

# Polyporenic Acids from The Mushroom *Buglossoporus quercinus* Possess Chemosensitizing and Efflux Pump Inhibitory Activities on Colo 320 Adenocarcinoma Cells

Kristóf Felegyi<sup>1</sup>, Zsófia Garádi<sup>1,2</sup>, Bálint Rácz<sup>3</sup>, Gábor Tóth<sup>3,4</sup>, Viktor Papp<sup>5</sup>, Imre Boldizsár<sup>1,6</sup>, András Dancsó<sup>2</sup>, Gabriella Spengler<sup>3</sup>, Szabolcs Béni<sup>1,7</sup> and Attila Ványolós<sup>1,\*</sup>

- <sup>1</sup> Department of Pharmacognosy, Semmelweis University, 1085 Budapest, Hungary; felegyi.kristof@pharma.semmelweis-univ.hu (K.F.); garadi.zsofia@pharma.semmelweis-univ.hu (Z.G.); boldizsar.imre@semmelweis.hu (I.B.); beni.szabolcs@semmelweis.hu (S.B.)
  - <sup>2</sup> Directorate of Drug Substance Development, Egis Pharmaceuticals Plc., 1475 Budapest, Hungary; dancso.andras@egis.hu
  - <sup>3</sup> Albert Szent-Györgyi Health Center, Department of Medical Microbiology, Albert Szent-Györgyi Medical School, University of Szeged, 6725 Szeged, Hungary; racz.balint@med.u-szeged.hu (B.R.); toth.gabor.1@med.u-szeged.hu (G.T.); spengler.gabriella@med.u-szeged.hu (G.S.)
  - <sup>4</sup> ELKH-USZ Biologically Active Natural Products Research Group, University of Szeged, 6720 Szeged, Hungary
  - <sup>5</sup> Department of Botany, Hungarian University of Agriculture and Life Sciences, 1118 Budapest, Hungary; papp.viktor@uni-mate.hu
  - <sup>6</sup> Department of Plant Anatomy, Institute of Biology, Eötvös Loránd University, 1117 Budapest, Hungary
  - <sup>7</sup> Department of Analytical Chemistry, Institute of Chemistry, Eötvös Loránd University, 1117 Budapest, Hungary
- \* Correspondence: vanyolos.attila@semmelweis.hu

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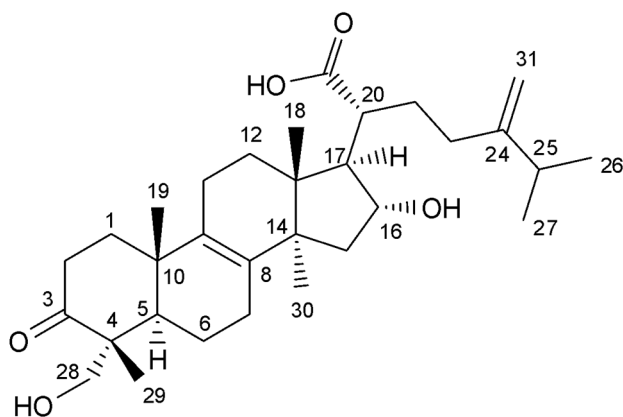


Table S2. NMR Spectroscopic Data (600 MHz, CDCl<sub>3</sub><sup>a</sup>, pyridine-*d*<sub>5</sub><sup>b</sup>, tetrahydrofuran-*d*<sub>8</sub><sup>c</sup>, or methanol-*d*:pyridine-*d*<sub>5</sub> 19:1<sup>d</sup>, methanol-*d*<sup>e</sup>) for compounds **10-12** 70

Table S3. Chemosensitizing Activity of Compounds **3-4**, and **7-12** on Colo 320 Adenocarcinoma Cells 71

Table S4. P-gp Efflux Pump Inhibitory Activity of Compounds **1-12** on MDR Colo 320 Colon Adenocarcinoma Cell Line 73

## Spectra and spectral data on compound 1



HR-ESI-MS (+)  $m/z$  501.3568  $[M + H]^+$  (501.3575 calcd. for  $C_{31}H_{49}O_5$ ;  $\Delta$  -1.3 ppm); HR-ESI-MSMS (CID = 15%, 30%, 45%) 483.3460, 465.3365, 453.3355

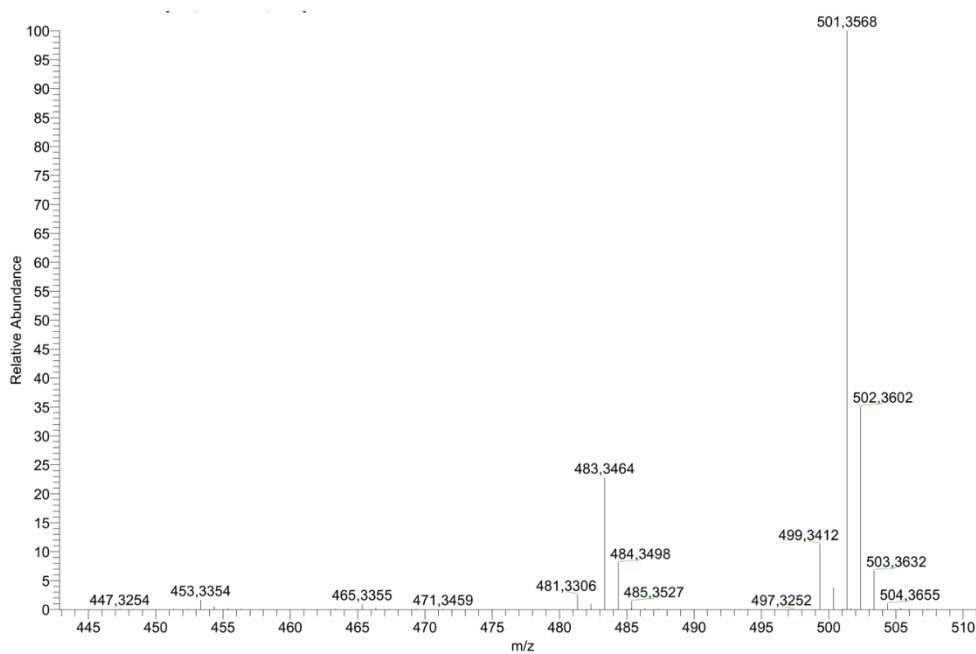


Figure S1. HR-ESI-MS spectrum of compound 1

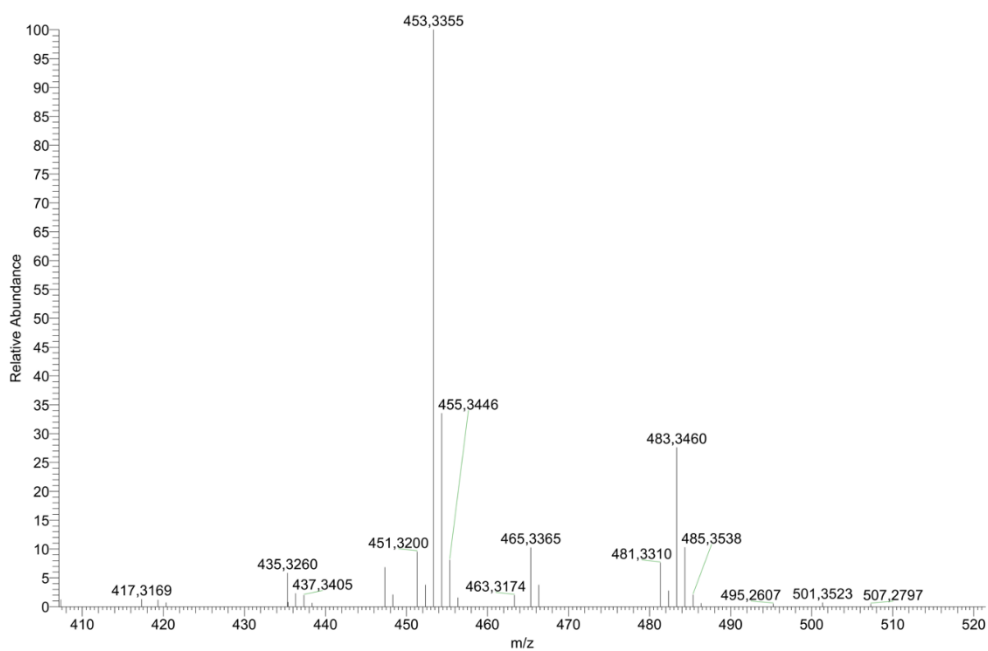


Figure S2. MS-MS spectrum of compound 1

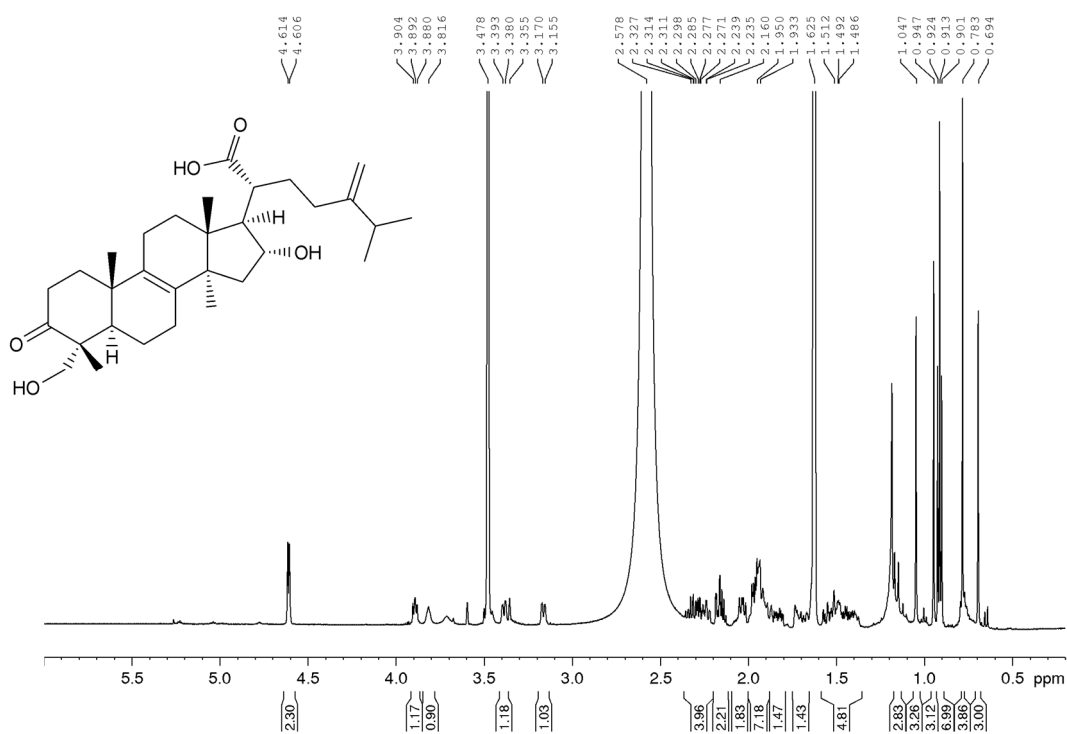


Figure S3. <sup>1</sup>H spectrum of compound 1 (600 MHz, THF-d<sub>8</sub>, 295 K)

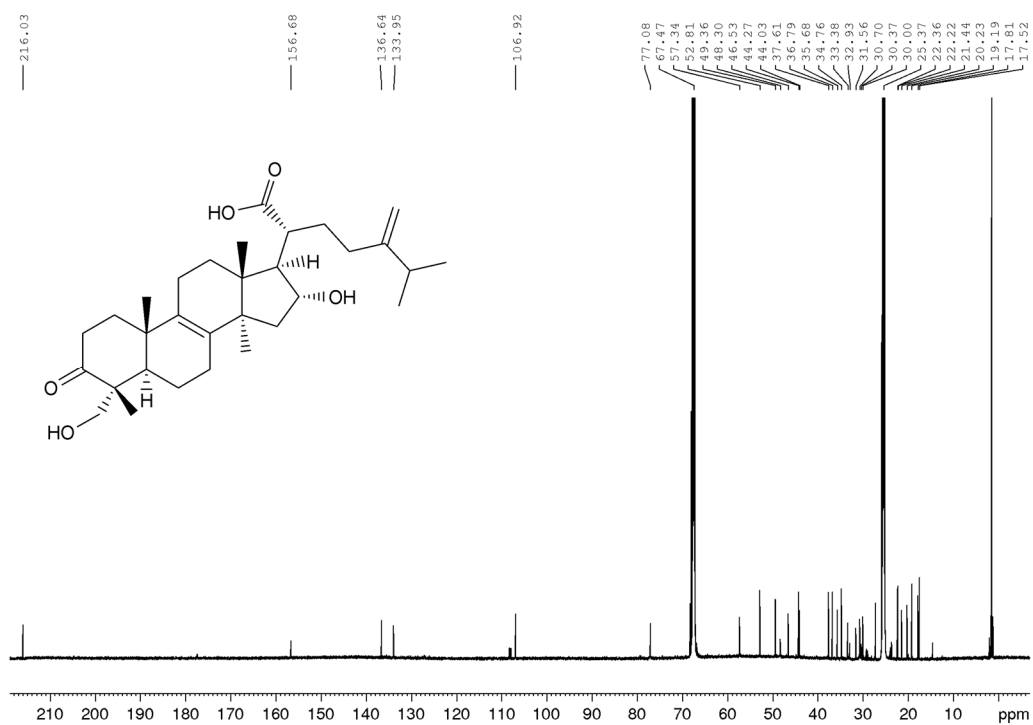


Figure S4.  $^{13}\text{C}$  spectrum of compound 1 (150 MHz,  $\text{THF-d}_8$ , 295 K)

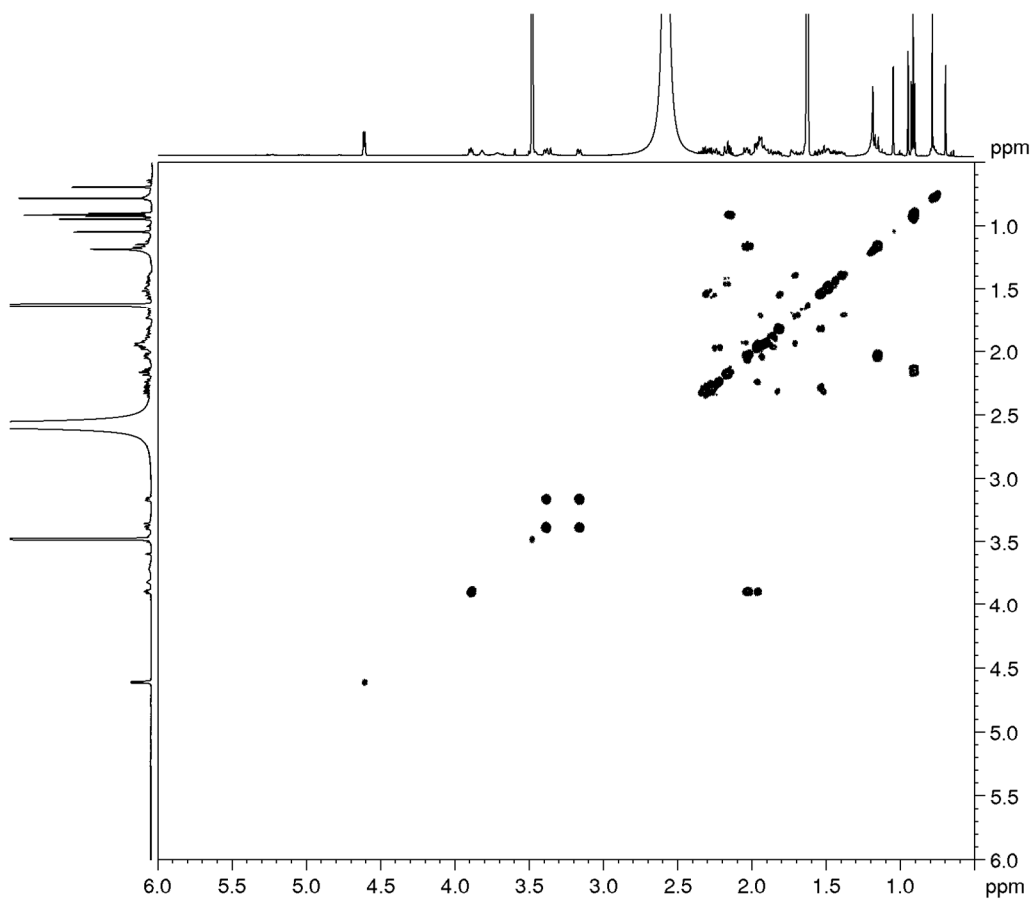


Figure S5. COSY spectrum of compound 1 (600 MHz,  $\text{THF-d}_8$ , 295 K)

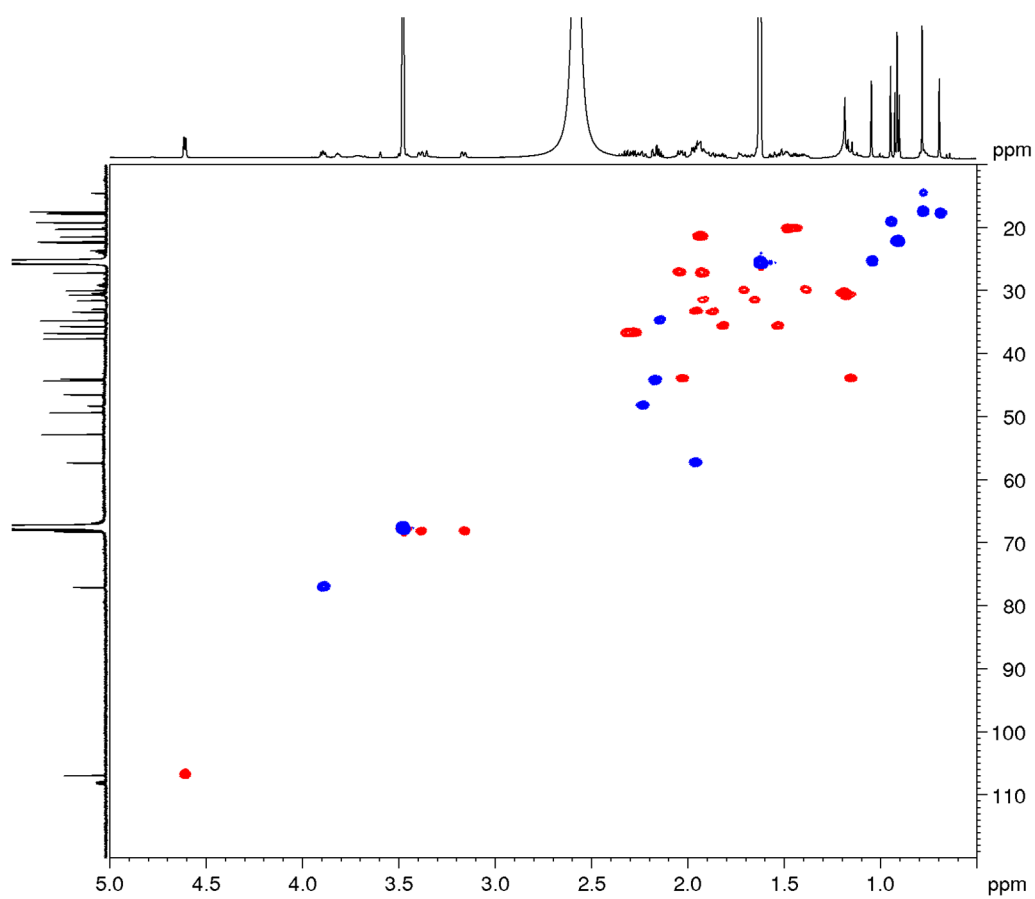


Figure S6. DEPT-edited HSQC spectrum of compound **1** (600 MHz, THF- $d_8$ , 295 K)

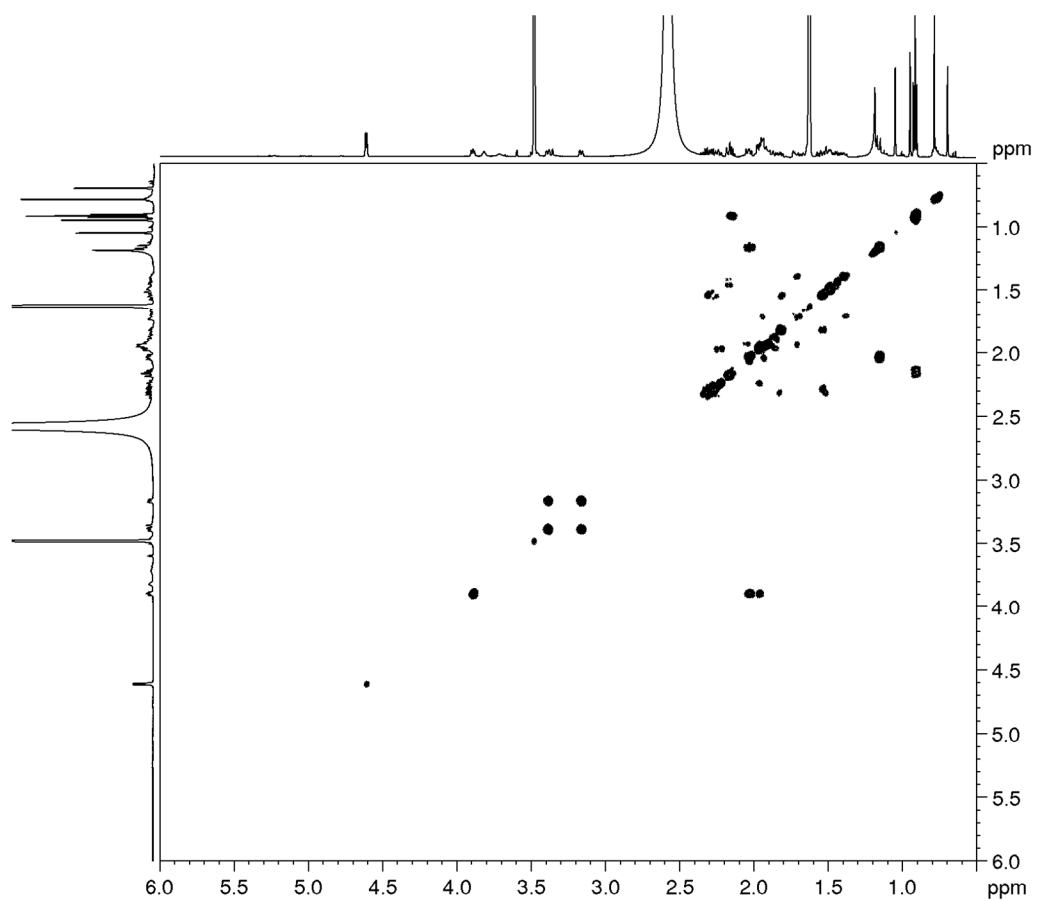


Figure S7. HMBC spectrum of compound **1** (600 MHz,  $\text{THF-}d_8$ , 295 K)

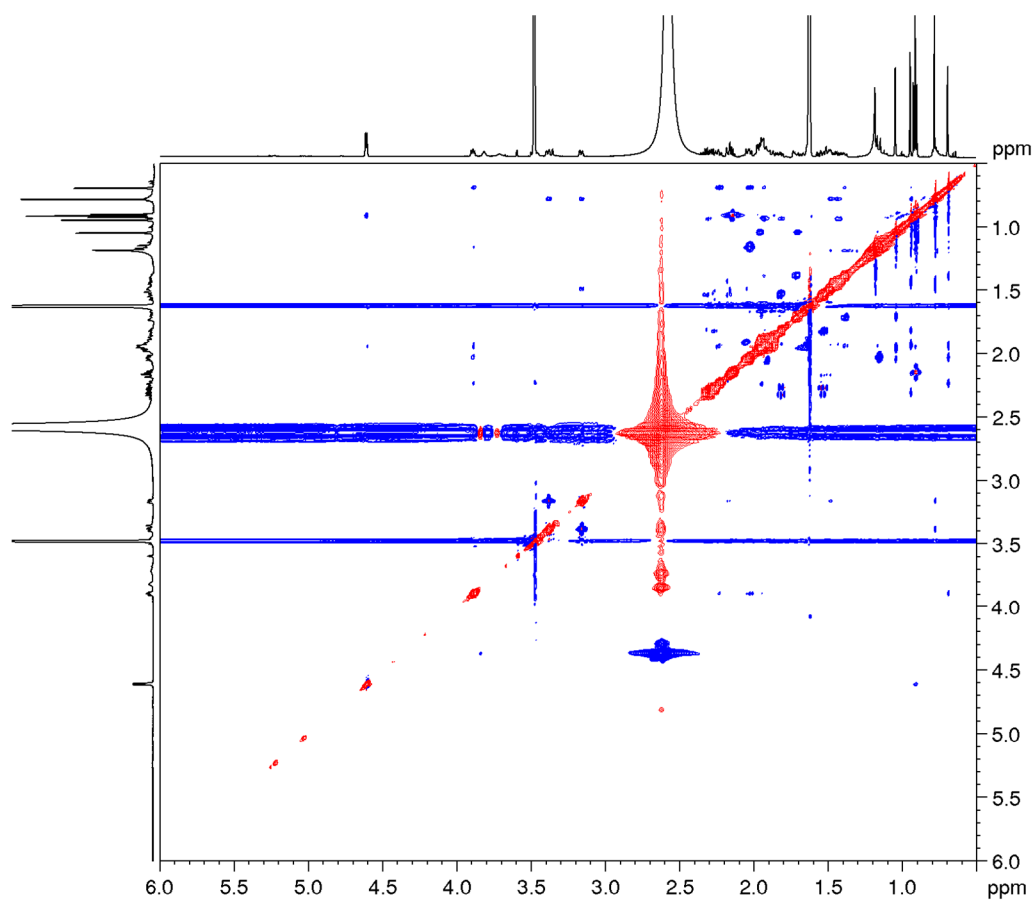


Figure S8. NOESY spectrum of compound **1** (600 MHz, THF-*d*<sub>8</sub>, 295 K)

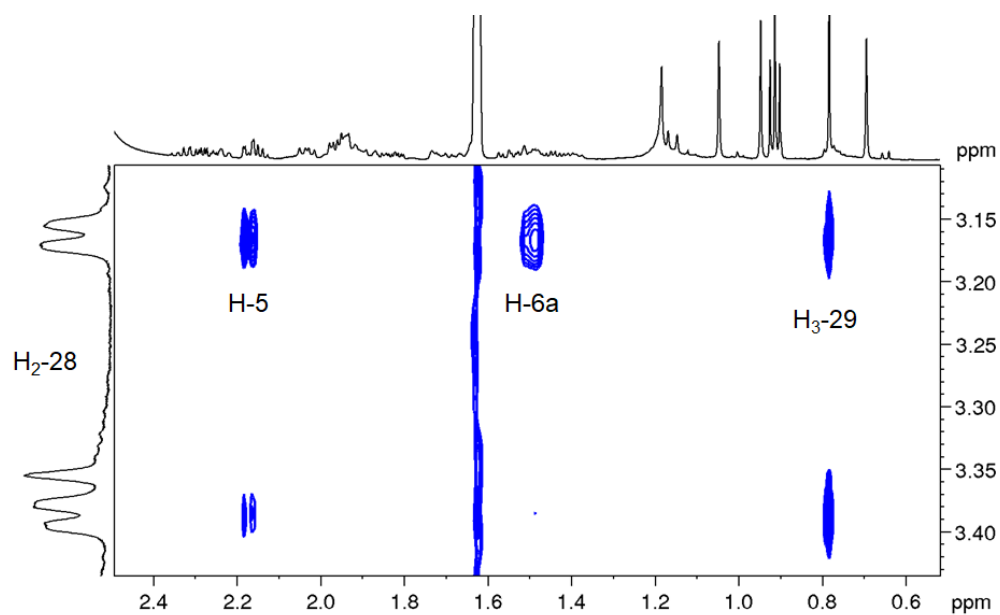
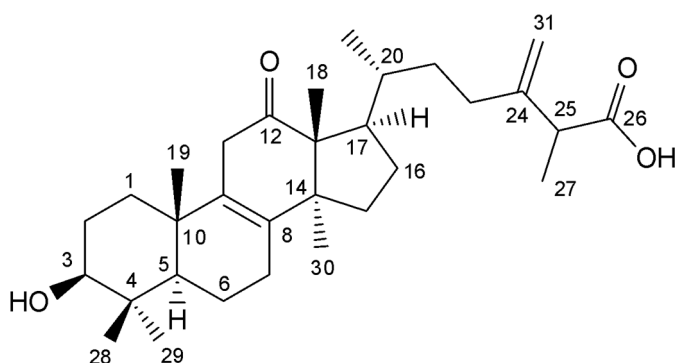


Figure S9. Selected region of the NOESY spectrum of compound **1** (600 MHz, THF-*d*<sub>8</sub>, 295 K)

## Spectra and spectral data on compound 2



HR-ESI-MS (+)  $m/z$  485.3620  $[M + H]^+$  (485.3625 calcd. for  $C_{31}H_{49}O_4$ ;  $\Delta$  -1.0 ppm); HR-ESI-MSMS (CID = 15%, 30%, 45%) 468.9432, 454.8377

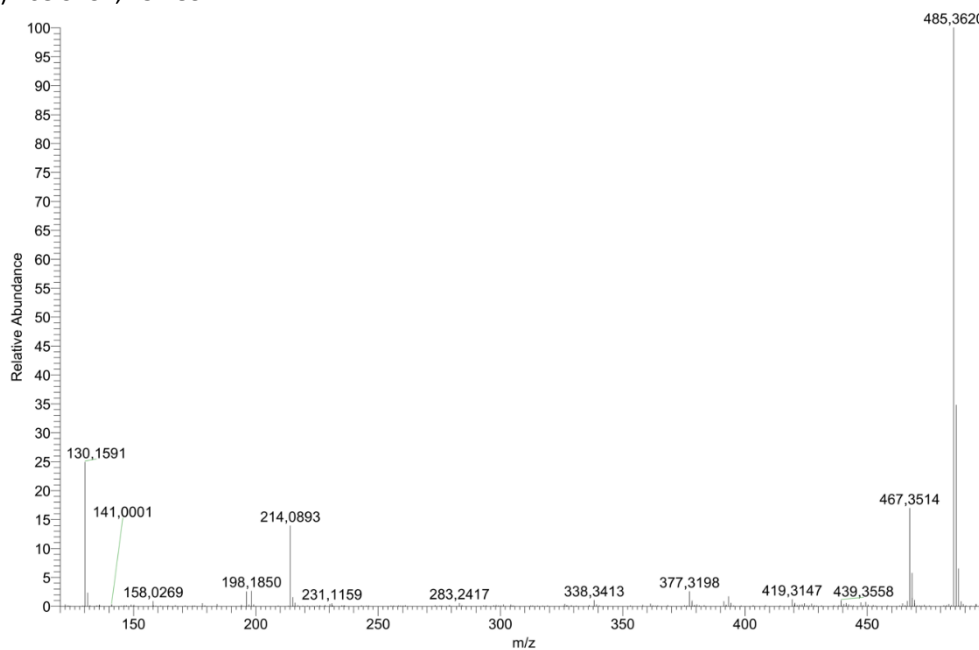


Figure S10. HR-ESI-MS spectrum of compound 2



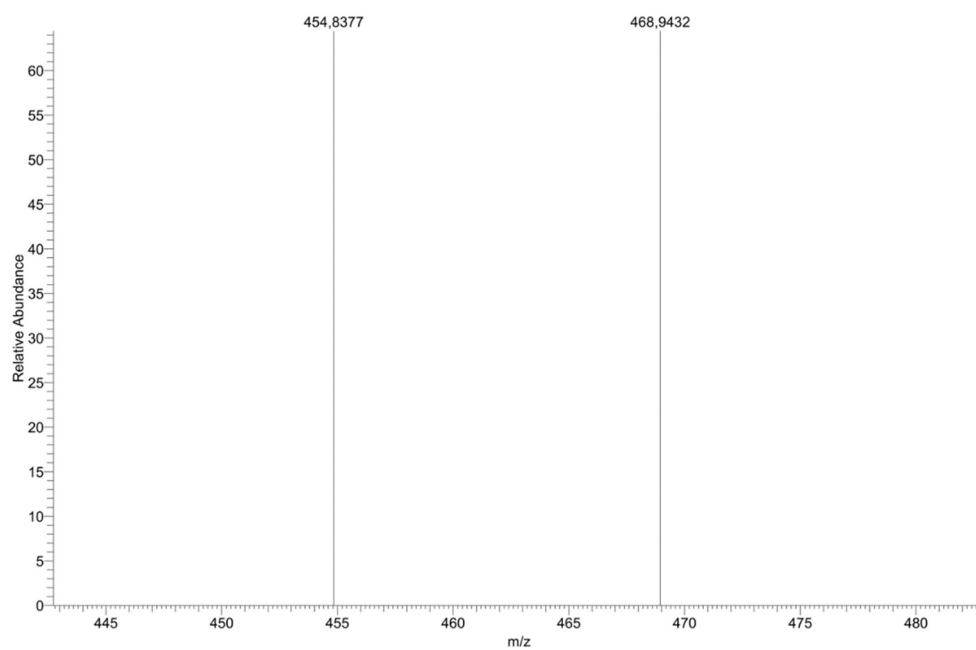


Figure S11. MS-MS spectrum of compound 2

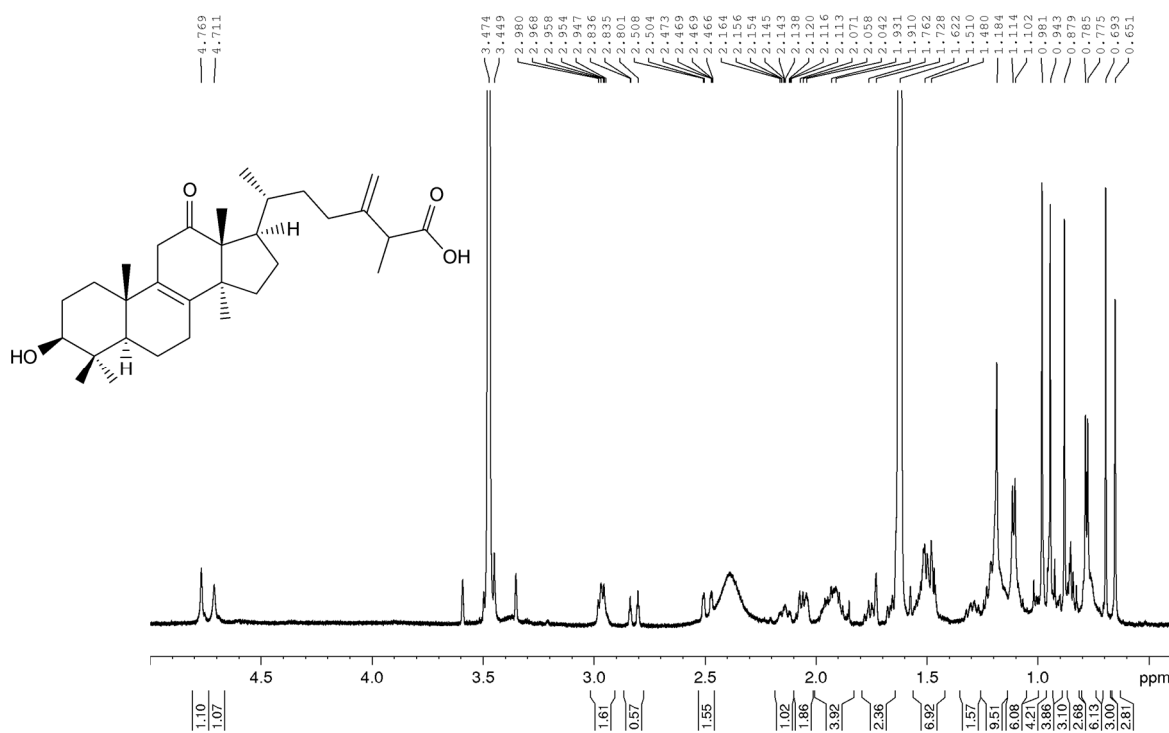


Figure S12. <sup>1</sup>H spectrum of compound 2 (600 MHz, THF-*d*<sub>8</sub>, 295 K)

