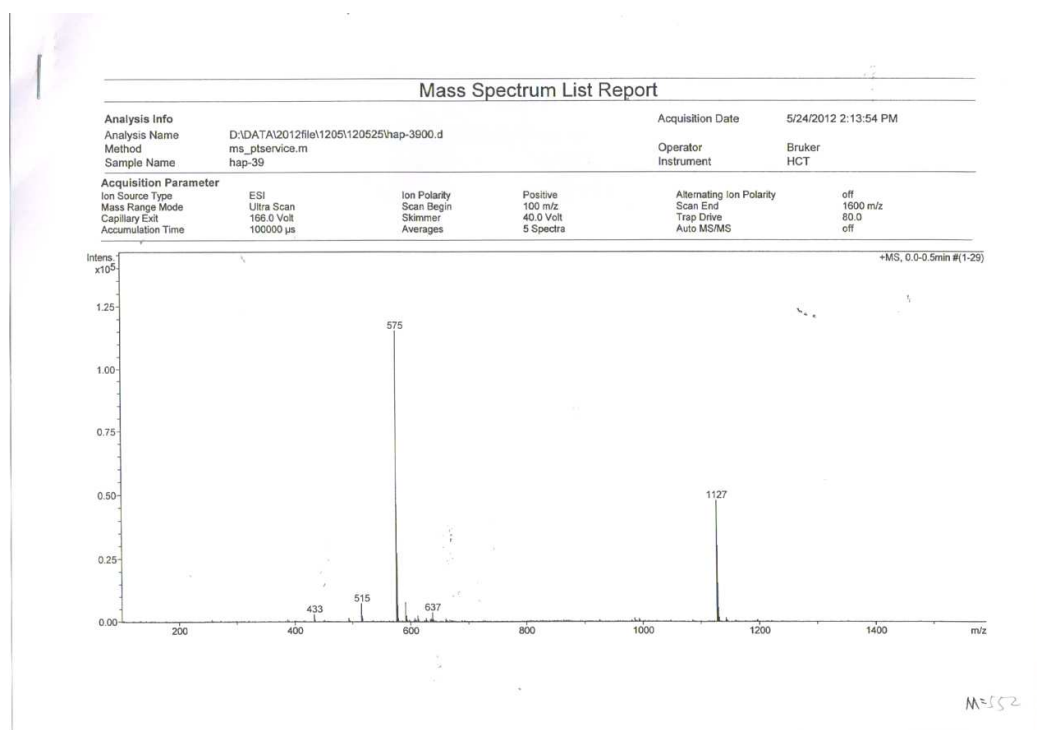


Figure S40. HR-EI (+) MS of aphanamixoid F (4)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
28 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 7-10

hap-39

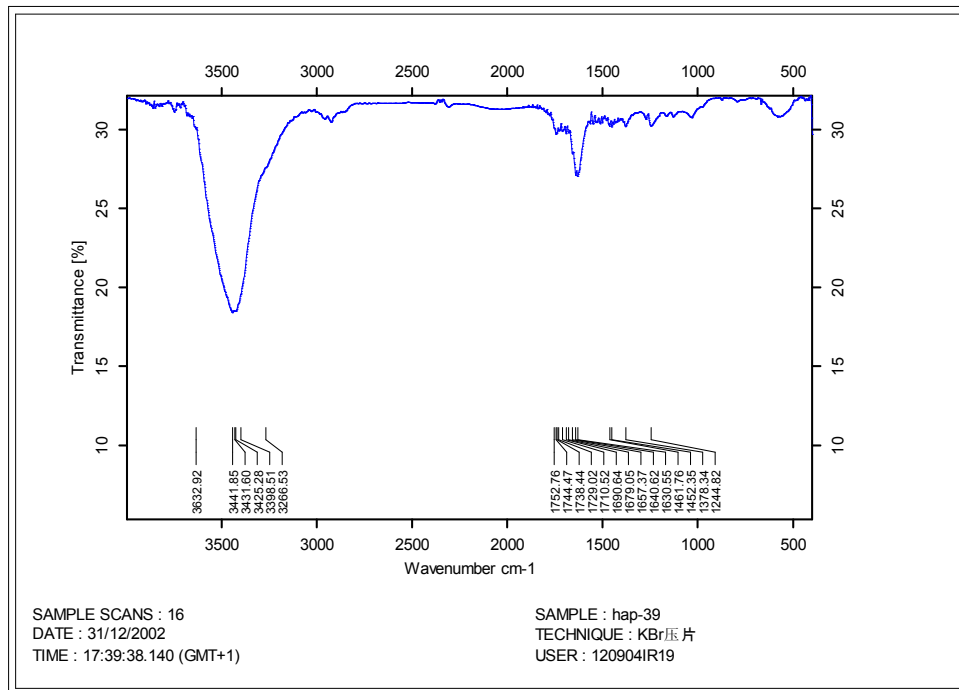
13.36.08 04-Sep-2012

Voltage EI+

KIB
M120905EA-15AFAMM 23 (2.111)

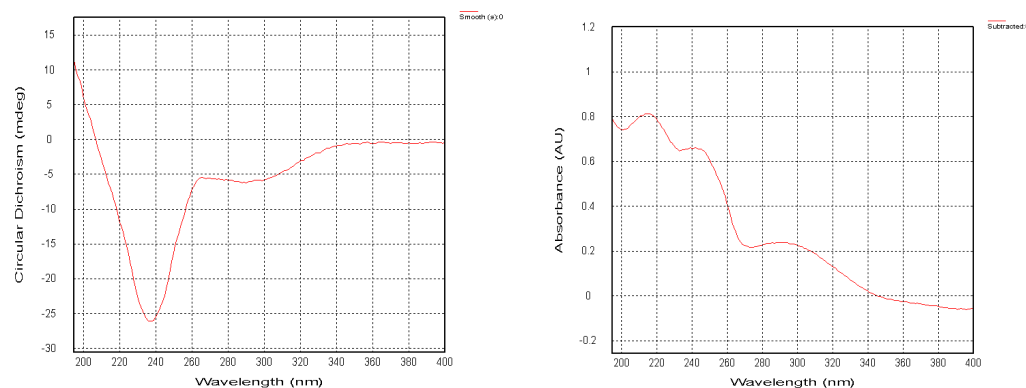
Autospec Premier
P776
157

Figure S41. IR spectrum of aphanamixoid F (4)



Wavenumber	Abs_Intensity	Rel_Intensity	Width	Found if Threshold <	Shoulder
568.214	0.308	0.001	9.208	0.412869	0
581.766	0.308	0.013	35.033	9.105393	0
1031.219	0.307	0.005	11.133	3.022829	0
1037.314	0.308	0.000	6.770	0.008037	0
1128.992	0.308	0.003	19.044	2.131382	0
1244.823	0.302	0.010	36.044	6.613341	0
1271.219	0.306	0.004	14.674	2.543186	0
1359.792	0.306	0.000	3.919	0.129007	0
1378.335	0.302	0.006	14.484	4.080581	0
1390.657	0.304	0.001	3.481	0.492850	0
1401.899	0.306	0.001	2.868	0.340796	0
1414.505	0.305	0.002	6.726	1.147572	0
1424.377	0.305	0.001	6.051	0.377137	0
1432.722	0.304	0.002	3.779	1.574908	0
1441.859	0.303	0.002	5.608	0.883020	0
1452.347	0.301	0.011	5.191	7.094265	0
1461.762	0.302	0.004	4.111	2.675691	0
1467.913	0.303	0.001	4.072	0.451230	0
1479.510	0.306	0.002	9.694	1.277295	0
1493.620	0.307	0.001	3.922	0.627265	0
1501.975	0.304	0.004	4.952	2.946802	0
1512.421	0.303	0.006	7.246	3.923683	0
1529.435	0.304	0.003	6.520	2.015777	0
1535.215	0.304	0.002	4.261	0.354394	0
1549.773	0.303	0.007	11.554	3.999601	0
1564.866	0.303	0.004	5.773	1.358535	0
1572.757	0.304	0.001	3.541	0.570202	0
1630.552	0.270	0.050	22.908	35.675121	0
1640.622	0.271	0.003	11.656	2.130035	0
1657.374	0.284	0.002	5.544	1.098871	0
1679.046	0.297	0.003	4.856	1.294347	0
1690.638	0.297	0.005	7.916	3.539030	0
1710.520	0.299	0.004	11.173	2.477825	0
1729.015	0.299	0.003	11.556	1.314266	0
1738.437	0.297	0.001	3.658	0.219826	0
1744.469	0.297	0.008	5.520	5.071515	0
1752.756	0.300	0.000	5.831	0.105590	0
1765.547	0.306	0.001	5.731	0.451361	0
2923.912	0.304	0.009	21.302	5.963810	0
2958.175	0.306	0.003	21.933	1.512718	0
3104.719	0.308	0.000	15.158	0.135610	0
3112.531	0.308	0.001	4.370	0.312101	0
3134.362	0.305	0.001	14.941	0.350397	0
3147.446	0.304	0.000	7.788	0.223454	0
3266.531	0.276	0.000	31.412	0.133612	0
3398.509	0.195	0.000	16.961	0.138108	0
3425.277	0.185	0.001	23.910	0.350408	0
3431.602	0.185	0.000	3.661	0.065448	0
3441.846	0.184	0.136	180.602	99.204567	0
3632.916	0.300	0.001	16.767	0.647250	0
3653.662	0.307	0.002	3.900	1.309552	0
3664.712	0.308	0.001	5.336	0.598028	0

Figure S42. CD spectrum of aphanamixoid F (4)



File: CD HAP-39-1mm(195-400)12090420.dsx

ProBinaryX

Attributes :

- Time Stamp :Tue Sep 04 16:35:11 2012

- File ID : {A07D8115-1B23-47a0-AC18-4F99046C5FC8}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.3150mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Chemical structure of compound 10:

CC(=C)OC(=O)C1=C(C)C(=C(C)C(=O)O1C(=O)OC)C=C2C=CC(=C2)C3=C(C)C(=O)OC3C4=CC=CC=C4

¹H NMR spectrum (CDCl₃):

Chemical Shift (ppm)	Integration
7.3555	0.09
7.2598	0.02
7.1825	0.02
6.7412	0.94
6.7274	1.04
6.7129	1.01
6.6994	1.01
6.3247	1.01
6.1863	1.01
5.9229	1.01
5.8325	1.01
5.8156	1.01
5.5381	1.01
5.4884	1.01
5.4712	1.01
3.7829	3.13
3.4029	1.02
3.3860	1.02
3.3820	1.02
3.3650	1.02
2.9602	1.12
2.9378	1.12
2.9263	1.12
2.8441	1.12
2.8337	1.12
2.6784	1.12
2.6784	1.12
2.3958	1.12
2.3861	1.12
2.3522	1.12
2.0862	1.12
1.9702	1.12
1.8214	1.12
1.8071	1.12
1.7224	1.12
1.6153	1.12
1.4928	1.12
1.5600	1.12

Chemical structure of compound 10a is shown. The ^{13}C NMR spectrum (ppm) is displayed below the structure, with peaks labeled as follows:

173.20, 170.86, 168.36, 167.57, 144.58, 142.16, 140.40, 140.28, 138.14, 137.03, 133.03, 131.63, 128.16, 126.54, 126.32, 123.29, 118.15, 111.08, 81.13, 77.97, 77.35, 77.03, 76.72, 72.36, 52.16, 51.28, 49.04, 45.17, 38.18, 34.74, 28.67, 26.13, 25.95, 21.04, 14.60, 14.39, 11.72.

Figure S45. HSQC spectrum of aphanamixoid G (**5**) in CDCl₃

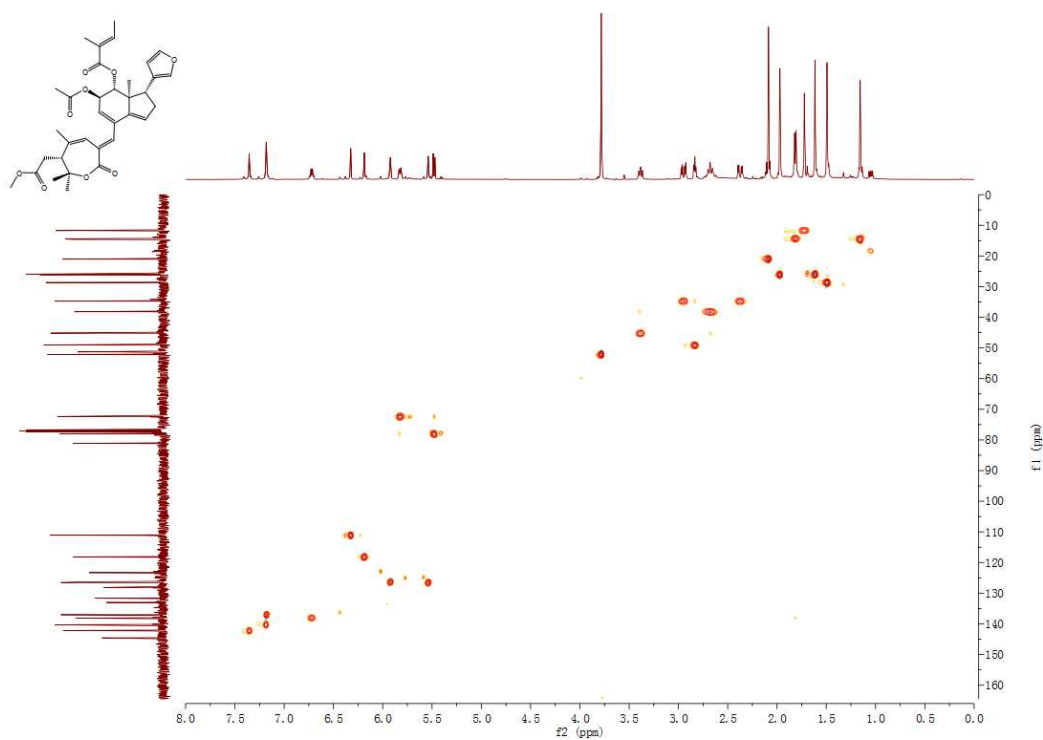


Figure S46. HMBC spectrum of aphanamixoid G (**5**) in CDCl₃

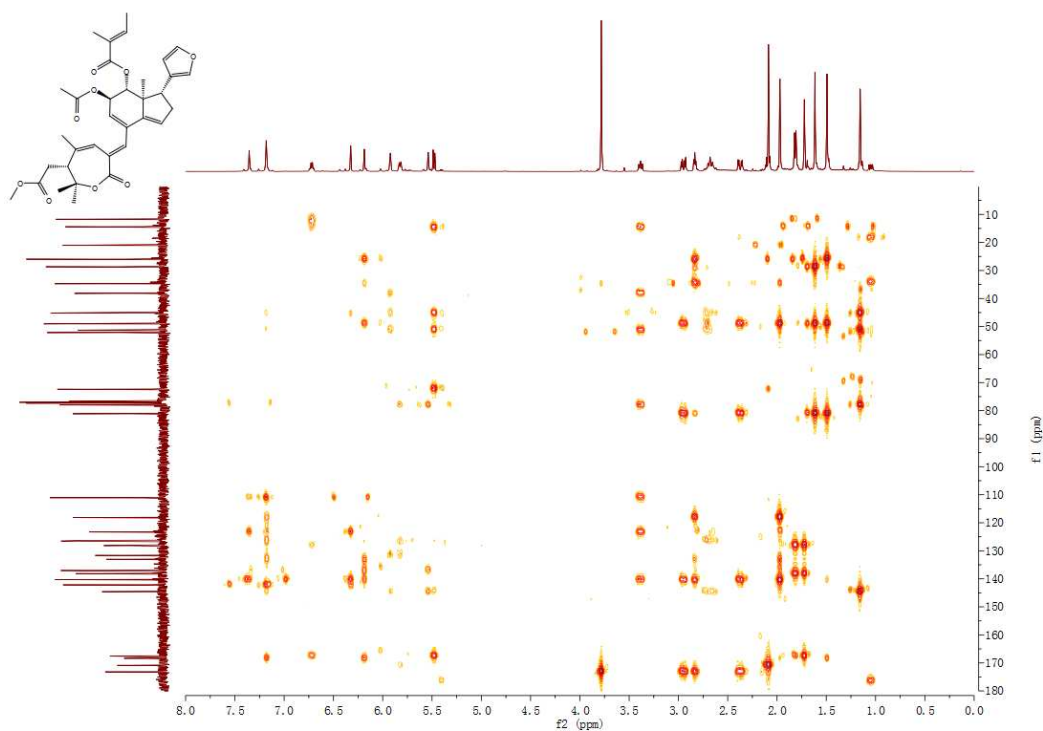


Figure S47. ^1H - ^1H COSY spectrum of aphanamixoid G (**5**) in CDCl_3

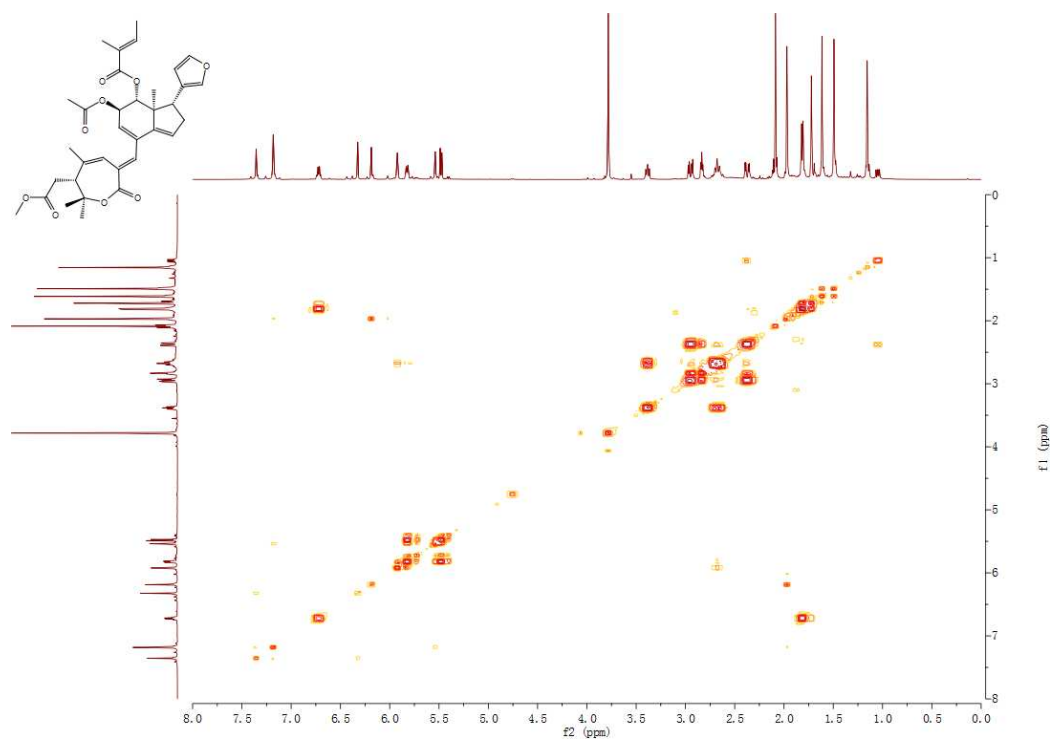


Figure S48. ROESY spectrum of aphanamixoid G (**5**) in CDCl_3

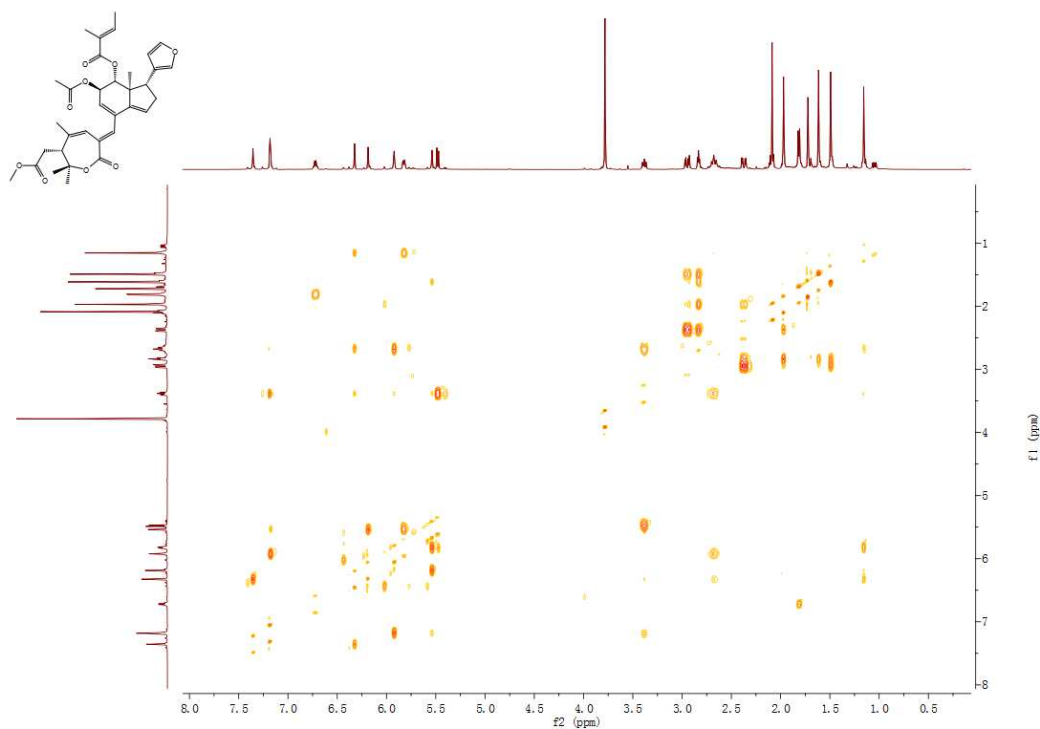


Figure S49. ESI (+) MS of aphanamixoid G (5)

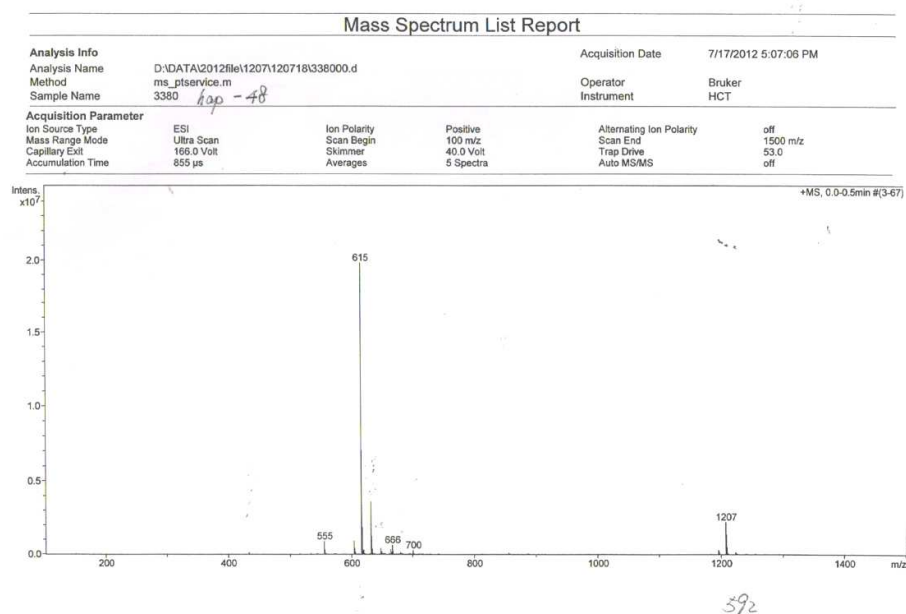


Figure S50. HR-EI (+) MS of aphanamixoid G (5)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

31 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

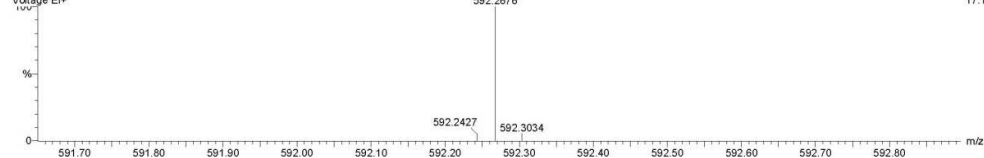
Elements Used:

C: 0-200 H: 0-400 O: 7-10

hap-48

13:59:44 04-Sep-2012

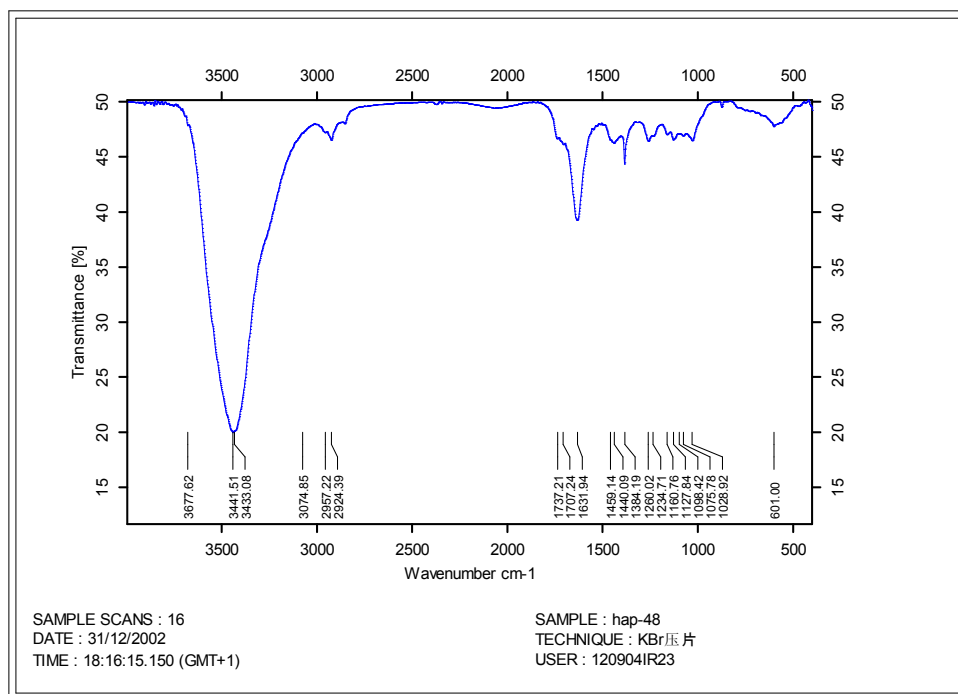
Voltage EI+



Autospec Premier
P776
17.1

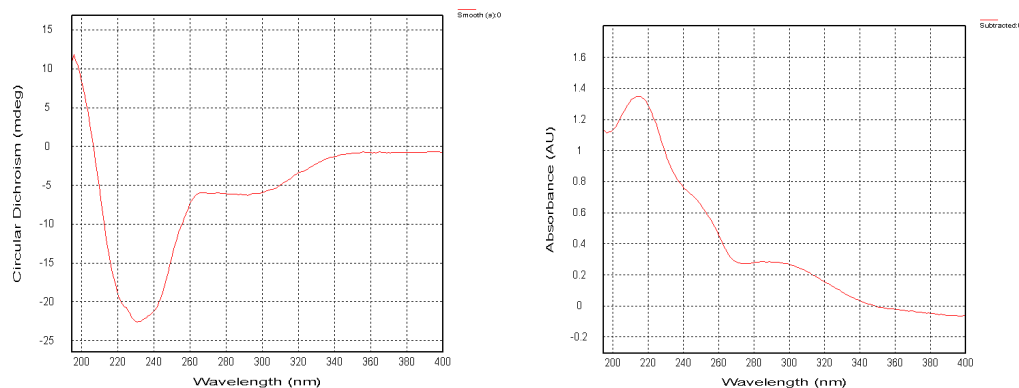
Minimum:				-10.0		
Maximum:	100.0	10.0		120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
592.2676	592.2672	0.4	0.7	15.0	5546029.5	C34 H40 O9

Figure S51. IR spectrum of aphanamixoid G (5)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
600.996	0.477	0.024	25.436	7.703007	0
1028.915	0.465	0.019	33.485	4.846217	0
1075.778	0.469	0.002	14.350	0.567102	0
1098.419	0.471	0.000	4.548	0.043993	0
1127.835	0.465	0.010	19.876	1.913461	0
1160.759	0.470	0.005	19.321	0.836307	0
1234.708	0.469	0.002	16.026	0.121571	0
1260.024	0.464	0.019	22.188	5.892594	0
1384.187	0.443	0.040	10.393	12.434483	0
1440.086	0.462	0.011	23.024	2.306371	0
1459.139	0.465	0.001	12.271	0.065095	0
1631.943	0.392	0.109	58.086	35.859497	0
1707.237	0.461	0.002	12.401	0.332431	0
1737.213	0.466	0.002	17.080	0.483604	0
2924.388	0.465	0.018	23.263	5.005702	0
2957.223	0.472	0.002	18.516	0.256059	0
3074.853	0.471	0.000	7.166	0.016901	0
3433.079	0.201	0.000	52.861	0.027299	0
3441.506	0.200	0.302	169.426	100.005142	0
3677.618	0.478	0.001	7.576	0.289891	0

Figure S52. CD spectrum of aphanamixoid G (5)



File: CD HAP-48-1mm(195-400)12090427.dsx

ProBinaryX

Attributes :

- Time Stamp :Tue Sep 04 17:45:20 2012

- File ID : {A5AEF20B-414D-4b49-B41F-9C128064939D}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.3450mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Chemical structure of compound 10 is shown. The ¹H NMR spectrum (CDCl₃) displays peaks at the following chemical shifts (ppm): 7.3425, 7.1989, 6.3432, 6.3012, 5.9404, 5.6955, 5.5911, 5.5871, 5.5710, 5.5670, 5.4995, 5.3501, 5.3295, 3.7044, 3.3234, 3.2993, 3.2770, 2.9049, 2.8905, 2.8631, 2.8482, 2.7477, 2.7354, 2.7222, 2.5837, 2.5603, 2.2800, 2.2691, 2.2375, 2.2262, 2.0418, 1.8926, 1.8465, 1.6137, 1.3988, and 1.0473. Integration values are provided below the peaks: 1.04, 1.04, 1.01, 1.00, 0.91, 1.00, 1.02, 1.00, 1.00, 3.03, 1.02, 1.02, 1.01, 2.05, 1.02, 3.13, 3.04, 3.10, 3.10, 3.02, and 3.01.

Chemical structure of compound 10a is shown in the top left corner. The ¹³C NMR spectrum (CDCl₃) is displayed below the structure, with the following chemical shifts (ppm) labeled:

173.25, 170.95, 170.76, 165.93, 144.07, 142.32, 139.98, 139.95, 136.01, 134.86, 132.85, 125.06, 124.47, 123.98, 122.80, 111.20, 81.05, 78.52, 76.99, 72.45, 52.16, 51.61, 49.02, 45.36, 38.41, 34.71, 28.86, 25.84, 25.60, 21.05, 20.98, 13.73.

