

Supporting Information

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Cytotoxic Constituents from the Rhizomes of *Monstera deliciosa*

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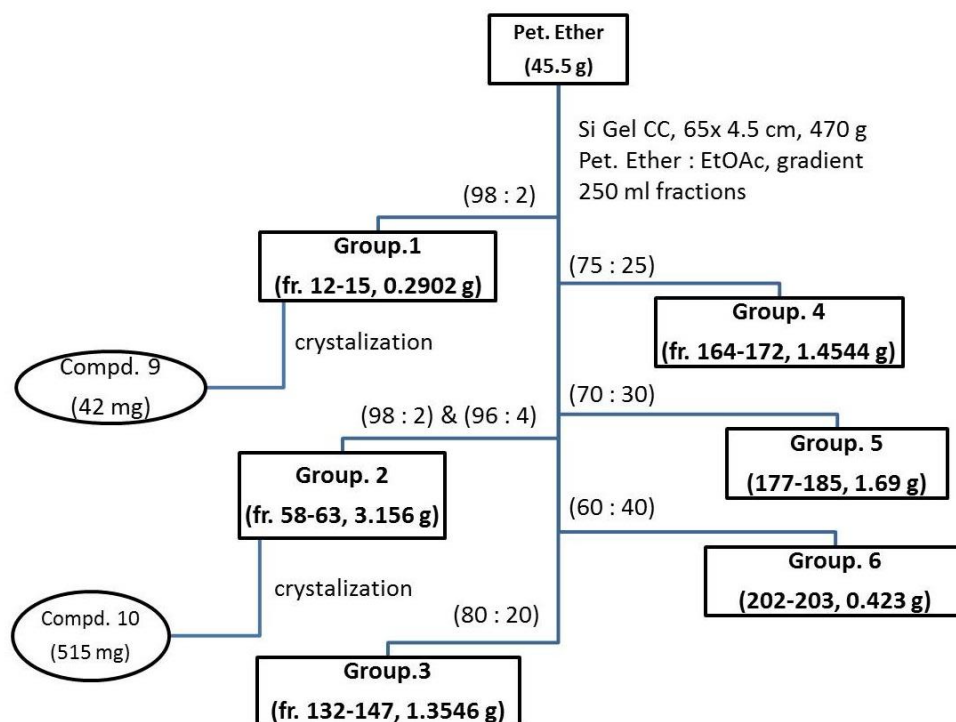


Figure S1: Scheme for chromatographic fractionation of the pet. ether extract & separation of **9** (β -sitosteryl palmitate) and **10** (β -sitosterol).

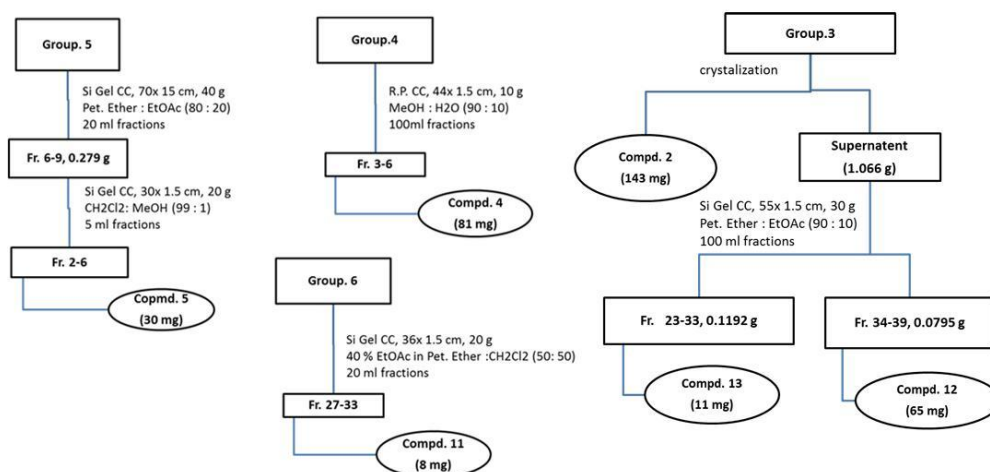


Figure S2: Scheme for chromatographic separation of **2** (propiosyringone), **4** (sesartemin), **5** (yangambin), **11** (7-oxo- β -sitosterol-3-O- β -D-glucopyranoside)-6'-palmitate), **12** (5α , 8α -epi-dioxyergosta-6, 22-dien-3 β -ol), and **13** (oleanolic acid).

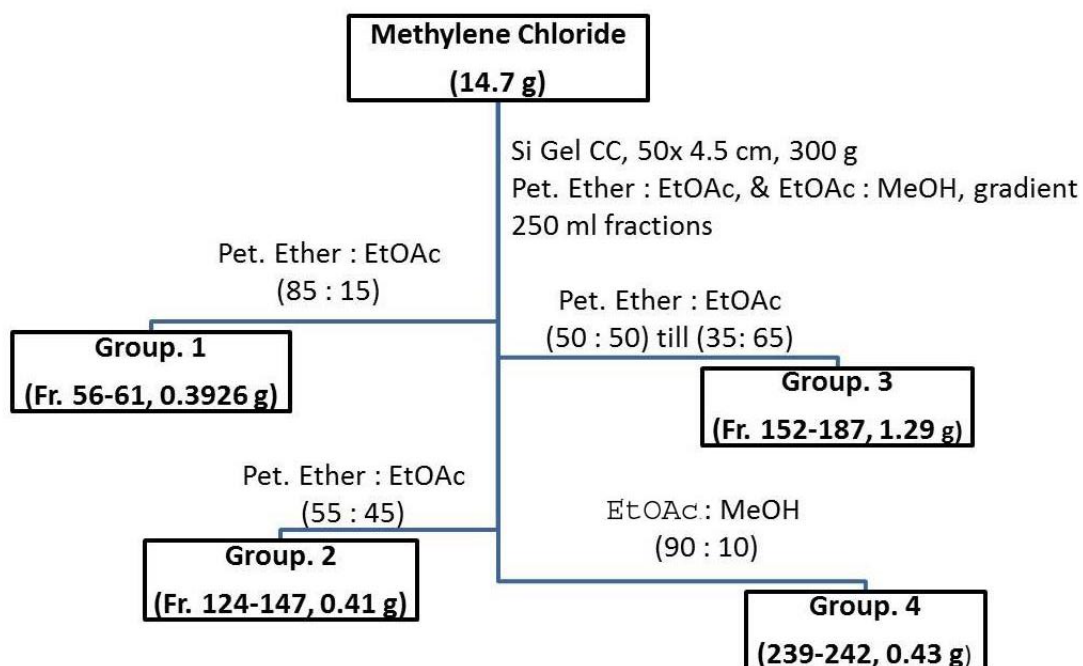


Figure S3: Scheme for chromatographic fractionation of the methylene chloride extract

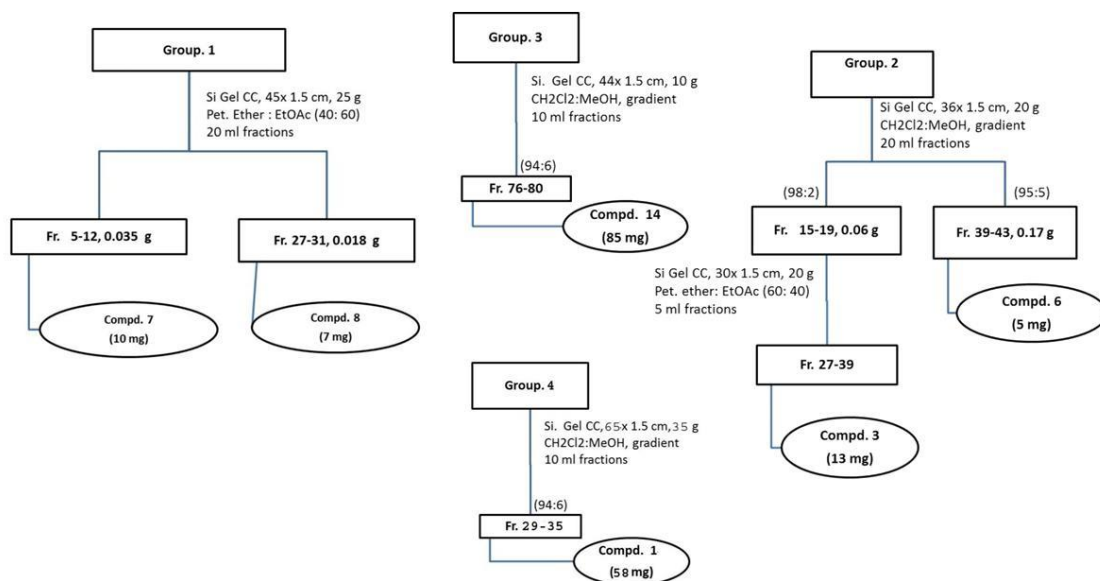


Figure S4: Scheme for chromatographic separation of compounds **1**(propiosyringone- β -D-glucopyranoside), **3** (ceplignan), **6** (syringaresinol), **7** (protocatechuic aldehyde), **8** (3-methyl thio-indole) and **14** (9, 12, 13-trihydroxy-10-octadecenoic acid).

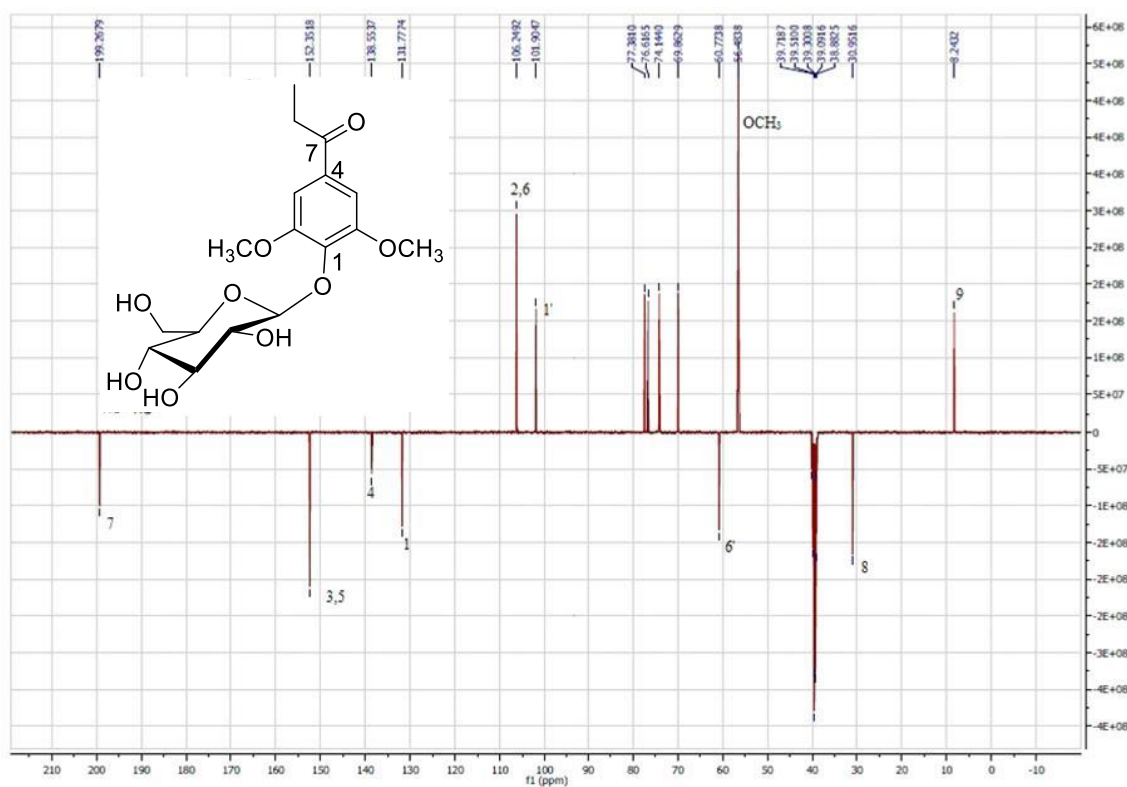


Figure S6: APT (100 MHz, DMSO- d_6) spectrum of **1** (propiosyringone- β -D-glucopyranoside)

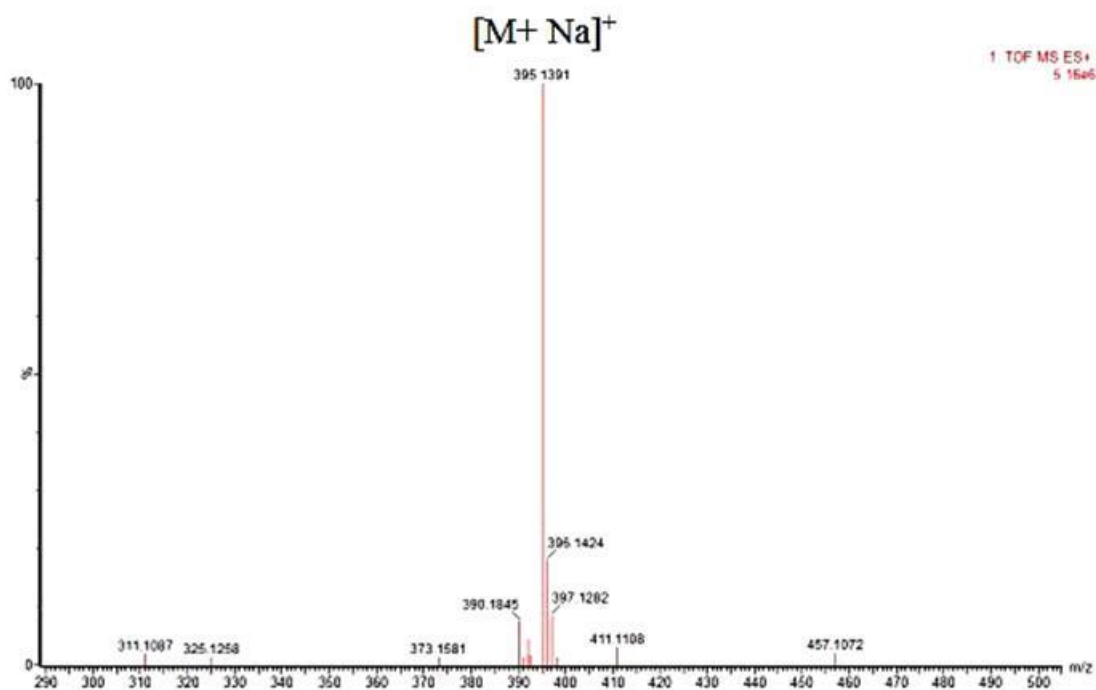


Figure S7: Positive ESI/TOF-MS spectrum of **1** (propiosyringone- β -D-glucopyranoside)

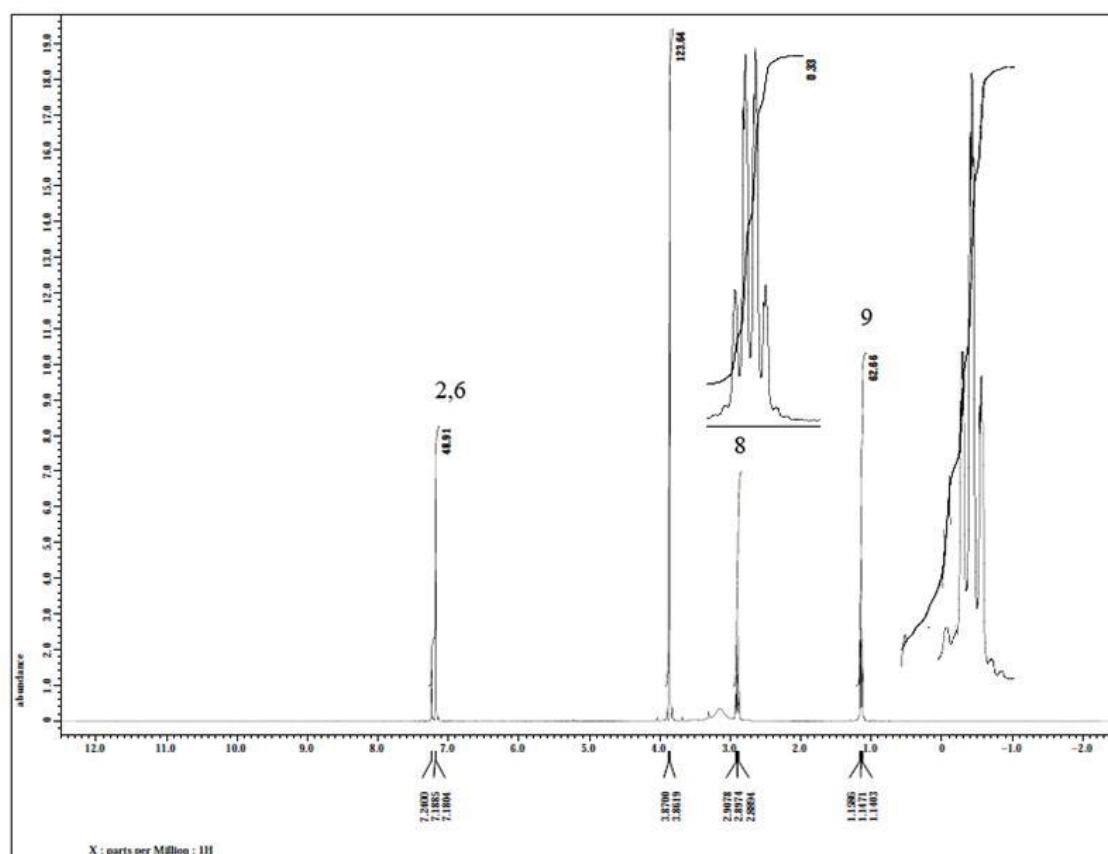


Figure S8: ^1H -NMR (400 MHz, CDCl_3) spectrum of **2** (propiosyringone)

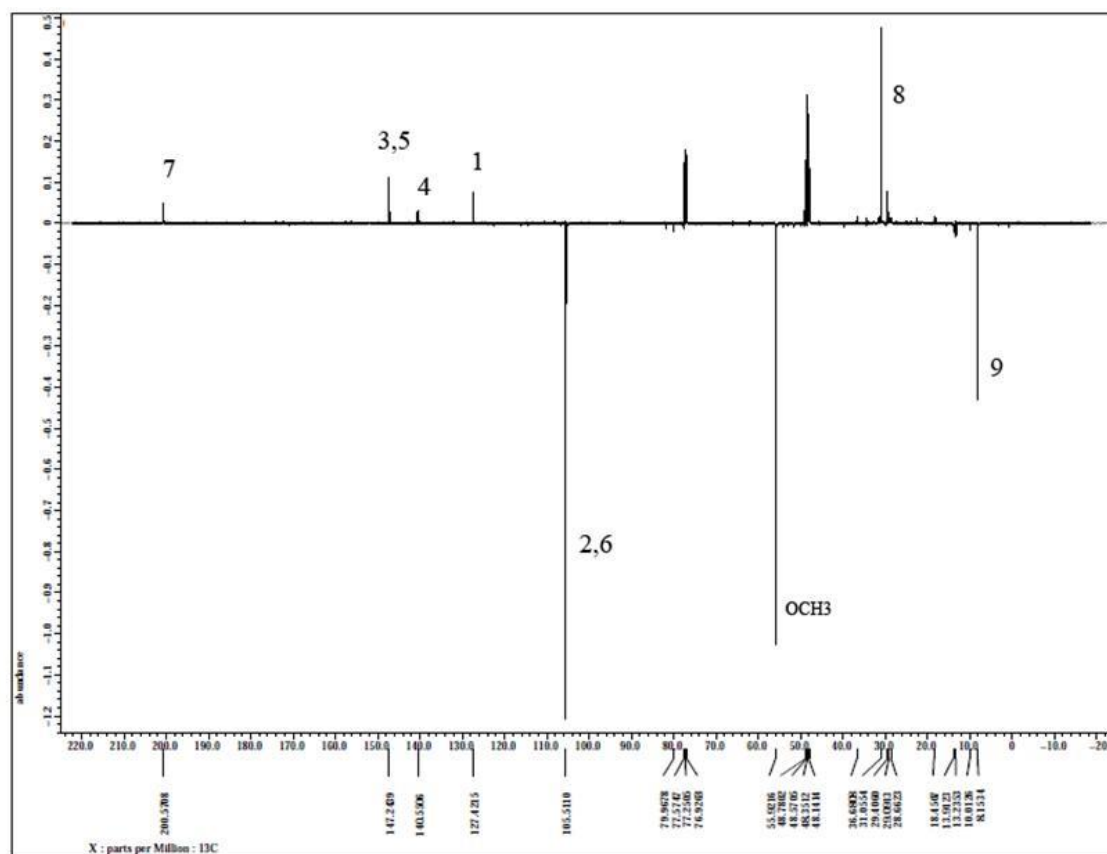


Figure S9: APT (100 MHz, CDCl_3) spectrum of **2** (propiosyringone)

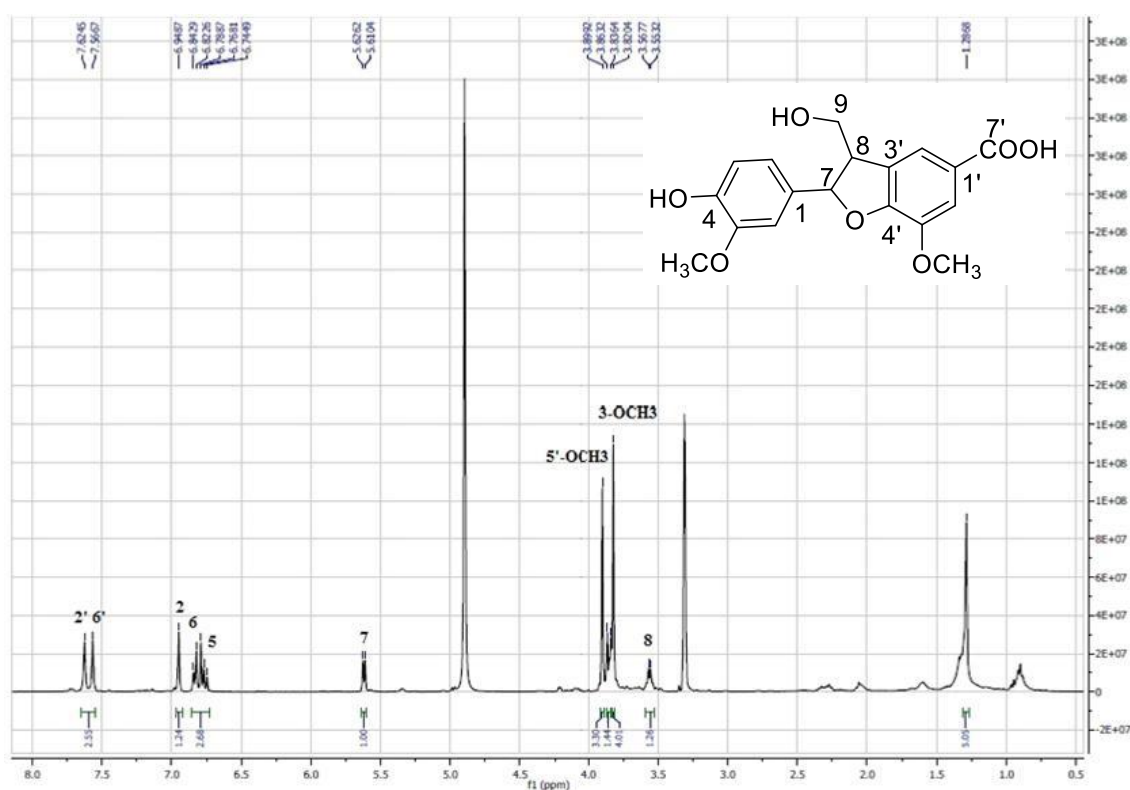


Figure S10: ¹H-NMR (400 MHz, CD₃OD) spectrum of **3** (ceplignan)

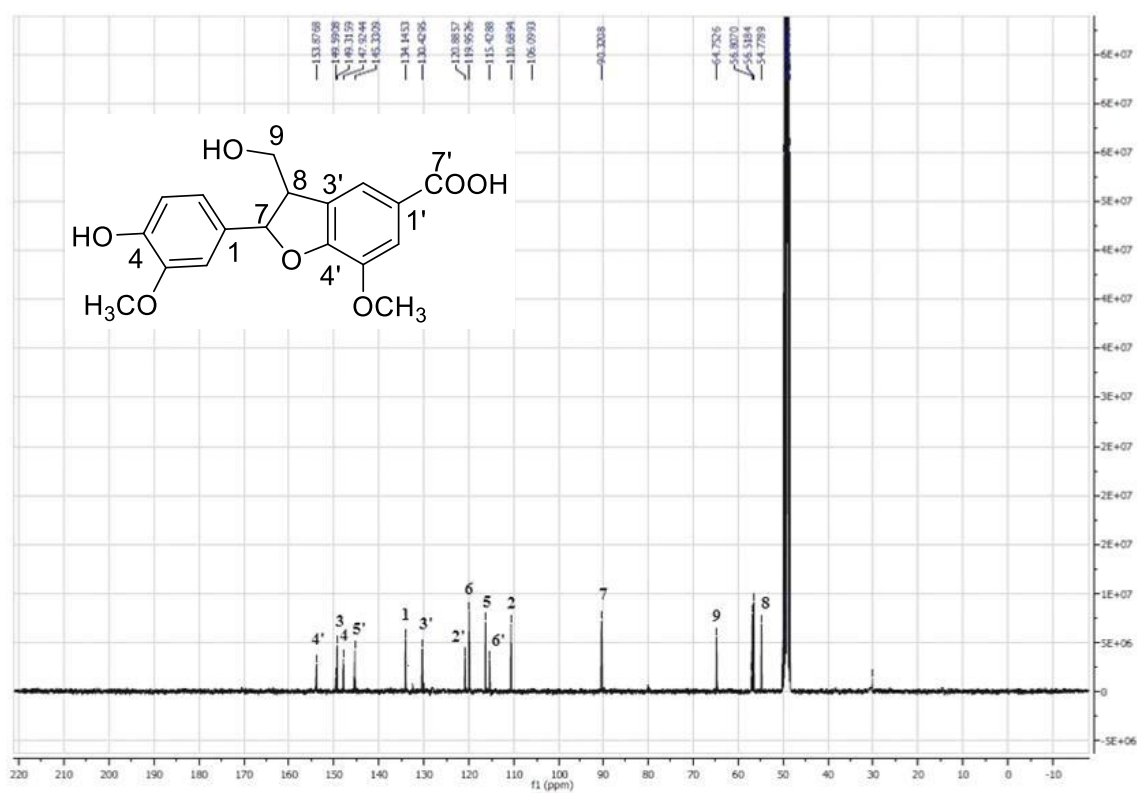


Figure S11: ^{13}C -NMR (100 MHz, CD_3OD) spectrum of **3** (ceplignan)

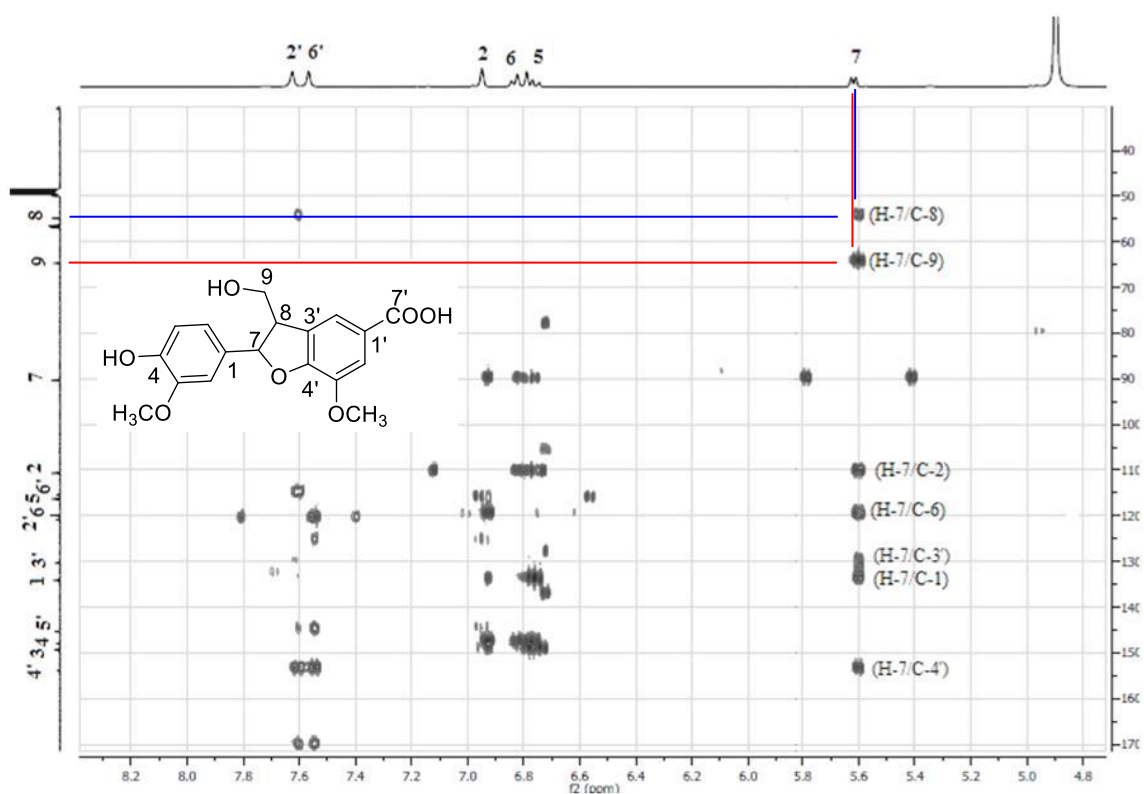
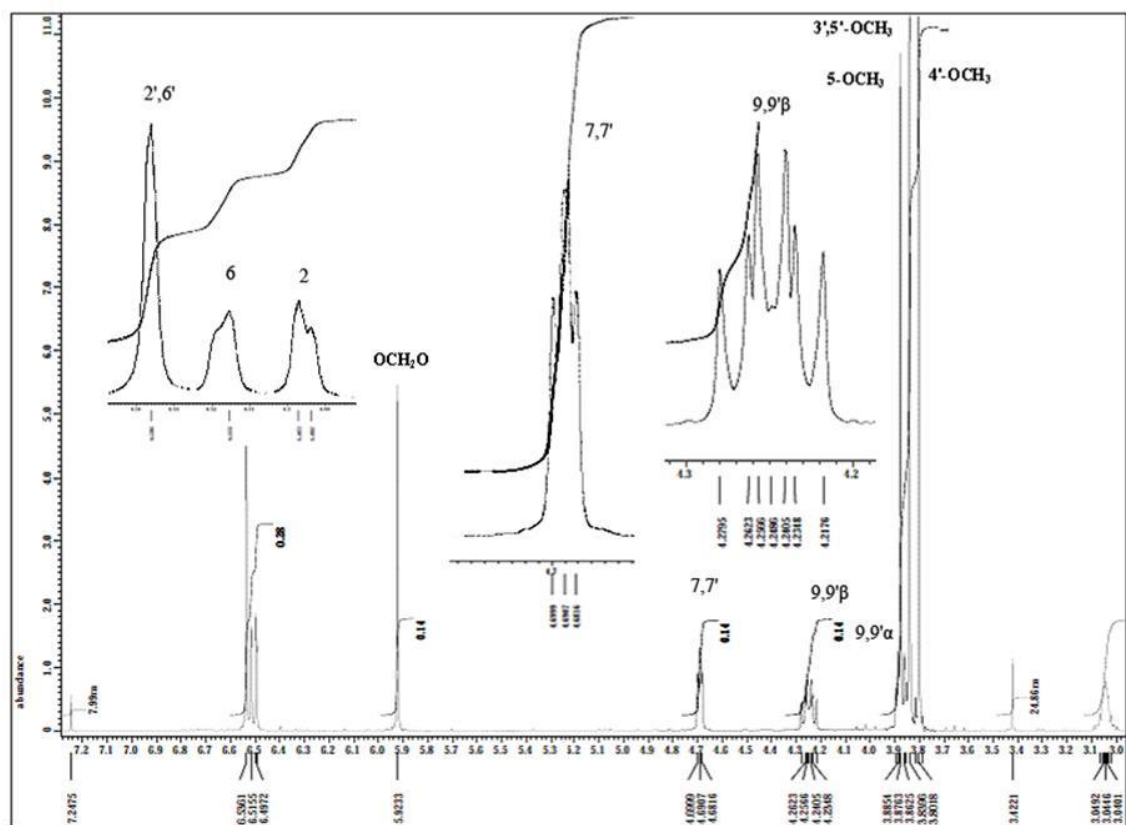


Figure S12: HMBC spectrum of **3** (ceplignan)



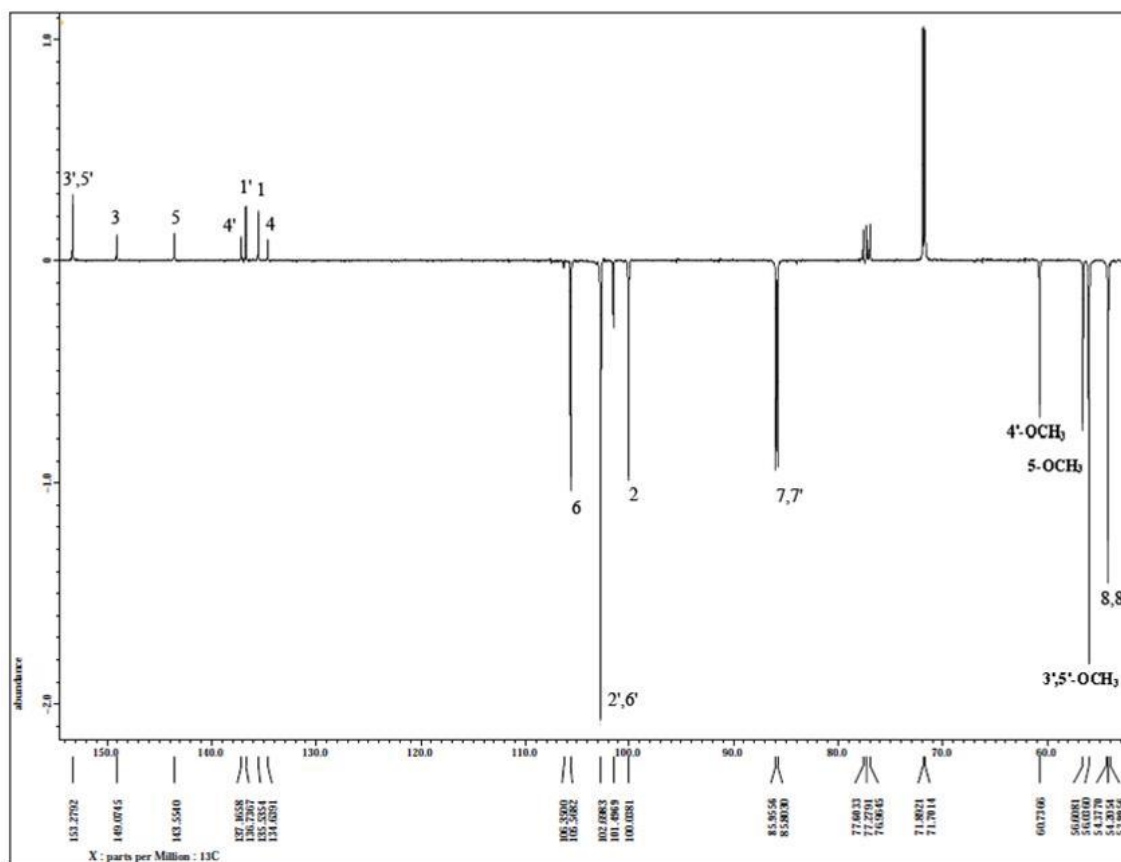


Figure S14:APT (100 MHz, CDCl_3) spectrum of **4** (sesartemin)

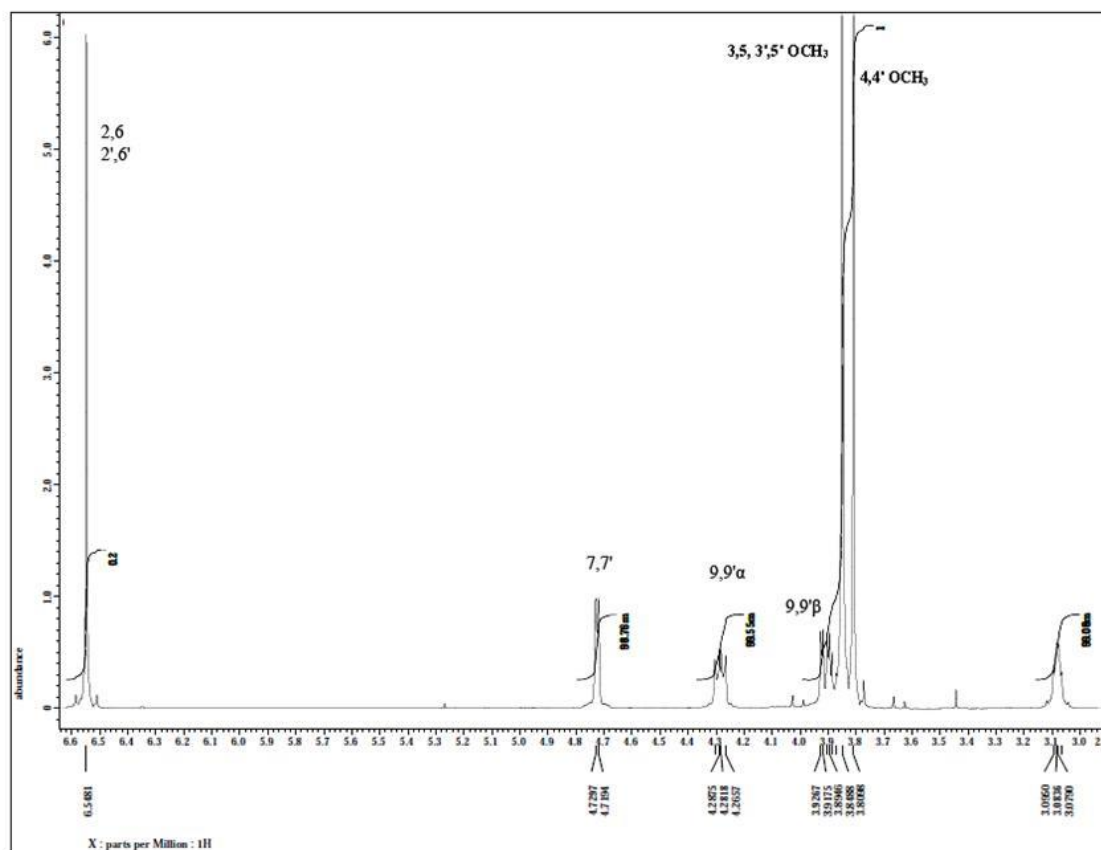


Figure S15: ^1H -NMR (400 MHz, CDCl_3) spectrum of 5 (yangambin)

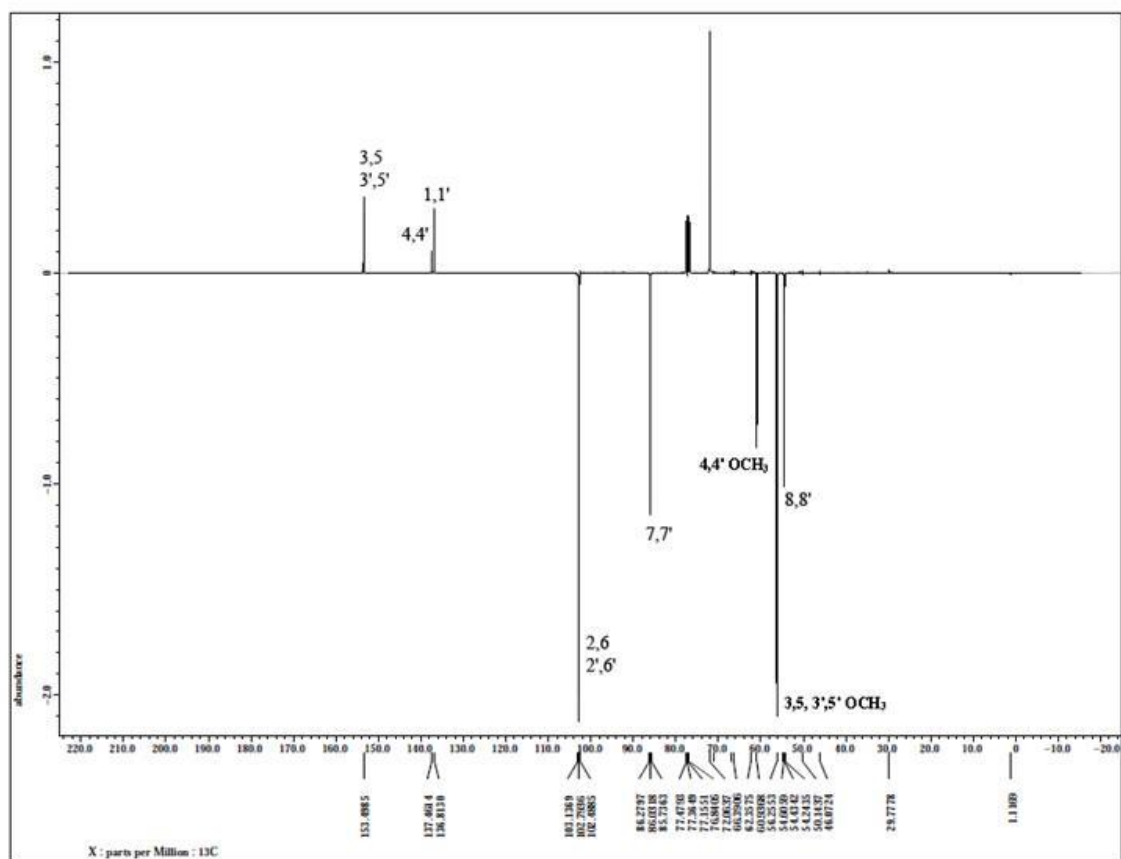


Figure S16: APT (100 MHz, CDCl₃) spectrum of 5 (yangambin)

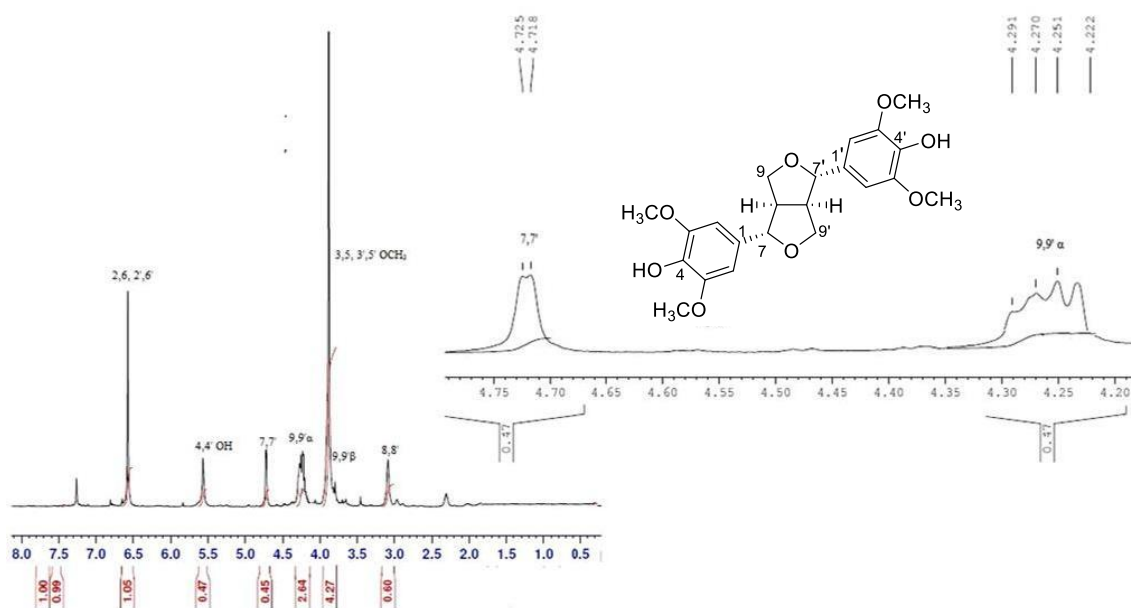


Figure S17: ^1H -NMR (400 MHz, CDCl_3) spectrum of **6** (syringaresinol)

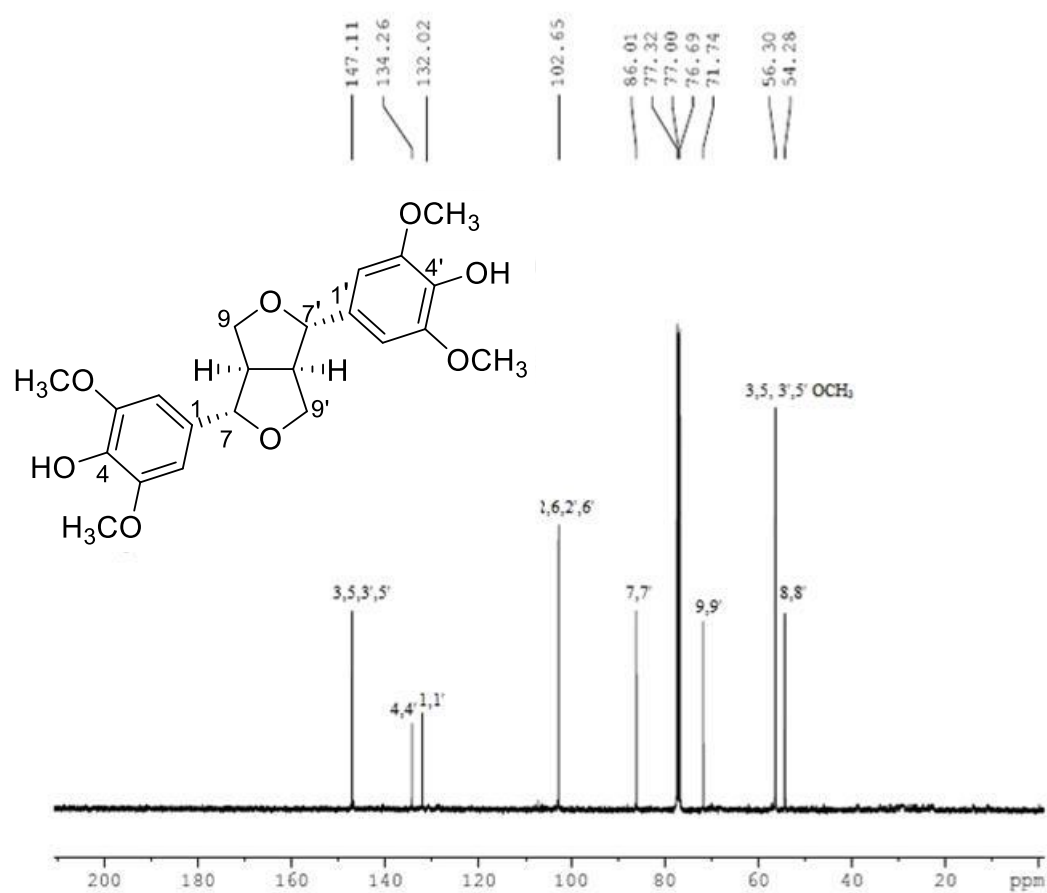


Figure S18: ¹³C-NMR (100 MHz, CDCl₃) spectrum of **6** (syringaresinol)

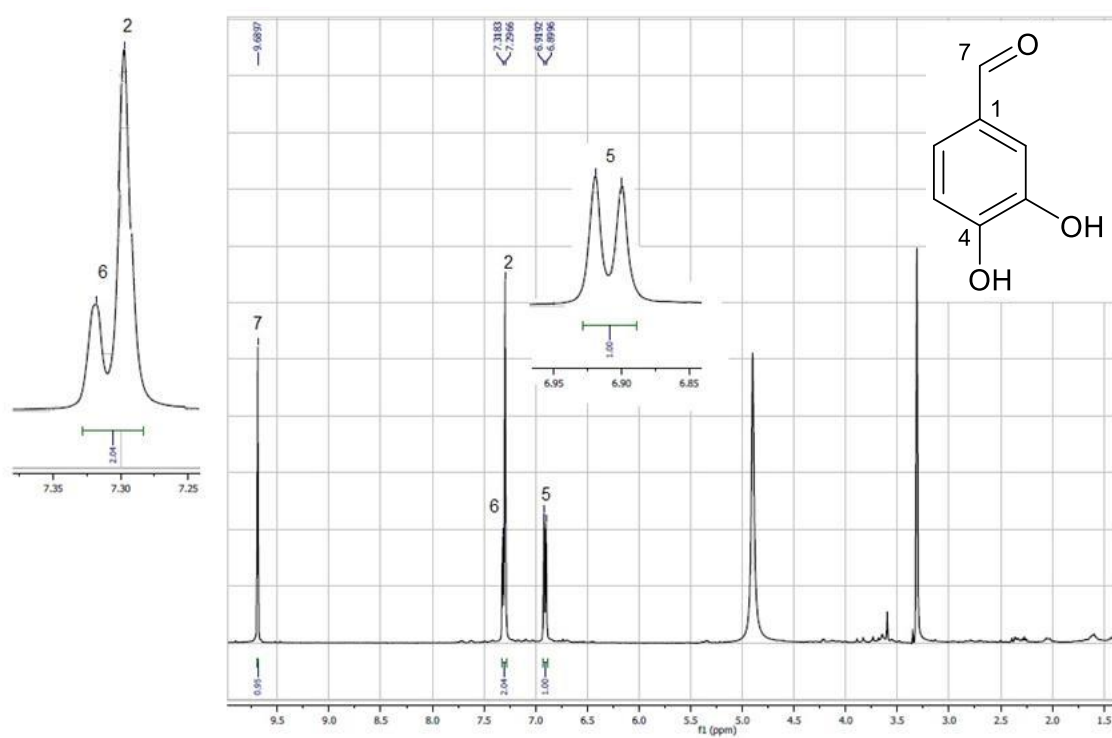


Figure S19: ^1H -NMR (400 MHz, CD_3OD) spectrum of 7 (protocatechuic aldehyde)

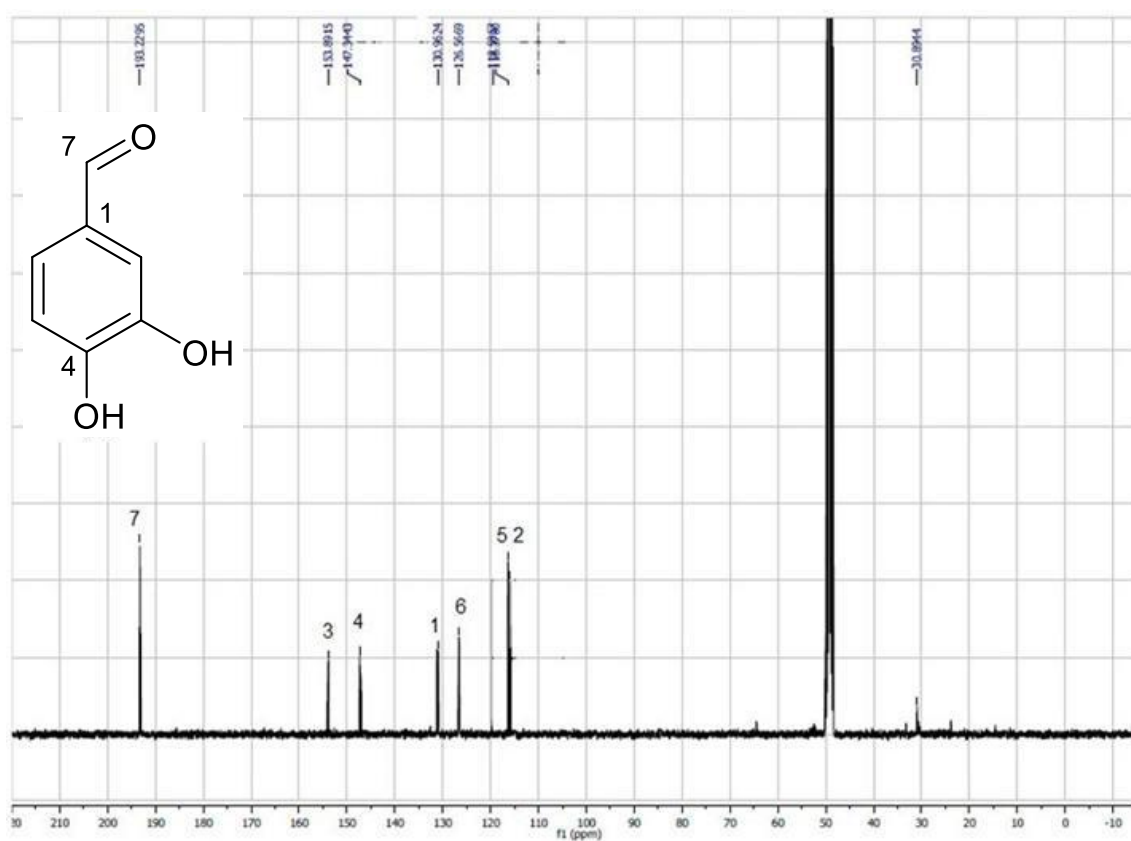


Figure S20: ^{13}C -NMR (100 MHz, CD_3OD) spectrum of 7 (protocatechuic aldehyde)

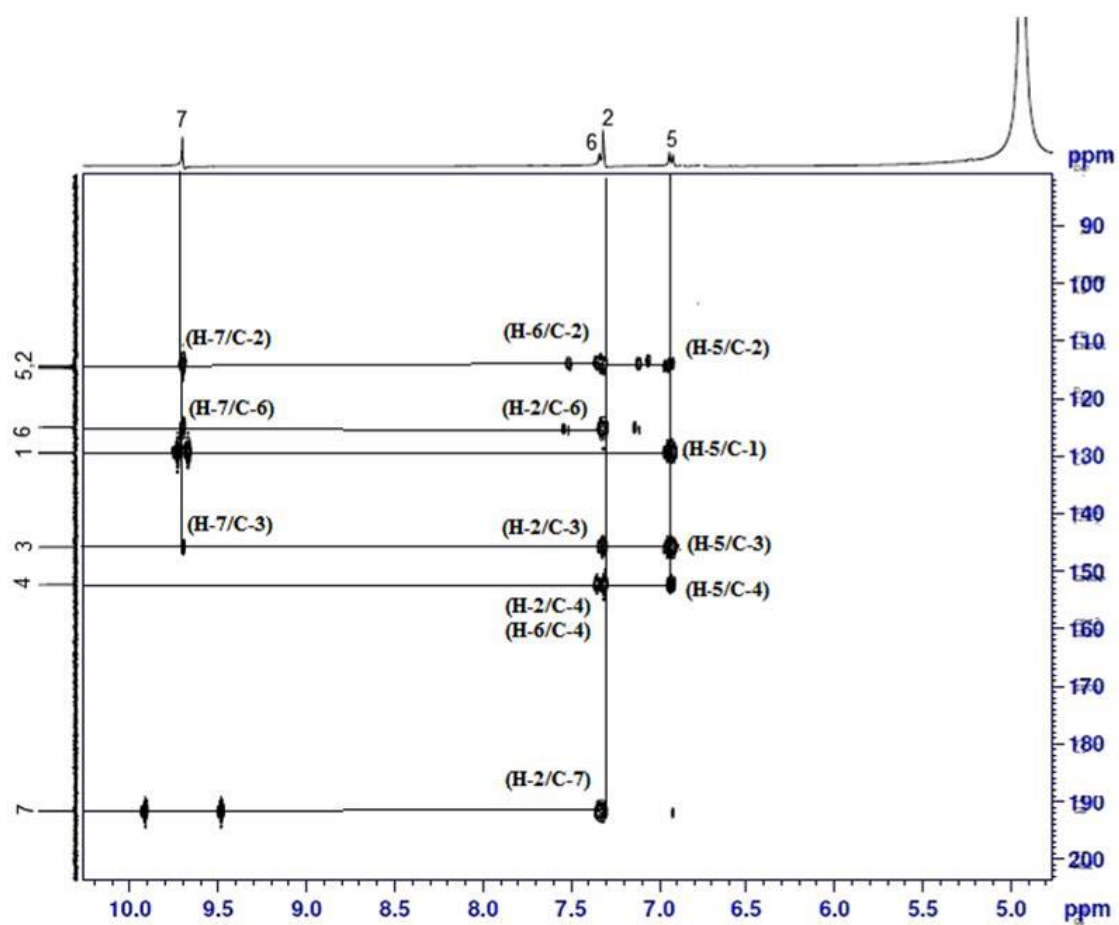


Figure S21: HMBC spectrum of 7 (protocatechuic aldehyde)

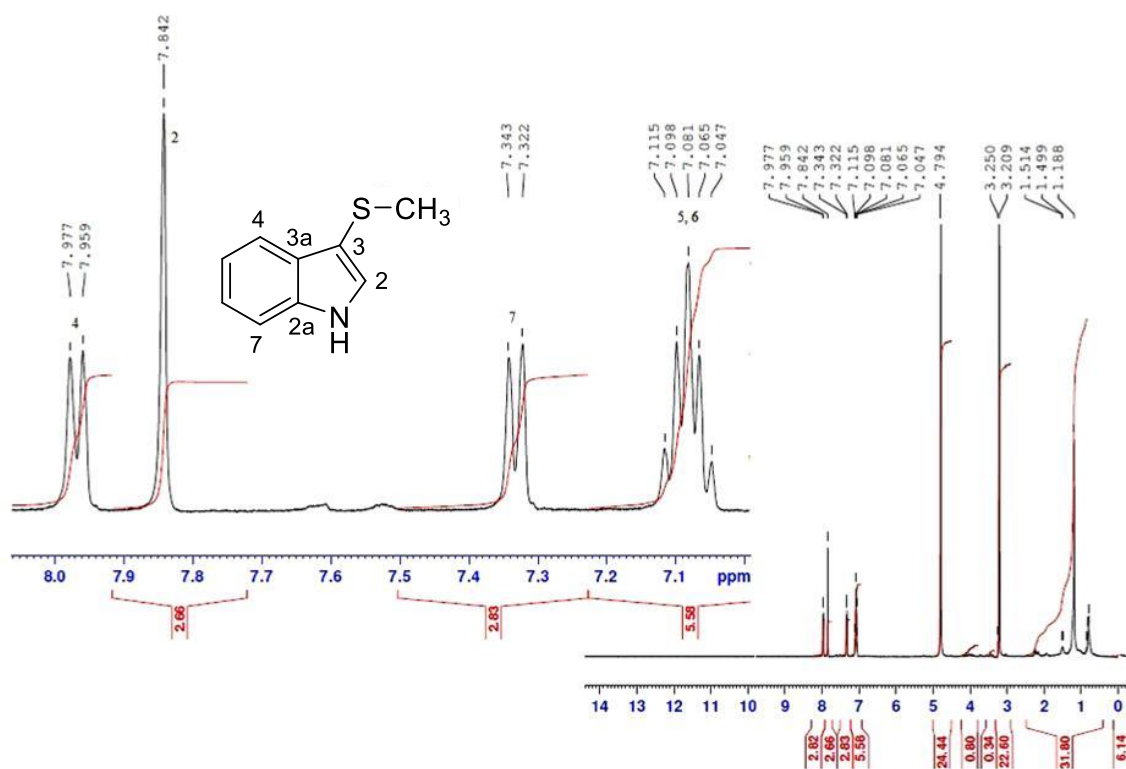


Figure S22: ¹H-NMR (400 MHz, CD₃OD) spectrum of **8** (3-methyl thio-indole)

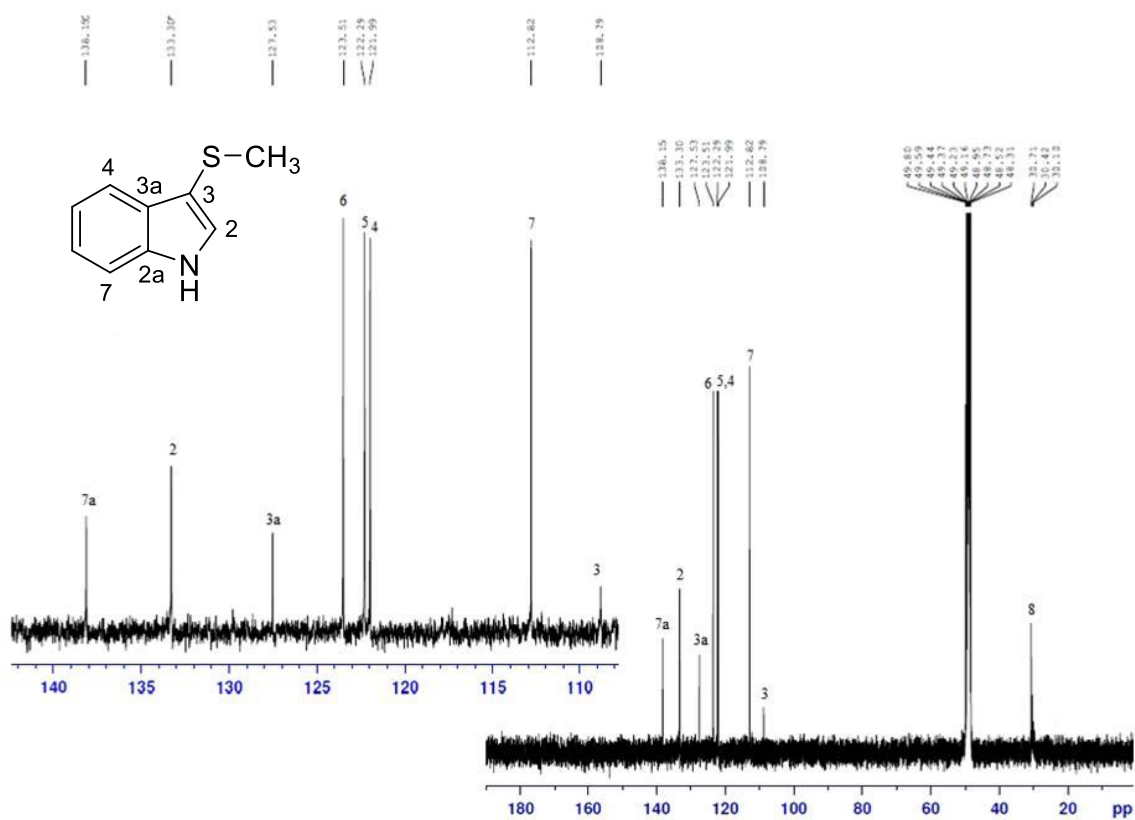


Figure S23: ^{13}C -NMR (100 MHz, CD_3OD) spectrum of **8** (3-methyl thio-indole)

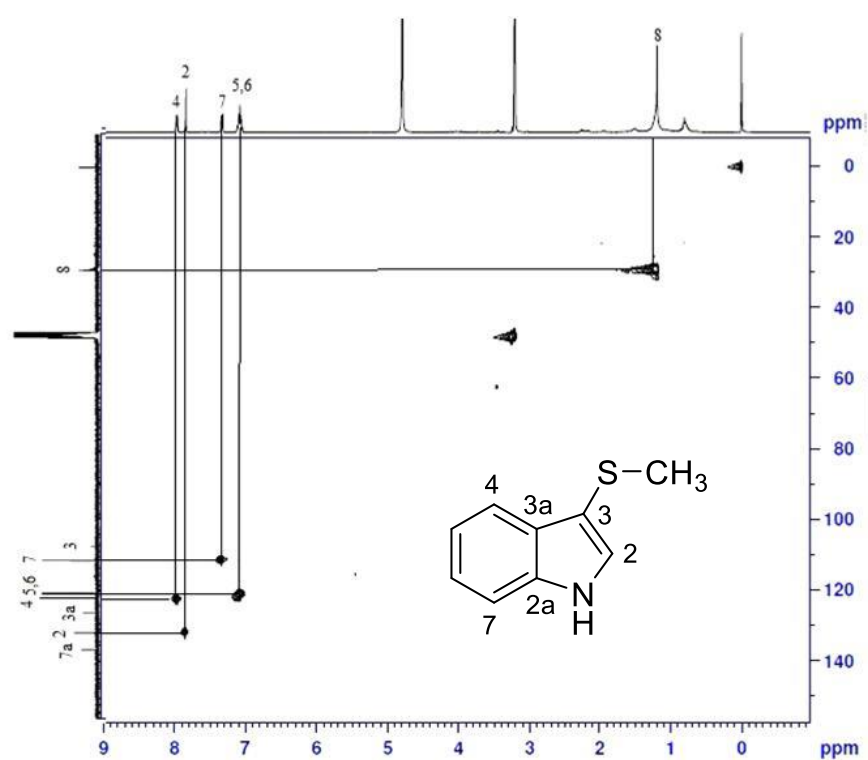


Figure S24: HSQC spectrum of **8** (3-methyl thio-indole)

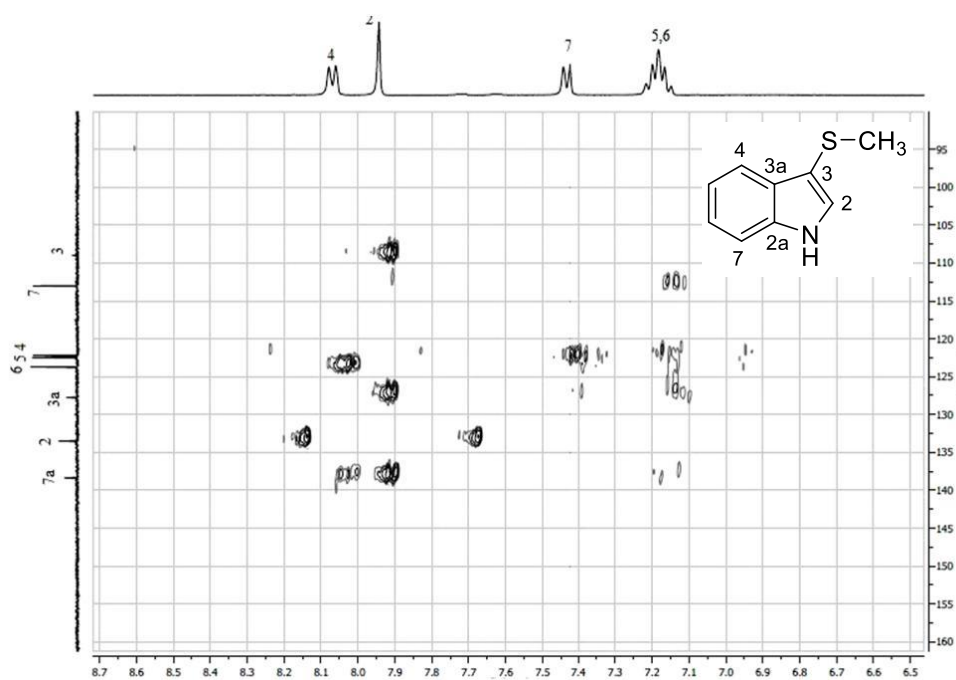


Figure S25: HMBC spectrum of **8** (3-methyl thio-indole)

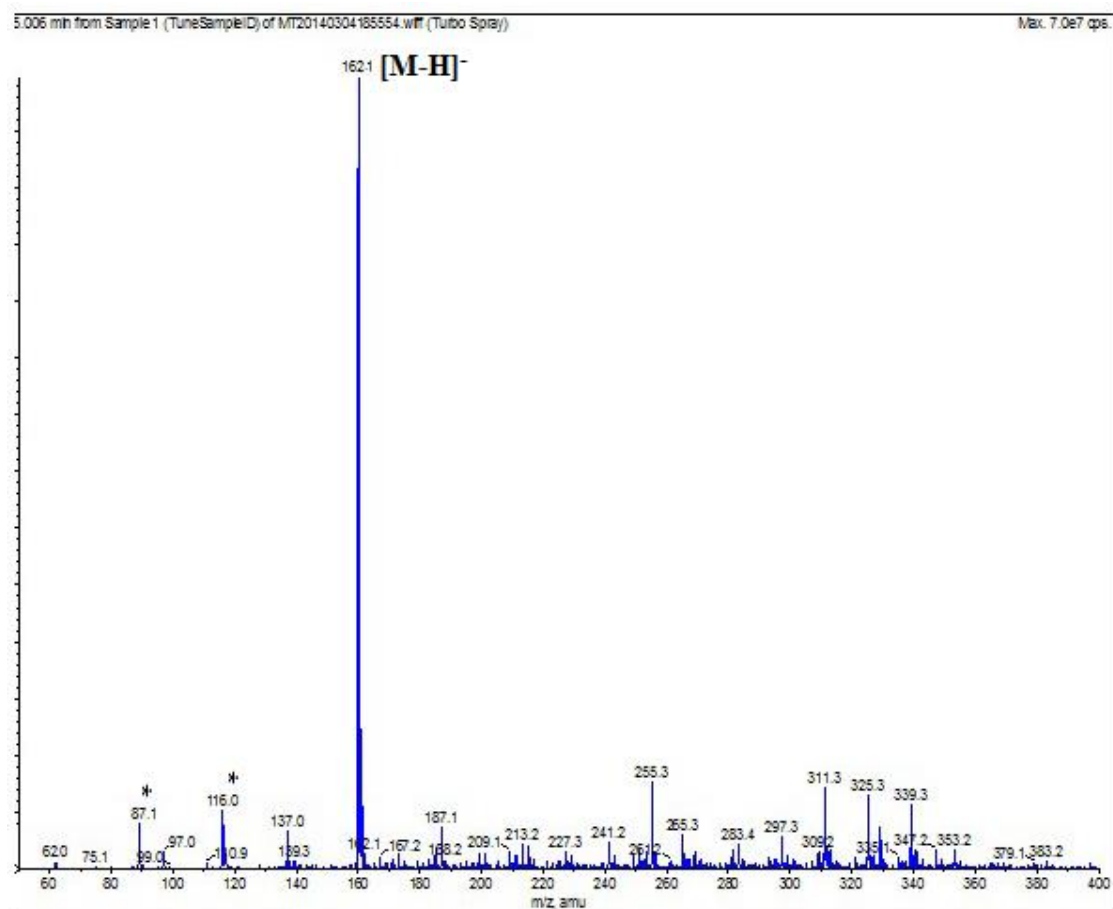
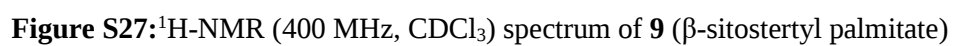


Figure S26: Negative ESI/MS spectrum of **8** (3-methyl thio-indole)



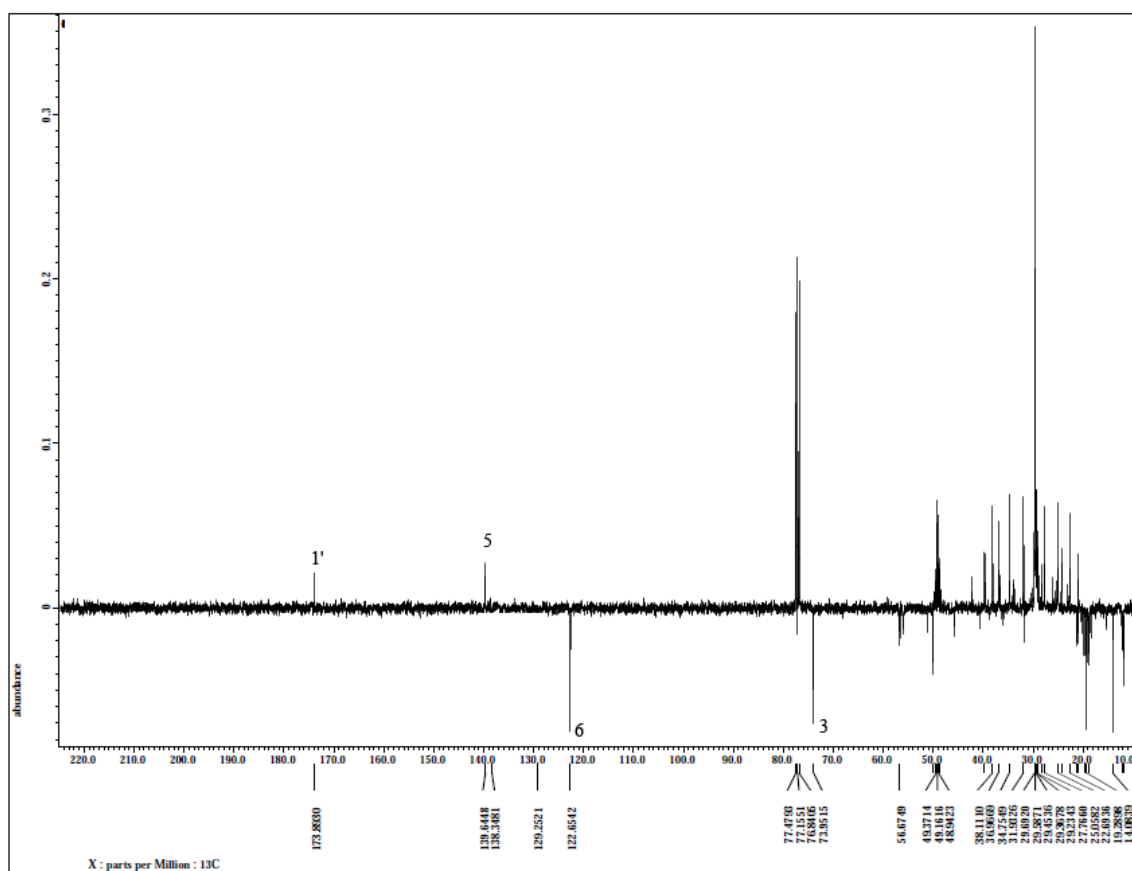


Figure S28: APT (100 MHz, CDCl₃) spectrum of **9** (β-sitosteryl palmitate)

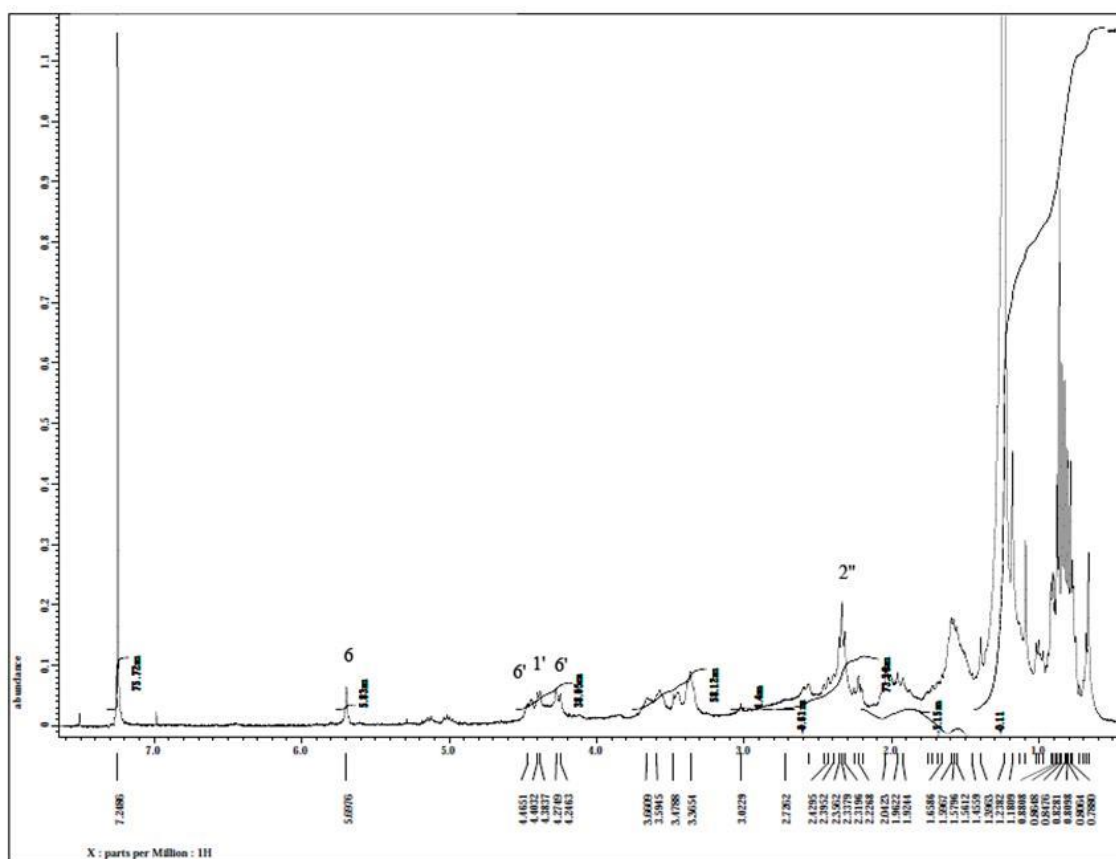


Figure S29: ¹H-NMR (400 MHz, CDCl₃) spectrum of **11** (7-oxo- β-sitosterol-3-O-β-D-glucopyranoside)-6'-palmitate)

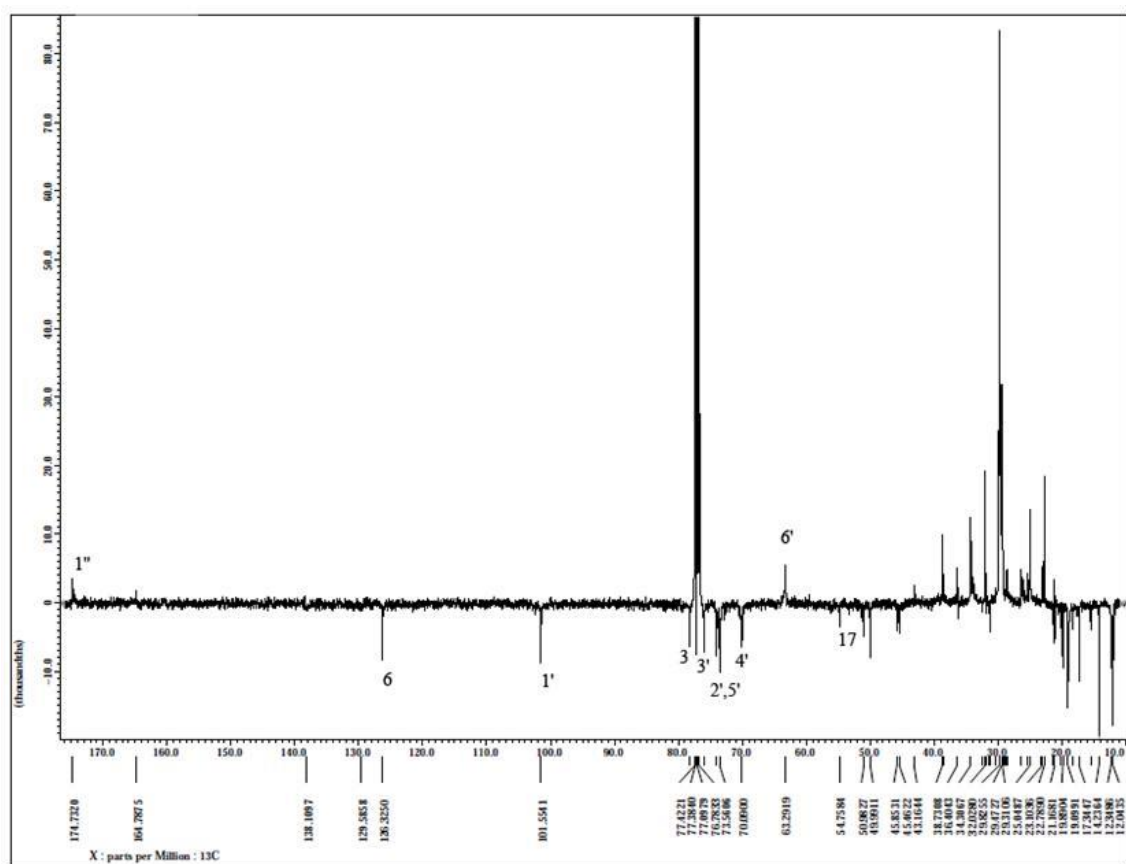


Figure S30: APT (100 MHz, CDCl₃) spectrum of **11** (7-oxo- β-sitosterol-3-O-β-D-glucopyranoside)-6'-palmitate)

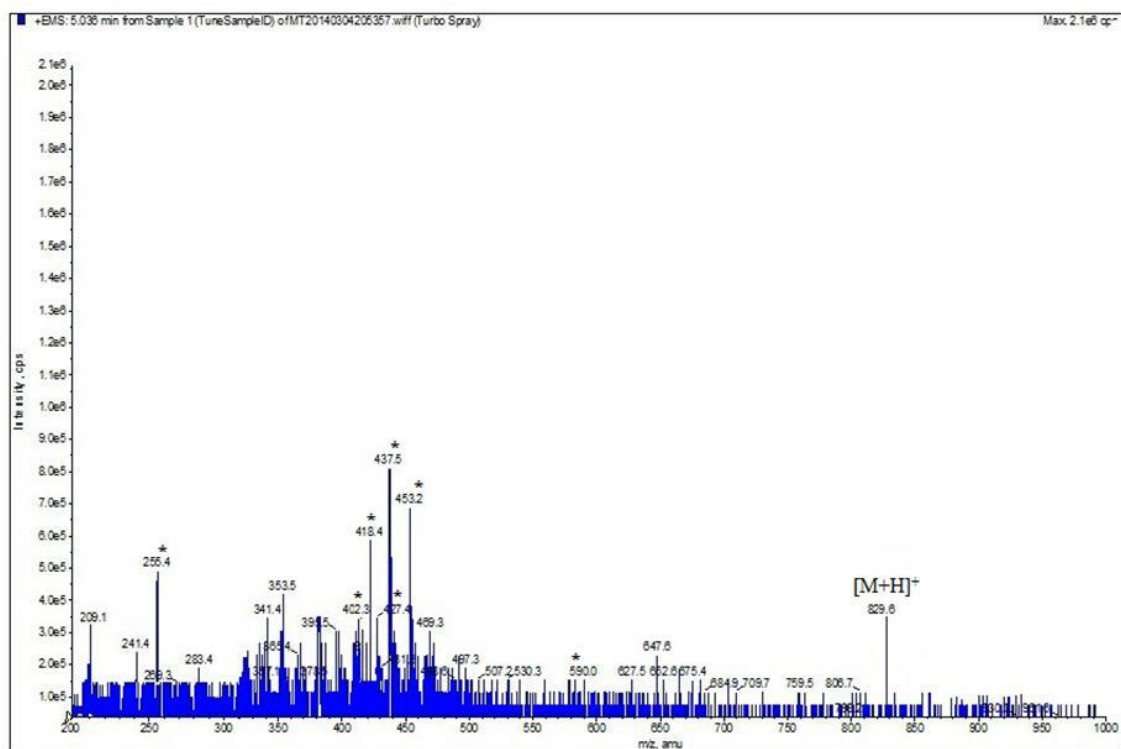


Figure S31: Positive ESI/EMS spectrum of **11** (7-oxo- β -sitosterol-3-O- β -D-glucopyranoside)-6'-palmitate)

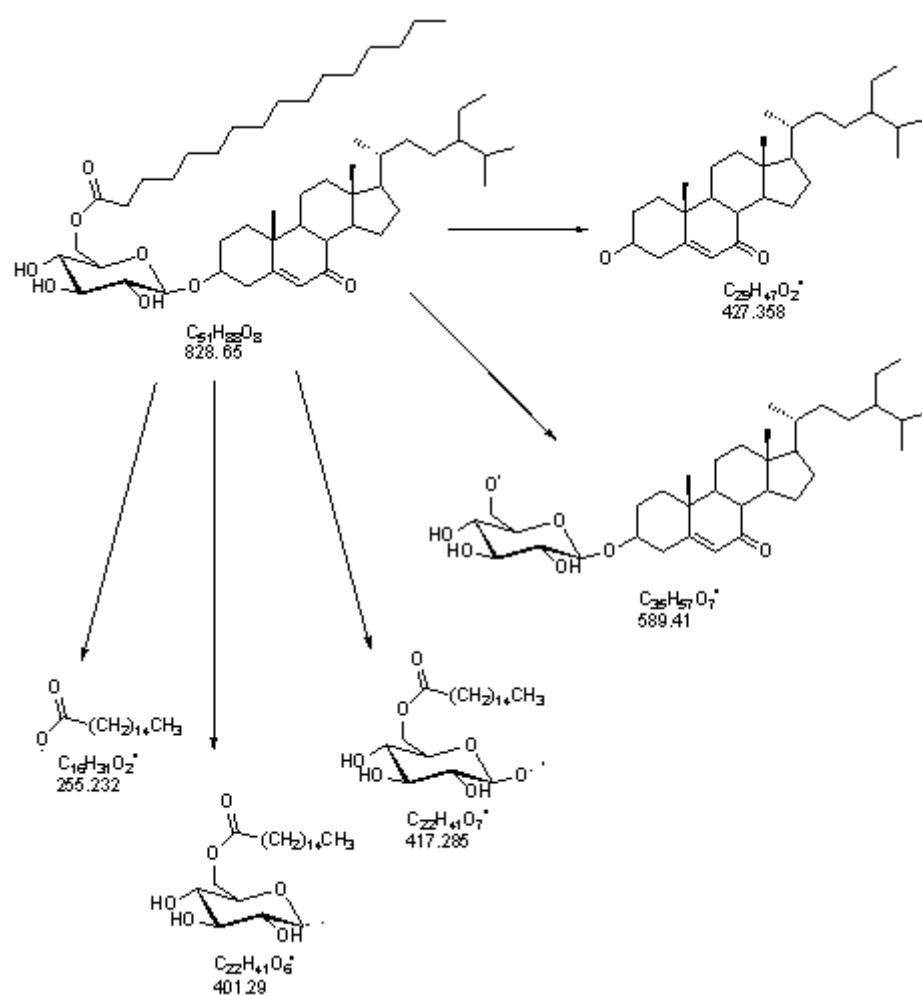


Figure S32: Some possible fragmentation patterns of **11** (7-oxo- β-sitosterol-3-O-β-D-glucopyranoside)-6'-palmitate)

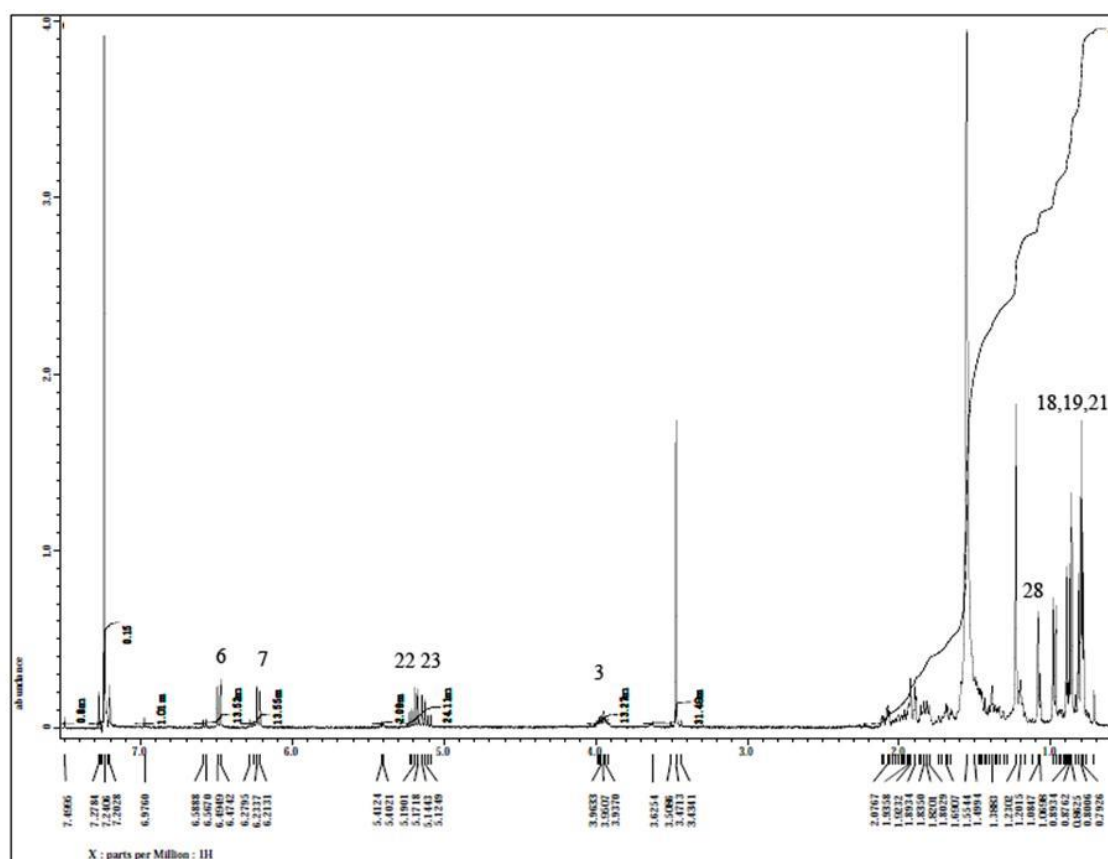


Figure S33: ^1H -NMR (400 MHz, CDCl_3) spectrum of **12** ($5\alpha, 8\alpha$ -epi-dioxyergosta-6, 22-dien- 3β -ol)

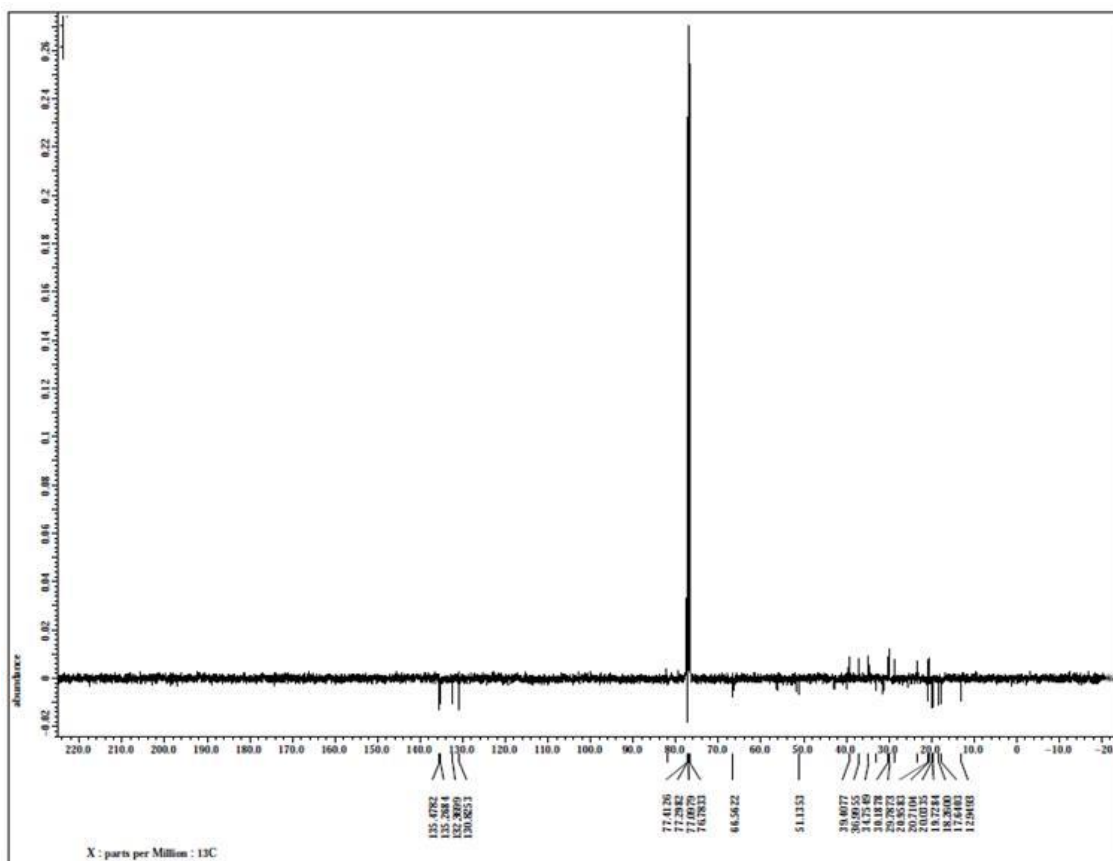


Figure S34: APT (100 MHz, CDCl_3) spectrum of **12** (5α , 8α -epi-dioxyergosta-6, 22-dien- 3β -ol)

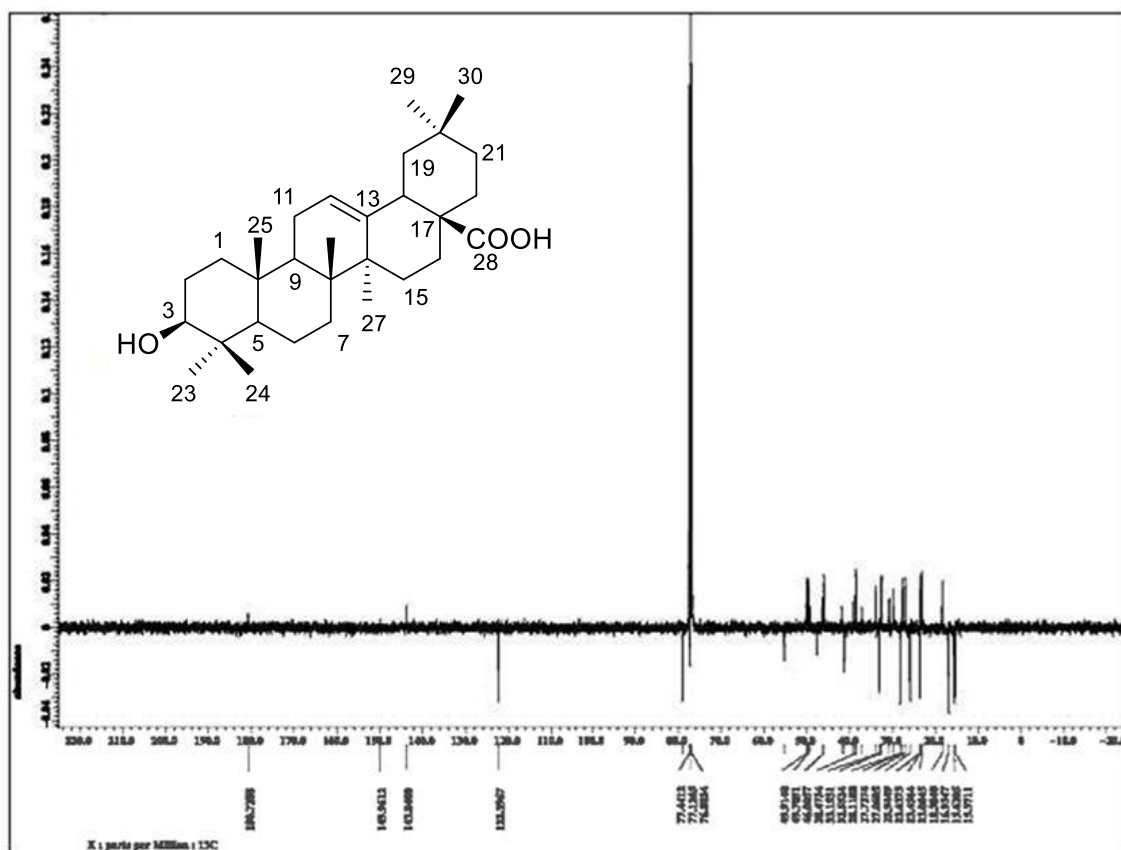


Figure S36: APT (100 MHz, CDCl₃) spectrum of **13** (oleanolic acid)

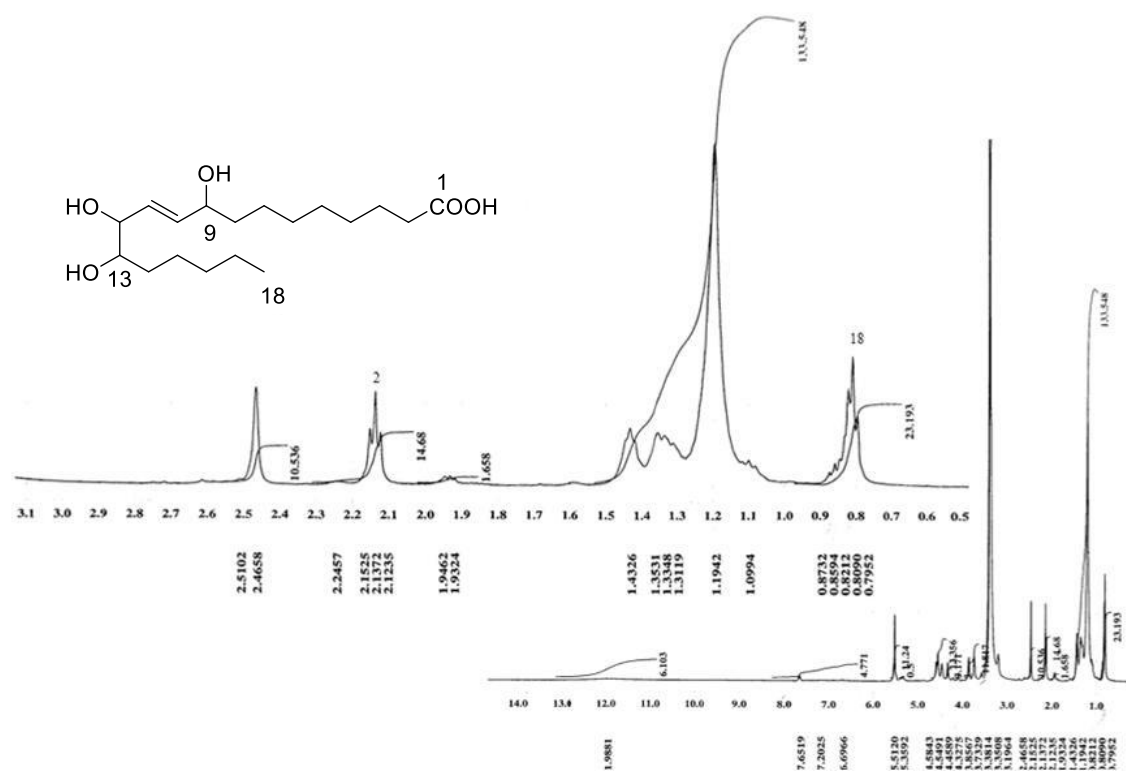


Figure S37: ^1H -NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of **14** (9, 12, 13-trihydroxy-10-octadecenoic acid)

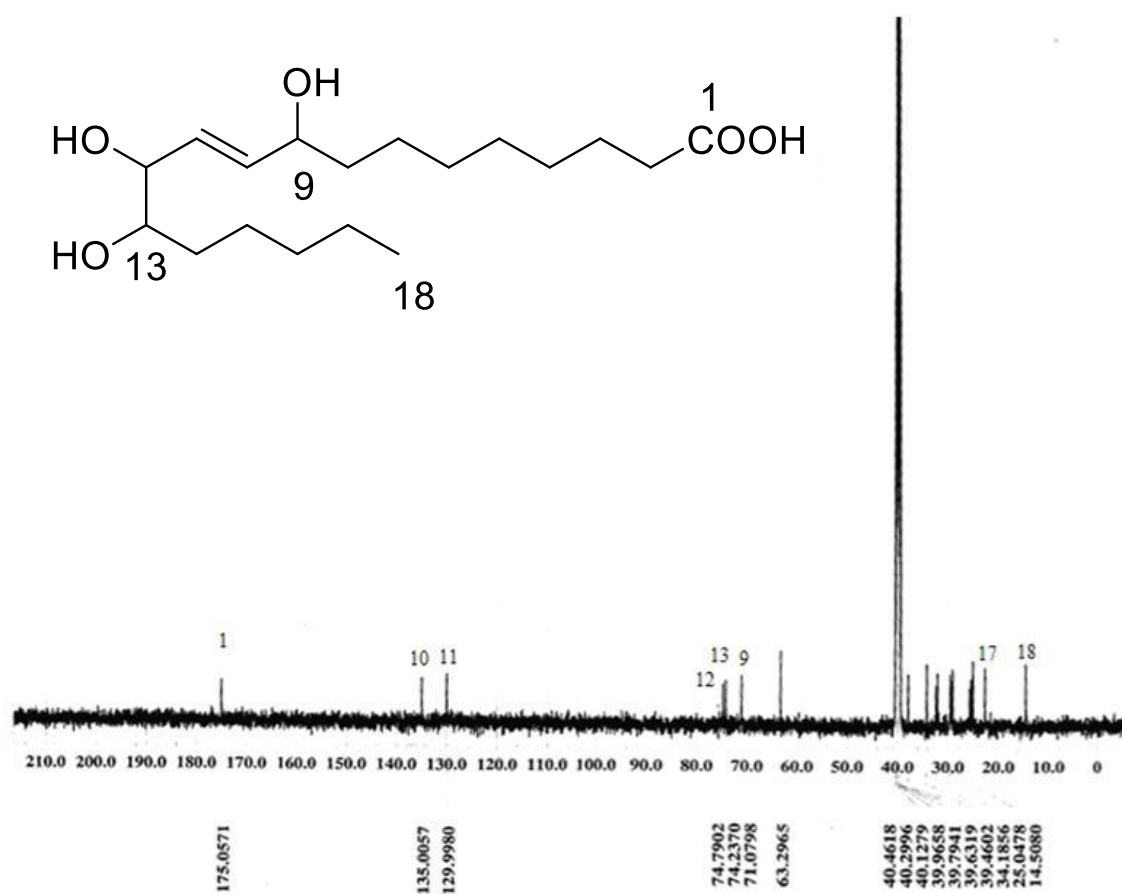


Figure S38: APT (125 MHz, DMSO- d_6) spectrum of **14** (9, 12, 13-trihydroxy-10-octadecenoic acid)

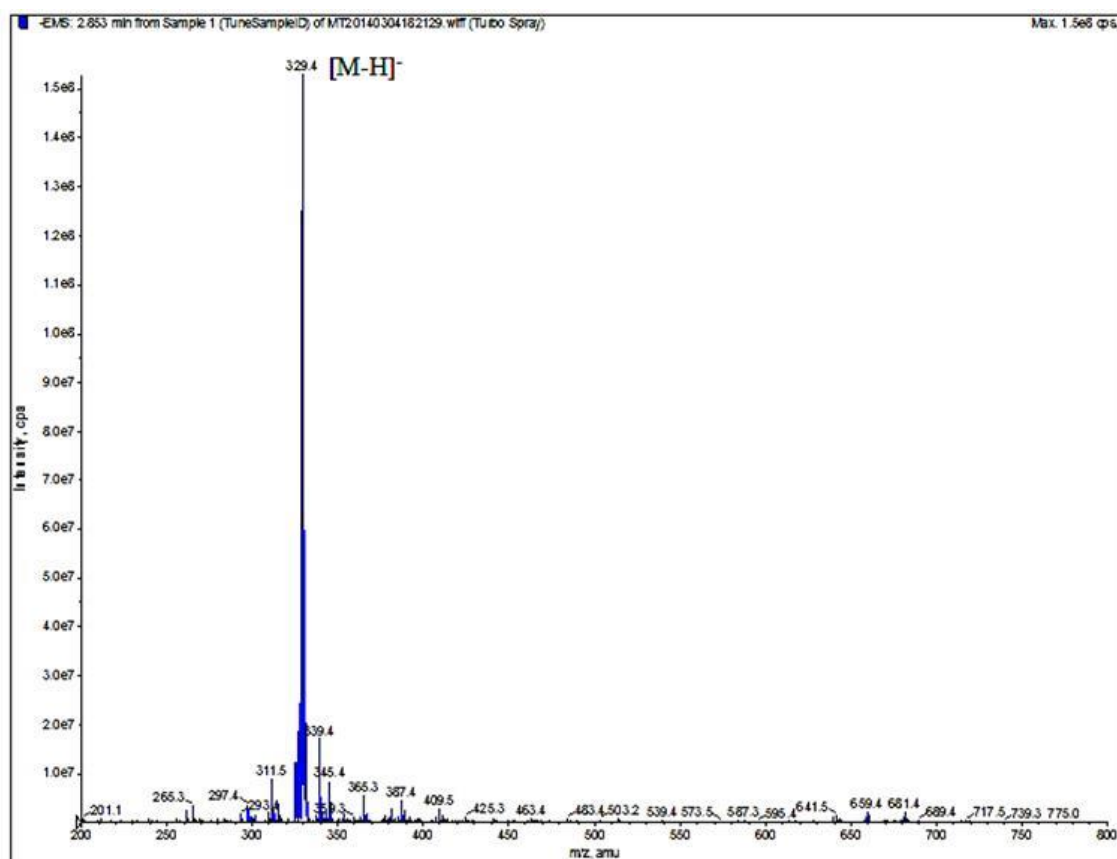


Figure S39: Negative ESI/EMS spectrum of **14** (9, 12, 13-trihydroxy-10-octadecenoic acid)

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

#	1		2		3	
	¹ H-NMR (400 MHz, DMSO- <i>d</i> ₆)	APT (100 MHz, DMSO- <i>d</i> ₆)	¹ H-NMR (400 MHz, CDCl ₃)	APT (100 MHz, CDCl ₃)	¹ H-NMR (400 MHz, CD ₃ OD)	¹³ C-NMR (100 MHz, CD ₃ OD)
1		131.7	--	128.1	--	134.1
2	7.25 (s, 2H)	106.2	7.18 (2H, s)	105.5	6.94 (H, br.s)	110.6
3	--	152.3	--	147.0	--	149.3
4	--	138.5	--	139.9	--	147.9
5	--	152.3	--	147.0	6.77 (H, <i>d</i> , <i>J</i> =8.2)	116.3
6	7.25 (s, 2H)	106.2	7.18 (2H, s)	105.5	6.83 (H, <i>d</i> , <i>J</i> =8.1)	119.9
7	--	199.2	--	200.0	5.4 (H, <i>d</i> , <i>J</i> =6.3)	90.3
8	7.25 (s, 2H)	30.9	2.89 (2H, <i>q</i>)	31.3	3.55 (H, <i>d</i> , <i>J</i> =5.8)	54.7
9	1.07 (3H, t)	8.2	1.14 (3H, <i>t</i>)	8.5	3.86 (9a), 3.83 (9b)	64.7
OCH₃	3.79 (6H, s)	56.9	3.86 (6H, s)	56.4	3.82 (3H, s)	56.5
1'	5.07 (H, <i>d</i> , <i>J</i> =7.6)	101.9	--	--	--	**
2'	3.00-3.59	74.1	--	--	7.62 (H, br.s)	120.8
3'	3.00-3.59	76.6	--	--	--	130.4
4'	3.00-3.59	69.8	--	--	--	153.8.
5'	3.00-3.59	77.3	--	--	--	145.3
6'	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.s)	115.4
7'	--	--	--	--	--	170.1
5'- OCH₃	--	--	--	--	3.89 (3H, s)	56.8

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

*H-6'a should appear at δ 3.84 (Güvenalp and Demirezer, 2005) but it is masked by the (OCH₃) signal, H-6'b should appear at δ 4.20 (H, *dd*) [1] instead it appeared at δ 4.31 (H, *t*).

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

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

4			5		
#	¹ H-NMR (400 MHz, CDCl ₃)	APT (100 MHz, CDCl ₃)	#	¹ H-NMR (400 MHz, CDCl ₃)	APT (100 MHz, CDCl ₃)
1	--	135.5	1,1'	--	136.8
2	6.49 (H, br.s)	100.0	2, 6, 2', 6'	6.45 (4H, s)	102.7
3	--	149.0	3, 5, 3', 5'	--	153.4
4	--	134.6	4,4'	--	137.4
5	--	143.5	7, 7'	4.72 (2H, <i>d</i>)	86.0
6	6.51 (H, br.s)	105.5	8, 8'	3.08 (2H, <i>m</i>)	54.2
7	4.69 (H, <i>d</i>)	85.9	9, 9'	α 4.28 (2H, <i>dd</i>) β 3.92 (2H, <i>dd</i>)	72.0
8	3.04 (H, <i>m</i>)	54.2	3,5, 3',5' OCH₃	3.84(12H, s)	56.2
9	α 3.86-3.88 (H, <i>dd</i>) β 4.21-4.27 (H, <i>dd</i>)	71.7	4,4' OCH₃	3.80 (6H,s)	60.9
1'	--	136.7			
2', 6'	6.53 (2H, s)	102.6			
3', 5'	--	153.2			
4'	--	137.1			
7'	4.69 (H, <i>d</i>)	85.8			
8'	3.04 (H, <i>m</i>)	54.2			
9'	α 3.86-3.88 (H, <i>dd</i>) β 4.21-4.27 (H, <i>dd</i>)	71.8			
OCH₂O	5.92 (2H,s)	101.4			
5-OCH₃	3.93 (3H,s)	56.6			
4'-OCH₃	3.85 (3H,s)	60.7			
3',5'-OCH₃	3.88 (6H,s)	56.0			

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

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

6			7			8		
#	¹ H-NMR (400 MHz, CDCl ₃)	¹³ C- NMR (100 MHz, CDCl ₃)	#	¹ H-NMR (400 MHz, CD ₃ OD)	¹³ C-NMR (100 MHz, CD ₃ OD)	#	¹ H-NMR (400 MHz, CD ₃ OD)	¹³ C-NMR (100 MHz, CD ₃ OD)
1,1'	--	132.0	1	--	130.9	2	7.84 (H, s)	133.3
2, 6, 2', 6'	6.57 (4H, s)	102.6	2	7.29 (H, s)	115.9	3	--	108.7
3, 5, 3', 5'	--	147.1	3	--	147.3	3a	--	127.5
4,4'	--	134.2	4	--	153.8	4	7.96 (H, <i>d</i> , <i>J</i> =7.3)	121.9
7, 7'	4.72 (2H, <i>d</i>)	86.1	5	6.90 (H, <i>d</i> , <i>J</i> =7.3)	116.3	5	7.08 (2H, <i>dd</i>)	122.2
8, 8'	3.1 (2H, <i>m</i>)	54.2	6	7.30 (H, <i>d</i> , <i>J</i> =8.6)	126.5	6	7.08 (2H, <i>dd</i>)	123.5
9, 9'	α 4.27 (2H, <i>br.</i>) β 3.90 (2H) *	71.7	7	9.86 (H, s)	193.2	7	7.33 (H, <i>d</i> , <i>J</i> =8.4)	112.8
3,5, 3',5' OCH₃	3.90 (12H, s) *	56.3				7a	--	138.1
4, 4' OH	5.56(2H, s)					8	1.2 (3H, s)	30.7

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

* 9β, 9'β protons (2H, δ 3.90) are masked by the methoxy protons (12H, δ 3.90), they appear collectively at δ 3.90 (14H, s)

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

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

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

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

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

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

* *J* value couldn't be calculated.

Table S6: ¹H-NMR and APT spectral data of **12** (5 α , 8 α -epi-dioxyergosta-6, 22-dien-3 β -ol).

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

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

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

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

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

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

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

The chemical shift (δ) 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% CO₂ 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 1.0×10^4 cells/ well at 37°C for 24 hr under 5% CO₂. 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® microplate reader (Winooski, VT, USA). The relative cell viability in percentage was calculated as $(A_{570 \text{ nm}} \text{ of treated samples} / A_{570 \text{ nm}} \text{ of untreated sample}) \times 100$. Statistical analysis of the data was performed using Microsoft Excel software version 2010.

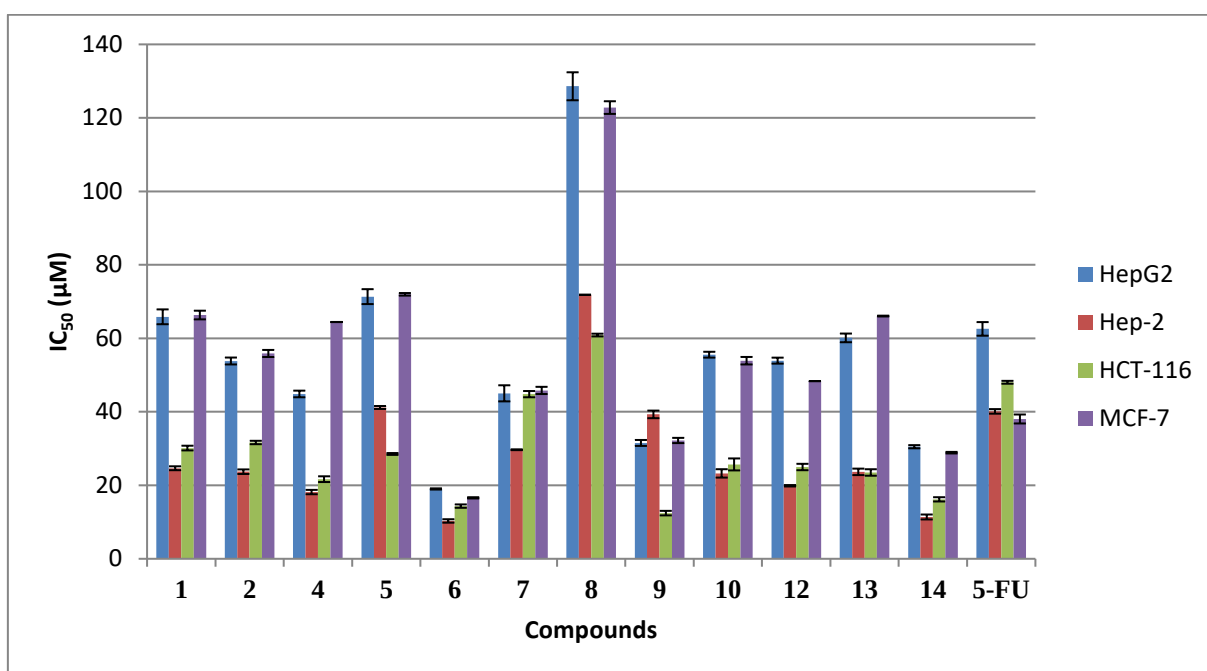


Figure S40. Calculated IC_{50} (μM) for the *in vitro* cytotoxicity of **1-14**

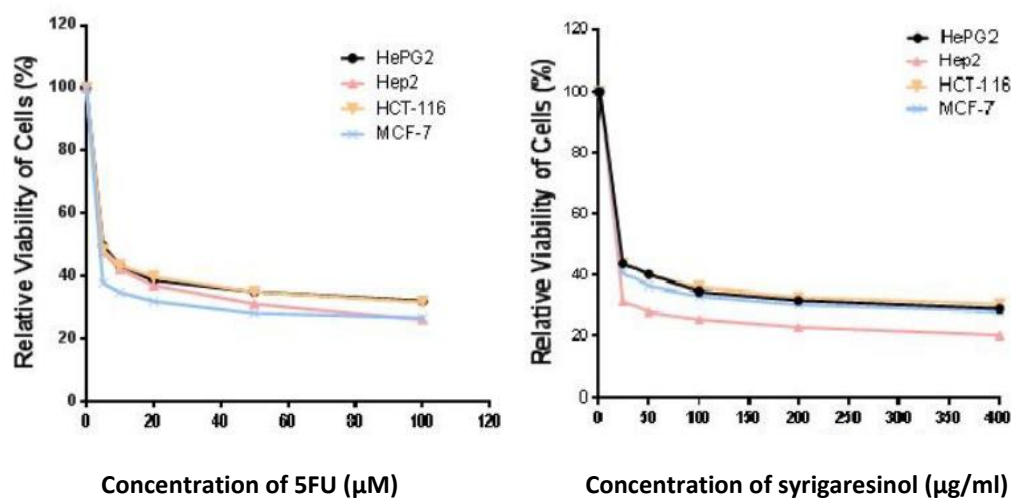


Figure S41: The log concentration- cell viability graph of 5FU and **6** (syringaresinol).

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