

## Supporting Information

*Rec. Nat. Prod.* 17:2 (2023) 372-376

### Cytotoxic Constituents from the Rhizomes of *Monstera deliciosa*

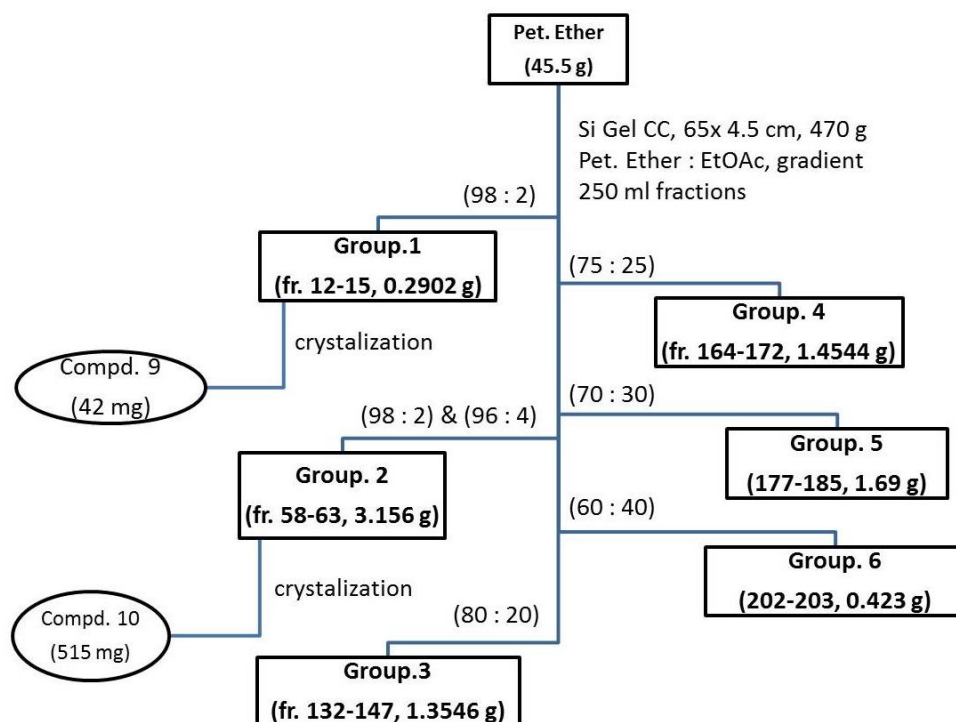
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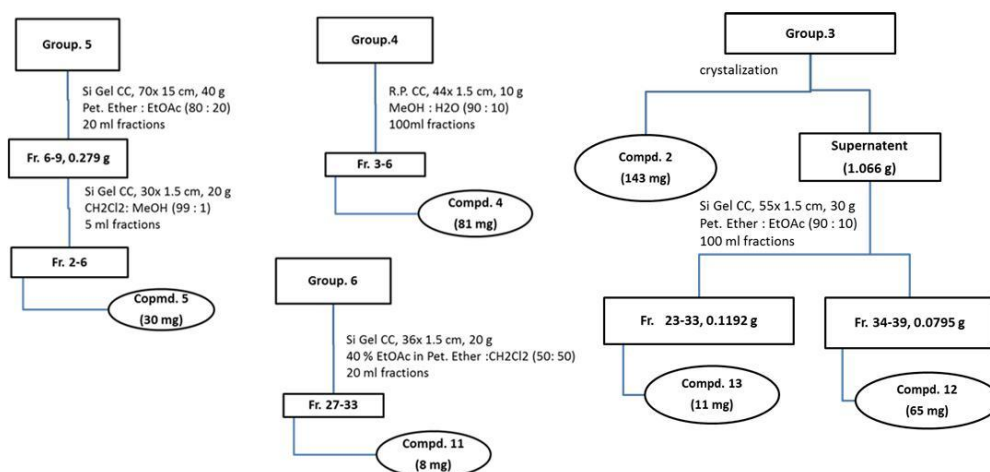
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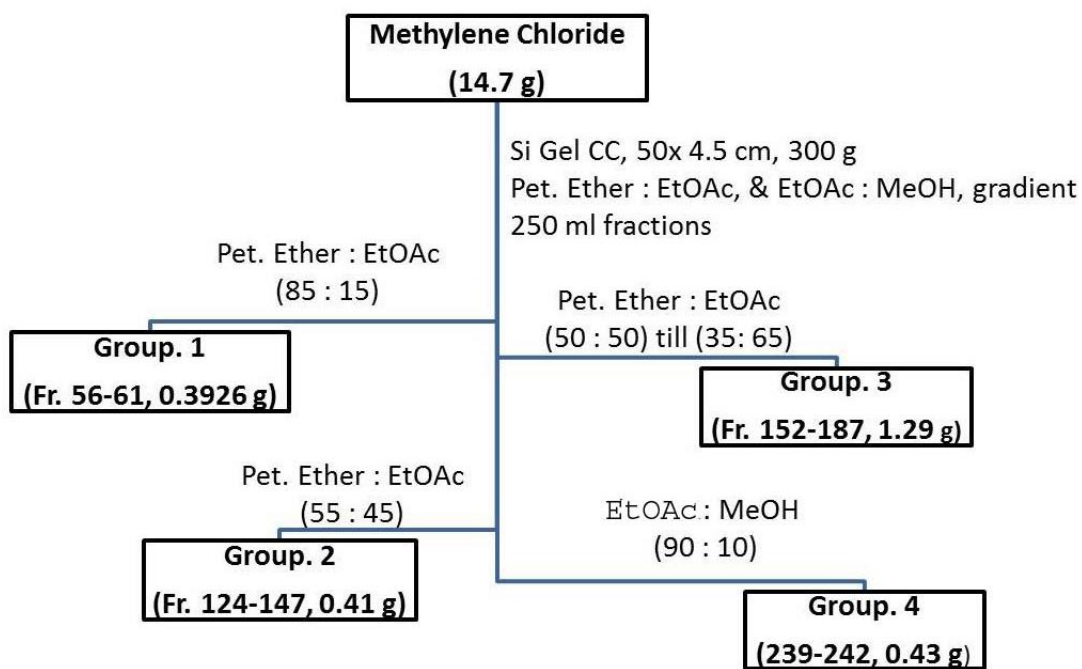
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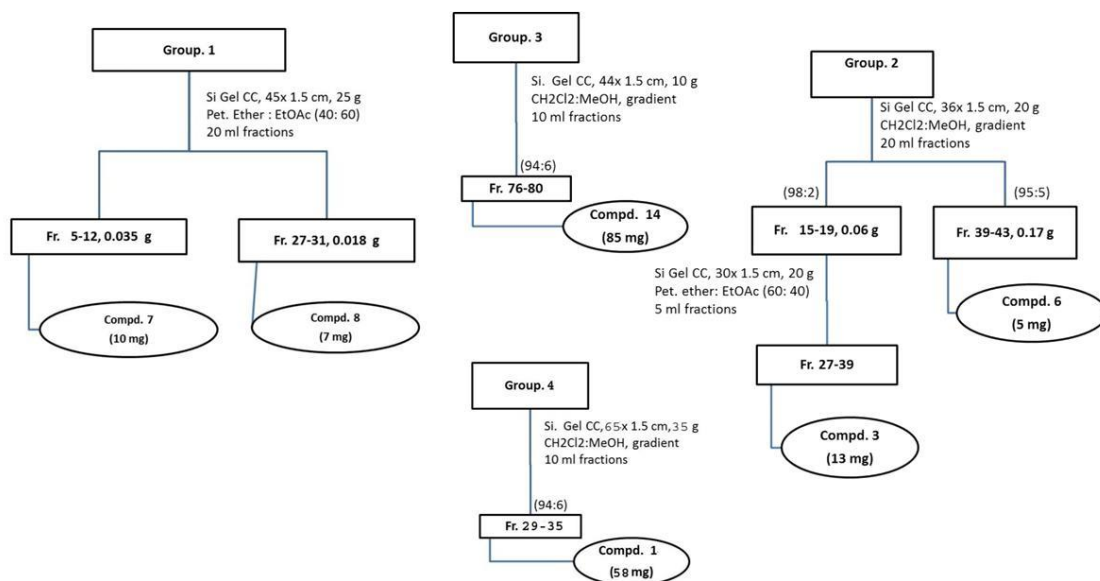
**Figure S1:** Scheme for chromatographic fractionation of the pet. ether extract & separation of **9** ( $\beta$ -sitosteryl palmitate) and **10** ( $\beta$ -sitosterol).



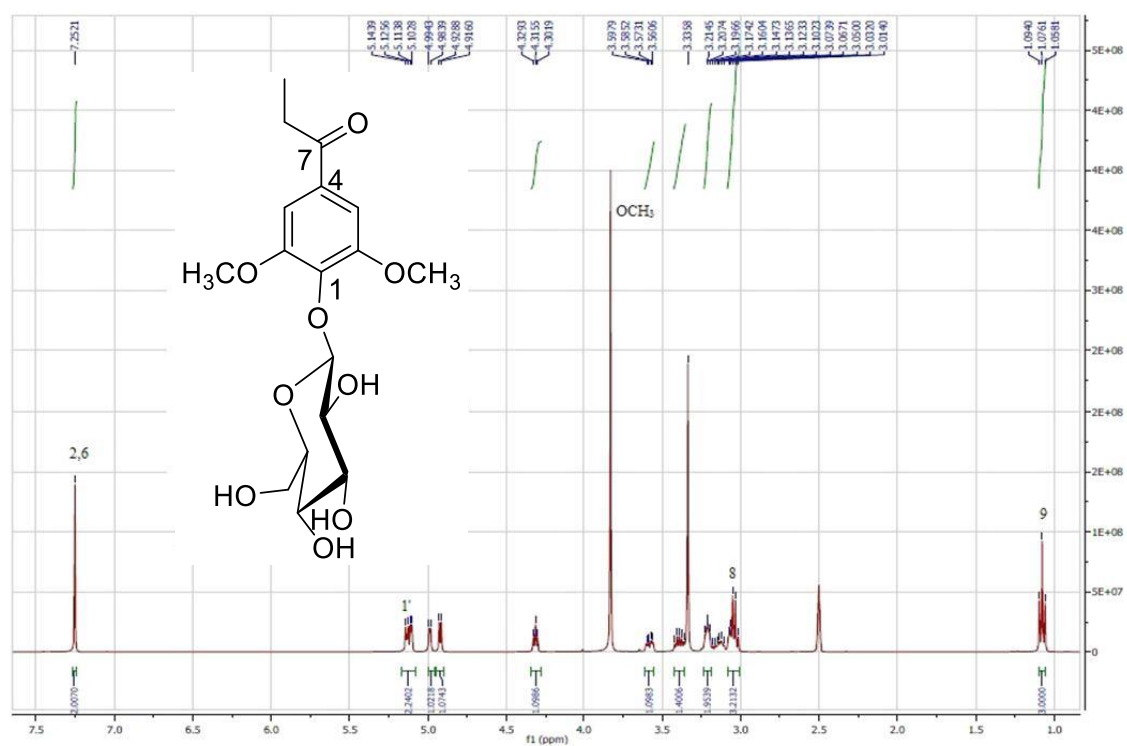
**Figure S2:** Scheme for chromatographic separation of **2** (propiosyringone), **4** (sesartemin), **5** (yangambin), **11** (7-oxo-  $\beta$ -sitosterol-3-O- $\beta$ -D-glucopyranoside)-6'-palmitate), **12** ( $5\alpha$ ,  $8\alpha$ -epi-dioxyergosta-6, 22-dien-3 $\beta$ -ol), and **13** (oleanolic acid).



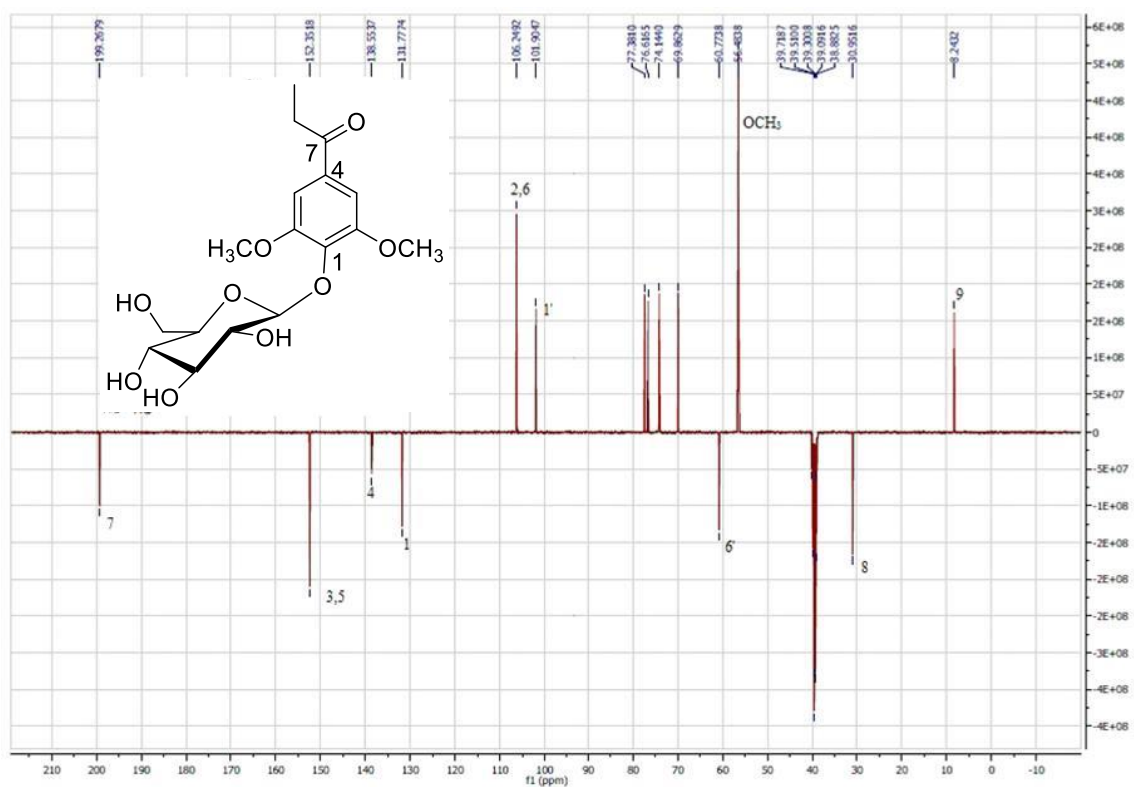
**Figure S3:** Scheme for chromatographic fractionation of the methylene chloride extract



**Figure S4:** Scheme for chromatographic separation of compounds **1**(propiosyringone- $\beta$ -D-glucopyranoside), **3** (ceplignan), **6** (syringaresinol), **7** (protocatechuic aldehyde ), **8** (3-methyl thio-indole) and **14** (9, 12, 13-trihydroxy-10-octadecenoic acid).