Figure S55. HSQC spectrum of aphanamixoid H (**6**) in CDCl₃

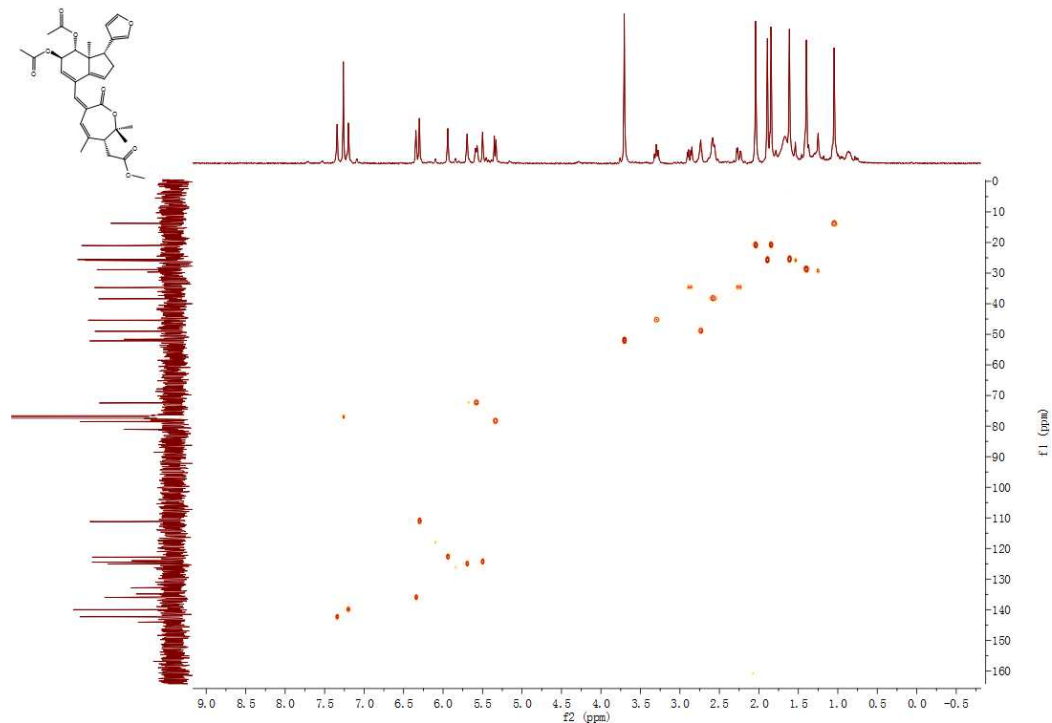


Figure S56. HMBC spectrum of aphanamixoid H (**6**) in CDCl₃

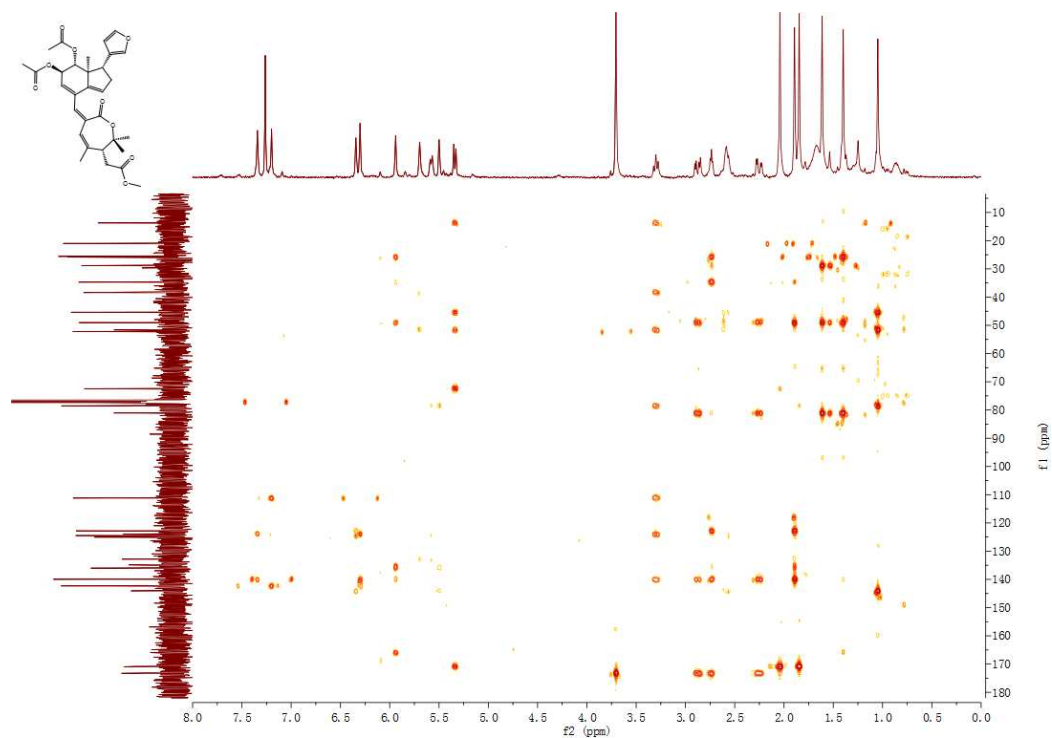


Figure S57. ^1H - ^1H COSY spectrum of aphanamixoid H (**6**) in CDCl_3

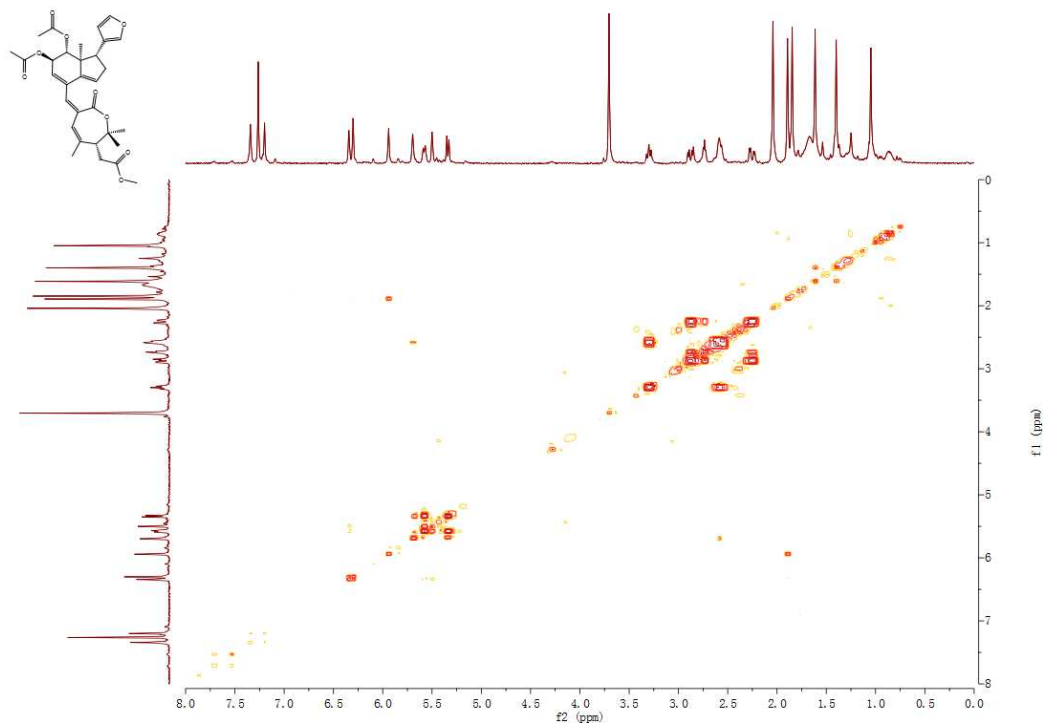


Figure S58. ROESY spectrum of aphanamixoid H (**6**) in CDCl_3

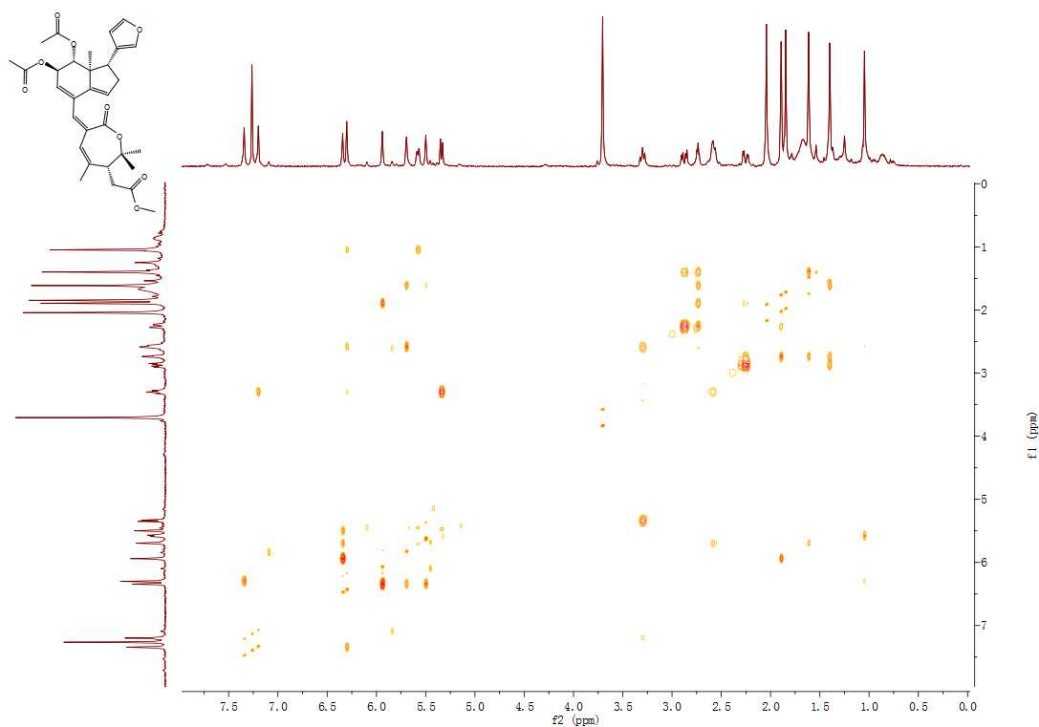


Figure S59. ESI (+) MS of aphanamixoid H (6)

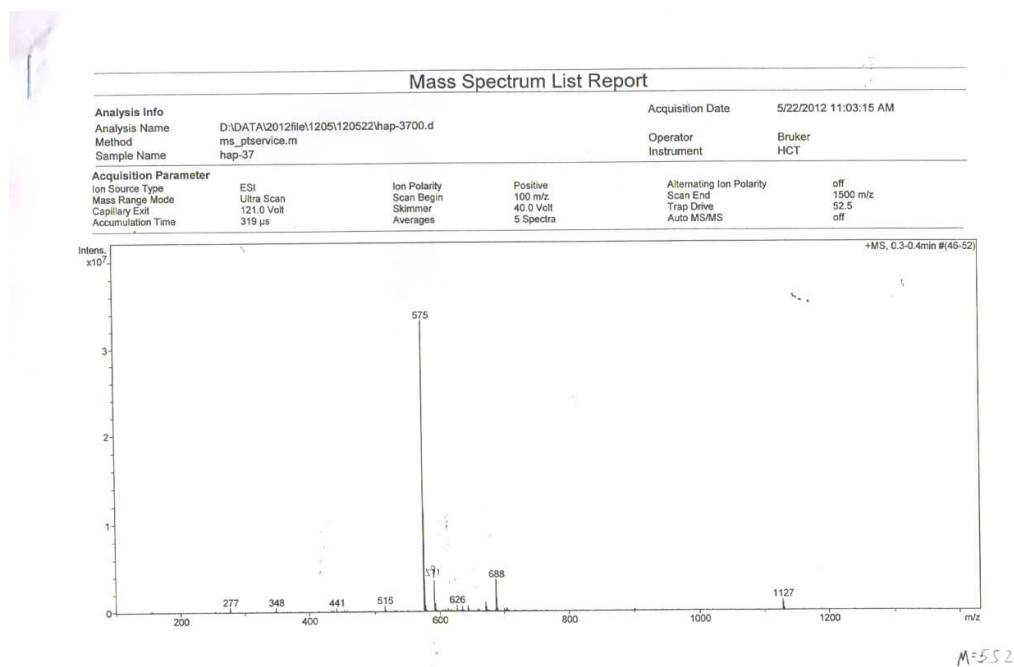


Figure S58. HR-EI (+) MS of aphanamixoid H (6)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

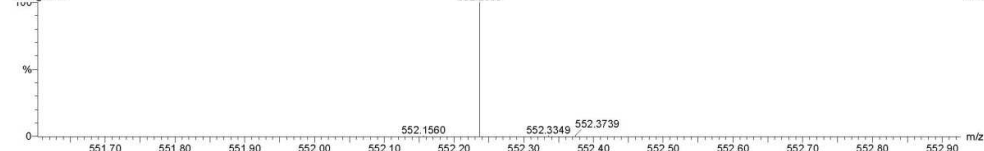
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
28 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:
C: 0-200 H: 0-400 O: 7-10

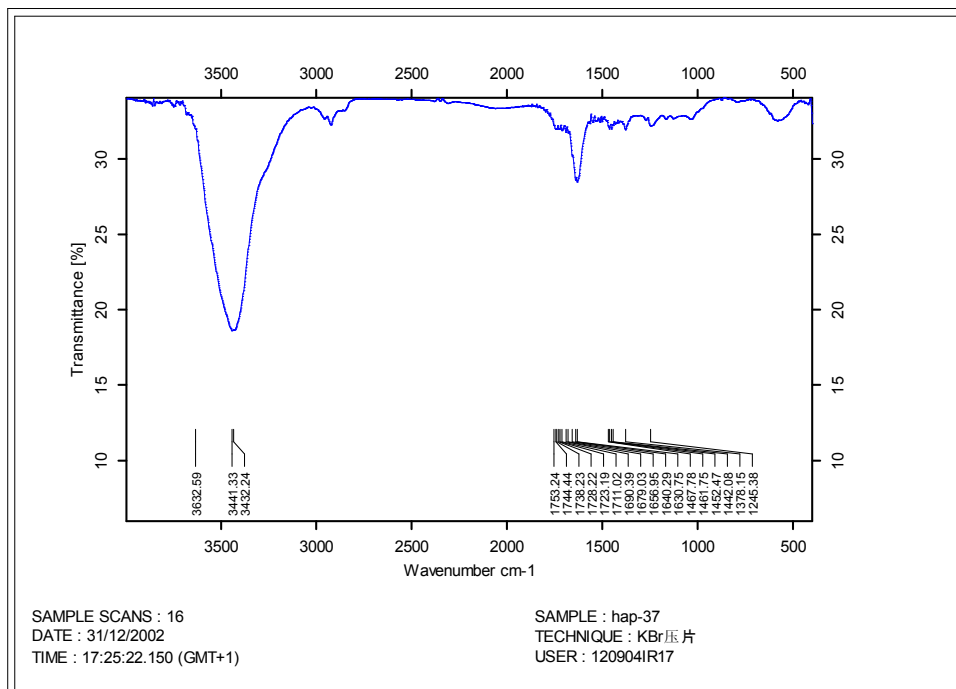
hap-37
13.25.57 04-Sep-2012

Voltage El+



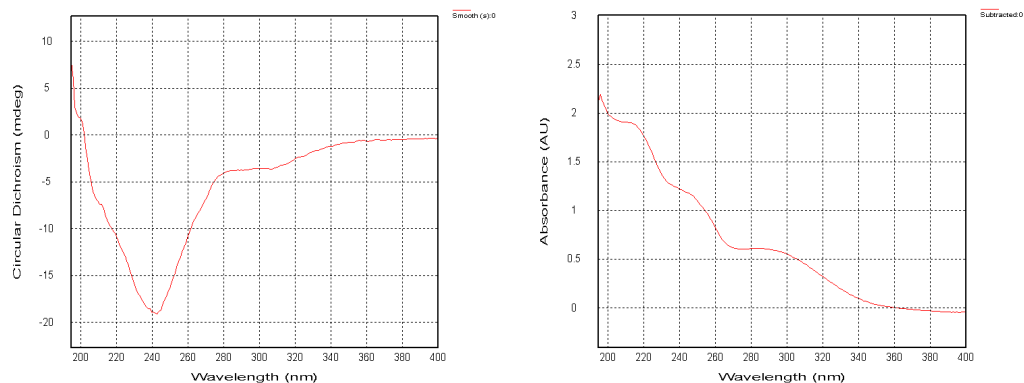
Minimum:				-10.0	
Maximum:	100.0	10.0		120.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT Formula
552.2365	552.2359	0.6	1.1	14.0	5546061.0 C31 H36 O9

Figure S61. IR spectrum of aphanamixoid H (6)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
567.402	0.326	0.001	8.211	0.134617	0
582.341	0.325	0.015	6.549	9.766092	0
1245.380	0.322	0.008	39.278	4.516885	0
1270.975	0.325	0.002	13.445	1.220646	0
1359.750	0.325	0.000	4.041	0.111698	0
1378.150	0.319	0.013	13.526	6.808423	0
1390.622	0.323	0.001	3.222	0.323046	0
1401.859	0.324	0.001	3.163	0.319840	0
1414.465	0.324	0.002	6.300	0.795016	0
1424.208	0.324	0.001	5.847	0.362994	0
1432.825	0.323	0.002	3.755	1.224623	0
1442.083	0.322	0.001	5.605	0.459806	0
1452.470	0.320	0.007	5.202	4.022692	0
1461.746	0.320	0.004	4.198	2.261783	0
1467.776	0.321	0.001	4.121	0.268712	0
1478.409	0.325	0.001	10.012	0.502728	0
1501.990	0.325	0.004	4.948	2.235736	0
1512.563	0.324	0.004	7.438	2.687587	0
1529.354	0.325	0.001	6.597	0.263345	0
1535.499	0.325	0.003	4.246	1.525812	0
1551.123	0.324	0.005	11.746	2.784881	0
1564.885	0.323	0.003	5.672	0.903663	0
1573.042	0.324	0.001	3.575	0.341427	0
1630.747	0.284	0.056	22.443	36.063702	0
1640.285	0.286	0.002	12.404	1.161273	0
1656.952	0.302	0.001	5.067	0.391049	0
1679.025	0.317	0.001	4.755	0.734079	0
1690.394	0.318	0.004	7.870	2.332586	0
1711.017	0.319	0.004	10.823	2.261358	0
1723.189	0.320	0.003	4.540	1.542900	0
1728.215	0.320	0.001	5.205	0.075630	0
1738.227	0.320	0.001	3.631	0.317388	0
1744.441	0.319	0.004	5.379	2.018210	0
1753.239	0.322	0.000	5.900	0.185880	0
1765.520	0.326	0.001	5.820	0.381299	0
2923.139	0.323	0.013	21.886	7.714441	0
2957.656	0.327	0.003	24.380	1.191375	0
3135.167	0.327	0.000	13.947	0.073275	0
3432.240	0.186	0.000	51.091	0.116409	0
3441.328	0.186	0.154	180.946	99.799782	0
3632.587	0.319	0.001	16.682	0.421402	0

Figure S65. CD spectrum of aphanamixoid H (6)



File: CD HAP-37-1mm(195-400)12090416.dsx

ProBinaryX

Attributes :

- Time Stamp :Tue Sep 04 16:00:02 2012

- File ID : {2676664F-67B3-4965-B142-B6BE998B2110}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.6500mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Chemical structure of compound 10:

CCOC(=O)C1=CC(=C(C=C1)C2=CC(=C(C=C2)C3C(C(C3)O)C4C(=C(C=C4)C5C(=C(C=C5)C6C(=C(C=C6)C7C(=C(C=C7)C8C(=C(C=C8)C9C(=C(C=C9)C10C(=C(C=C10)C11C(=C(C=C11)C12C(=C(C=C12)C13C(=C(C=C13)C14C(=C(C=C14)C15C(=C(C=C15)C16C(=C(C=C16)C17C(=C(C=C17)C18C(=C(C=C18)C19C(=C(C=C19)C20C(=C(C=C20)C21C(=C(C=C21)C22C(=C(C=C22)C23C(=C(C=C23)C24C(=C(C=C24)C25C(=C(C=C25)C26C(=C(C=C26)C27C(=C(C=C27)C28C(=C(C=C28)C29C(=C(C=C29)C30C(=C(C=C30)C31C(=C(C=C31)C32C(=C(C=C32)C33C(=C(C=C33)C34C(=C(C=C34)C35C(=C(C=C35)C36C(=C(C=C36)C37C(=C(C=C37)C38C(=C(C=C38)C39C(=C(C=C39)C40C(=C(C=C40)C41C(=C(C=C41)C42C(=C(C=C42)C43C(=C(C=C43)C44C(=C(C=C44)C45C(=C(C=C45)C46C(=C(C=C46)C47C(=C(C=C47)C48C(=C(C=C48)C49C(=C(C=C49)C50C(=C(C=C50)C51C(=C(C=C51)C52C(=C(C=C52)C53C(=C(C=C53)C54C(=C(C=C54)C55C(=C(C=C55)C56C(=C(C=C56)C57C(=C(C=C57)C58C(=C(C=C58)C59C(=C(C=C59)C60C(=C(C=C60)C61C(=C(C=C61)C62C(=C(C=C62)C63C(=C(C=C63)C64C(=C(C=C64)C65C(=C(C=C65)C66C(=C(C=C66)C67C(=C(C=C67)C68C(=C(C=C68)C69C(=C(C=C69)C70C(=C(C=C70)C71C(=C(C=C71)C72C(=C(C=C72)C73C(=C(C=C73)C74C(=C(C=C74)C75C(=C(C=C75)C76C(=C(C=C76)C77C(=C(C=C77)C78C(=C(C=C78)C79C(=C(C=C79)C80C(=C(C=C80)C81C(=C(C=C81)C82C(=C(C=C82)C83C(=C(C=C83)C84C(=C(C=C84)C85C(=C(C=C85)C86C(=C(C=C86)C87C(=C(C=C87)C88C(=C(C=C88)C89C(=C(C=C89)C90C(=C(C=C90)C91C(=C(C=C91)C92C(=C(C=C92)C93C(=C(C=C93)C94C(=C(C=C94)C95C(=C(C=C95)C96C(=C(C=C96)C97C(=C(C=C97)C98C(=C(C=C98)C99C(=C(C=C99)C100C(=C(C=C100)C101C(=C(C=C101)C102C(=C(C=C102)C103C(=C(C=C103)C104C(=C(C=C104)C105C(=C(C=C105)C106C(=C(C=C106)C107C(=C(C=C107)C108C(=C(C=C108)C109C(=C(C=C109)C110C(=C(C=C110)C111C(=C(C=C111)C112C(=C(C=C112)C113C(=C(C=C113)C114C(=C(C=C114)C115C(=C(C=C115)C116C(=C(C=C116)C117C(=C(C=C117)C118C(=C(C=C118)C119C(=C(C=C119)C120C(=C(C=C120)C121C(=C(C=C121)C122C(=C(C=C122)C123C(=C(C=C123)C124C(=C(C=C124)C125C(=C(C=C125)C126C(=C(C=C126)C127C(=C(C=C127)C128C(=C(C=C128)C129C(=C(C=C129)C130C(=C(C=C130)C131C(=C(C=C131)C132C(=C(C=C132)C133C(=C(C=C133)C134C(=C(C=C134)C135C(=C(C=C135)C136C(=C(C=C136)C137C(=C(C=C137)C138C(=C(C=C138)C139C(=C(C=C139)C140C(=C(C=C140)C141C(=C(C=C141)C142C(=C(C=C142)C143C(=C(C=C143)C144C(=C(C=C144)C145C(=C(C=C145)C146C(=C(C=C146)C147C(=C(C=C147)C148C(=C(C=C148)C149C(=C(C=C149)C150C(=C(C=C150)C151C(=C(C=C151)C152C(=C(C=C152)C153C(=C(C=C153)C154C(=C(C=C154)C155C(=C(C=C155)C156C(=C(C=C156)C157C(=C(C=C157)C158C(=C(C=C158)C159C(=C(C=C159)C160C(=C(C=C160)C161C(=C(C=C161)C162C(=C(C=C162)C163C(=C(C=C163)C164C(=C(C=C164)C165C(=C(C=C165)C166C(=C(C=C166)C167C(=C(C=C167)C168C(=C(C=C168)C169C(=C(C=C169)C170C(=C(C=C170)C171C(=C(C=C171)C172C(=C(C=C172)C173C(=C(C=C173)C174C(=C(C=C174)C175C(=C(C=C175)C176C(=C(C=C176)C177C(=C(C=C177)C178C(=C(C=C178)C179C(=C(C=C179)C180C(=C(C=C180)C181C(=C(C=C181)C182C(=C(C=C182)C183C(=C(C=C183)C184C(=C(C=C184)C185C(=C(C=C185)C186C(=C(C=C186)C187C(=C(C=C187)C188C(=C(C=C188)C189C(=C(C=C189)C190C(=C(C=C190)C191C(=C(C=C191)C192C(=C(C=C192)C193C(=C(C=C193)C194C(=C(C=C194)C195C(=C(C=C195)C196C(=C(C=C196)C197C(=C(C=C197)C198C(=C(C=C198)C199C(=C(C=C199)C200C(=C(C=C200)C201C(=C(C=C201)C202C(=C(C=C202)C203C(=C(C=C203)C204C(=C(C=C204)C205C(=C(C=C205)C206C(=C(C=C206)C207C(=C(C=C207)C208C(=C(C=C208)C209C(=C(C=C209)C210C(=C(C=C210)C211C(=C(C=C211)C212C(=C(C=C212)C213C(=C(C=C213)C214C(=C(C=C214)C215C(=C(C=C215)C216C(=C(C=C216)C217C(=C(C=C217)C218C(=C(C=C218)C219C(=C(C=C219)C220C(=C(C=C220)C221C(=C(C=C221)C222C(=C(C=C222)C223C(=C(C=C223)C224C(=C(C=C224)C225C(=C(C=C225)C226C(=C(C=C226)C227C(=C(C=C227)C228C(=C(C=C228)C229C(=C(C=C229)C230C(=C(C=C230)C231C(=C(C=C231)C232C(=C(C=C232)C233C(=C(C=C233)C234C(=C(C=C234)C235C(=C(C=C235)C236C(=C(C=C236)C237C(=C(C=C237)C238C(=C(C=C238)C239C(=C(C=C239)C240C(=C(C=C240)C241C(=C(C=C241)C242C(=C(C=C242)C243C(=C(C=C243)C244C(=C(C=C244)C245C(=C(C=C245)C246C(=C(C=C246)C247C(=C(C=C247)C248C(=C(C=C248)C249C(=C(C=C249)C250C(=C(C=C250)C251C(=C(C=C251)C252C(=C(C=C252)C253C(=C(C=C253)C254C(=C(C=C254)C255C(=C(C=C255)C256C(=C(C=C256)C257C(=C(C=C257)C258C(=C(C=C258)C259C(=C(C=C259)C260C(=C(C=C260)C261C(=C(C=C261)C262C(=C(C=C262)C263C(=C(C=C263)C264C(=C(C=C264)C265C(=C(C=C265)C266C(=C(C=C266)C267C(=C(C=C267)C268C(=C(C=C268)C269C(=C(C=C269)C270C(=C(C=C270)C271C(=C(C=C271)C272C(=C(C=C272)C273C(=C(C=C273)C274C(=C(C=C274)C275C(=C(C=C275)C276C(=C(C=C276)C277C(=C(C=C277)C278C(=C(C=C278)C279C(=C(C=C279)C280C(=C(C=C280)C281C(=C(C=C281)C282C(=C(C=C282)C283C(=C(C=C283)C284C(=C(C=C284)C285C(=C(C=C285)C286C(=C(C=C286)C287C(=C(C=C287)C288C(=C(C=C288)C289C(=C(C=C289)C290C(=C(C=C290)C291C(=C(C=C291)C292C(=C(C=C292)C293C(=C(C=C293)C294C(=C(C=C294)C295C(=C(C=C295)C296C(=C(C=C296)C297C(=C(C=C297)C298C(=C(C=C298)C299C(=C(C=C299)C300C

Chemical structure of compound 10b is shown. The ^{13}C NMR spectrum (CDCl₃) displays the following chemical shifts (ppm): 173.38, 171.11, 170.74, 168.56, 142.81, 141.40, 140.52, 134.05, 133.62, 133.39, 132.17, 122.29, 118.22, 111.46, 81.37, 77.44, 77.23, 77.02, 76.28, 72.89, 69.37, 60.12, 52.47, 51.80, 49.43, 45.15, 37.26, 34.75, 33.01, 29.92, 28.89, 26.18, 26.10, 21.28, 21.09, and 13.03.