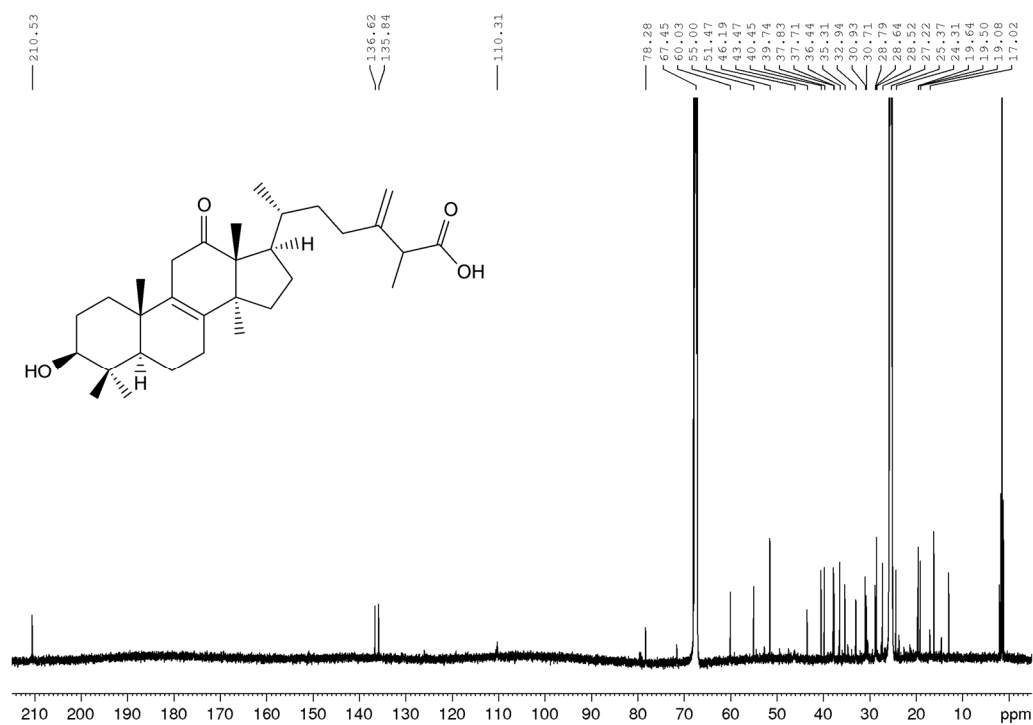


Figure S13.  $^{13}\text{C}$  spectrum of compound **2** (150 MHz,  $\text{THF}-d_8$ , 295 K)

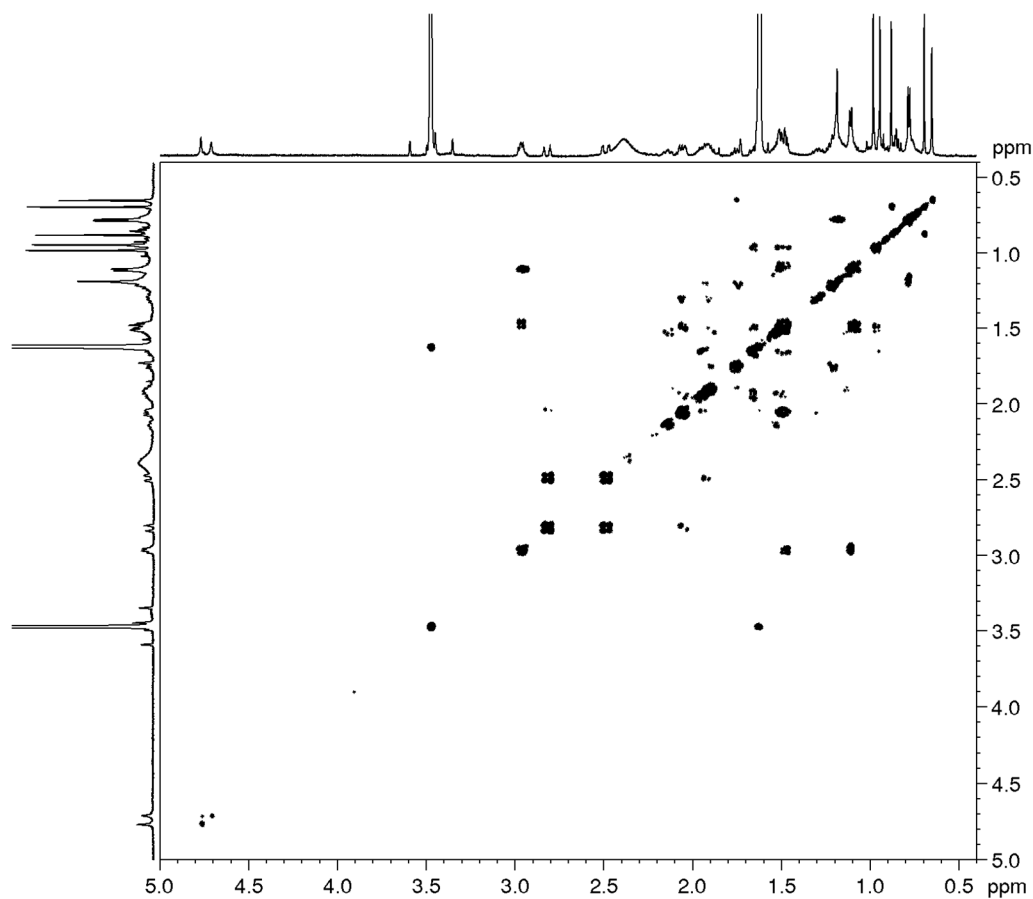


Figure S14. COSY spectrum of compound **2** (600 MHz,  $\text{THF}-d_8$ , 295 K)

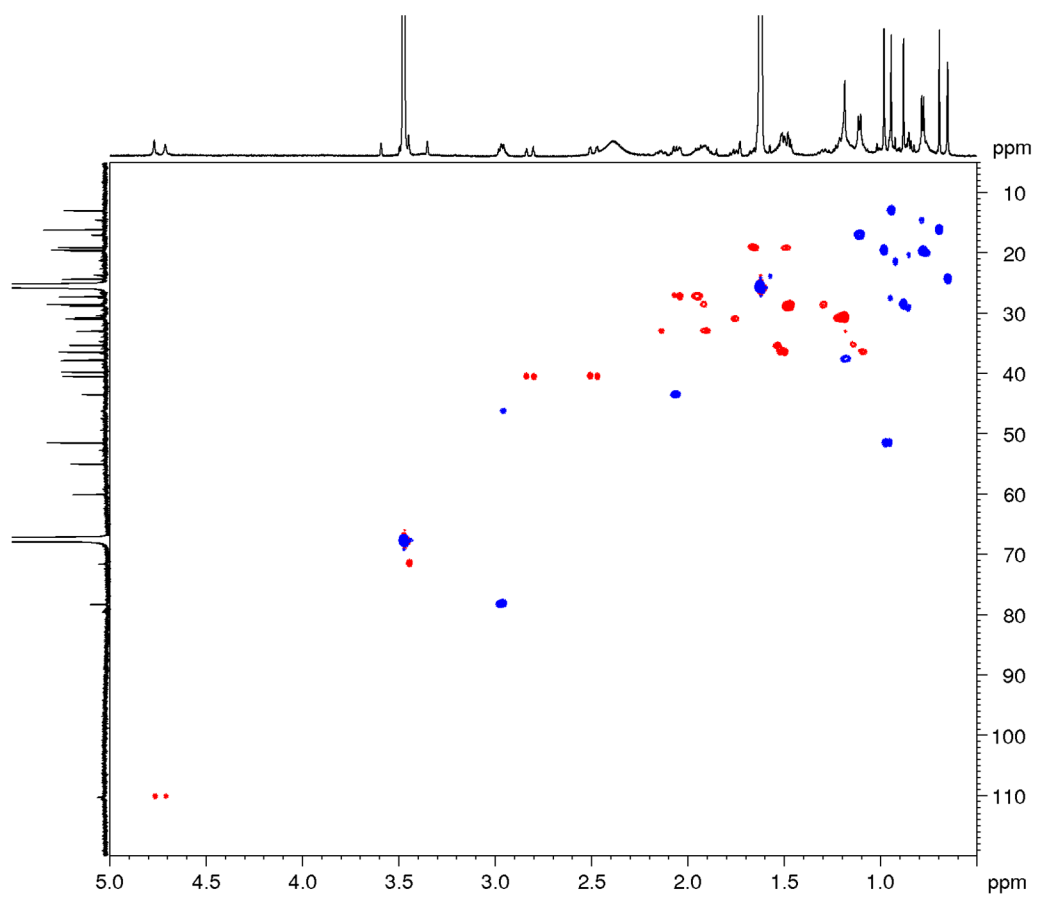


Figure S15. DEPT-edited HSQC spectrum of compound **2** (600 MHz, THF-*d*<sub>8</sub>, 295 K)

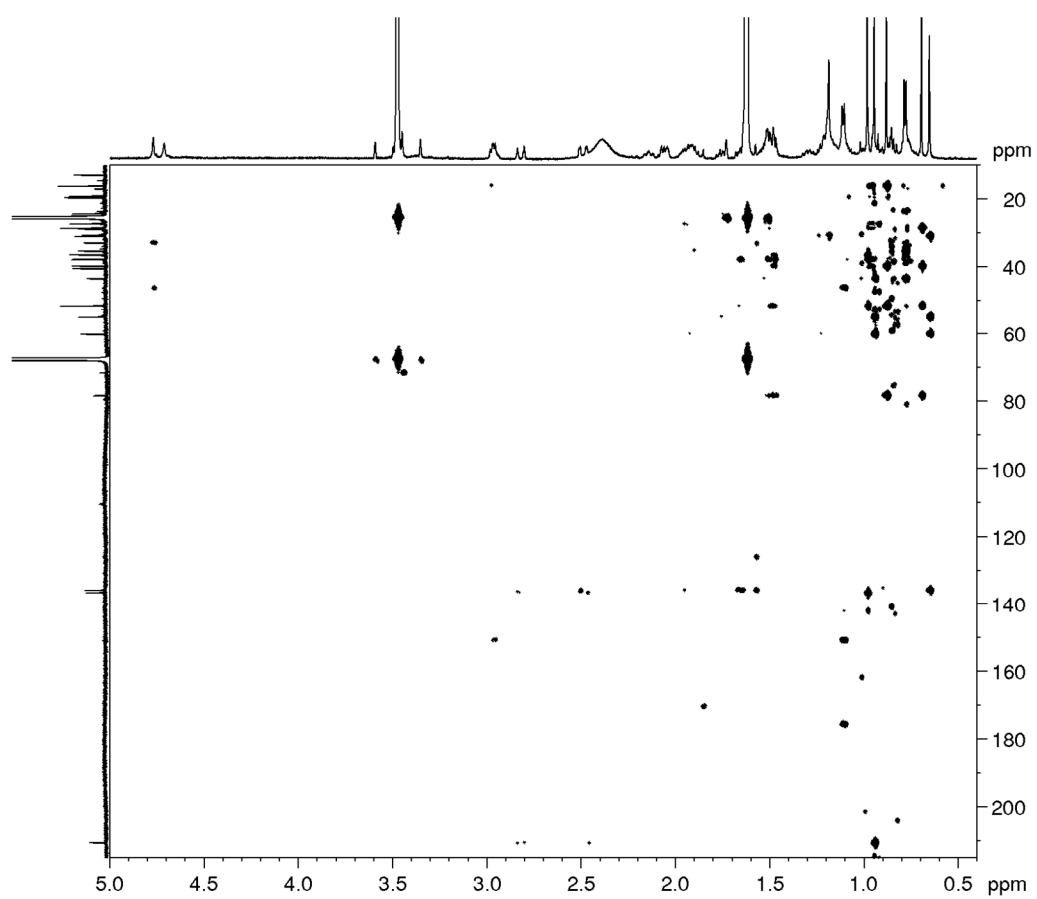


Figure S16. HMBC spectrum of compound **2** (600 MHz,  $\text{THF-}d_8$ , 295 K)

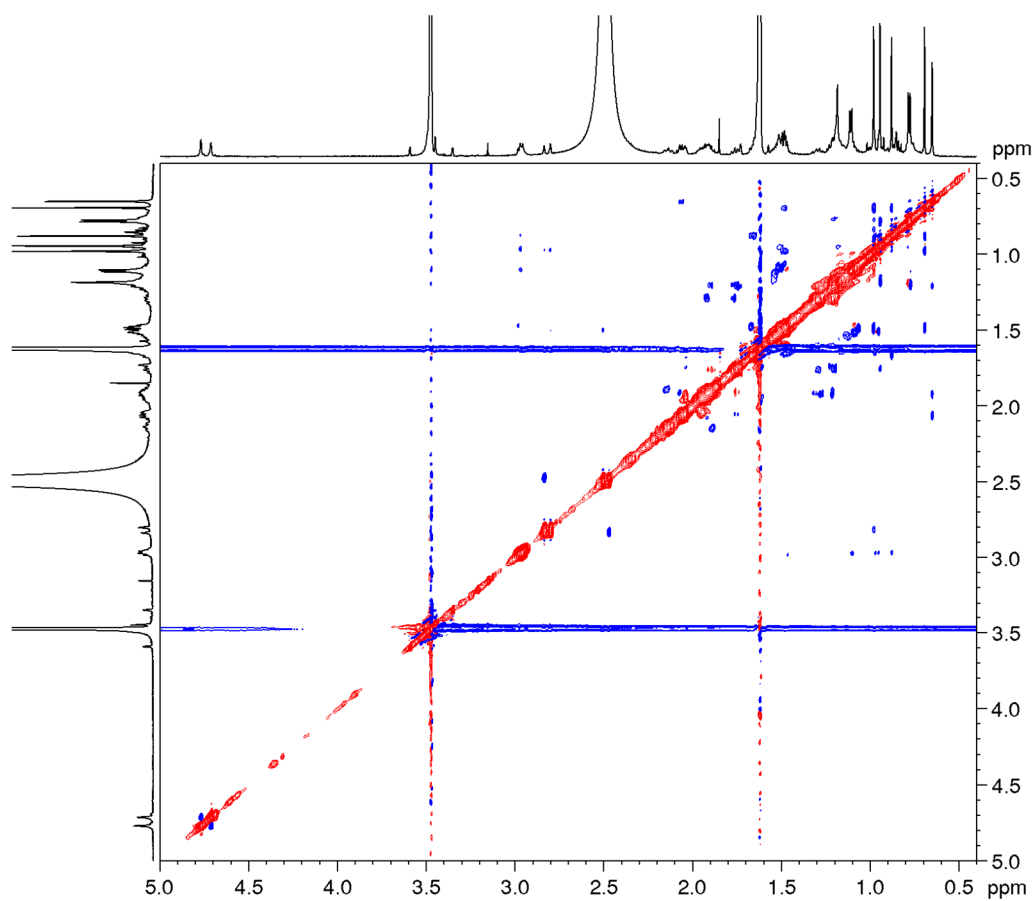


Figure S17. NOESY spectrum of compound **2** (600 MHz, THF- $d_8$ , 295 K)

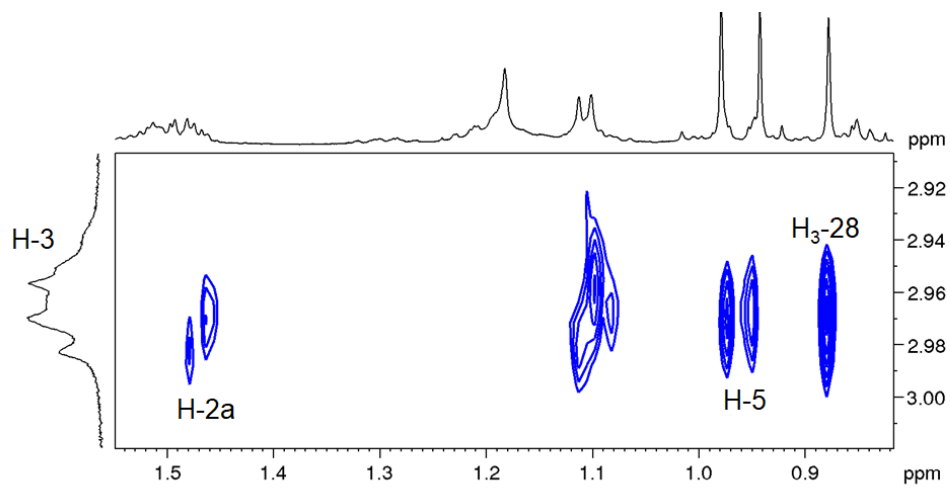
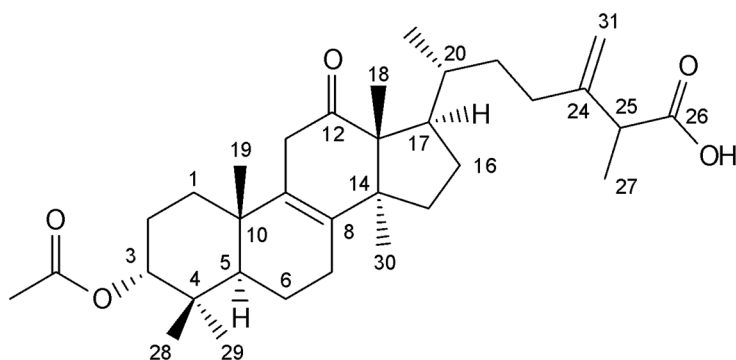


Figure S18. Selected region of the NOESY spectrum of compound **2** (600 MHz, THF- $d_8$ , 295 K)

### Spectra and spectral data on compound 3



HR-ESI-MS (+)  $m/z$  527.3721  $[M + H]^+$  (527.3731 calcd. for  $C_{33}H_{51}O_5$ ;  $\Delta$  -2.0 ppm); HR-ESI-MSMS (CID = 15%, 30%, 45%) 509.3611, 481.3671, 467.3504, 449.3400, 421.3456

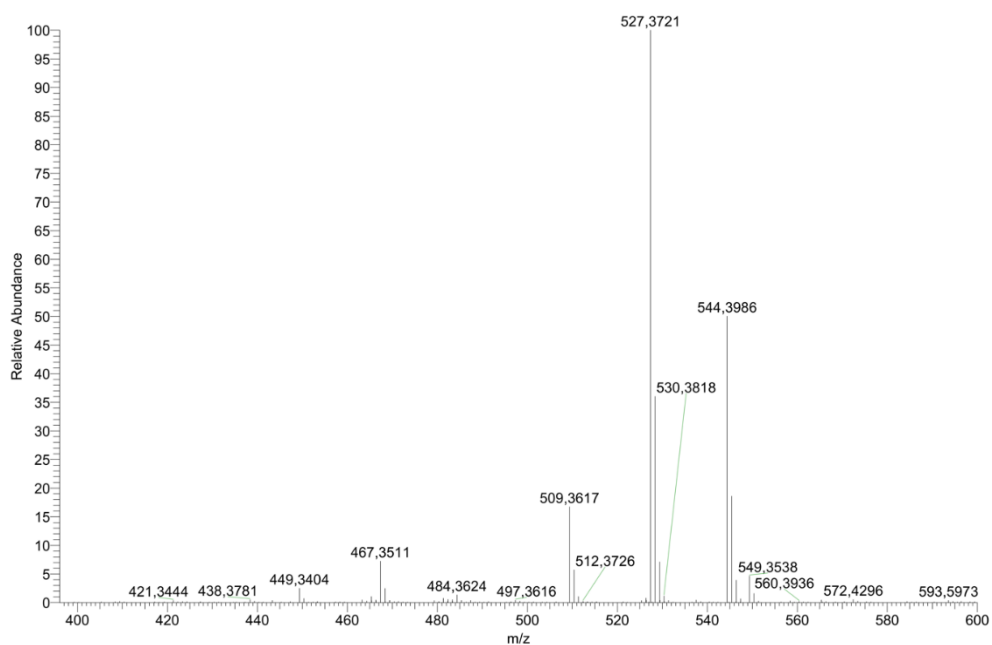


Figure S19. HR-ESI-MS spectrum of compound 3

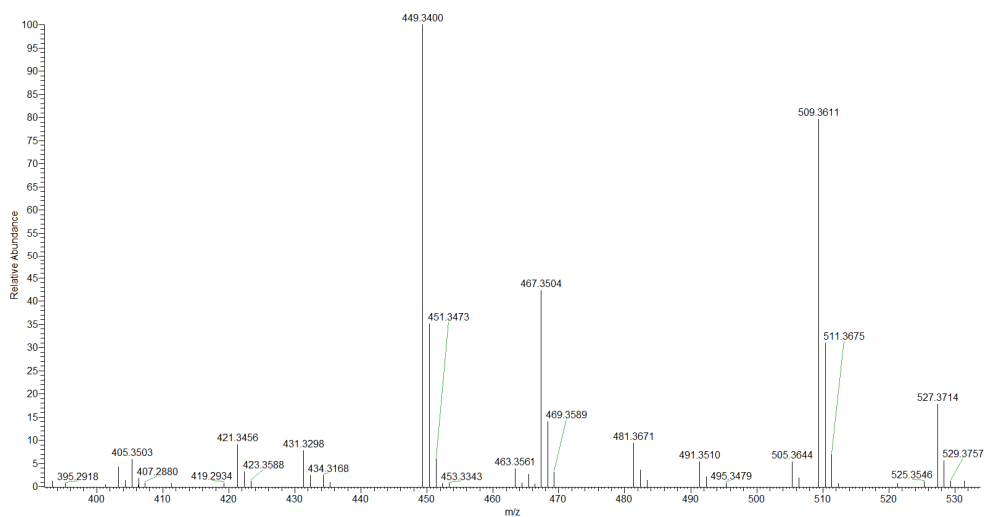


Figure S20. MS-MS spectrum of compound 3

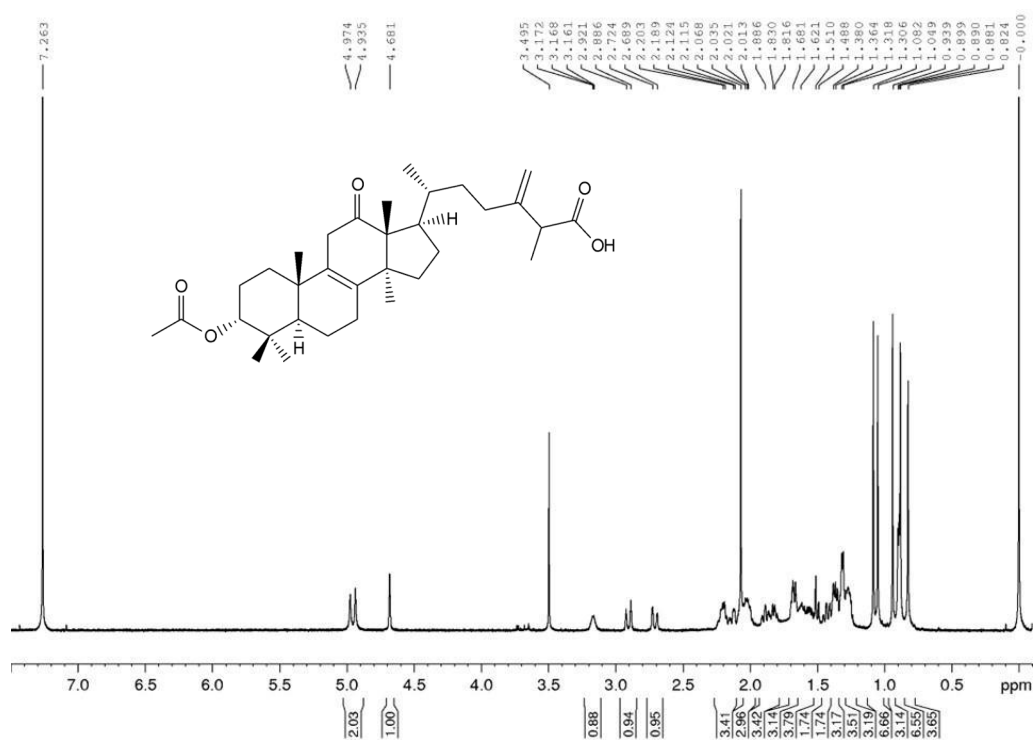


Figure S21. <sup>1</sup>H spectrum of compound 3 (600 MHz, CDCl<sub>3</sub>, 295 K)

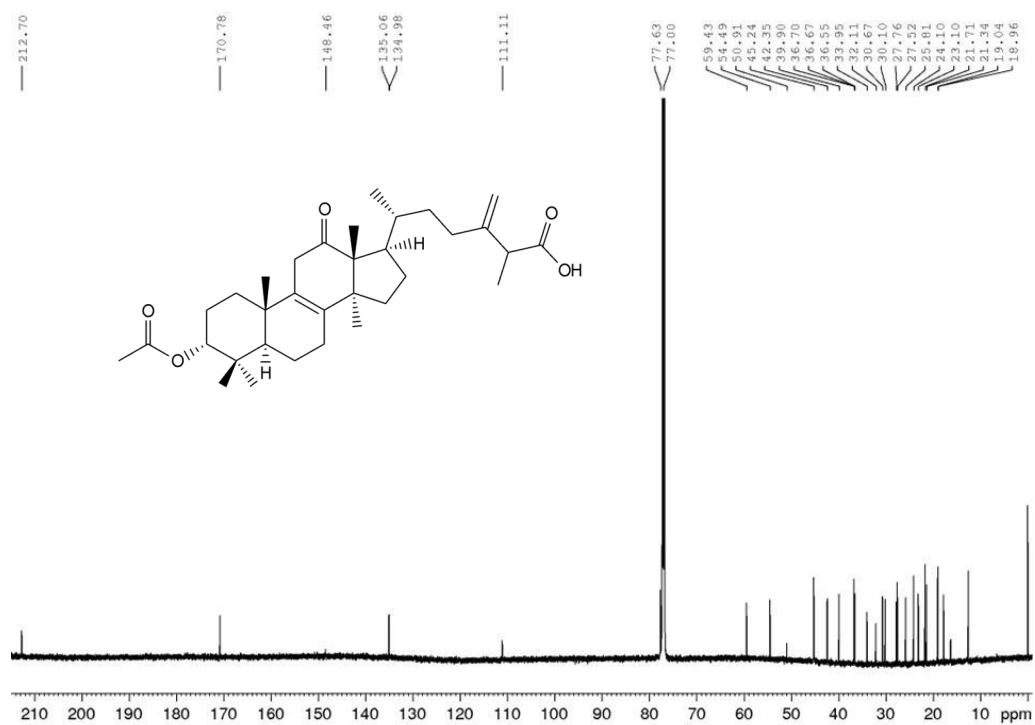


Figure S22.  $^{13}\text{C}$  spectrum of compound **3** (150 MHz,  $\text{CDCl}_3$ , 295 K)

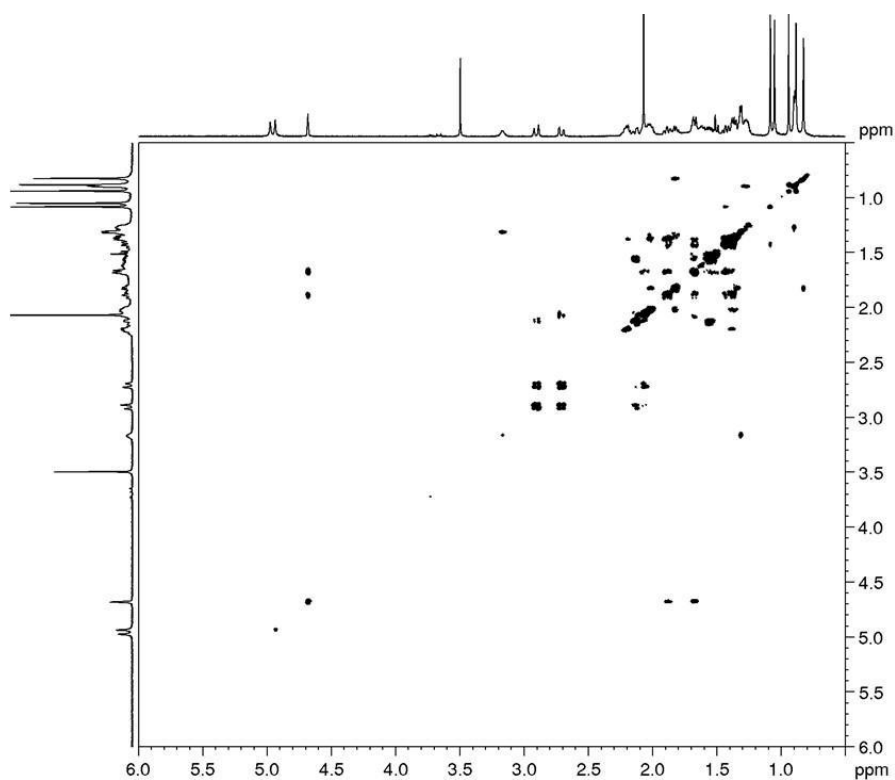


Figure S23. COSY spectrum of compound **3** (600 MHz,  $\text{CDCl}_3$ , 295 K)



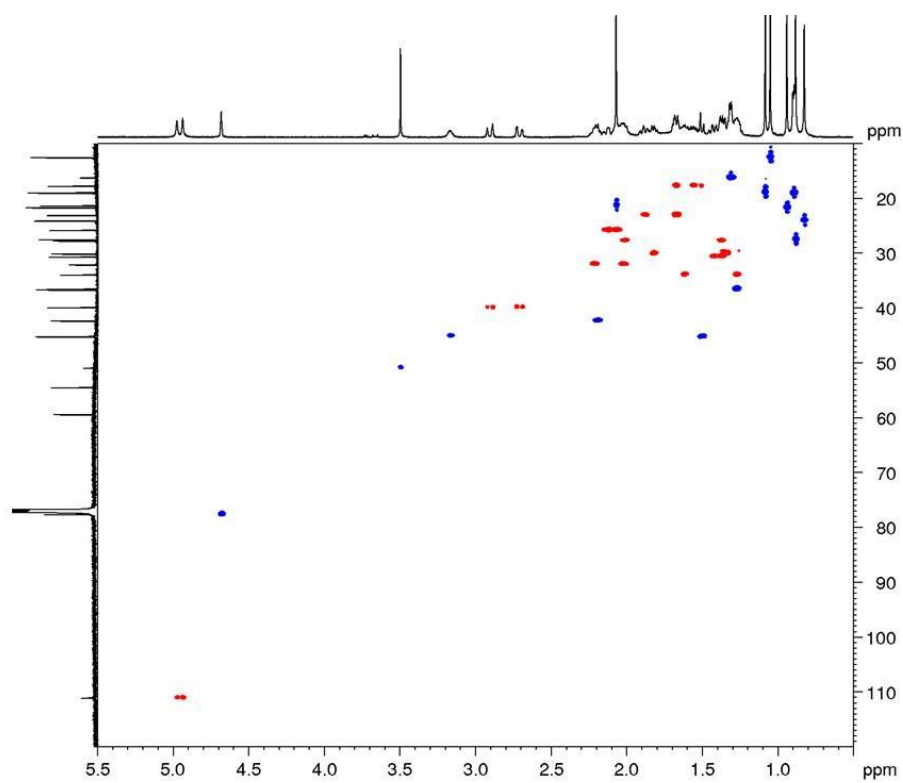


Figure S24. DEPT-edited HSQC spectrum of compound **3** (600 MHz, CDCl<sub>3</sub>, 295 K)

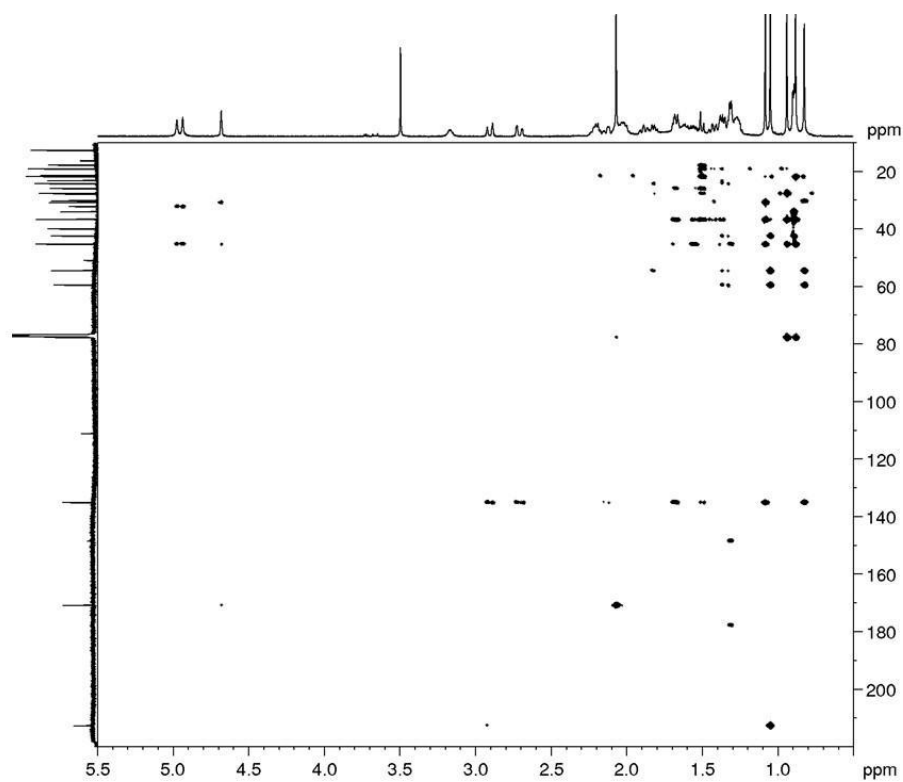


Figure S25. HMBC spectrum of compound **3** (600 MHz, CDCl<sub>3</sub>, 295 K)