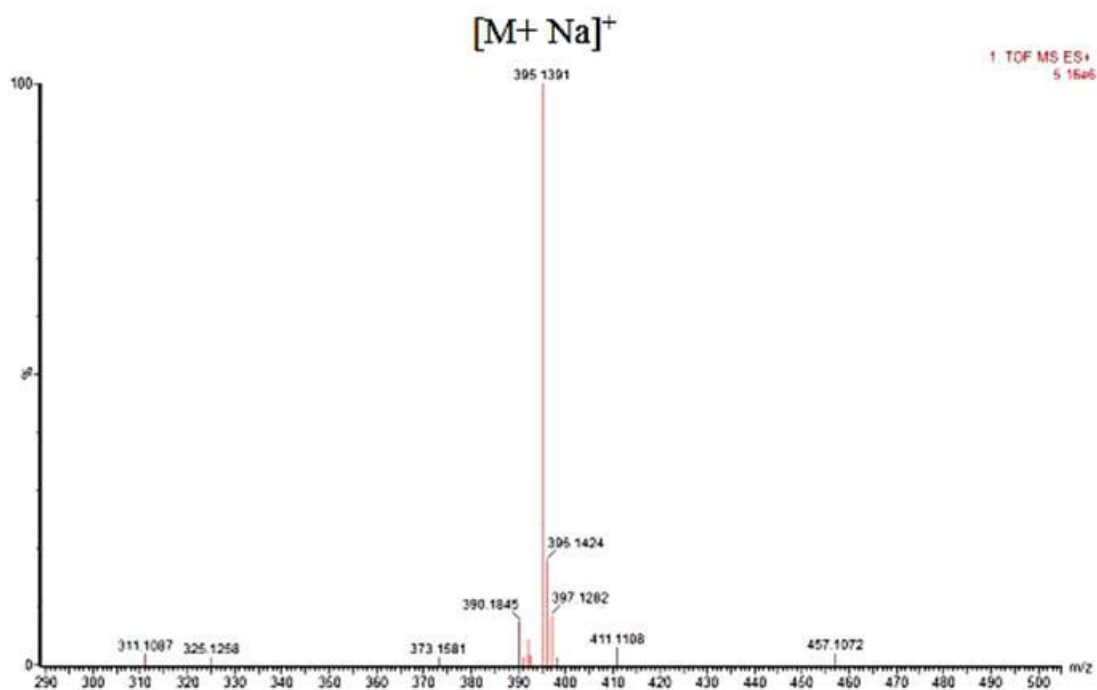


**Figure S5:** <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of **1** (propiosyringone-β-D-glucopyranoside)

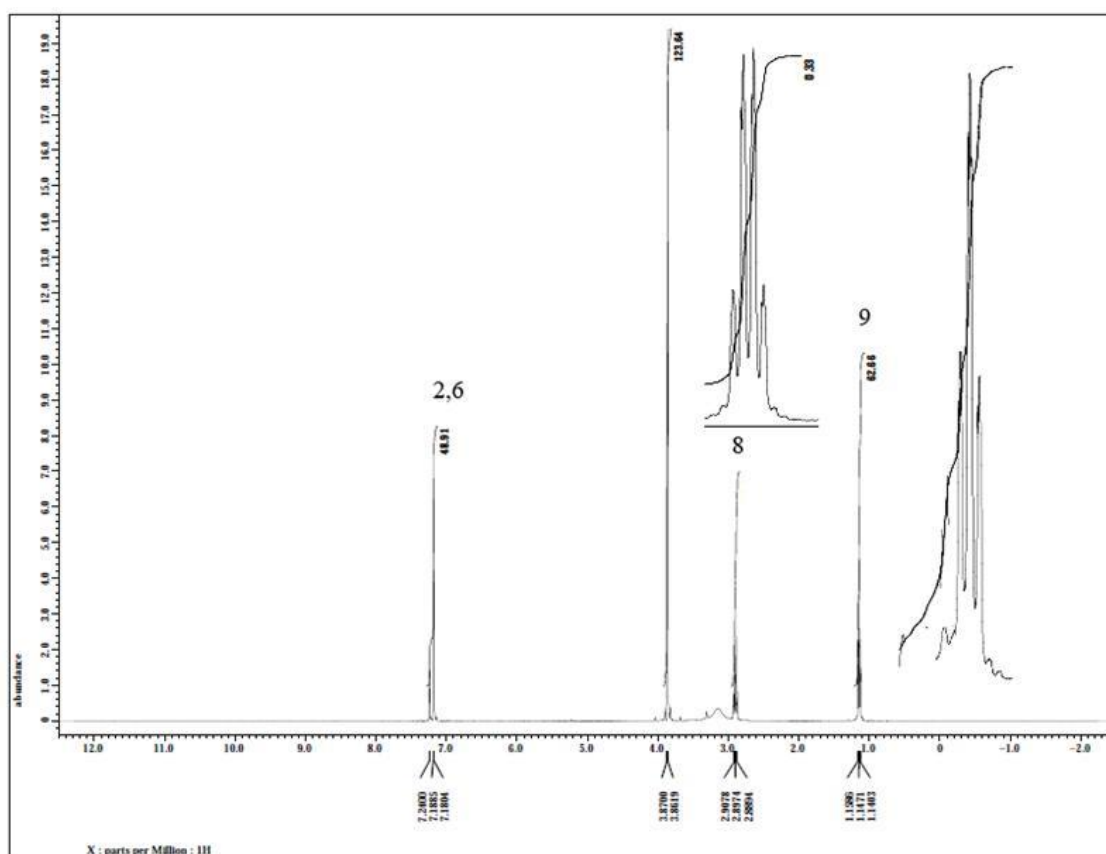


**Figure S6:** APT (100 MHz, DMSO-*d*<sub>6</sub>) spectrum of **1** (propiosyringone-β-D-glucopyranoside)

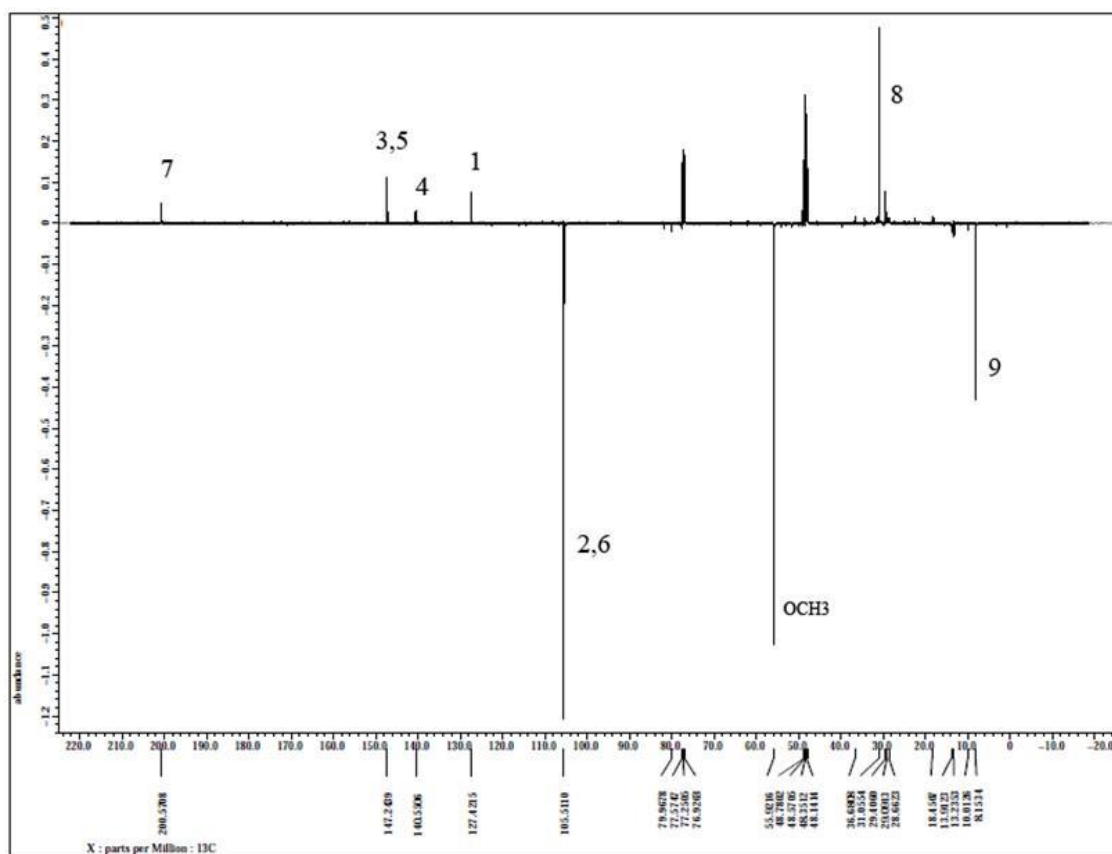




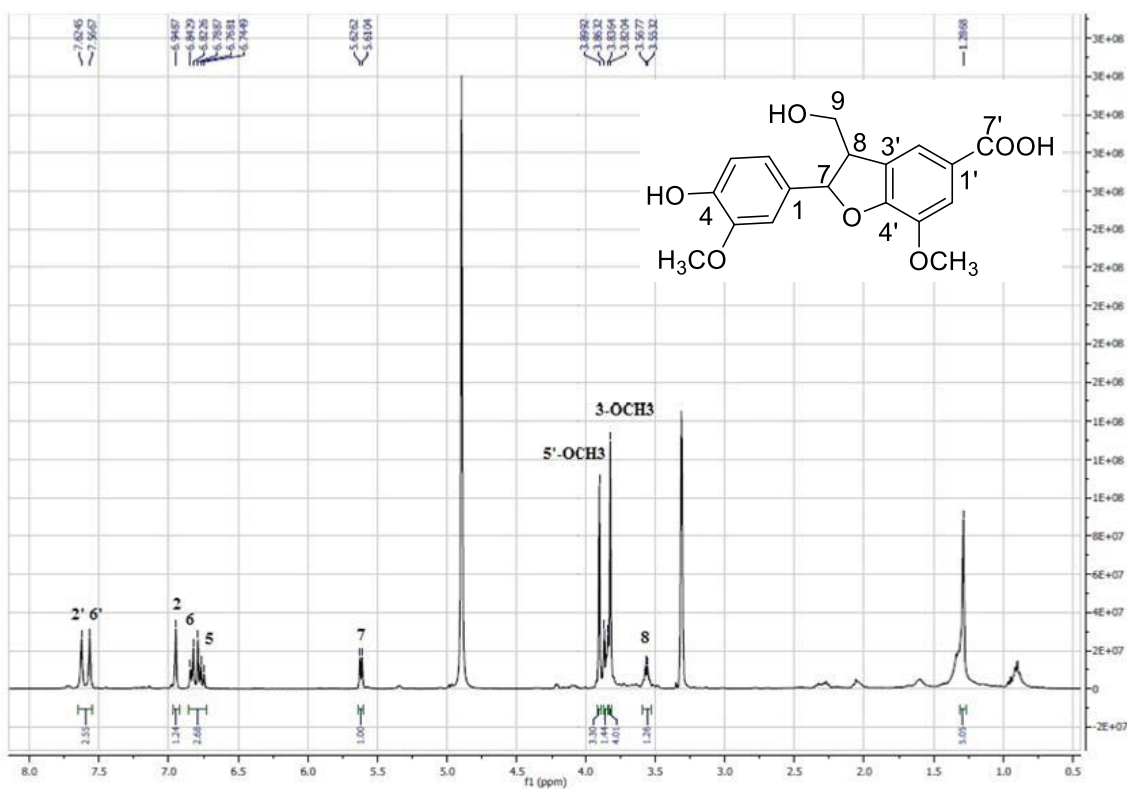
**Figure S7:** Positive ESI/TOF-MS spectrum of **1** (propiosyringone- $\beta$ -D-glucoopyranoside)



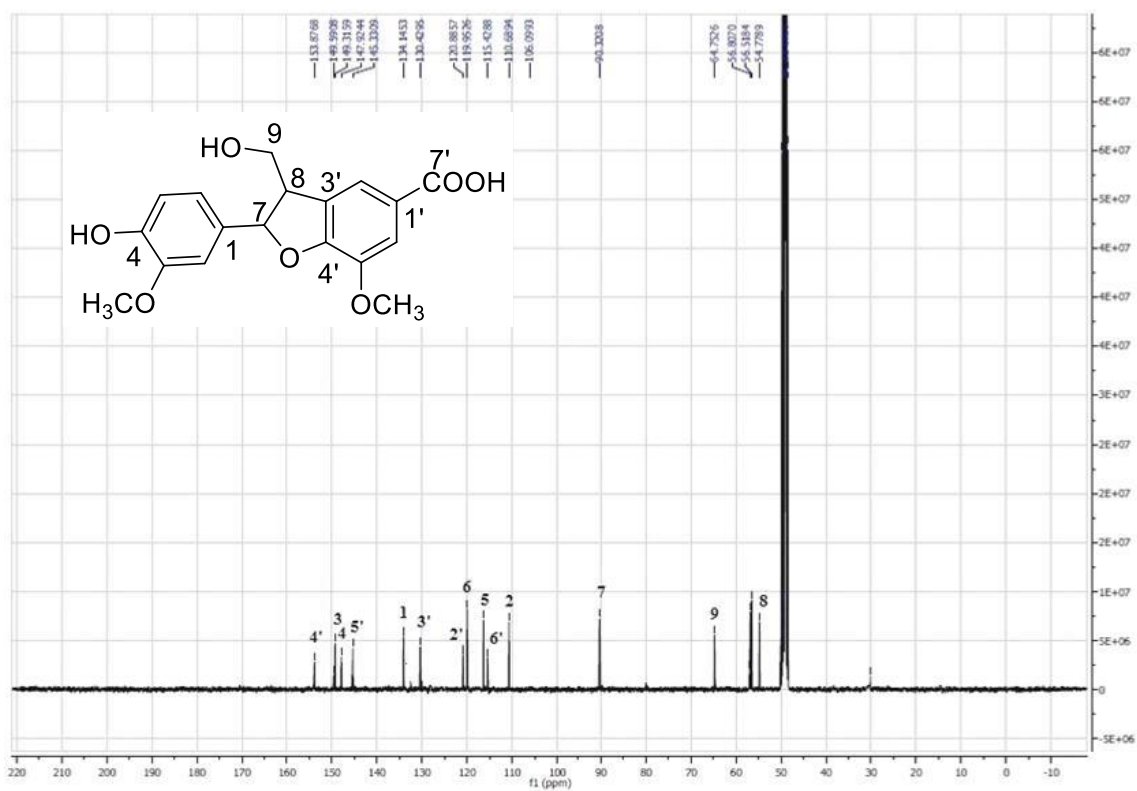
**Figure S8:**  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectrum of **2** (propiosyringone)



**Figure S9:** APT (100 MHz, CDCl<sub>3</sub>) spectrum of **2** (propiosyringone)



**Figure S10:**  $^1\text{H-NMR}$  (400 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of **3** (ceplignan)



**Figure S11:** <sup>13</sup>C-NMR (100 MHz, CD<sub>3</sub>OD) spectrum of **3** (ceplignan)

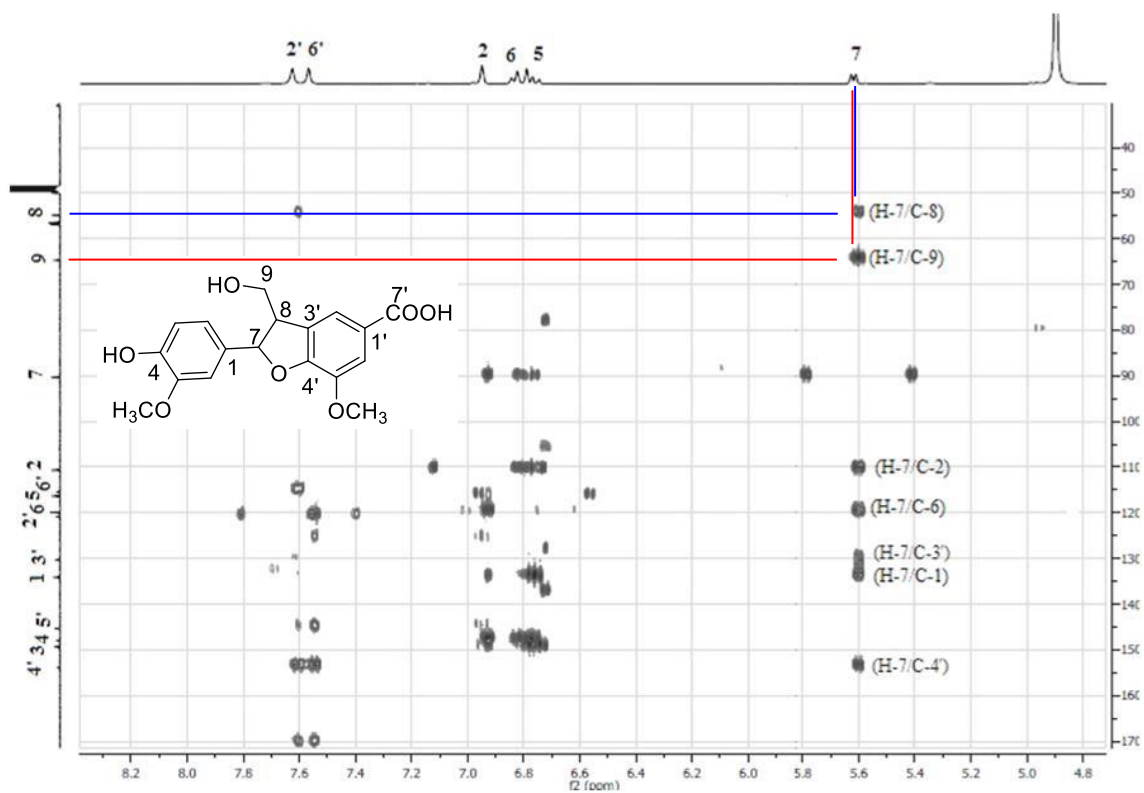
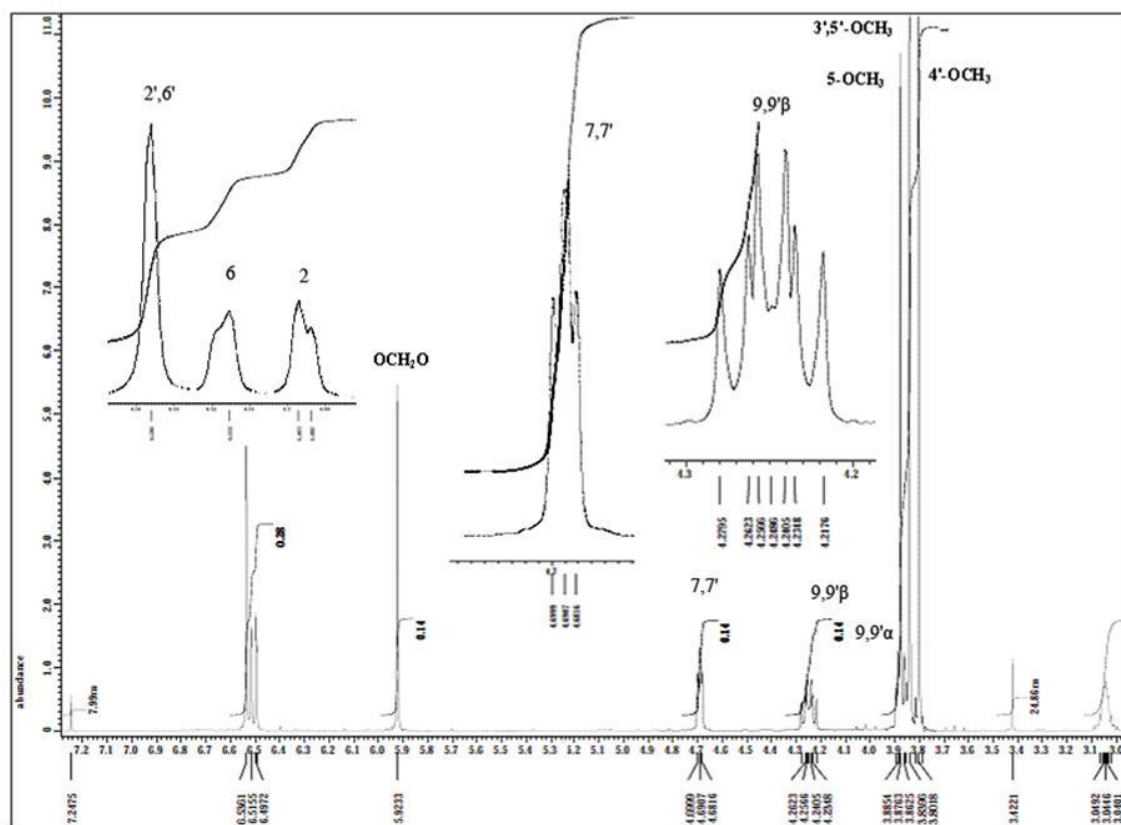