Figure S65. HSQC spectrum of aphanamixoid I (**7**) in CDCl₃

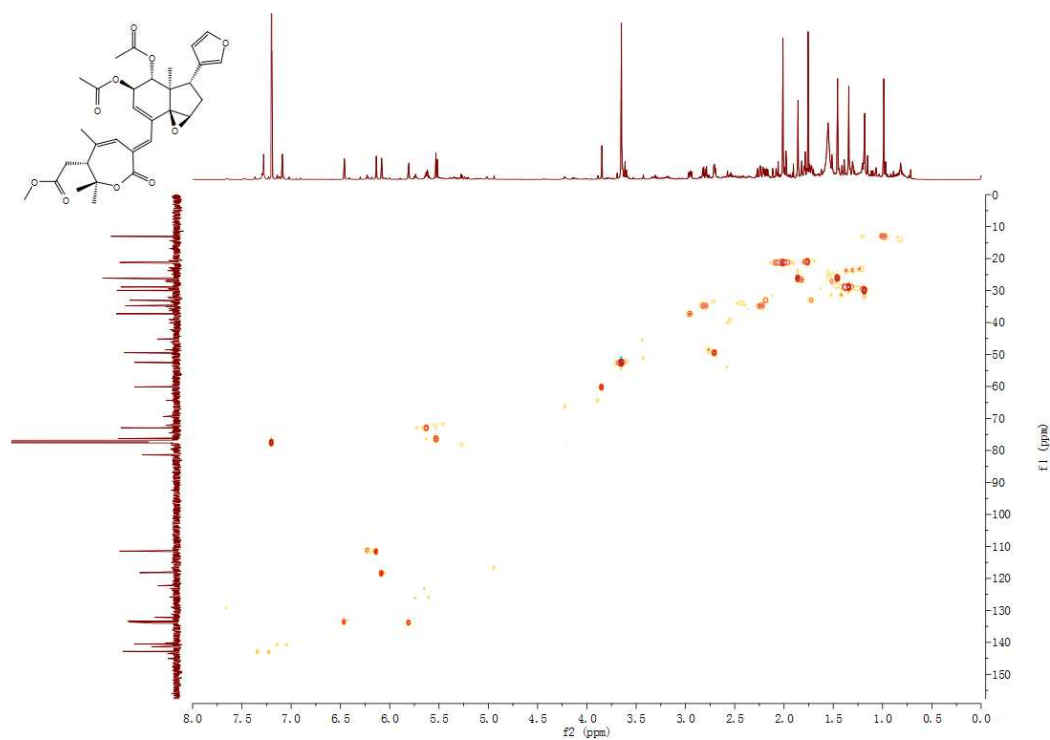


Figure S66. HMBC spectrum of aphanamixoid I (**7**) in CDCl₃

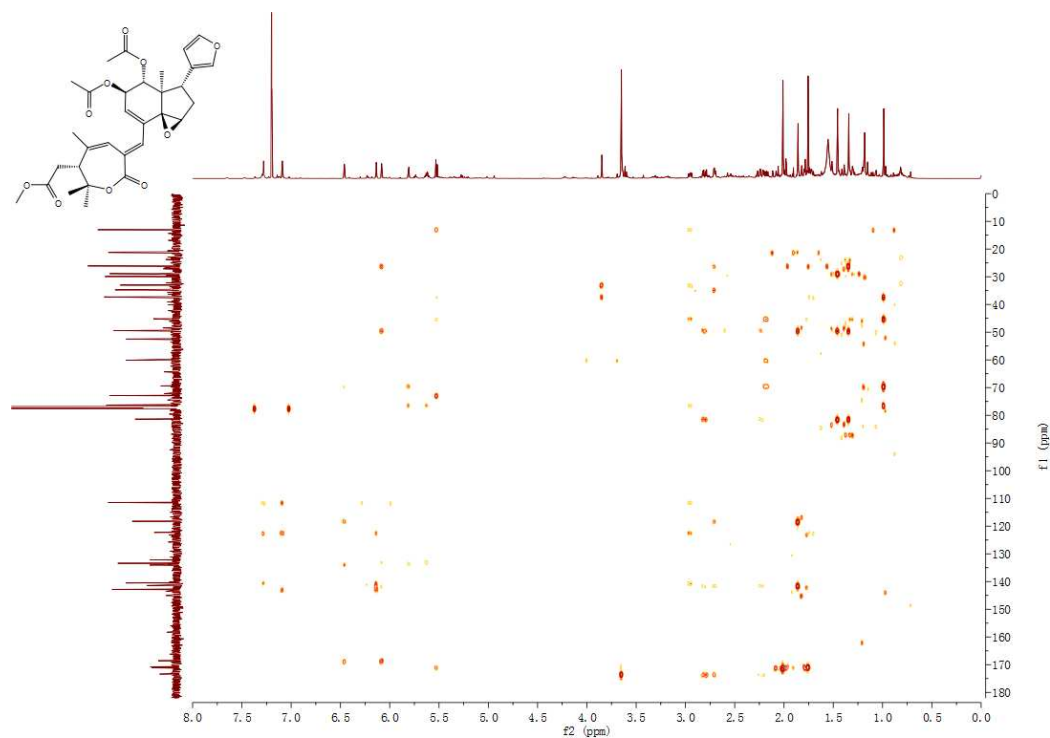


Figure S67. ^1H - ^1H COSY spectrum of aphanamixoid I (7) in CDCl_3

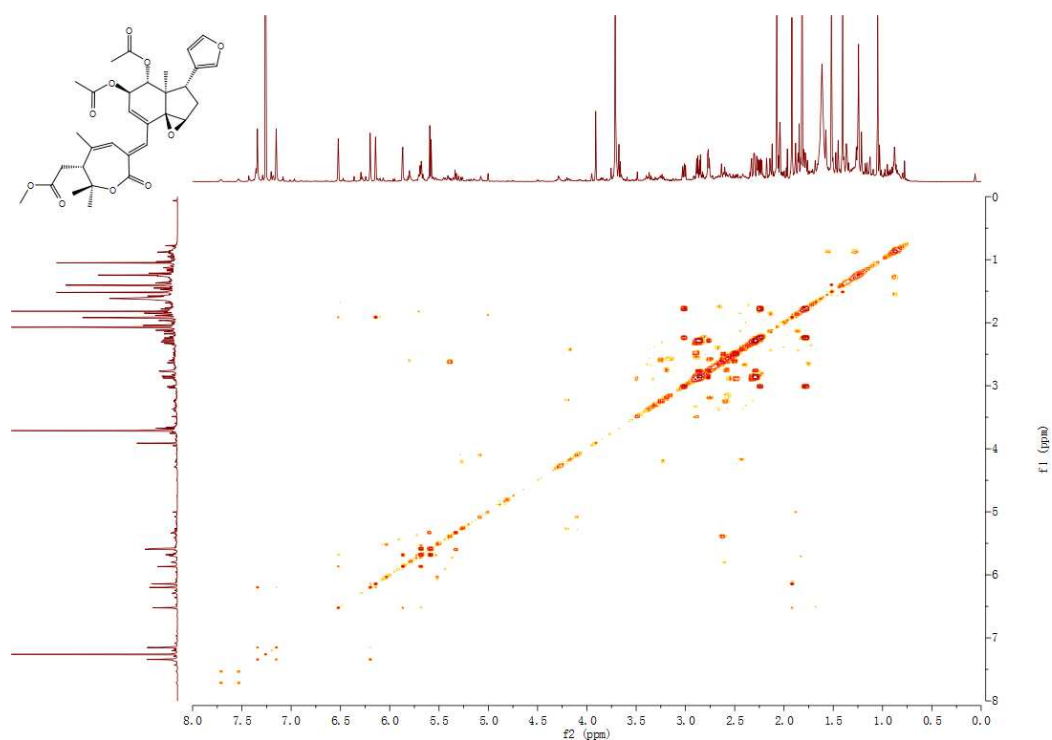


Figure S68. ROESY spectrum of aphanamixoid I (7) in CDCl_3

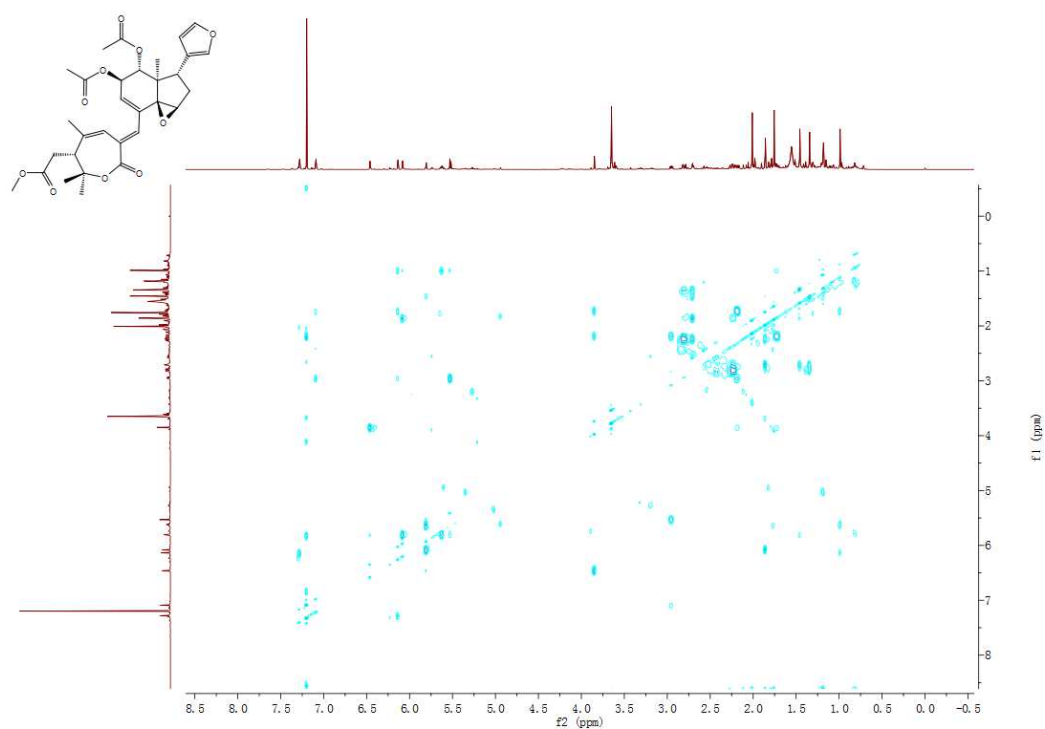


Figure S69. ESI (+) MS of aphanamixoid I (7)

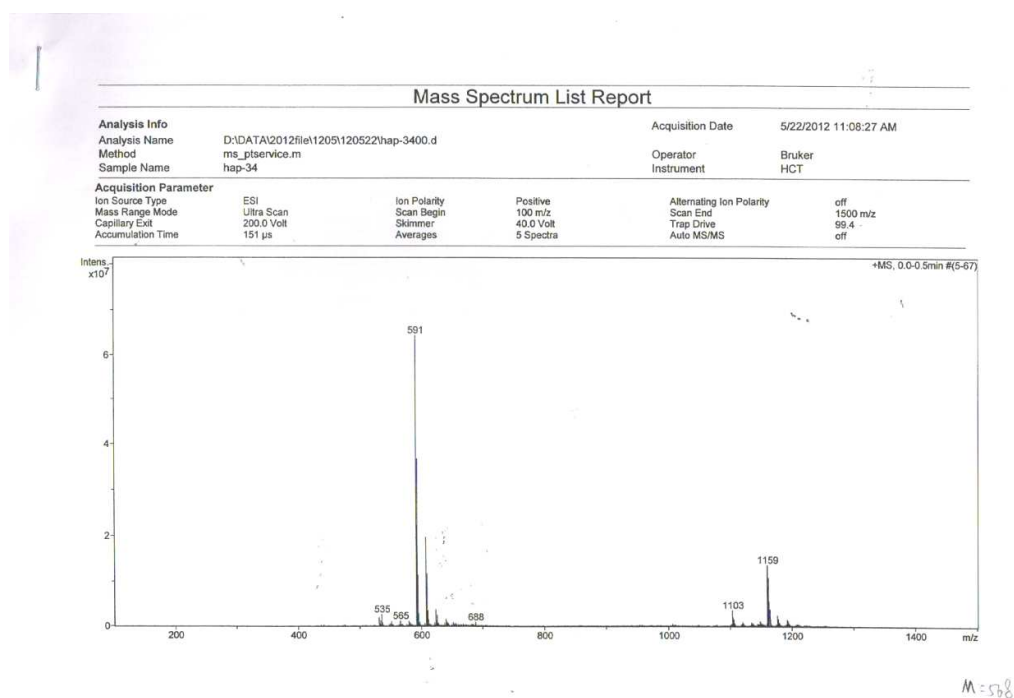


Figure S70. HR-EI (+) MS of aphanamixoid I (7)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

29 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

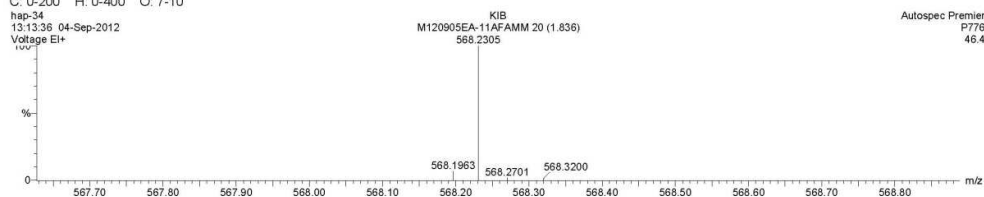
Elements Used:

C: 0-200 H: 0-400 O: 7-10

hap-34

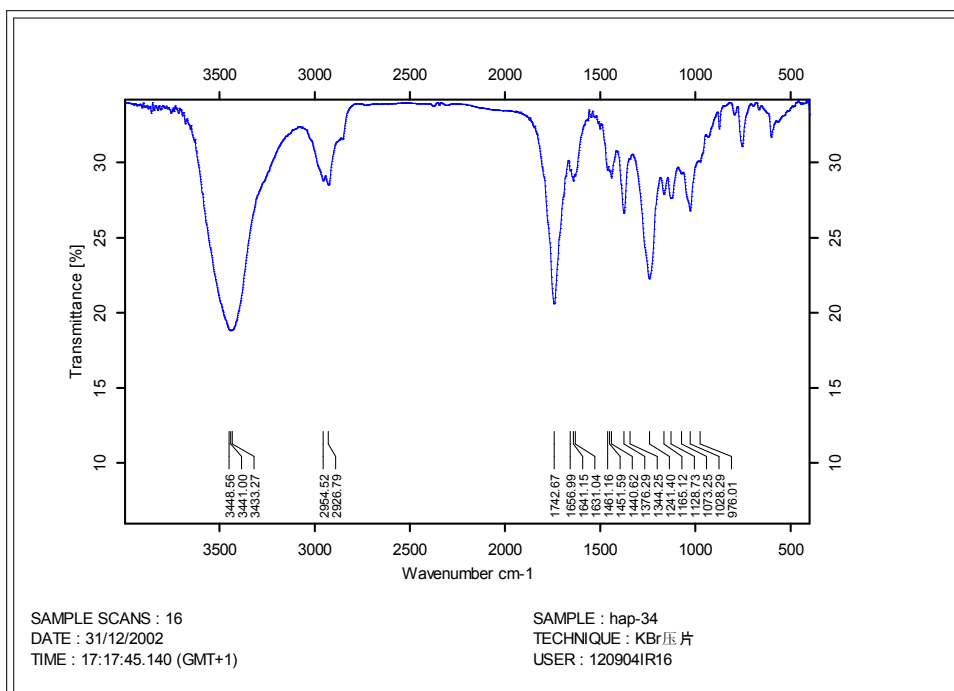
13:13:36 04-Sep-2012

Voltage EI+



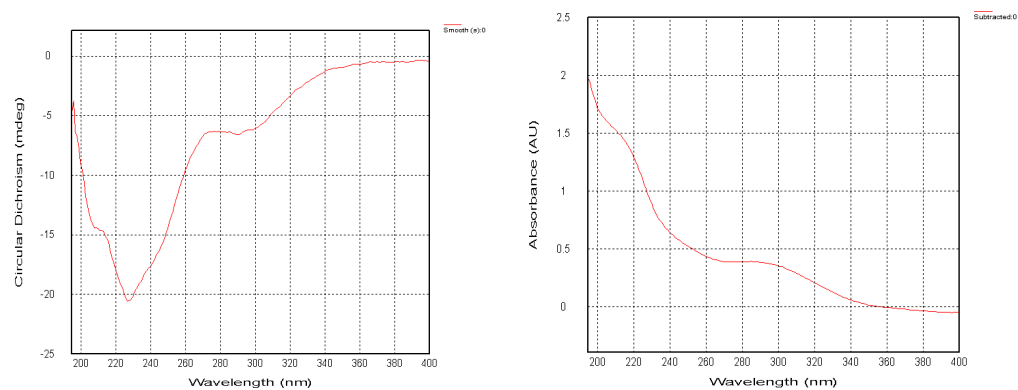
Minimum:						
Maximum:	100.0	10.0	-10.0			
			120.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
568.2305	568.2308	-0.3	-0.5	14.0	5546042.5	C31 H36 O10

Figure S71. IR spectrum of aphanamixoid I (7)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
566.509	0.327	0.002	23.434	0.730121	0
601.531	0.317	0.024	15.196	15.109008	0
754.645	0.311	0.030	25.806	19.110735	0
794.561	0.332	0.007	16.857	3.596402	0
873.726	0.322	0.012	8.646	7.301173	0
933.111	0.317	0.004	29.793	1.037559	0
976.005	0.300	0.001	24.553	0.487406	0
1028.288	0.268	0.033	34.590	18.897408	0
1073.254	0.293	0.002	14.908	0.505345	0
1128.726	0.276	0.018	27.054	9.189581	0
1165.122	0.279	0.011	18.611	7.319848	0
1241.397	0.222	0.115	64.289	73.285919	0
1344.245	0.302	0.001	5.112	0.187349	0
1376.289	0.266	0.045	27.222	25.657572	0
1414.648	0.307	0.001	3.812	0.415845	0
1440.616	0.290	0.023	13.273	11.824325	0
1451.587	0.294	0.002	4.809	0.504454	0
1461.162	0.295	0.005	12.680	2.031492	0
1631.039	0.291	0.004	14.843	0.924386	0
1641.154	0.288	0.022	12.667	9.080729	0
1656.987	0.294	0.002	4.281	0.759645	0
1742.671	0.206	0.135	65.708	87.315880	0
1832.453	0.319	0.000	11.110	0.098043	0
2853.958	0.315	0.001	10.455	0.746336	0
2926.790	0.285	0.043	21.609	25.438162	0
2954.521	0.288	0.006	40.397	2.167369	0
3147.898	0.317	0.000	7.682	0.097675	0
3433.273	0.188	0.000	51.936	0.018530	0
3441.004	0.188	0.152	6.199	98.873955	0
3448.564	0.189	0.000	178.780	0.027276	0
3632.215	0.314	0.002	13.616	1.285446	0

Figure S72. CD spectrum of aphanamixoid I (7)



File: CD HAP-34-1mm(195-400)12090415.dsx

ProBinaryX

Attributes :

- Time Stamp :Tue Sep 04 15:50:01 2012

- File ID : {88623781-C993-4a27-B45C-2410B8A0323F}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.6300mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Chemical structure of compound 10 is shown in the upper left. The ^1H NMR spectrum (CDCl₃) shows peaks at the following chemical shifts (ppm): 7.2869, 7.0696, 6.6144, 6.6028, 6.5661, 6.1820, 5.9080, 5.7864, 5.7707, 5.7692, 5.7658, 5.6969, 5.6809, 3.9422, 3.7391, 3.0645, 3.0569, 2.9191, 2.9075, 2.8850, 2.8735, 2.8018, 2.7922, 2.7813, 2.3400, 2.3313, 2.3060, 2.2974, 2.2792, 2.2652, 2.2513, 2.2370, 2.0691, 1.9435, 1.8465, 1.8244, 1.8189, 1.7966, 1.7530, 1.7388, 1.6353, 1.5489, 1.4353, 1.1020.

Chemical structure of compound 10a is shown in the top left corner. The ¹³C NMR spectrum (CDCl₃) is displayed below, with the following chemical shifts (ppm) labeled:

Chemical Shift (ppm)
173.06
170.77
168.13
167.21
142.26
141.13
140.61
137.99
133.80
133.56
133.44
132.07
128.19
121.89
118.17
111.23
81.10
77.23
76.97
76.72
76.09
72.90
69.27
59.90
52.10
49.43
45.30
37.15
34.68
32.74
28.71
25.95
25.90
20.95
14.27
12.98
11.61

Figure S75. HSQC spectrum of aphanamixoid J (**8**) in CDCl₃

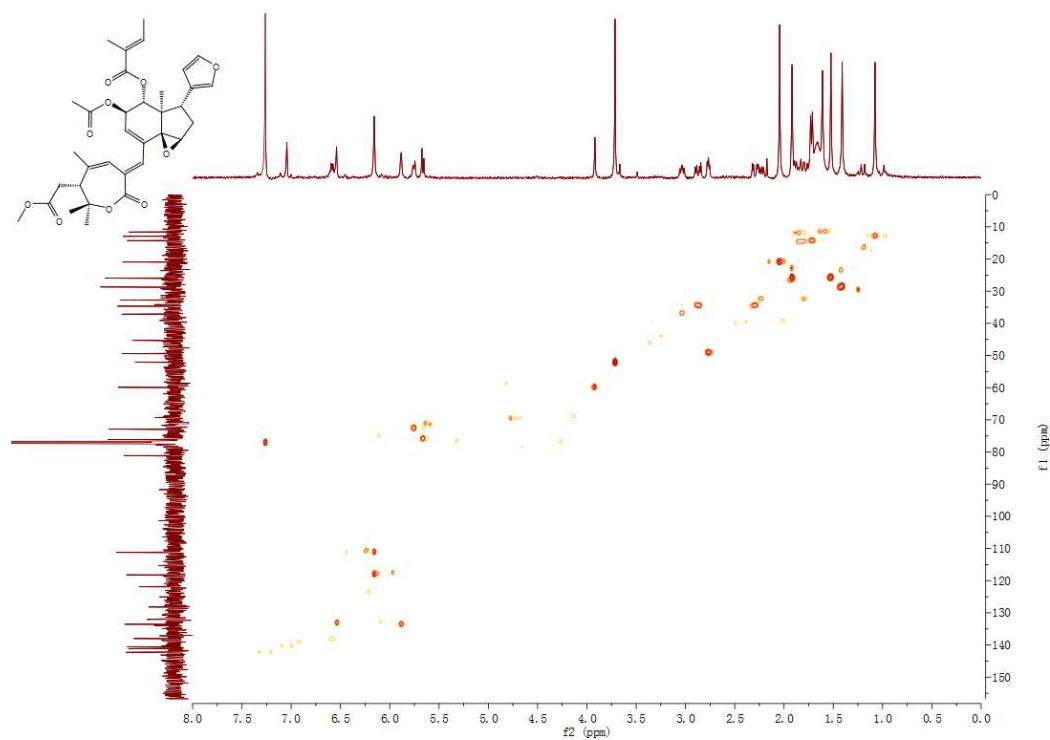


Figure S76. HMBC spectrum of aphanamixoid J (**8**) in CDCl₃

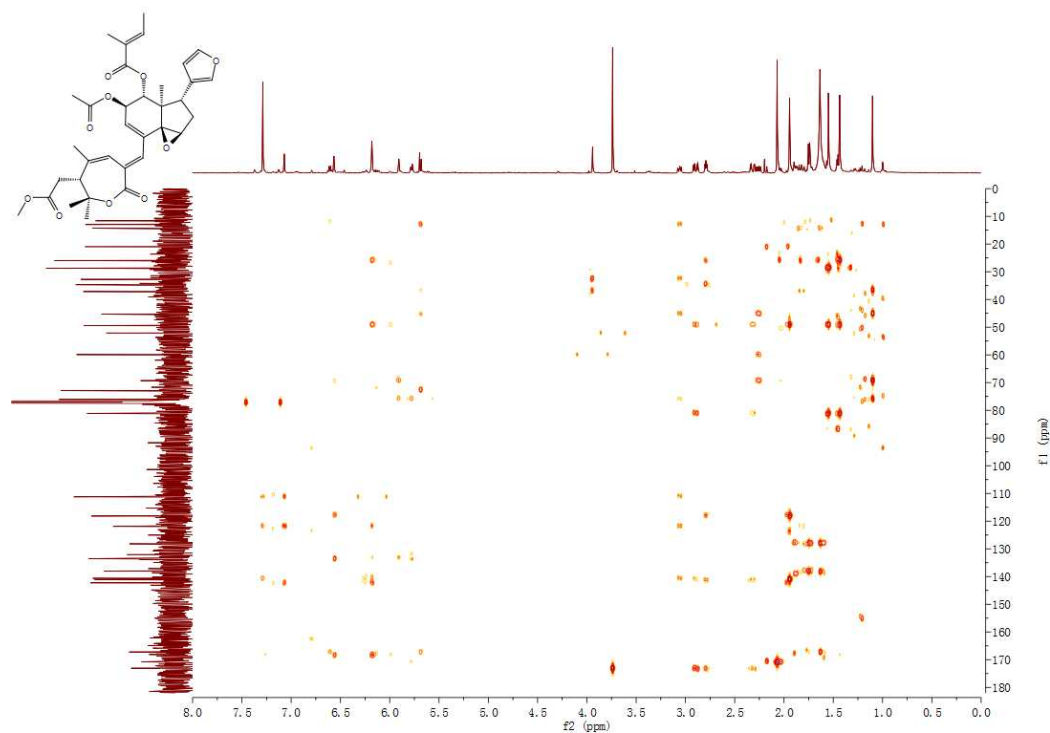


Figure S77. ^1H - ^1H COSY spectrum of aphanamixoid J (**8**) in CDCl_3

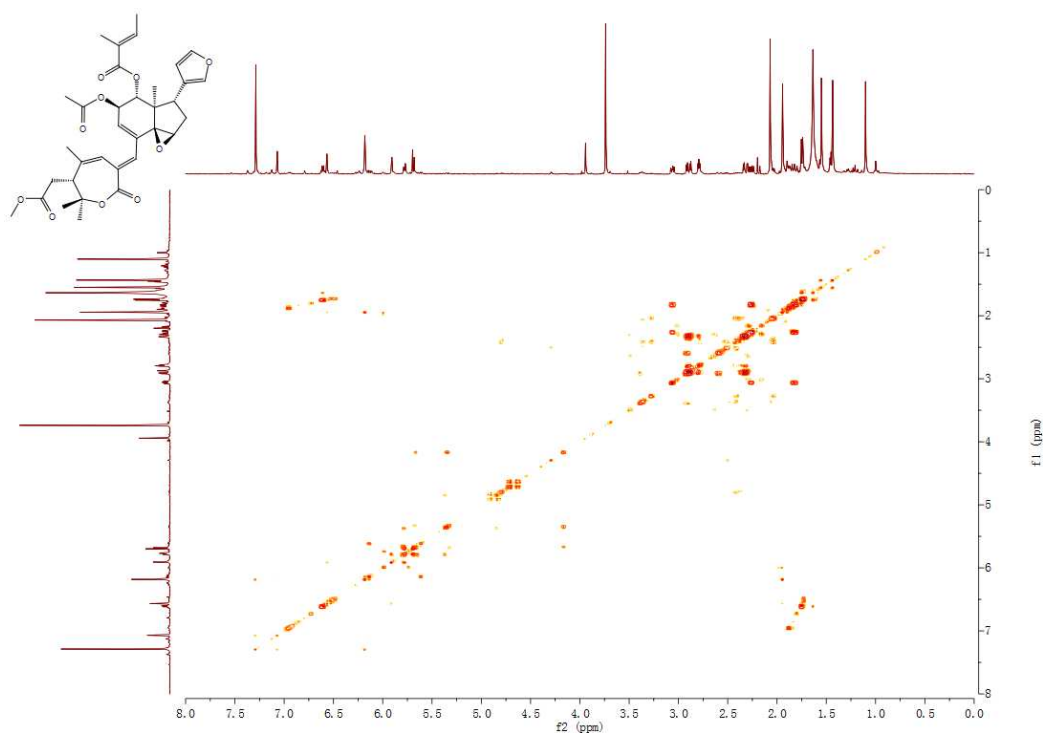


Figure S78. ROESY spectrum of aphanamixoid J (**8**) in CDCl_3

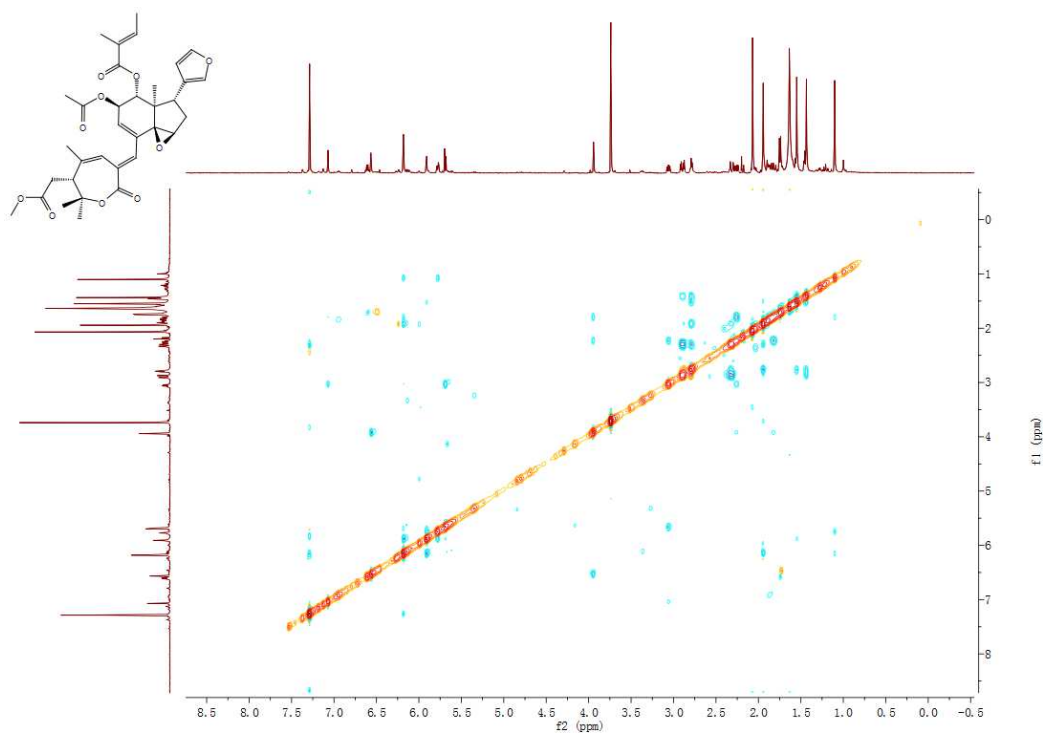


Figure S79. ESI (+) MS of aphanamixoid J (8)

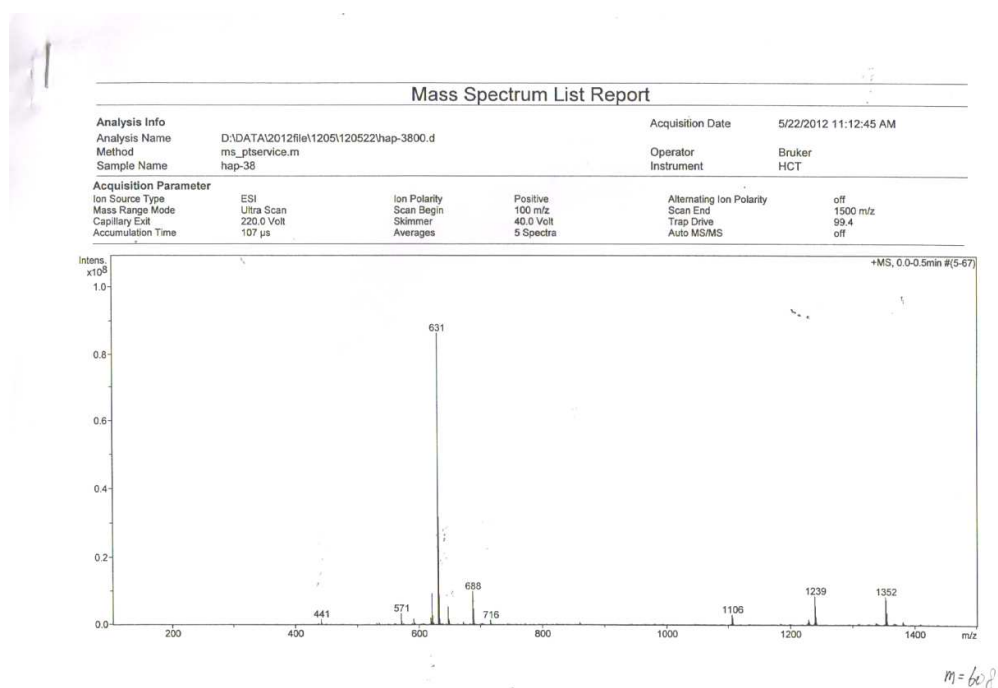


Figure S80. HR-EI (+) MS of aphanamixoid J (8)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

31 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

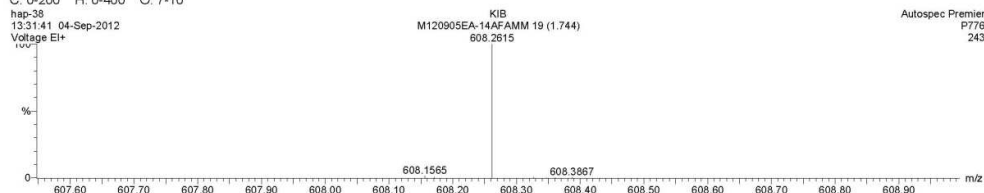
Elements Used:

C: 0-200 H: 0-400 O: 7-10

hap-38

13.31.41 04-Sep-2012

Voltage EI+

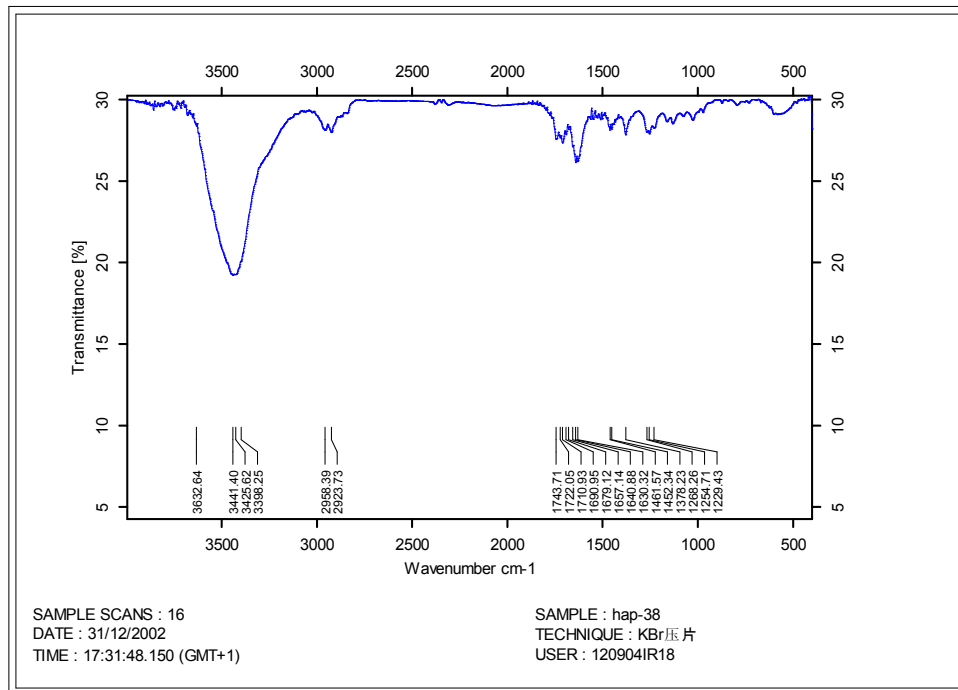


Autospec Premier
P776
243

Minimum: -10.0
Maximum: 100.0 10.0 120.0

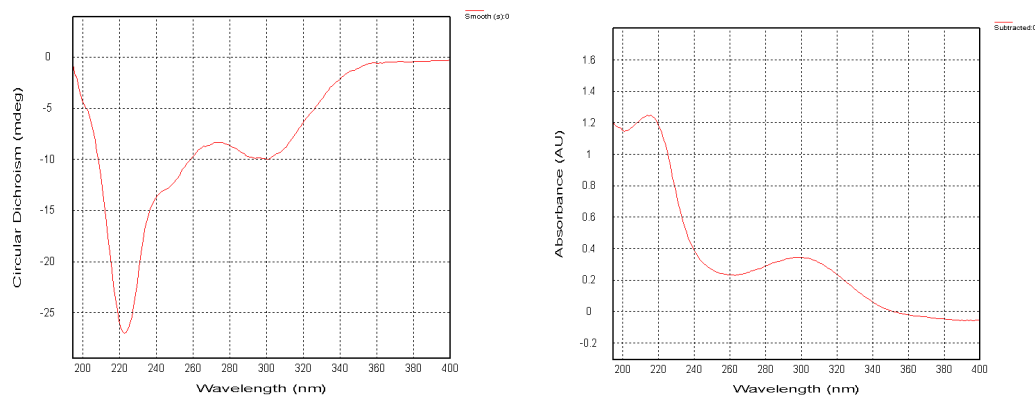
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
608.2615	608.2621	-0.6	-1.0	15.0	5546141.0	C34 H40 O10

Figure S81. IR spectrum of aphanamixoid J (8)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
582.625	0.291	0.010	7.695	8.611174	0
602.088	0.291	0.002	12.828	0.723808	0
623.513	0.295	0.001	7.394	0.573596	0
795.805	0.296	0.004	10.032	3.294452	0
974.425	0.292	0.002	14.987	2.019695	0
1000.452	0.292	0.001	9.183	0.390389	0
1027.897	0.287	0.006	21.109	4.789096	0
1076.025	0.290	0.002	17.437	1.898821	0
1131.653	0.285	0.007	18.888	5.893352	0
1163.792	0.286	0.004	18.846	2.331362	0
1229.429	0.282	0.002	15.886	1.244092	0
1254.708	0.279	0.015	9.621	12.756756	0
1268.258	0.280	0.003	9.737	1.017297	0
1359.312	0.287	0.001	4.480	0.346666	0
1378.225	0.278	0.018	11.347	14.938067	0
1433.152	0.286	0.002	3.633	1.128446	0
1441.736	0.285	0.002	5.442	0.630430	0
1452.337	0.282	0.004	5.278	3.215676	0
1461.574	0.281	0.011	4.338	8.706665	0
1630.315	0.262	0.003	16.777	2.991292	0
1640.880	0.261	0.040	11.962	35.270714	0
1657.143	0.271	0.001	4.996	1.233581	0
1679.118	0.281	0.003	4.758	1.978519	0
1690.953	0.278	0.004	7.609	2.047164	0
1710.925	0.273	0.012	11.492	10.250178	0
1722.050	0.276	0.002	10.170	1.581927	0
1743.712	0.275	0.005	7.625	4.169638	0
2923.726	0.280	0.015	22.174	12.592999	0
2958.390	0.281	0.005	28.292	3.255254	0
3398.248	0.201	0.000	17.161	0.240556	0
3425.616	0.193	0.001	24.306	0.268215	0
3441.401	0.192	0.108	25.882	98.069359	0
3632.640	0.283	0.002	15.139	1.716102	0

Figure S82. CD spectrum of aphanamixoid J (8)



File: CD HAP-38-1mm(195-400)12090418.dsx

ProBinaryX

Attributes :

- Time Stamp :Tue Sep 04 16:19:25 2012

- File ID : {FF769333-431F-4276-8496-BDB84A2BE7B8}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.3400mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Figure S83. ^1H NMR spectrum of aphanamixoid K (**9**) in CDCl_3

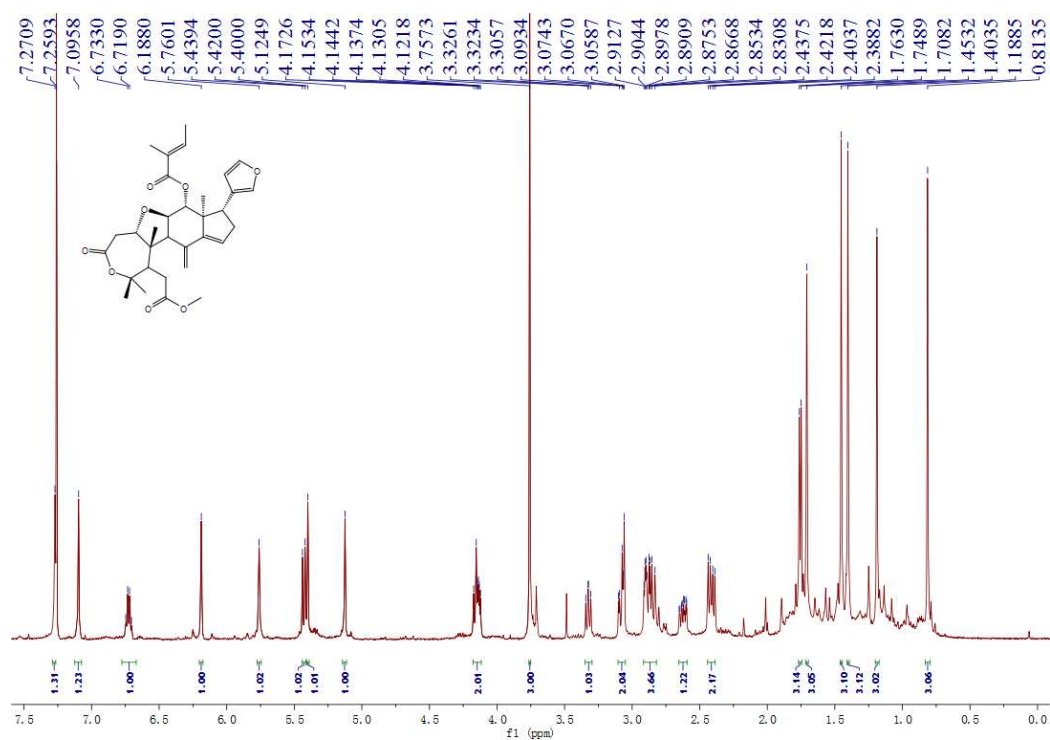


Figure S84. ^{13}C NMR spectrum of aphanamixoid K (**9**) in CDCl_3

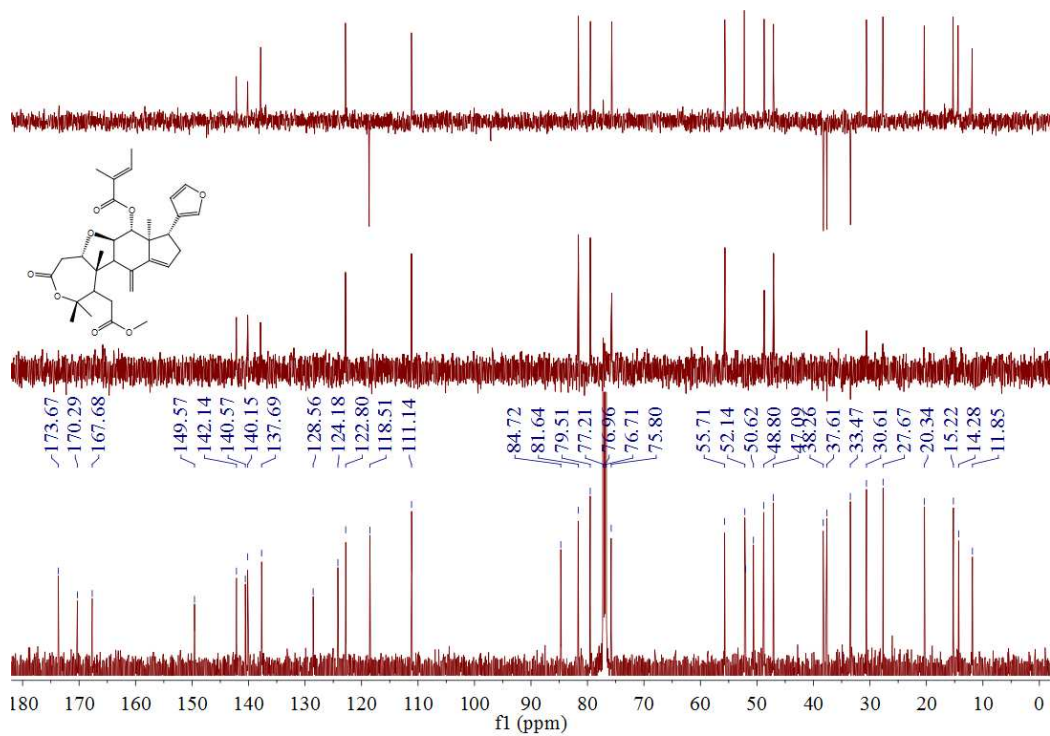


Figure S85. HSQC spectrum of aphanamixoid K (**9**) in CDCl₃

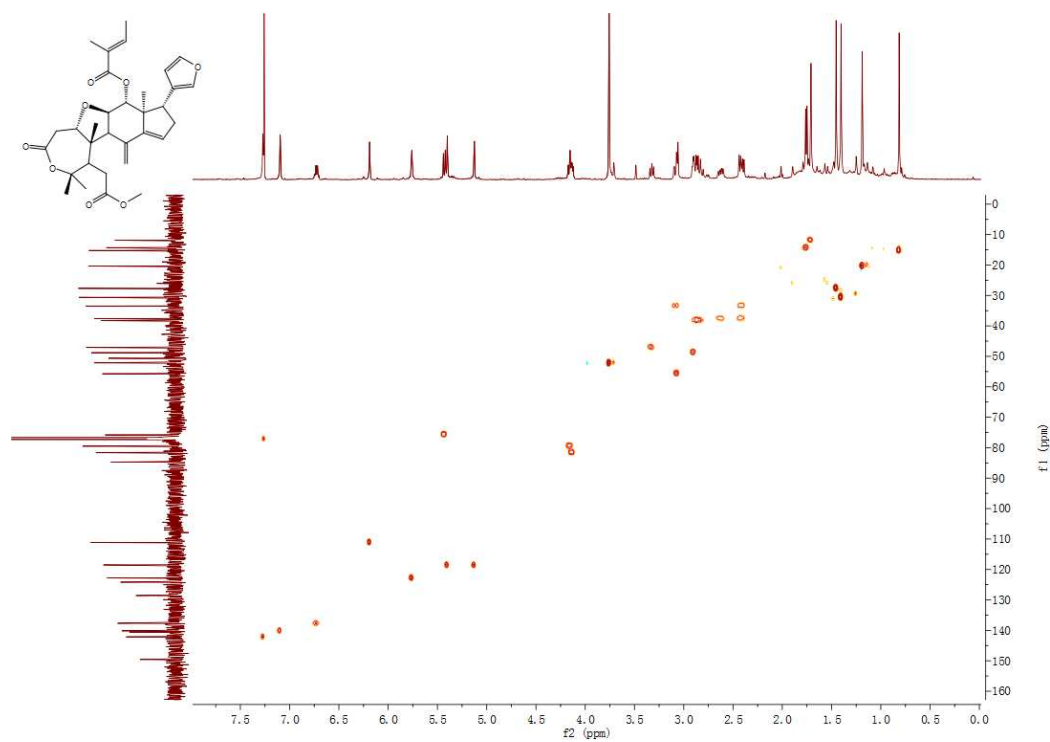


Figure S86. HMBC spectrum of aphanamixoid K (**9**) in CDCl₃

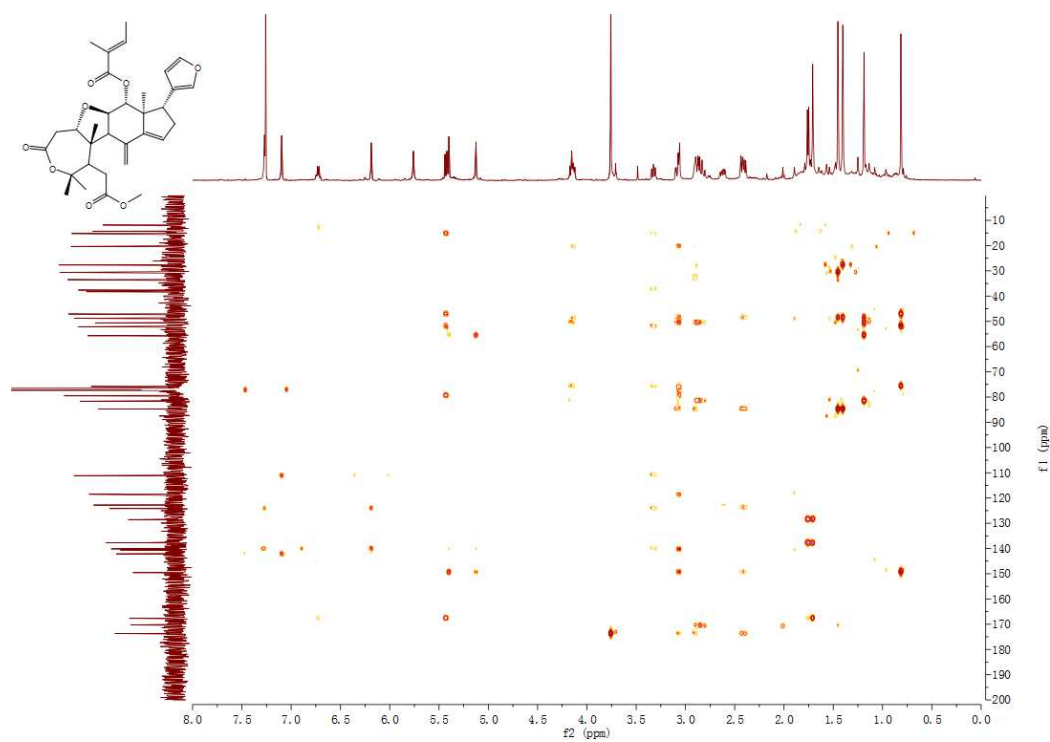


Figure S87. ^1H - ^1H COSY spectrum of aphanamixoid K (9) in CDCl_3

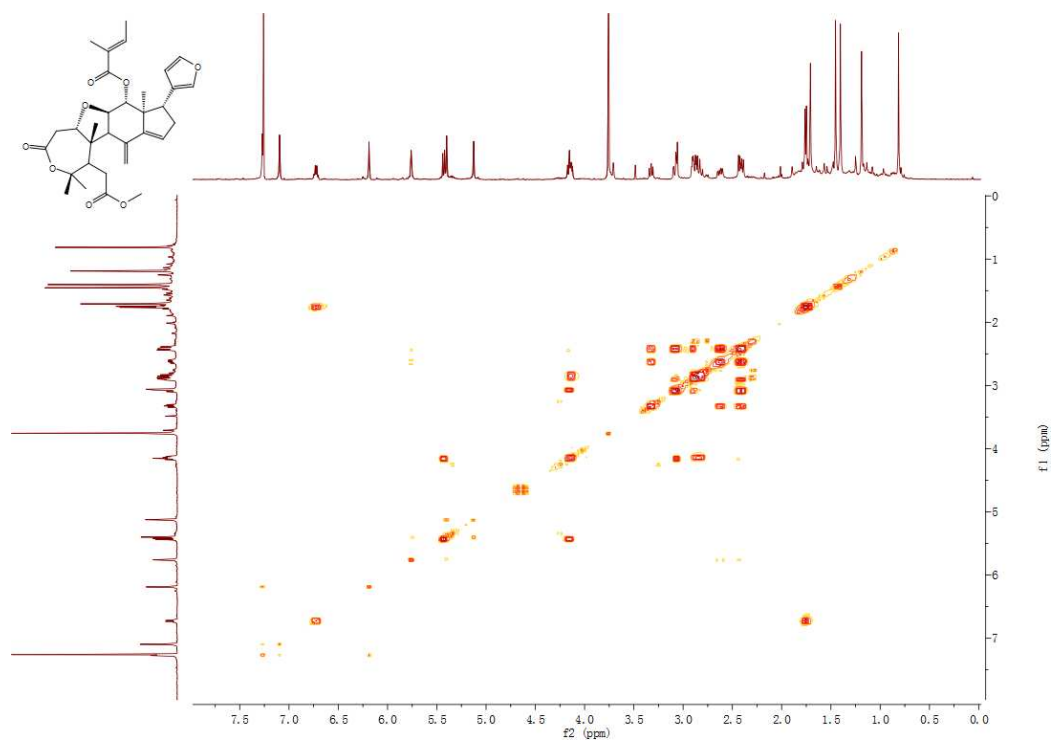


Figure S88. ROESY spectrum of aphanamixoid K (9) in CDCl_3

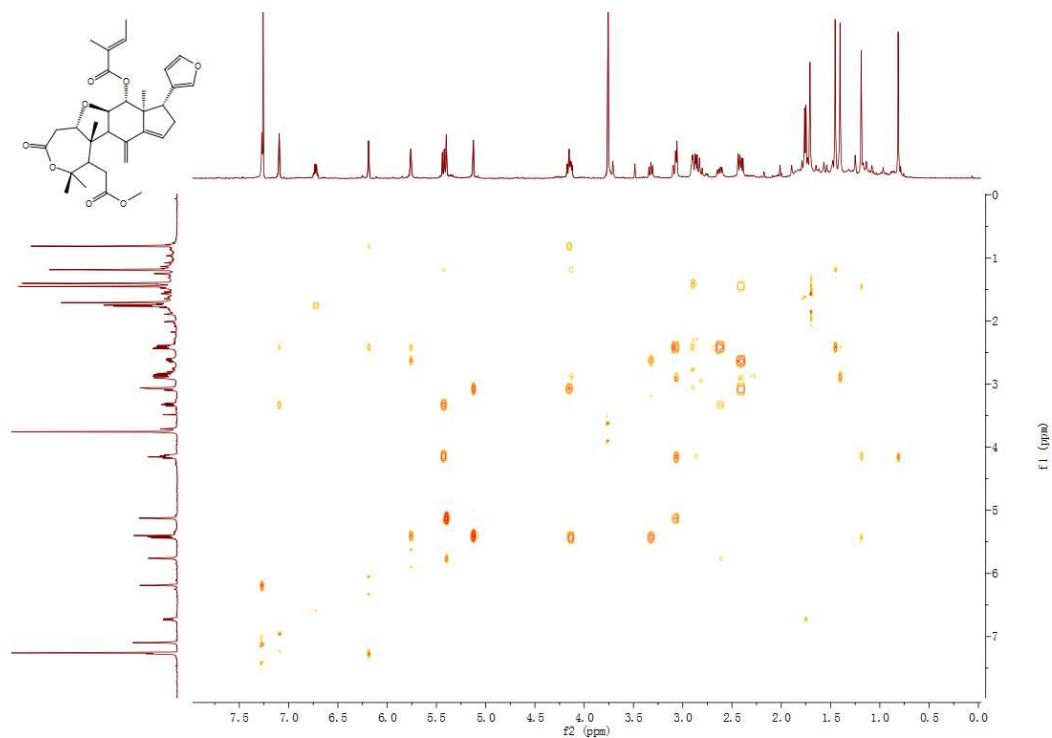


Figure S89. ESI (+) MS of aphanamixoid K (9)

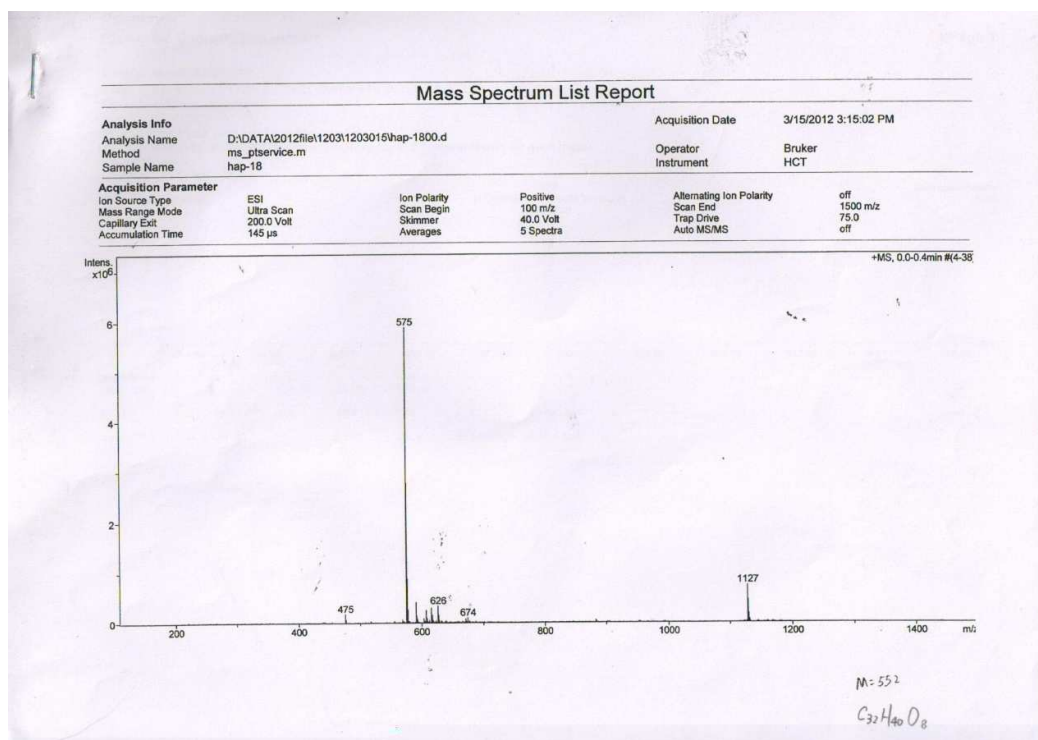


Figure S90. HR-EI (+) MS of aphanamixoid K (9)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

20 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 6-9

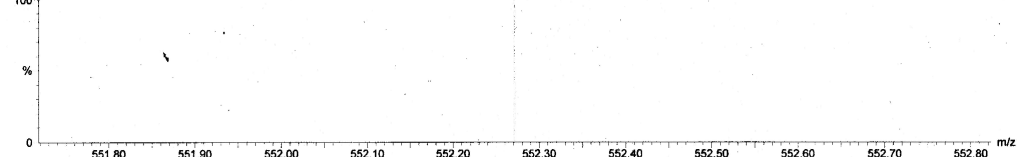
hap-18

15.14.34 05-Sep-2012

Voltage EI+

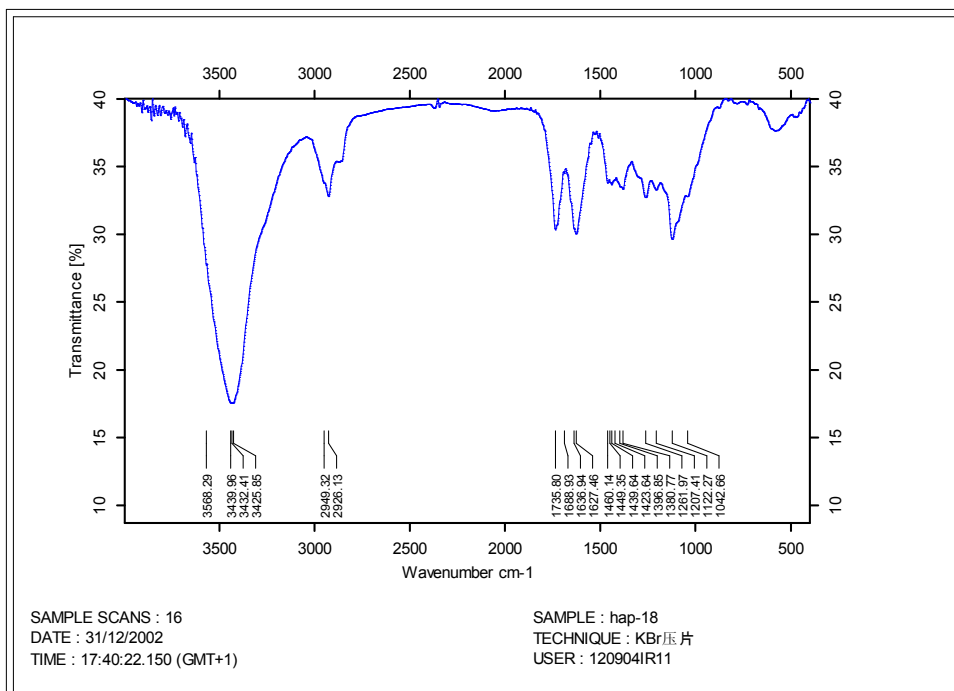
KIB
M120906EA-17AFMM 33 (3.029)
552.2709

Autospec Premier
P776
1



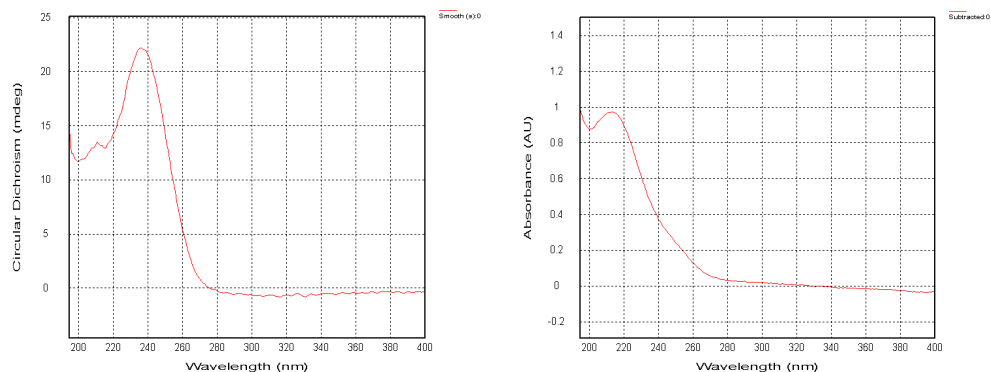
Minimum:				-10.0		
Maximum:	100.0	10.0	120.0			
Mass	Calc. Mass	mDa	PPM	DBE	1-FIT	Formula
552.2709	552.2723	-1.4	-2.5	13.0	5546026.0	C ₃₂ H ₄₀ O ₈

Figure S91. IR spectrum of aphanamixoid K (9)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
567.640	0.377	0.001	41.052	0.036824	0
583.308	0.376	0.024	14.614	10.569580	0
604.859	0.378	0.001	10.194	0.072799	0
1042.662	0.328	0.004	38.430	0.326232	0
1122.270	0.296	0.104	52.283	46.187241	0
1207.413	0.333	0.006	23.637	2.361092	0
1261.965	0.327	0.016	31.839	5.595063	0
1380.771	0.333	0.026	13.395	9.143389	0
1396.854	0.335	0.001	8.895	0.119989	0
1423.643	0.340	0.001	5.548	0.032317	0
1439.641	0.336	0.013	6.772	2.473884	0
1449.351	0.338	0.001	4.863	0.088865	0
1460.143	0.338	0.005	13.606	1.130831	0
1627.461	0.300	0.079	52.080	33.710754	0
1636.942	0.304	0.001	8.477	0.030342	0
1688.925	0.345	0.002	6.385	0.486094	0
1735.800	0.303	0.049	44.821	20.089136	0
2857.260	0.354	0.001	7.877	0.111930	0
2870.153	0.353	0.002	12.321	0.338666	0
2926.130	0.328	0.049	22.299	19.595989	0
2949.321	0.338	0.001	13.295	0.075053	0
3425.854	0.176	0.000	34.241	0.012911	0
3432.411	0.175	0.225	4.320	100.012260	0
3439.961	0.176	0.002	123.441	0.069525	0
3568.287	0.277	0.002	14.749	0.504520	0
3631.094	0.353	0.005	12.998	2.053776	0

Figure S92. CD spectrum of aphanamixoid K (9)



File: CD HAP-18-1mm(195-400)12052505.dsx

ProBinaryX

Attributes :

- Time Stamp :Fri May 25 13:44:00 2012

- File ID : {5E75909A-2670-4d05-B654-F52B1B197A85}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.4200mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Chemical structure of compound 10 is shown in the top left. The ^1H NMR spectrum (CDCl₃) shows peaks at the following chemical shifts (ppm): 7.3090, 7.1778, 6.2560, 5.7676, 5.3998, 5.3535, 5.3295, 5.1189, 4.1042, 4.0501, 3.7517, 3.3351, 3.0464, 3.0260, 2.9131, 2.9029, 2.8958, 2.8872, 2.8527, 2.8428, 2.8283, 2.4344, 2.4165, 2.3919, 2.3746, 2.2598, 2.2424, 1.5803, 1.5642, 1.5276, 1.4467, 1.3989, 1.3669, 1.3499, 1.3323, 1.3152, 1.1654, 0.9526, 0.9351, 0.8816, 0.8629, 0.8443, 0.8280.