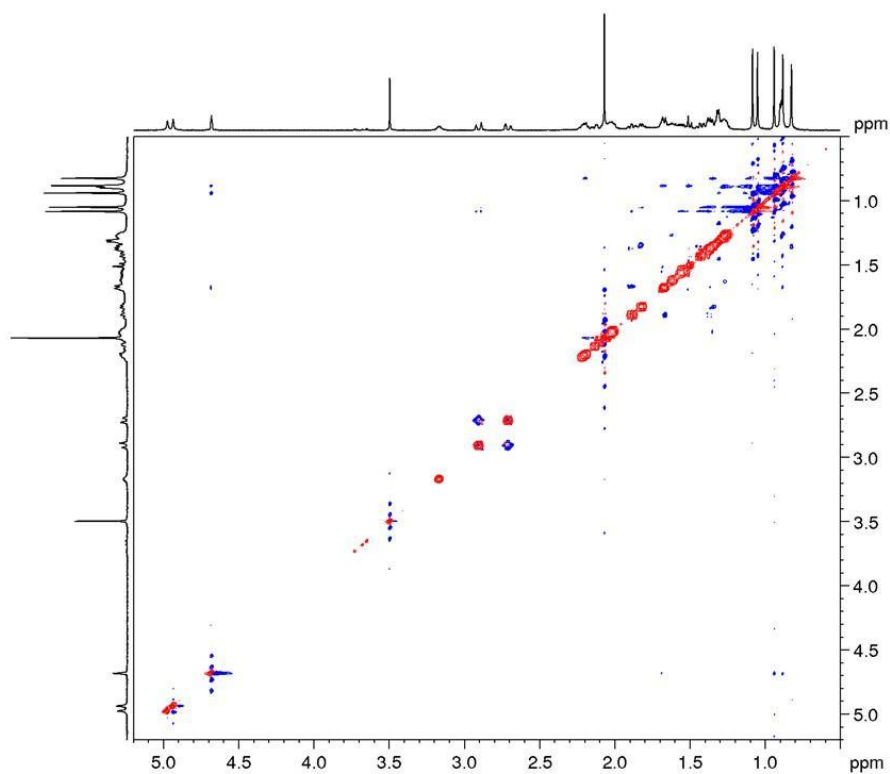
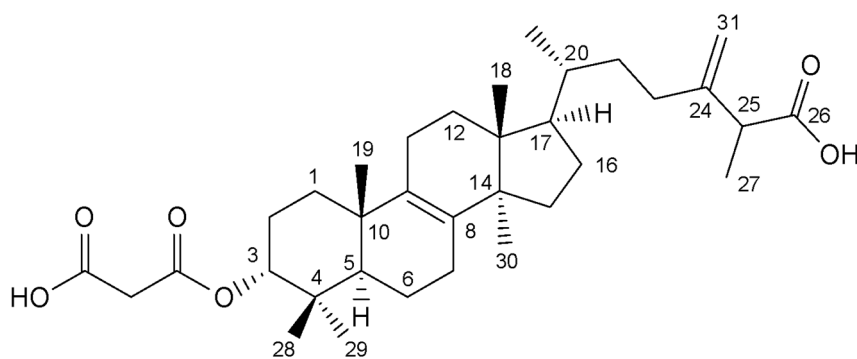


Figure S26. NOESY spectrum of compound **3** (600 MHz, CDCl<sub>3</sub>, 295 K)

#### Spectra and spectral data on compound **4**



HR-ESI-MS (-)  $m/z$  555.3694 [ $M - H$ ]<sup>-</sup> (555.3680 calcd. for C<sub>34</sub>H<sub>51</sub>O<sub>6</sub>;  $\Delta$  2.6 ppm); HR-ESI-MSMS (CID = 15%, 30%, 45%)  $m/z$  511.3787

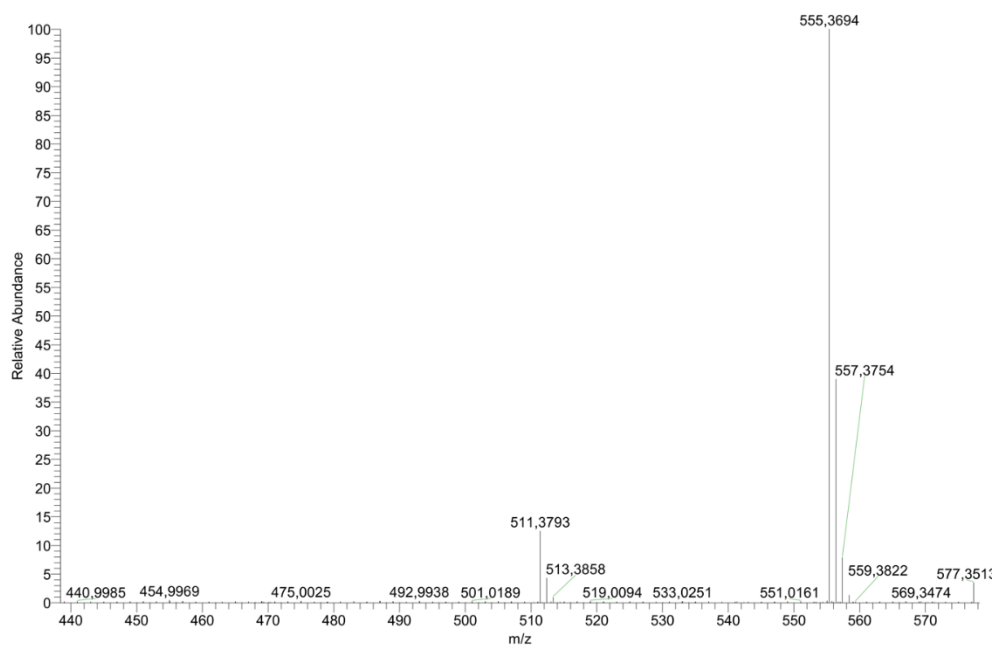


Figure S27. HR-ESI-MS spectrum of compound 4

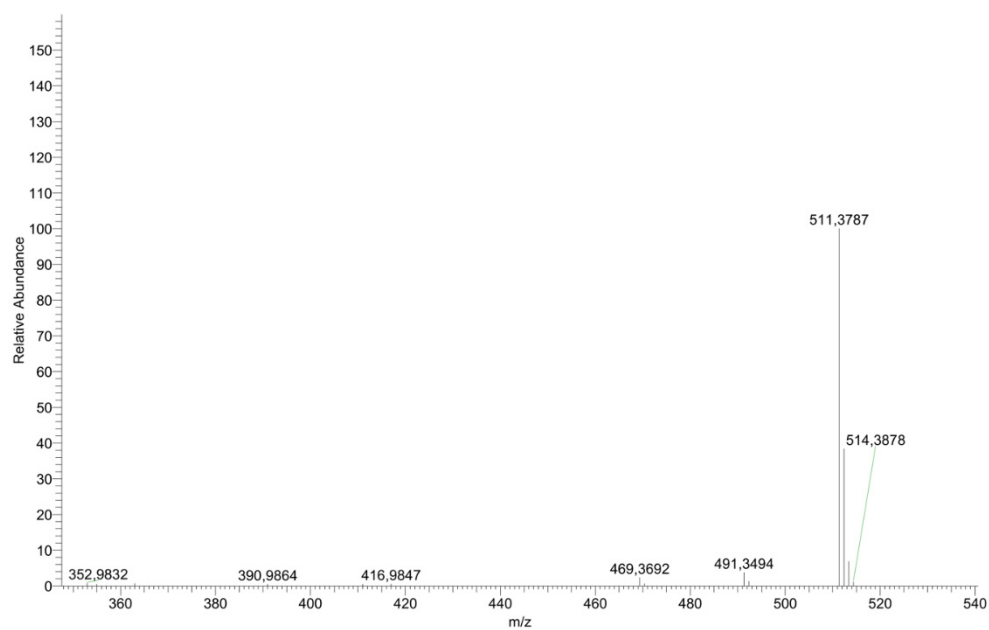
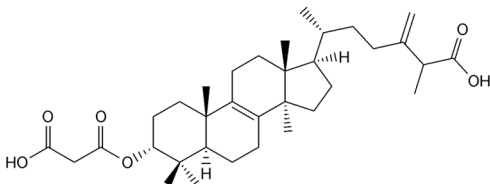


Figure S28. MS-MS spectrum of compound 4



Chemical structure of compound 1 is shown above the spectrum. The structure is a complex steroid derivative with a carboxylic acid group and a methyl group. The spectrum displays peaks corresponding to the carbon atoms in the molecule, with the following chemical shifts (ppm) labeled above the peaks:

- 179.64
- 167.24
- 149.31
- 134.34
- 134.23
- 111.38
- 80.63
- 77.00
- 50.27
- 49.85
- 45.29
- 45.01
- 44.45
- 40.67
- 36.80
- 36.75
- 36.29
- 34.40
- 33.65
- 30.94
- 30.78
- 30.64
- 28.19
- 27.63
- 25.94
- 24.24
- 23.16
- 21.71
- 18.32
- 18.22
- 18.63
- 17.97

24

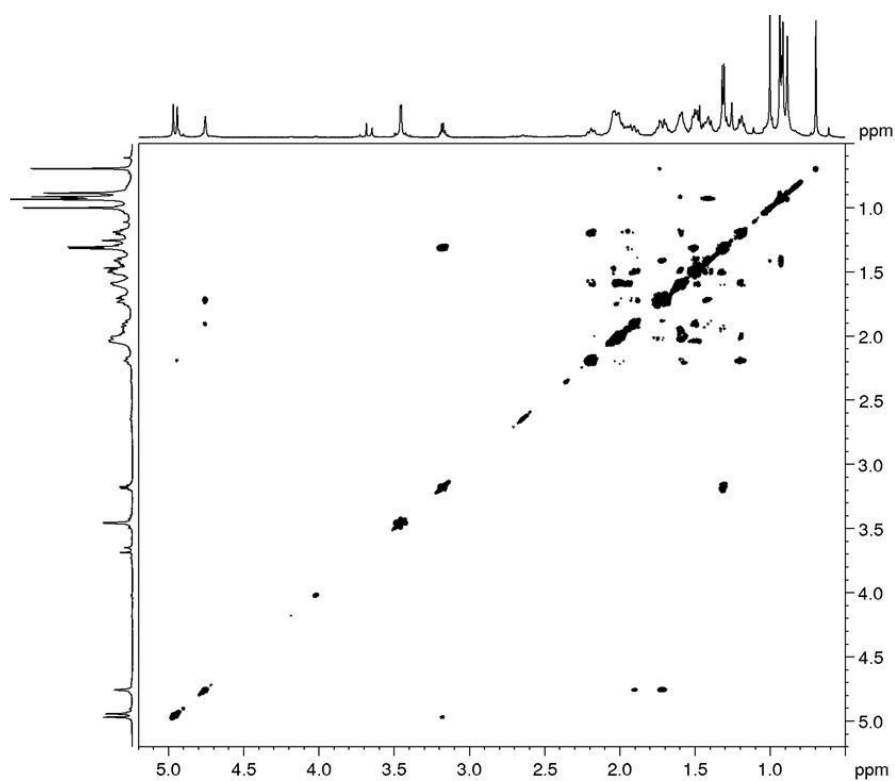


Figure S31. COSY spectrum of compound **4** (600 MHz, CDCl<sub>3</sub>, 295 K)

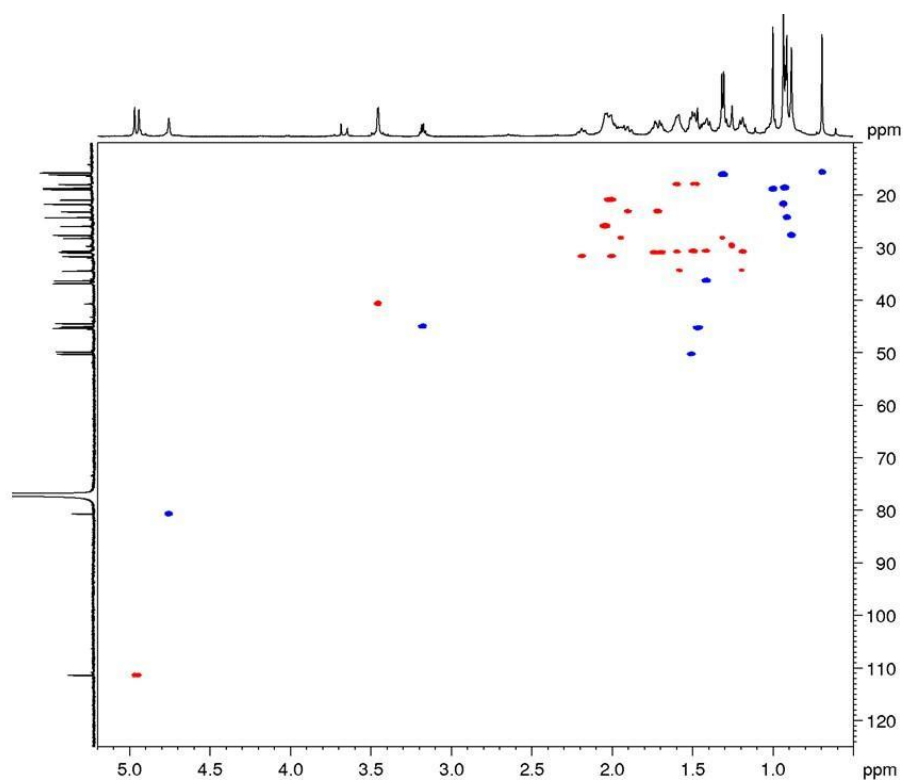


Figure S32. DEPT-edited HSQC spectrum of compound **4** (600 MHz, CDCl<sub>3</sub>, 295 K)

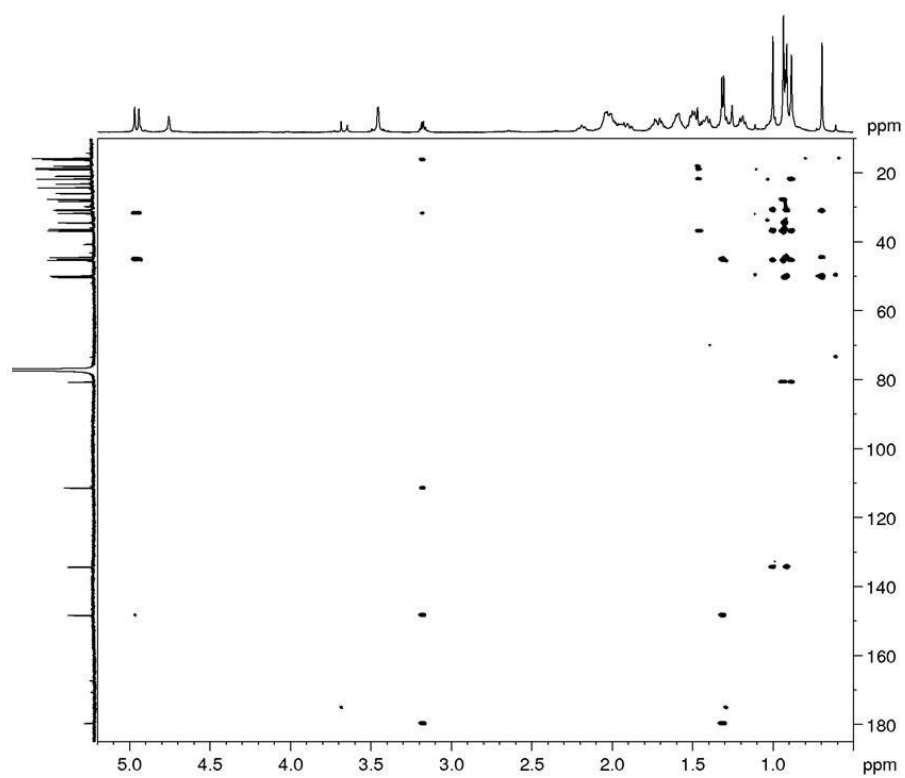


Figure S33. HMBC spectrum of compound **4** (600 MHz,  $\text{CDCl}_3$ , 295 K)

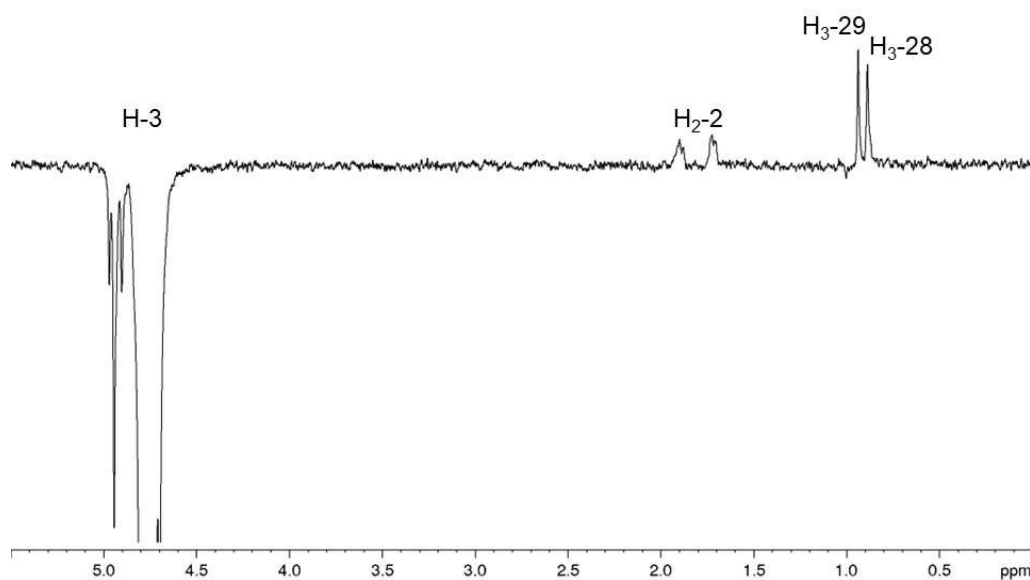
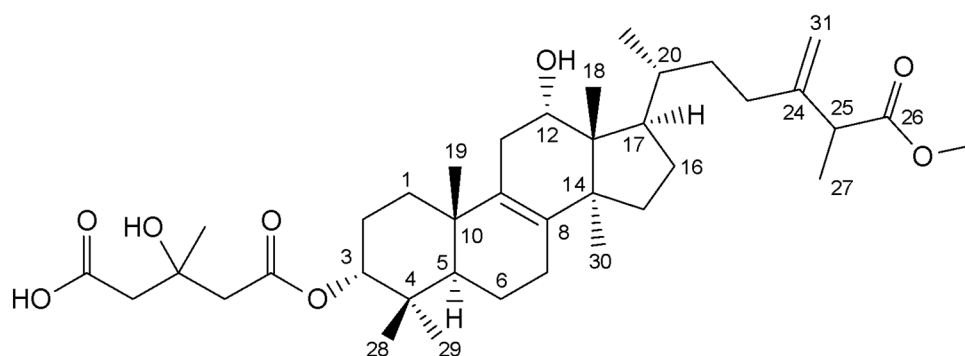


Figure S34. Selective gradient NOESY spectrum of compound **4** (600 MHz,  $\text{CDCl}_3$ , 295 K)

## Spectra and spectral data on compound 5



HR-ESI-MS (+)  $m/z$  645.4343  $[M + H]^+$  (645.4361 calcd. for  $C_{38}H_{61}O_8$ ;  $\Delta$  2.8 ppm); HR-ESI-MSMS (CID = 15%, 30%, 45%) 627.4243, 465.3715

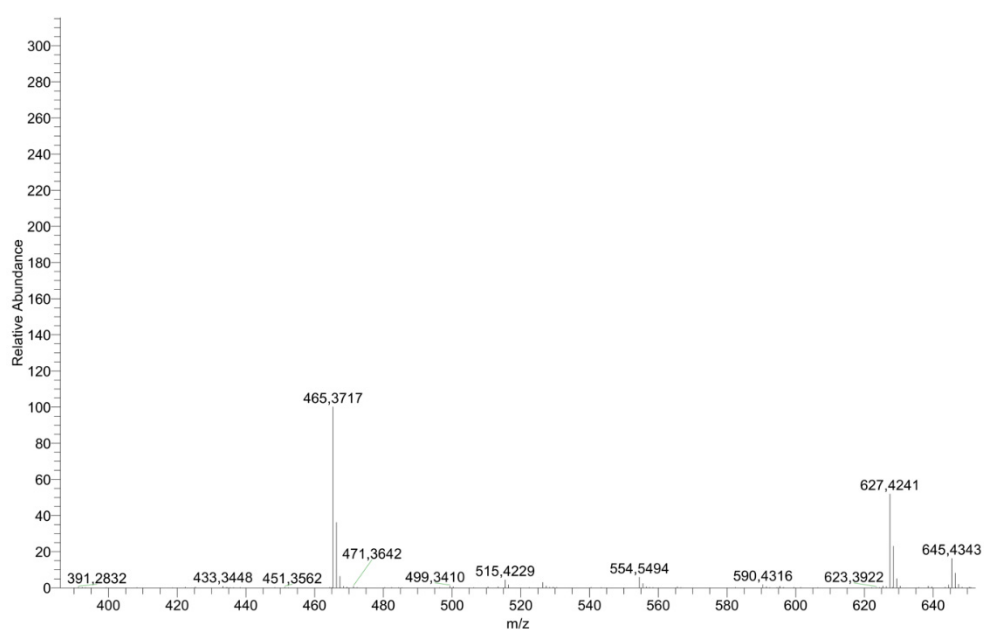


Figure S35. HR-ESI-MS spectrum of compound 5

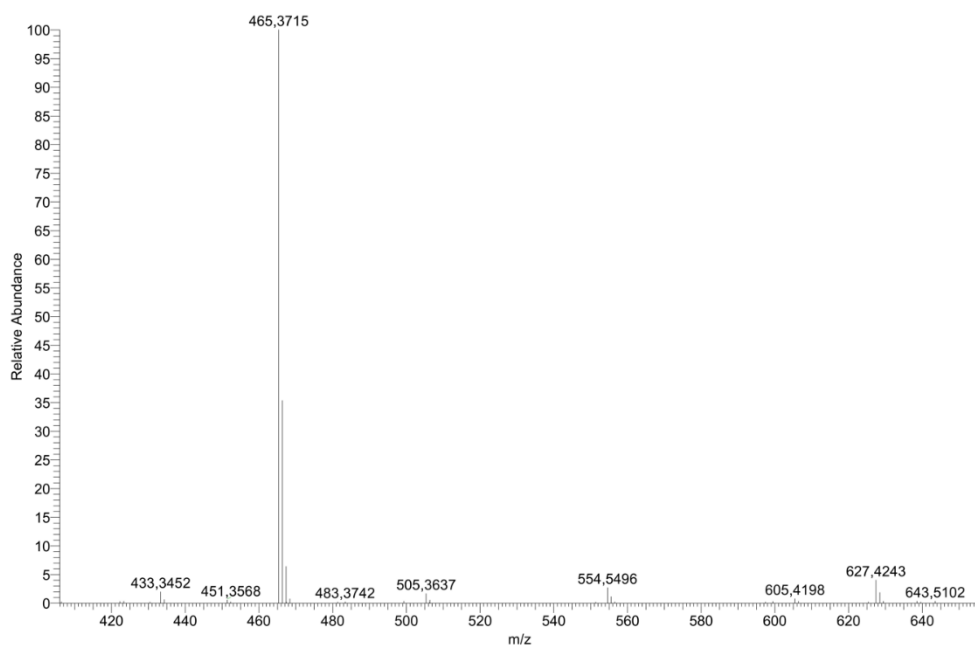


Figure S36. MS-MS spectrum of compound 5

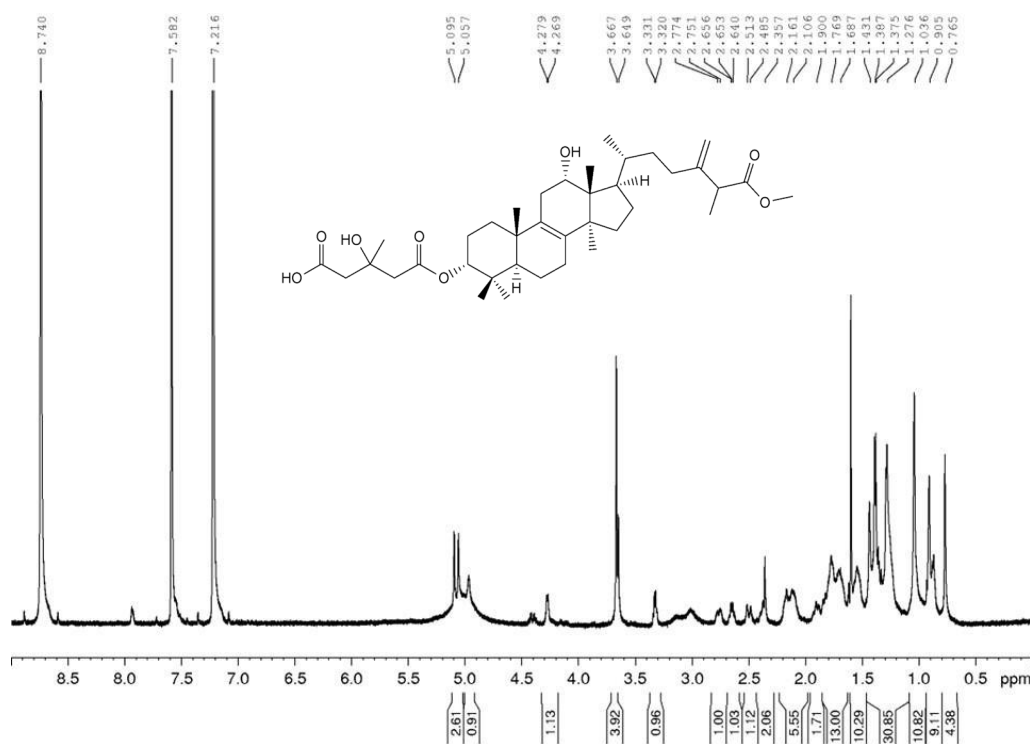


Figure S37. <sup>1</sup>H spectrum of compound 5 (600 MHz, pyridine-d<sub>5</sub>, 295 K)



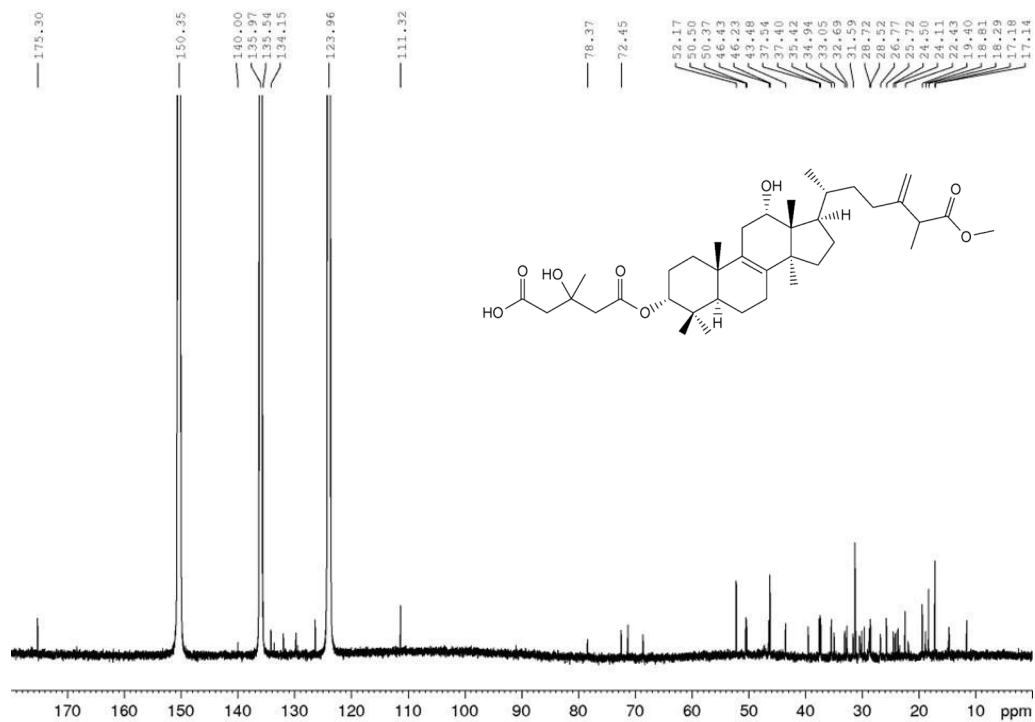


Figure S38.  $^{13}\text{C}$  spectrum of compound **5** (150 MHz, pyridine- $d_5$ , 295 K)

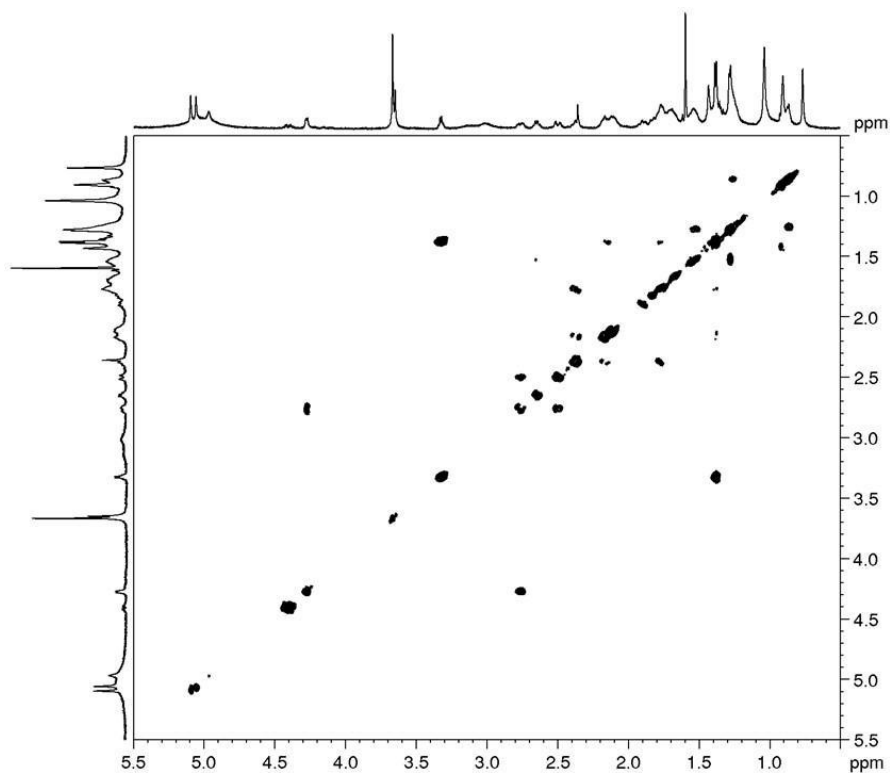


Figure S39. COSY spectrum of compound **5** (600 MHz, pyridine- $d_5$ , 295 K)

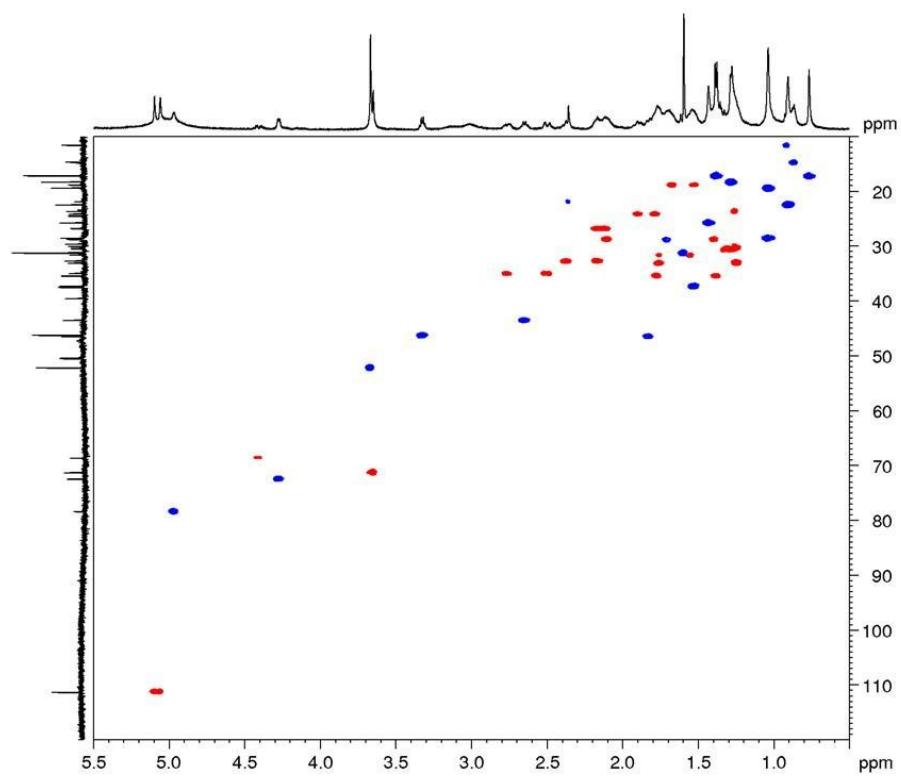


Figure S40. DEPT-edited HSQC spectrum of compound **5** (600 MHz, pyridine-*d*<sub>5</sub>, 295 K)