Figure S12: HMBC spectrum of **3** (ceplignan)



**Figure S13:**  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectrum of **4** (sesartemin)

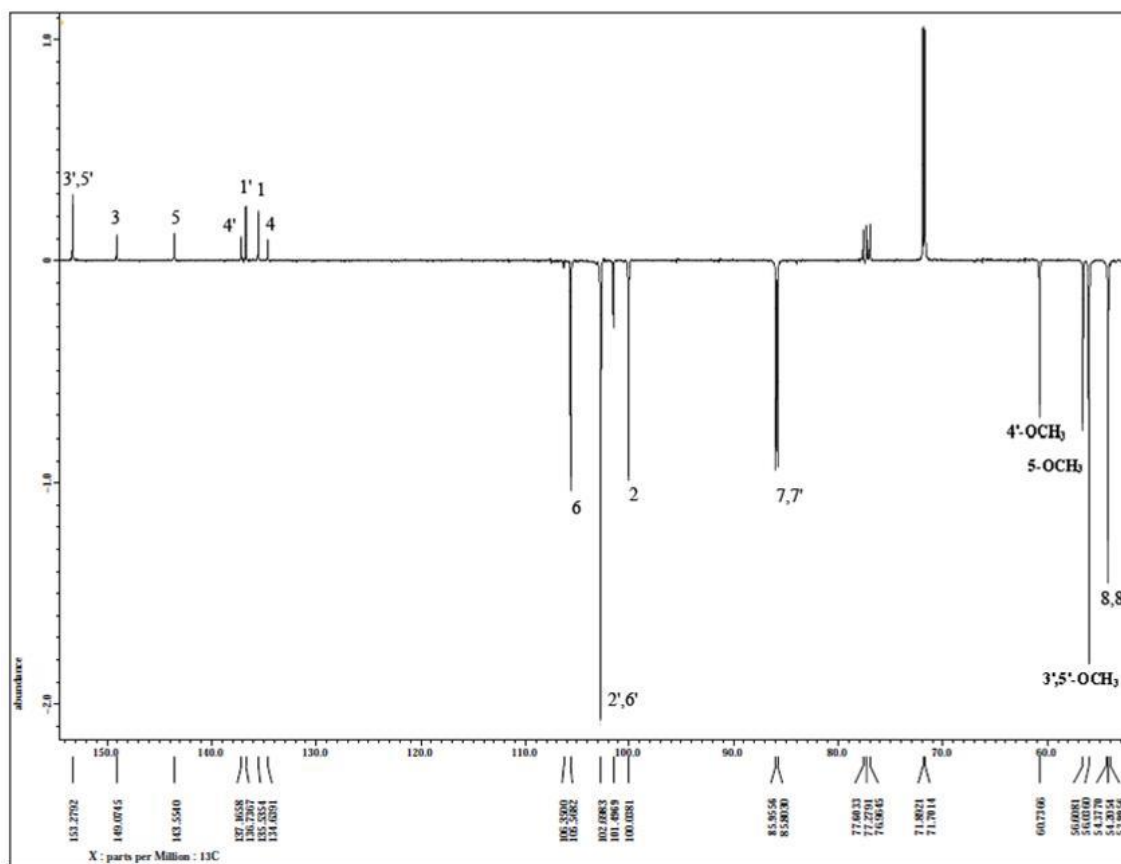
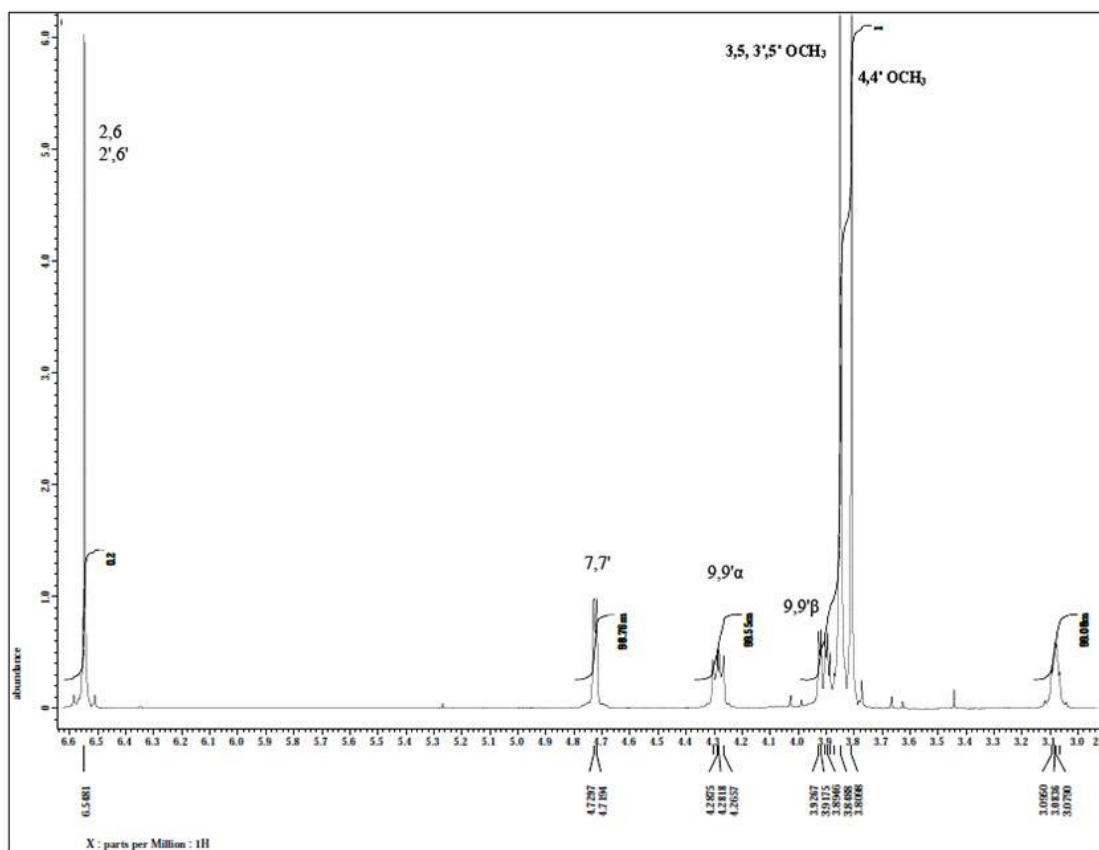
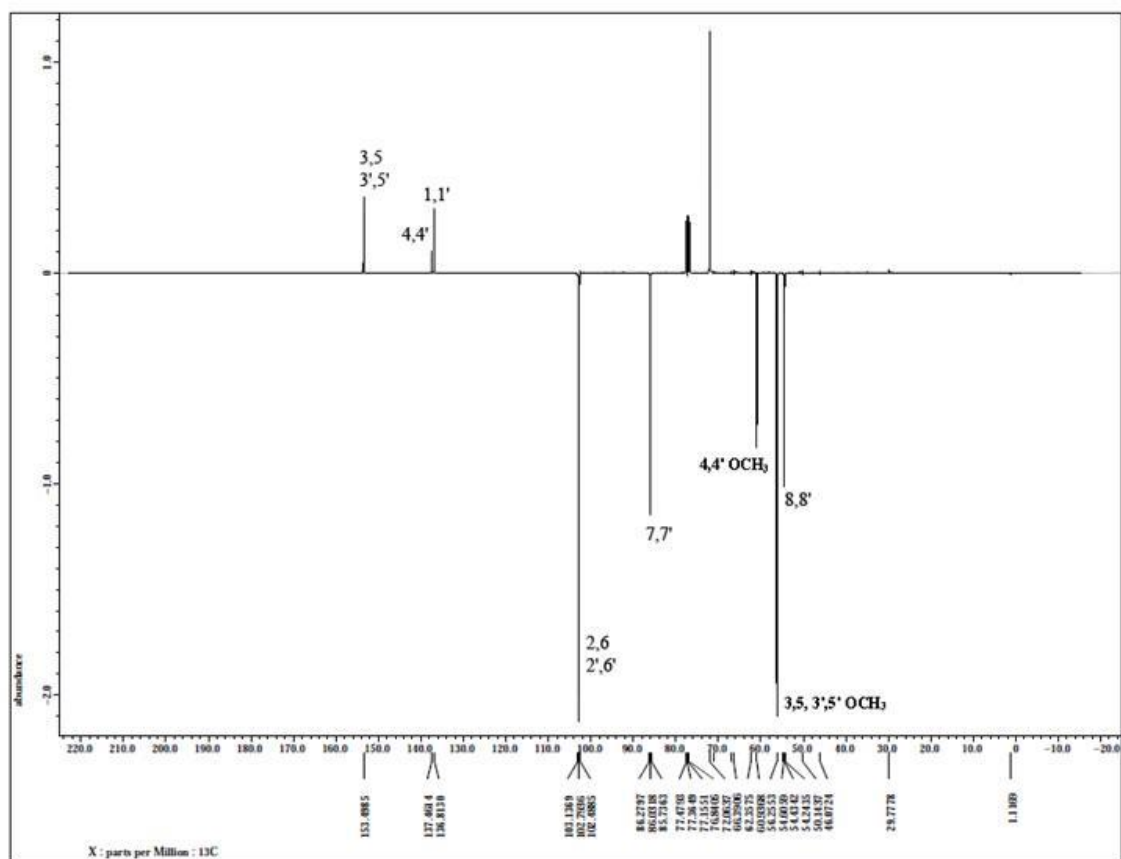


Figure S14:APT (100 MHz, CDCl<sub>3</sub>) spectrum of **4** (sesartemin)

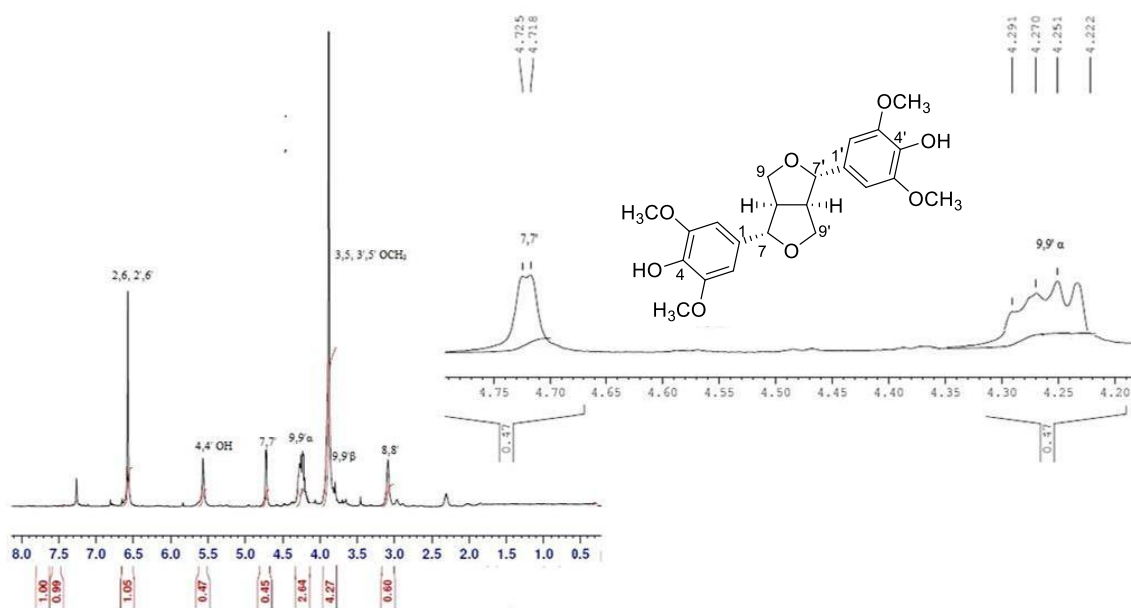




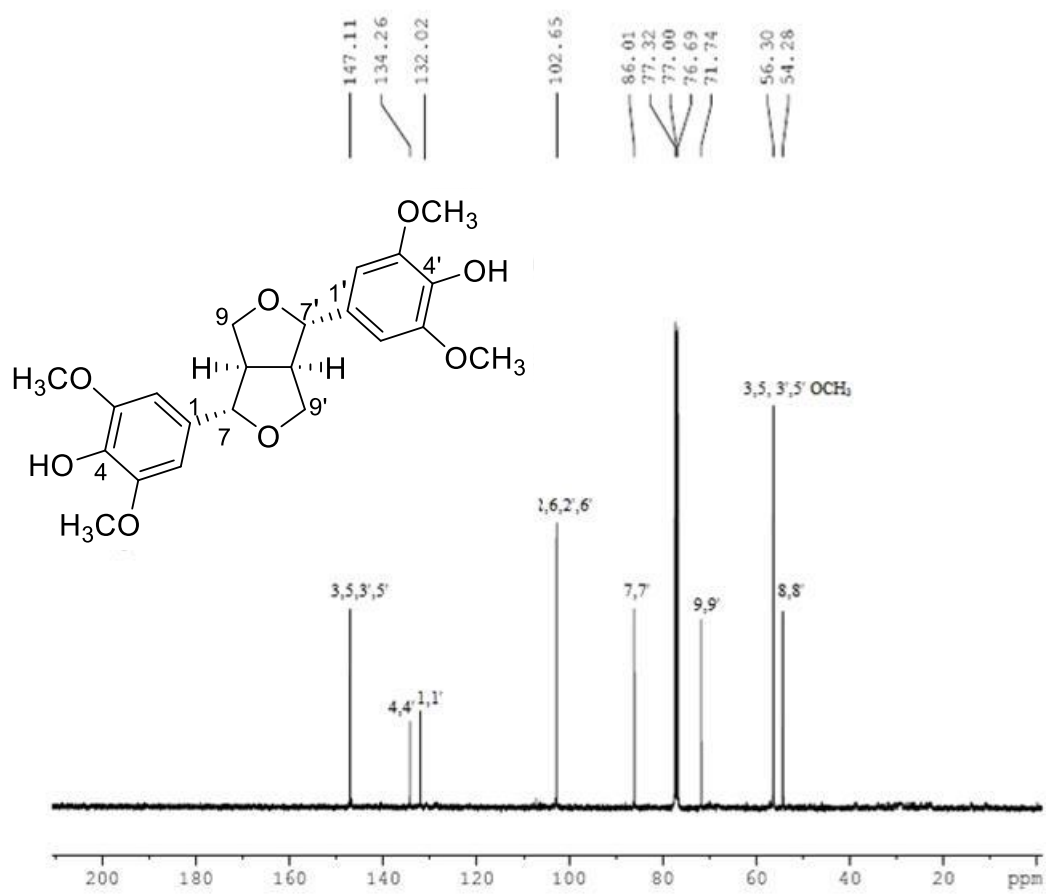
**Figure S15:**  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectrum of **5** (yangambin)



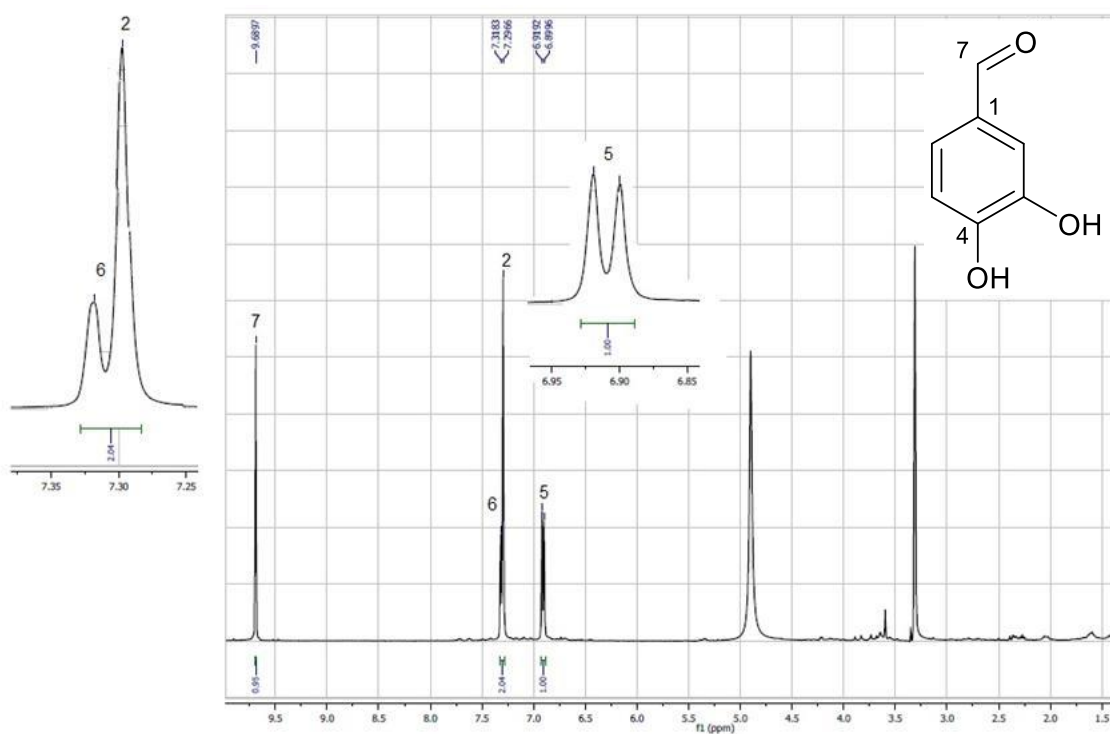
**Figure S16:** APT (100 MHz,  $\text{CDCl}_3$ ) spectrum of **5** (yangambin)



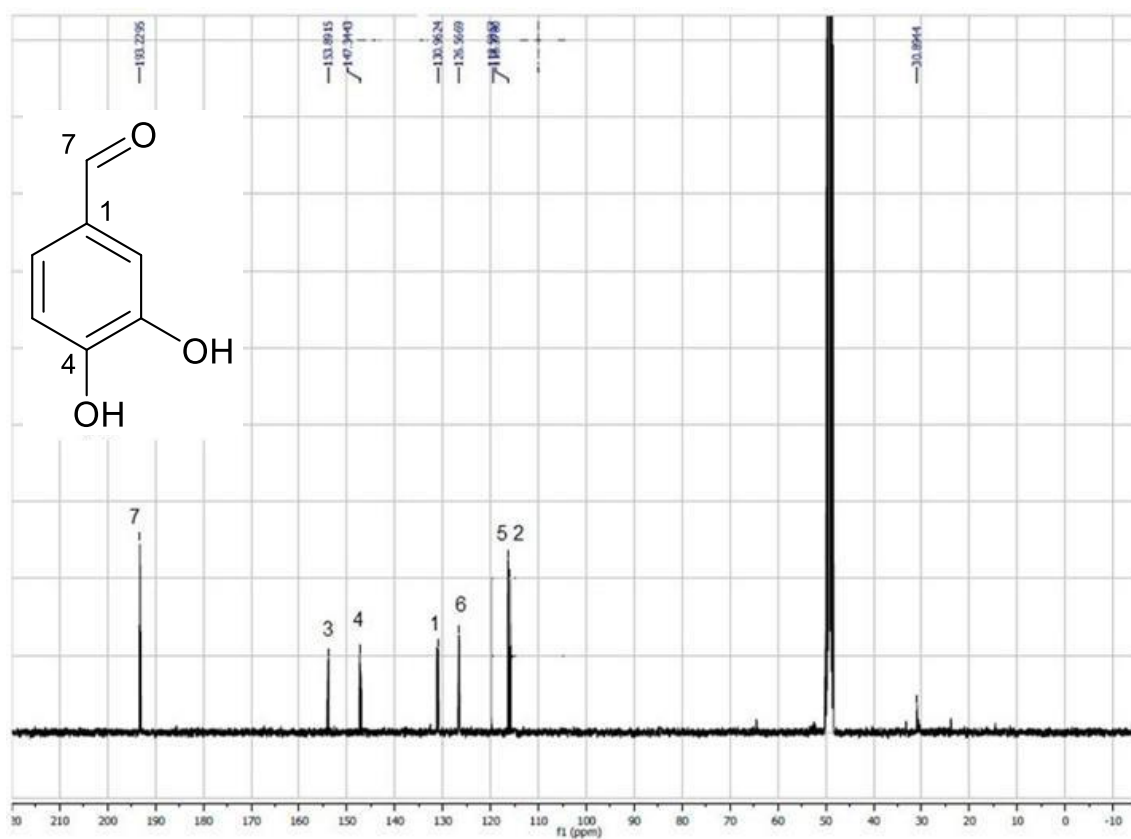
**Figure S17:** <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) spectrum of **6** (syringaresinol)



**Figure S18:** <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) spectrum of **6** (syringaresinol)



**Figure S19:** <sup>1</sup>H-NMR (400 MHz, CD<sub>3</sub>OD) spectrum of **7** (protocatechuic aldehyde)



**Figure S20:**  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of **7** (protocatechuic aldehyde)

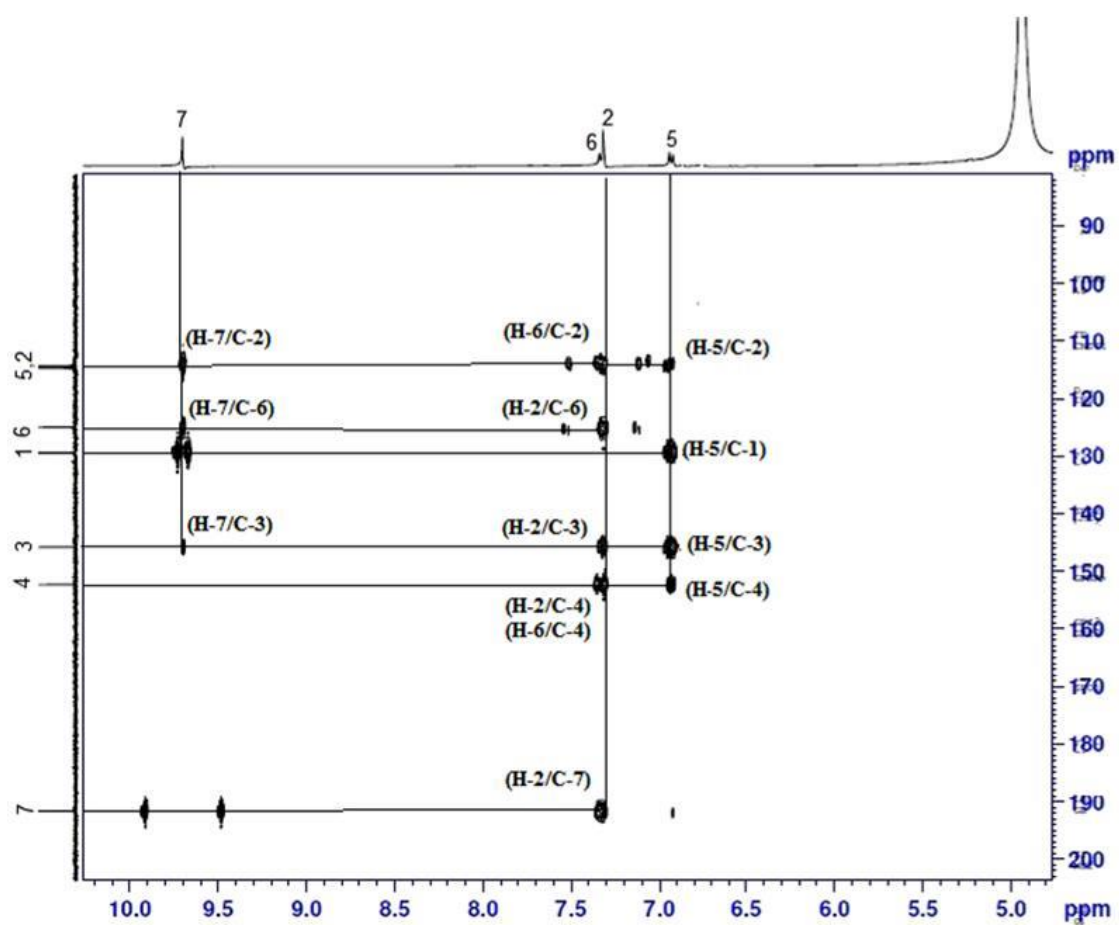
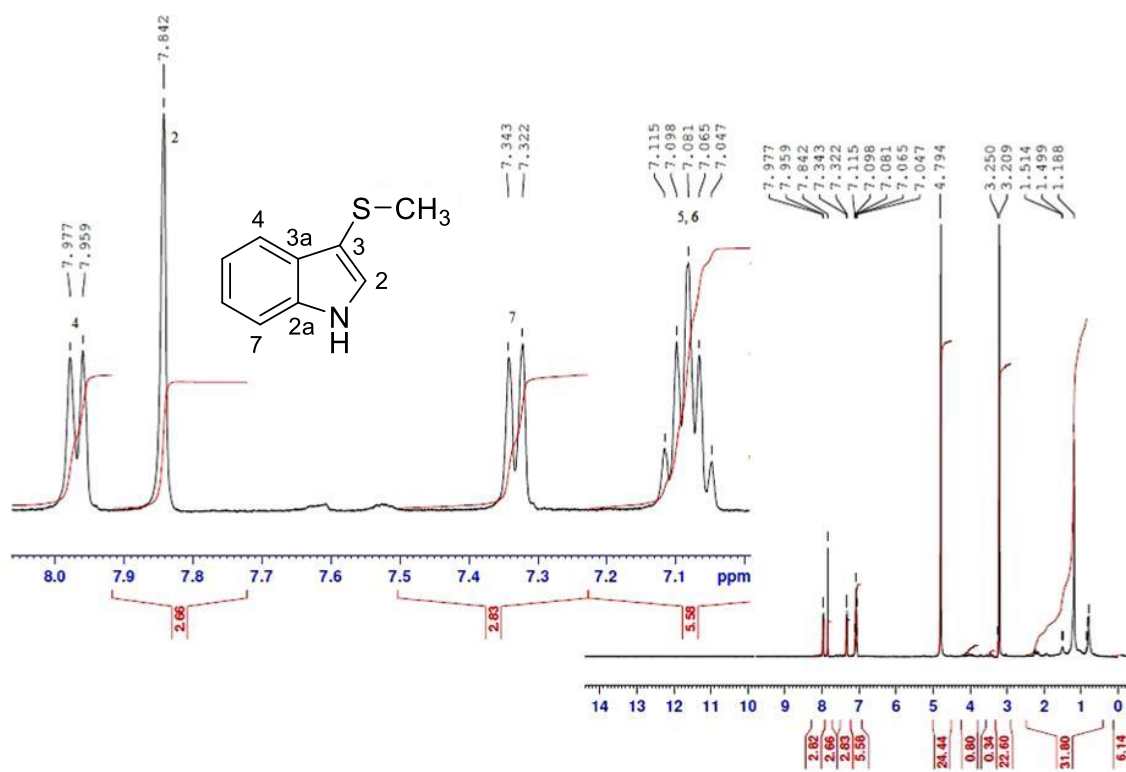
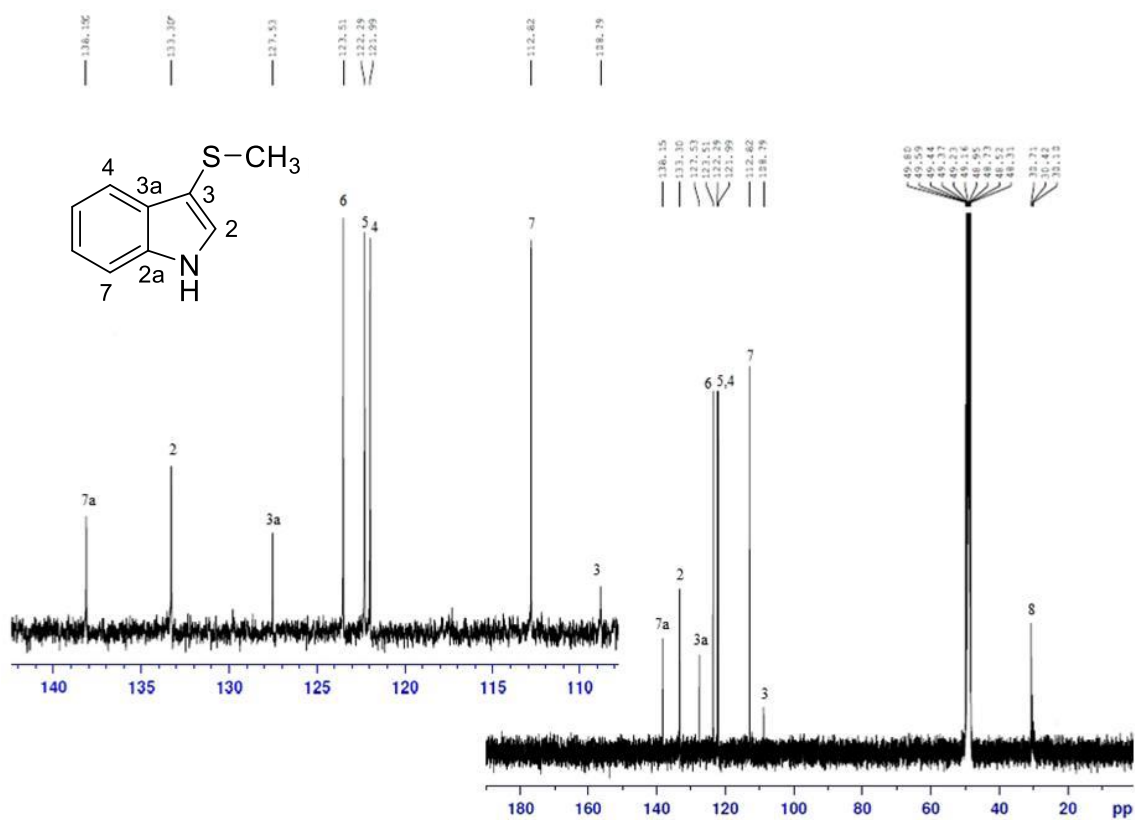


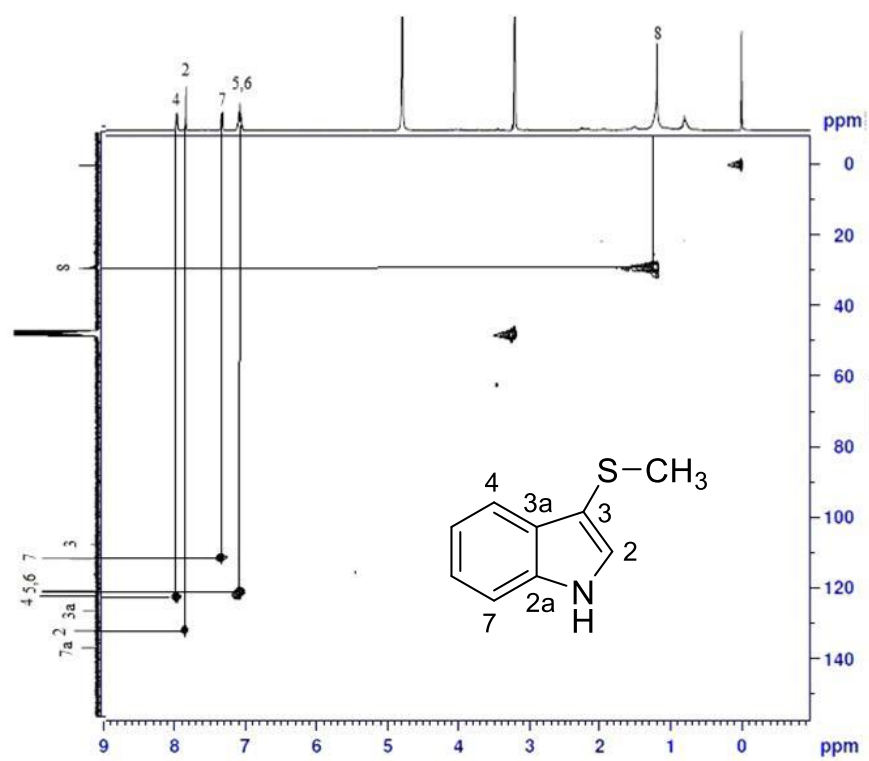
Figure S21: HMBC spectrum of 7 (protocatechuic aldehyde)



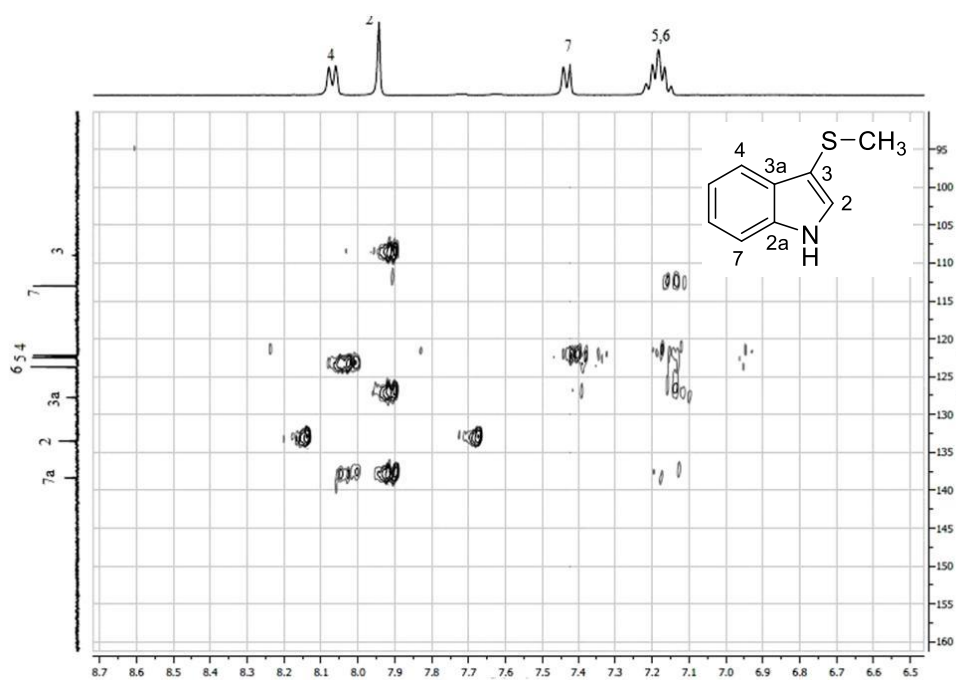
**Figure S22:** <sup>1</sup>H-NMR (400 MHz, CD<sub>3</sub>OD) spectrum of **8** (3-methyl thio-indole)



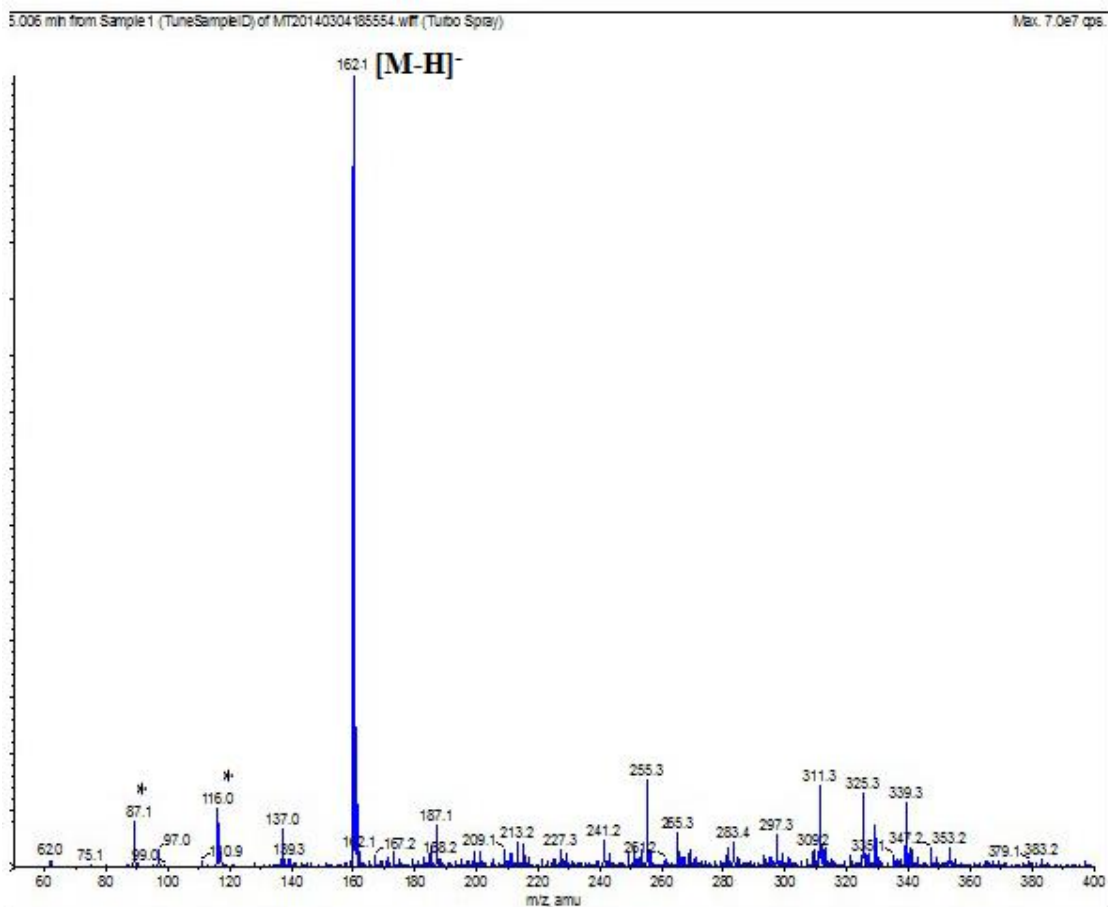




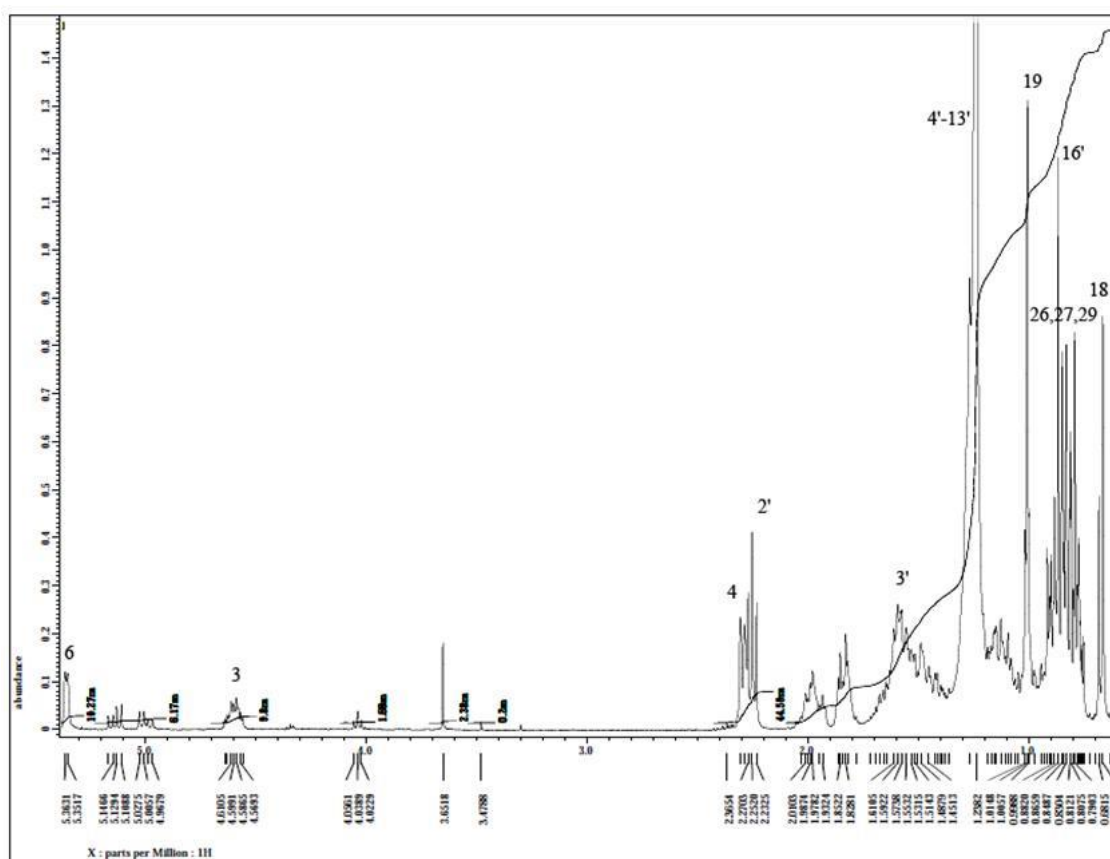
**Figure S24:** HSQC spectrum of **8** (3-methyl thio-indole)



**Figure S25:** HMBC spectrum of **8** (3-methyl thio-indole)



**Figure S26:** Negative ESI/EMS spectrum of **8** (3-methyl thio-indole)



**Figure S27:** <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) spectrum of **9** (β-sitosteryl palmitate)

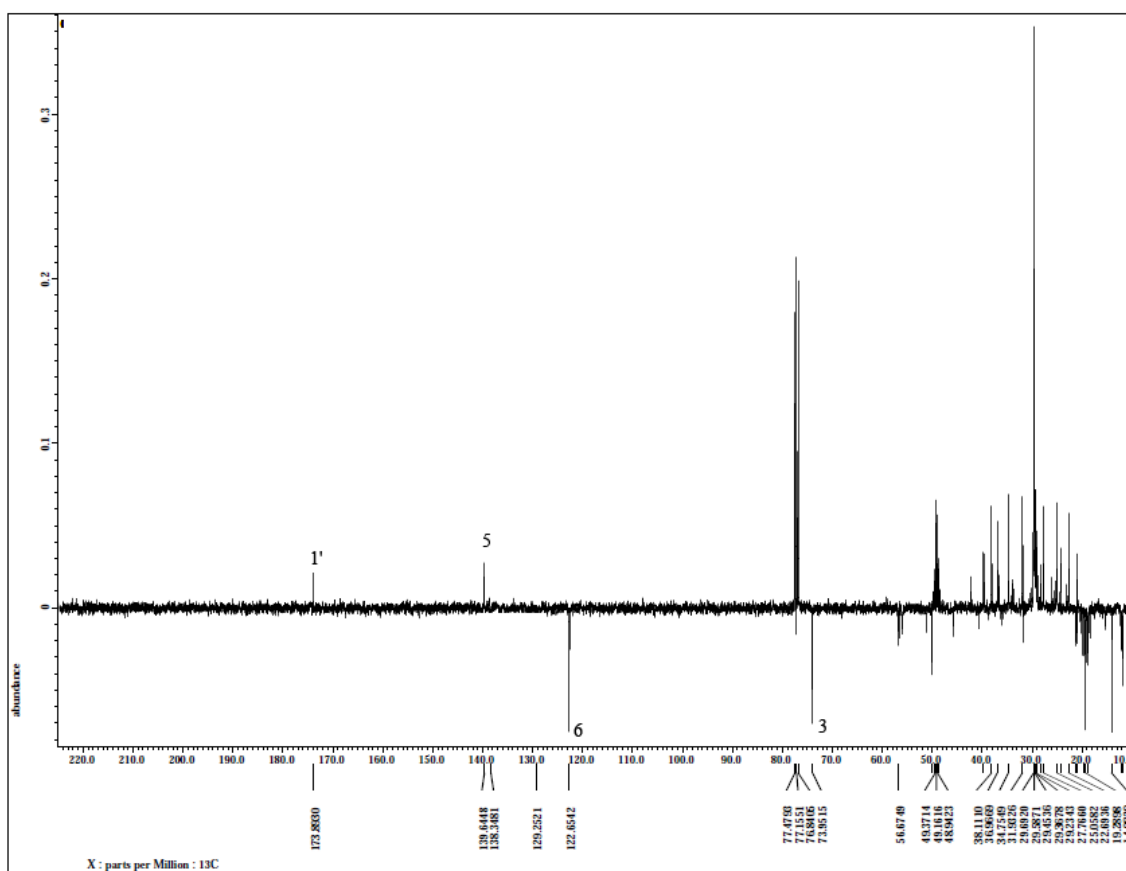
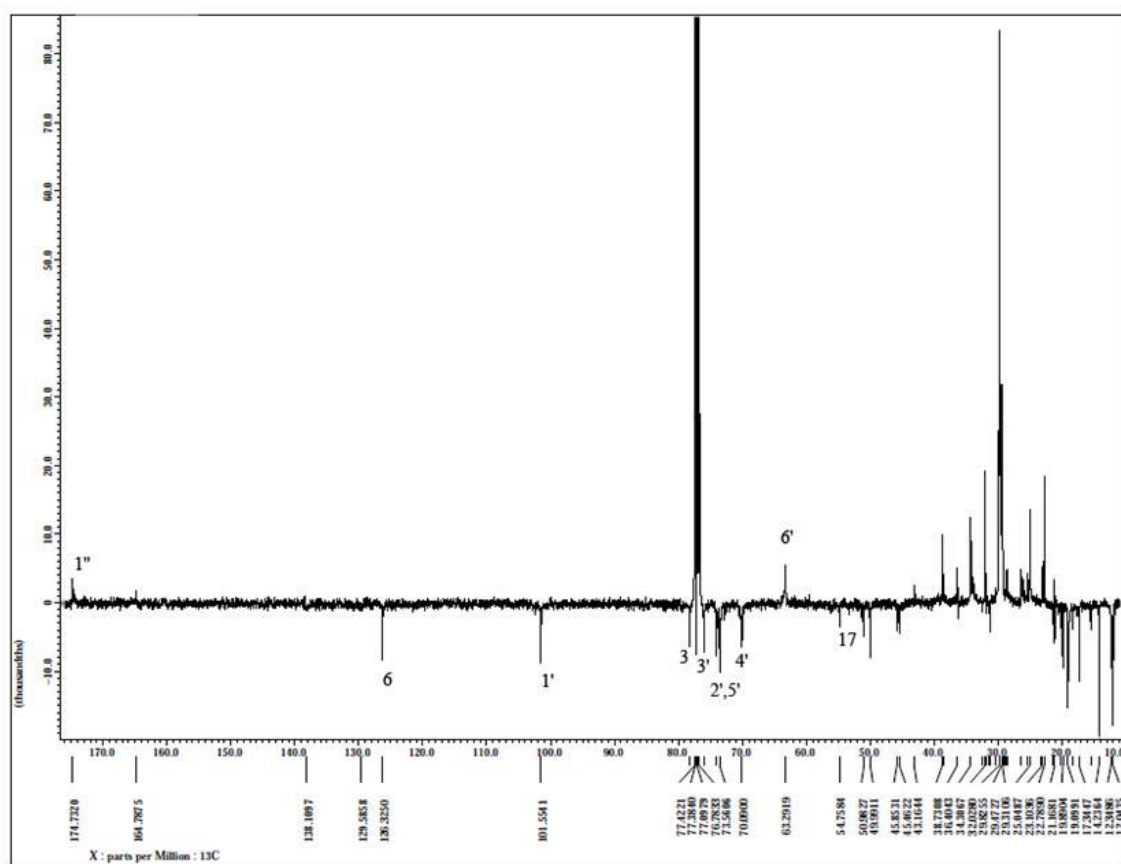


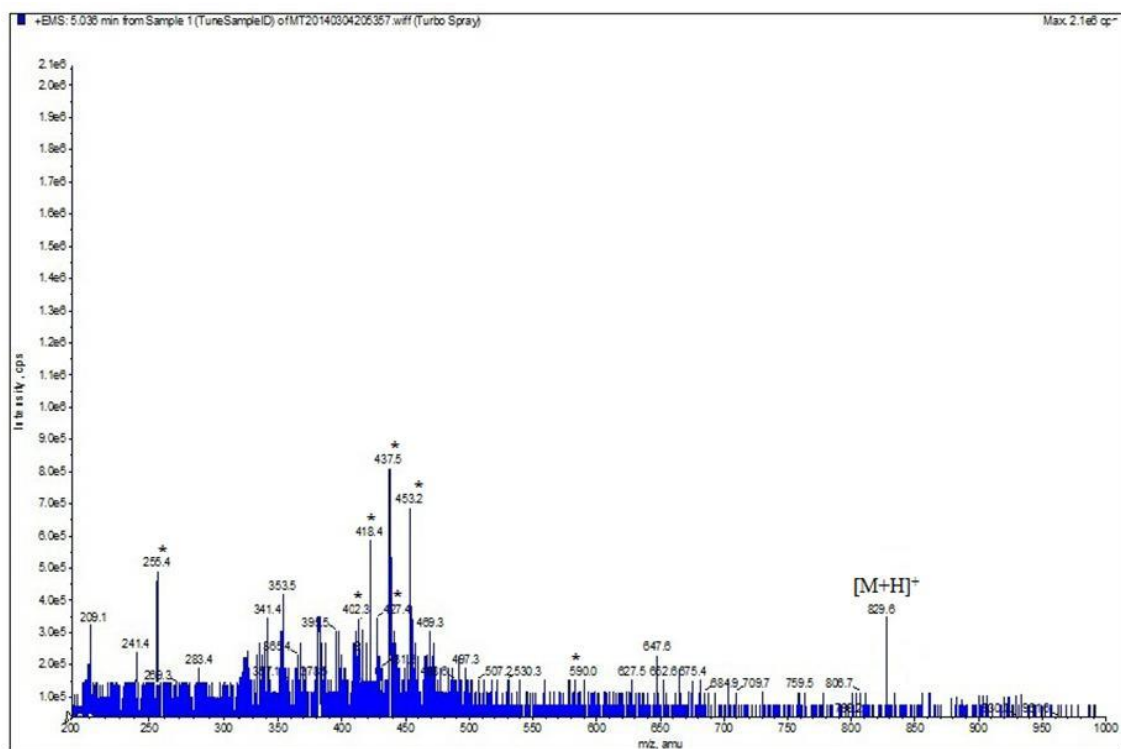
Figure S28: APT (100 MHz, CDCl<sub>3</sub>) spectrum of **9** ( $\beta$ -sitosteryl palmitate)



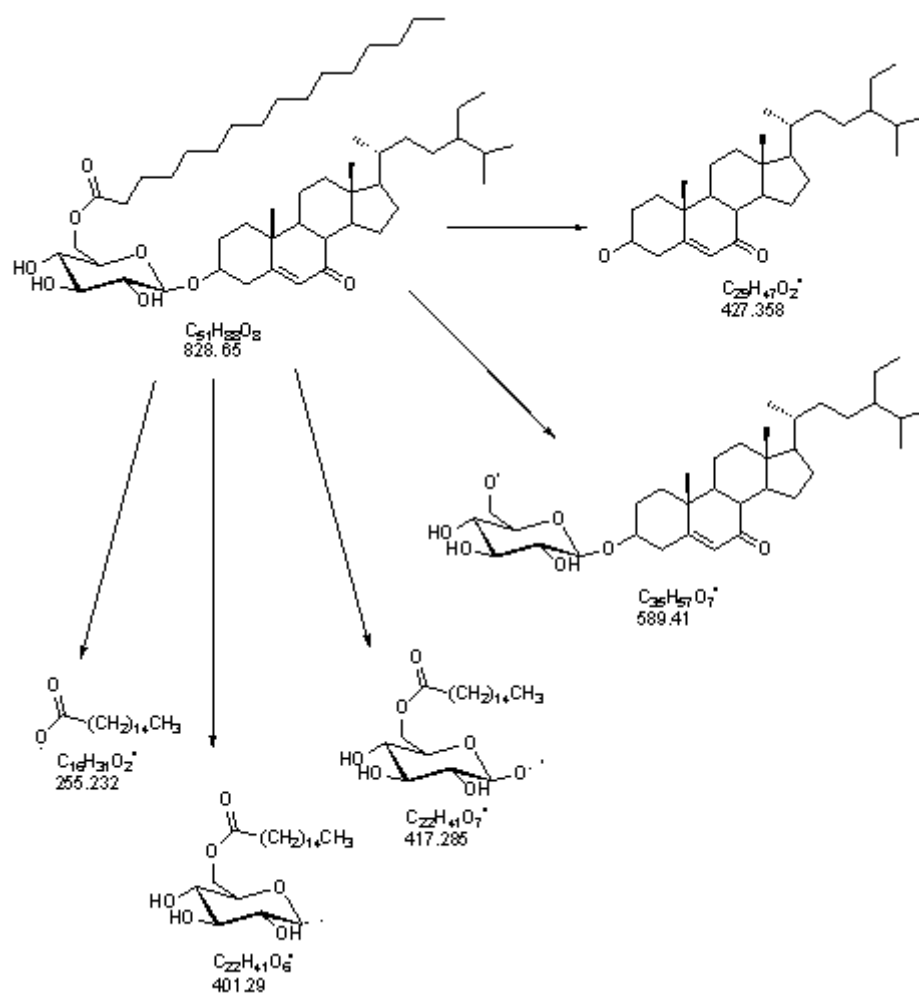


**Figure S30:** APT (100 MHz, CDCl<sub>3</sub>) spectrum of **11** (7-oxo- β-sitosterol-3-O-β-D-glucopyranoside)-6'-palmitate)

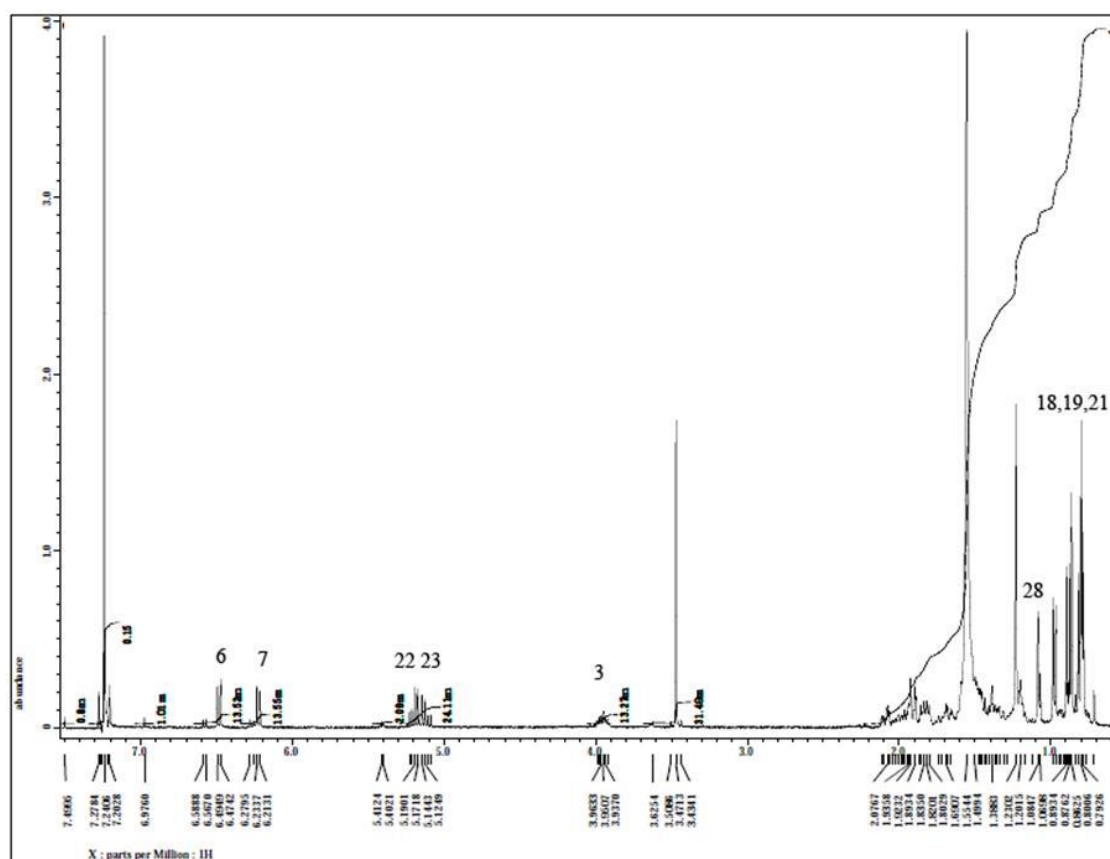




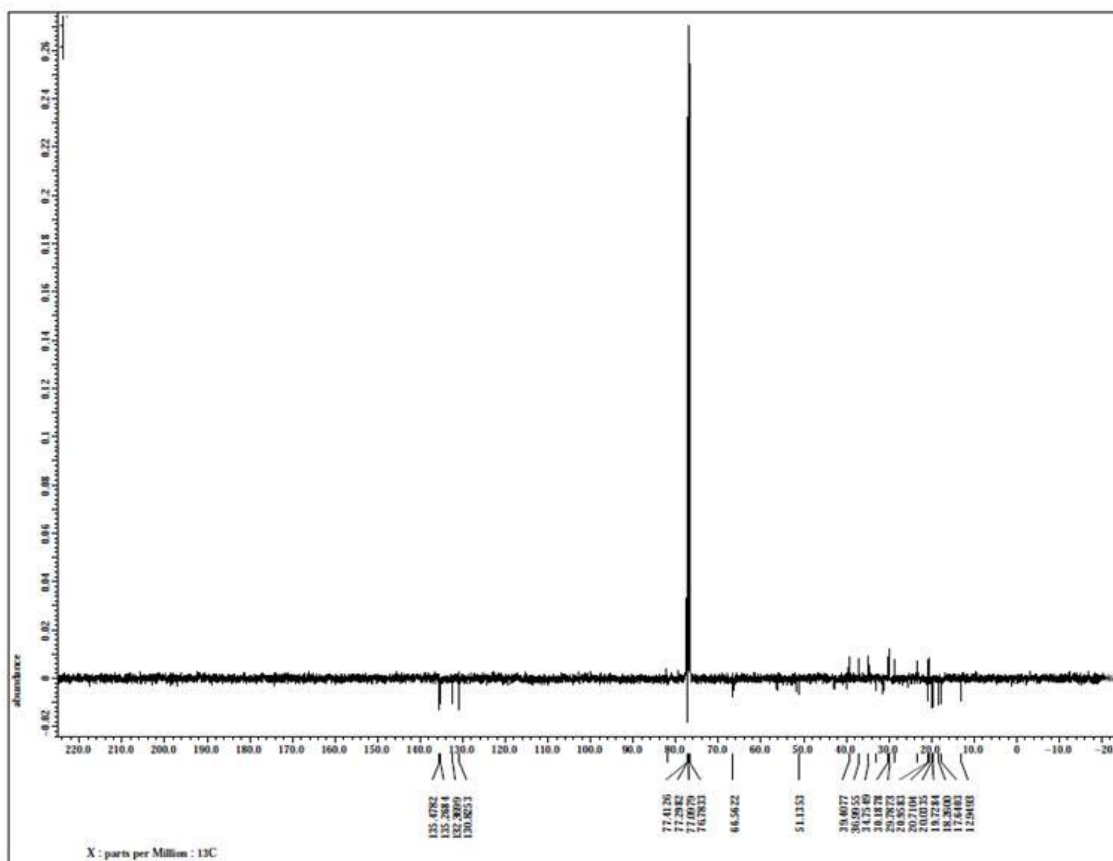
**Figure S31:** Positive ESI/EMS spectrum of **11** (7-oxo-  $\beta$ -sitosterol-3-O- $\beta$ -D-glucopyranoside)-6'-palmitate)



**Figure S32:** Some possible fragmentation patterns of **11** (7-oxo-β-sitosterol-3-O-β-D-glucopyranoside)-6'-palmitate)



**Figure S33:**  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ ) spectrum of **12** ( $5\alpha$ ,  $8\alpha$ -epi-dioxyergosta-6, 22-dien- $3\beta$ -ol)



**Figure S34:** APT (100 MHz, CDCl<sub>3</sub>) spectrum of **12** (5 $\alpha$ , 8 $\alpha$ -epi-dioxyergosta-6, 22-dien-3 $\beta$ -ol)

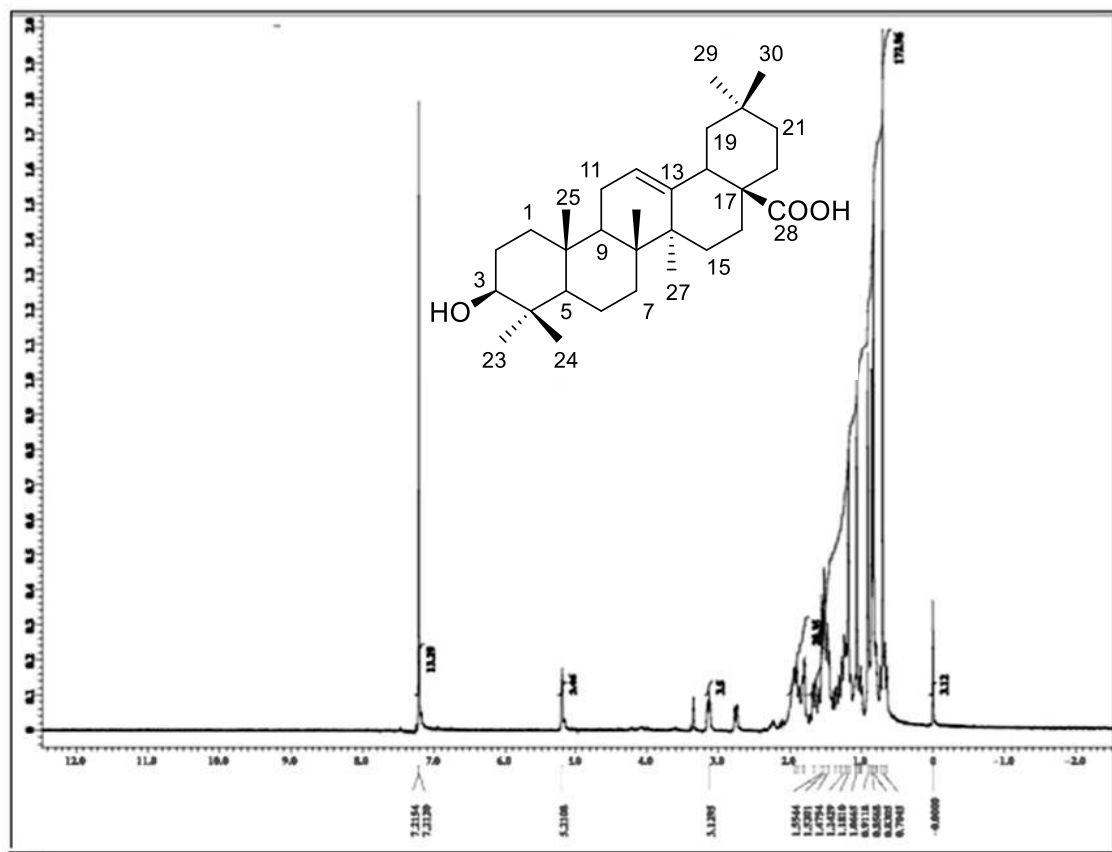


Figure S35: <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) spectrum of **13** (oleanolic acid)

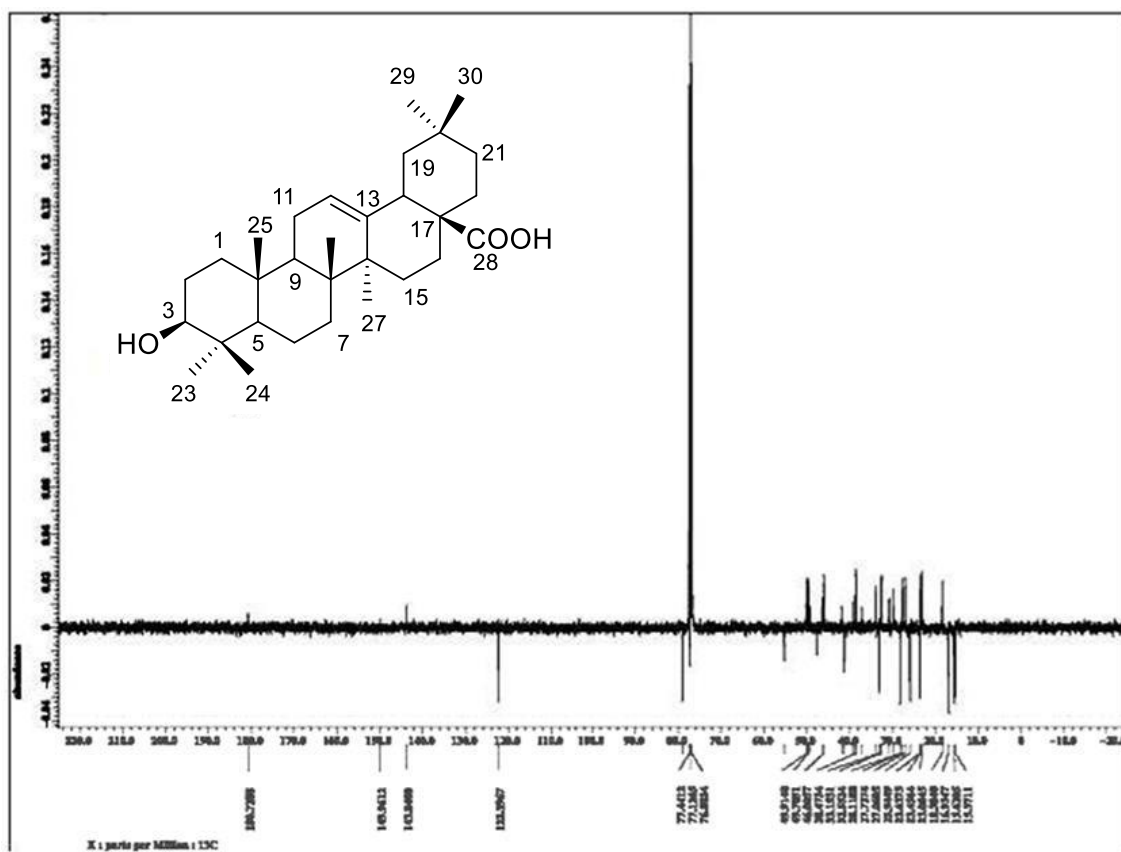
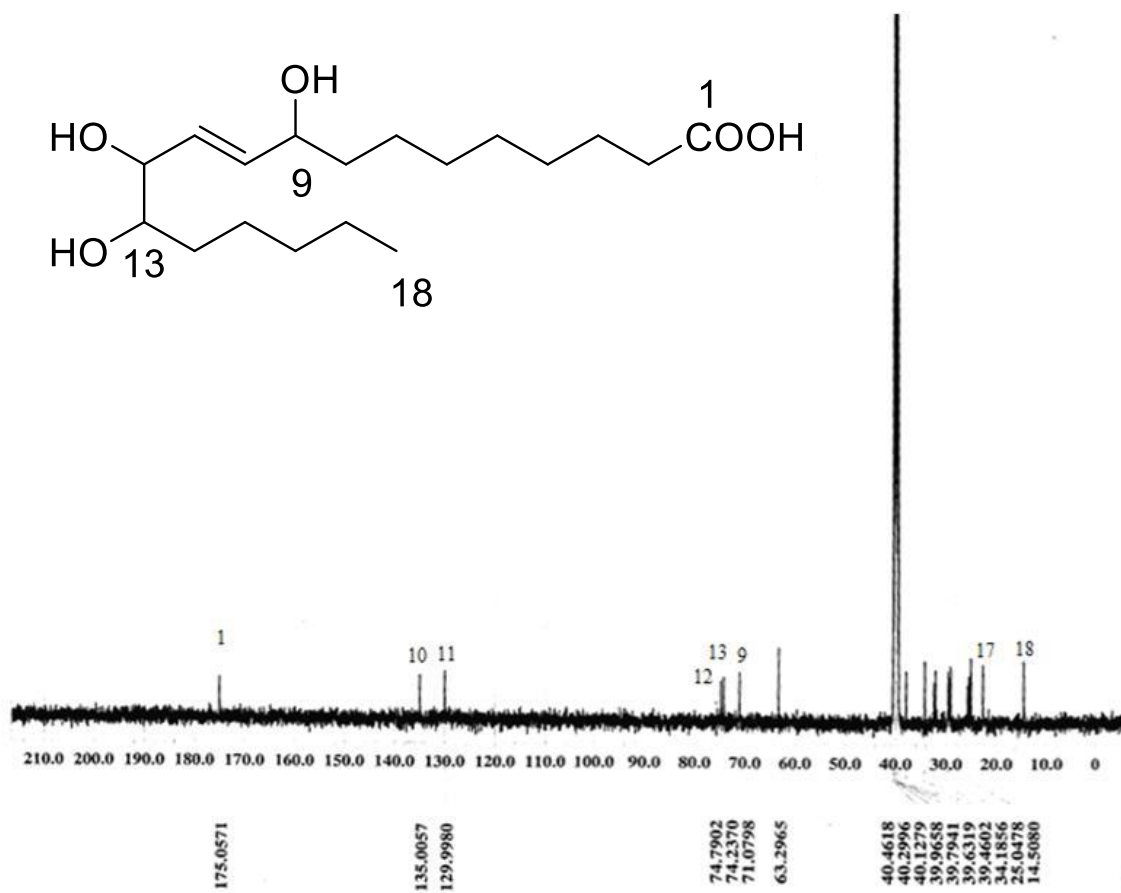


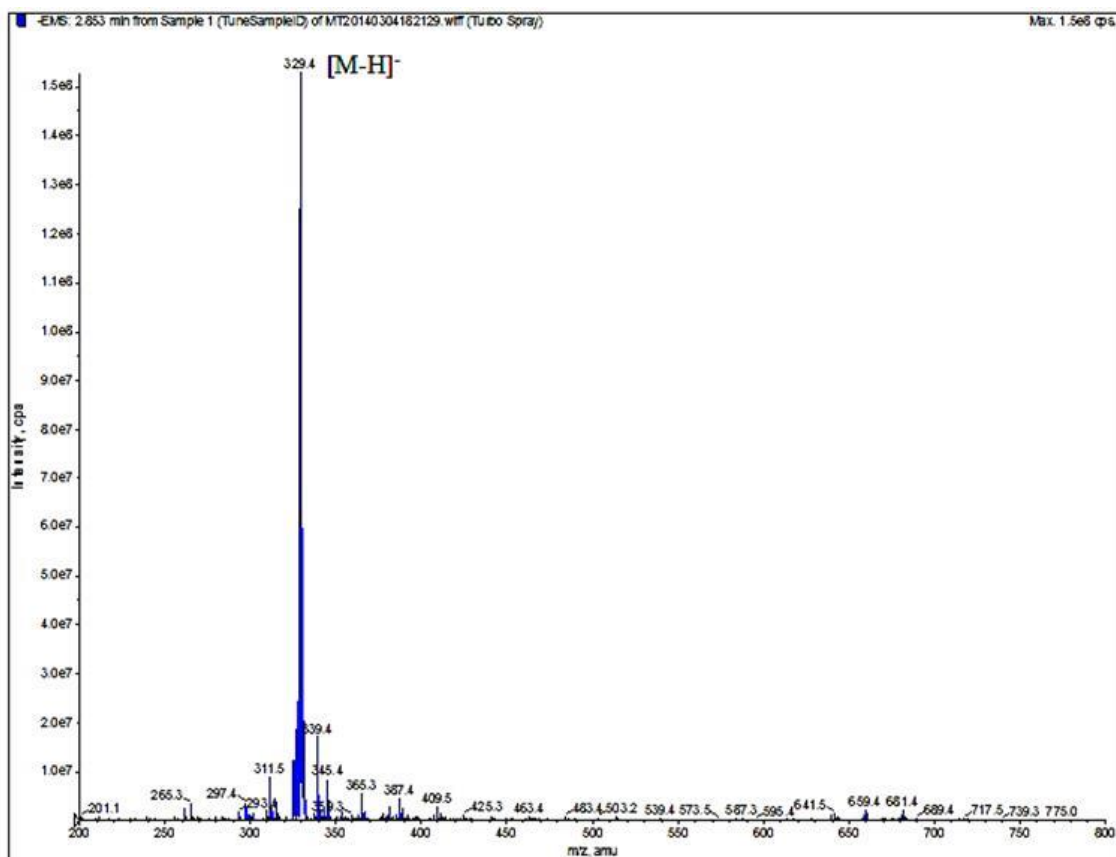
Figure S36: APT (100 MHz,  $\text{CDCl}_3$ ) spectrum of **13** (oleanolic acid)





**Figure S38:** APT (125 MHz, DMSO- $d_6$ ) spectrum of **14** (9, 12, 13-trihydroxy-10-octadecenoic acid)





**Figure S39:** Negative ESI/EMS spectrum of **14** (9, 12, 13-trihydroxy-10-octadecenoic acid)

**Table S1:** <sup>1</sup>H-NMR and APT spectral data of **1** (propiosyringone-β-D-glucopyranoside), **2** (propiosyringone) and **3** (ceplignan).

#	<b>1</b>		<b>2</b>		<b>3</b>	
	<sup>1</sup> H-NMR (400 MHz, DMSO- <i>d</i> <sub>6</sub> )	APT (100 MHz, DMSO- <i>d</i> <sub>6</sub> )	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> )	APT (100 MHz, CDCl <sub>3</sub> )	<sup>1</sup> H-NMR (400 MHz, CD <sub>3</sub> OD)	<sup>13</sup> C-NMR (100 MHz, CD <sub>3</sub> OD)
<b>1</b>		131.7	--	128.1	--	134.1
<b>2</b>	7.25 ( <i>s</i> , 2H)	106.2	7.18 (2H, <i>s</i> )	105.5	6.94 (H, br. <i>s</i> )	110.6
<b>3</b>	--	152.3	--	147.0	--	149.3
<b>4</b>	--	138.5	--	139.9	--	147.9
<b>5</b>	--	152.3	--	147.0	6.77 (H, <i>d</i> , <i>J</i> =8.2)	116.3
<b>6</b>	7.25 ( <i>s</i> , 2H)	106.2	7.18 (2H, <i>s</i> )	105.5	6.83 (H, <i>d</i> , <i>J</i> =8.1)	119.9
<b>7</b>	--	199.2	--	200.0	5.4 (H, <i>d</i> , <i>J</i> =6.3)	90.3
<b>8</b>	7.25 ( <i>s</i> , 2H)	30.9	2.89 (2H, <i>q</i> )	31.3	3.55 (H, <i>d</i> , <i>J</i> =5.8)	54.7
<b>9</b>	1.07 (3H, <i>t</i> )	8.2	1.14 (3H, <i>t</i> )	8.5	3.86 (9a), 3.83 (9b)	64.7
<b>OCH<sub>3</sub></b>	3.79 (6H, <i>s</i> )	56.9	3.86 (6H, <i>s</i> )	56.4	3.82 (3H, <i>s</i> )	56.5
<b>1'</b>	5.07 (H, <i>d</i> , <i>J</i> =7.6)	101.9	--	--	--	**
<b>2'</b>	3.00-3.59	74.1	--	--	7.62 (H, br. <i>s</i> )	120.8
<b>3'</b>	3.00-3.59	76.6	--	--	--	130.4
<b>4'</b>	3.00-3.59	69.8	--	--	--	153.8.
<b>5'</b>	3.00-3.59	77.3	--	--	--	145.3
<b>6'</b>	H-6'a* H-6'b* 3.57 (H, <i>dd</i> , <i>J</i> =12.3, 6.25)	60.7	--	--	7.56 (H, br. <i>s</i> )	115.4
<b>7'</b>	--	--	--	--	--	170.1
<b>5'-</b>	--	--	--	--	3.89 (3H, <i>s</i> )	56.8
<b>OCH<sub>3</sub></b>						

The chemical shift ( $\delta$ ) is expressed in ppm and coupling constants (*J*) in Hz

\*H-6'a should appear at  $\delta$  3.84 (Güvenalp and Demirezer, 2005) but it is masked by the (OCH<sub>3</sub>) signal, H-6'b should appear at  $\delta$  4.20 (H, *dd*) [1] instead it appeared at  $\delta$  4.31 (H, *t*).

\*\* Signal didn't appear (should appear at 125.2, [2]).

**Table S2:** <sup>1</sup>H-NMR and APT spectral data of **4** (sesartemin) and **5** (yangambin).

<b>4</b>			<b>5</b>		
#	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> )	APT (100 MHz, CDCl <sub>3</sub> )	#	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> )	APT (100 MHz, CDCl <sub>3</sub> )
<b>1</b>	--	135.5	<b>1,1'</b>	--	136.8
<b>2</b>	6.49 (H, br. <i>s</i> )	100.0	<b>2, 6, 2', 6'</b>	6.45 (4H, <i>s</i> )	102.7
<b>3</b>	--	149.0	<b>3, 5, 3', 5'</b>	--	153.4
<b>4</b>	--	134.6	<b>4,4'</b>	--	137.4
<b>5</b>	--	143.5	<b>7, 7'</b>	4.72 (2H, <i>d</i> )	86.0
<b>6</b>	6.51 (H, br. <i>s</i> )	105.5	<b>8, 8'</b>	3.08 (2H, <i>m</i> )	54.2
<b>7</b>	4.69 (H, <i>d</i> )	85.9	<b>9, 9'</b>	α 4.28 (2H, <i>dd</i> ) β 3.92 (2H, <i>dd</i> )	72.0
<b>8</b>	3.04 (H, <i>m</i> )	54.2	<b>3,5, 3',5'</b> <b>OCH<sub>3</sub></b>	3.84(12H, <i>s</i> )	56.2
<b>9</b>	α 3.86-3.88 (H, <i>dd</i> ) β 4.21-4.27 (H, <i>dd</i> )	71.7	<b>4,4' OCH<sub>3</sub></b>	3.80 (6H, <i>s</i> )	60.9
<b>1'</b>	--	136.7			
<b>2', 6'</b>	6.53 (2H, <i>s</i> )	102.6			
<b>3', 5'</b>	--	153.2			
<b>4'</b>	--	137.1			
<b>7'</b>	4.69 (H, <i>d</i> )	85.8			
<b>8'</b>	3.04 (H, <i>m</i> )	54.2			
<b>9'</b>	α 3.86-3.88 (H, <i>dd</i> ) β 4.21-4.27 (H, <i>dd</i> )	71.8			
<b>OCH<sub>2</sub>O</b>	5.92 (2H, <i>s</i> )	101.4			
<b>5-OCH<sub>3</sub></b>	3.93 (3H, <i>s</i> )	56.6			
<b>4'-OCH<sub>3</sub></b>	3.85 (3H, <i>s</i> )	60.7			
<b>3',5'- OCH<sub>3</sub></b>	3.88 (6H, <i>s</i> )	56.0			

The chemical shift ( $\delta$ ) is expressed in ppm and coupling constants ( $J$ ) in Hz

**Table S3:** <sup>1</sup>H and <sup>13</sup>C-NMR spectral data of **6** (syringaresinol), **7** (protocatechuic aldehyde), and **8** (3-methyl thio-indole).

<b>6</b>			<b>7</b>			<b>8</b>		
#	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> )	<sup>13</sup> C- NMR (100 MHz, CDCl <sub>3</sub> )	#	<sup>1</sup> H-NMR (400 MHz, CD <sub>3</sub> OD)	<sup>13</sup> C-NMR (100 MHz, CD <sub>3</sub> OD)	#	<sup>1</sup> H-NMR (400 MHz, CD <sub>3</sub> OD)	<sup>13</sup> C-NMR (100 MHz, CD <sub>3</sub> OD)
<b>1,1'</b>	--	132.0	<b>1</b>	--	130.9	<b>2</b>	7.84 (H, <i>s</i> )	133.3
<b>2, 6, 2', 6'</b>	6.57 (4H, <i>s</i> )	102.6	<b>2</b>	7.29 (H, <i>s</i> )	115.9	<b>3</b>	--	108.7
<b>3, 5, 3', 5'</b>	--	147.1	<b>3</b>	--	147.3	<b>3a</b>	--	127.5
<b>4,4'</b>	--	134.2	<b>4</b>	--	153.8	<b>4</b>	7.96 (H, <i>d, J=7.3</i> )	121.9
<b>7, 7'</b>	4.72 (2H, <i>d</i> )	86.1	<b>5</b>	6.90 (H, <i>d, J=7.3</i> )	116.3	<b>5</b>	7.08 (2H, <i>dd</i> )	122.2
<b>8, 8'</b>	3.1 (2H, <i>m</i> )	54.2	<b>6</b>	7.30 (H, <i>d, J=8.6</i> )	126.5	<b>6</b>	7.08 (2H, <i>dd</i> )	123.5
<b>9, 9'</b>	α 4.27 (2H, <i>br.</i> ) β 3.90 (2H) *	71.7	<b>7</b>	9.86 (H, <i>s</i> )	193.2	<b>7</b>	7.33 (H, <i>d, J=8.4</i> )	112.8
<b>3,5, 3',5' OCH<sub>3</sub></b>	3.90 (12H, <i>s</i> ) *	56.3				<b>7a</b>	--	138.1
<b>4, 4' OH</b>	5.56(2H, <i>s</i> )					<b>8</b>	1.2 (3H, <i>s</i> )	30.7

The chemical shift ( $\delta$ ) is expressed in ppm and coupling constants ( $J$ ) in Hz

\* 9 $\beta$ , 9' $\beta$  protons (2H,  $\delta$  3.90) are masked by the methoxy protons (12H,  $\delta$  3.90), they appear collectively at  $\delta$  3.90 (14H, *s*)

**Table S4:** <sup>1</sup>H-NMR (400 MHz) and APT (100 MHz) spectral data of **9** (β-sitosteryl palmitate).

#	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> )	APT (100 MHz, CDCl <sub>3</sub> )	#	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> )	APT (100 MHz, CDCl <sub>3</sub> )
<b>1</b>		36.9	<b>21</b>	0.9 (3H, <i>d</i> )	18.7
<b>2</b>		27.7	<b>22</b>		33.9
<b>3</b>	4.5 (H, <i>m</i> )	73.9	<b>23</b>		26.1
<b>4</b>	2.3 (2H, <i>m</i> )	38.1	<b>24</b>		45.8
<b>5</b>		139.6	<b>25</b>		29.2
<b>6</b>	5.3 (H, br. <i>d</i> )	122.6	<b>26</b>	0.75-0.92	19.2
<b>7</b>		32.0	<b>27</b>	0.75-0.92	19.7
<b>8</b>		31.9	<b>28</b>		23.0
<b>9</b>		50.0	<b>29</b>	0.75-0.92	11.8
<b>10</b>		36.7	<b>1'</b>		173.8
<b>11</b>		21.0	<b>2'</b>	2.25 (2H <i>t</i> , <i>J</i> =7.8)	34.7
<b>12</b>		39.7	<b>3'</b>	1.57 (2H, <i>m</i> )	25.0
<b>13</b>		42.3	<b>4'-</b> <b>13'</b>	1.21-1.31 (20 H, br. <i>s</i> )	29.2-29.7
<b>14</b>		56.6	<b>14'</b>		31.9
<b>15</b>		24.2	<b>15'</b>		22.7
<b>16</b>		27.7	<b>16'</b>	0.86 (3H, <i>t</i> , <i>J</i> =6.4)	14.0
<b>17</b>		56.0			
<b>18</b>	0.66 (3H, <i>s</i> )	11.9			
<b>19</b>	0.99 (3H, <i>s</i> )	18.9			
<b>20</b>		36.3			

The chemical shift (δ) is expressed in ppm and coupling constants (*J*) in Hz

**Table S5:** <sup>1</sup>H-NMR and APT spectral data of **11** (7-oxo- β-sitosterol-3-O-β-D-glucopyranoside)-6'-palmitate).

#	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> )	APT (100 MHz, CDCl <sub>3</sub> )	#	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> )	APT (100 MHz, CDCl <sub>3</sub> )
<b>1</b>	--	36.4	<b>22</b>	--	34.3
<b>2</b>	--	32.0	<b>23</b>	--	26.3
<b>3</b>	--	78.4	<b>24</b>	--	45.8
<b>4</b>	--	42.9	<b>25</b>	--	29.2
<b>5</b>	--	164.7	<b>26</b>	0.79 (3H, <i>d</i> , <i>J</i> =7.3)	19.8
<b>6</b>	5.69 (H, <i>s</i> )	126.3	<b>27</b>	0.78 (3H, <i>d</i> , <i>J</i> =5.4)	18.3
<b>7</b>	--	202.7	<b>28</b>	--	23.1
<b>8</b>	--	45.4	<b>29</b>	0.82 (3H, <i>t</i> , <i>J</i> =6.5)	12.3
<b>9</b>	--	49.9	<b>1'</b>	4.39 (H, <i>d</i> , <i>J</i> =7.8)	101.5
<b>10</b>	--	38.5	<b>2'</b>	--	73.5
<b>11</b>	--	21.5	<b>3'</b>	--	77.3
<b>12</b>	--	38.7	<b>4'</b>	--	70.0
<b>13</b>	--	43.1	<b>5'</b>	--	73.5
<b>14</b>	--	49.9	<b>6'</b>	4.26 (H <sub>a</sub> , <i>d</i> , <i>J</i> =11.5)	63.2
				4.44 (H <sub>b</sub> , <i>dd</i> , <i>J</i> =*)	
<b>15</b>	--	23.1	<b>1''</b>	--	174.0
<b>16</b>	--	28.6	<b>2''</b>	2.37 (H, <i>t</i> , <i>J</i> =6.5)	34.0
<b>17</b>	--	54.7	<b>3''</b>	--	25.0
<b>18</b>	0.66 (3H, <i>s</i> )	12.0	<b>4''-</b> <b>13''</b>	1.19-1.35	29.3-29.8
<b>19</b>	1.18 (3H, <i>s</i> )	17.3	<b>14''-</b>	--	32.0
<b>20</b>	--	36.2	<b>15''</b>	--	22.7
<b>21</b>	0.91 (3H, <i>d</i> , <i>J</i> =5.9)	19.0	<b>16''</b>	0.88 (3H, <i>t</i> , <i>J</i> =6.4)	14.1

The chemical shift ( $\delta$ ) is expressed in ppm and coupling constants (*J*) in Hz

\* *J* value couldn't be calculated.

**Table S6:** <sup>1</sup>H-NMR and APT spectral data of **12** (5 $\alpha$ , 8 $\alpha$ -epi-dioxyergosta-6, 22-dien-3 $\beta$ -ol).

#	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> )	APT (100 MHz, CDCl <sub>3</sub> )	#	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> )	APT (100 MHz, CDCl <sub>3</sub> )
<b>1</b>	--	34.7	<b>15</b>	--	20.7
<b>2</b>	--	30.1	<b>16</b>	--	28.7
<b>3</b>	3.94 (H, <i>m</i> )	66.5	<b>17</b>	--	56.2
<b>4</b>	--	36.9	<b>18</b>	0.78-.86 (9H,18,19,21)	12.9
<b>5</b>	--	81.9	<b>19</b>	0.78-.86 (9H,18,19,21)	18.2
<b>6</b>	6.48 (H, <i>d</i> , <i>J</i> = 8.2)	135.4	<b>20</b>	--	39.4
<b>7</b>	6.22 (H, <i>d</i> , <i>J</i> = 8.2)	130.8	<b>22</b>	5.11 (H, <i>dd</i> , <i>J</i> =15.6, 8.2)	132.3
<b>8</b>	--	79.5	<b>23</b>	--	42.9
<b>9</b>	--	51.1	<b>24</b>	--	33.1
<b>10</b>	--	36.9	<b>25</b>	0.88 (3H, <i>d</i> , <i>J</i> = 7.2)	19.7
<b>11</b>	--	23.4	<b>26</b>	0.97 (3H, <i>d</i> , <i>J</i> = 6.4)	20.0
<b>12</b>	--	39.4	<b>27</b>	1.07 (3H, <i>d</i> , <i>J</i> =5.9)	17.6
<b>13</b>	--	44.6	<b>28</b>	5.19(H, <i>dd</i> , <i>J</i> =15.1, 7.3)	135.2
<b>14</b>	--	51.7			

The chemical shift ( $\delta$ ) is expressed in ppm and coupling constants (*J*) in Hz

**Table S7:** <sup>1</sup>H-NMR and APT spectral data of **13** (oleanolic acid).

#	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> )	APT (100 MHz, CDCl <sub>3</sub> )	#	<sup>1</sup> H-NMR (400 MHz, CDCl <sub>3</sub> )	APT (100 MHz, CDCl <sub>3</sub> )
<b>1</b>	--	38.4	<b>16</b>	--	23.4
<b>2</b>	--	27.0	<b>17</b>	--	46.4
<b>3</b>	3.13 (H, <i>dd.</i> , <i>J</i> = 5.04, 11.44 )	77.4	<b>18</b>	2.74 (H, <i>m</i> )	41.2
<b>4</b>	--	38.7	<b>19</b>	--	46.0
<b>5</b>	--	55.2	<b>20</b>	--	30.7
<b>6</b>	--	18.3	<b>21</b>	--	33.9
<b>7</b>	--	32.7	<b>22</b>	--	32.5
<b>8</b>	--	39.2	<b>23</b>	1.06 (3H, <i>s</i> )	28.1
<b>9</b>	--	47.0	<b>24</b>	0.70 (3H, <i>s</i> )	15.6
<b>10</b>	--	37.0	<b>25</b>	0.85 (3H, <i>s</i> )	15.3
<b>11</b>	--	23.0	<b>26</b>	0.70 (3H, <i>s</i> )	16.9
<b>12</b>	5.19 (H, <i>br.s</i> )	122.3	<b>27</b>	1.18 (3H, <i>s</i> )	25.9
<b>13</b>	--	143.8	<b>28</b>	--	180.7
<b>14</b>	--	41.7	<b>29</b>	0.91 (3H, <i>s</i> )	23.1
<b>15</b>	--	27.7	<b>30</b>	0.83 (3H, <i>s</i> )	23.6

The chemical shift ( $\delta$ ) is expressed in ppm and coupling constants (*J*) in Hz



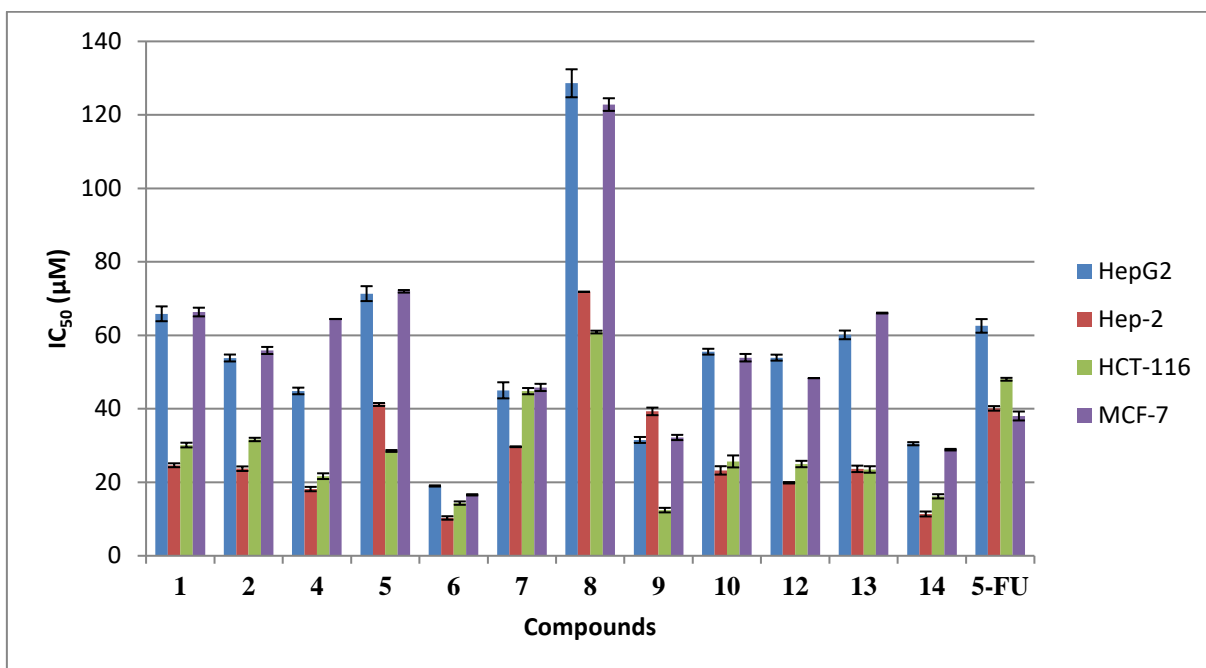
**Table S8:**  $^1\text{H}$ -,  $^{13}\text{C}$ -NMR, HSQC, and HMBC spectral data of **14** (9, 12, 13-trihydroxy-10-octadecenoic acid).

#	$^1\text{H}$ -NMR (500 MHz, DMSO- $d_6$ )	$^{13}\text{C}$ -NMR (125 MHz, DMSO- $d_6$ )	HSQC	HMBC correlations
<b>1</b>		175.0	C-1	
<b>2</b>	2,13 (2H, <i>t</i> )	34.1	C-2	C-1, C-3, C-4
<b>3</b>	1.43, <i>m</i>	25.0	C-3	C-1, C-2, C-4
<b>4</b>	1.19, <i>br.</i>	29.5	C-4	
<b>5,6</b>	1.19, <i>br.</i>	25.4	C-5,C-6	
<b>7</b>	1.34, <i>m</i>	25.7	C-7	C-9
<b>8</b>	1.34, <i>m</i>	37.9	C-8	
<b>9</b>	3.9	71.0	C-9	C-8, C-10, C-11
<b>10</b>	5.51, <i>d</i>	135.0	C-10	C-9, C-11, C-12
<b>11</b>	5.51, <i>d</i>	129.9	C-11	C-9, C-10, C-12
<b>12</b>	3.78	74.7	C-12	C-10, C-11, C-13, C-14
<b>13</b>	3.25	74.2	C-13	C-11, C-12, C-15
<b>14</b>	1.34, <i>m</i>	32.3	C-14	
<b>15</b>	1.19, <i>br.</i>	29.6	C-15	
<b>16</b>	1.19, <i>br.</i>	32.0	C-16	
<b>17</b>	1.19, <i>br.</i>	22.6	C-17	
<b>18</b>	0.82 (2H, <i>t</i> )	14.5	C-18	C-16, C-17

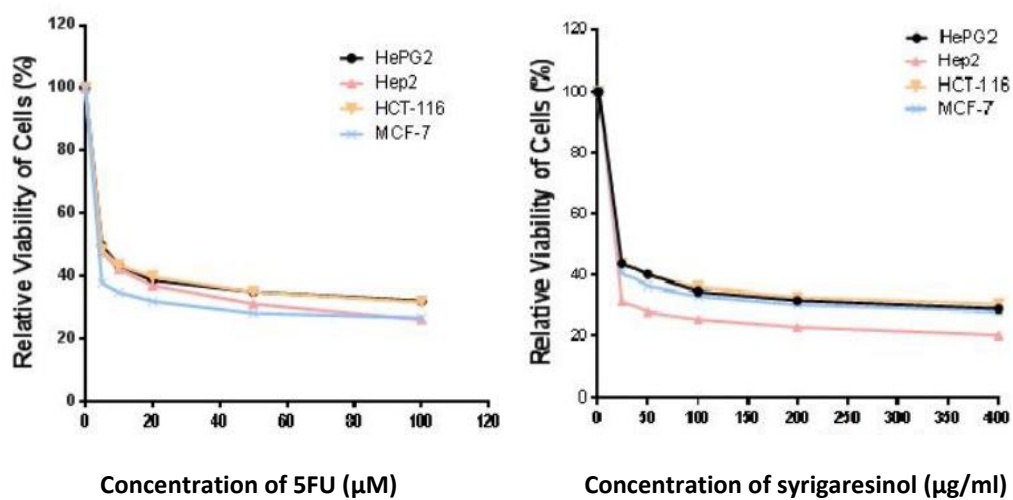
The chemical shift ( $\delta$ ) is expressed in ppm and coupling constants ( $J$ ) in Hz

## **S1: MTT Assay**

Human cancer cell lines from liver (HePG-2), larynx (Hep-2), colon (HCT-116), or breast (MCF-7) originated from ATCC (Manassas, VA, USA) and were obtained from VACSERA, Cairo, Egypt. Cells were observed under an inverted microscope (Olympus 1x 70, Tokyo, Japan). MTT (3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyltetrazolium bromide), dimethylsulfoxide (DMSO), 5-fluorouracil (5-FU), and RPMI-1640 medium were obtained from Sigma-Aldrich (St. Louis, MO, USA), 10% fetal bovine serum from GIBCO, Paisely, UK). The assay was carried out according to Mauceri et. al.,1998 [3]. The cell lines were cultured in RPMI-1640 medium with 10% fetal bovine serum. The antibiotics added are 100 units/mL penicillin and 100 µg/mL streptomycin at 37°C in a 5% CO<sub>2</sub> incubator. The samples were dissolved in DMSO and diluted with phosphate buffer solution (PBS) 5-fluorouracil was used as a standard anticancer drug for comparison. The cells (HePG2, Hep2, HCT116 and MCF-7) were seeded in a 96-well plate at a density of 1.0 x 10<sup>4</sup> cells/ well at 37°C for 24 hr under 5% CO<sub>2</sub>. Samples of different concentration were added to each well and cultured for 48 hr. The treated cells were washed with PBS and 100 µl of MTT solution (5mg/ml MTT stock in PBS diluted to 1 mg/ml with 10% RPMI-1640 medium) was added to each well and incubated for 4hr at 37°C. Finally, 100 µL of DMSO was added and optical densities at 570 nm were measured using a A BioTeck<sup>®</sup> microplate reader (Winooski, VT, USA). The relative cell viability in percentage was calculated as ( $A_{570\text{ nm}}$  of treated samples/ $A_{570\text{ nm}}$  of untreated sample) X 100. Statistical analysis of the data was performed using Microsoft Excel software version 2010.



**Figure S40.** Calculated IC<sub>50</sub> (µM) for the *in vitro* cytotoxicity of 1-14



**Figure S41:** The log concentration- cell viability graph of 5FU and 6 (syringaresinol).

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