Chemical structure of compound 10 is shown. The ^{13}C NMR spectrum (ppm) is displayed below the structure, with peaks labeled with their chemical shifts:

- 175.92
- 173.70
- 170.45
- 149.52
- 142.25
- 140.26
- 140.04
- 124.23
- 123.05
- 118.67
- 111.15
- 84.85
- 81.55
- 79.55
- 77.31
- 77.00
- 76.68
- 75.31
- 55.58
- 52.26
- 51.74
- 50.49
- 48.61
- 47.41
- 41.63
- 38.21
- 37.94
- 33.34
- 30.54
- 27.68
- 26.41
- 20.33
- 16.16
- 15.16
- 11.61

Figure S95. HSQC spectrum of aphanamixoid L (**10**) in CDCl₃

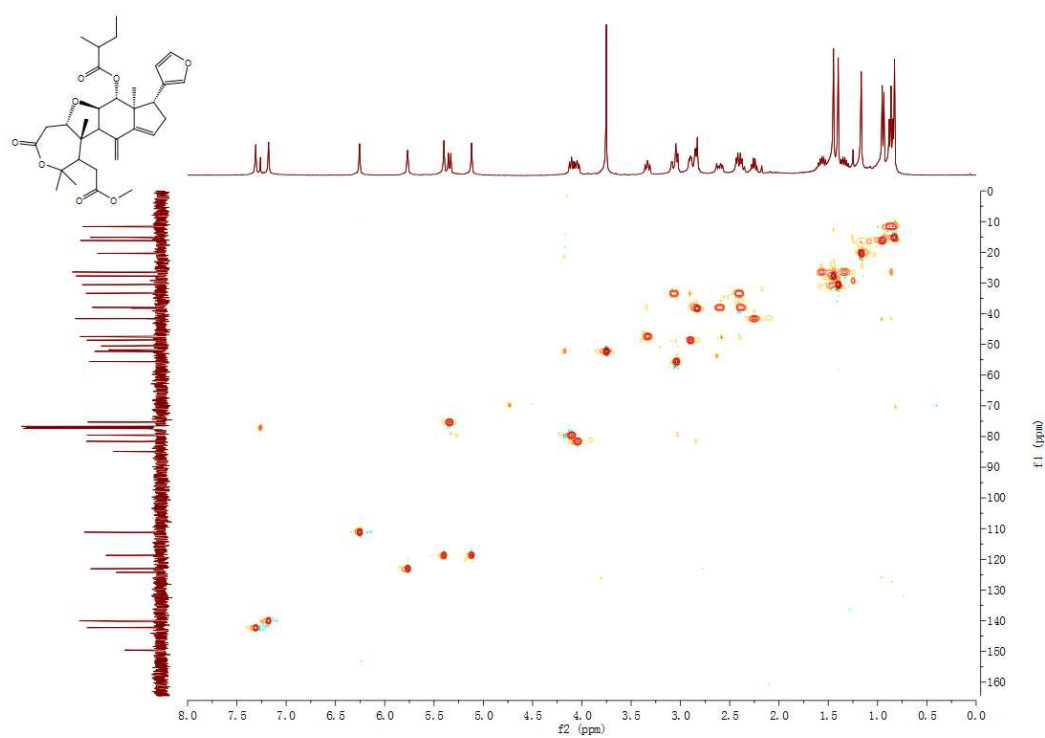


Figure S96. HMBC spectrum of aphanamixoid L (**10**) in CDCl₃

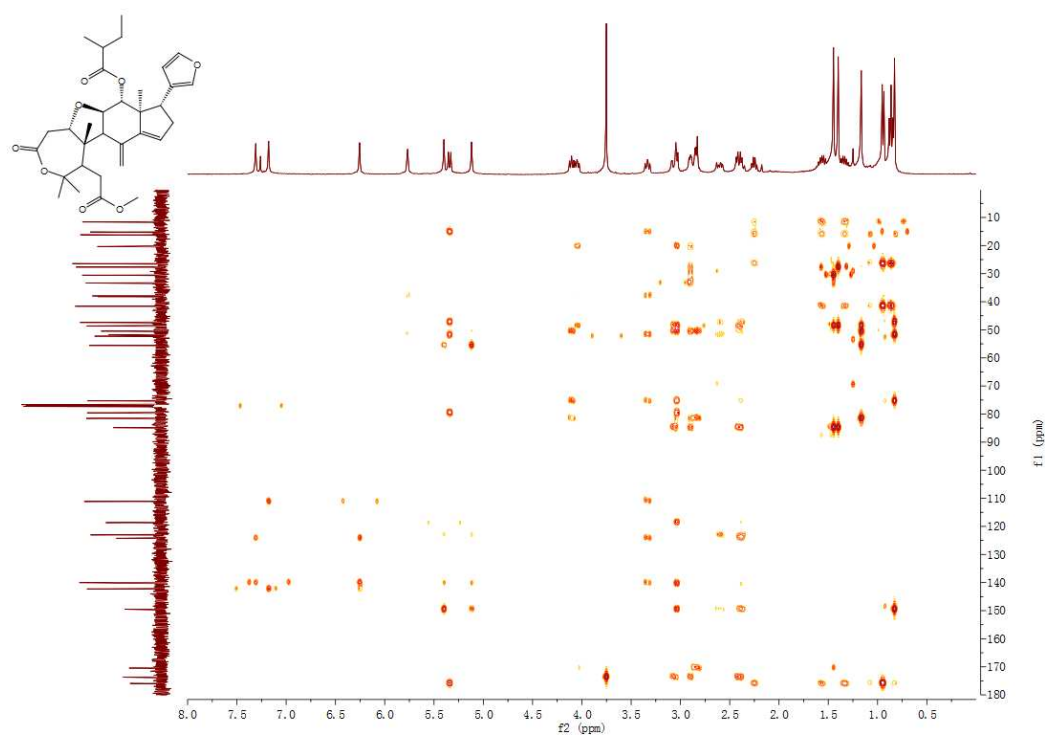


Figure S97. ^1H - ^1H COSY spectrum of aphanamixoid L (**10**) in CDCl_3

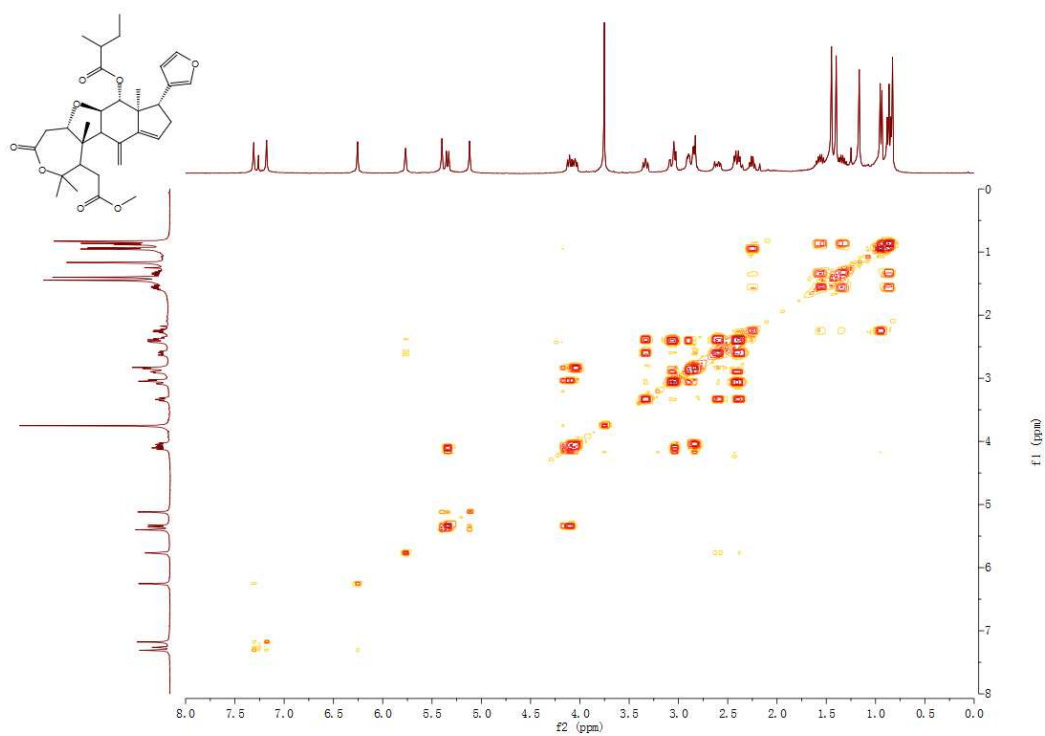


Figure S98. ROESY spectrum of aphanamixoid L (**10**) in CDCl_3

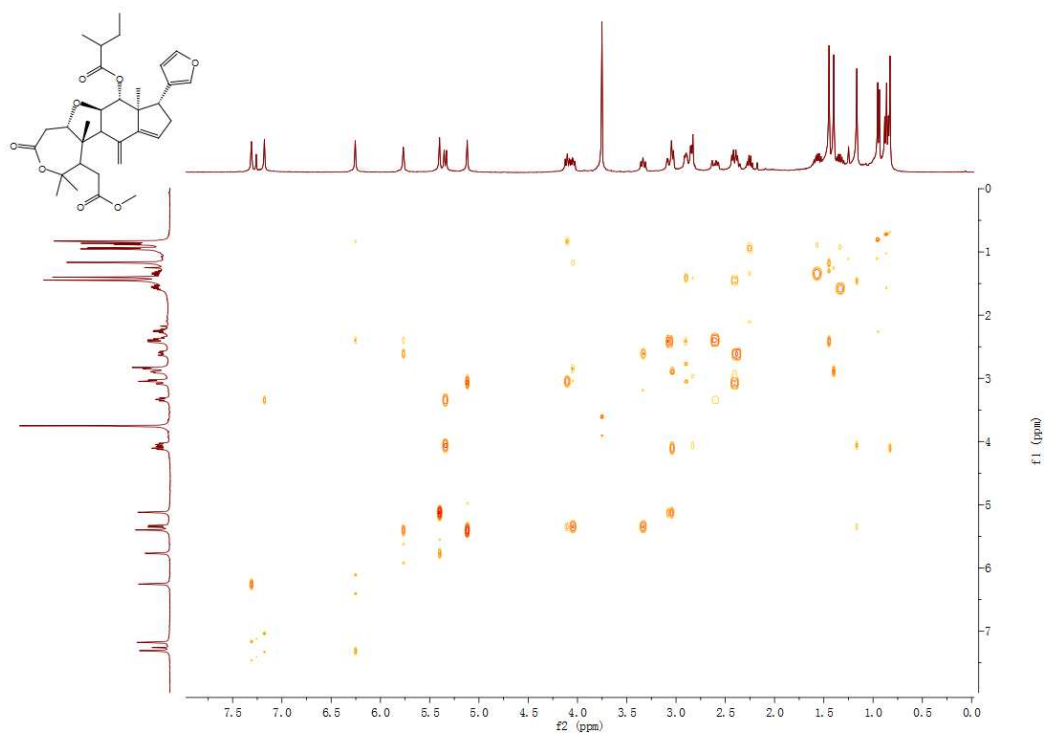


Figure S99. ESI (+) MS of aphanamixoid L (10)

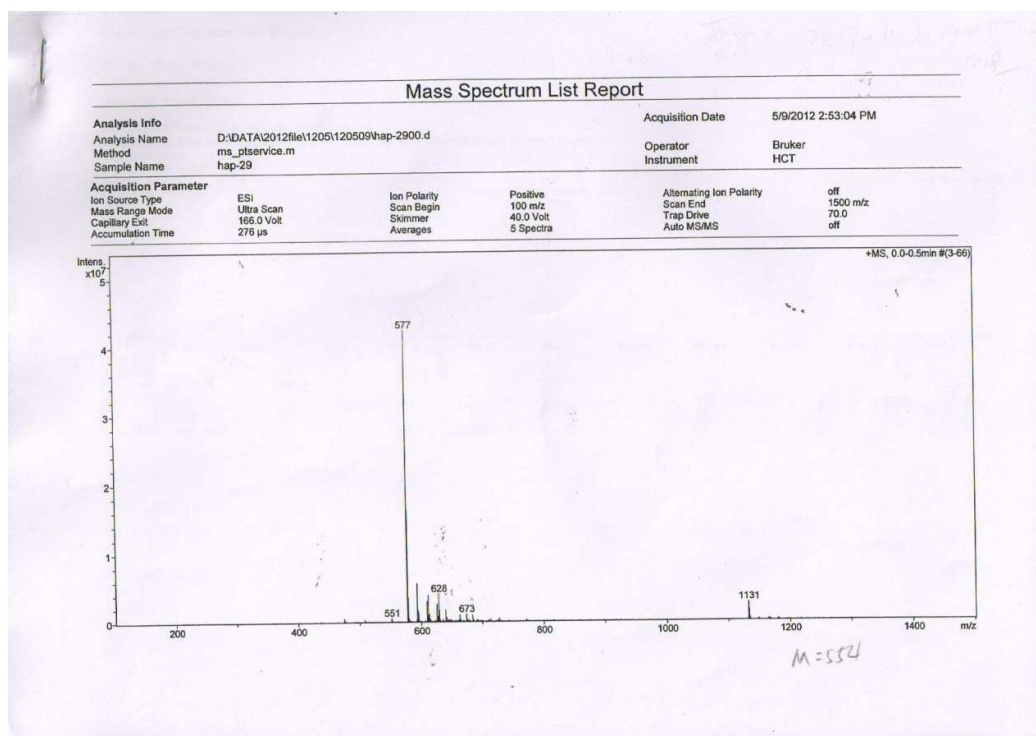


Figure S100. HR-EI (+) MS of aphanamixoid L (10)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

69 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 1-9

hap-29

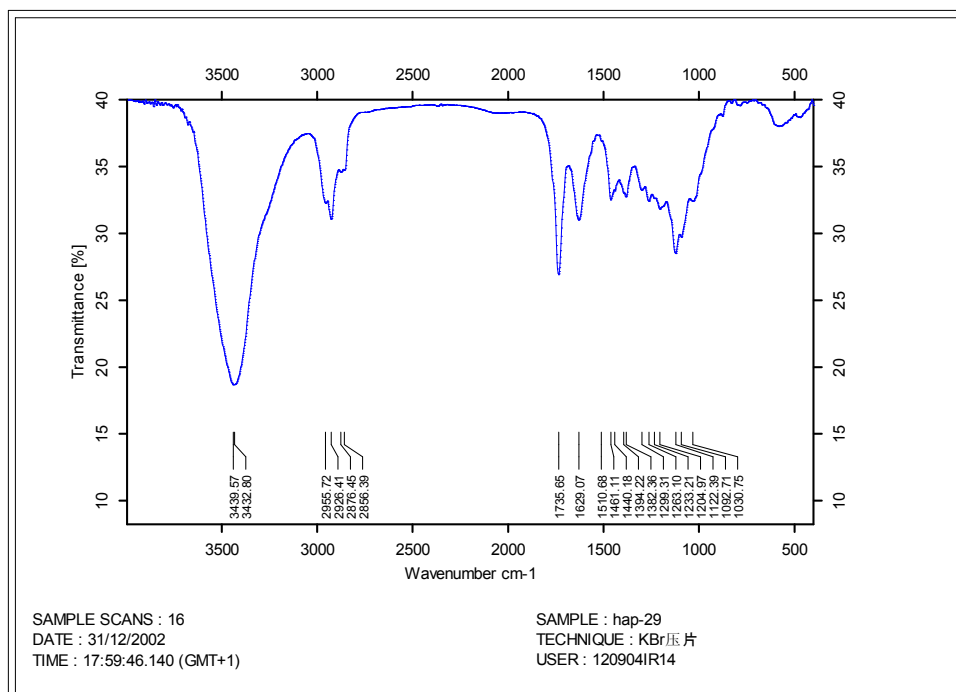
10:18:35 04-Sep-2012

Voltage EI+

KIB
M120905EA-09AFAMM 43 (3.947)
554.2892

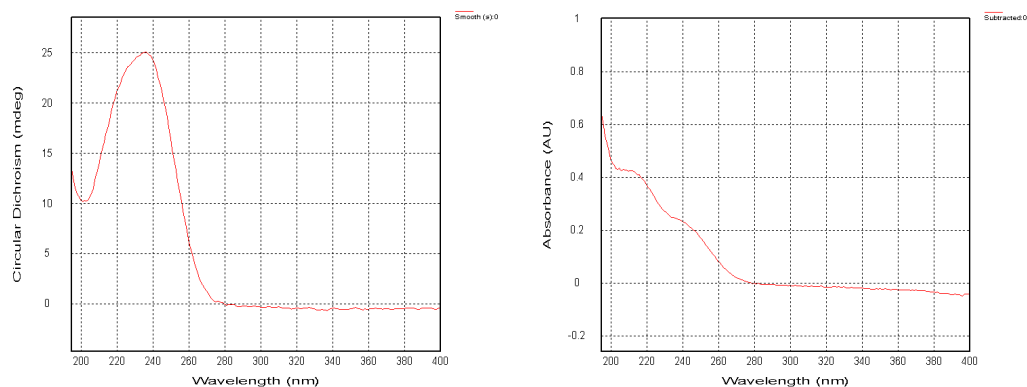
Autospec Premier
P776
2.14

Figure S101. IR spectrum of aphanamixoid L (10)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
428.850	0.393	0.001	8.997	0.205299	0
450.181	0.390	0.000	5.135	0.013070	0
470.321	0.387	0.006	14.302	1.355528	0
478.591	0.387	0.001	4.483	0.183255	0
485.499	0.387	0.000	5.306	0.013014	0
498.910	0.389	0.000	6.037	0.089531	0
514.748	0.386	0.001	5.665	0.207913	0
525.798	0.385	0.001	6.248	0.033115	0
540.383	0.383	0.001	8.079	0.214063	0
568.219	0.380	0.001	16.805	0.109632	0
581.820	0.380	0.020	46.961	9.379220	0
645.981	0.394	0.000	7.582	0.006724	0
661.626	0.396	0.000	3.781	0.030668	0
669.804	0.396	0.001	5.137	0.295626	0
785.093	0.395	0.005	9.938	2.151297	0
797.921	0.396	0.001	9.450	0.055298	0
875.704	0.388	0.002	11.350	0.837158	0
894.054	0.389	0.000	5.761	0.085156	0
1030.747	0.324	0.004	38.736	0.858755	0
1092.713	0.297	0.003	26.839	0.967743	0
1122.394	0.285	0.098	25.231	41.670940	0
1204.965	0.318	0.010	31.474	2.629297	0
1233.212	0.326	0.001	9.227	0.210303	0
1263.100	0.324	0.008	17.927	2.400138	0
1299.305	0.332	0.007	27.037	1.359512	0
1382.359	0.327	0.017	13.696	5.948814	0
1394.224	0.330	0.001	8.553	0.060596	0
1440.178	0.332	0.002	8.128	0.263518	0
1461.107	0.325	0.040	19.811	11.803261	0
1510.676	0.369	0.001	7.101	0.268816	0
1629.071	0.310	0.050	56.869	19.212648	0
1735.652	0.269	0.129	38.083	59.932129	0
2856.388	0.347	0.001	9.602	0.387128	0
2876.450	0.346	0.003	12.601	0.978227	0
2926.408	0.311	0.068	23.281	30.190926	0
2955.716	0.323	0.007	23.139	0.833957	0
3432.796	0.187	0.000	51.084	0.059918	0
3439.567	0.187	0.213	173.565	100.011894	0

Figure S102. CD spectrum of aphanamixoid L (**10**)



File: CD HAP-29-1mm(195-400)12052508.dsx

ProBinaryX

Attributes :

- Time Stamp :Fri May 25 14:16:16 2012

- File ID : {BB717B15-0C29-4938-9A15-051140659AA4}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 269.516 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.4200mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Figure S103. ^1H NMR spectrum of aphanamixoid M (**11**) in CDCl_3

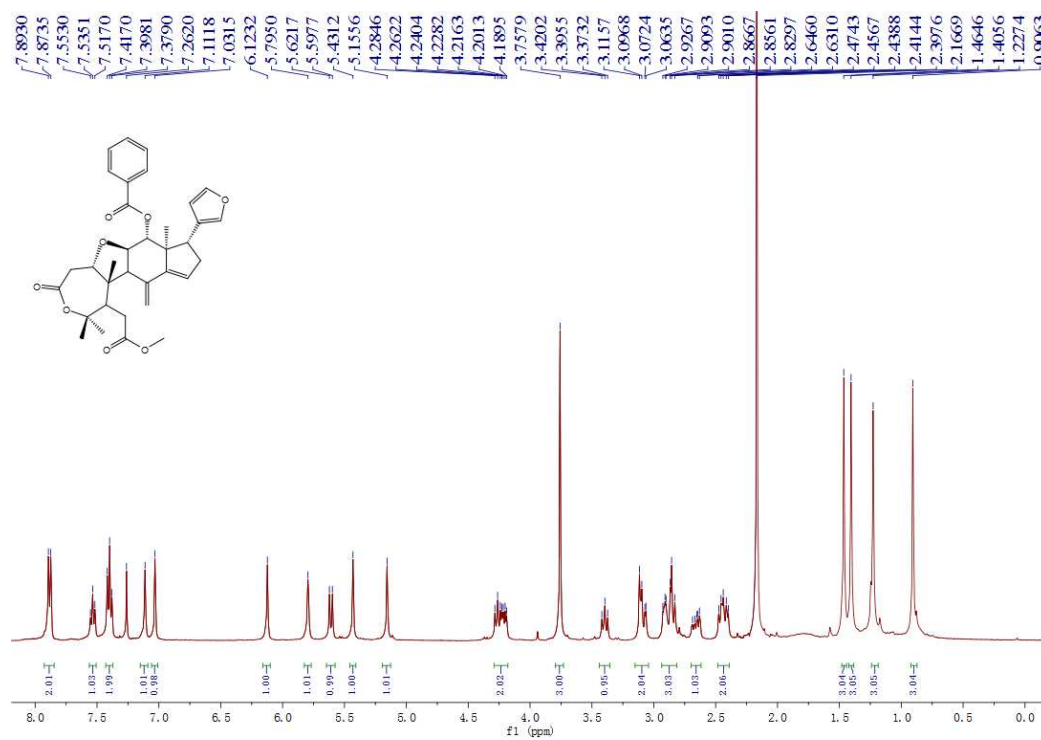


Figure S104. ^{13}C NMR spectrum of aphanamixoid M (**11**) in CDCl_3

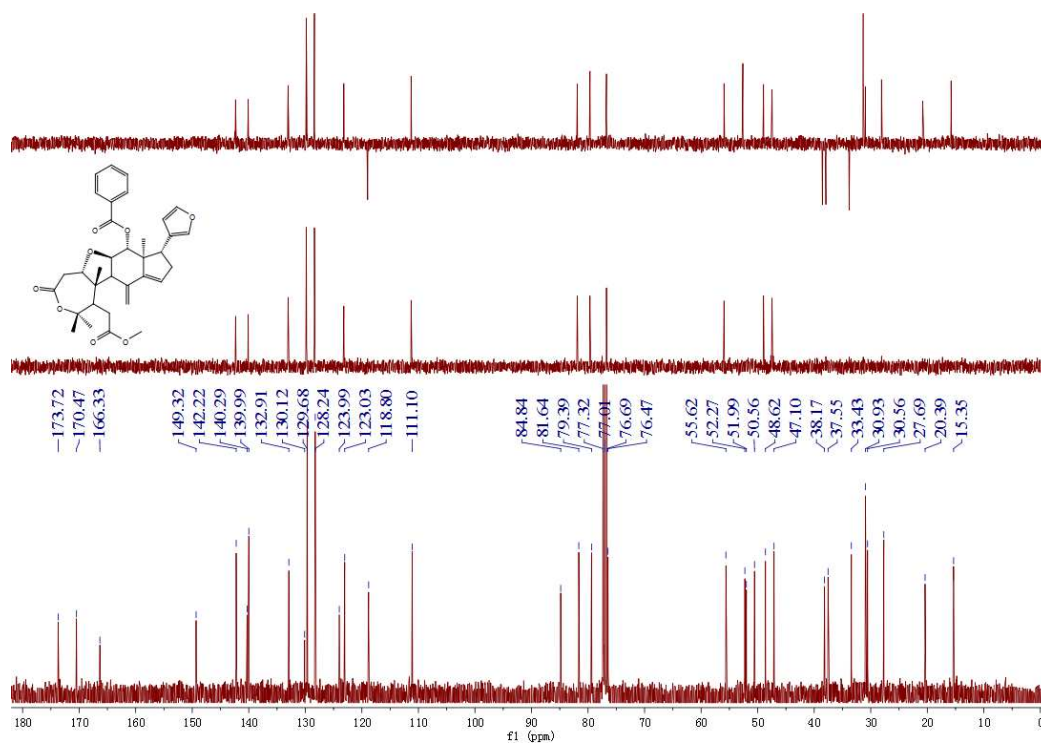


Figure S105. HSQC spectrum of aphanamixoid M (**11**) in CDCl₃

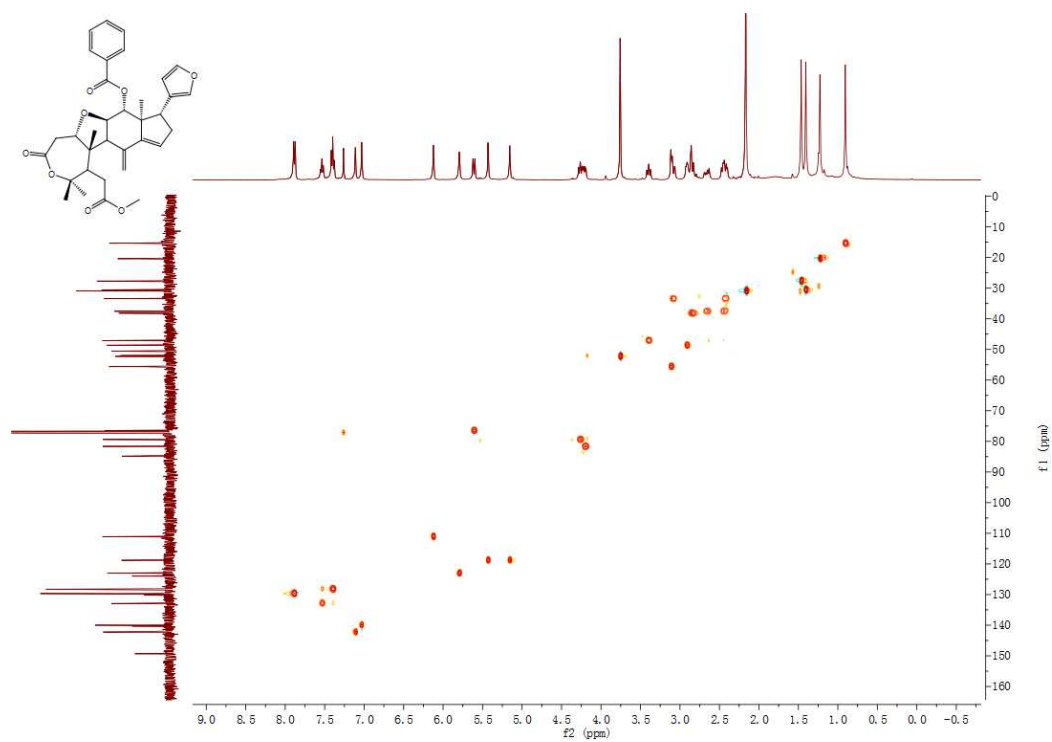


Figure S106. HMBC spectrum of aphanamixoid M (**11**) in CDCl₃

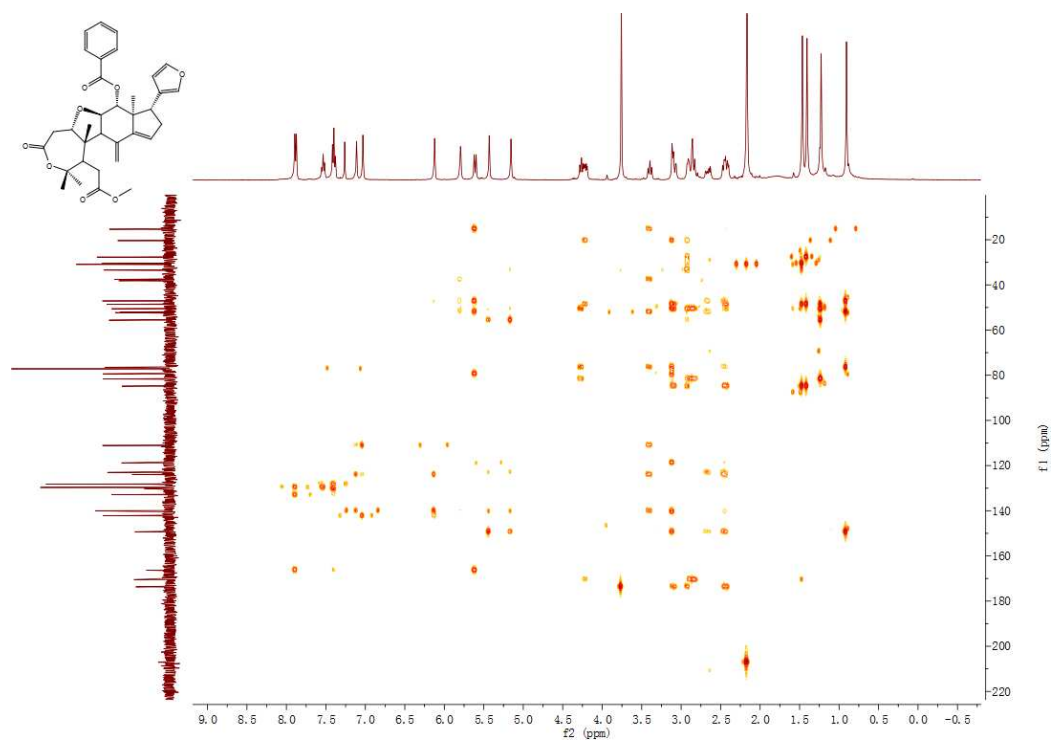


Figure S107. ^1H - ^1H COSY spectrum of aphanamixoid M (**11**) in CDCl_3

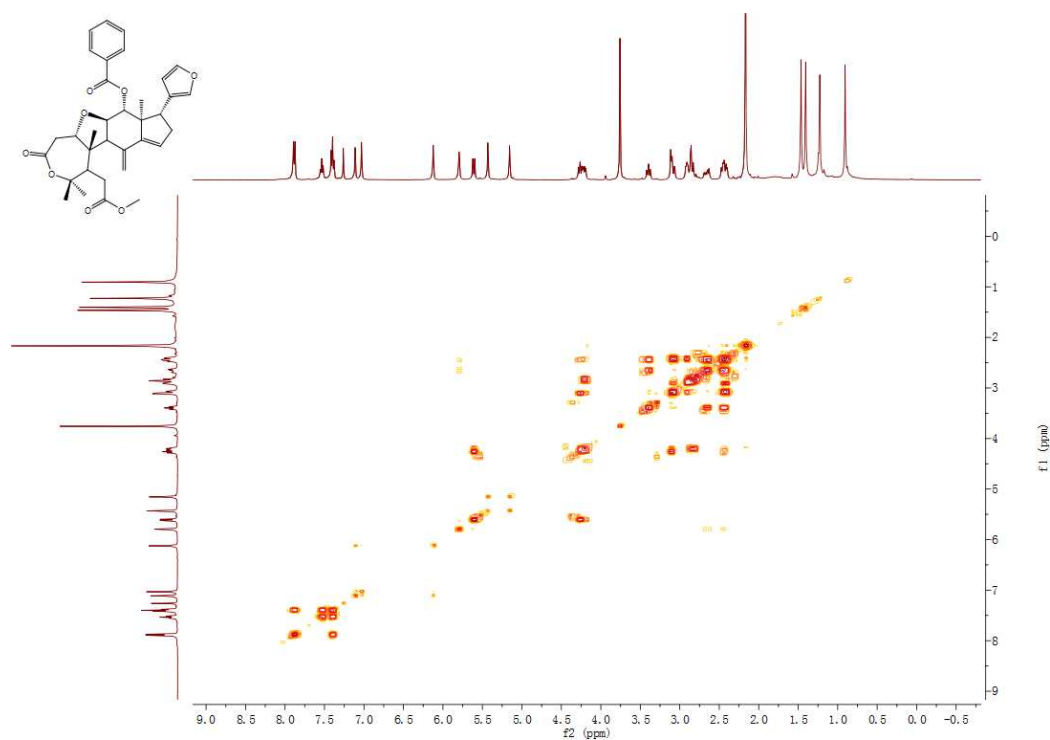


Figure S108. ROESY spectrum of aphanamixoid M (**11**) in CDCl_3

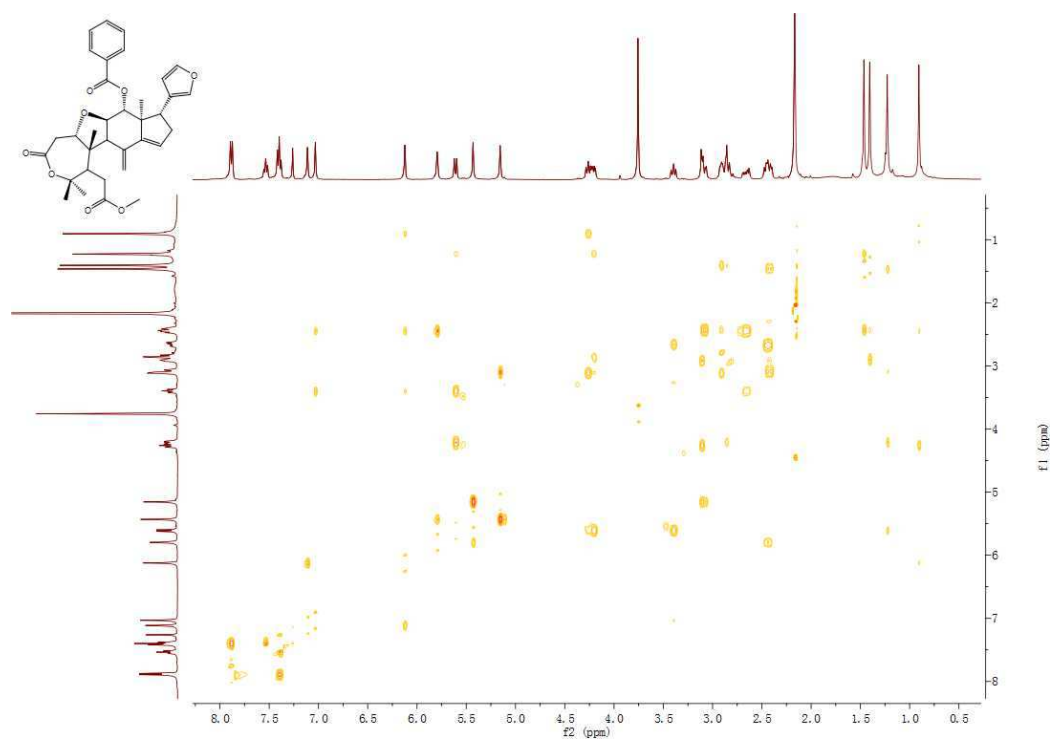


Figure S109. ESI (+) MS of aphanamixoid M (**11**)