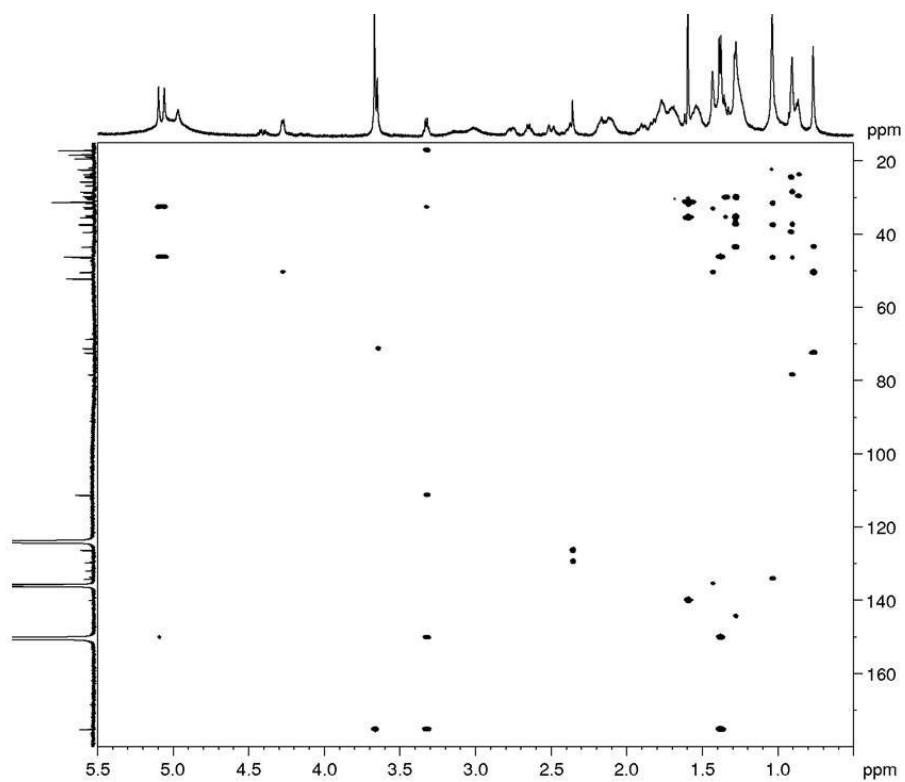


Figure S41. HMBC spectrum of compound **5** (600 MHz, pyridine-*d*<sub>5</sub>, 295 K)

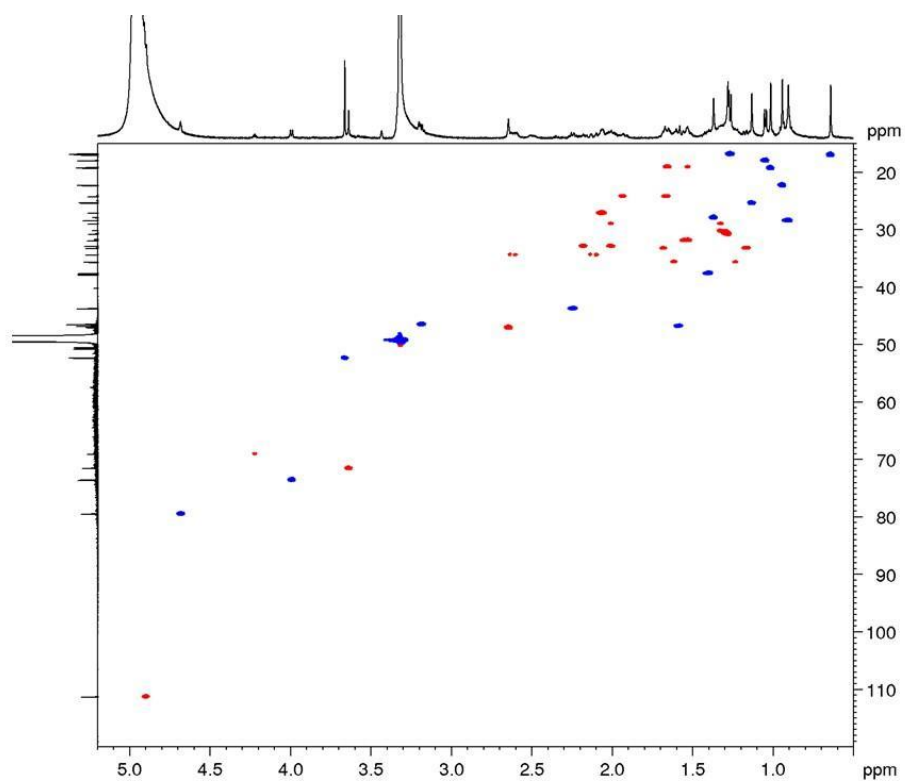


Figure S42. DEPT-edited HSQC spectrum of compound **5** (600 MHz, CD<sub>3</sub>OD:pyridine-*d*<sub>5</sub> (19:1), 295 K)

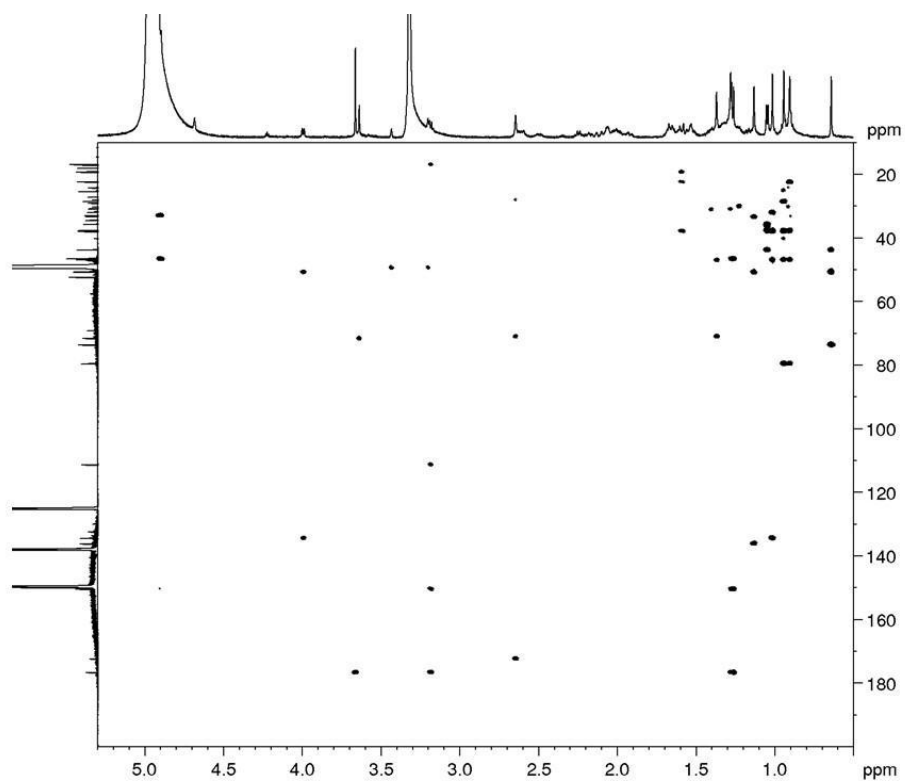


Figure S43. HMBC spectrum of compound **5** (600 MHz, CD<sub>3</sub>OD: pyridine-*d*<sub>5</sub> (19:1), 295 K)

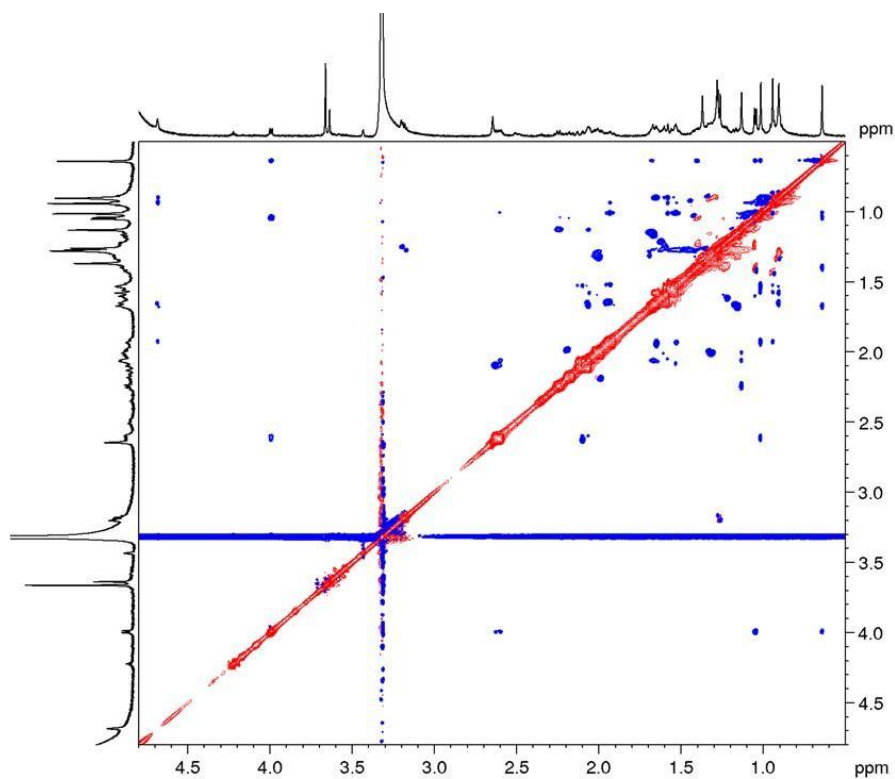
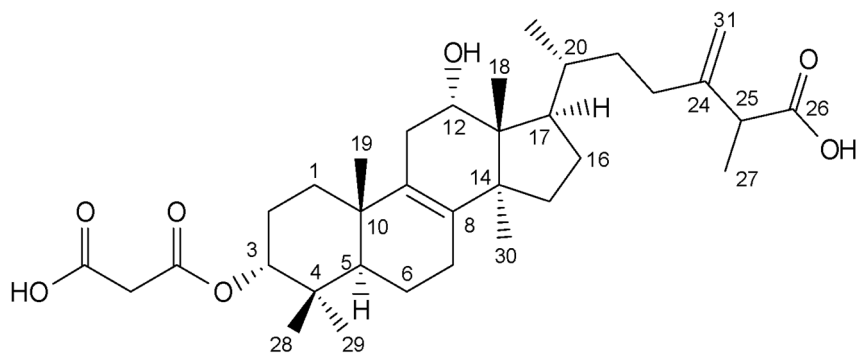


Figure S44. ROESY spectrum of compound **5** (600 MHz, CD<sub>3</sub>OD:pyridine-*d*<sub>5</sub> (19:1), 295 K)

#### Spectra and spectral data on compound **6**



HR-ESI-MS (-)  $m/z$  571.3642 [ $M - H$ ]<sup>-</sup> (571.3629 calcd. for C<sub>34</sub>H<sub>51</sub>O<sub>7</sub>;  $\Delta$  2.2 ppm;); HR-ESI-MSMS (CID = 15%, 30%, 45%) 527.3740, 483.3840, 441.3737

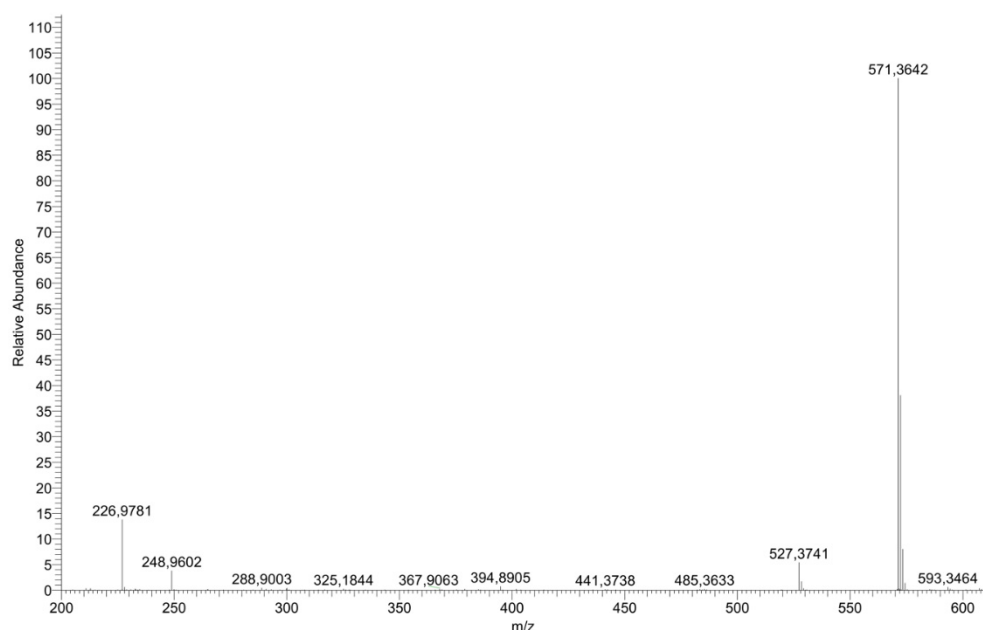


Figure S45. HR-ESI-MS spectrum of compound 6

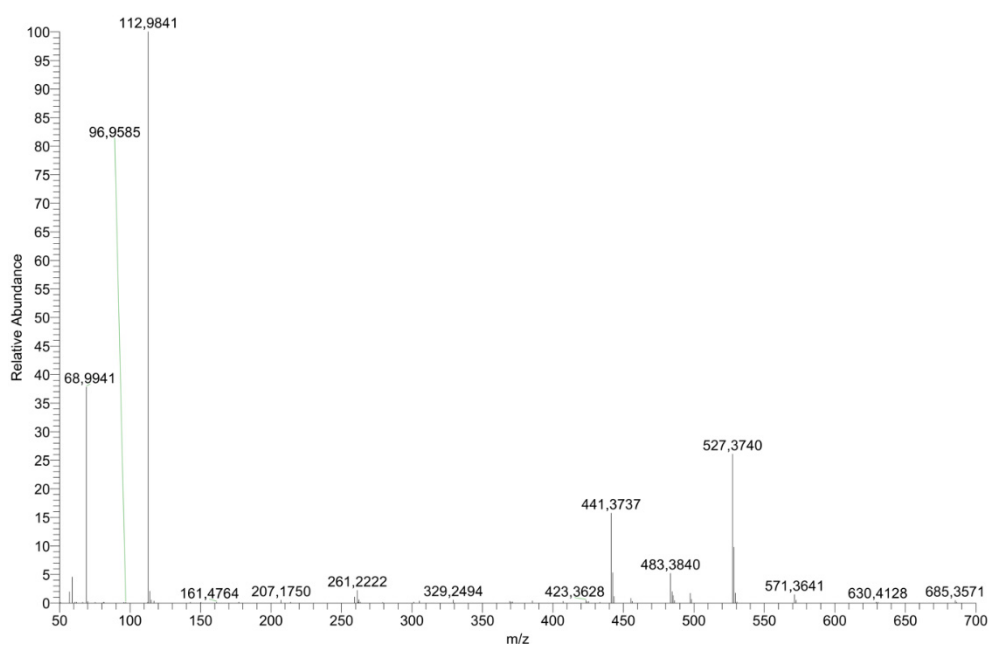


Figure S46. MS-MS spectrum of compound 6

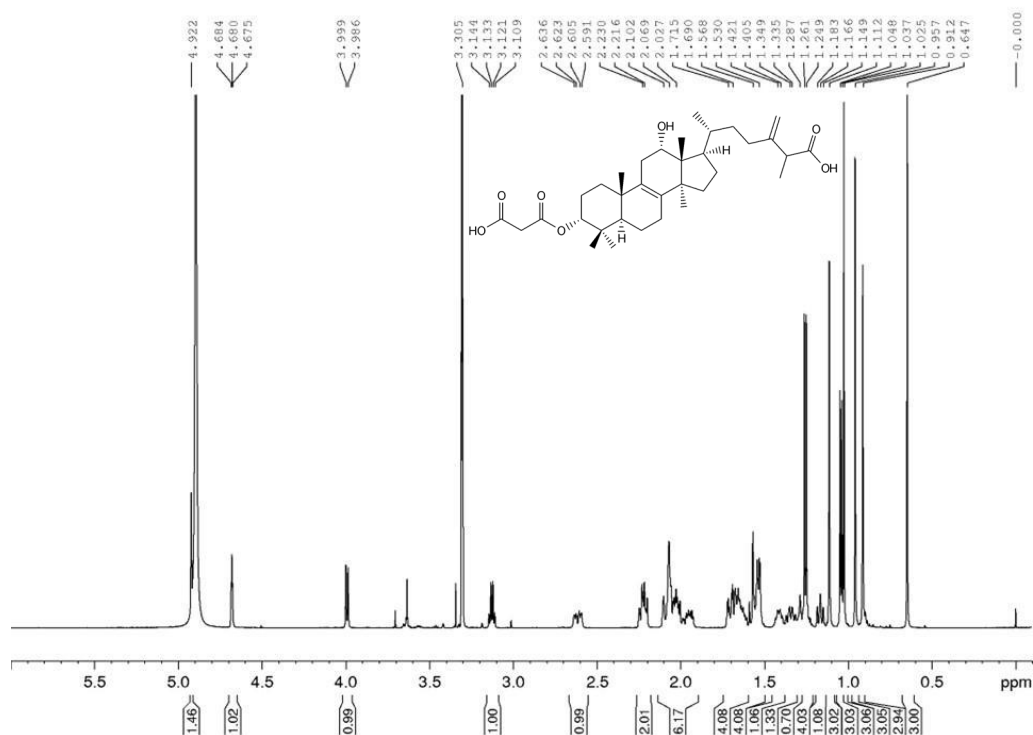


Figure S47. <sup>1</sup>H spectrum of compound 6 (150 MHz, CD<sub>3</sub>OD, 295 K)

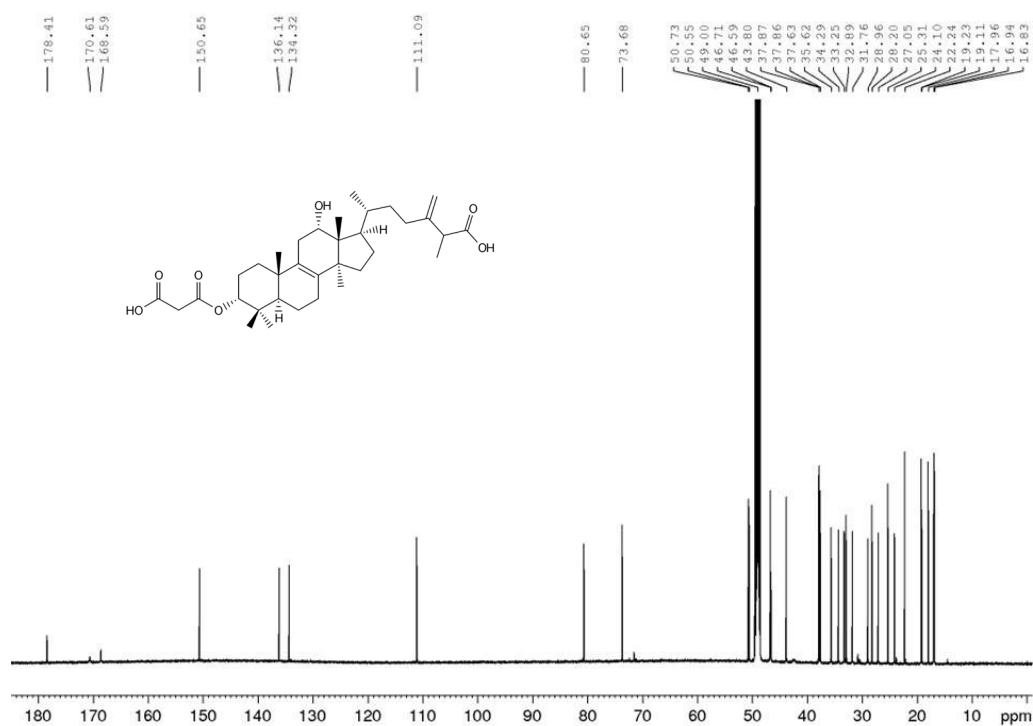


Figure S48. <sup>13</sup>C spectrum of compound 6 (600 MHz, CD<sub>3</sub>OD, 295 K)

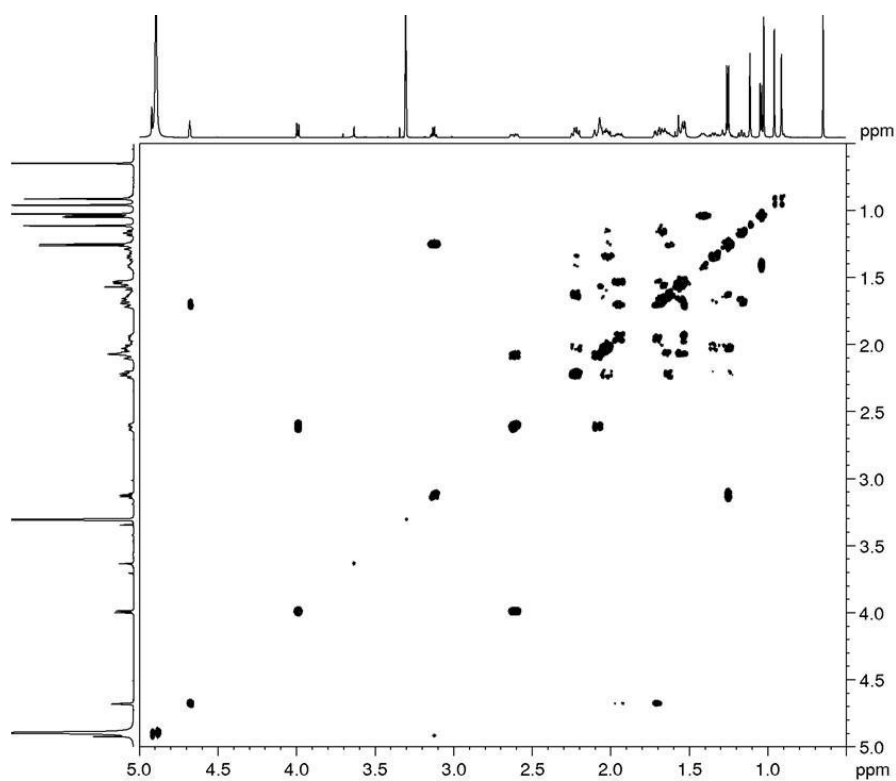


Figure S49. COSY spectrum of compound **6** (600 MHz, CD<sub>3</sub>OD, 295 K)

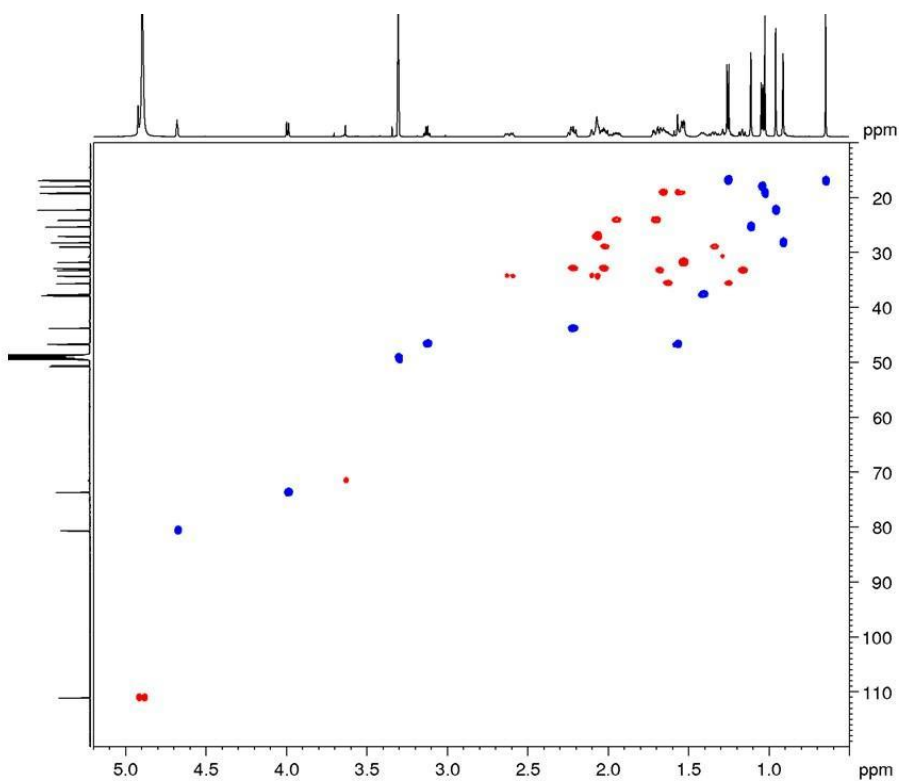


Figure S50. DEPT-edited HSQC spectrum of compound **6** (600 MHz CD<sub>3</sub>OD, 295 K)

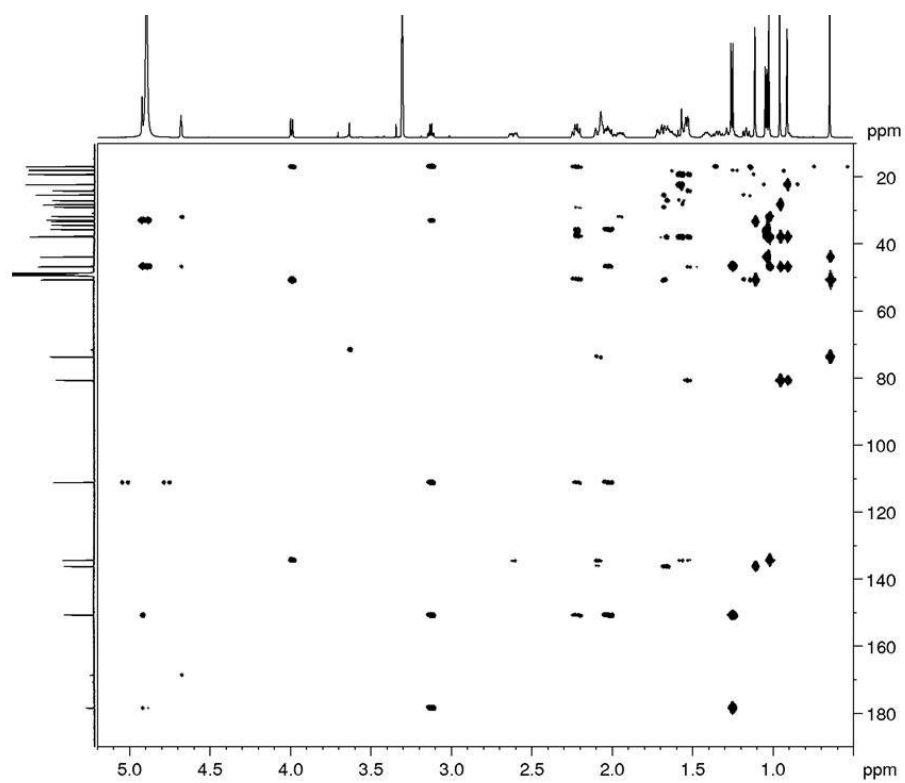


Figure S51. HMBC spectrum of compound **6** (600 MHz,  $\text{CD}_3\text{OD}$ , 295 K)

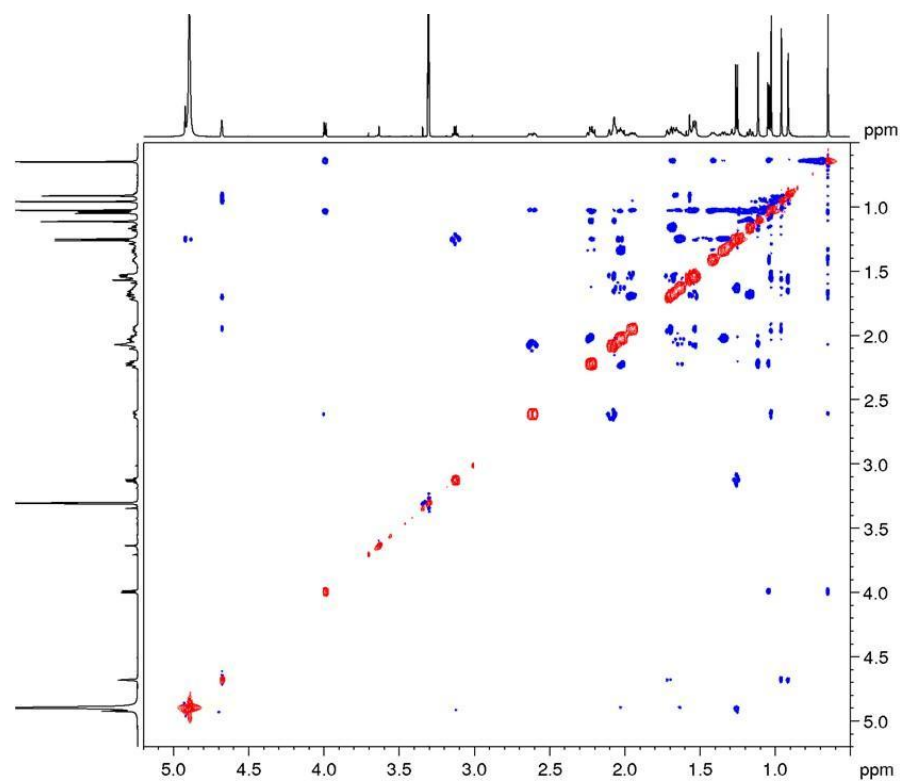


Figure S52. NOESY spectrum of compound **6** (600 MHz,  $\text{CD}_3\text{OD}$ , 295 K)



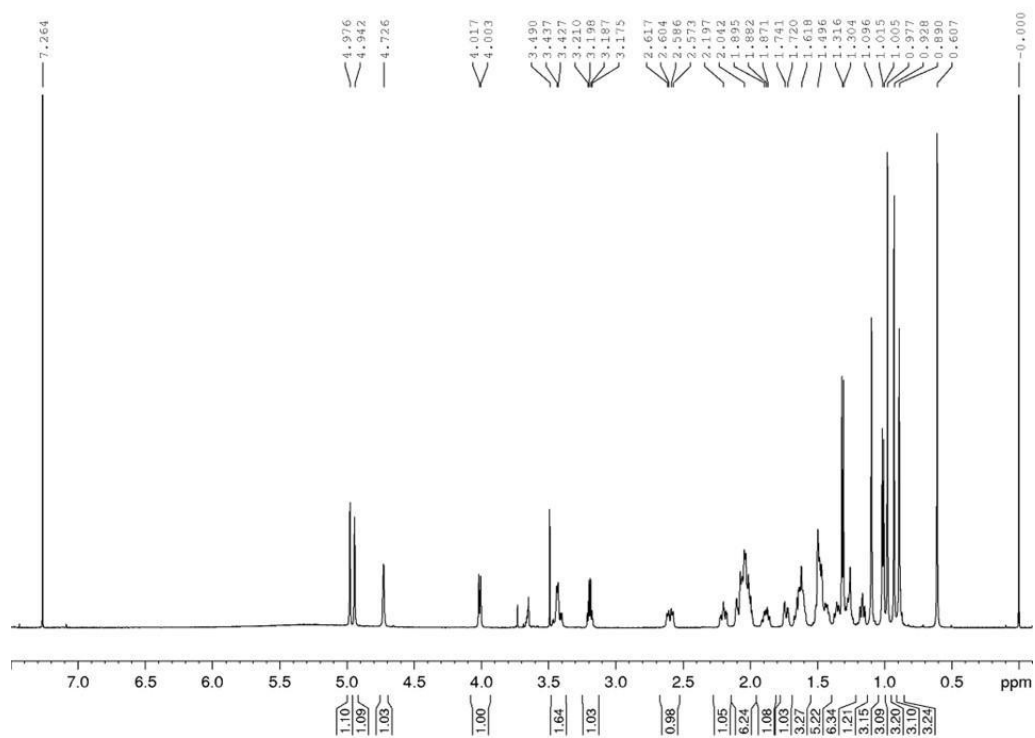


Figure S53.  $^1\text{H}$  spectrum of compound **6** (600 MHz,  $\text{CDCl}_3$ , 295 K)

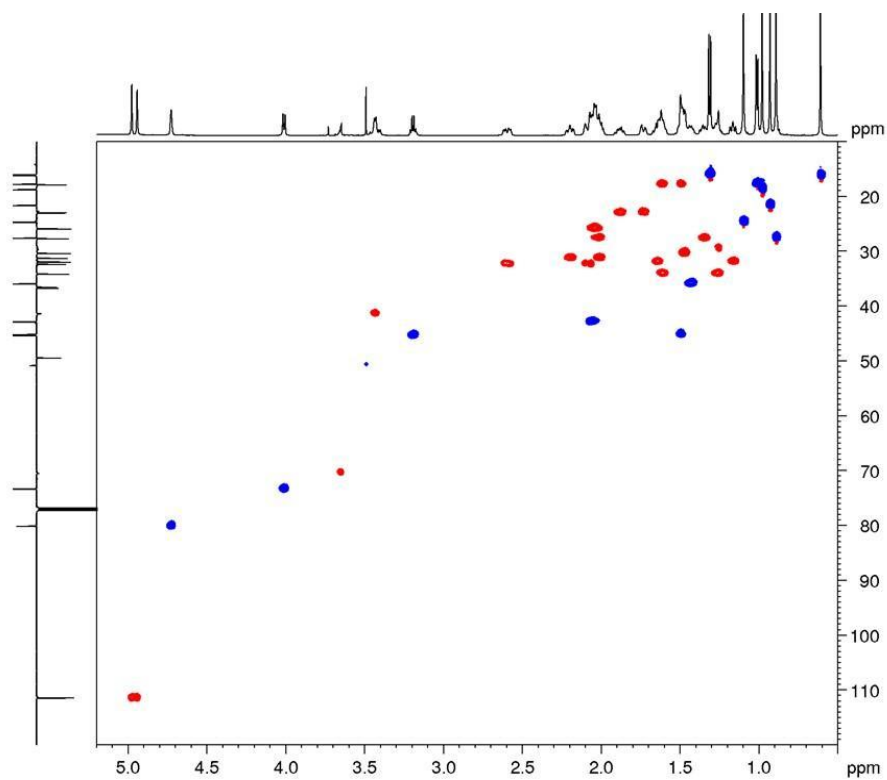


Figure S54. DEPT-edited HSQC spectrum of compound **6** (600 MHz,  $\text{CDCl}_3$ , 295 K)