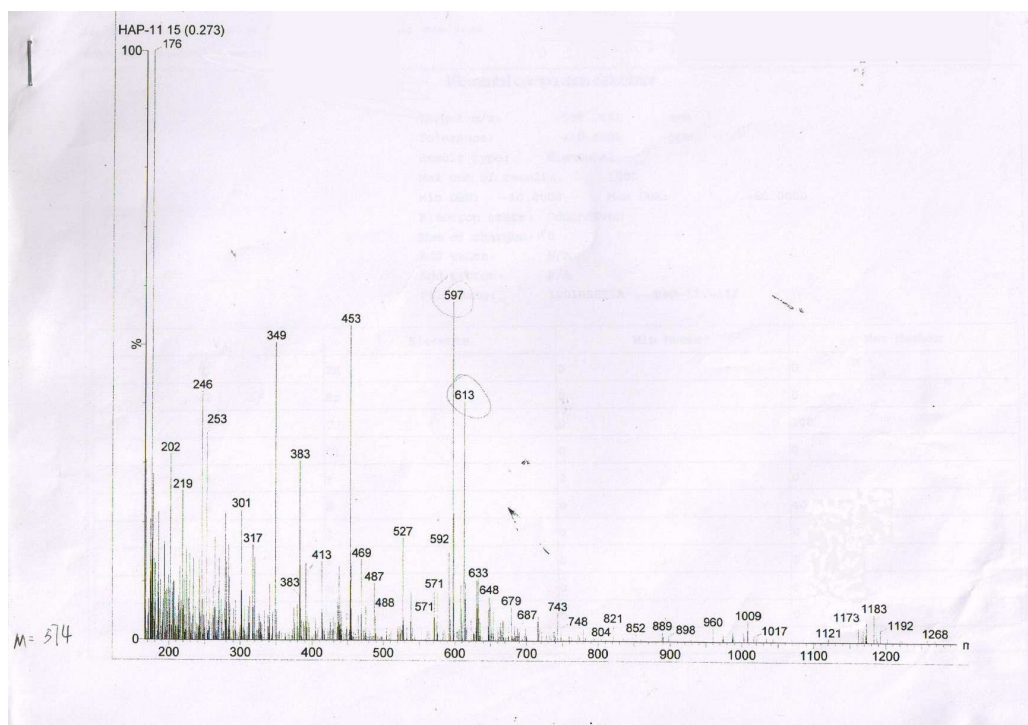


Figure S110. HR-EI (+) MS of aphanamixoid M (**11**)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

65 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 1-8

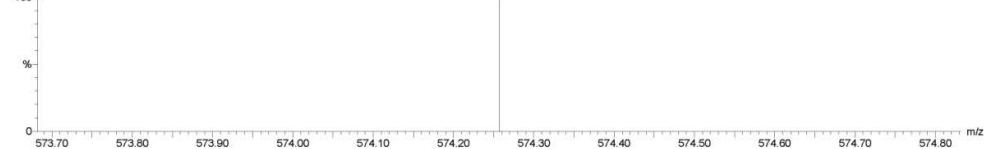
hap-15

08:50:55 04-Sep-2012

Voltage EI+

KIB
M120905EA-03AFAMM 80 (7.343)
574.2571

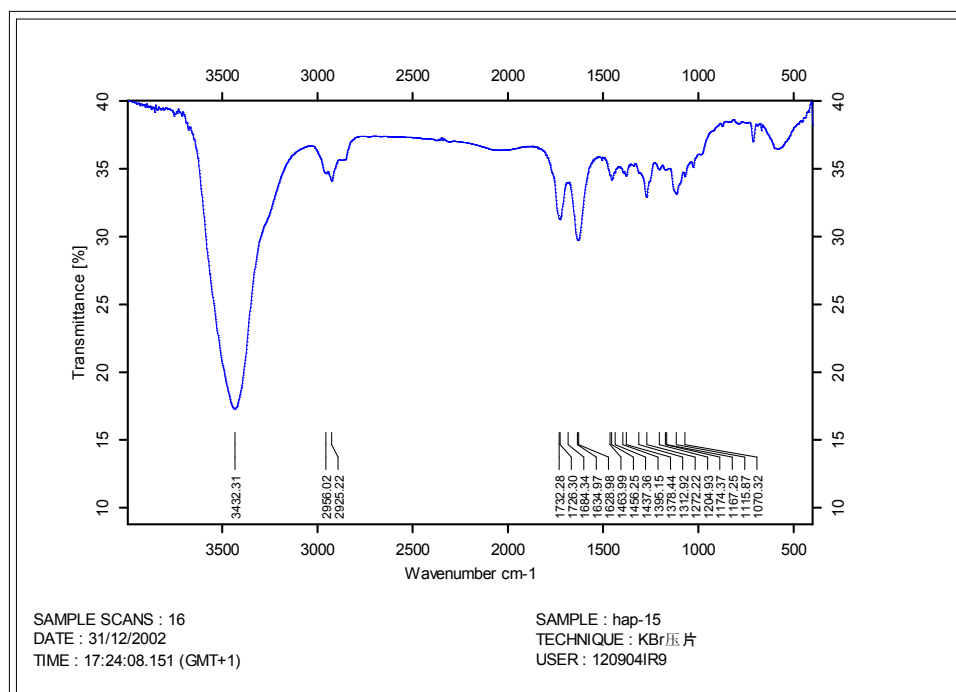
Autospec Premier
P776
24.2



Minimum: -10.0
Maximum: 100.0 10.0 120.0

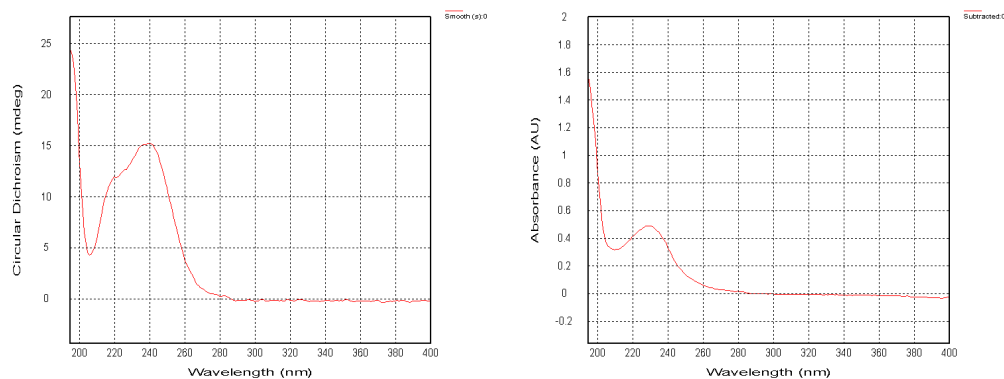
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
574.2571	574.2567	0.4	0.7	16.0	5546032.5	C34 H38 O8

Figure S111. IR spectrum of aphanamixoid M (11)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
492.595	0.381	0.001	4.191	0.042655	0
526.910	0.372	0.001	5.112	0.097911	0
581.081	0.364	0.030	46.494	9.676296	0
599.306	0.365	0.001	10.950	0.210744	0
668.545	0.378	0.005	5.121	2.051030	0
689.126	0.382	0.001	8.255	0.448381	0
711.950	0.370	0.014	13.428	5.876683	0
874.429	0.381	0.003	8.517	1.015028	0
987.416	0.360	0.001	18.378	0.174625	0
998.059	0.361	0.000	3.918	0.039348	0
1027.126	0.351	0.005	9.954	1.904939	0
1070.323	0.344	0.004	10.573	1.465286	0
1115.872	0.331	0.030	40.211	10.272658	0
1167.245	0.349	0.000	10.946	0.002756	0
1174.367	0.349	0.002	9.724	0.568420	0
1204.925	0.349	0.004	18.874	1.424717	0
1272.215	0.329	0.039	31.599	13.225202	0
1312.922	0.347	0.002	9.146	0.216217	0
1340.326	0.352	0.002	4.299	0.611547	0
1346.050	0.352	0.000	4.873	0.035542	0
1362.952	0.352	0.001	3.779	0.144254	0
1378.442	0.345	0.008	13.116	3.211061	0
1395.149	0.347	0.002	6.315	0.571202	0
1419.133	0.351	0.001	3.723	0.369068	0
1437.361	0.347	0.001	3.879	0.340810	0
1456.246	0.342	0.015	12.309	5.387274	0
1463.990	0.345	0.001	4.152	0.139201	0
1628.984	0.297	0.000	16.950	0.112938	0
1634.971	0.297	0.089	14.425	33.855331	0
1684.335	0.339	0.001	3.857	0.396735	0
1726.297	0.313	0.029	17.813	12.172623	0
1732.277	0.313	0.000	9.470	0.023953	0
2854.950	0.356	0.001	9.064	0.251838	0
2870.867	0.356	0.002	13.952	0.275882	0
2925.216	0.341	0.028	22.477	11.449226	0
2956.017	0.346	0.004	22.111	0.701688	0
3432.306	0.173	0.227	231.974	99.974861	0

Figure S112. CD spectrum of aphanamixoid M (**11**)



File: CD HAP-15-1mm(195-400)12052503.dsx

ProBinaryX

Attributes :

- Time Stamp :Fri May 25 13:30:04 2012

- File ID : {A16A837B-47F0-435f-9467-9E5F2D8C48C6}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.1500mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Figure S113. ^1H NMR spectrum of aphanamixoid N (**12**) in CDCl_3

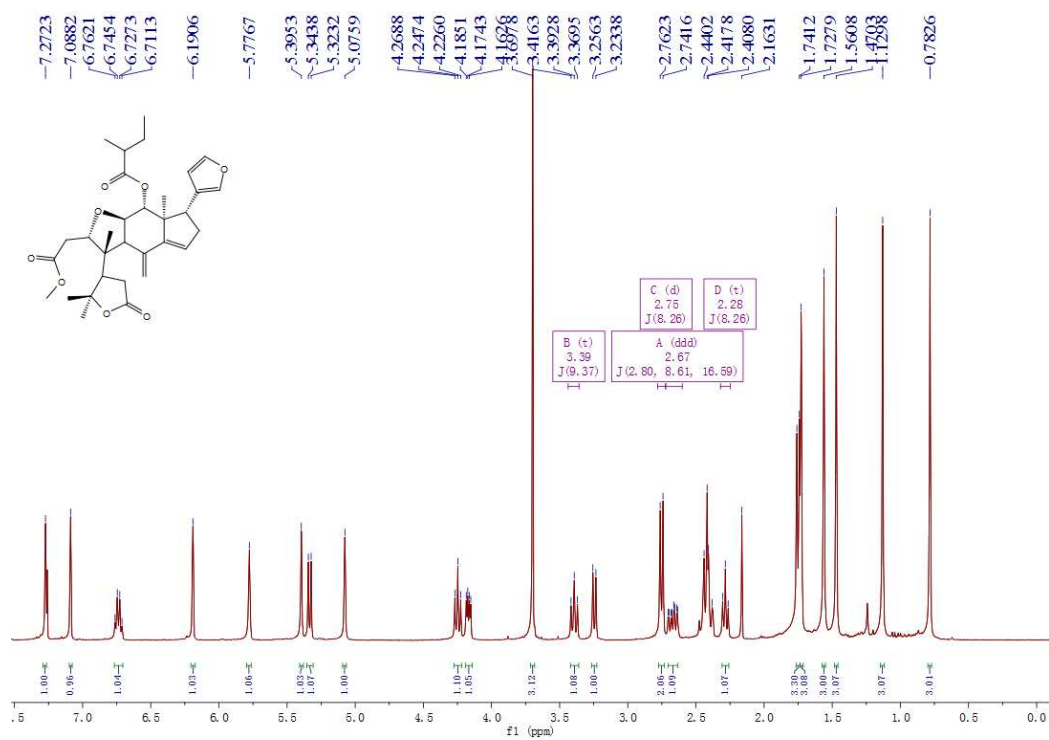


Figure S114. ^{13}C NMR spectrum of aphanamixoid N (**12**) in CDCl_3

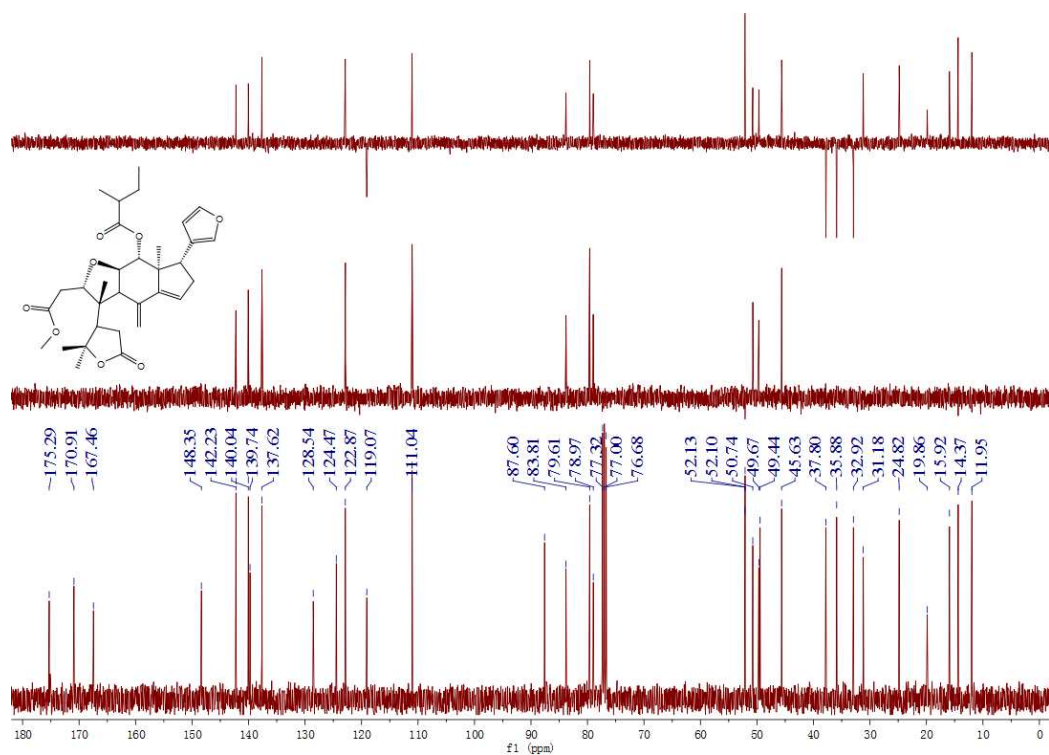


Figure S115. HSQC spectrum of aphanamixoid N (**12**) in CDCl₃

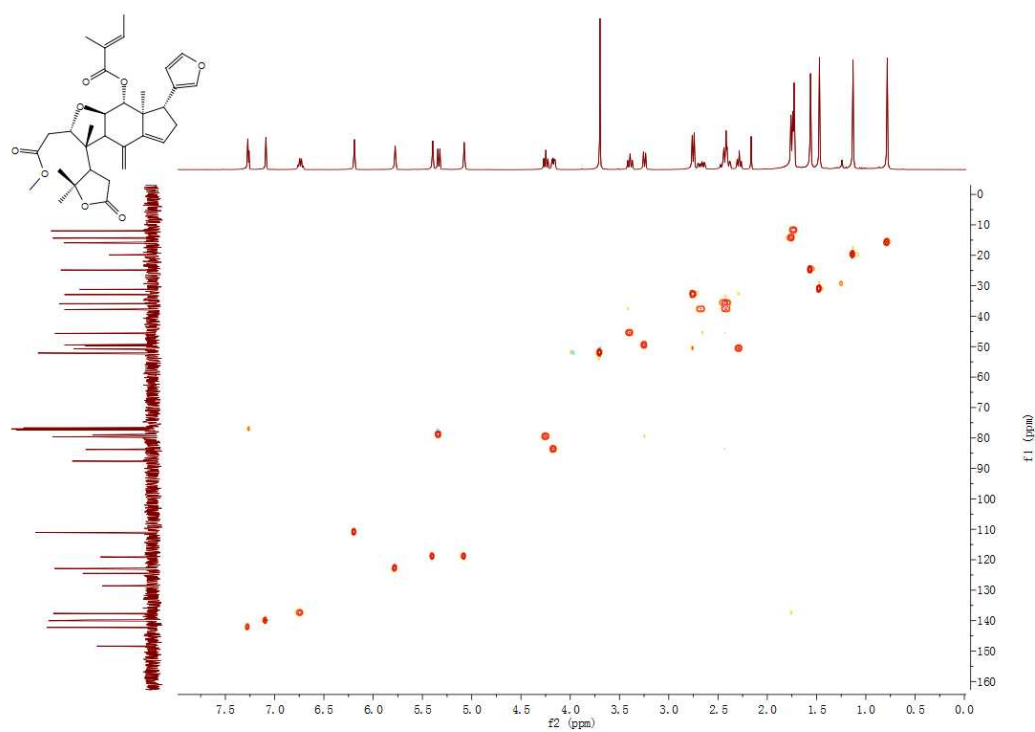


Figure S116. HMBC spectrum of aphanamixoid N (**12**) in CDCl₃

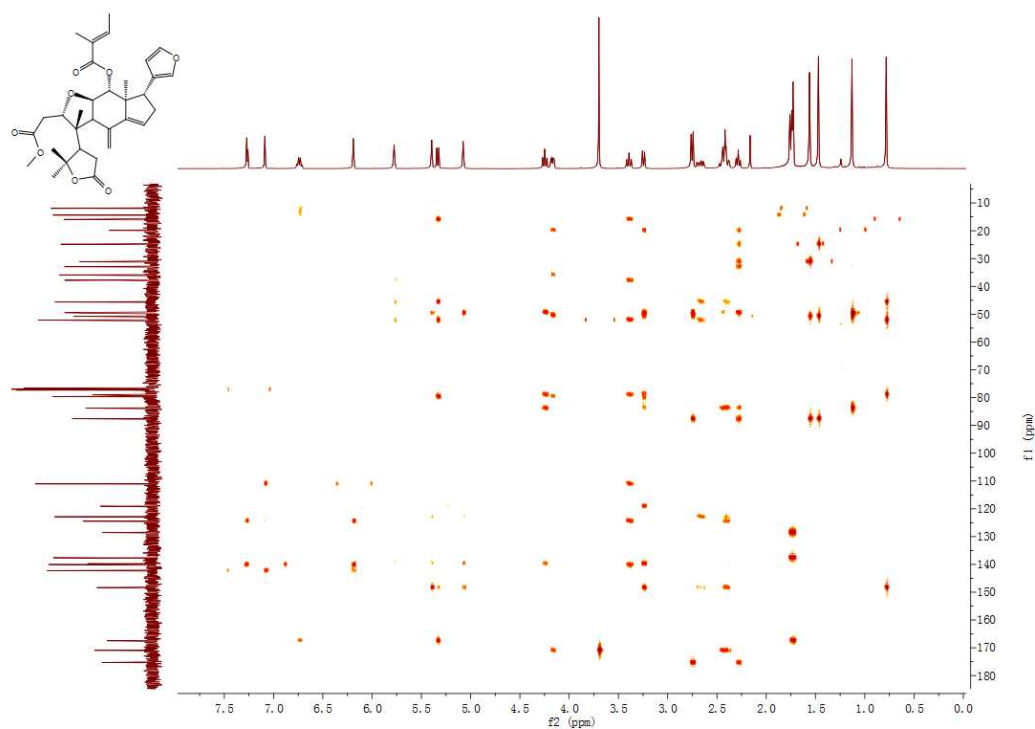


Figure S117. ^1H - ^1H COSY spectrum of aphanamixoid N (**12**) in CDCl_3

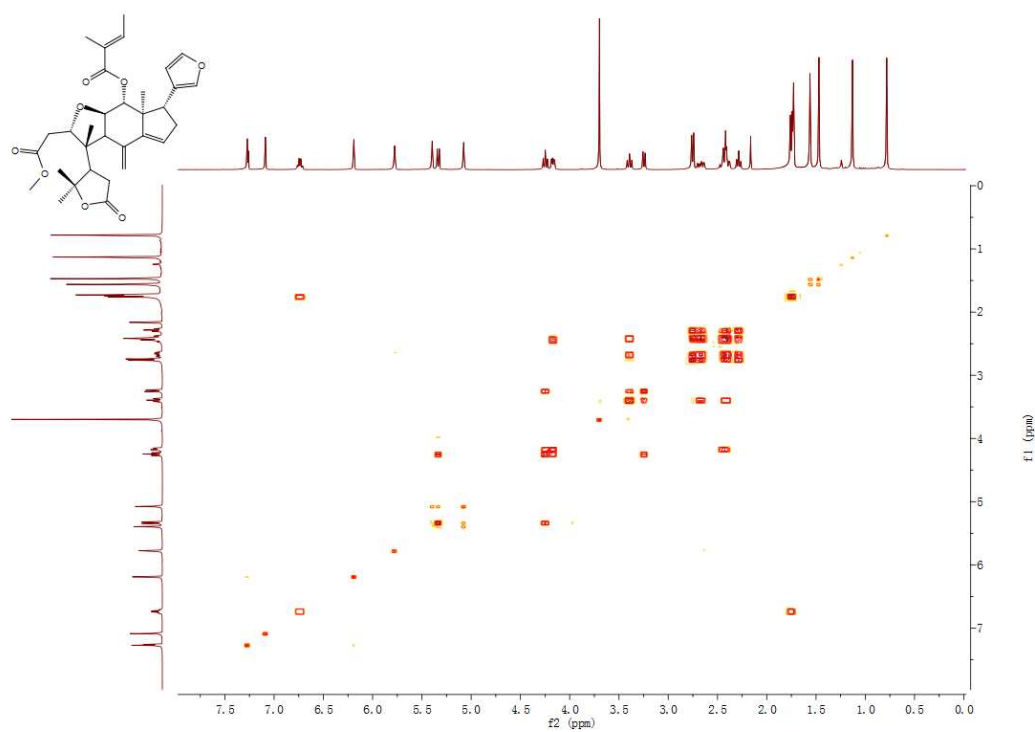


Figure S118. ROESY spectrum of aphanamixoid N (**12**) in CDCl_3

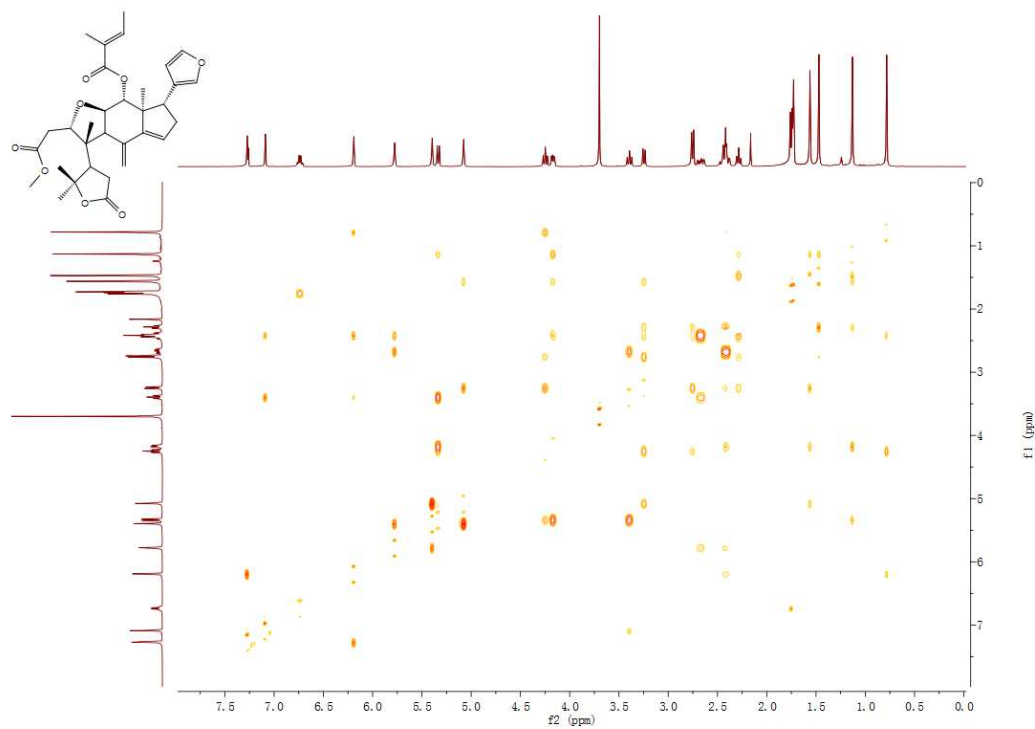


Figure S119. ESI (+) MS of aphanamixoid N (12)

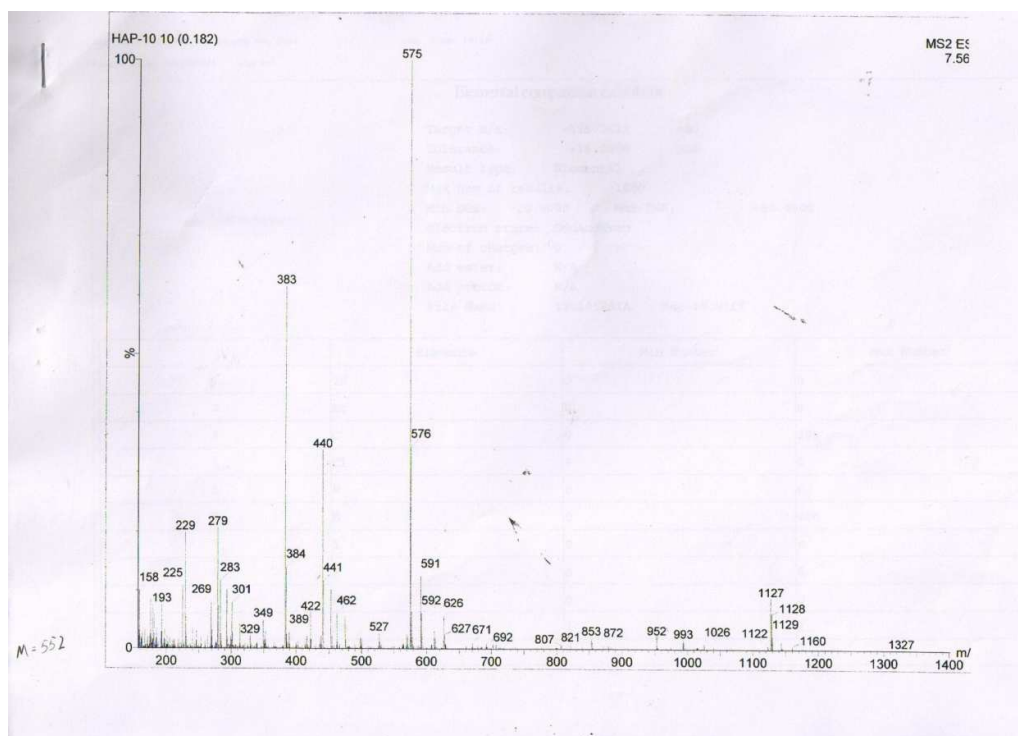


Figure S120. HR-ESI (+) MS of aphanamixoid N (12)