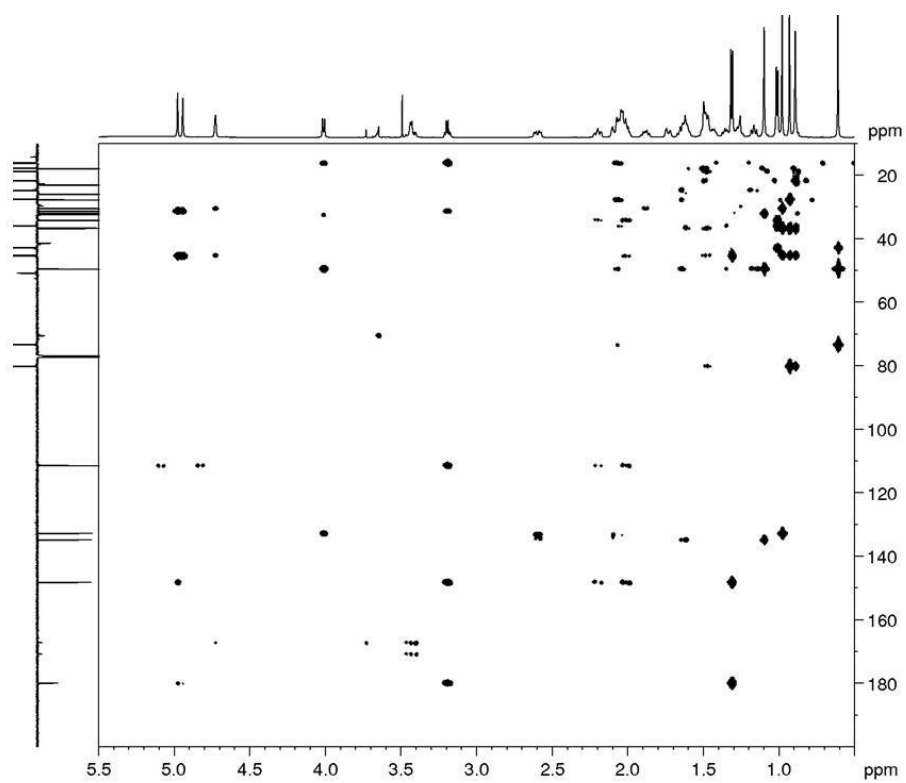
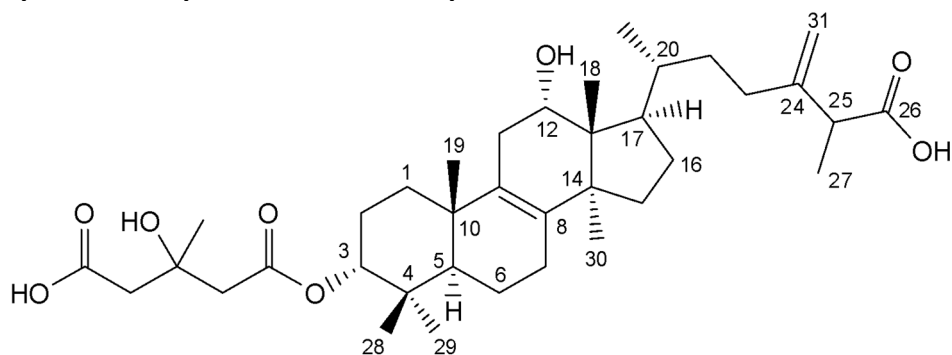


Figure S55. HMBC spectrum of compound **6** (600 MHz, CDCl<sub>3</sub>, 295 K)

## Spectra and spectral data on compound 7



HR-ESI-MS (-)  $m/z$  629.4063 [ $M - H$ ]<sup>-</sup> (629.4048 calcd. for  $C_{37}H_{57}O_8$   $\Delta$  2.3 ppm;); HR-ESI-MSMS (CID = 15%, 30%, 45%) 567.4055, 527.3735, 485.3621, 483 (27), 441.3735

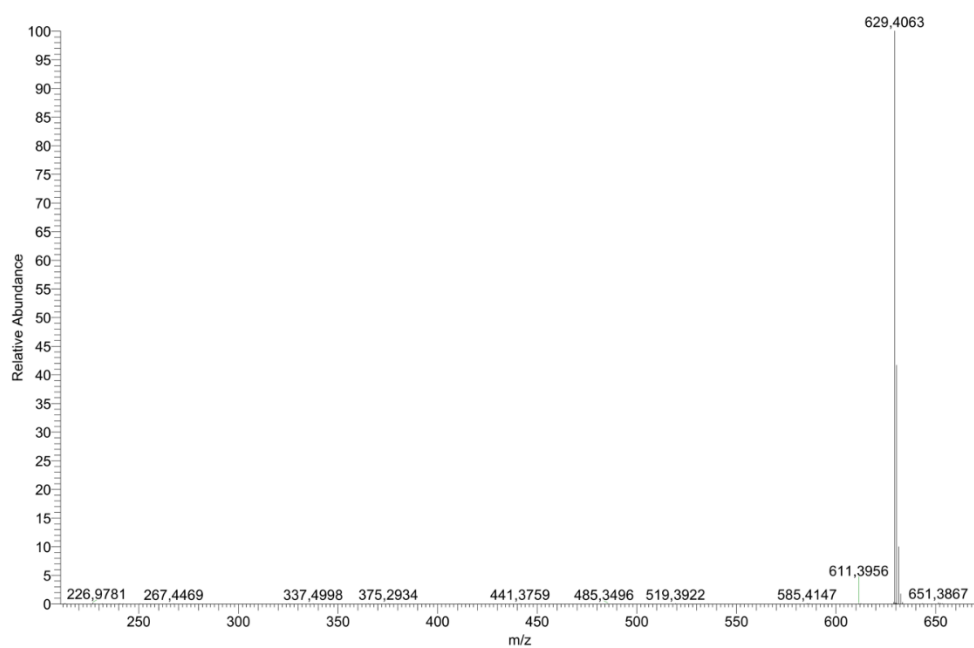


Figure S56. HR-ESI-MS spectrum of compound 7

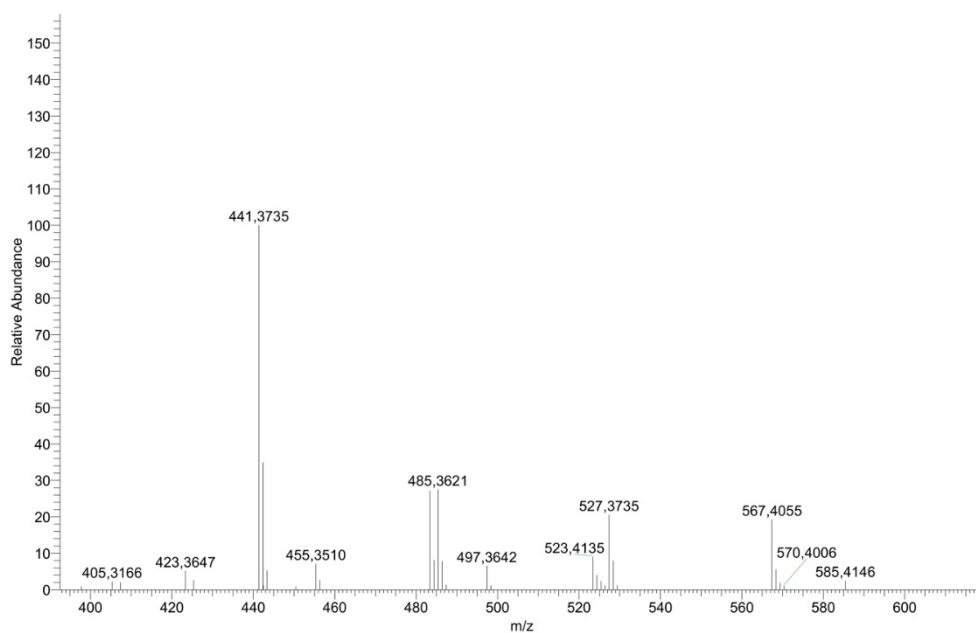


Figure S57. MS-MS spectrum of compound 7

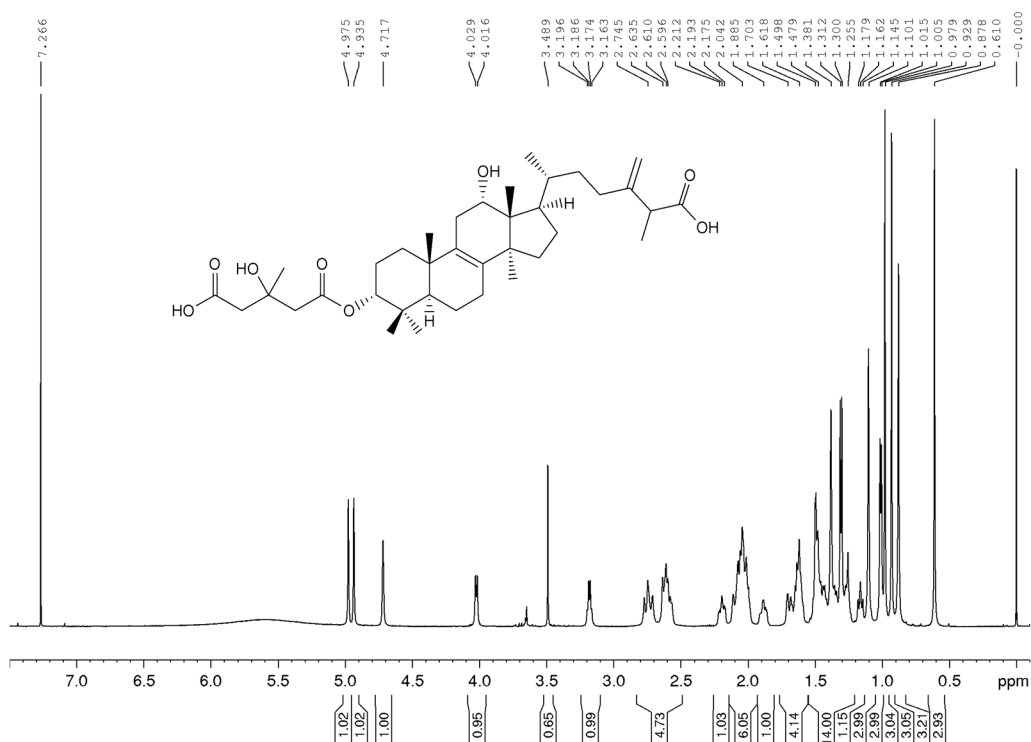


Figure S58. <sup>1</sup>H spectrum of compound 7 (600 MHz, CDCl<sub>3</sub>, 295 K)

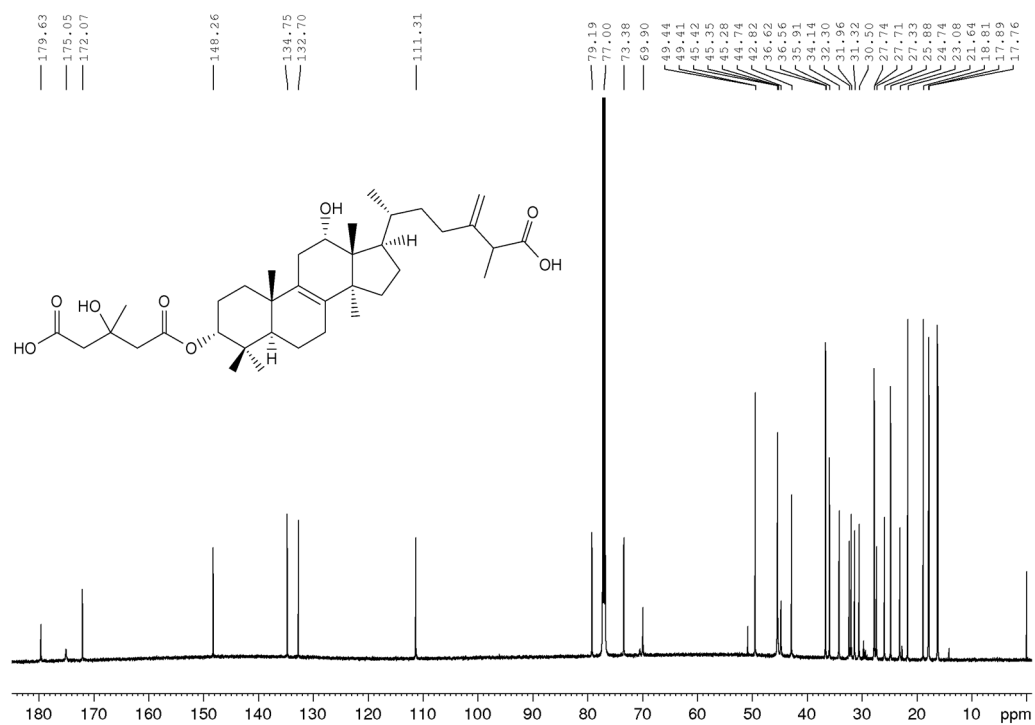


Figure S59.  $^{13}\text{C}$  spectrum of compound **7** (150 MHz,  $\text{CDCl}_3$ , 295 K),

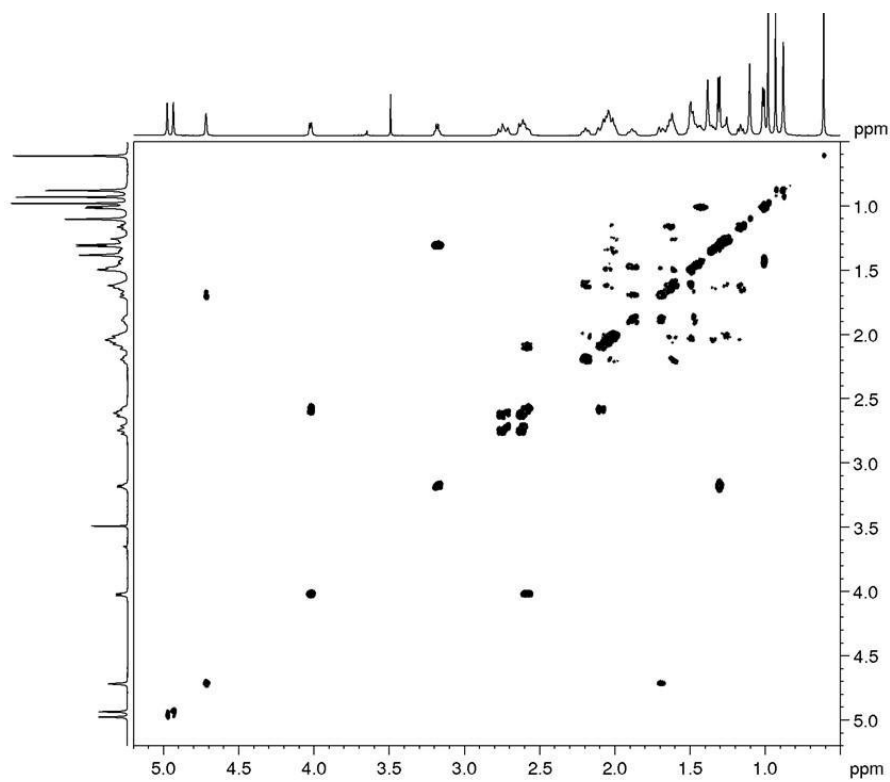


Figure S60. COSY spectrum of compound **7** (600 MHz,  $\text{CDCl}_3$ , 295 K)

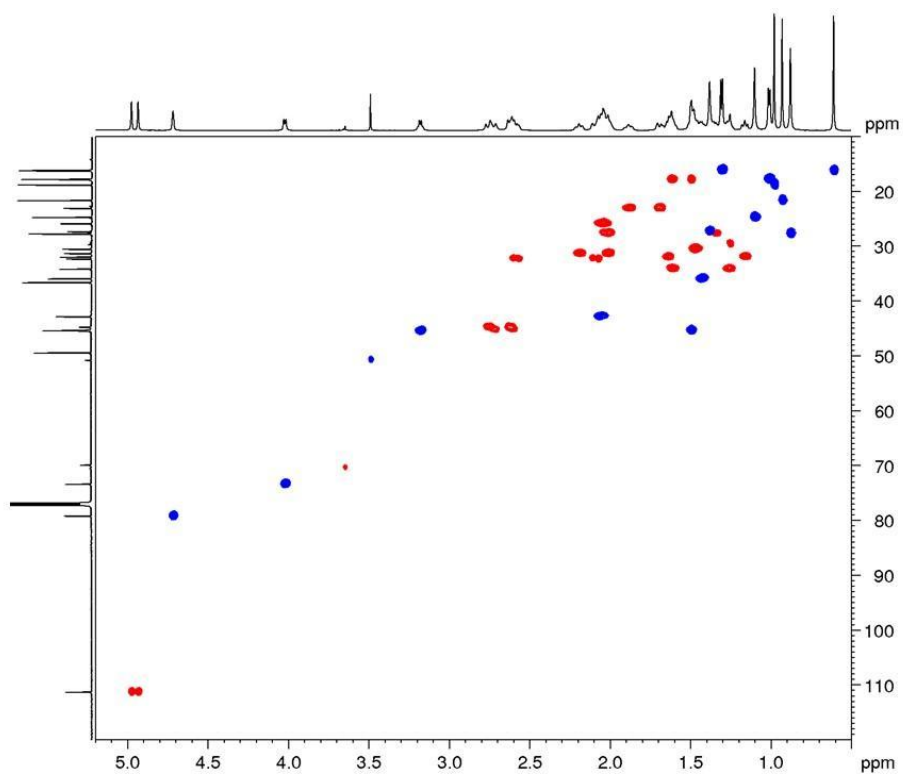


Figure S61. DEPT-edited HSQC spectrum of compound **7** (600 MHz,  $\text{CDCl}_3$ , 295 K)

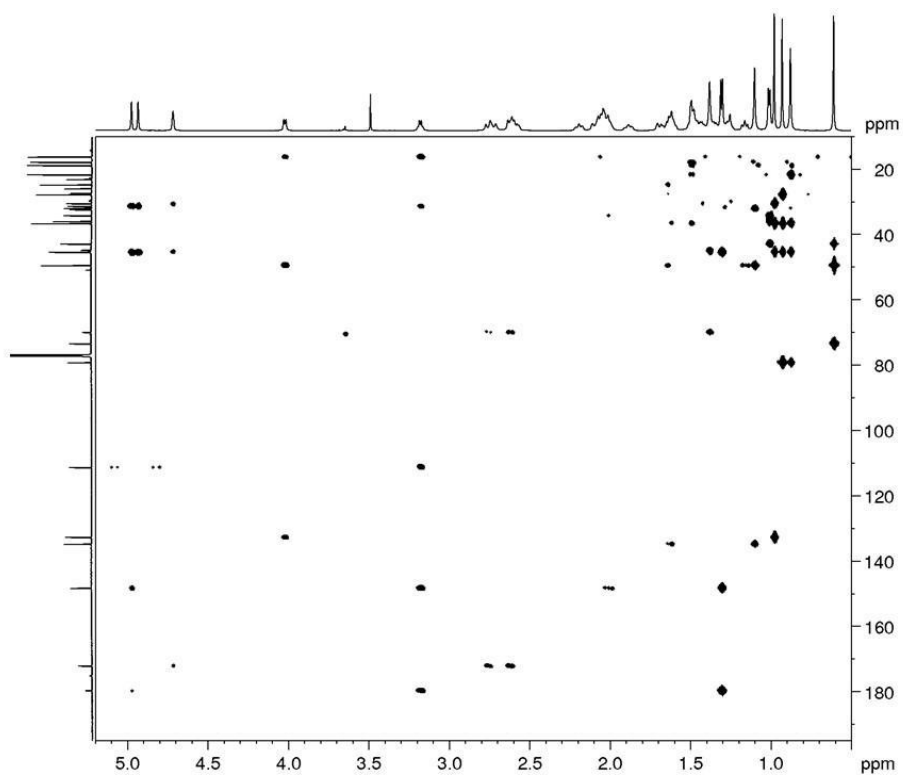


Figure S62. HMBC spectrum of compound **7** (600 MHz,  $\text{CDCl}_3$ , 295 K)

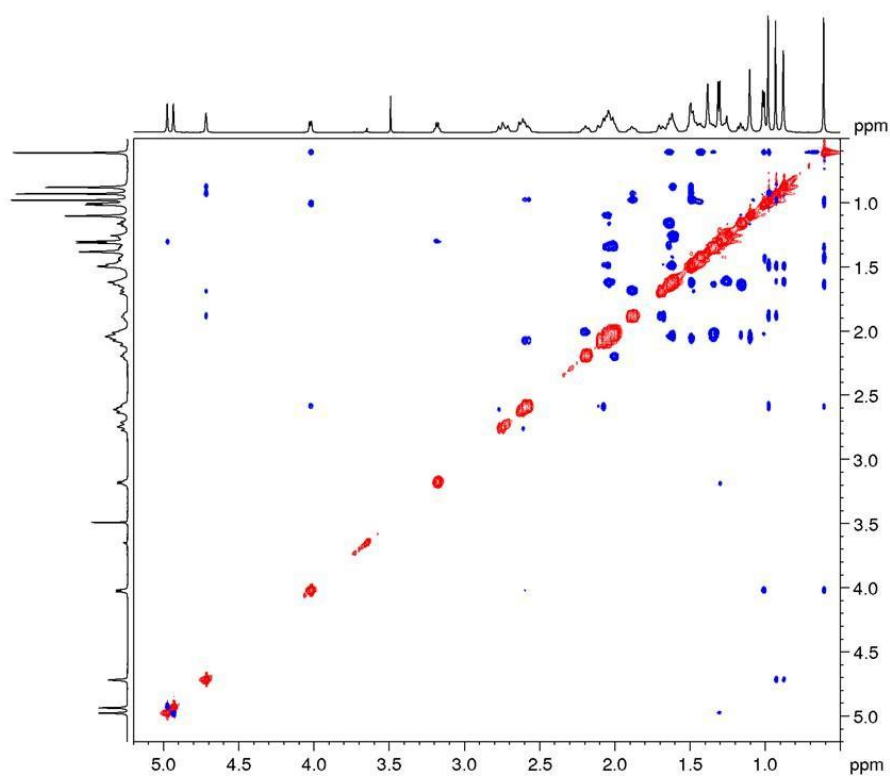
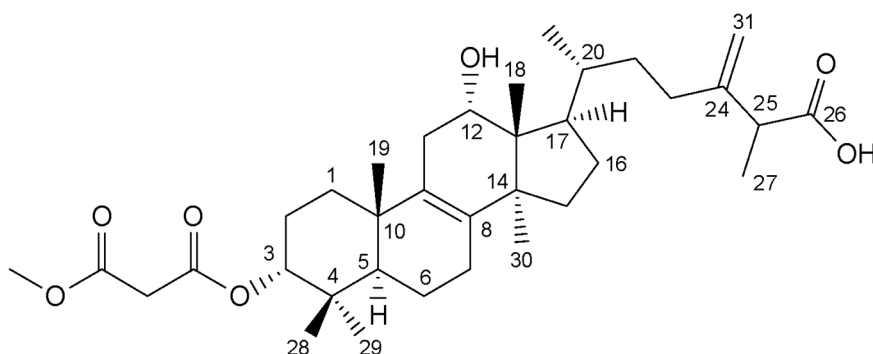


Figure S63. ROESY spectrum of compound **7** (600 MHz, CDCl<sub>3</sub>, 295 K)

## Spectra and spectral data on compound 8



HR-ESI-MS (-)  $m/z$  585.3798 [ $M - H$ ]<sup>-</sup> (585.3786 calcd. for  $C_{35}H_{53}O_7$ ;  $\Delta$  2.1 ppm); HR-ESI-MSMS (CID = 15%, 30%, 45%) 541.3893, 509.3629, 441.3734

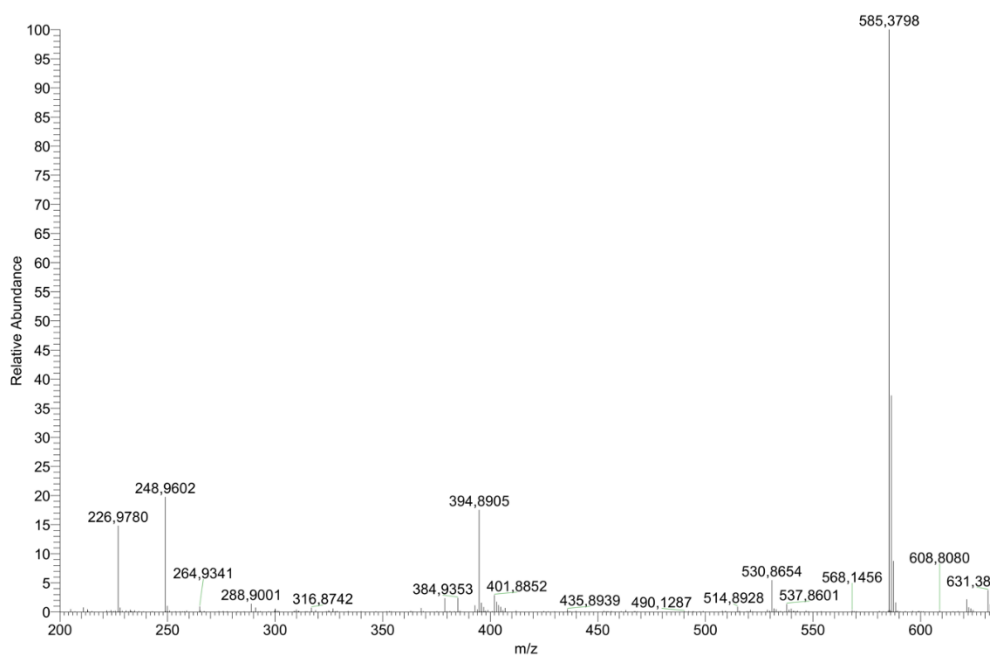


Figure S64. HR-ESI-MS spectrum of compound 8



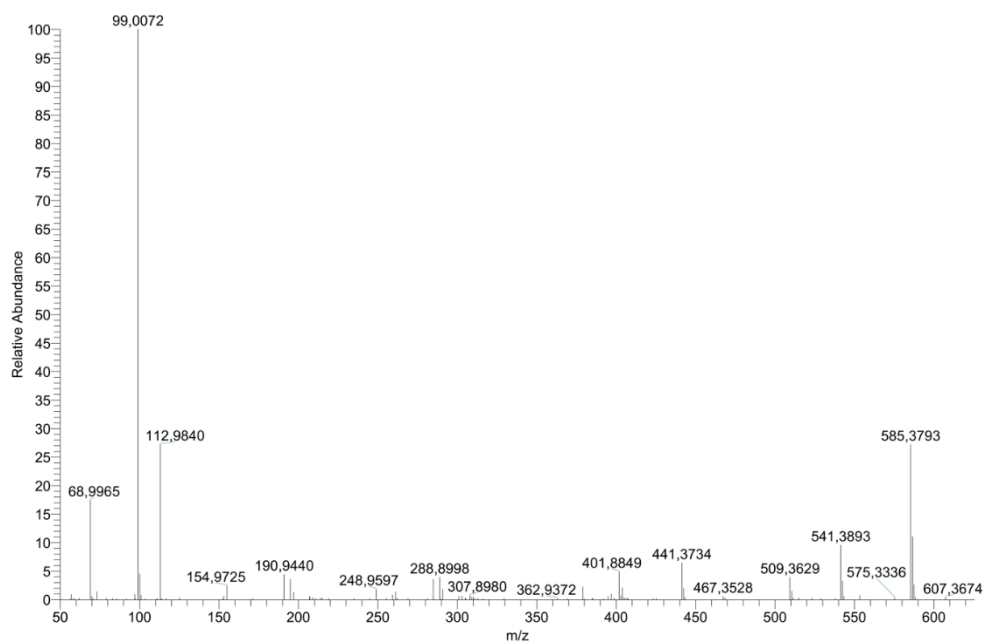


Figure S65. MS-MS spectrum of compound **8**

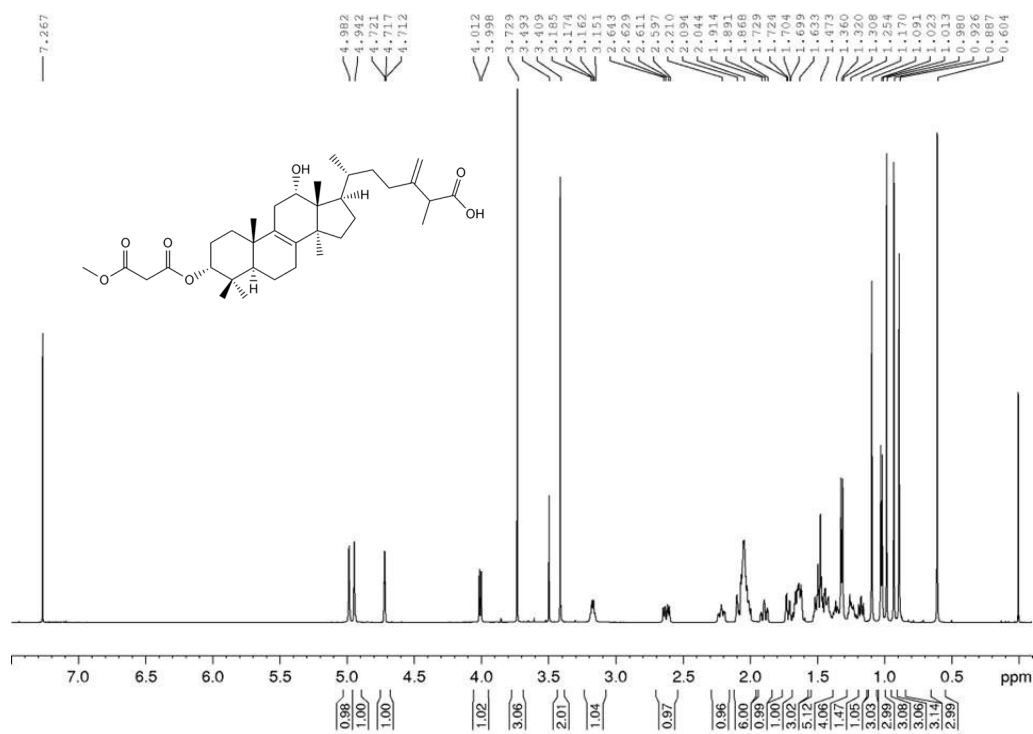


Figure S66. <sup>1</sup>H spectrum of compound **8** (600 MHz, CDCl<sub>3</sub>, 295 K)

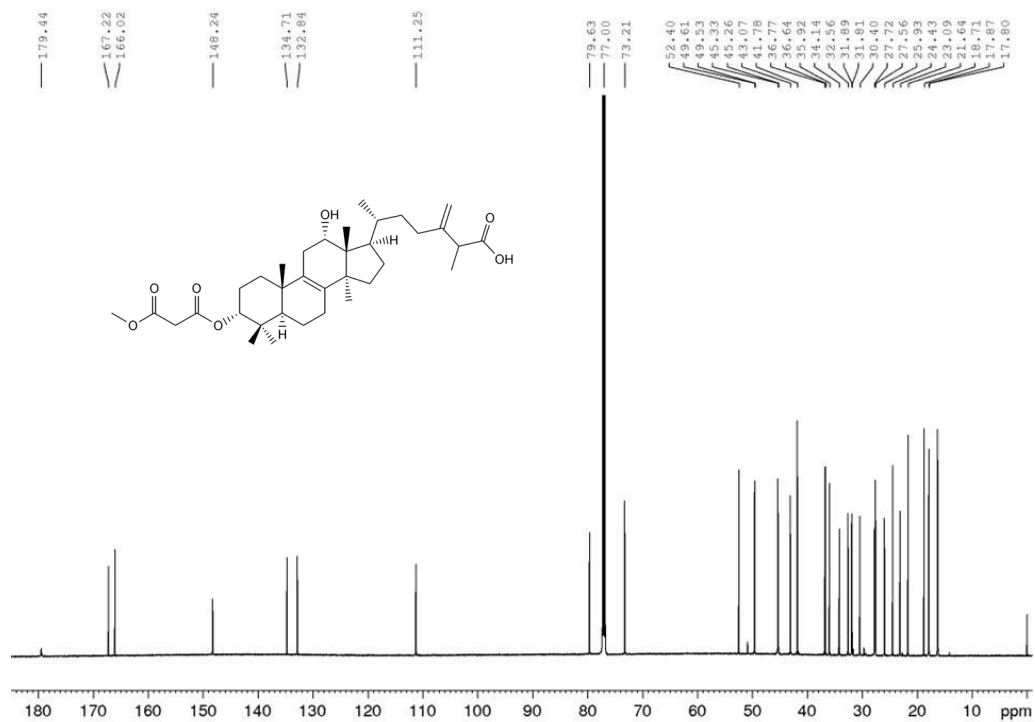


Figure S67.  $^{13}\text{C}$  spectrum of compound **8** (150 MHz,  $\text{CDCl}_3$ , 295 K)

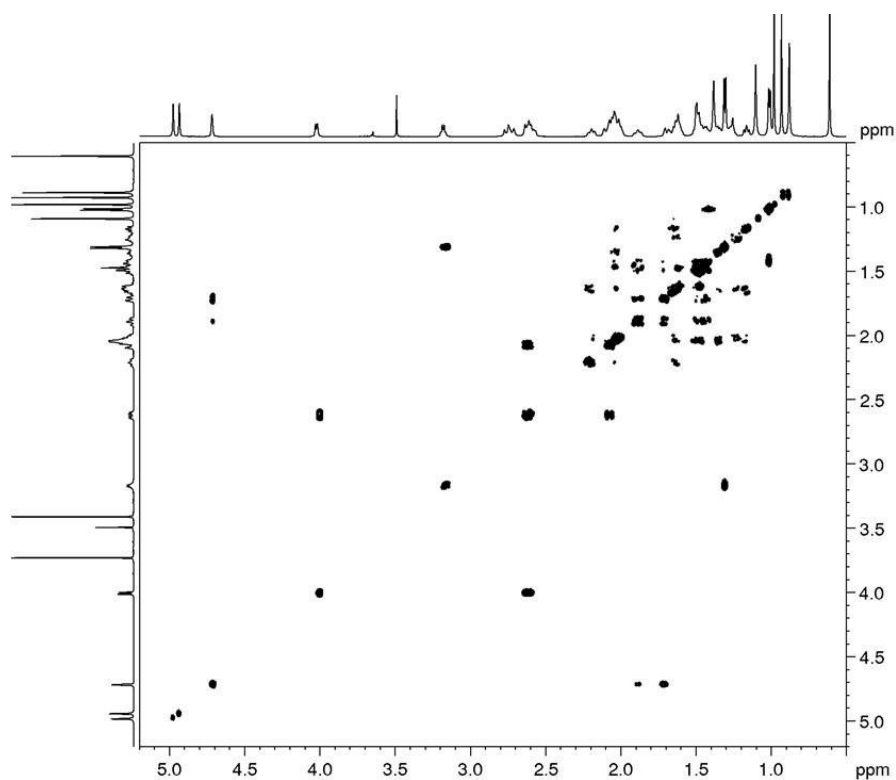


Figure S68. COSY spectrum of compound **8** (600 MHz,  $\text{CDCl}_3$ , 295 K)

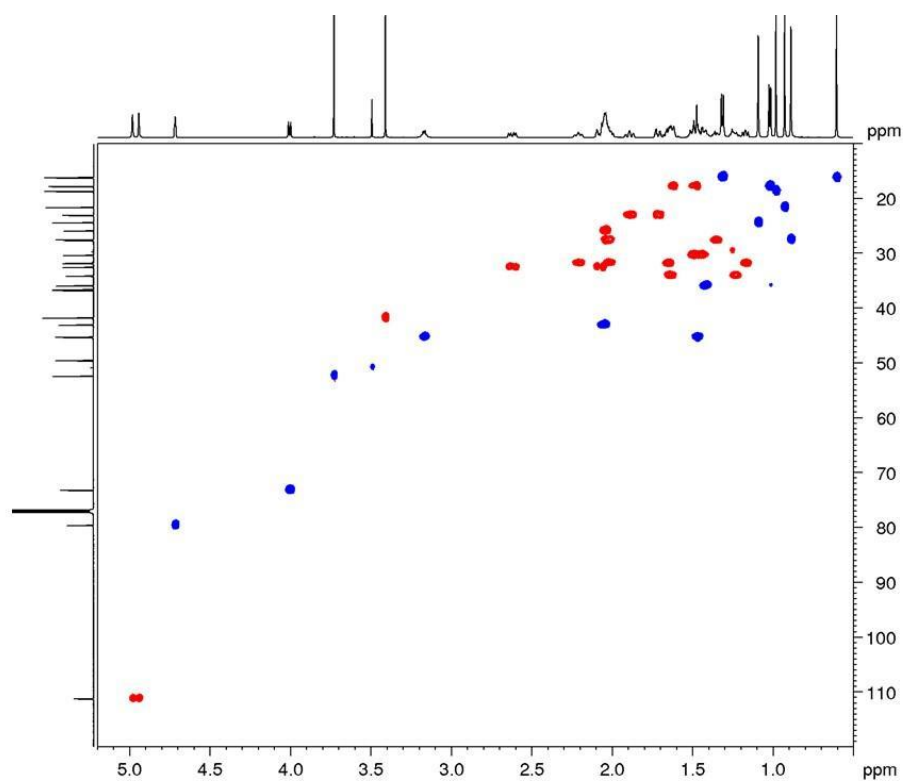


Figure S69. DEPT-edited HSQC spectrum of compound **8** (600 MHz,  $\text{CDCl}_3$ , 295 K)

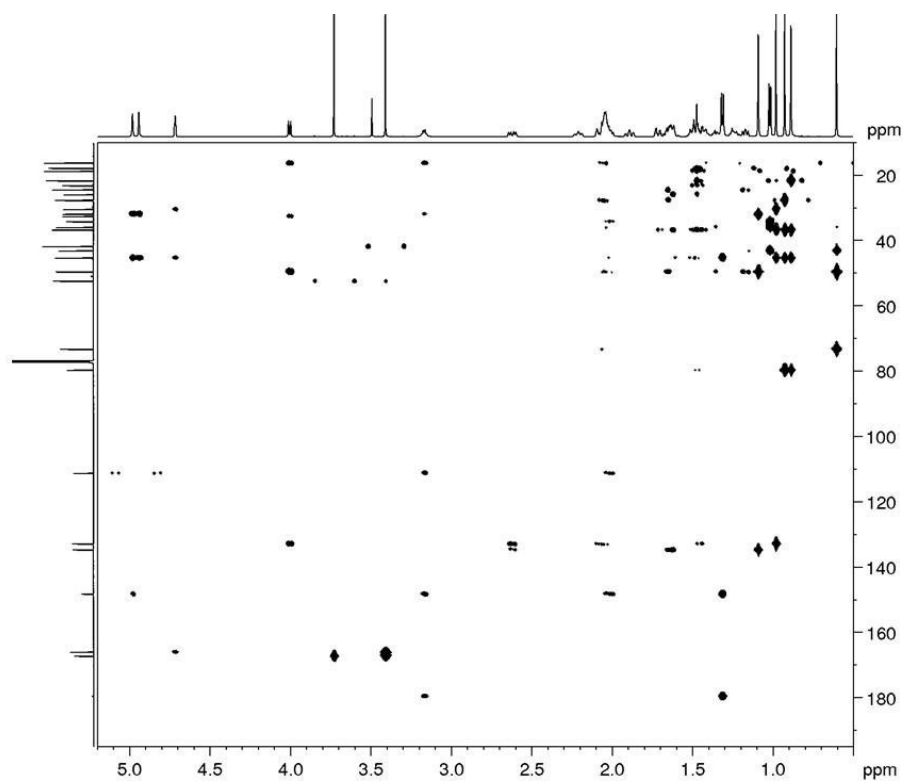


Figure S70. HMBC spectrum of compound **8** (600 MHz,  $\text{CDCl}_3$ , 295 K)

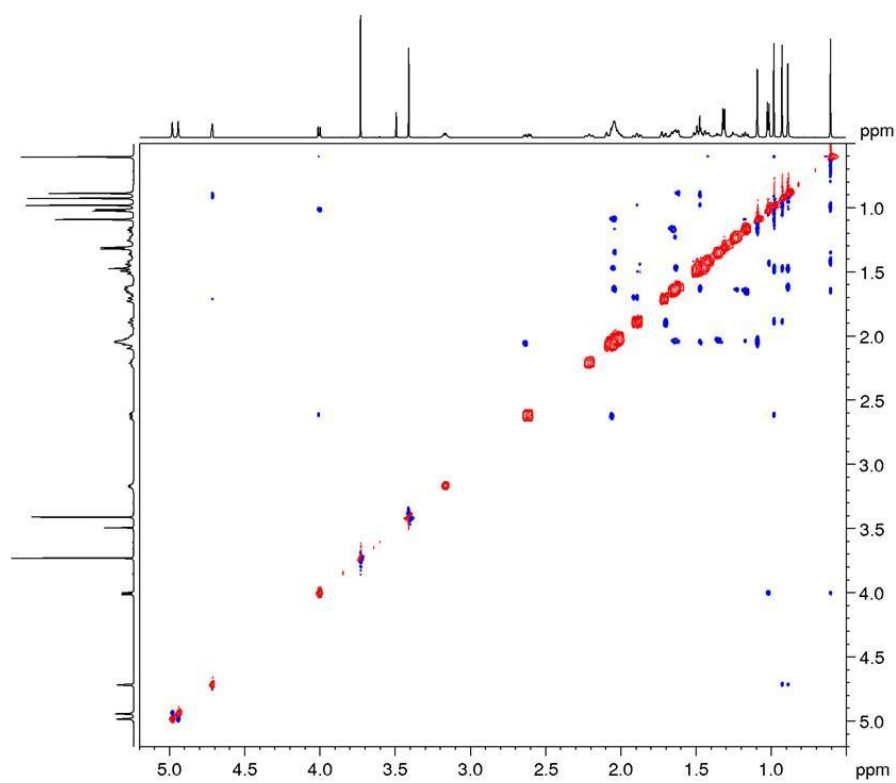
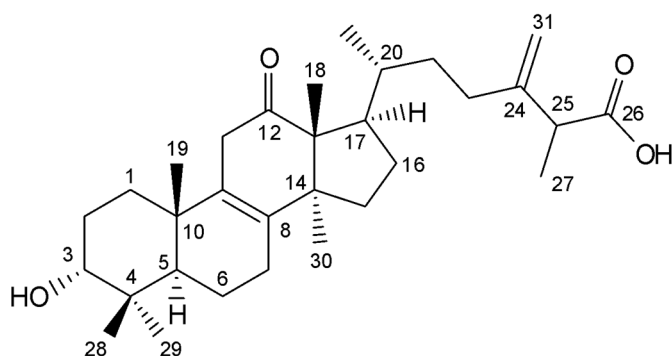


Figure S71. ROESY spectrum of compound **8** (600 MHz, CDCl<sub>3</sub>, 295 K)

## Spectra and spectral data on compound 9



HR-ESI-MS (+)  $m/z$  485.3616  $[M + H]^+$  (485.3625 calcd. for  $C_{31}H_{49}O_4$ ;  $\Delta$  -1.9 ppm); HR-ESI-MSMS (CID = 15%, 30%, 45%) 467.3510, 449.3404

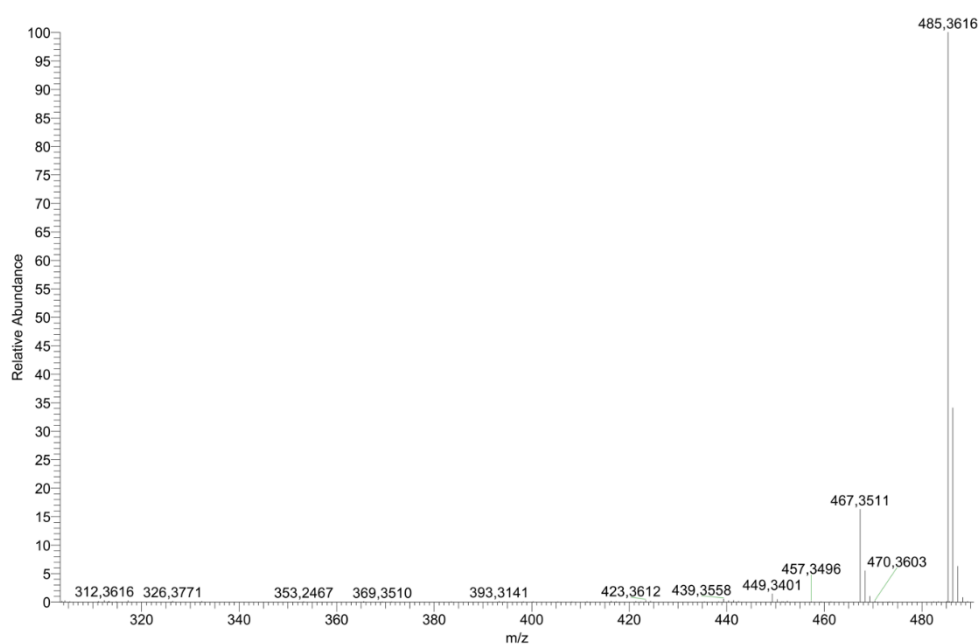


Figure S72. HR-ESI-MS spectrum of compound 9

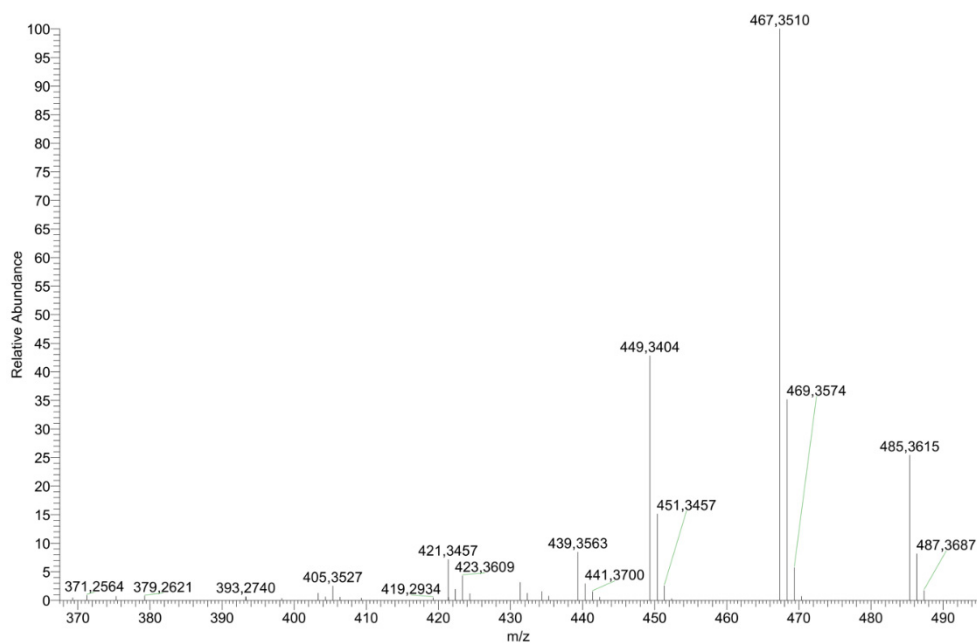


Figure S73. MS-MS spectrum of compound 9

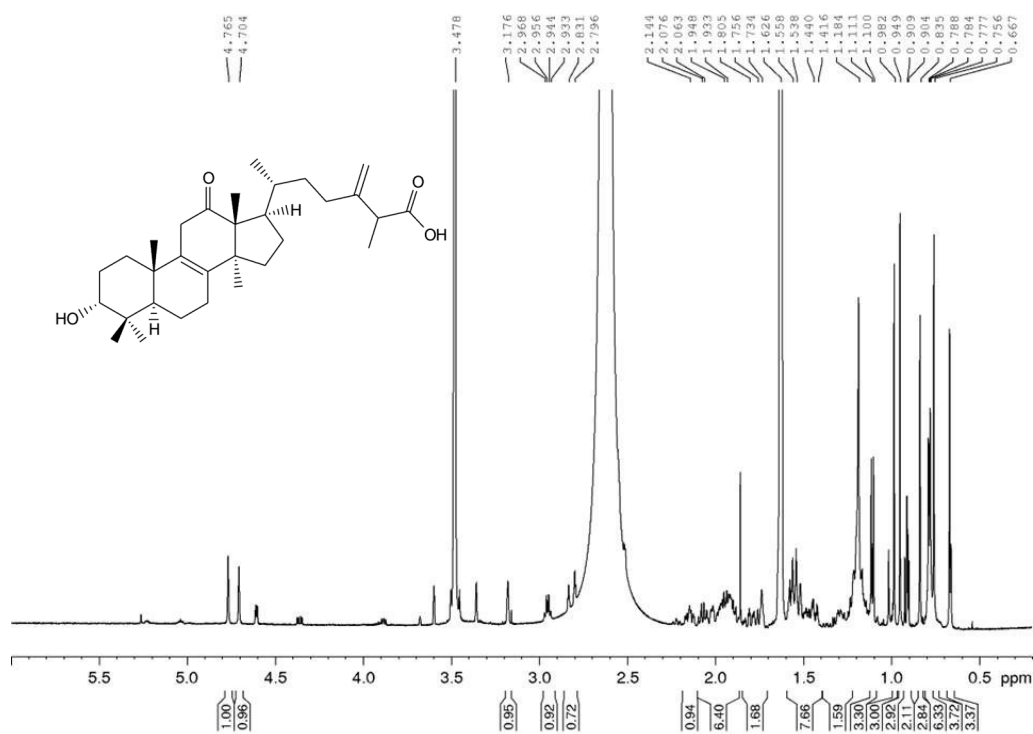


Figure S74. <sup>1</sup>H spectrum of compound 9 (600 MHz, CDCl<sub>3</sub>, 295 K)

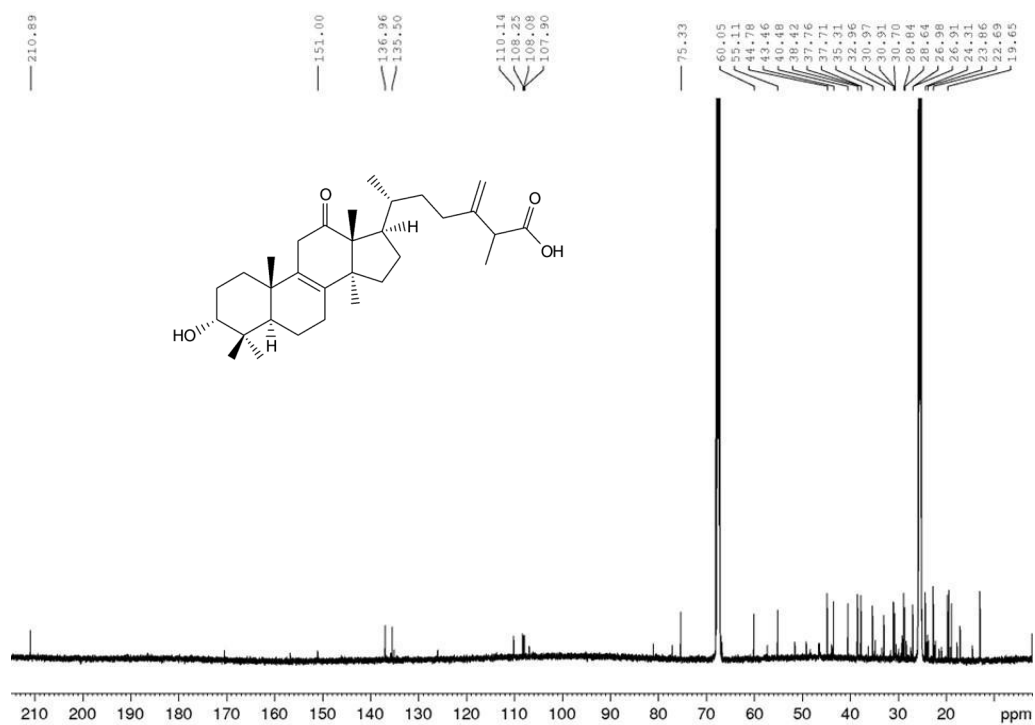


Figure S75.  $^{13}\text{C}$  spectrum of compound 9 (150 MHz,  $\text{CDCl}_3$ , 295 K)

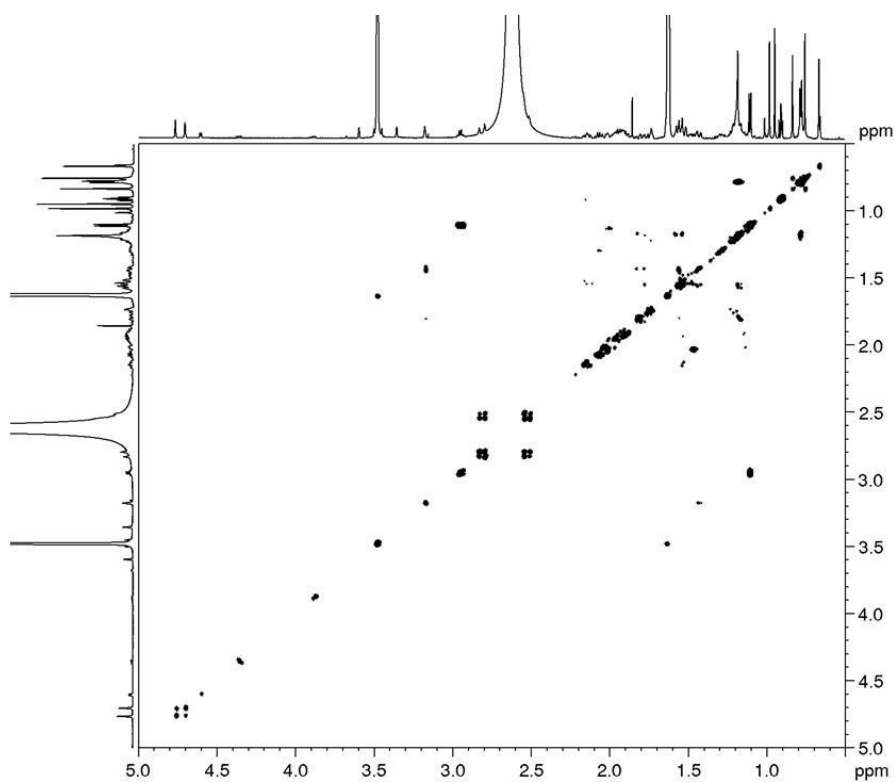


Figure S76. COSY spectrum of compound 9 (600 MHz,  $\text{CDCl}_3$ , 295 K)

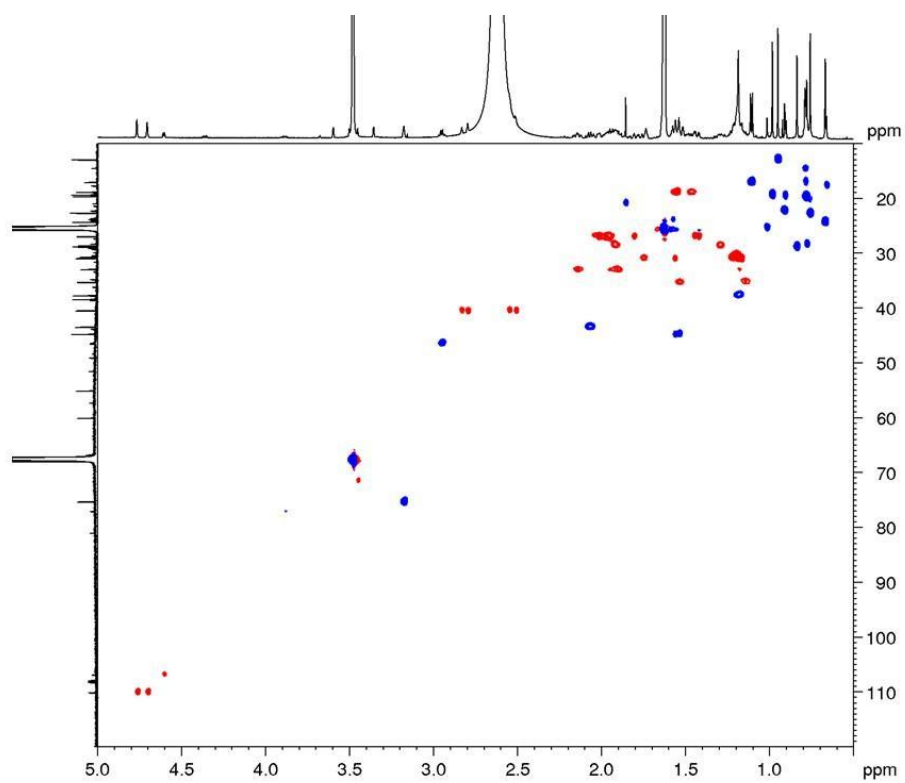


Figure S77. DEPT-edited HSQC spectrum of compound **9** (600 MHz, CDCl<sub>3</sub>, 295 K)

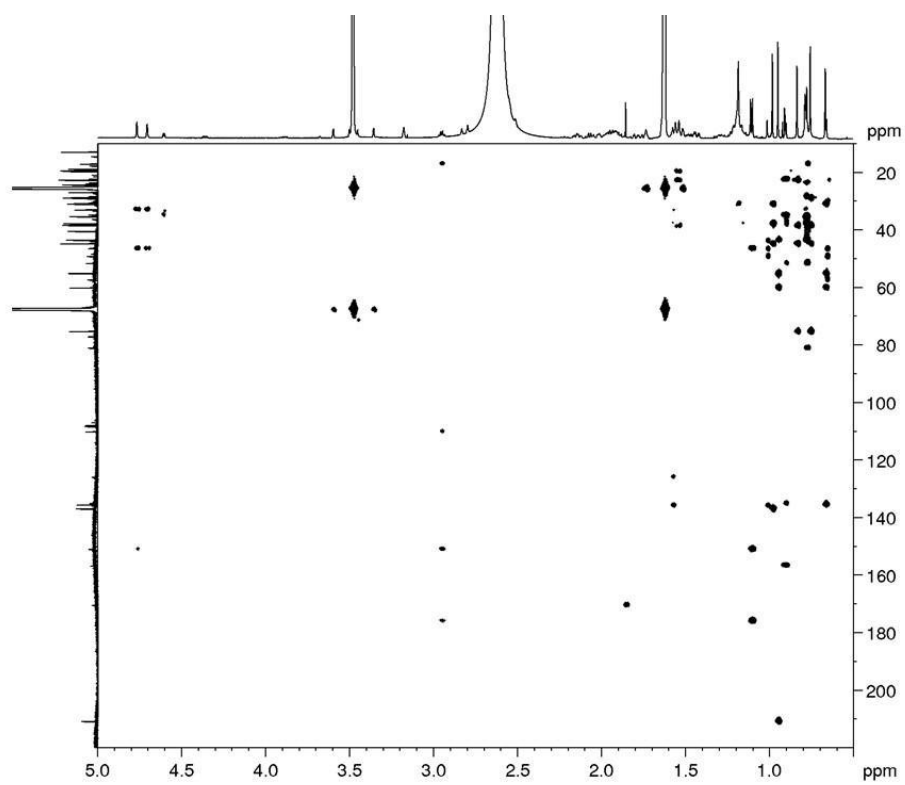


Figure S78. HMBC spectrum of compound **9** (600 MHz, CDCl<sub>3</sub>, 295 K)



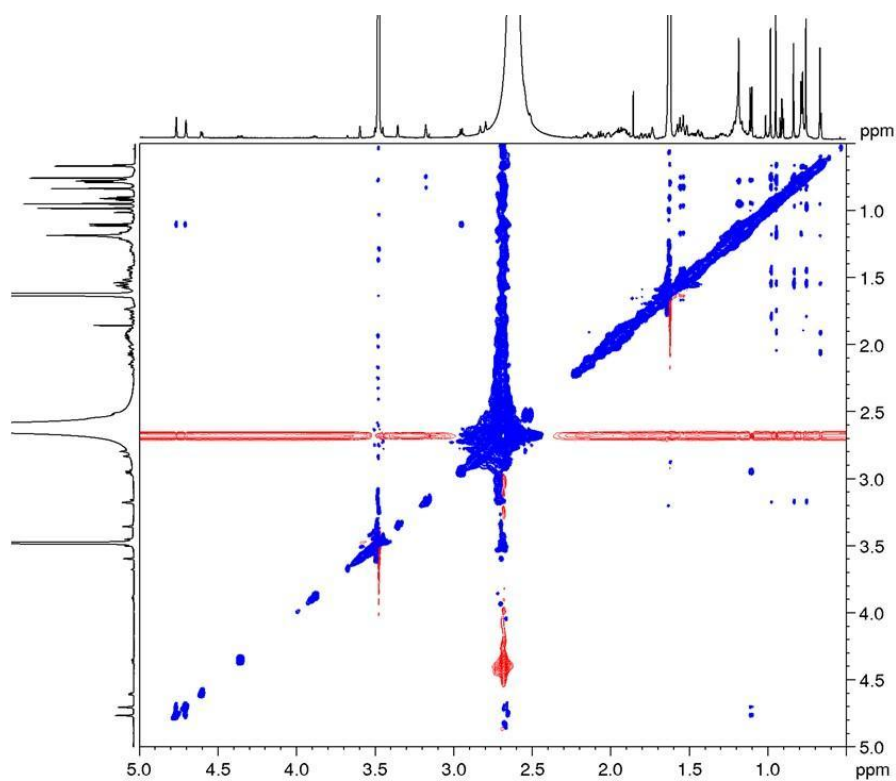


Figure S79. NOESY spectrum of compound **9** (600 MHz,  $\text{CDCl}_3$ , 295 K)

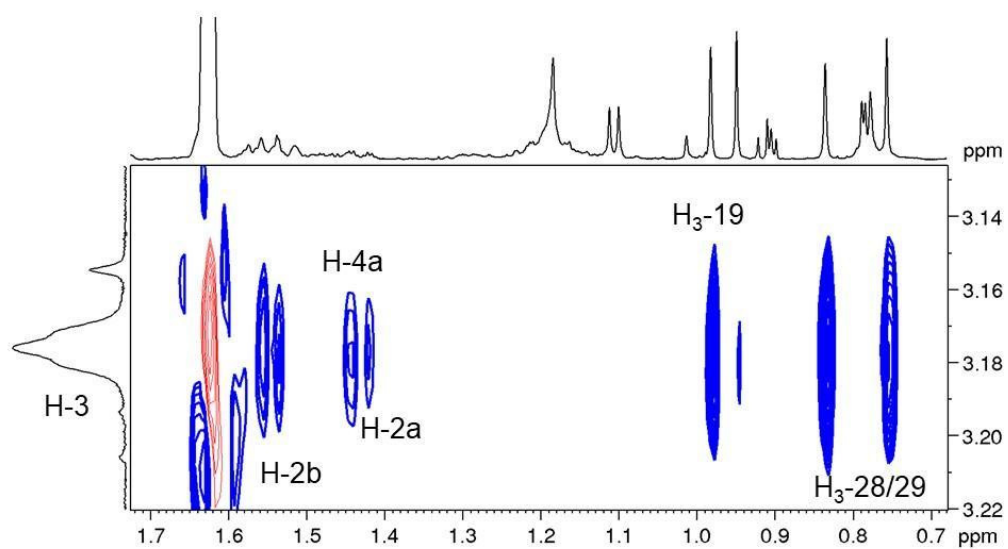
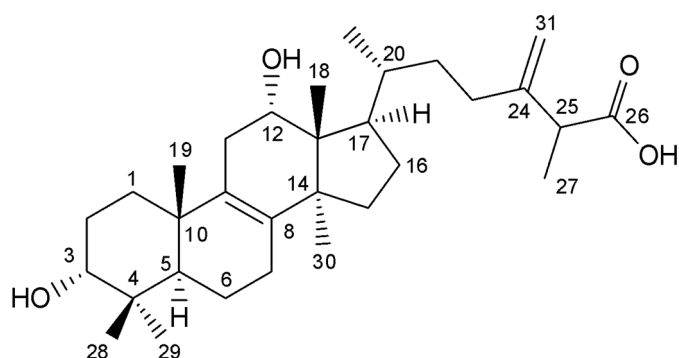


Figure S80. NOESY spectrum of compound **9** (600 MHz,  $\text{CDCl}_3$ , 295 K)

## Spectra and spectral data on compound **10**



HR-ESI-MS (-)  $m/z$  485.3638 [ $M - H$ ]<sup>-</sup> (485.3625 calcd. for  $C_{31}H_{49}O_4$ ;  $\Delta$  2.6 ppm); HR-ESI-MSMS (CID = 15%, 30%, 45%) 455.3529, 441.3736, 423.3636

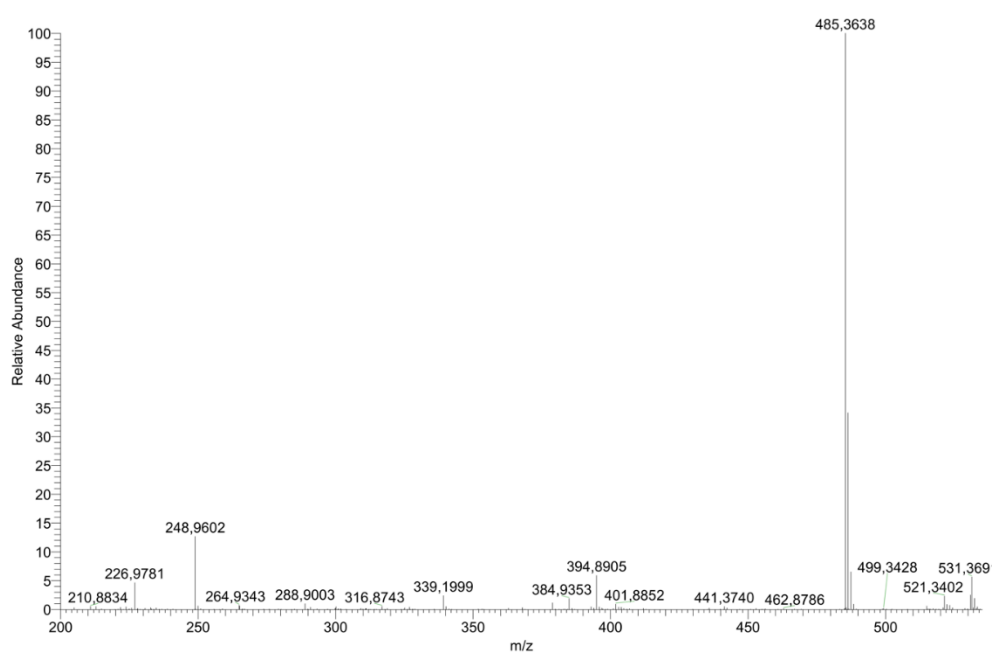


Figure S81. HR-ESI-MS spectrum of compound **10**

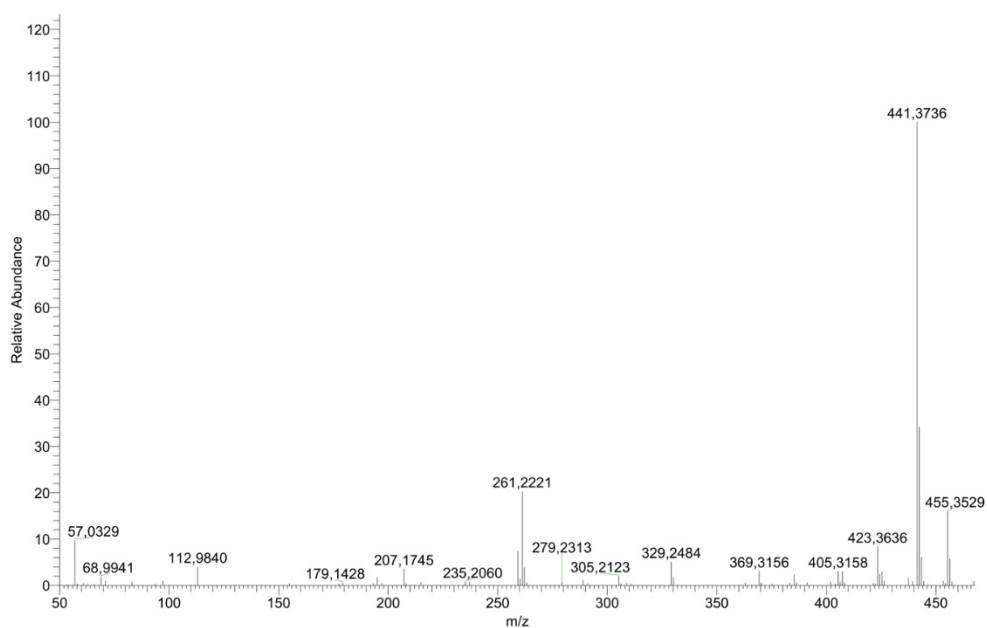


Figure S82. MS-MS spectrum of compound **10**

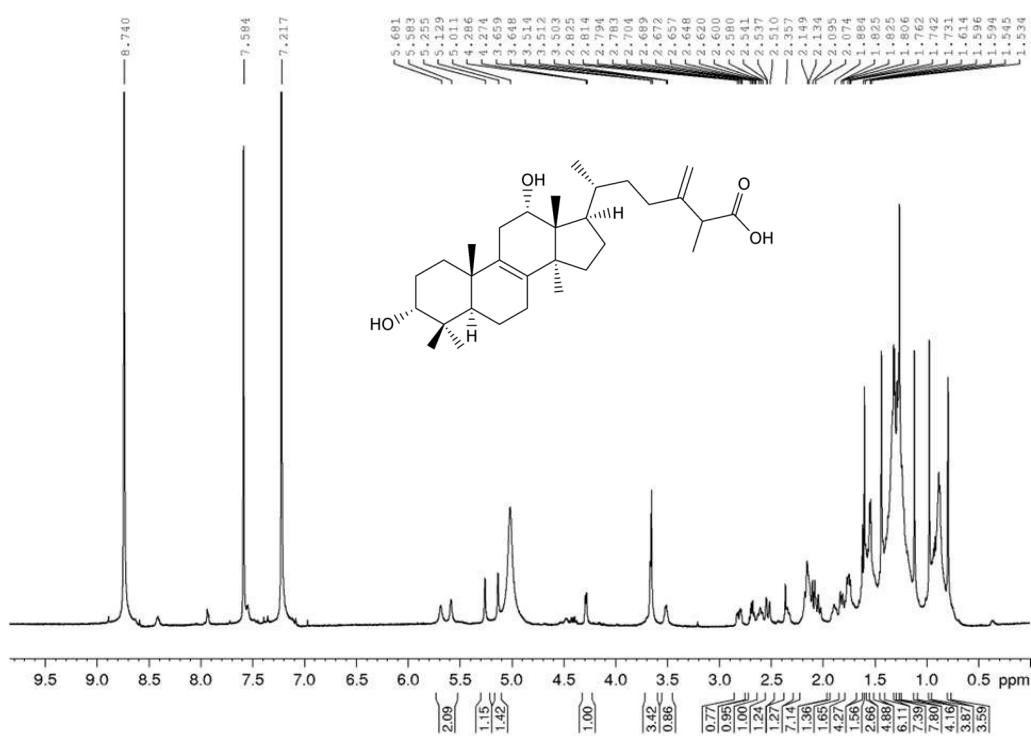


Figure S83. <sup>1</sup>H spectrum of compound **10** (600 MHz, pyridine-*d*<sub>5</sub>, 295 K)