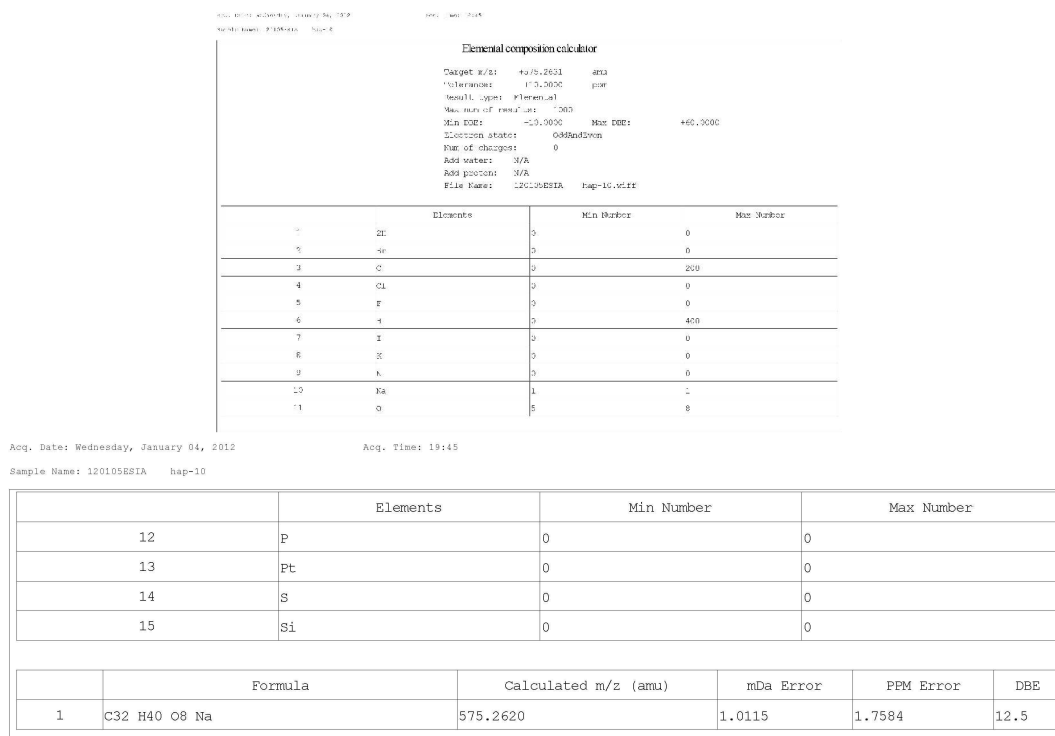
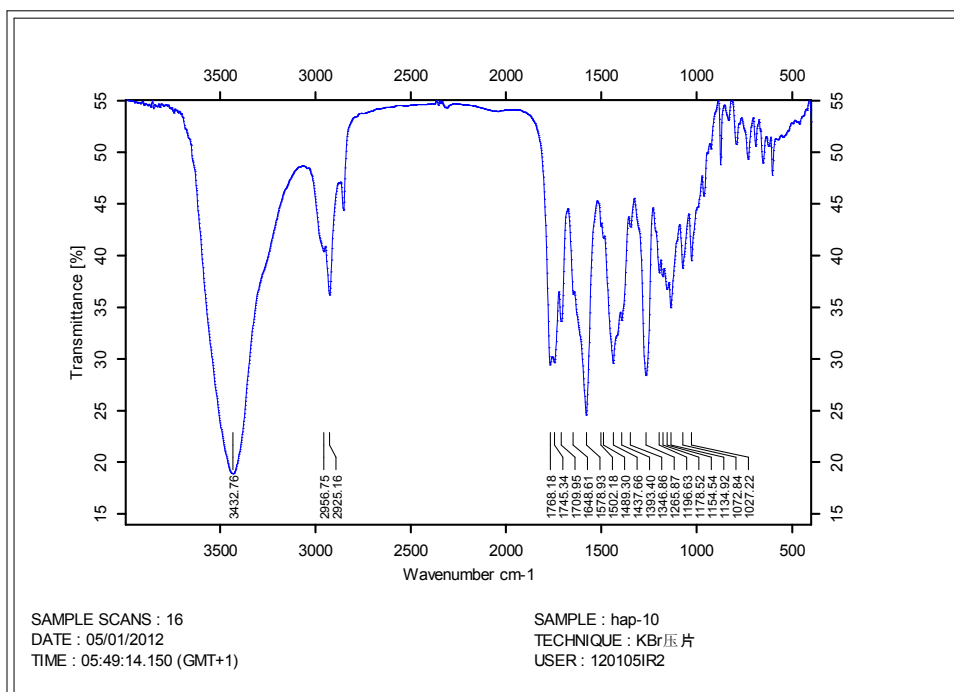
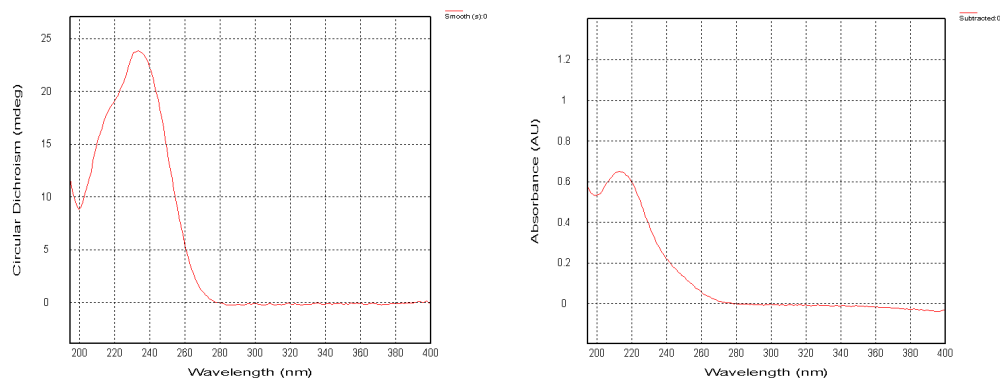


Figure S121. IR spectrum of aphanamixoid N (**12**)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
459.869	0.527	0.010	8.663	1.099586	0
473.483	0.529	0.001	8.727	0.172872	0
494.641	0.528	0.002	8.538	0.154895	0
518.792	0.521	0.001	7.507	0.028449	0
546.483	0.514	0.005	22.208	0.686703	0
572.612	0.512	0.004	10.379	0.293182	0
581.461	0.512	0.000	4.489	0.034898	0
601.821	0.478	0.072	8.958	19.989674	0
621.275	0.505	0.009	11.083	2.495686	0
651.066	0.489	0.029	13.954	7.087254	0
667.363	0.520	0.004	3.965	0.398881	0
690.729	0.505	0.027	12.175	7.196003	0
730.224	0.493	0.045	20.256	11.268280	0
775.222	0.527	0.002	6.674	0.237439	0
791.360	0.507	0.034	15.879	7.150435	0
833.303	0.531	0.017	19.209	4.073959	0
873.558	0.488	0.062	8.531	17.178211	0
925.101	0.503	0.012	9.396	1.548158	0
942.223	0.499	0.004	7.276	0.273565	0
961.086	0.458	0.029	12.780	5.348363	0
993.032	0.447	0.003	14.006	0.047638	0
1027.222	0.395	0.055	17.204	12.653017	0
1072.836	0.388	0.053	21.883	11.654660	0
1134.918	0.349	0.125	17.291	26.805845	0
1154.536	0.368	0.014	12.458	1.793043	0
1178.521	0.380	0.015	7.415	2.279366	0
1196.629	0.383	0.024	13.309	3.512679	0
1265.874	0.284	0.185	40.527	47.560997	0
1346.857	0.428	0.016	12.087	2.730568	0
1393.404	0.337	0.019	25.620	2.312532	0
1437.658	0.296	0.159	43.078	43.588474	0
1489.304	0.417	0.007	6.529	0.699740	0
1502.177	0.428	0.008	6.094	1.043133	0
1578.928	0.245	0.305	42.559	84.267281	0
1648.613	0.363	0.015	8.665	0.665799	0
1709.948	0.336	0.051	18.892	7.971789	0
1745.340	0.296	0.029	19.001	1.640152	0
1768.184	0.294	0.165	11.488	41.844437	0
2852.272	0.444	0.030	13.173	7.602767	0
2873.351	0.470	0.001	6.047	0.220724	0
2925.161	0.362	0.138	24.262	34.696106	0
2956.753	0.404	0.012	38.943	1.530157	0
3044.333	0.484	0.001	9.011	0.161492	0
3082.119	0.485	0.001	7.499	0.062110	0
3432.759	0.189	0.361	253.758	99.925224	0

Figure S122. CD spectrum of aphanamixoid N (**12**)



File: CD HAP-10-1mm(195-400)11122906.dsx

ProBinaryX

Attributes :

- Time Stamp :Thu Dec 29 15:30:29 2011

- File ID : {22DD87D1-8BDC-4613-84AA-3D04AA979FC5}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.1575mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Figure S123. ^1H NMR spectrum of aphanamixoid O (**13**) in CDCl_3

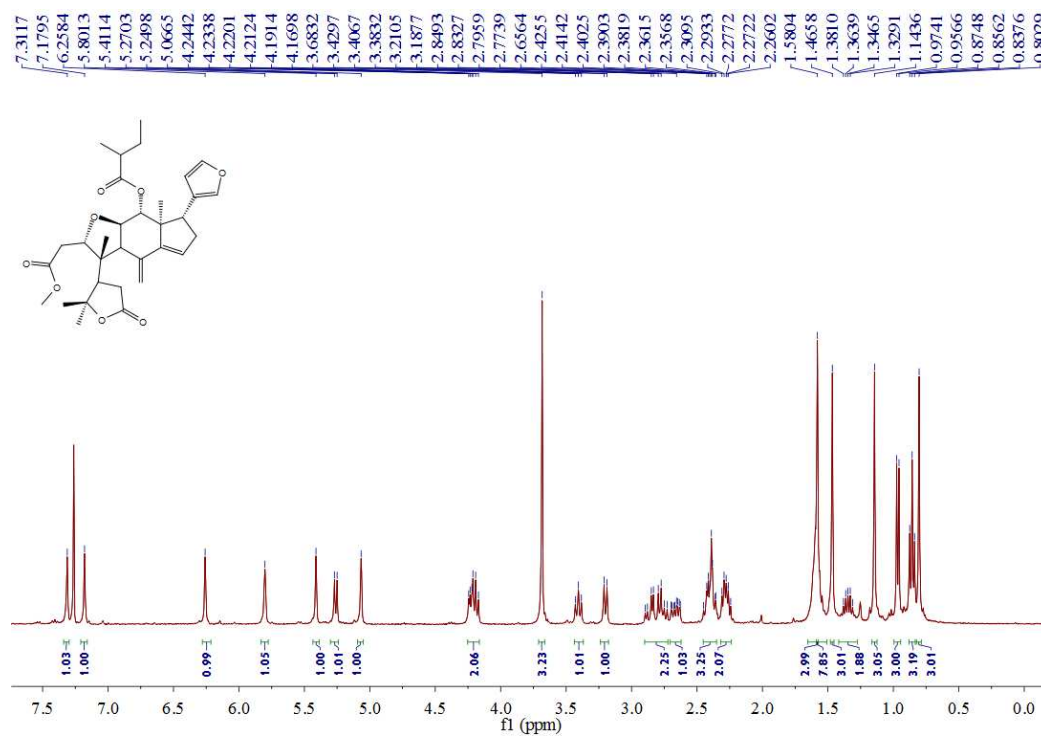


Figure S124. ^{13}C NMR spectrum of aphanamixoid O (**13**) in CDCl_3

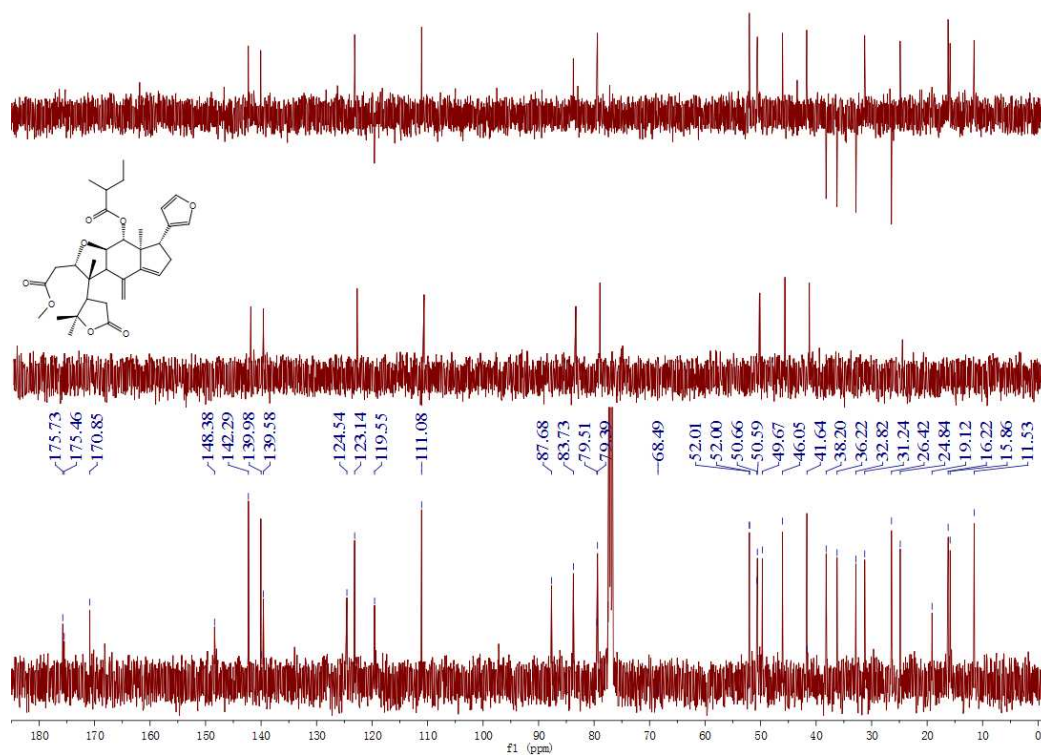


Figure S125. HSQC spectrum of aphanamixoid O (**13**) in CDCl₃

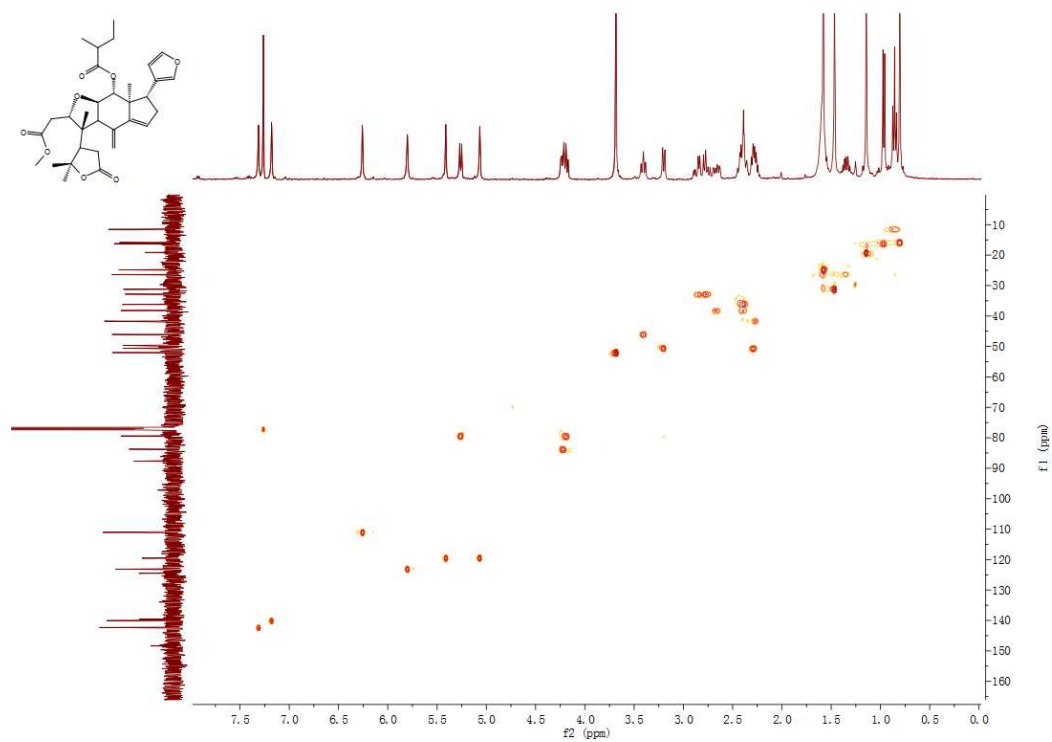


Figure S126. HMBC spectrum of aphanamixoid O (**13**) in CDCl₃

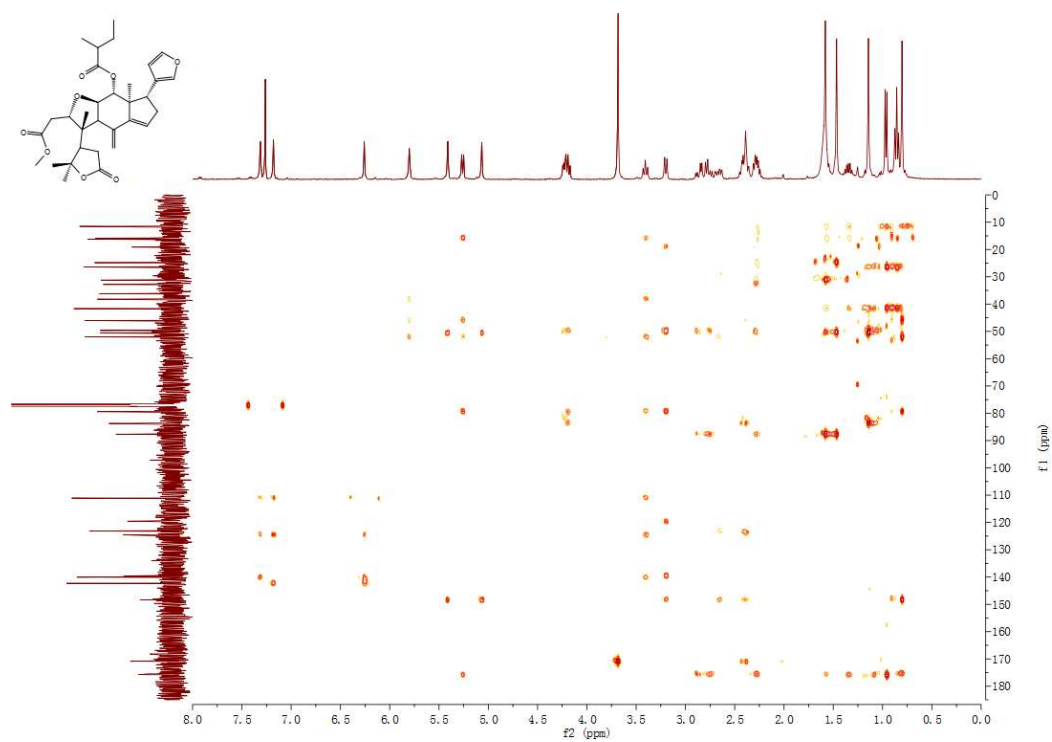


Figure S127. ^1H - ^1H COSY spectrum of aphanamixoid O (**13**) in CDCl_3

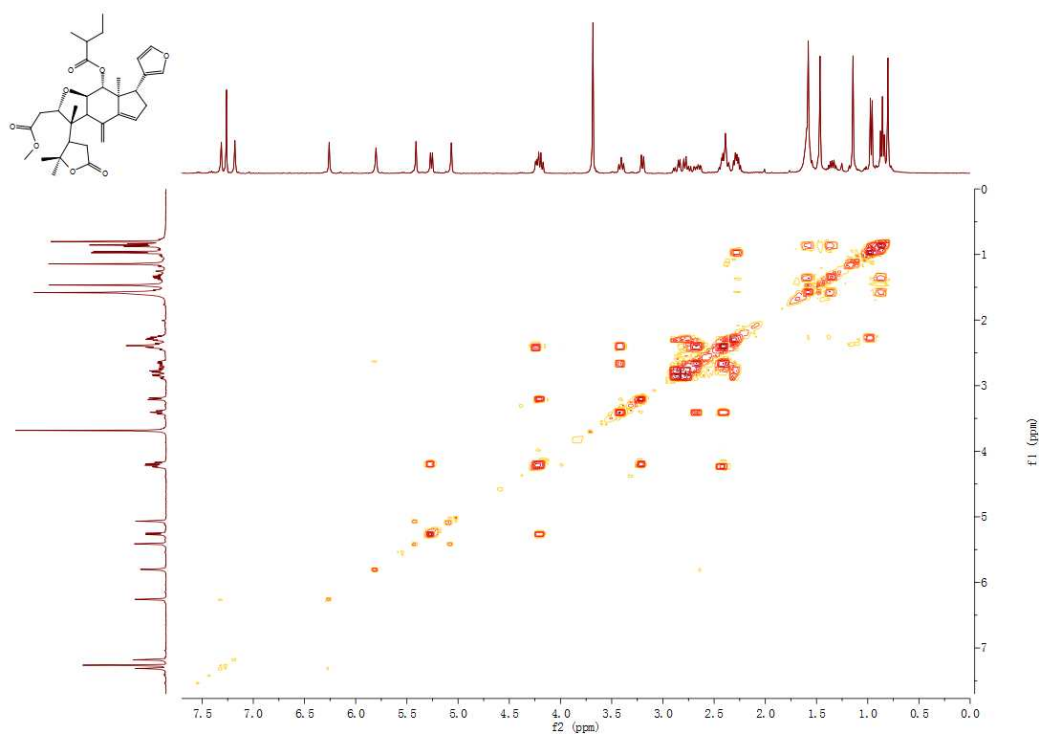


Figure S128. ROESY spectrum of aphanamixoid O (**13**) in CDCl_3

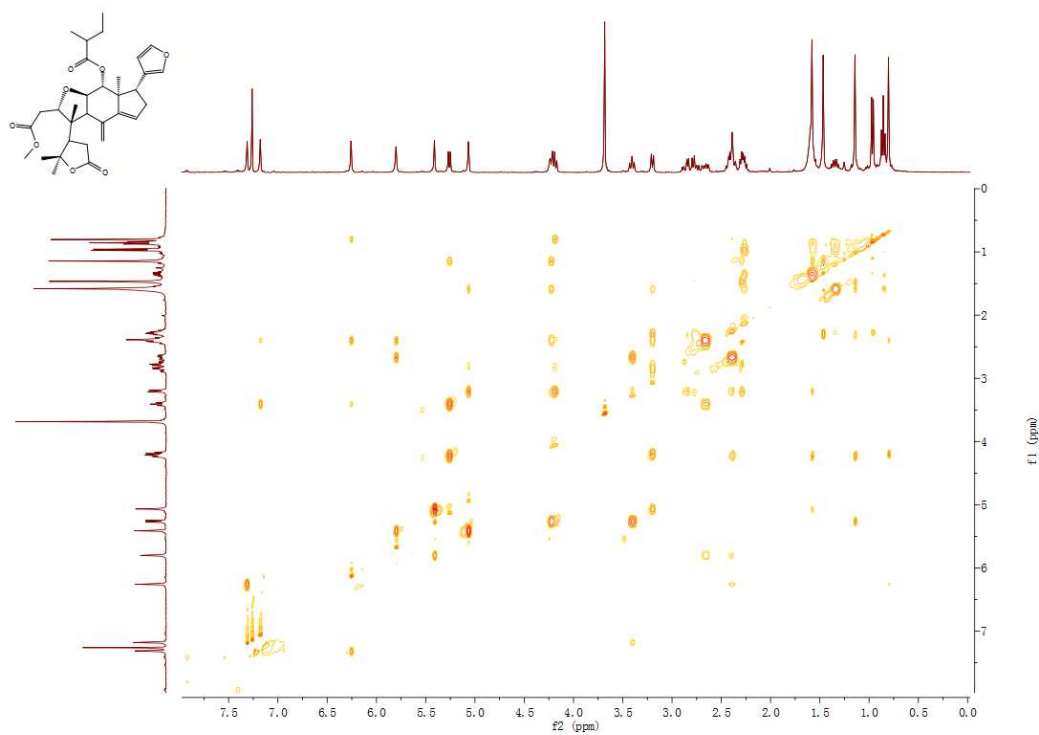


Figure S129. ESI (+) MS of aphanamixoid O (13)

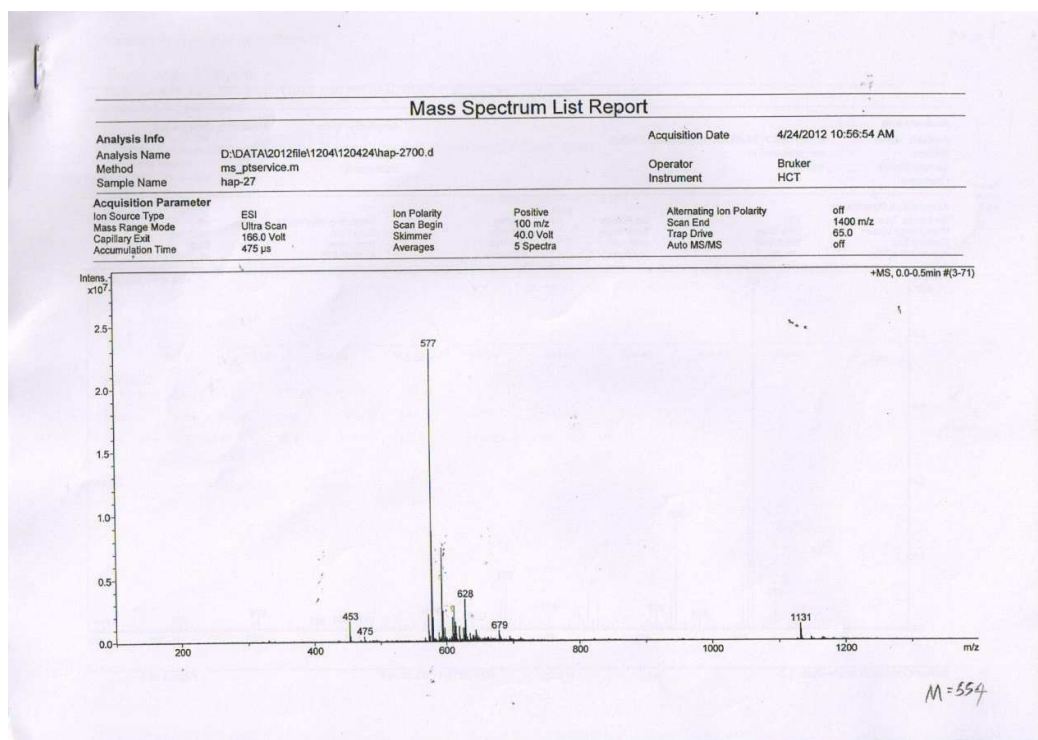


Figure S130. HR-EI (+) MS of aphanamixoid O (13)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

29 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 6-9

hap-27

09:36:47 04-Sep-2012

Voltage E+

100V

%

0

553.80

553.90

554.00

554.10

554.20

554.30

554.40

554.50

554.60

554.70

554.80

m/z

Minimum:

Maximum:

Mass

554.2889

Calc. Mass

554.2880

mDa

0.9

PPM

1.6

DBE

12.0

i-FIT

5546025.5

Formula

C32 H42 O8

M120905EA-06AFAMM 37 (3.397)

K1B

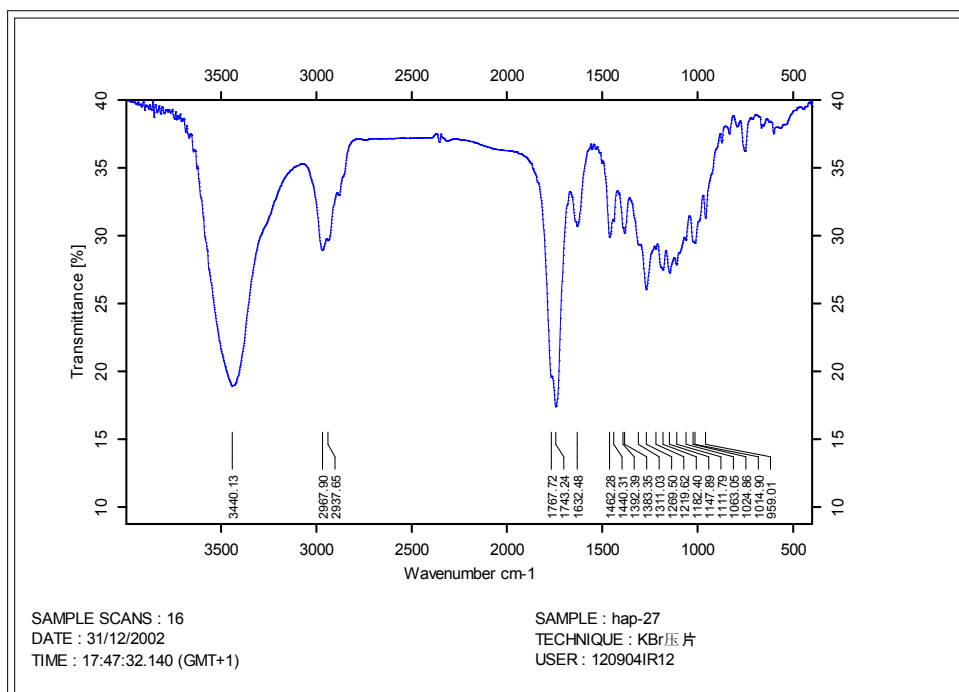
554.2889

Autospec Premier

P776

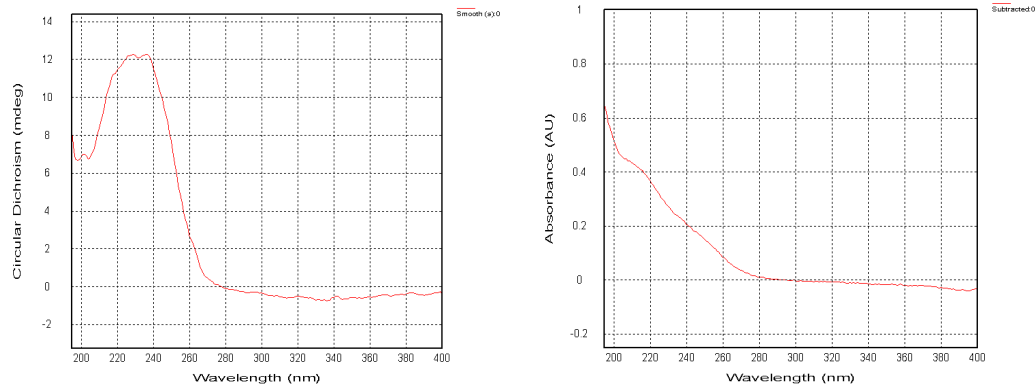
1.89

Figure S131. IR spectrum of aphanamixoid O (13)



Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
542.110	0.382	0.001	24.125	0.196633	0
566.355	0.379	0.003	14.229	0.397930	0
584.943	0.380	0.000	2.690	0.004282	0
589.695	0.380	0.000	2.869	0.030565	0
601.969	0.375	0.018	9.368	6.370305	0
657.370	0.381	0.002	11.041	0.415874	0
666.856	0.379	0.009	5.251	3.172189	0
752.950	0.362	0.028	24.189	11.665393	0
794.863	0.380	0.006	18.111	1.896465	0
834.099	0.375	0.010	15.259	2.636609	0
873.796	0.368	0.008	7.106	3.007939	0
959.006	0.313	0.019	16.039	7.562804	0
1014.904	0.294	0.024	12.742	8.962687	0
1024.863	0.295	0.003	9.296	0.157478	0
1063.048	0.297	0.006	10.038	0.975590	0
1111.787	0.278	0.007	12.963	2.353655	0
1147.887	0.272	0.030	19.701	9.557183	0
1182.403	0.275	0.016	28.029	6.439275	0
1219.624	0.290	0.003	8.709	0.920295	0
1269.501	0.260	0.116	28.443	47.535782	0
1311.027	0.293	0.002	14.222	0.159981	0
1383.353	0.302	0.028	12.925	11.591720	0
1392.392	0.306	0.001	7.580	0.049458	0
1416.038	0.331	0.001	4.623	0.220229	0
1440.312	0.310	0.007	9.930	0.657064	0
1462.279	0.299	0.044	19.759	15.274588	0
1503.401	0.354	0.003	5.927	0.692675	0
1632.483	0.307	0.038	44.545	11.415178	0
1743.237	0.174	0.226	33.740	100.005371	0
1767.722	0.196	0.002	15.039	0.359374	0
1840.725	0.339	0.000	4.564	0.066835	0
2880.797	0.330	0.003	12.995	0.847057	0
2937.647	0.296	0.003	23.429	0.823395	0
2967.897	0.289	0.067	31.570	28.227734	0
3440.125	0.189	0.203	218.504	82.281624	0

Figure S132. CD spectrum of aphanamixoid O (**13**)



File: CD HAP-27-1mm(195-400)12052506.dsx

ProBinaryX

Attributes :

- Time Stamp :Fri May 25 13:51:39 2012

- File ID : {38C74302-66F6-4469-856C-B675B27926E9}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.3850mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

¹H NMR spectrum of compound 10 in CDCl₃.