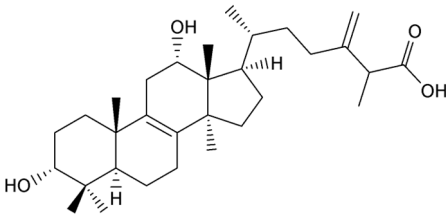


Figure S84.  $^{13}\text{C}$  spectrum of compound **10** (150 MHz, pyridine- $d_5$ , 295 K)

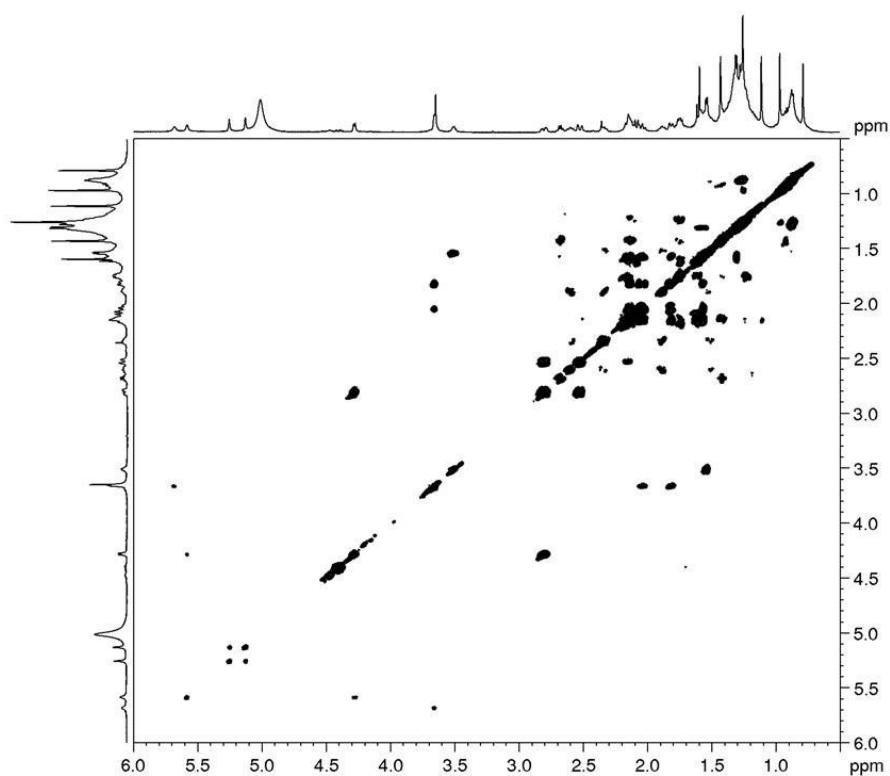


Figure S85. COSY spectrum of compound **10** (600 MHz, pyridine-*d*<sub>5</sub>, 295 K)

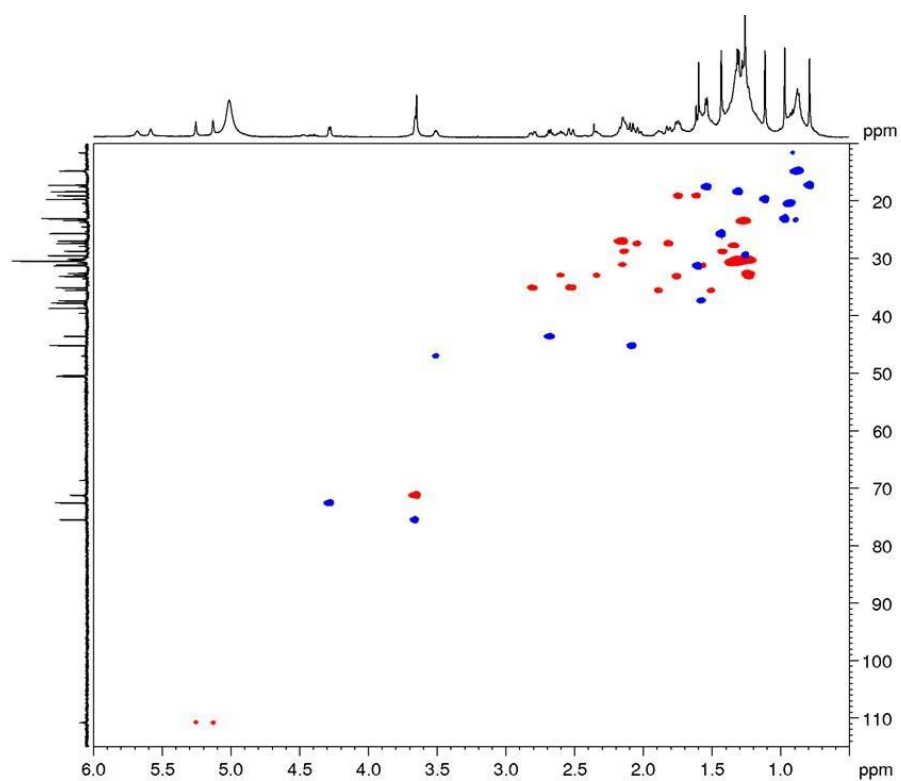


Figure S86. DEPT-edited HSQC spectrum of compound **10** (600 MHz, pyridine- $d_5$ , 295 K)

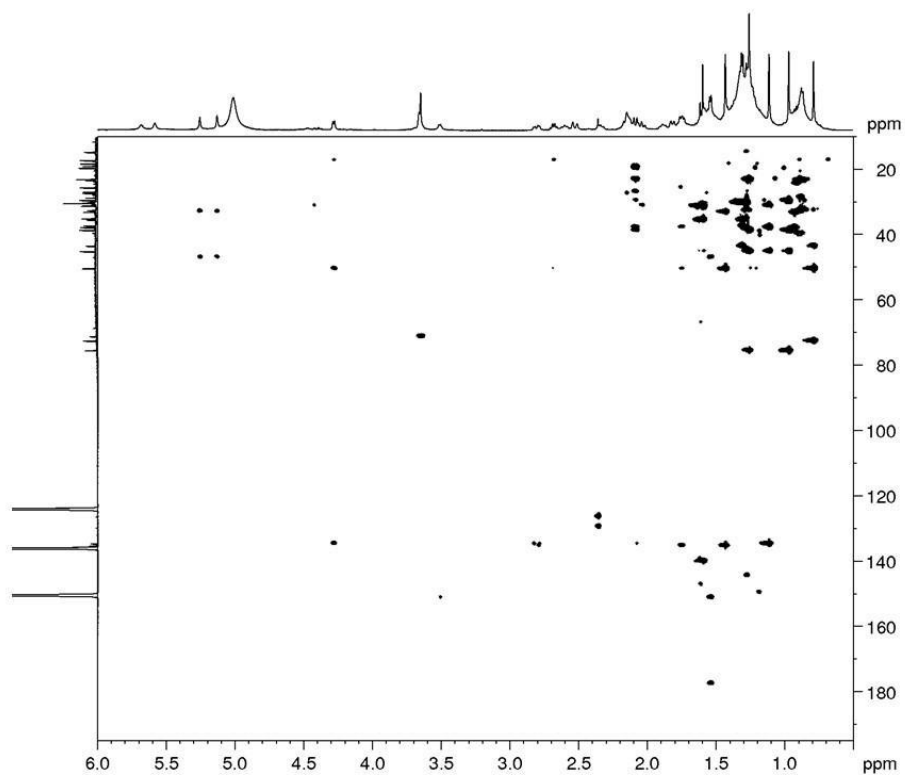


Figure S87. HMBC spectrum of compound **10** (600 MHz, pyridine- $d_5$ , 295 K)

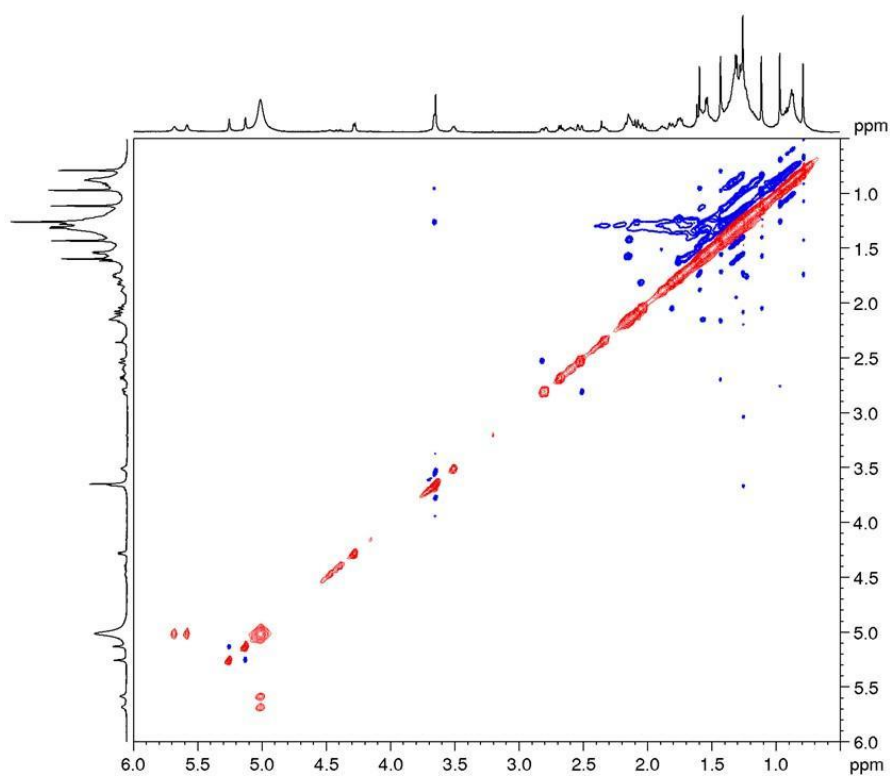
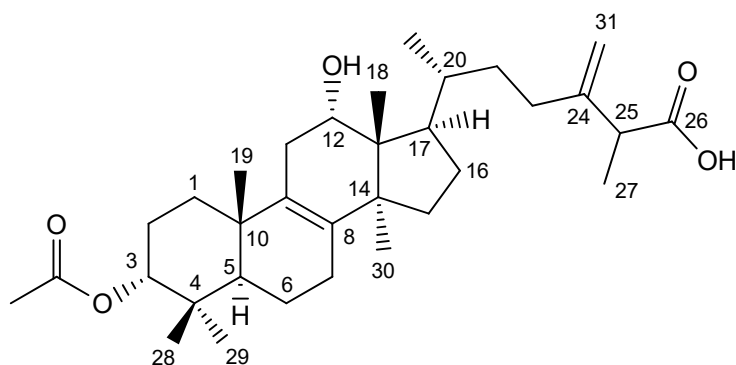


Figure S88. NOESY spectrum of compound **10** (600 MHz, pyridine-*d*<sub>5</sub>, 295 K)

## Spectra and spectral data on compound **11**



HR-ESI-MS (-)  $m/z$  527.3743 [ $M - H$ ] (527.3731 calcd. for  $C_{34}H_{51}O_5$   $\Delta$  2.3 ppm); HR-ESI-MSMS (CID = 15%, 30%, 45%) 497.3636, 483.3841, 441.3736

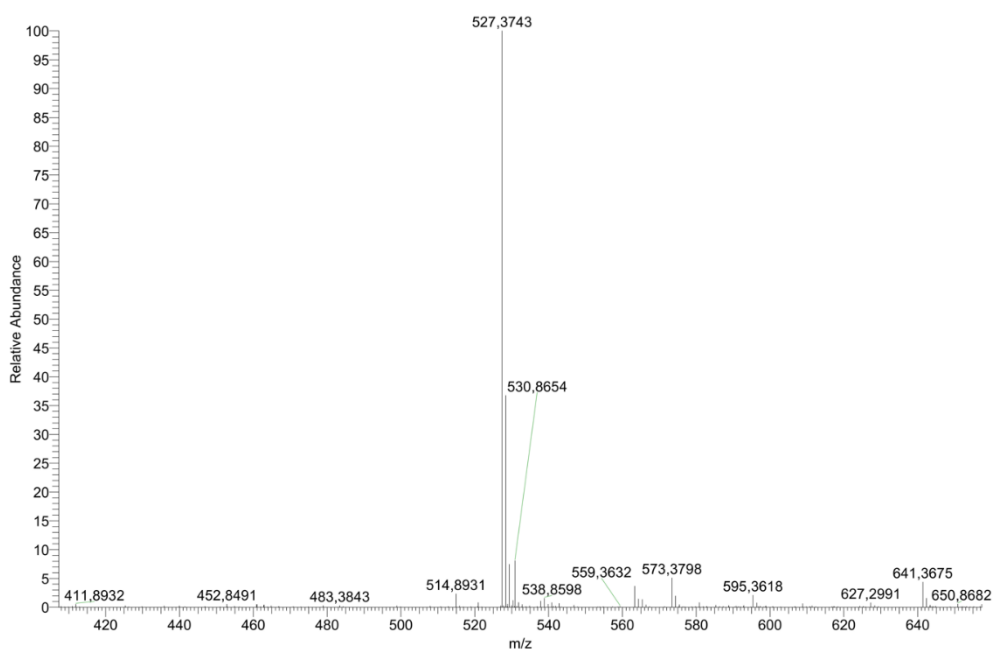


Figure S89. HR-ESI-MS spectrum of compound **11**

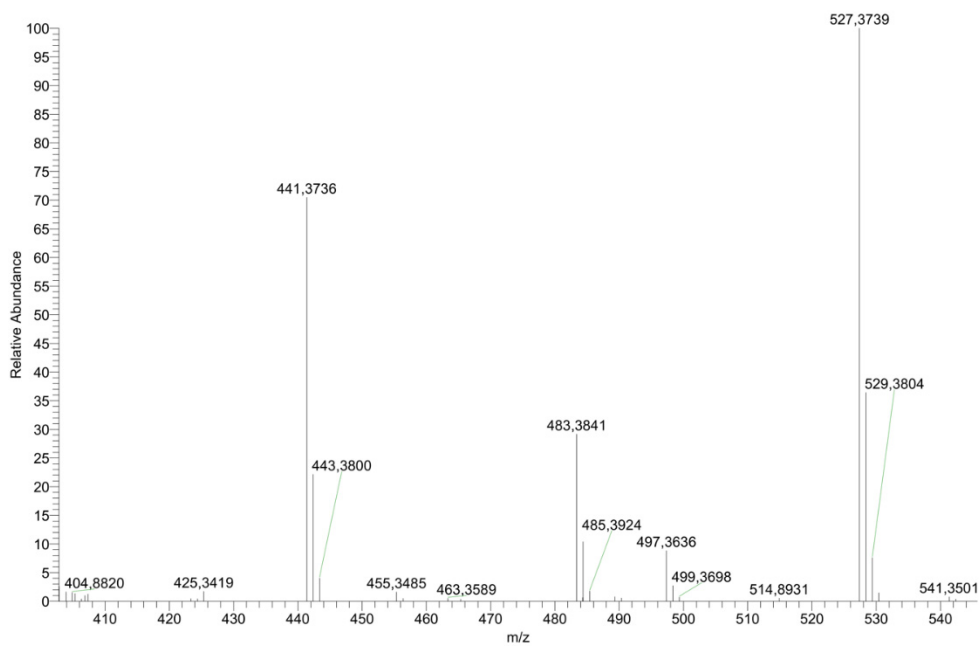


Figure S90. MS-MS spectrum of compound **11**

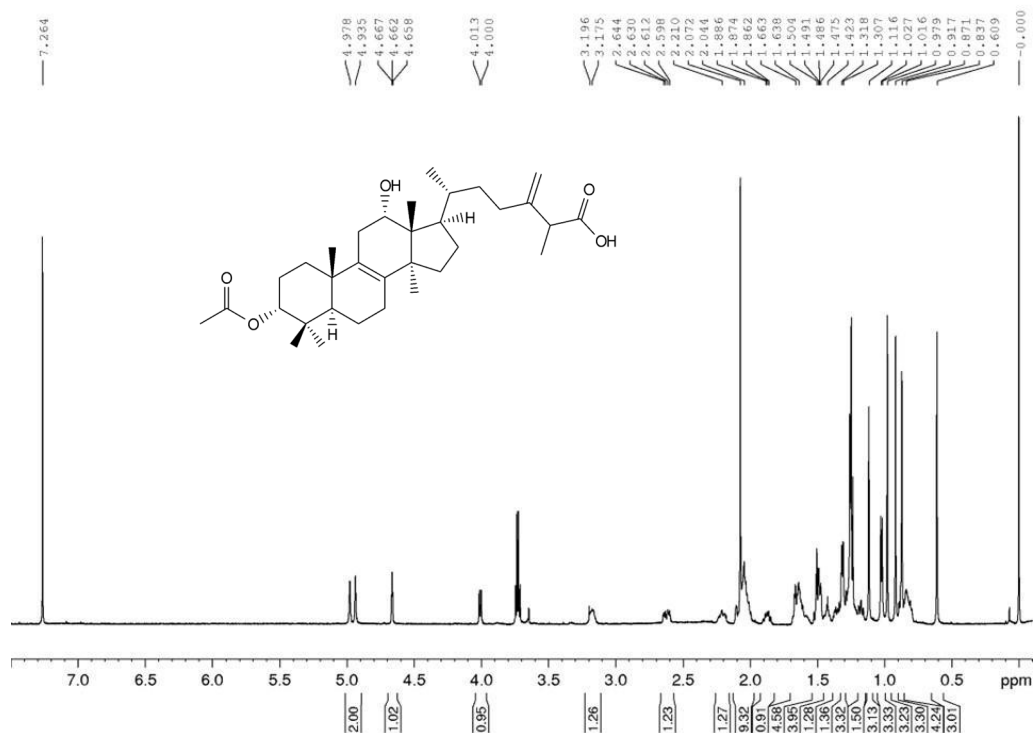


Figure S91. <sup>1</sup>H spectrum of compound **11** (600 MHz, CDCl<sub>3</sub>, 295 K)



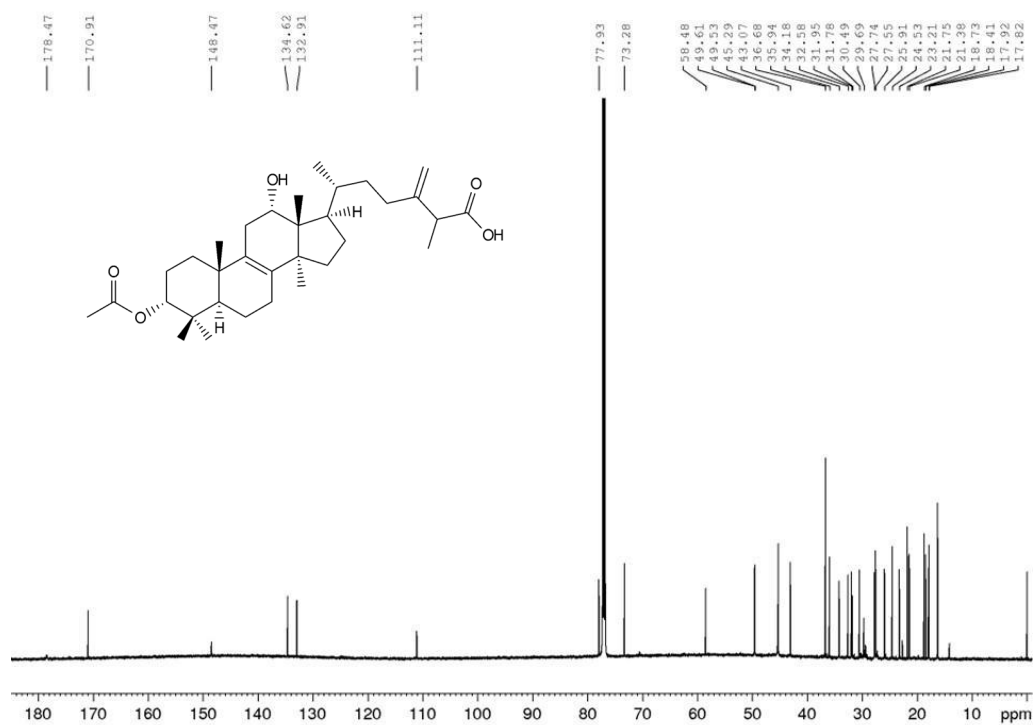


Figure S92.  $^{13}\text{C}$  spectrum of compound **11** (150 MHz, CDCl<sub>3</sub>, 295 K)

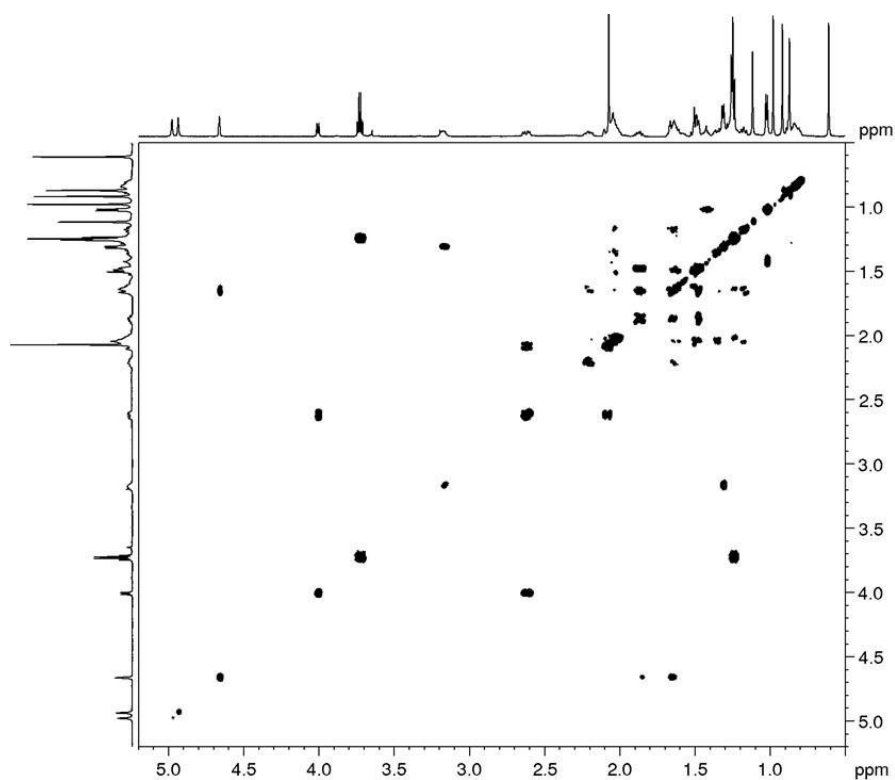


Figure S93. COSY spectrum of compound **11** (600 MHz, CDCl<sub>3</sub>, 295 K)

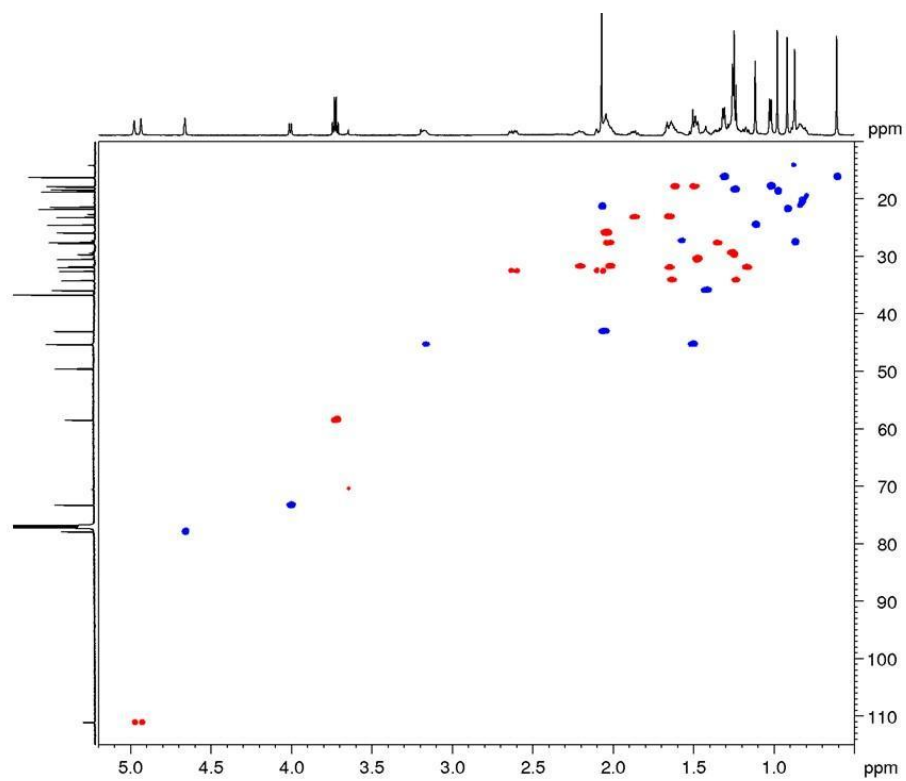


Figure S94. DEPT-edited HSQC spectrum of compound **11** (600 MHz, CDCl<sub>3</sub>, 295 K)

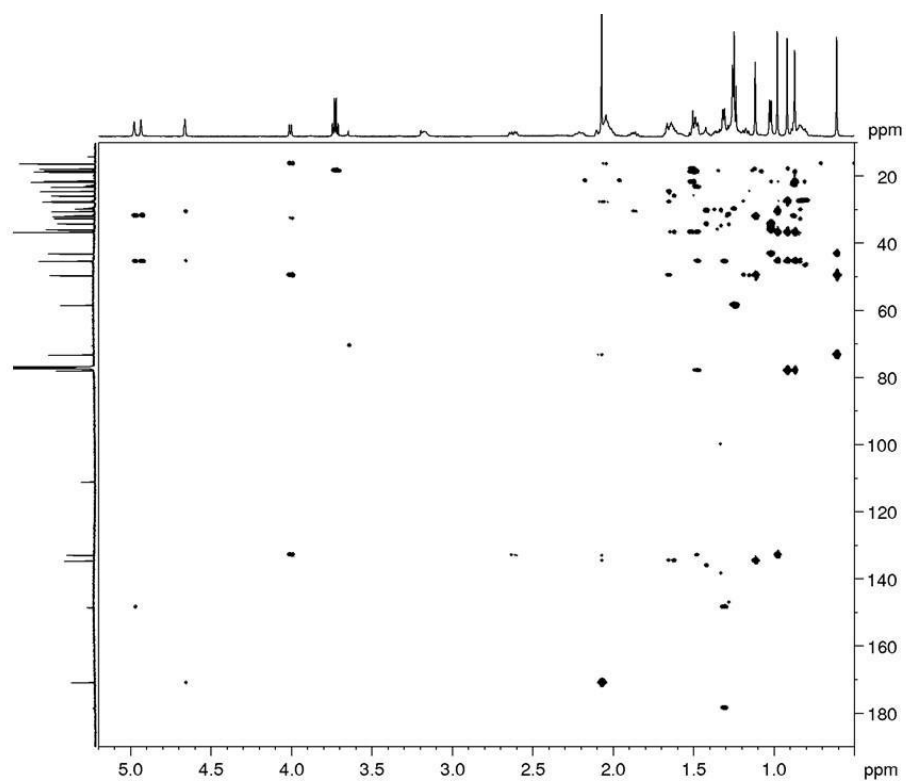


Figure S95. HMBC spectrum of compound **11** (600 MHz, CDCl<sub>3</sub>, 295 K)

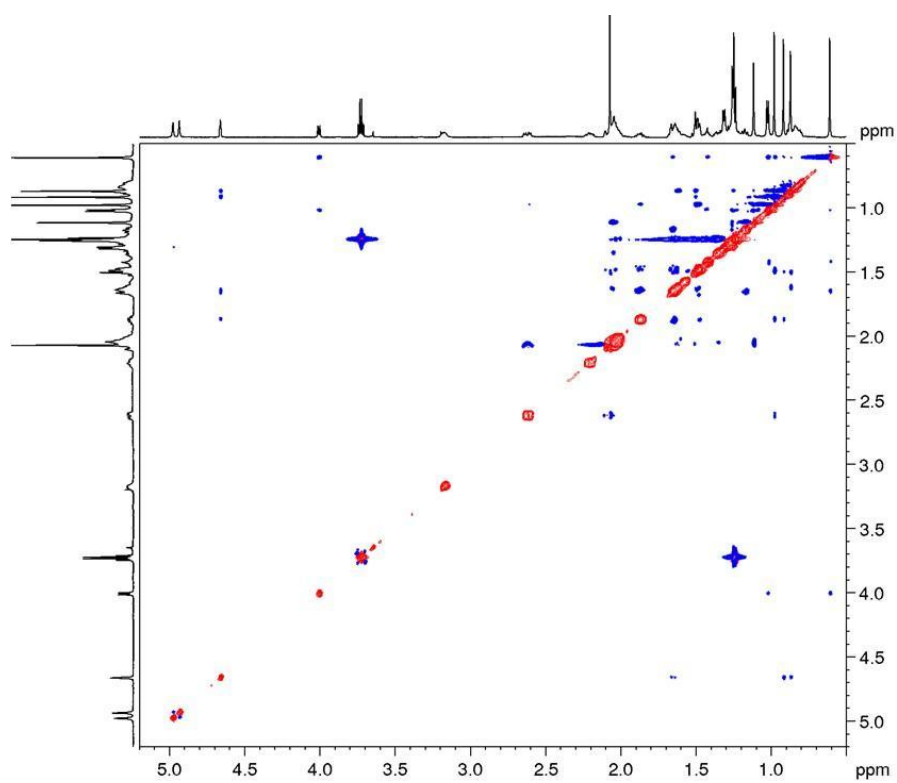
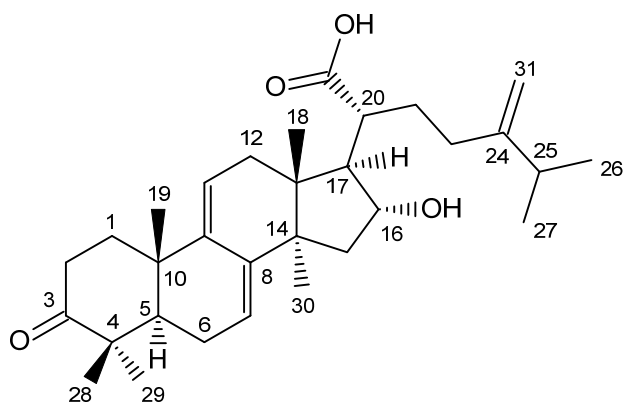


Figure S96. NOESY spectrum of compound **11** (600 MHz, CDCl<sub>3</sub>, 295 K)

## Spectra and spectral data on compound **12**



HR-ESI-MS (+)  $m/z$  483.3461  $[M + H]^+$  (483.3469 calcd. for  $C_{31}H_{47}O_4$ ;  $\Delta$  -1.6 ppm); HR-ESI-MSMS (CID = 15%, 30%, 45%) 465.3354, 309.2205

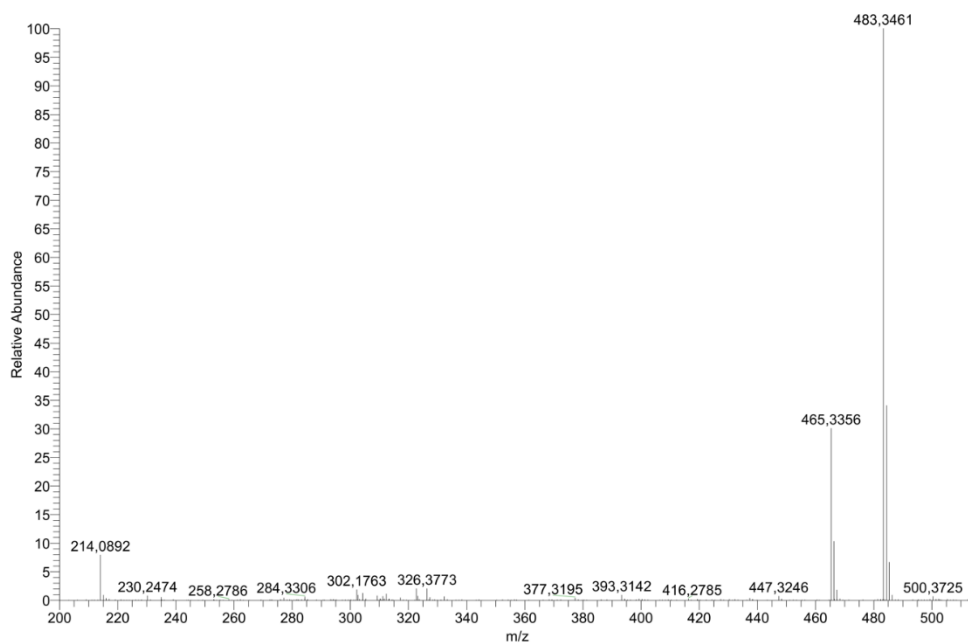


Figure S97. HR-ESI-MS spectrum of compound **12**

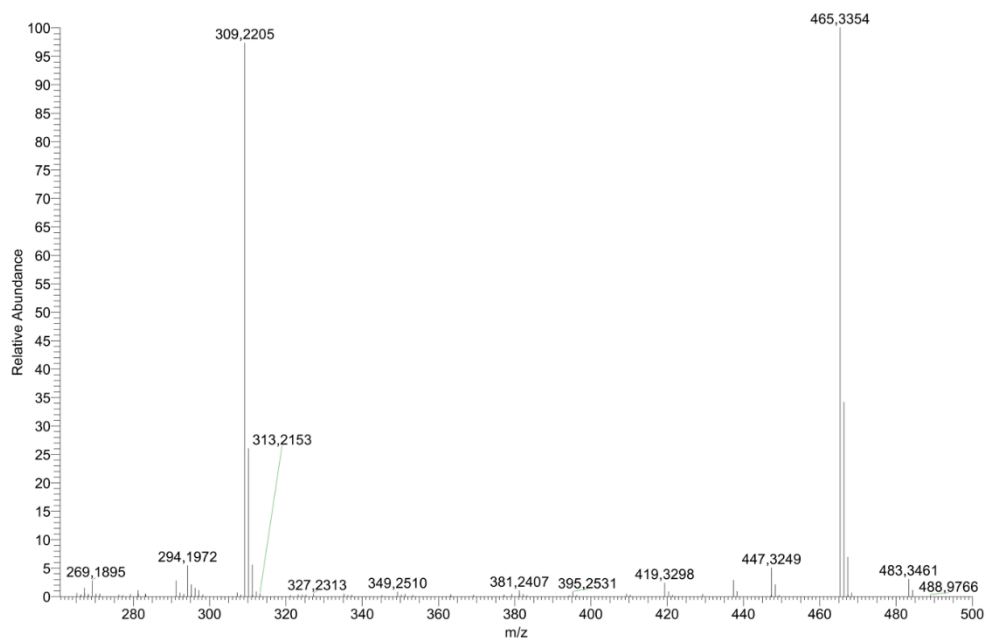


Figure S98. MS-MS spectrum of compound **12**

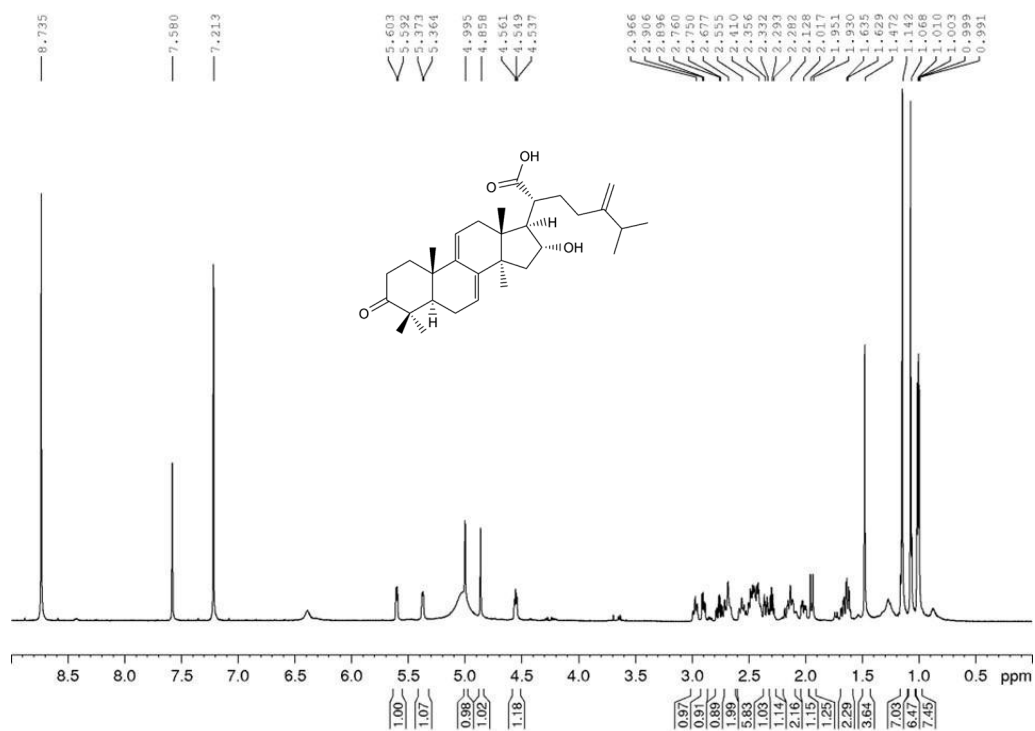


Figure S99. <sup>1</sup>H spectrum of compound **12** (600 MHz, pyridine-*d*<sub>5</sub>, 295 K)

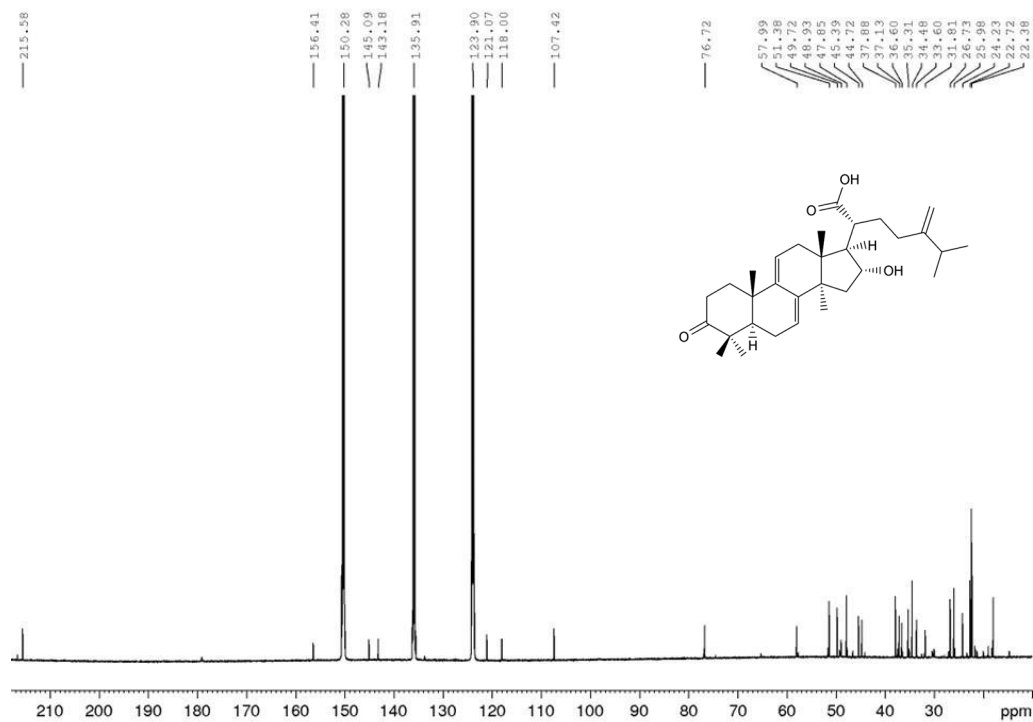


Figure S100.  $^{13}\text{C}$  spectrum of compound **12** (150 MHz, pyridine- $d_5$ , 295 K)

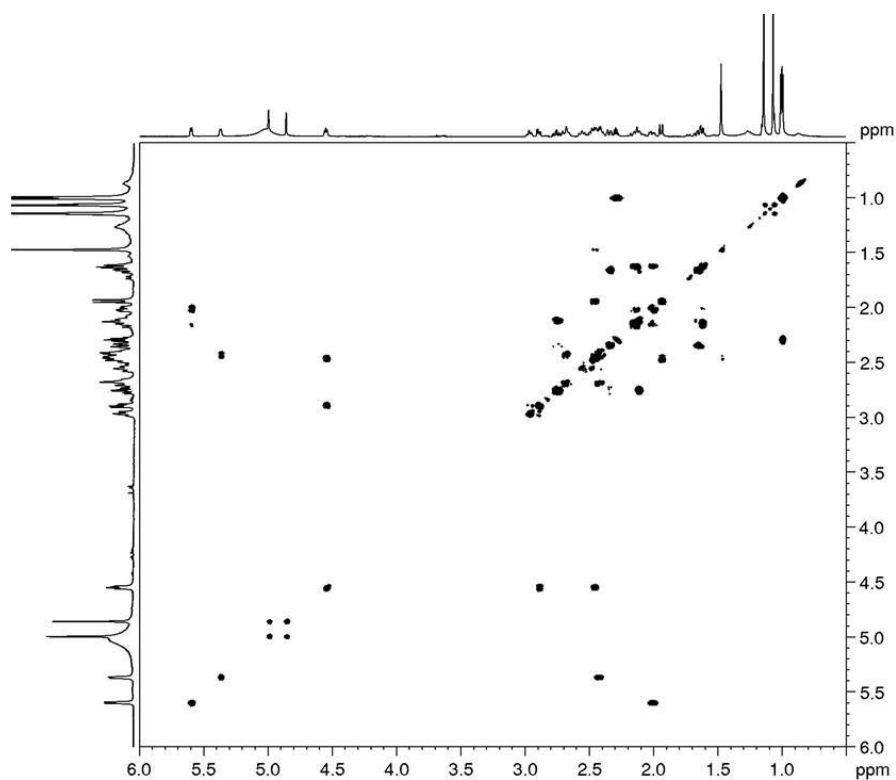


Figure S101. COSY spectrum of compound **12** (600 MHz, pyridine- $d_5$ , 295 K)

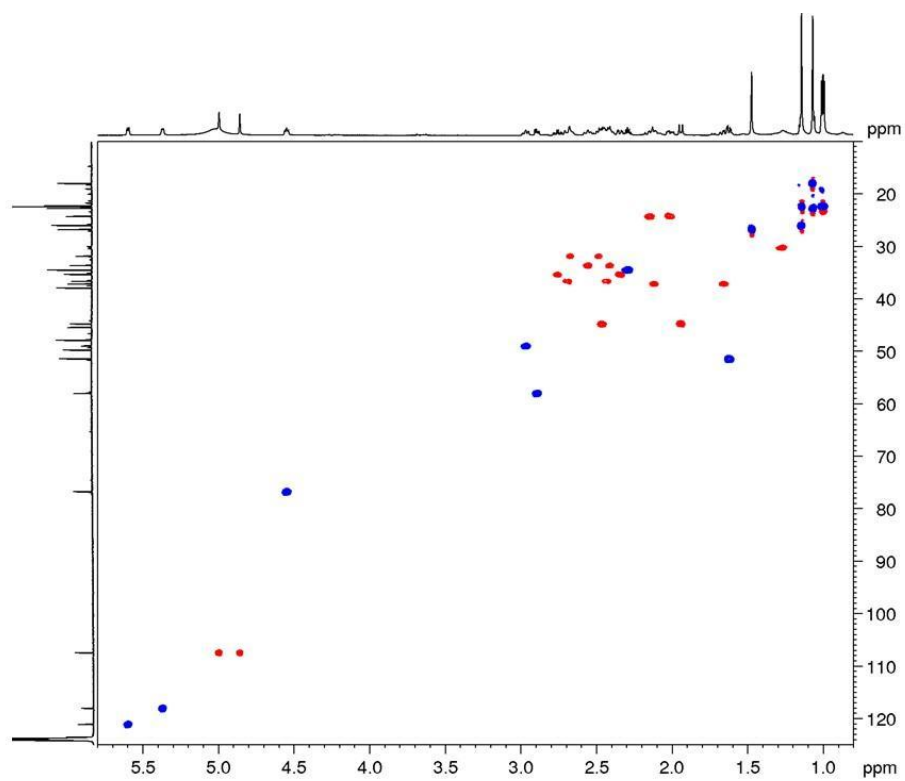


Figure S102. DEPT-edited HSQC spectrum of compound **12** (600 MHz, pyridine-*d*<sub>5</sub>, 295 K)

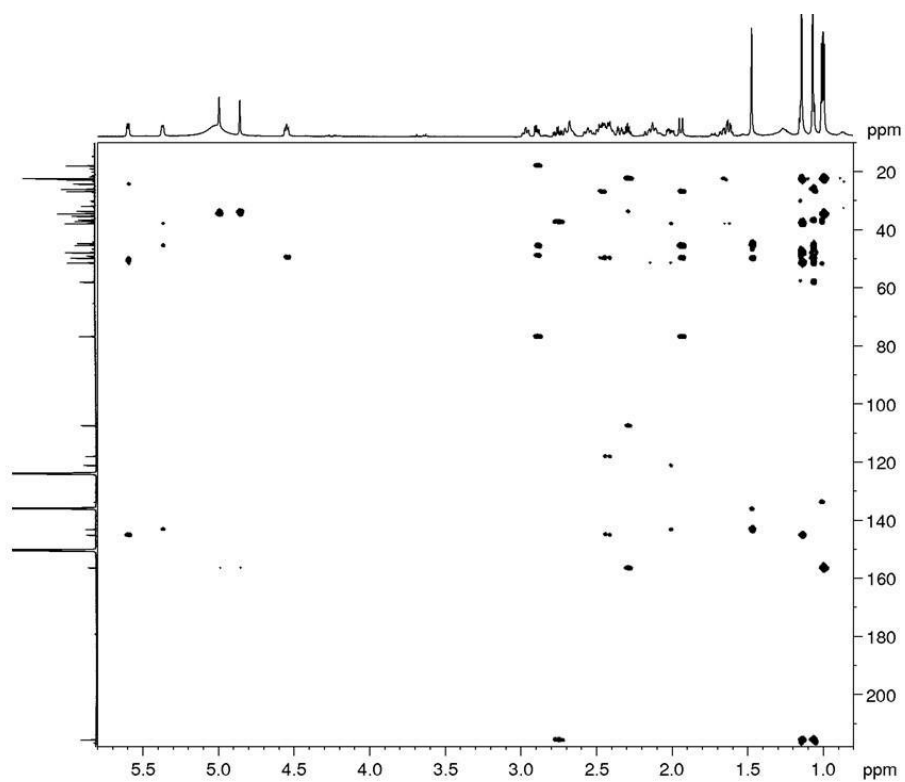


Figure S103. HMBC spectrum of compound **12** (600 MHz, pyridine-*d*<sub>5</sub>, 295 K)

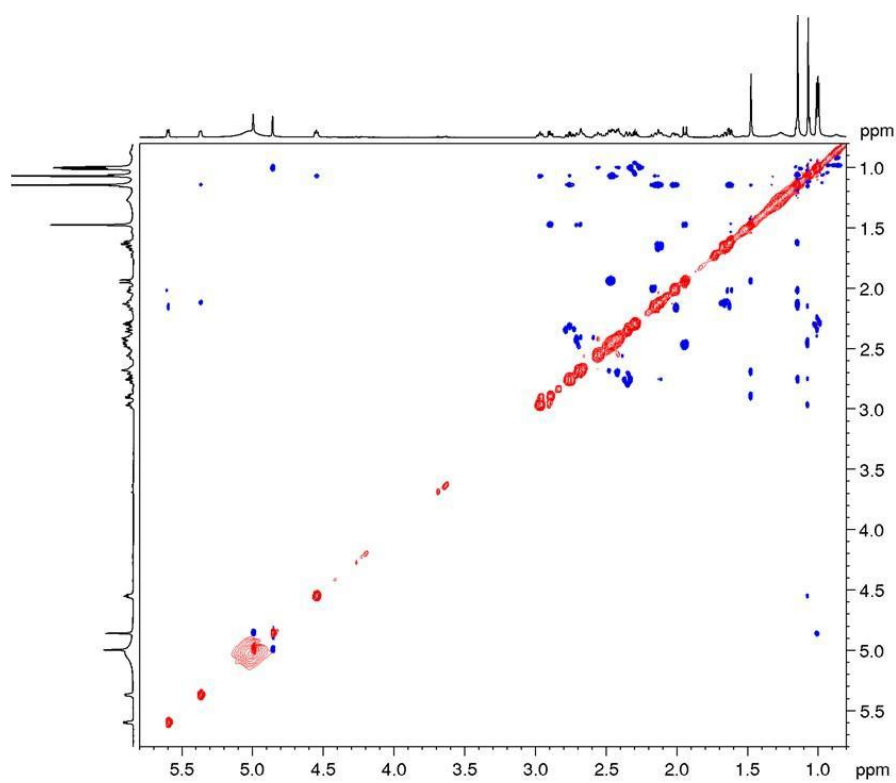


Figure S104. NOESY spectrum of compound **12** (600 MHz, pyridine-*d*<sub>5</sub>, 295 K)



Table S1. NMR Spectroscopic Data (600 MHz, CDCl<sub>3</sub><sup>a</sup>, pyridine-*d*<sub>5</sub><sup>b</sup>, tetrahydrofuran-*d*<sub>8</sub><sup>c</sup>, or methanol-*d*:pyridine-*d*<sub>5</sub> 19:1<sup>d</sup>, methanol-*d*<sup>e</sup>) for compounds **6-9**

1 <sup>c</sup>			2 <sup>c</sup>			3 <sup>a</sup>			4 <sup>a</sup>			5 <sup>b</sup>			
position	δ <sub>c</sub> type		δ <sub>H</sub> (J in Hz)	δ <sub>c</sub> type		δ <sub>H</sub> (J in Hz)	δ <sub>c</sub> type		δ <sub>H</sub> (J in Hz)	δ <sub>c</sub> type		δ <sub>H</sub> (J in Hz)	δ <sub>c</sub> type		δ <sub>H</sub> (J in Hz)
1	35.7	CH <sub>2</sub>	1.82, m	36.4	CH <sub>2</sub>	1.51, m	30.7	CH <sub>2</sub>	1.43, m	30.6	CH <sub>2</sub>	1.49, m	31.6	CH <sub>2</sub>	1.75, m
			1.54, m			1.09, m			1.37, m			1.41, m			1.55, m
			2.31, dd, (10.0, 8.0)			1.48, m			1.87, m			1.90, m			1.90, m
2	36.8	CH <sub>2</sub>	2.28, dd, (8.0, 3.4)	28.8	CH <sub>2</sub>	1.67, m	23.1	CH <sub>2</sub>	1.67, m	23.2	CH <sub>2</sub>	1.72, m	24.1	CH <sub>2</sub>	1.78, m
			4.76, br s			4.68, br s			4.76, br s			4.97, br s			
3	216.0	C		78.3	CH	2.97, m	77.6	CH		80.6	CH		78.4	CH	
4	52.8	C		39.7	C		36.7	C		36.8	C		37.4	C	
5	44.3	CH	2.17, m	51.5	CH	0.96, m	45.2	CH	1.50, m	45.3	CH	1.47, m	46.4	CH	1.83, m
6	20.2	CH <sub>2</sub>	1.49, m	19.1	CH <sub>2</sub>	1.65, m	17.8	CH <sub>2</sub>	1.67, m	18.0	CH <sub>2</sub>	1.59, m	18.8	CH <sub>2</sub>	1.62, m
			1.44, m			1.49, m			1.56, m			1.49, m			1.52, m
			2.03, m			2.06, m			2.12, m			2.04, m			2.17, m
7	27.2	CH <sub>2</sub>	1.93, m	27.2	CH <sub>2</sub>	1.95, m	25.8	CH <sub>2</sub>	2.07, m	25.9	CH <sub>2</sub>	2.04, m	26.8	CH <sub>2</sub>	2.12, m
8	136.6	C		135.8	C		135.0	C		134.2	C		135.5	C	
9	134.0	C		136.6	C		135.1	C		134.3	C		134.2	C	
10	37.6	C		37.8	C		36.7	C		36.8	C		37.5	C	
11	21.4	CH <sub>2</sub>	1.94, m	40.5	CH <sub>2</sub>	2.82, m	39.9	CH <sub>2</sub>	2.90, m	20.9	CH <sub>2</sub>	2.01, m	34.9	CH <sub>2</sub>	2.76, m
			2.49, m			2.71, m						2.50, m			
12	30.0	CH <sub>2</sub>	1.71, m	210.5	C		212.7	C		30.9	CH <sub>2</sub>	1.74, m	72.5	CH	4.27, d (7.6)
			1.39, m						1.69, m						
13	46.5	C		55.0	C		54.5	C		44.5	C		50.5	C	
14	49.4	C		60.0	C		59.4	C		49.9	C		50.4	C	
15	44.0	CH <sub>2</sub>	2.03, m	30.9	CH <sub>2</sub>	1.75, m	30.1	CH <sub>2</sub>	1.82, m	30.8	CH <sub>2</sub>	1.60, m	33.1	CH <sub>2</sub>	1.76, m
			1.15, m			1.20, m			1.35, m			1.18, m			1.25, m
						1.91, m			2.01, m			1.94, m			2.11, m
16	77.1	CH	3.89, m	28.6	CH <sub>2</sub>	1.29, m	27.8	CH <sub>2</sub>	1.37, m	28.2	CH <sub>2</sub>	1.31, m	28.7	CH <sub>2</sub>	1.40, m
17	57.3	CH	1.96, m	43.5	CH	2.06, m	42.4	CH	2.19, m	50.3	CH	1.50, m	43.5	CH	2.65, m
18	17.8	CH <sub>3</sub>	0.69, s	12.9	CH <sub>3</sub>	0.94, s	12.6	CH <sub>3</sub>	1.05, s	15.7	CH <sub>3</sub>	0.69, s	17.2	CH <sub>3</sub>	0.77, s
19	19.2	CH <sub>3</sub>	0.95, s	19.5	CH <sub>3</sub>	0.98, s	19.0	CH <sub>3</sub>	1.08, s	18.9	CH <sub>3</sub>	1.00, s	19.4	CH <sub>3</sub>	1.03, s
20	48.3	CH	2.24, m	37.7	CH	1.18, m	36.6	CH	1.27, m	36.3	CH	1.41, m	37.3	CH	1.53, m
21	177.4	C		19.6	CH <sub>3</sub>	0.78, d (6.4)	19.0	CH <sub>3</sub>	0.89, d (5.8)	18.6	CH <sub>3</sub>	0.93, m	18.3	CH <sub>3</sub>	1.28, m
			1.53, m			1.62, m			1.58, m			1.77, m			
22	31.6	CH <sub>2</sub>	1.92, m	35.3	CH <sub>2</sub>	1.14, m	34.0	CH <sub>2</sub>	1.27, m	34.2	CH <sub>2</sub>	1.19, m	35.4	CH <sub>2</sub>	1.38, m
			1.64, m												
23	33.4	CH <sub>2</sub>	1.96, m	32.9	CH <sub>2</sub>	2.14, m	32.1	CH <sub>2</sub>	2.21	31.7	CH <sub>2</sub>	2.19, m	32.7	CH <sub>2</sub>	2.37, m
			1.87, m			1.09, m			2.02			2.00, m			2.17, m
24	156.7	C		150.9	C		148.5	C		148.3	C		150.2	C	
25	34.8	CH	2.14, m	46.2	CH	2.96, m	45.1	CH	3.17, m	45.0	CH	3.18, q (7.0)	46.2	CH	3.32, q (7.1)
26	22.4	CH <sub>3</sub>	0.91, d (6.9)	175.6	C		177.7	C		179.6	C		175.3	C	
27	22.2	CH <sub>3</sub>	0.92, d (6.9)	17.0	CH <sub>3</sub>	1.10, d (7.4)	16.3	CH <sub>3</sub>	1.31, d (6.7)	16.1	CH <sub>3</sub>	1.31, d (7.0)	17.1	CH <sub>3</sub>	1.38, d (7.1)
28	68.3	CH <sub>2</sub>	3.39, dd (10.2, 2.4)	28.5	CH <sub>3</sub>	0.88, s	27.5	CH <sub>3</sub>	0.88, s	27.6	CH <sub>3</sub>	0.88, s	28.5	CH <sub>3</sub>	1.04, s

			3.16, dd (10.2, 2.4)											
29	17.5	CH <sub>3</sub>	0.78, s	16.1	CH <sub>3</sub>	0.69, s	21.7	CH <sub>3</sub>	0.94, s	21.7	CH <sub>3</sub>	0.93, m	22.4	CH <sub>3</sub> 0.91, s
30	25.3	CH <sub>3</sub>	1.05, s	24.3	CH <sub>3</sub>	0.65, s	24.1	CH <sub>3</sub>	0.82, s	24.2	CH <sub>3</sub>	0.91, s	25.7	CH <sub>3</sub> 1.43, s
31	106.9	CH <sub>2</sub>	4.61, br s	110.3	CH <sub>2</sub>	4.77, br s 4.71, br s	111.1	CH <sub>2</sub>	4.97, br s 4.94, br s	111.4	CH <sub>2</sub>	4.97, br s 4.94, br s	111.3	CH <sub>2</sub> 5.10, br s 5.06, br s
1'							170.8	C		167.2	C		172.4 <sup>d</sup>	C
2'										40.2	CH <sub>2</sub>	3.64, m	47.0 <sup>d</sup>	CH <sub>2</sub> 2.64 <sup>d</sup> , m
3'										170.6	C		71.0 <sup>d</sup>	C
4'													47.0 <sup>d</sup>	CH <sub>2</sub> 2.64 <sup>d</sup> , m
5'													172.4 <sup>d</sup>	C
1'-CH <sub>3</sub>							21.3	CH <sub>3</sub>	2.07, s					
3'-CH <sub>3</sub>													27.9 <sup>d</sup>	CH <sub>3</sub> 1.37 <sup>d</sup> , m
26-CH <sub>3</sub>													52.3 <sup>d</sup>	CH <sub>3</sub> 3.67 <sup>d</sup> , m

Table S2. NMR Spectroscopic Data (600 MHz, CDCl<sub>3</sub><sup>a</sup>, pyridine-*d*<sub>5</sub><sup>b</sup>, tetrahydrofuran-*d*<sub>8</sub><sup>c</sup>, or methanol-*d*:pyridine-*d*<sub>5</sub> 19:1<sup>d</sup>, methanol-*d*<sup>e</sup>) for compounds **10-12**

position	10 <sup>b</sup>			11 <sup>a</sup>			12 <sup>b</sup>		
	δ <sub>c</sub>	type	δ <sub>H</sub> (J in Hz)	δ <sub>c</sub>	type	δ <sub>H</sub> (J in Hz)	δ <sub>c</sub>	type	δ <sub>H</sub> (J in Hz)
1	31.1	CH <sub>2</sub>	2.14, m	30.5	CH <sub>2</sub>	1.48, m	37.1	CH <sub>2</sub>	2.12, m 1.66, m
2	27.4	CH <sub>2</sub>	2.05, m 1.82, m	23.2	CH <sub>2</sub>	1.87, m 1.65, m	35.3	CH <sub>2</sub>	2.75, m 2.34, m
3	75.5	CH	3.66, br s	77.9	CH	4.66, br s	215.6	C	
4	38.6	C		36.7	C		47.9	C	
5	45.1	CH	2.08, m	45.3	CH	1.50, m	51.4	CH	1.62, m
6	19.1	CH <sub>2</sub>	1.74, m 1.61, m	17.9	CH <sub>2</sub>	1.62, m 1.50, m	24.2	CH <sub>2</sub>	2.15, m 2.01, m
7	27.0	CH <sub>2</sub>	2.15, m	25.9	CH <sub>2</sub>	2.04, m	121.1	CH	5.60, d (6.4)
8	135.3	C		134.6	C		143.2	C	
9	134.7	C		132.9	C		145.1	C	
10	37.8	C		36.7	C		37.9	C	
11	35.1	CH <sub>2</sub>	2.81, m 2.52, m	32.6	CH <sub>2</sub>	2.62, m 2.09, m	118.0	CH	5.37, d (6.0)
12	72.5	CH	4.28, d (7.5)	73.2	CH	4.00, d (8.0)	36.6	C	2.69, m 2.43, m
13	50.5	C		49.5	C		45.4	C	
14	50.4	C		49.6	C		49.7	C	
15	33.1	CH <sub>2</sub>	1.76, m	32.0	CH <sub>2</sub>	1.65, m 1.17, m	44.7	CH <sub>2</sub>	2.46, m 1.94, m
16	28.8	CH <sub>2</sub>	2.14, m 1.43, m	27.7	CH <sub>2</sub>	2.02, m 1.35, m	76.7	CH	4.55, m
17	43.6	CH	2.68, m	43.1	CH	2.06, m	58.0	CH	2.89, m
18	17.2	CH <sub>3</sub>	0.79, s	16.2	CH <sub>3</sub>	0.61, s	18.0	CH <sub>3</sub>	1.07, s
19	19.7	CH <sub>3</sub>	1.11, s	18.7	CH <sub>3</sub>	0.98, s	22.4	CH <sub>3</sub>	1.14, s
20	37.3	CH	1.58, m	35.9	CH	1.42, m	48.9	CH	2.97, m
21	18.4	CH	1.31, d (6.1)	17.8	CH <sub>3</sub>	1.02, d (6.4)	179.1	C	
22	35.5	CH <sub>2</sub>	1.89, m 1.51, m	34.2	CH <sub>2</sub>	1.63, m 1.24, m	31.8	CH <sub>2</sub>	2.67, m 2.49, m
23	32.9	CH <sub>2</sub>	2.60, m 2.34, m	31.8	CH <sub>2</sub>	2.21, m 2.02, m	33.6	CH <sub>2</sub>	2.56, m 2.41, m
24	151.1	C		148.5	C		156.4	C	
25	46.9	CH	3.51, m	45.3	CH	3.18, m	34.5	CH	2.29, m
26	177.4	C		178.5	C		22.2	CH <sub>3</sub>	1.00, d (6.8)
27	17.5	CH <sub>3</sub>	1.54, d (6.7)	16.2	CH <sub>3</sub>	1.31, d (6.9)	22.2	CH <sub>3</sub>	1.00, d (6.8)
28	29.5	CH <sub>3</sub>	1.26, s	27.6	CH <sub>3</sub>	0.87, s	26.0	CH <sub>3</sub>	1.14, s
29	23.1	CH <sub>3</sub>	0.97, s	21.8	CH <sub>3</sub>	0.92, s	22.7	CH <sub>3</sub>	1.07, s
30	25.6	CH <sub>3</sub>	1.43, s	24.5	CH <sub>3</sub>	1.12, s	26.7	CH <sub>3</sub>	1.47, s
31	110.8	CH <sub>2</sub>	5.25, br s 5.13, br s	111.1	CH <sub>2</sub>	4.98, br s 4.94, br s	107.4	CH <sub>2</sub>	5.00, br s 4.86, br s
1'				170.9	C				
1'-CH <sub>3</sub>				21.4	CH <sub>3</sub>	2.07, m			

Table S3. Chemosensitizing Activity of Compounds 3-4, and 7-12 on Colo 320 Adenocarcinoma Cells

Compound	c(IC <sub>50</sub> *4) [uM]	Drug:Doxo ratio	CI	SD	type
<b>3</b>	119.13	13.82:1	0.907	0.12	Nearly additive
		27.64:1	0.601	0.0495	Synergism
		55.28:1	0.972	0.081	Nearly additive
		110.56:1	1.027	0.1133	Nearly additive
		221.12:1	0.944	0.1212	Nearly additive
		442.24:1	1.471	0.3143	Strong antagonism
<b>4</b>	276.66	32.08:1	0.816	0.2102	Moderate synergism
		64.16:1	0.691	0.0705	Synergism
		128.32:1	0.734	0.0845	Moderate synergism
		256.64:1	0.739	0.092	Moderate synergism
		513.28:1	0.904	0.1805	Nearly additive
		1026.56:1	1.421	0.2691	Antagonism
<b>7</b>	246.84	28.63:1	1.002	0.0372	Nearly additive
		57.26:1	0.972	0.1029	Nearly additive
		114.52:1	0.419	0.0697	Synergism
		229.04:1	1.371	0.1618	Antagonism
		458.08:1	1.347	0.2608	Antagonism
		916.16:1	1.295	0.1921	Antagonism
<b>8</b>	144.74	16.8:1	0.905	0.0877	Nearly additive
		33.6:1	0.889	0.0332	Slight synergism
		67.2:1	0.574	0.0698	Synergism
		134.4:1	0.713	0.0972	Moderate synergism
		268.8:1	0.64	0.0956	Synergism
		537.6:1	1.042	0.0934	Nearly additive
<b>9</b>	157.84	18.23:1	1.316	0.21	Antagonism
		36.64:1	0.656	0.0528	Synergism
		73.28:1	0.653	0.0839	Synergism

		146.56:1	0.447	0.0534	Synergism
		293.12:1	0.559	0.0681	Synergism
		586.24:1	0.276	0.096	Strong synergism
<b>10</b>	195.9	22.72:1	1.258	0.3766	Antagonism
		45.44:1	1.09	0.1509	Nearly additive
		90.88:1	0.779	0.0819	Moderate synergism
		181.76:1	0.798	0.1561	Moderate synergism
		363.52:1	0.988	0.2678	Nearly additive
		727.04:1	1.438	0.3819	Antagonism
<b>11</b>	118.96	13.8:1	1.456	0.2324	Strong antagonism
		27.6:1	0.841	0.14	Moderate synergism
		55.2:1	0.911	0.2554	Nearly additive
		110.4:1	1.491	0.2423	Strong antagonism
		220.8:1	1.89	0.3337	Strong antagonism
		441.6:1	1.938	0.3863	Strong antagonism
<b>12</b>	82.85	9.62:1	1.992	0.3279	Strong antagonism
		19.24:1	1.42	0.2308	Antagonism
		38.48:1	0.608	0.0324	Synergism
		76.96:1	0.895	0.0678	Slight synergism
		153.92:1	0.736	0.0458	Moderate synergism
		307.84:1	0.824	0.2692	Moderate synergism

Range	Description
<0.1	Very strong synergism
0.1-0.3	Strong synergism
0.3-0.7	Synergism
0.7-0.85	Moderate Synergism

0.85-0.9	Slight synergism
0.9-1.1	Nearly additive
1.1-1.2	Moderate antagonism
1.2-1.45	Antagonism
1.45-3.3	Strong antagonism
3.3-10	Very strong antagonism

Doxo: doxorubicin, CI: combination index, SD: standard deviation

Table S4. P-gp Efflux Pump Inhibitory Activity of Compounds **1–12** on MDR Colo 320 Colon Adenocarcinoma Cell Line

Samples	conc. $\mu\text{M}$	FSC	SSC	FL-1	FAR
Tariquidar	0.2	1557	1038	45.800	15.091
Compound <b>1</b>	20	1696	898	2.350	0.774
Compound <b>2</b>	20	1603	947	3.190	1.051
Compound <b>3</b>	20	1239	889	13.500	<b>4.448</b>
Compound <b>4</b>	20	1349	930	4.060	1.338
Compound <b>5</b>	20	1332	1012	23.100	<b>7.611</b>
Compound <b>6</b>	20	1681	845	1.170	0.386
Compound <b>7</b>	20	1593	865	1.800	0.593
Compound <b>8</b>	20	1356	916	6.310	<b>2.079</b>
Compound <b>9</b>	20	1427	928	2.860	0.942
Compound <b>10</b>	20	1383	902	11.600	<b>3.822</b>
Compound <b>11</b>	20	1463	940	7.560	<b>2.491</b>
Compound <b>12</b>	20	1420	1007	6.880	<b>2.267</b>
DMSO	2%	1654	675	1.220	0.402

FSC: forward scatter count; SSC: side scatter count; FL-1: mean fluorescence; FAR: fluorescence activity ratios