Chemical structure of compound 10: COC(=O)C1C(=C(C=C1)C2C(=C(C=C2)OC(=O)C3C(=C(C=C3)C4C(=C(C=C4)C5C(=C(C=C5)C6C(=C(C=C6)C7C(=C(C=C7)C8C(=C(C=C8)C9C(=C(C=C9)C10C(=C(C=C10)C11C(=C(C=C11)C12C(=C(C=C12)C13C(=C(C=C13)C14C(=C(C=C14)C15C(=C(C=C15)C16C(=C(C=C16)C17C(=C(C=C17)C18C(=C(C=C18)C19C(=C(C=C19)C20C(=C(C=C20)C21C(=C(C=C21)C22C(=C(C=C22)C23C(=C(C=C23)C24C(=C(C=C24)C25C(=C(C=C25)C26C(=C(C=C26)C27C(=C(C=C27)C28C(=C(C=C28)C29C(=C(C=C29)C30C(=C(C=C30)C31C(=C(C=C31)C32C(=C(C=C32)C33C(=C(C=C33)C34C(=C(C=C34)C35C(=C(C=C35)C36C(=C(C=C36)C37C(=C(C=C37)C38C(=C(C=C38)C39C(=C(C=C39)C40C(=C(C=C40)C41C(=C(C=C41)C42C(=C(C=C42)C43C(=C(C=C43)C44C(=C(C=C44)C45C(=C(C=C45)C46C(=C(C=C46)C47C(=C(C=C47)C48C(=C(C=C48)C49C(=C(C=C49)C50C(=C(C=C50)C51C(=C(C=C51)C52C(=C(C=C52)C53C(=C(C=C53)C54C(=C(C=C54)C55C(=C(C=C55)C56C(=C(C=C56)C57C(=C(C=C57)C58C(=C(C=C58)C59C(=C(C=C59)C60C(=C(C=C60)C61C(=C(C=C61)C62C(=C(C=C62)C63C(=C(C=C63)C64C(=C(C=C64)C65C(=C(C=C65)C66C(=C(C=C66)C67C(=C(C=C67)C68C(=C(C=C68)C69C(=C(C=C69)C70C(=C(C=C70)C71C(=C(C=C71)C72C(=C(C=C72)C73C(=C(C=C73)C74C(=C(C=C74)C75C(=C(C=C75)C76C(=C(C=C76)C77C(=C(C=C77)C78C(=C(C=C78)C79C(=C(C=C79)C80C(=C(C=C80)C81C(=C(C=C81)C82C(=C(C=C82)C83C(=C(C=C83)C84C(=C(C=C84)C85C(=C(C=C85)C86C(=C(C=C86)C87C(=C(C=C87)C88C(=C(C=C88)C89C(=C(C=C89)C90C(=C(C=C90)C91C(=C(C=C91)C92C(=C(C=C92)C93C(=C(C=C93)C94C(=C(C=C94)C95C(=C(C=C95)C96C(=C(C=C96)C97C(=C(C=C97)C98C(=C(C=C98)C99C(=C(C=C99)C100C(=C(C=C100)C101C(=C(C=C101)C102C(=C(C=C102)C103C(=C(C=C103)C104C(=C(C=C104)C105C(=C(C=C105)C106C(=C(C=C106)C107C(=C(C=C107)C108C(=C(C=C108)C109C(=C(C=C109)C110C(=C(C=C110)C111C(=C(C=C111)C112C(=C(C=C112)C113C(=C(C=C113)C114C(=C(C=C114)C115C(=C(C=C115)C116C(=C(C=C116)C117C(=C(C=C117)C118C(=C(C=C118)C119C(=C(C=C119)C120C(=C(C=C120)C121C(=C(C=C121)C122C(=C(C=C122)C123C(=C(C=C123)C124C(=C(C=C124)C125C(=C(C=C125)C126C(=C(C=C126)C127C(=C(C=C127)C128C(=C(C=C128)C129C(=C(C=C129)C130C(=C(C=C130)C131C(=C(C=C131)C132C(=C(C=C132)C133C(=C(C=C133)C134C(=C(C=C134)C135C(=C(C=C135)C136C(=C(C=C136)C137C(=C(C=C137)C138C(=C(C=C138)C139C(=C(C=C139)C140C(=C(C=C140)C141C(=C(C=C141)C142C(=C(C=C142)C143C(=C(C=C143)C144C(=C(C=C144)C145C(=C(C=C145)C146C(=C(C=C146)C147C(=C(C=C147)C148C(=C(C=C148)C149C(=C(C=C149)C150C(=C(C=C150)C151C(=C(C=C151)C152C(=C(C=C152)C153C(=C(C=C153)C154C(=C(C=C154)C155C(=C(C=C155)C156C(=C(C=C156)C157C(=C(C=C157)C158C(=C(C=C158)C159C(=C(C=C159)C160C(=C(C=C160)C161C(=C(C=C161)C162C(=C(C=C162)C163C(=C(C=C163)C164C(=C(C=C164)C165C(=C(C=C165)C166C(=C(C=C166)C167C(=C(C=C167)C168C(=C(C=C168)C169C(=C(C=C169)C170C(=C(C=C170)C171C(=C(C=C171)C172C(=C(C=C172)C173C(=C(C=C173)C174C(=C(C=C174)C175C(=C(C=C175)C176C(=C(C=C176)C177C(=C(C=C177)C178C(=C(C=C178)C179C(=C(C=C179)C180C(=C(C=C180)C181C(=C(C=C181)C182C(=C(C=C182)C183C(=C(C=C183)C184C(=C(C=C184)C185C(=C(C=C185)C186C(=C(C=C186)C187C(=C(C=C187)C188C(=C(C=C188)C189C(=C(C=C189)C190C(=C(C=C190)C191C(=C(C=C191)C192C(=C(C=C192)C193C(=C(C=C193)C194C(=C(C=C194)C195C(=C(C=C195)C196C(=C(C=C196)C197C(=C(C=C197)C198C(=C(C=C198)C199C(=C(C=C199)C200C(=C(C=C200)C201C(=C(C=C201)C202C(=C(C=C202)C203C(=C(C=C203)C204C(=C(C=C204)C205C(=C(C=C205)C206C(=C(C=C206)C207C(=C(C=C207)C208C(=C(C=C208)C209C(=C(C=C209)C210C(=C(C=C210)C211C(=C(C=C211)C212C(=C(C=C212)C213C(=C(C=C213)C214C(=C(C=C214)C215C(=C(C=C215)C216C(=C(C=C216)C217C(=C(C=C217)C218C(=C(C=C218)C219C(=C(C=C219)C220C(=C(C=C220)C221C(=C(C=C221)C222C(=C(C=C222)C223C(=C(C=C223)C224C(=C(C=C224)C225C(=C(C=C225)C226C(=C(C=C226)C227C(=C(C=C227)C228C(=C(C=C228)C229C(=C(C=C229)C230C(=C(C=C230)C231C(=C(C=C231)C232C(=C(C=C232)C233C(=C(C=C233)C234C(=C(C=C234)C235C(=C(C=C235)C236C(=C(C=C236)C237C(=C(C=C237)C238C(=C(C=C238)C239C(=C(C=C239)C240C(=C(C=C240)C241C(=C(C=C241)C242C(=C(C=C242)C243C(=C(C=C243)C244C(=C(C=C244)C245C(=C(C=C245)C246C(=C(C=C246)C247C(=C(C=C247)C248C(=C(C=C248)C249C(=C(C=C249)C250C(=C(C=C250)C251C(=C(C=C251)C252C(=C(C=C252)C253C(=C(C=C253)C254C(=C(C=C254)C255C(=C(C=C255)C256C(=C(C=C256)C257C(=C(C=C257)C258C(=C(C=C258)C259C(=C(C=C259)C260C(=C(C=C260)C261C(=C(C=C261)C262C(=C(C=C262)C263C(=C(C=C263)C264C(=C(C=C264)C265C(=C(C=C265)C266C(=C(C=C266)C267C(=C(C=C267)C268C(=C(C=C268)C269C(=C(C=C269)C270C(=C(C=C270)C271C(=C(C=C271)C272C(=C(C=C272)C273C(=C(C=C273)C274C(=C(C=C274)C275C(=C(C=C275)C276C(=C(C=C276)C277C(=C(C=C277)C278C(=C(C=C278)C279C(=C(C=C279)C280C(=C(C=C280)C281C(=C(C=C281)C282C(=C(C=C282)C283C(=C(C=C283)C284C(=C(C=C284)C285C(=C(C=C285)C286C(=C(C=C286)C287C(=C(C=C287)C288C(=C(C=C288)C289C(=C(C=C289)C290C(=C(C=C290)C291C(=C(C=C291)C292C(=C(C=C292)C293C(=C(C=C293)C294C(=C(C=C294)C295C(=C(C=C295)C296C(=C(C=C296)C297C(=C(C=C297)C29

Chemical structure of compound **1** is shown in the top left. The ¹H NMR spectrum (400 MHz, CDCl₃) is displayed above the ¹³C NMR spectrum (100 MHz, CDCl₃). The ¹H NMR spectrum shows peaks at 1.66, 1.71, 1.75, 1.87, 1.96, 2.07, 2.92, 3.14, 3.15, 3.61, 3.63, 4.45, 4.91, 4.97, 5.01, 5.09, 5.24, 5.26, 5.73, 7.80, 7.81, 7.82, 7.83, 7.84, 7.85, 7.86, 7.87, 7.88, 7.89, 7.90, 7.91, 7.92, 7.93, 7.94, 7.95, 7.96, 7.97, 7.98, 7.99, 8.00, 8.01, 8.02, 8.03, 8.04, 8.05, 8.06, 8.07, 8.08, 8.09, 8.10, 8.11, 8.12, 8.13, 8.14, 8.15, 8.16, 8.17, 8.18, 8.19, 8.20, 8.21, 8.22, 8.23, 8.24, 8.25, 8.26, 8.27, 8.28, 8.29, 8.30, 8.31, 8.32, 8.33, 8.34, 8.35, 8.36, 8.37, 8.38, 8.39, 8.40, 8.41, 8.42, 8.43, 8.44, 8.45, 8.46, 8.47, 8.48, 8.49, 8.50, 8.51, 8.52, 8.53, 8.54, 8.55, 8.56, 8.57, 8.58, 8.59, 8.60, 8.61, 8.62, 8.63, 8.64, 8.65, 8.66, 8.67, 8.68, 8.69, 8.70, 8.71, 8.72, 8.73, 8.74, 8.75, 8.76, 8.77, 8.78, 8.79, 8.80, 8.81, 8.82, 8.83, 8.84, 8.85, 8.86, 8.87, 8.88, 8.89, 8.90, 8.91, 8.92, 8.93, 8.94, 8.95, 8.96, 8.97, 8.98, 8.99, 9.00, 9.01, 9.02, 9.03, 9.04, 9.05, 9.06, 9.07, 9.08, 9.09, 9.10, 9.11, 9.12, 9.13, 9.14, 9.15, 9.16, 9.17, 9.18, 9.19, 9.20, 9.21, 9.22, 9.23, 9.24, 9.25, 9.26, 9.27, 9.28, 9.29, 9.30, 9.31, 9.32, 9.33, 9.34, 9.35, 9.36, 9.37, 9.38, 9.39, 9.40, 9.41, 9.42, 9.43, 9.44, 9.45, 9.46, 9.47, 9.48, 9.49, 9.50, 9.51, 9.52, 9.53, 9.54, 9.55, 9.56, 9.57, 9.58, 9.59, 9.60, 9.61, 9.62, 9.63, 9.64, 9.65, 9.66, 9.67, 9.68, 9.69, 9.70, 9.71, 9.72, 9.73, 9.74, 9.75, 9.76, 9.77, 9.78, 9.79, 9.80, 9.81, 9.82, 9.83, 9.84, 9.85, 9.86, 9.87, 9.88, 9.89, 9.90, 9.91, 9.92, 9.93, 9.94, 9.95, 9.96, 9.97, 9.98, 9.99, 10.00. The ¹³C NMR spectrum shows peaks at 16.31, 19.96, 25.07, 29.92, 31.44, 33.15, 36.13, 38.09, 45.91, 49.74, 50.11, 50.96, 52.41, 52.46, 79.73, 80.10, 84.10, 87.87, 111.24, 119.49, 123.36, 124.56, 128.53, 129.88, 130.48, 133.15, 139.88, 140.22, 142.54, 148.44, 166.36, 171.16, 175.55.

Figure S135. HSQC spectrum of aphanamixoid P (14) in CDCl₃

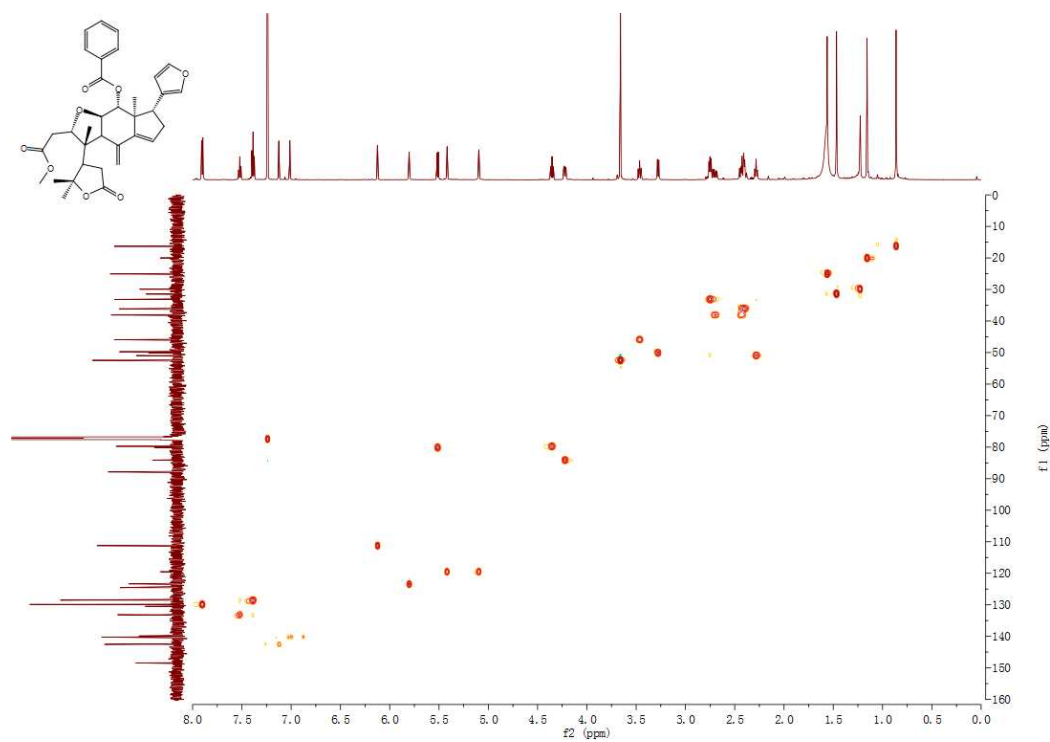


Figure S136. HMBC spectrum of aphanamixoid P (14) in CDCl₃

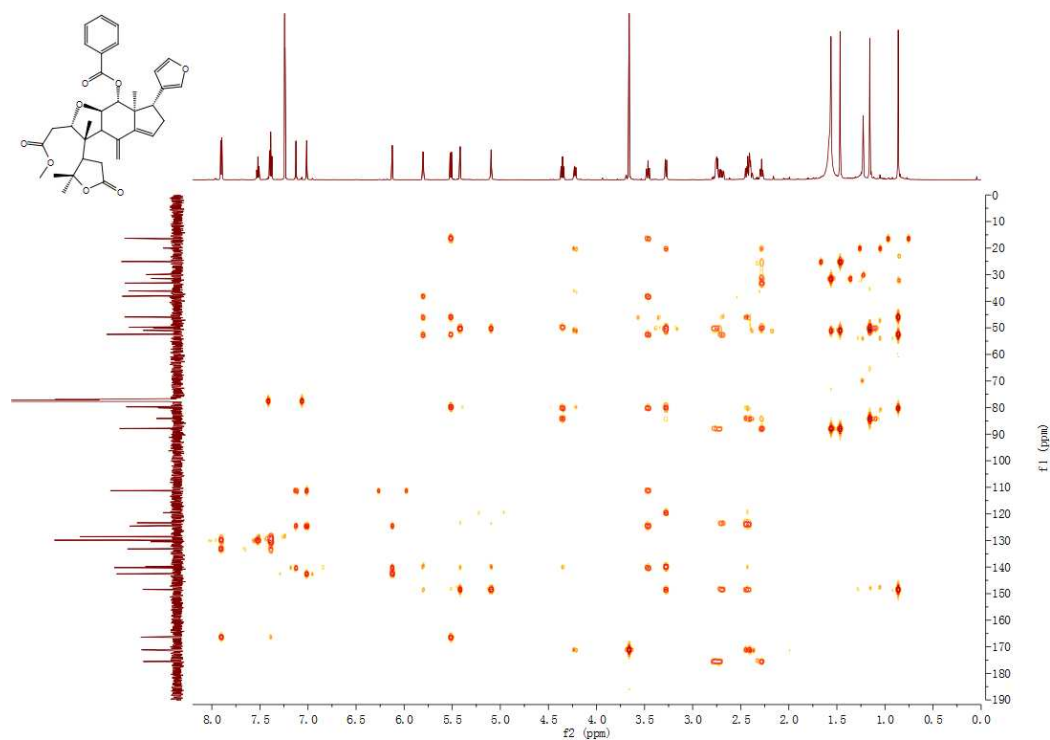


Figure S137. ^1H - ^1H COSY spectrum of aphanamixoid P (14) in CDCl_3

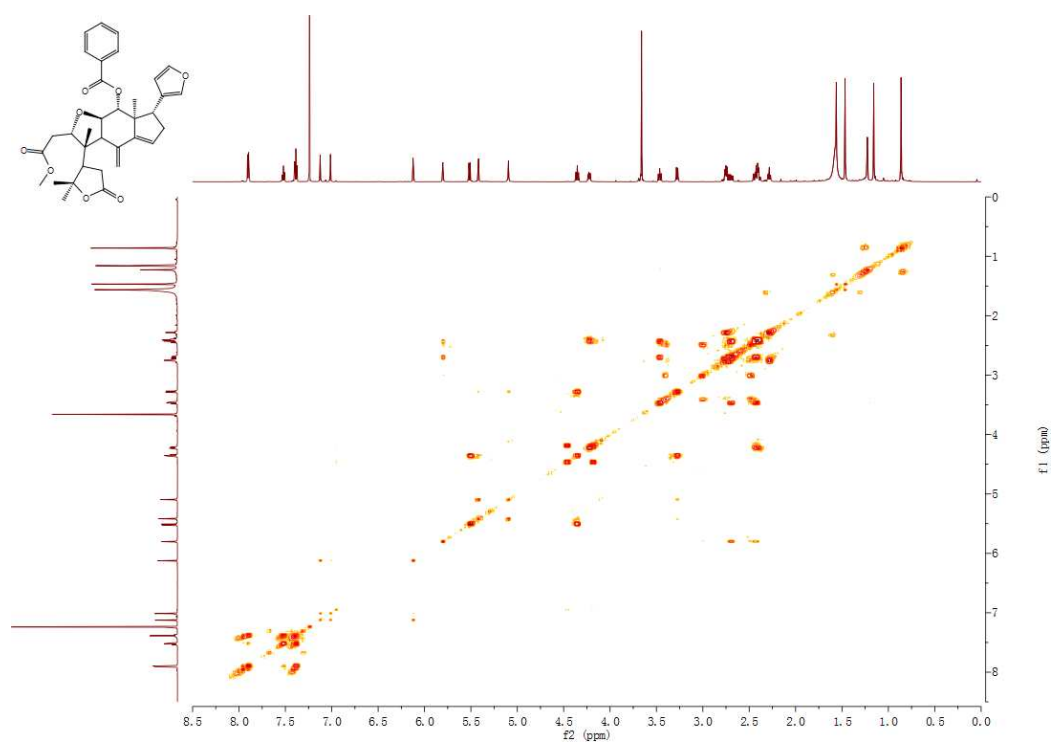


Figure S138. ROESY spectrum of aphanamixoid P (14) in CDCl_3

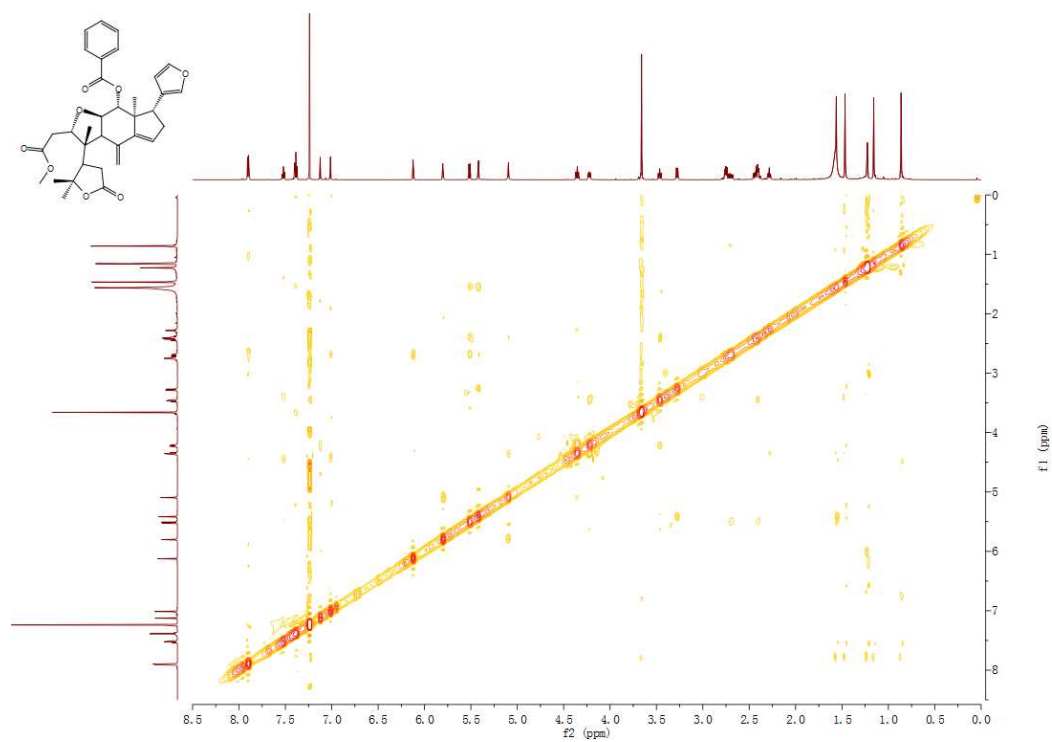


Figure S139. ESI (+) MS of aphanamixoid P (14)

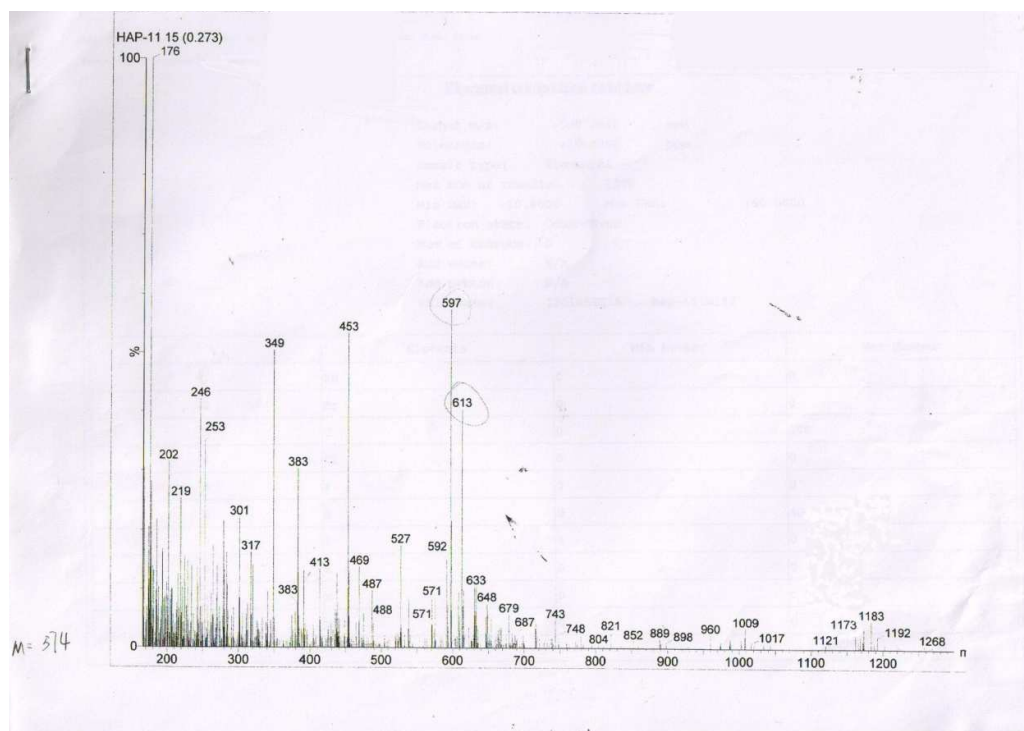


Figure S140. HR-ESI (+) MS of aphanamixoid P (14)

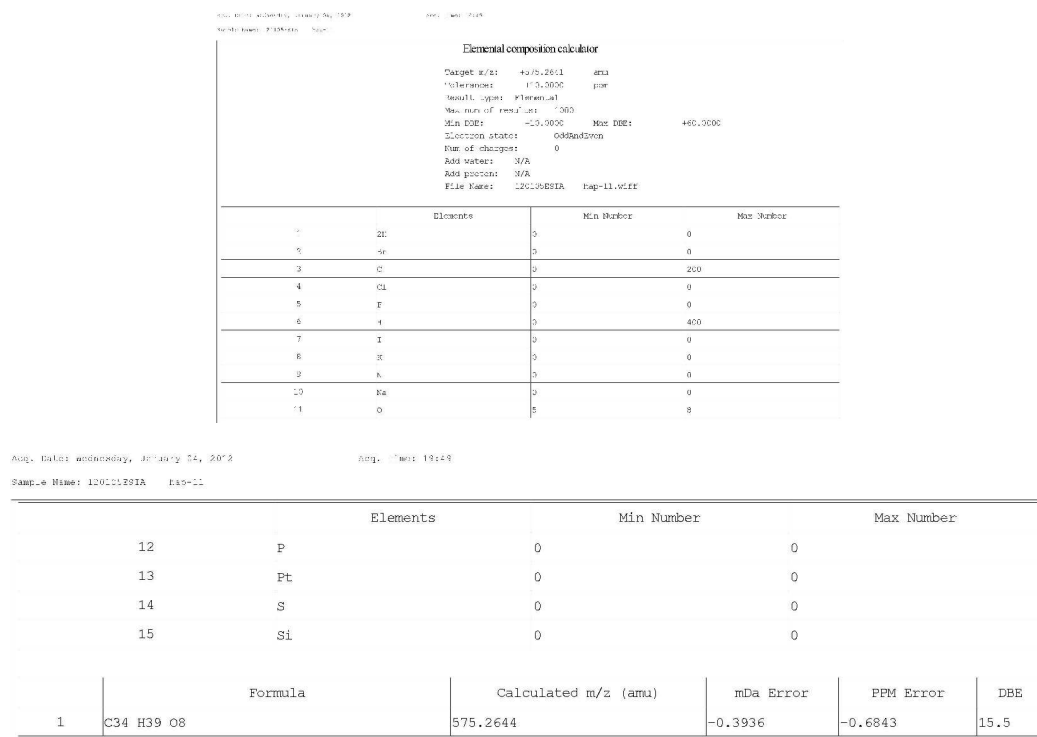
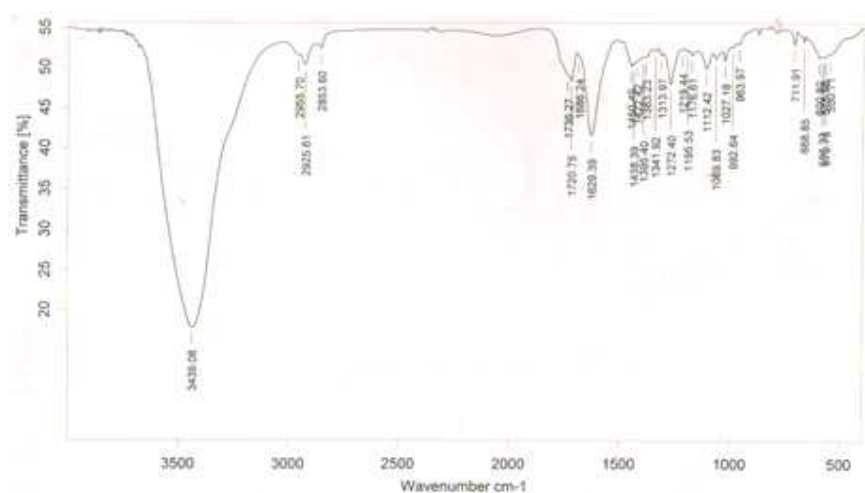


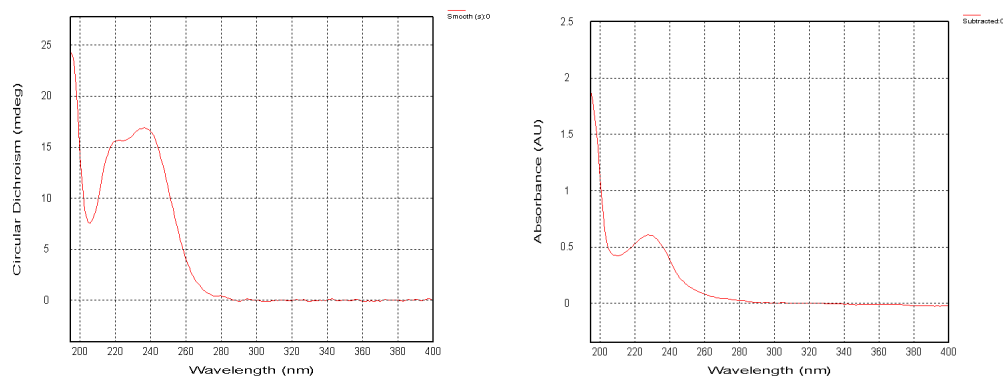
Figure S141. IR spectrum of aphanamixoid P (14)



Sample : hap-11		Frequency Range : 399.246 - 3996.32		Measured on : 09/01/2012	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27		Sample Scans : 16	
Customer : 120109IR12	Zerofilling : 2	Acquisition : Double Sided For			

Wavenumber	Abs. Intensity	Rel. Intensity	Width	Found if Threshold <	Shoulder
550.710	0.517	0.001	46.046	0.035276	0
570.730	0.514	0.001	5.101	0.028074	0
575.982	0.514	0.004	4.175	0.297771	0
585.323	0.514	0.000	4.975	0.060752	0
600.798	0.513	0.038	10.170	9.964440	0
668.848	0.532	0.009	5.259	2.148974	0
711.910	0.529	0.017	13.582	4.414880	0
963.967	0.530	0.003	12.169	0.523207	0
992.643	0.526	0.003	11.868	0.391568	0
1027.180	0.509	0.014	11.607	3.209902	0
1069.826	0.511	0.009	17.835	2.205313	0
1112.422	0.499	0.033	28.263	6.867225	0
1176.613	0.516	0.007	17.859	1.543999	0
1195.529	0.521	0.002	11.415	0.228112	0
1219.441	0.522	0.002	8.544	0.253430	0
1272.395	0.479	0.062	27.502	14.918269	0
1313.972	0.516	0.005	8.926	0.726336	0
1341.918	0.521	0.003	13.033	0.631312	0
1383.228	0.514	0.001	11.620	0.013256	0
1395.402	0.512	0.002	7.215	0.264328	0
1422.417	0.508	0.001	16.384	0.025764	0
1438.385	0.504	0.003	7.982	0.413492	0
1450.494	0.502	0.029	15.301	6.050733	0
1629.394	0.416	0.135	58.592	35.919525	0
1686.240	0.515	0.001	6.415	0.046461	0
1720.749	0.484	0.037	17.480	9.578664	0
1736.271	0.491	0.001	43.877	0.173653	0
2853.595	0.524	0.006	14.666	1.524306	0
2925.606	0.503	0.031	23.308	7.719439	0
2955.702	0.515	0.002	29.730	0.158007	0
3439.078	0.178	0.372	242.290	99.491318	0

Figure S142. CD spectrum of aphanamixoid P (14)



File: CD HAP-11-1mm(195-400)12010604.dsx

ProBinaryX

Attributes :

- Time Stamp :Fri Jan 06 16:17:03 2012

- File ID : {20DD912E-9AA8-460d-8BA2-7A47D5803945}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.1560mg/ml MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm