

Supporting information

Prenylated isoflavanones with antimicrobial potential from the root bark of *Dalbergia melanoxylon*

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(3*S*)-3,4',5,7-Tetrahydroxyl-2'-methoxy-3'-(4-hydroxyl-3-methylbut-2-enyl)-isoflavanone (1**)**

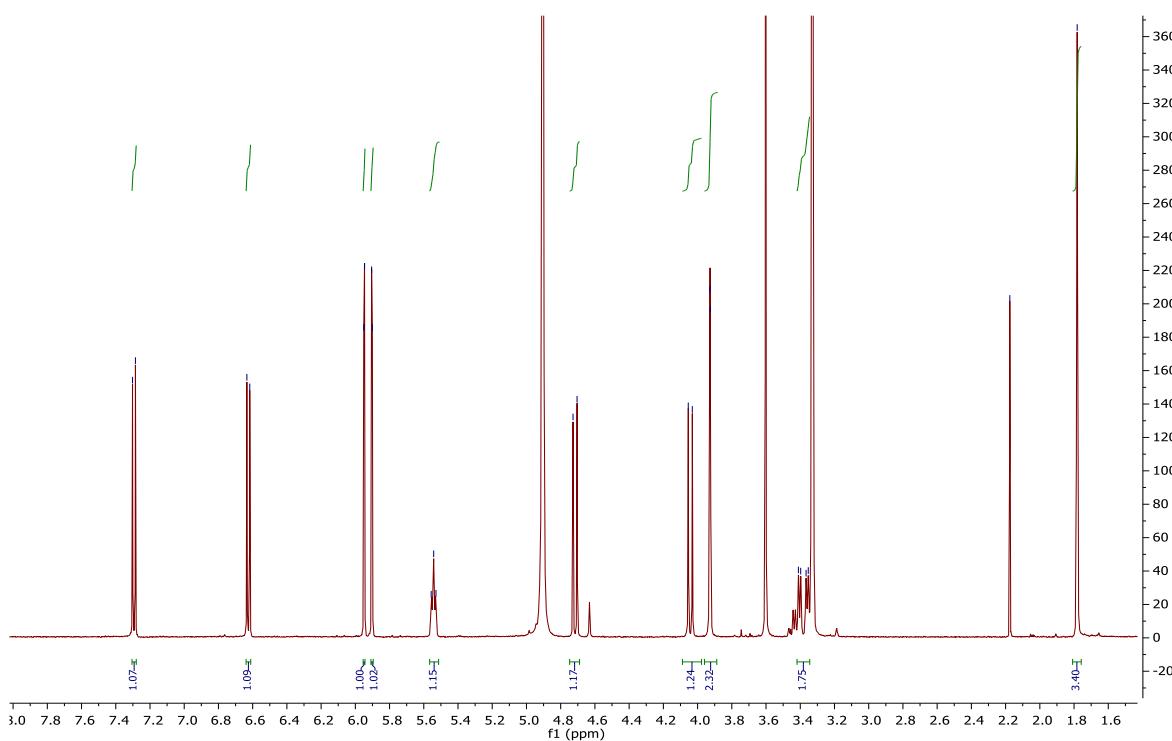


Figure S1_1: ^1H NMR spectrum (500 MHz, CD_3OD) of compound **1**

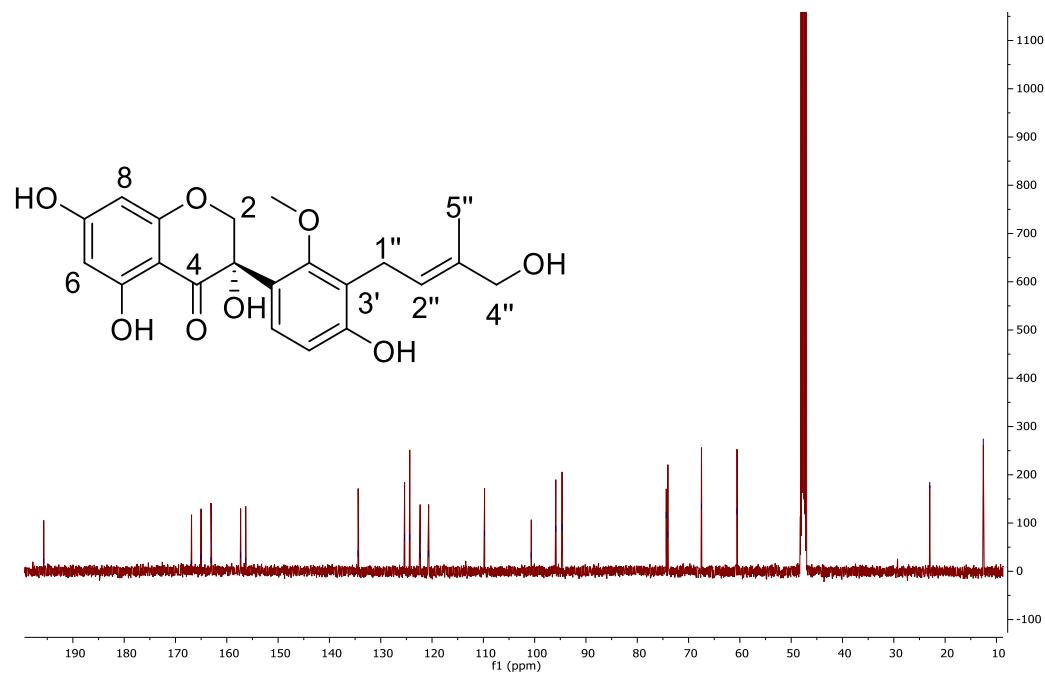


Figure S1_2: ^{13}C NMR spectrum (125 MHz, CD_3OD) of compound **1**

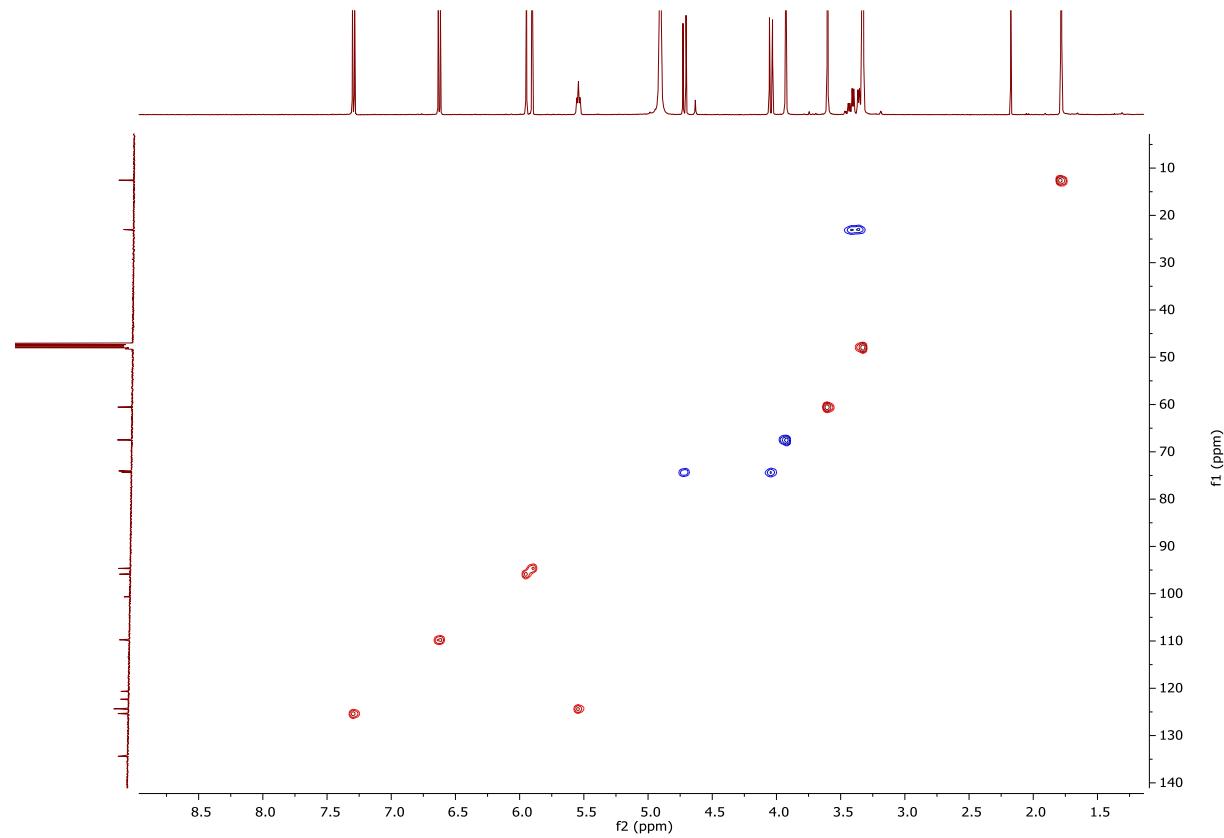


Figure S1_3: HSQCAD spectrum (125 MHz, CD₃OD) of compound **1**

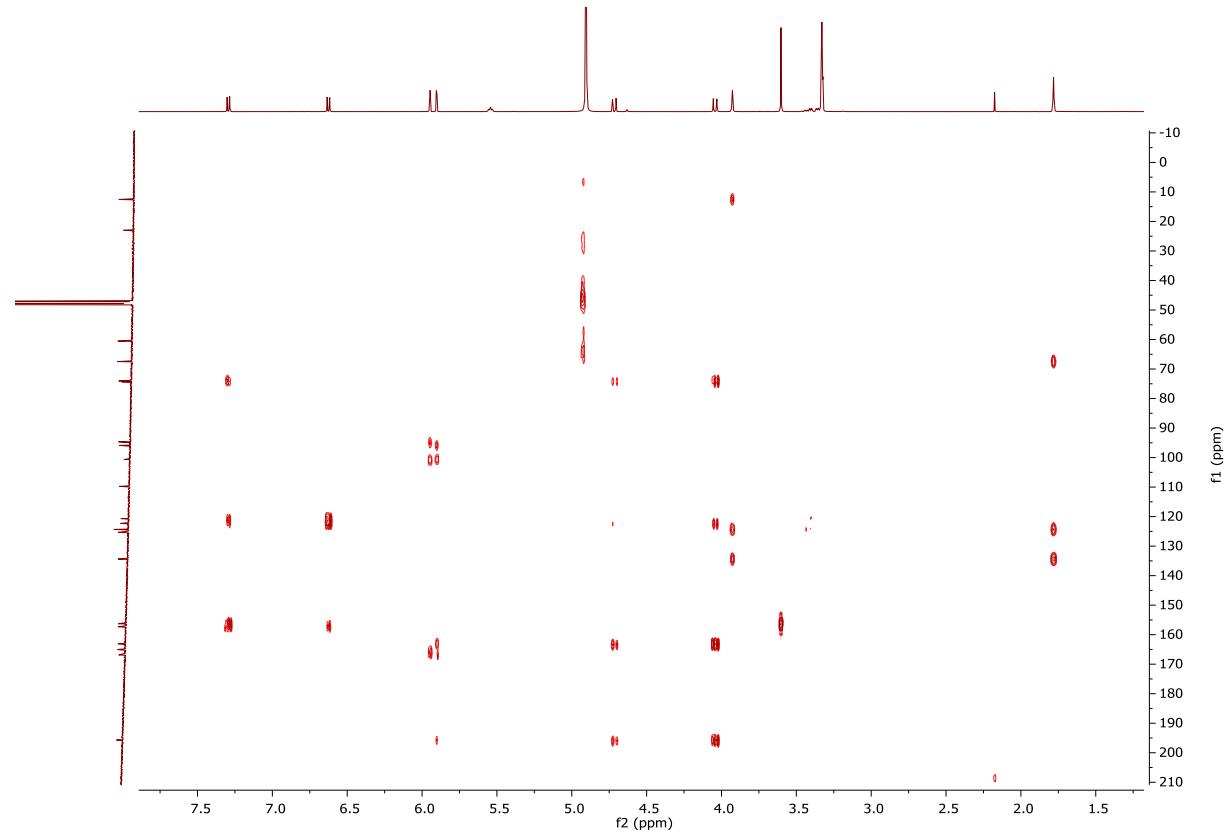


Figure S1_4: HMBC spectrum (125 MHz, CD₃OD) of compound **1**

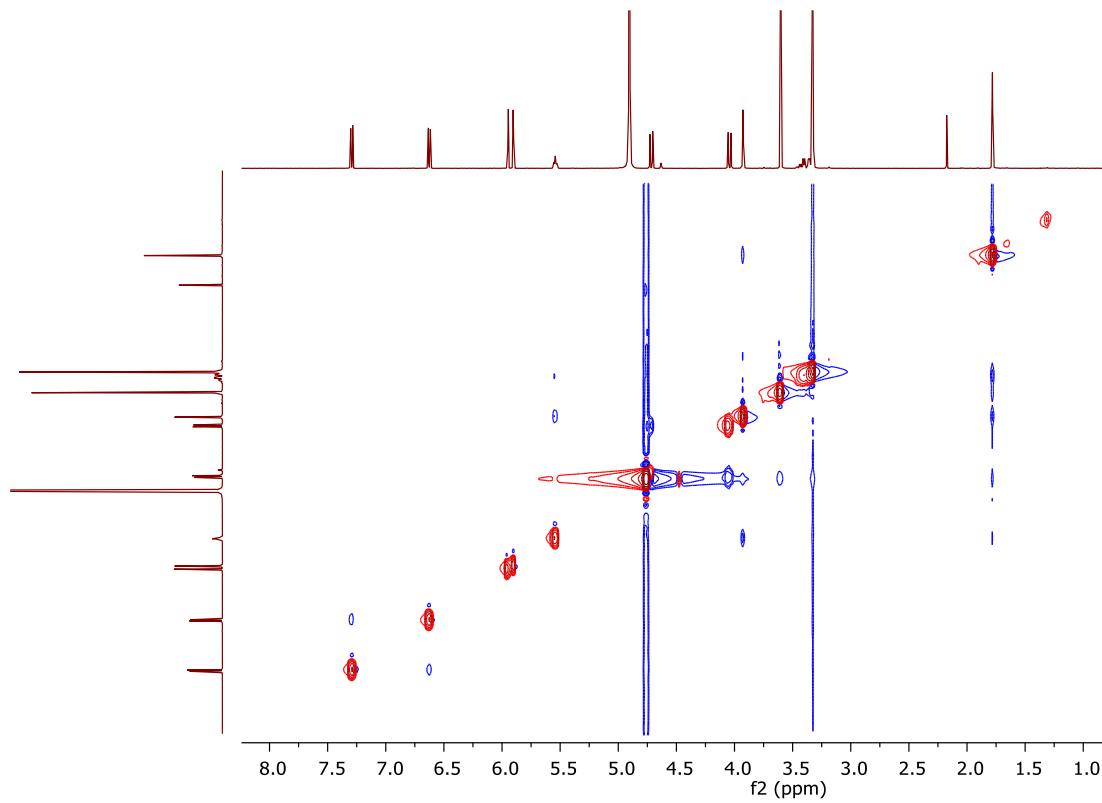


Figure S1_5: NOESY spectrum (125 MHz, CD₃OD) of compound **1**

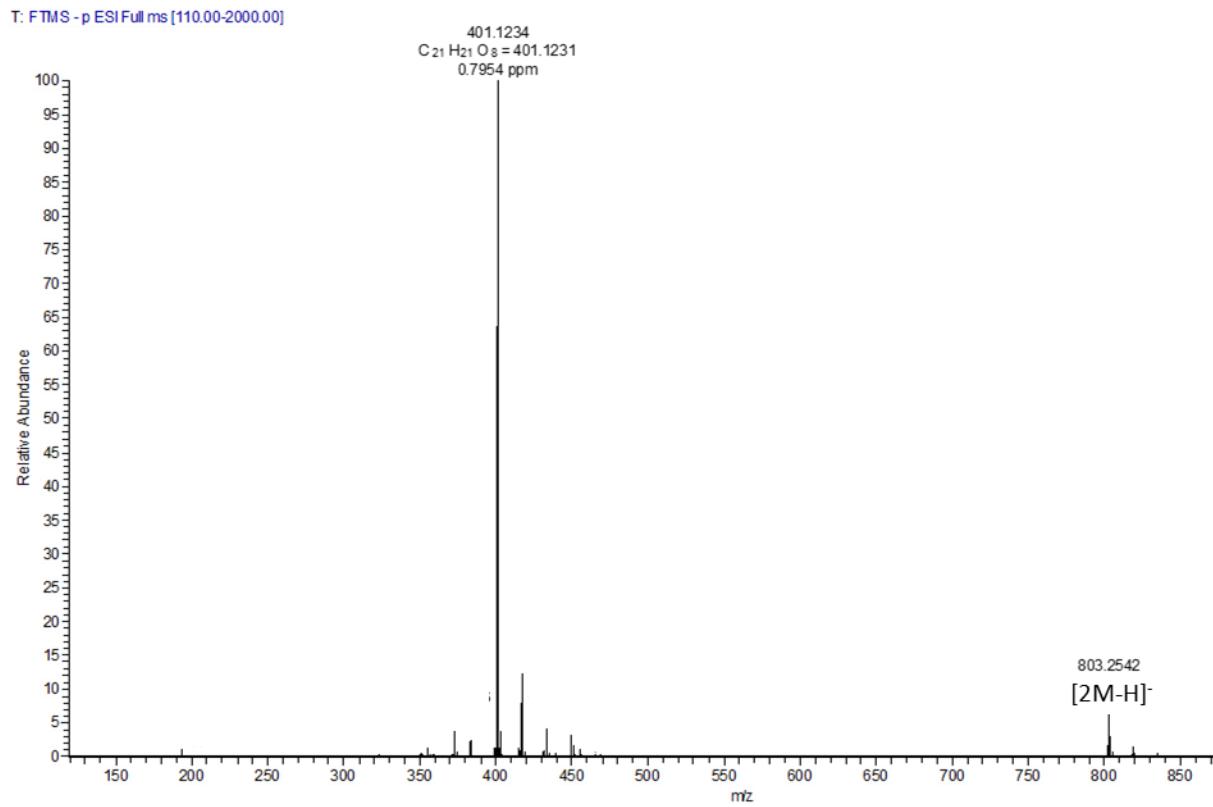


Figure S1_6: Negative ion ESI-HRMS spectrum of compound **1**

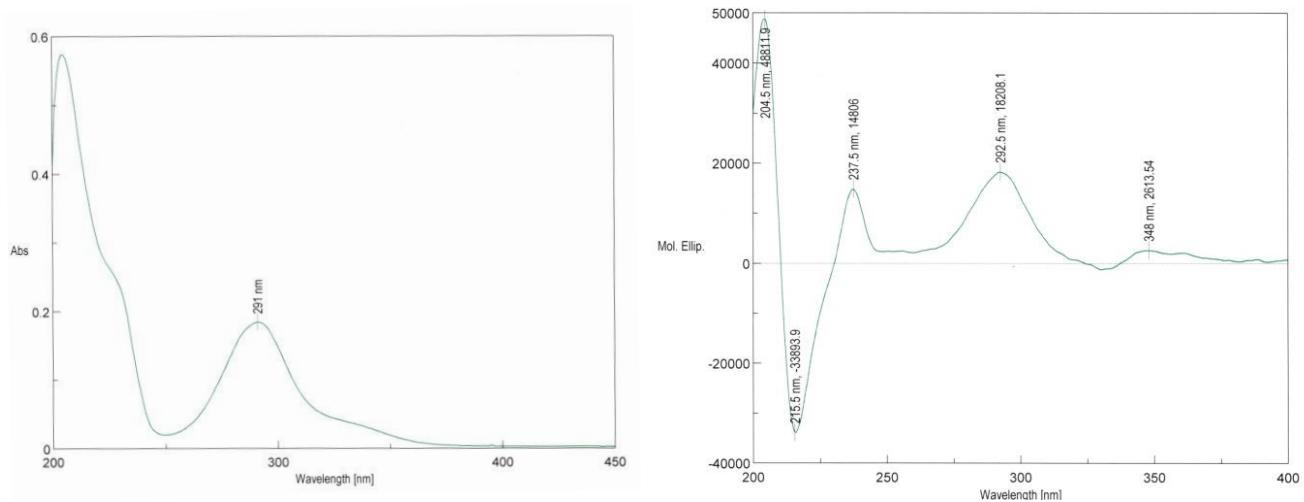


Figure S1_7: UV and CD spectra (MeOH) of compound **1**

Table S1: NMR data of compound **1**

No	δ_{H} ,* mult (J in Hz)	δ_{C}	HMBC	COSY	NOESY
2	A: 4.70, <i>d</i> (11.8) B: 4.03, <i>d</i> (11.8)	75.8	CH ₂ C2B, C3, C9, C1', C4 C2A, C3, C1', C9, C4	H2B H2A	H2B, 2'-OCH ₃ H2A
3		75.4	C		
4		197.1	C=O		
5		166.4	C		
6	5.93, <i>d</i> (2.0)	97.3	CH C8, C10,	H8	
7		168.3	C		
8	5.88, <i>d</i> (2.0)	96.1	CH C6, C10, C7, C4	H6	
9		164.5	C		
10		102.1	C		
1'		123.7	C		
2'		157.7	C		
3'		122.1	C		
4'		158.7	C		
5'	6.61, <i>d</i> (8.5)	111.2	CH C1', C3', C4'	H 6'	H6'
6'	7.27, <i>d</i> (8.5)	126.8	CH C3, C1', C2', C4', C3'	H 5'	H5'
1''	A: 3.40, <i>dd</i> (14.9/6.4) B: 3.33, <i>dd</i> (14.9/6.4)	24.4	CH ₂ C3', C2''	H 2''	
2''	5.52, <i>t-like</i> (6.4)	125.8	CH C4'', C5''	H 1''	H4''
3''		135.8	C		
4''	3.91, <i>s</i>	68.9	CH ₂ C5'', C2'', C3''		H5'', H2''
5''	1.76, <i>s</i>	14.0	CH ₃ C3'', C4'', C2''		H4''
2'-OCH ₃	3.58, <i>s</i>	62.0	CH ₃ C2'		H2A
5-OH	12.09, <i>s</i>				

*referenced to methanol-*d*4 solvent signal

(3*R*)-6-Geranyl-4',5,7-trihydroxyl-2'-methoxy-3'-prenylisoflavanone (2)

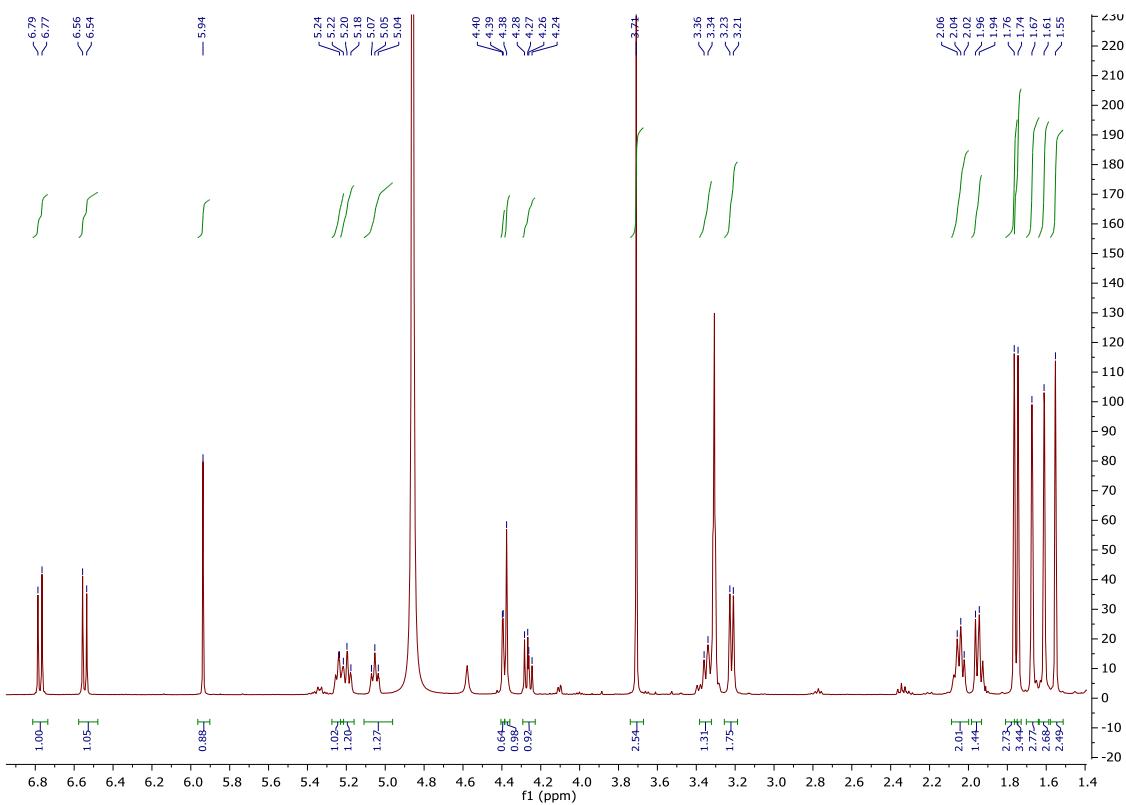


Figure S2_1: ^1H NMR spectrum (500 MHz, CD_3OD) of compound 2

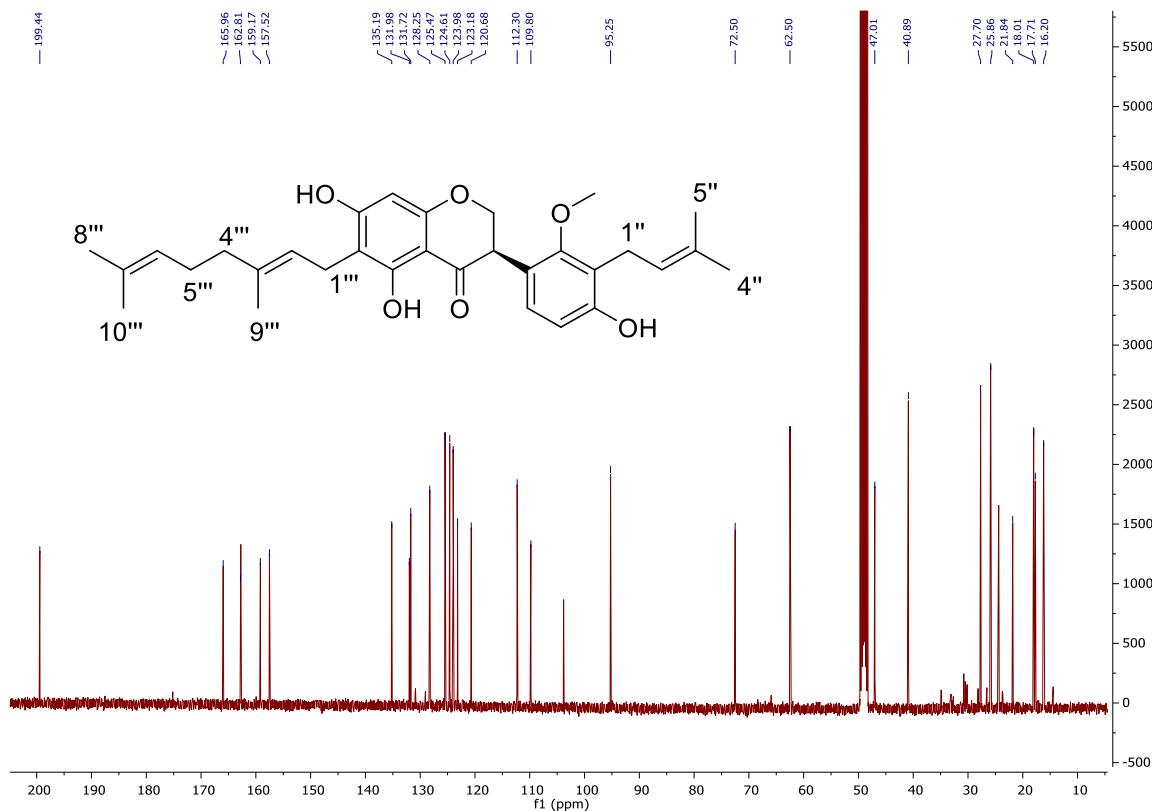


Figure S2-2: ^{13}C NMR spectrum (125 MHz, CD_3OD) of compound 2

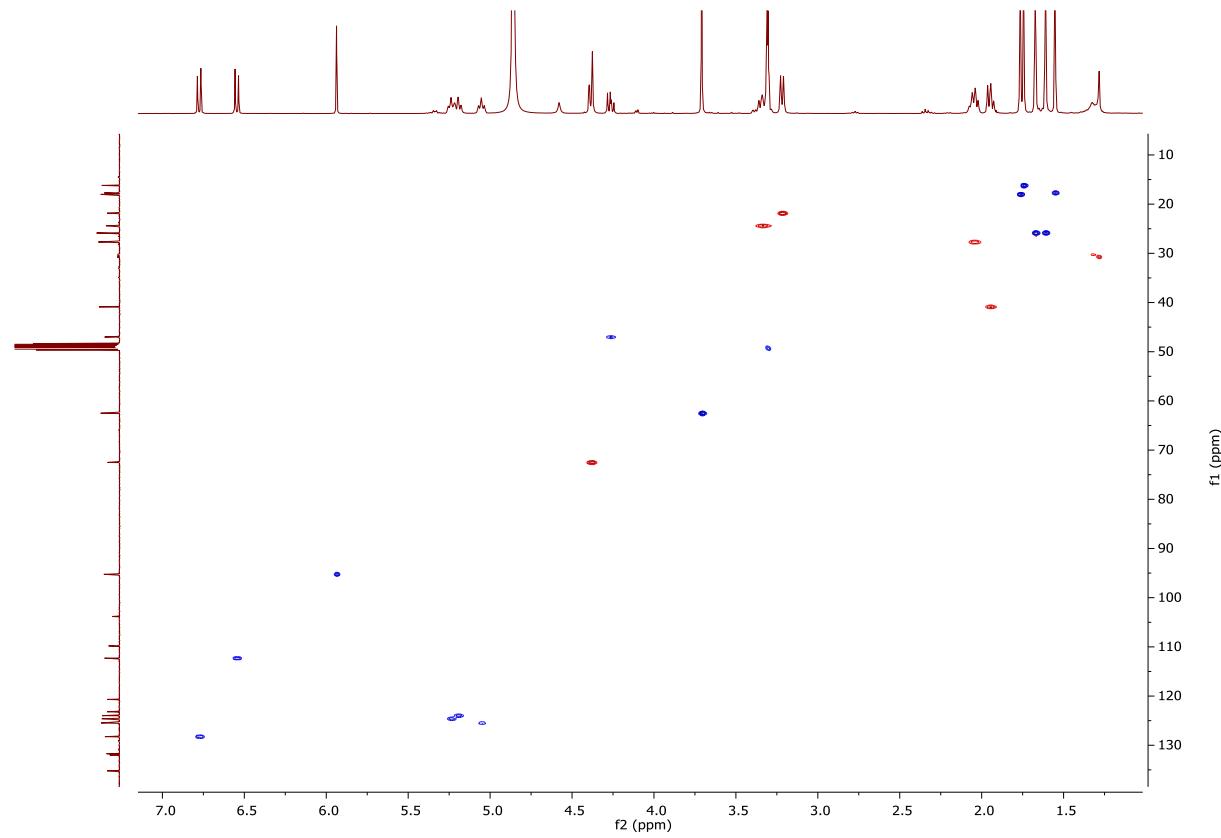


Figure S2_3: HSQCAD spectrum (125 MHz, CD_3OD) of compound 2

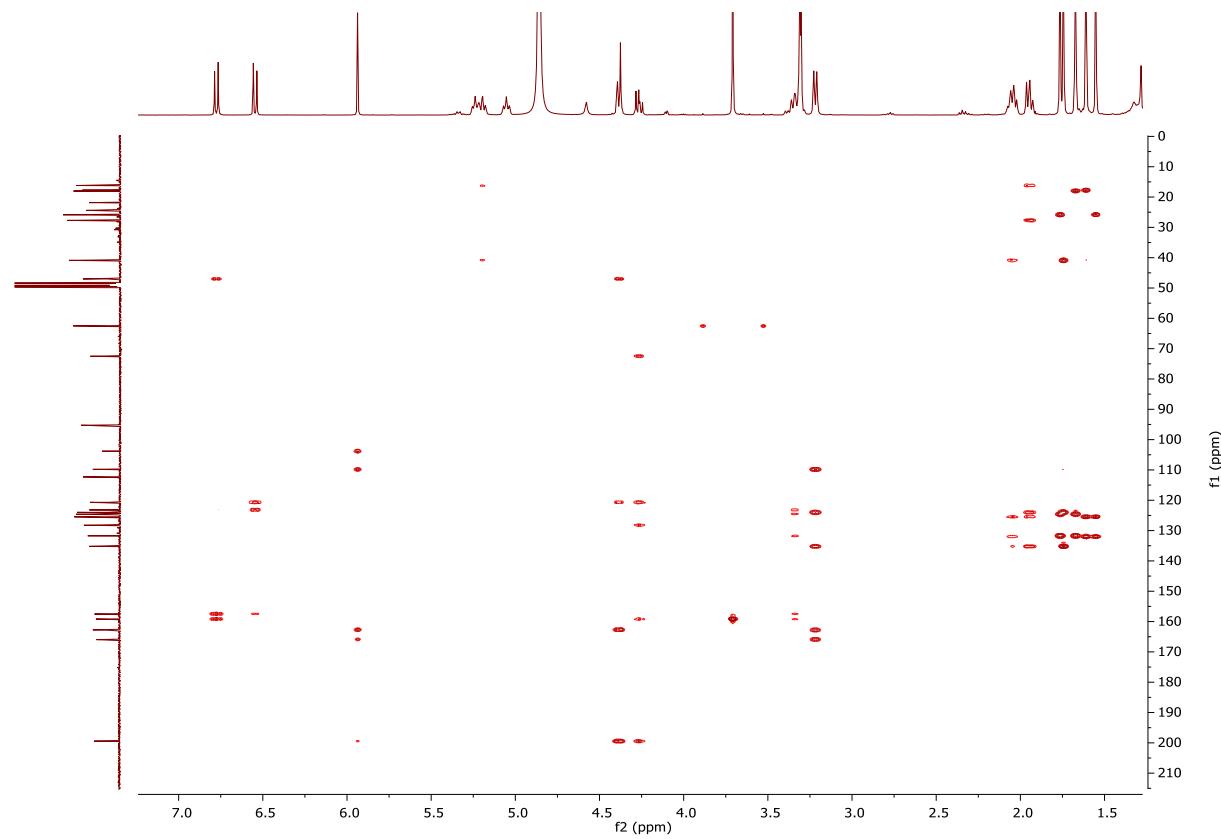


Figure S2_4: HMBC spectrum (125 MHz, CD_3OD) of compound 2

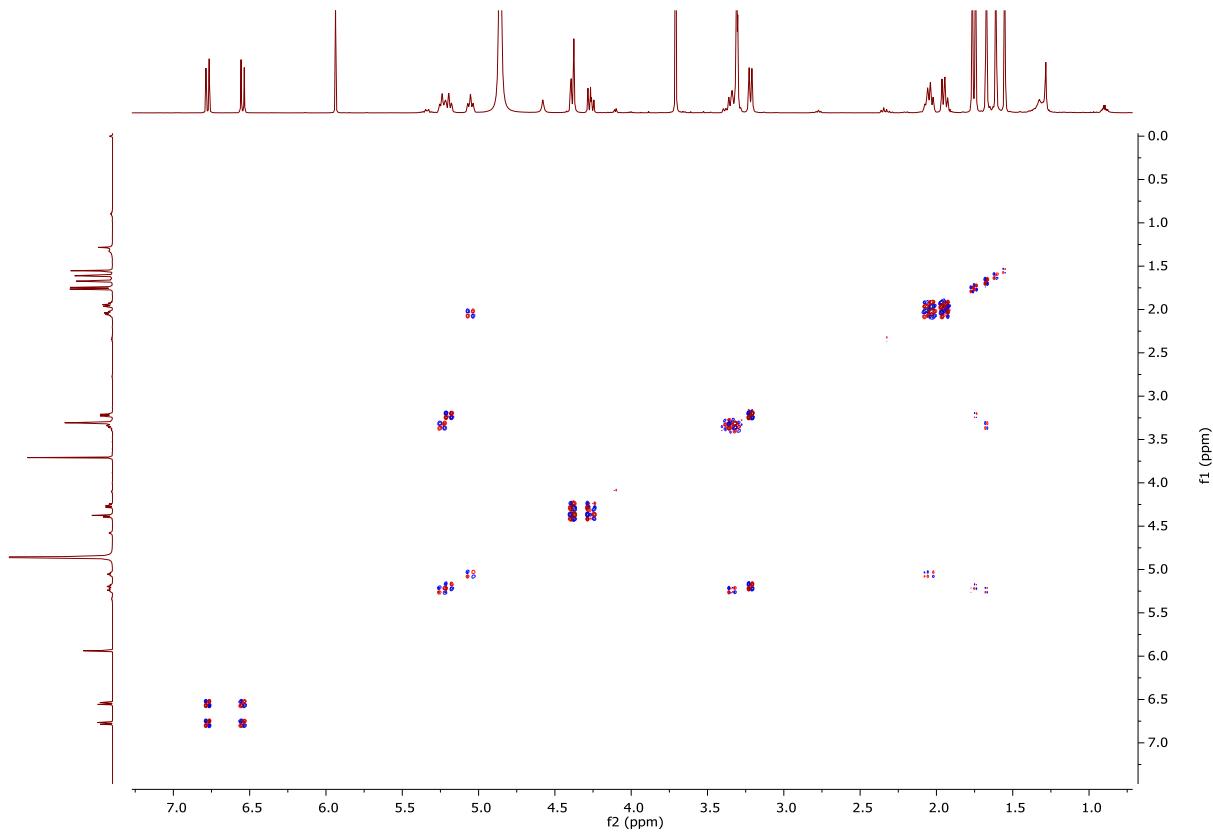


Figure S2_5: COSY spectrum of compound 2

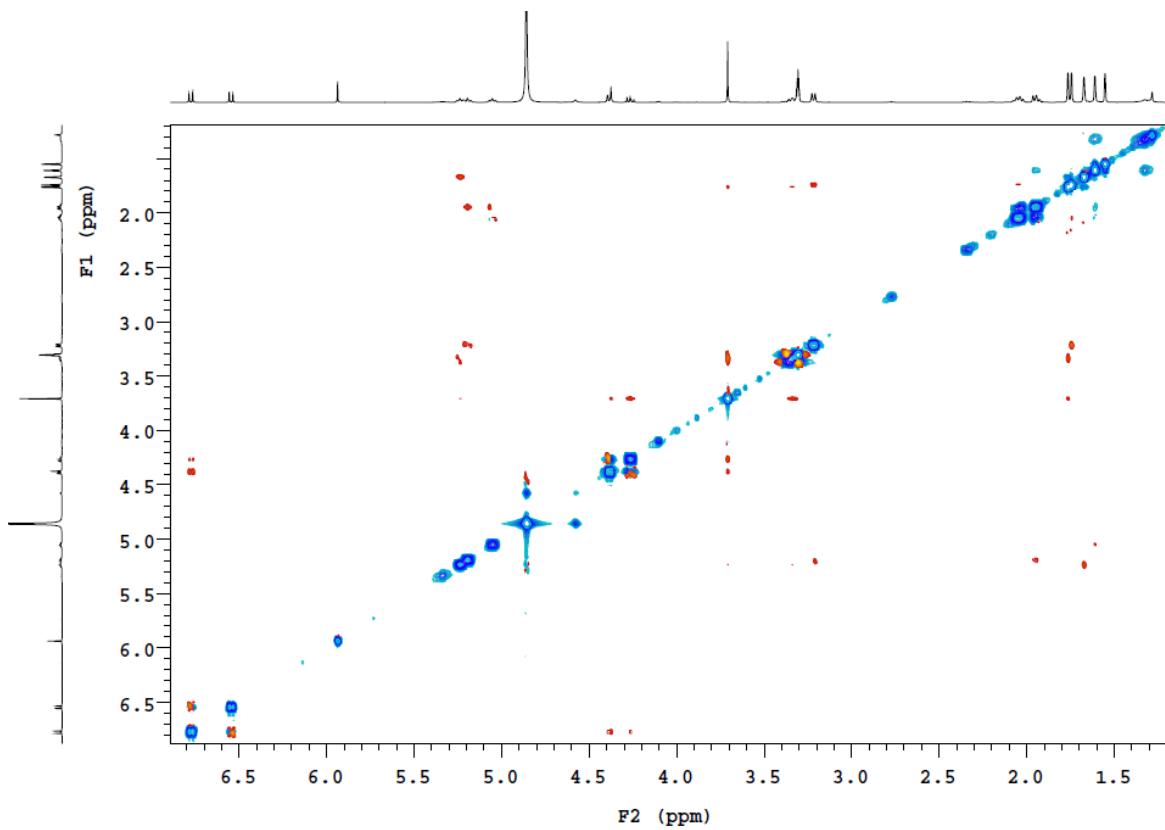


Figure S2_6: ROESY spectrum of compound 2

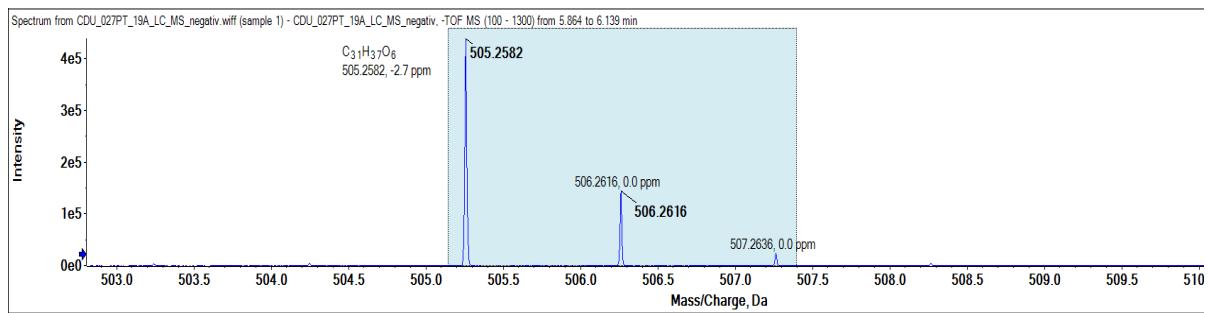


Figure S2_7: Negative ion ESI-HRMS spectrum of compound 2

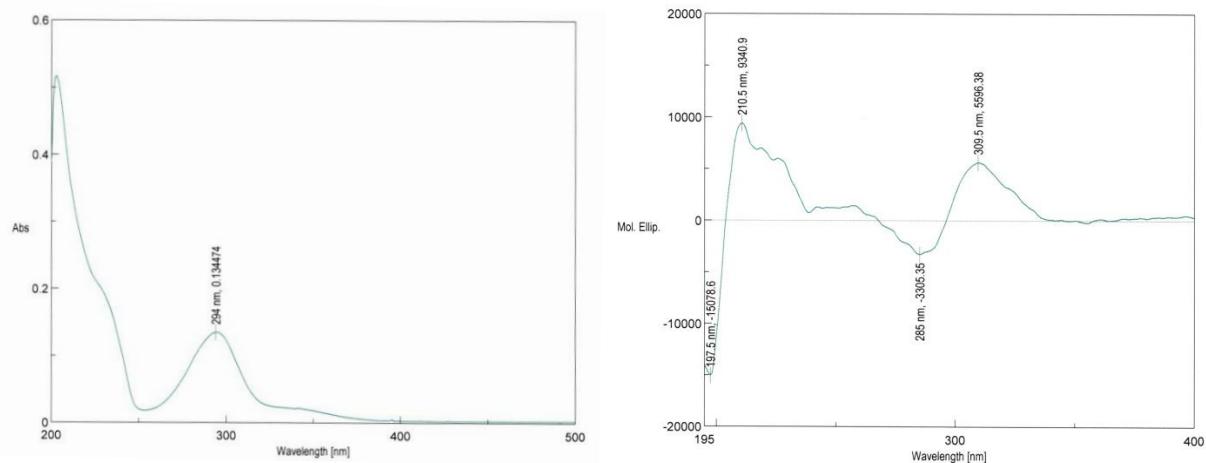


Figure S2_8: UV and CD spectra (MeOH) of compound 2

Table S2: NMR data of compound 2

No	δ_H , mult (J in Hz)	δ_C	HMBC (H → C)	COSY	NOESY
2	A: 4.40, <i>d</i> (8.9) B: 4.39, <i>d</i> (6.7)	72.5	CH ₂ C4, C3, C1', C9 C4, C3, C1', C9	H2B, H3 H2A, H3	H2B, H3 H2A, H3
3	4.26, <i>dd</i> (8.9/6.7)	47.0	CH C4, C2' C1', C6'	H2A/2B	H2A/2B
4		199.4	C=O		
5		162.8	C		
6		109.8	C		
7		166.0	C		
8	5.94, <i>s</i>	95.3	CH C9, C10, C6, C4, C7		
9		162.8	C		
10		103.8	C		
1'		120.7	C		
2'		159.2	C		
3'		123.2	C		
4'		157.5	C		
5'	6.55, <i>d</i> (8.4)	112.3	CH C1', C6', C3', C4'	H6'	H6'
6'	6.78, <i>d</i> (8.4)	128.3	CH C3, C5', C1', C4, C2'	H5'	H5'
1''	A: 3.37, <i>dd</i> (14.4/6.7) B: 3.30 (under solvent signal)	24.4	CH ₂ C4', C2', C2'', C3', C3''	H2''	H5''
2''	5.24, <i>t-like</i> (6.7)	124.6	CH C4'', C5''	H1''	H4''
3''		131.7	C		
4''	1.68, <i>s</i>	25.9	CH ₃		H2 ''
5''	1.76, <i>s</i>	18.0	CH ₃ C2'', C3''		H1''
1'''	3.22, <i>d</i> (7.2)	21.8	CH ₂ C7, C5, C3'', C2'', C6	H2'''	H9'''
2'''	5.20, <i>t-like</i> (7.2)	124.0	CH C9'', C4'', C1''	H1'''	H4'''
3'''		135.2	C		
4'''	1.95, <i>m</i>	40.9	CH ₂ C9'', C5'', C3'', C6'', C2''	H5'''	H2'', H5'', H6''
5'''	2.05, <i>m</i>	27.7	CH ₂ C4'', C6'', C3''	H6'', H4''	H4'', H6''
6'''	5.05, <i>br t</i> (6.8)	125.5	CH C8'', C10'', C5''	H5'''	H5'', H4'', H8''
7'''		132.0	C		
8'''	1.61, <i>s</i>	25.9	CH ₃ C10'', C6'', C7''		H6''
9'''	1.74, <i>s</i>	16.2	CH ₃ C4'', C3'', C2''		H1'''
10'''	1.55, <i>s</i>	17.7	CH ₃ C8'', C6'', C5''		
2''-OCH ₃	3.71, <i>s</i>	62.5	CH ₃ C2		H1'', H2'', H2B, H3
5-OH	12.41, <i>s</i>				

6-((2E,5E)-7-Hydroxyl-3,7-dimethyl-octa-2,5-dienyl)-4',5,7-trihydroxy-2'-methoxy-3'-prenylisoflavanone (3)

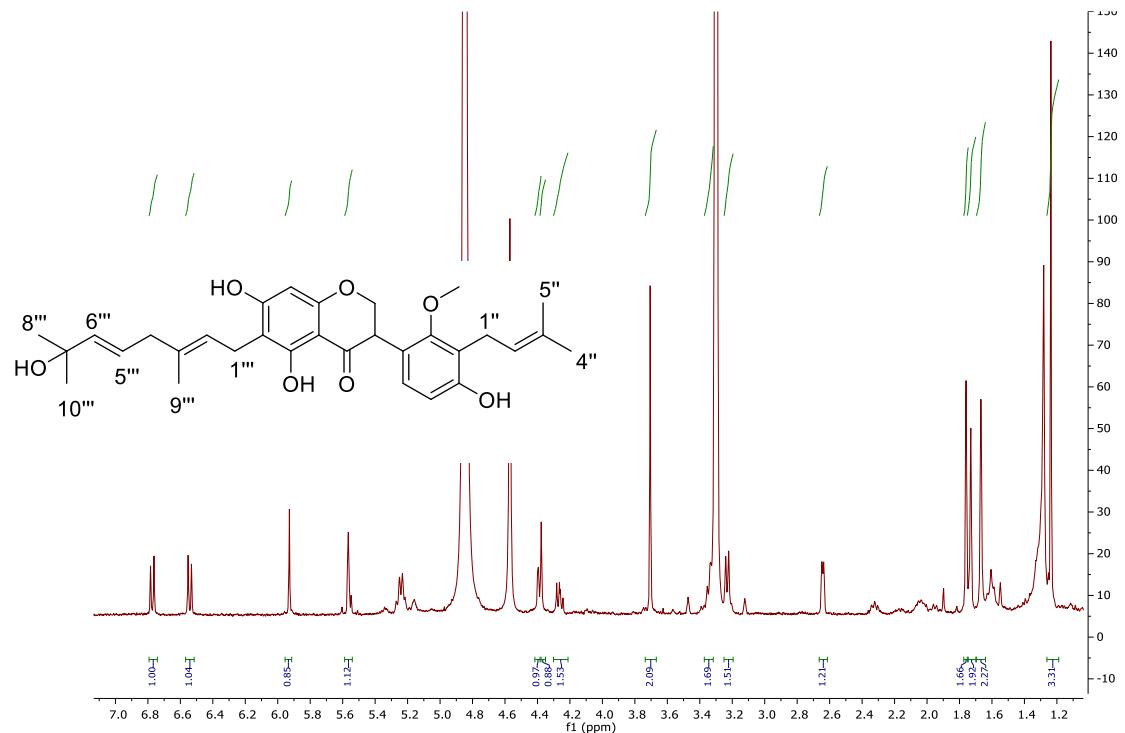


Figure S3_1: ¹H NMR spectrum (600 MHz, CD₃OD) of compound 3

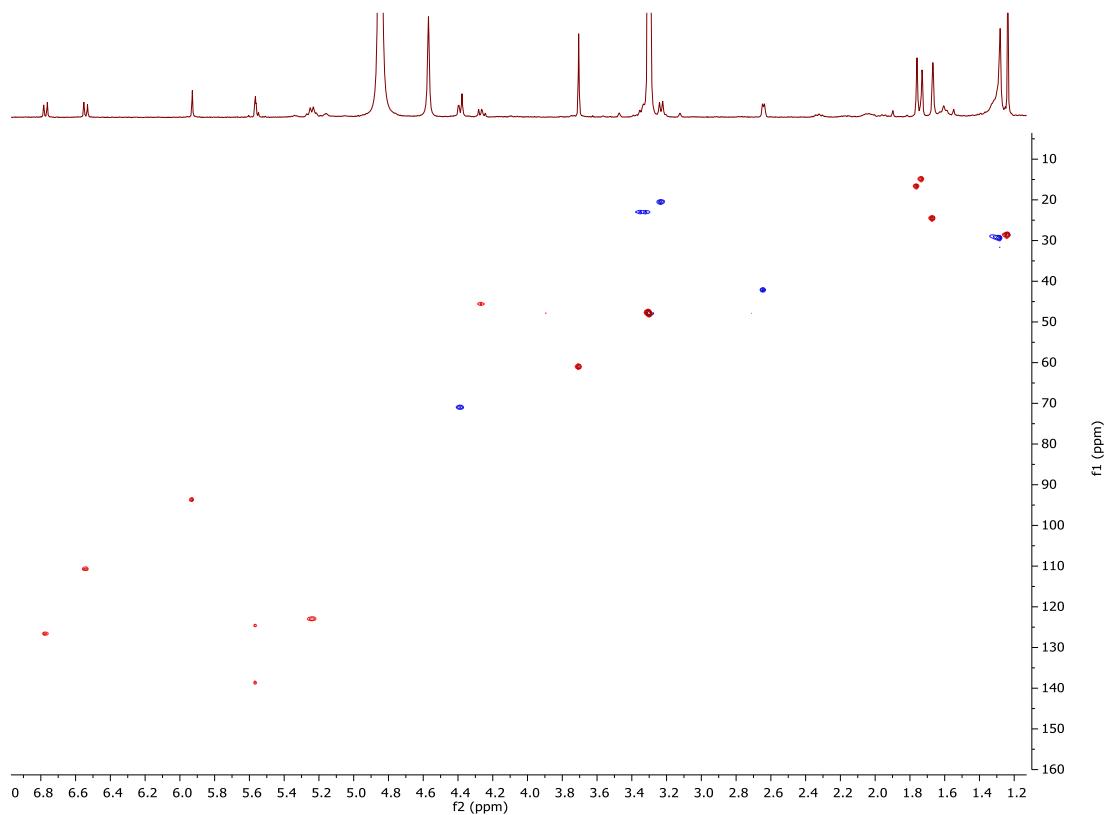


Figure S3_2: HSQCAD spectrum (125 MHz, CD₃OD) of compound 3

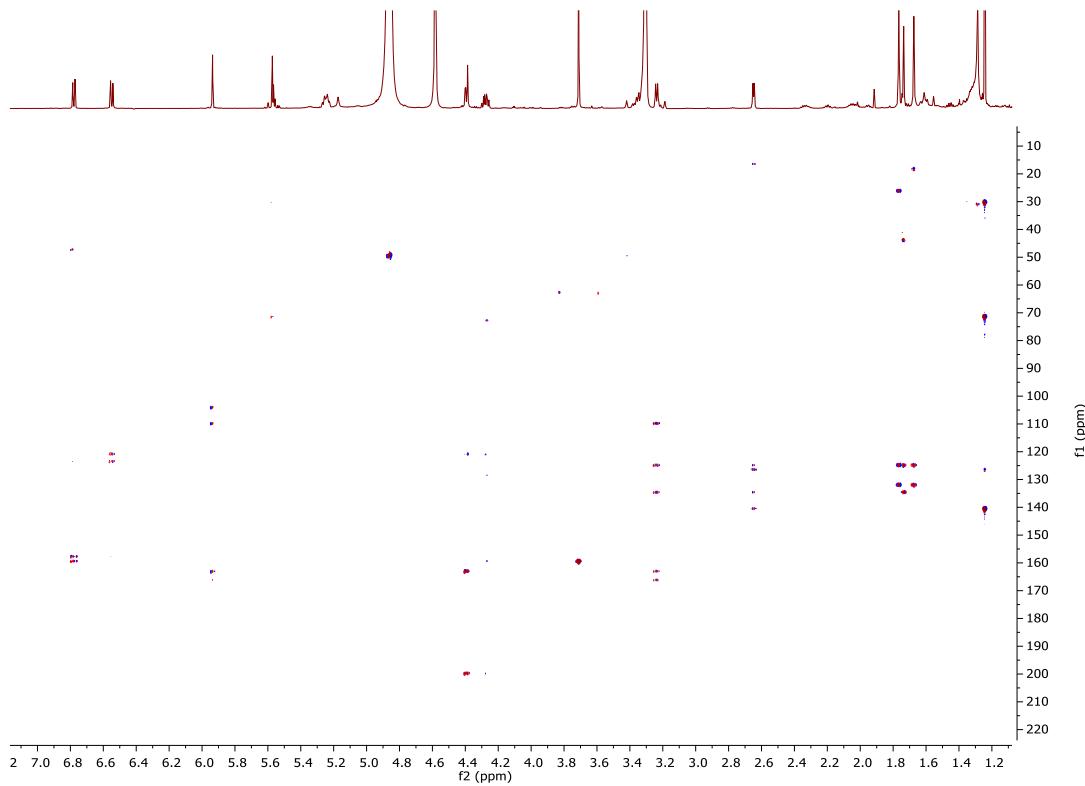


Figure S3_3: HMBC spectrum (125 MHz, CD_3OD) of compound 3

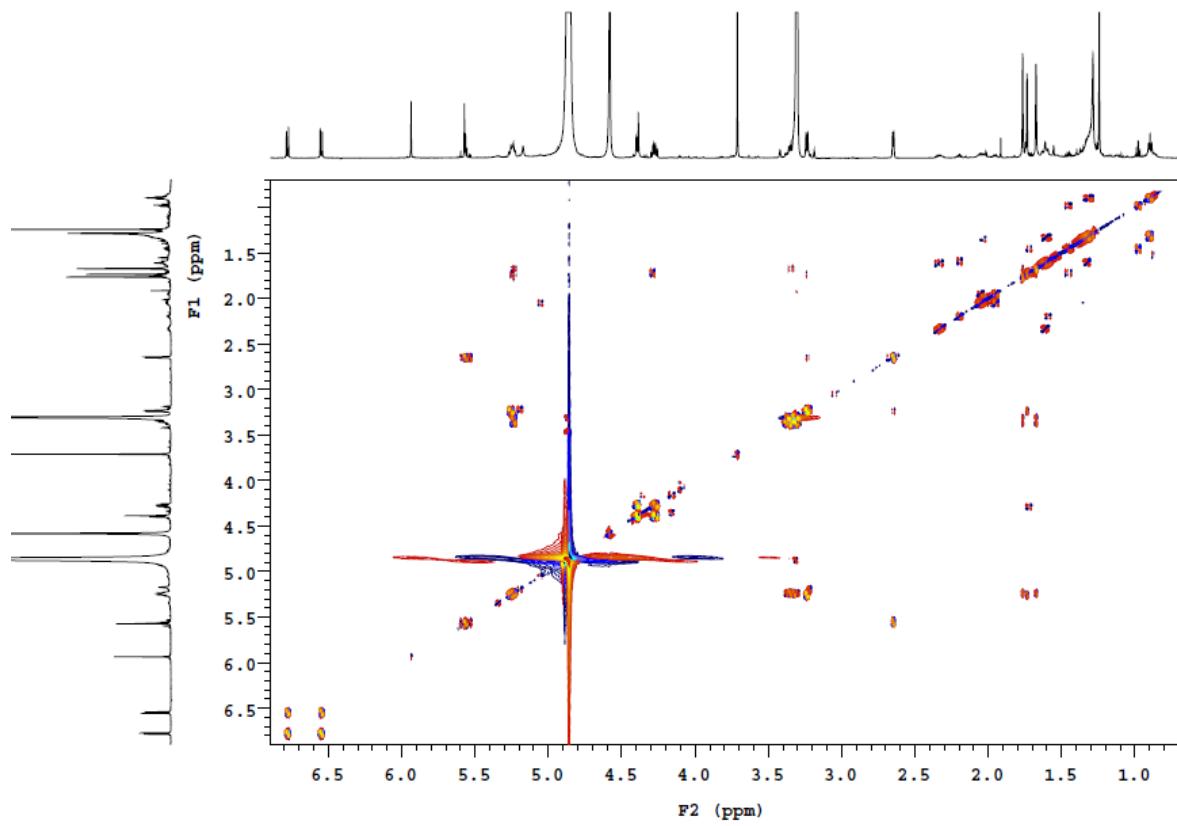


Figure S3_4: COSY spectrum (125 MHz, CD_3OD) of compound 3

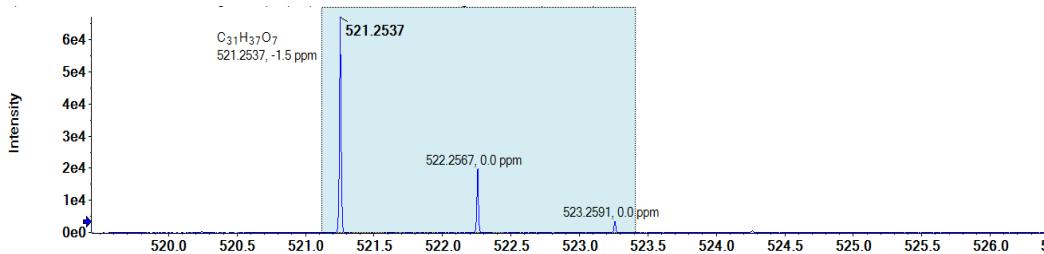


Figure S3_5: Negative ion ESI-HRMS spectrum of compound **3**

Table S3: NMR data of compound **3**

No	δ_H , mult (J in Hz)	δ_C	HMBC	COSY
2	A: 4.39, d (8.9) B: 4.38, d (6.8)	72.0 ^a	CH ₂ C9, C3, C4, C1' C9, C3, C4, C1'	H2B, H3 H2A, H3
3	4.24, dd (8.9/6.8)	46.8 ^a	CH C2', C4, C1', C2	H2A, H2B
4		199.6 ^b	C=O	
5		162.9 ^b	C	
6		109.8 ^b	C	
7		166.1 ^b	C	
8	5.94, s	94.8 ^a	CH C4, C6, C7	
9		162.9 ^b	C	
10		103.9 ^b	C	
1'		120.8 ^b	C	
2'		159.3 ^b	C	
3'		123.3 ^b	C	
4'		157.7 ^b	C	
5'	6.55, d (8.4)	111.9 ^a	CH C1', C3', C4', C2'	H6'
6'	6.78, d (8.4)	127.8 ^a	CH C3, C3', C4', C2'	H5'
1''	A: 3.36, dd (14.8/7.1) B: 3.32, under solvent	24.2 ^a	CH ₂ C3', C2', C4', C2'', C3''	H2''
2''	5.24, br t	124.2 ^a	CH	H1''
3''		131.4 ^b	C	
4''	1.67, s	25.6 ^a	CH ₃ C5'', C2'', C3''	
5''	1.77, s	17.8 ^a	CH ₃ C4'', C2'', C3''	
1'''	3.24, d (7.3)	21.7 ^a	CH ₂ C6, C2'', C3'', C7, C5	H2'''
2'''	5.25, br t	124.2 ^a	CH	H1'''
3'''		134.5 ^b	C	
4'''	2.65, br d (4.5)	43.4 ^a	CH ₂ C9'', C2'', C6'', C7''	H5'''
5'''	5.57, m	126.0 ^a	CH C4'',	H4'''
6'''	5.57, m	139.8 ^a	CH C4'', C7'', C8''/10''	
7'''		71.3 ^b	C	
8'''	1.24, s	29.6 ^a	CH ₃ C10'', C6'', C7''	
9'''	1.74, s	16.0	CH ₃ C4''	
10'''	1.24 s	29.6 ^a	CH ₃ C8'', C6'', C7''	
2''-OCH ₃	3.71, s	62.2 ^a	CH ₃ C2'	
5-OH	12.41, s			

Signals derived from ^aHSQC and ^bHMBC.

(E)-6-(6-Hydroxyl-3,7-dimethylocta-2,7-dienyl)-4',5,7-trihydroxyl-2'-methoxy-3'-prenylisoflavanone (4)

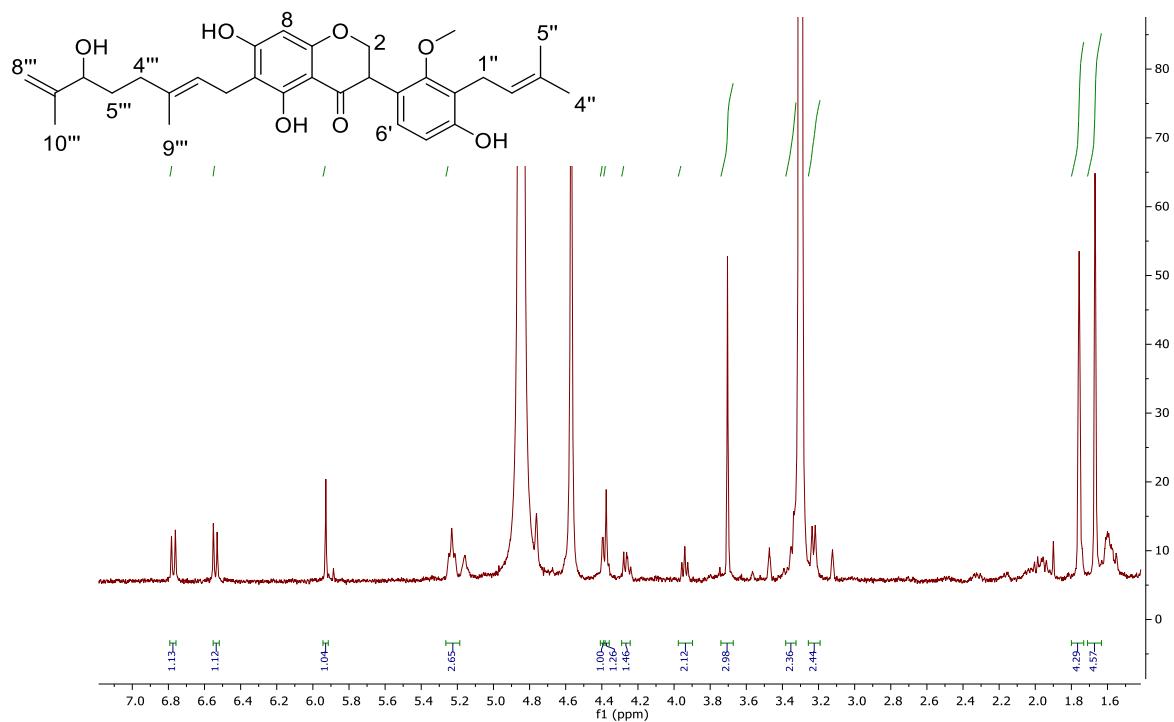


Figure S4_1: ¹H NMR spectrum (600 MHz, CD₃OD) of compound 4

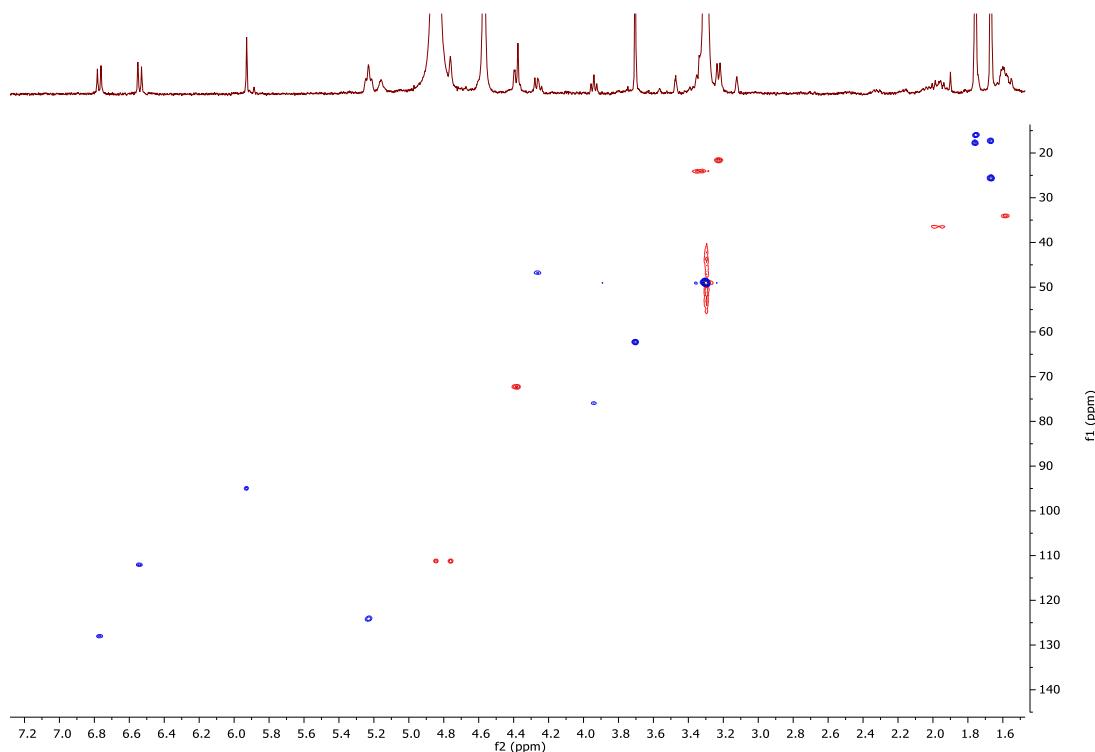


Figure S4_2: HSQCAD (NUS 50%) spectrum (600 MHz, CD₃OD) of compound 4

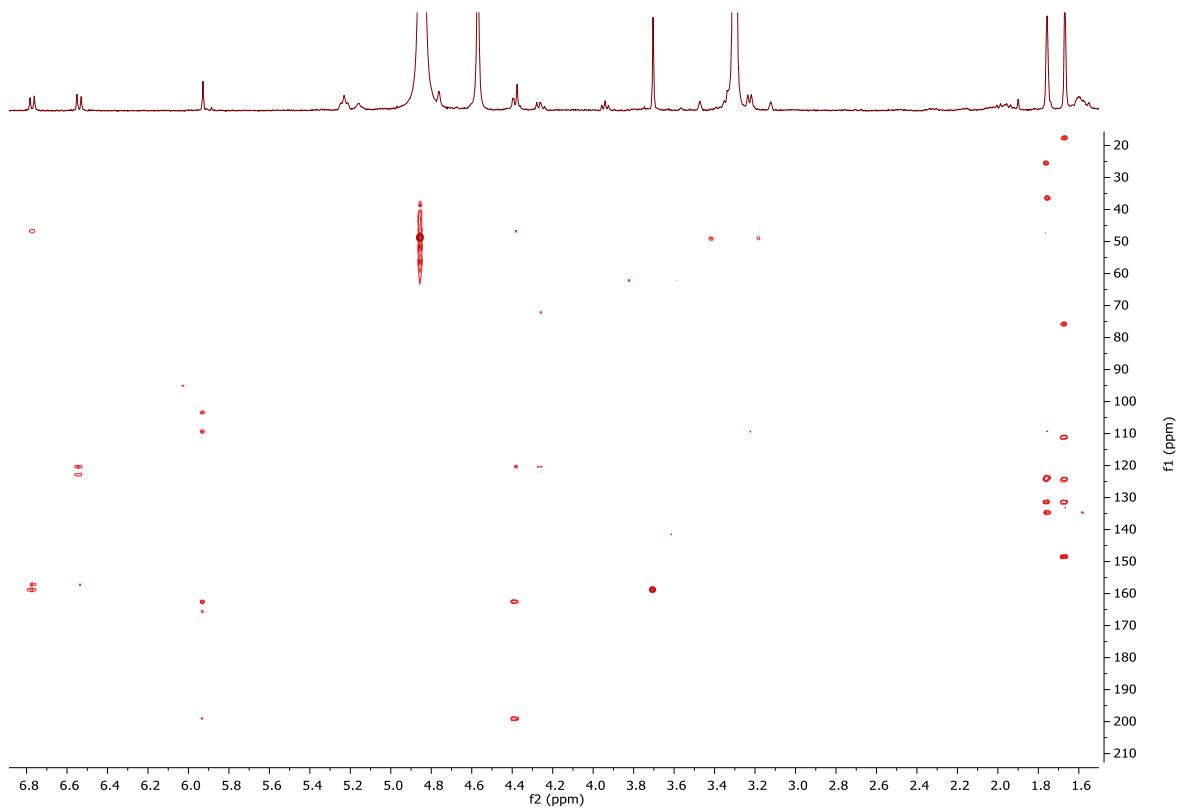


Figure S4_3: HMBC (NUS 50%) spectrum (600 MHz, CD₃OD) of compound 4

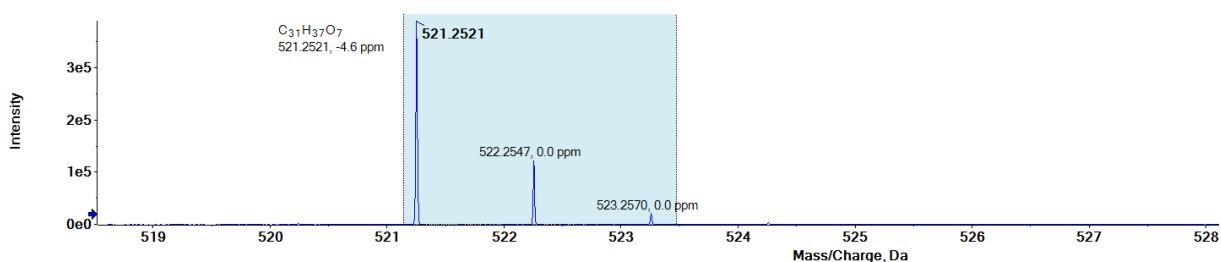


Figure S4_4: Negative ion ESI-HRMS spectrum of compound 4

Table S4: NMR data of compound 4

No	δ_{H} , mult (J in Hz)	δ_{C}		HMBC
2	A: 4.40, d (6.5) B: 4.39, d (9.1)	72.2 ^a	CH ₂	C4, C9, C3 C4, C9, C1'
3	4.27, dd (6.5/9.1)	46.8 ^a	CH	C2
4		199.2 ^b	C=O	
5		165.6 ^b	C	
6		109.4 ^b	C	
7		165.5 ^b	C	
8	5.93, s	95.0 ^a	CH	C10, C6, C7
9		162.5 ^b	C	
10		103.5 ^b	C	
1'		120.4 ^b	C	
2'		158.8 ^b	C	
3'		122.8 ^b	C	
4'		157.2 ^b	C	
5'	6.55, d (8.4)	112.1 ^a	CH	C3', C1'
6'	6.77, d (8.4)	128.0 ^a	CH	C3, C2', C3'
1''	3.34, m	24.1 ^a	CH ₂	
2''	5.24, br t	124.1 ^a	CH	
3''		131.4 ^b	C	
4''	1.67, s	25.6 ^a	CH ₃	C2'', C3'', C5''
5''	1.76, s	17.7 ^a	CH ₃	C3'', C2'', C4''
1'''	3.23, br d (6.5)	21.6 ^a	CH ₂	
2'''	5.24, br t (6.5)	124.3 ^a	CH	
3'''		134.7 ^b	C	
4'''	1.97, m	36.5 ^a	CH ₂	
5'''	1.59, m	34.1 ^a	CH ₂	C4'', C3'''
6'''	3.95, t (6.7)	75.9 ^a	CH	
7'''		148.4 ^b	C	
8'''	A: 4.85, m B: 4.76, m	111.2 ^a	=CH ₂	
9'''	1.77, s	16.0 ^a	CH ₃	C4'', C3'''
10'''	1.67, s	17.4 ^a	CH ₃	C6'', C7'', C8'''
2'-OCH ₃	3.70, s	62.2 ^a	CH ₃	C2'
5-OH	12.41, s			

Signals derived from ^aHSQC and ^bHMBC

6-Geranyl-4',5,7-trihydroxyl-2'-methoxy-3'-(2,3-epoxy-3-methyl-butyl)-isoflavanone (5),
contains compound **2** as impurity

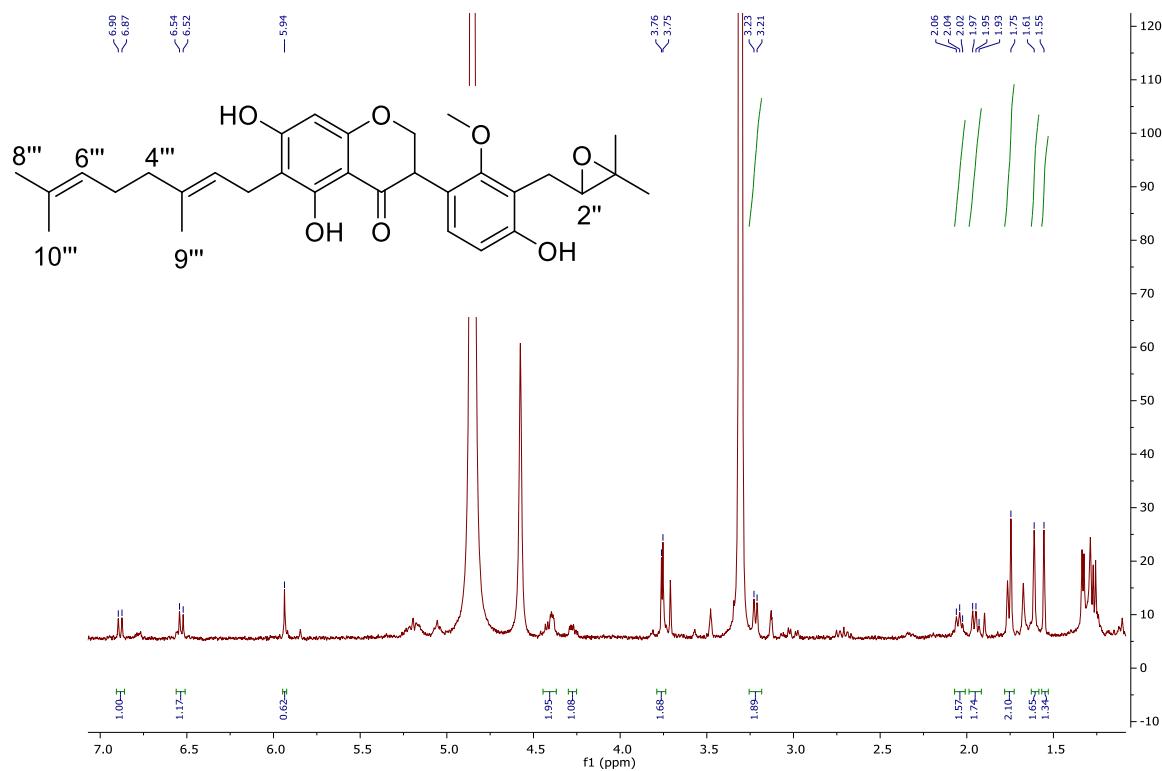


Figure S5_1: ^1H NMR spectrum (600 MHz, CD_3OD) of compound **5**

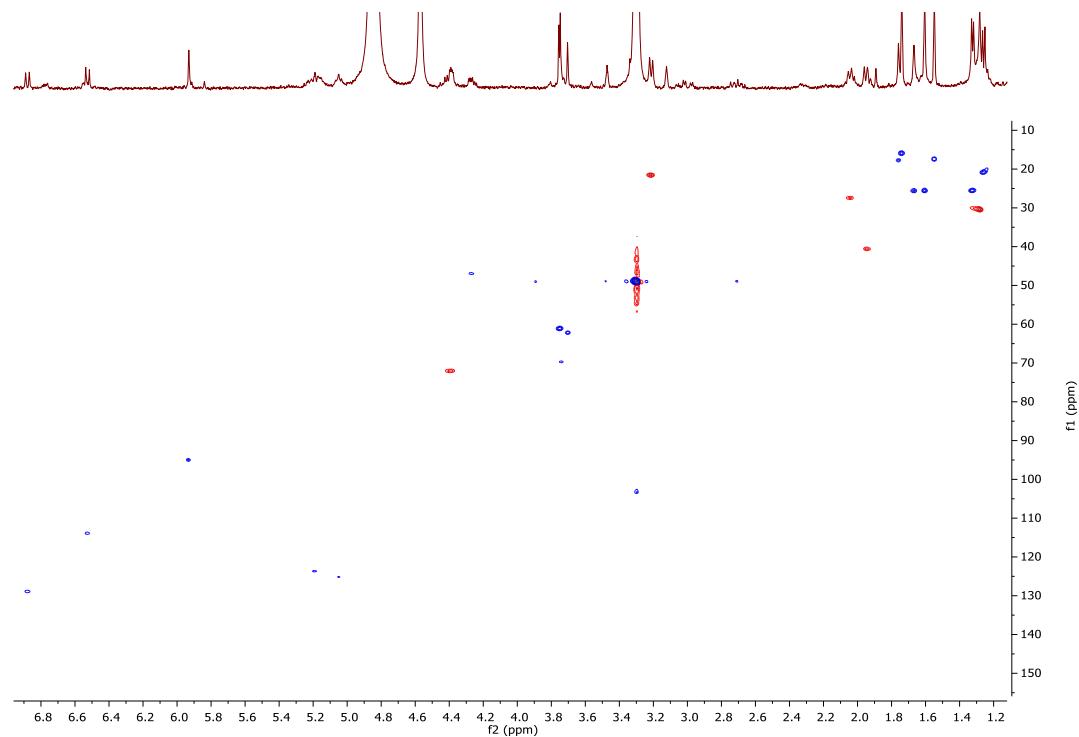


Figure S5_2: HSQCAD_ (NUS 50%) spectrum (600 MHz, CD_3OD) of compound **5**

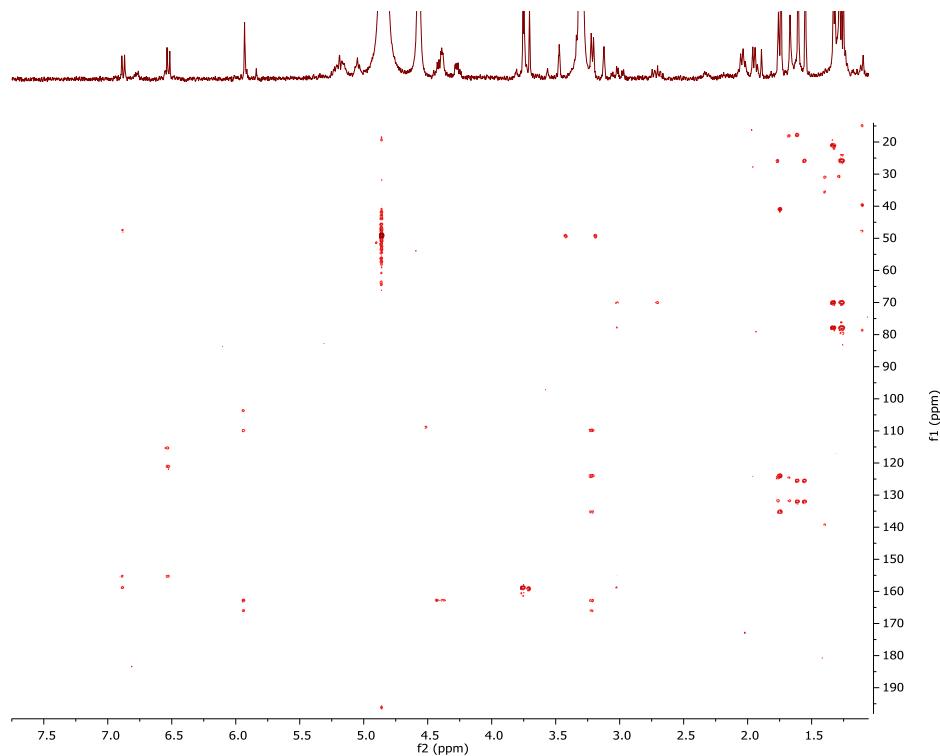


Figure S5_3: HMBC (NUS 50%) spectrum (600 MHz, CD₃OD) of compound **5**

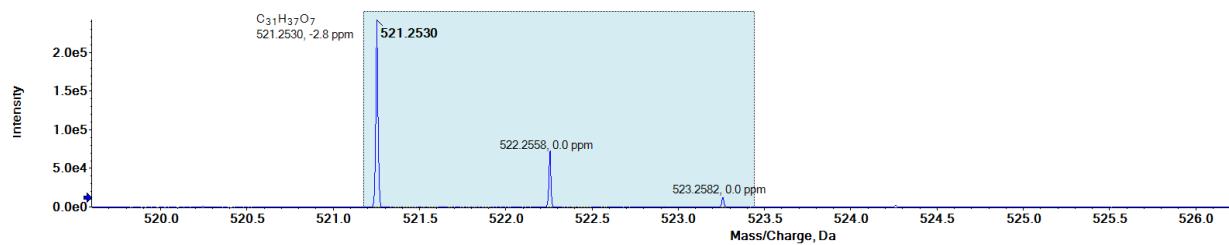


Figure S5_4: Negative ion ESI-HRMS spectrum of compound **5**

Table S5: NMR data of compound **5**

No	δ_{H} , mult (J in Hz)	δ_{C}		HMBC
2	A: 4.40, <i>m</i> B: 4.38, <i>m</i>	72.0 ^a	CH ₂	C4, C9, C4, C9,
3	4.27, <i>m</i>	46.9 ^a	CH	C2
4		199.1 ^b	C	
5		162.8 ^b	C	
6		109.8 ^b	C	
7		166.0 ^b	C	
8	5.94, <i>s</i>	95.3 ^a	CH	C9, C10, C6, C7, C4
9		162.8 ^b	C	
10		103.7 ^b	C	
1'		121.1 ^b	C	
2'		158.8 ^b	C	
3'		115.3 ^b	C	
4'		155.2 ^b	C	
5'	6.53, <i>d</i> (8.4)	113.9 ^a	CH	C2', C4', C3'
6'	6.88, <i>d</i> (8.4)	129.0 ^a	CH	C4', C1', C2'
1''	A: 3.02, <i>m</i> B: 2.70, <i>m</i>	27.6 ^a	CH ₂	C2'', C3'', C2'
2''	3.74, <i>m</i>	70.0 ^a	CH	
3''		77.8 ^a	C	
4''	1.32/1.34, <i>s</i>	25.6 ^a	CH ₃	C2'',
5''	1.26/1.27, <i>s</i>	20.8 ^a	CH ₃	C3'', C2''
1'''	3.22, <i>d</i> (7.2)	21.5 ^a	CH ₂	C7, C5, C6, C3''', C2''',
2'''	5.19, <i>br t</i>	123.6 ^a	CH	
3'''		135.2 ^b	C	
4'''	1.94, <i>d</i> (7.6)	40.7 ^a	CH ₂	
5'''	2.05, <i>m</i>	27.7 ^a	CH ₂	
6'''	5.05, <i>m</i>	125.2 ^a	CH	
7'''		132.0	C	
8'''	1.61, <i>s</i>	25.6 ^a	CH ₃	C10''', C6''', C7'''
9'''	1.74, <i>s</i>	16.0 ^a	CH ₃	C4''', C3''', C2'''
10'''	1.56, <i>s</i>	17.4 ^a	CH ₃	C8''', C6''', C7'''
2'-OCH ₃	3.76/3.75, <i>s</i>	61.1 ^a	CH ₃	C2'

Signals derived from ^aHSQC and ^bHMBC

(Z)-2',4',5,7-Tetrahydroxyl-8-(3,7-dimethylocta-2,6-dienyl)-isoflavanone (6),
contains kenusanone H (7) as impurity.

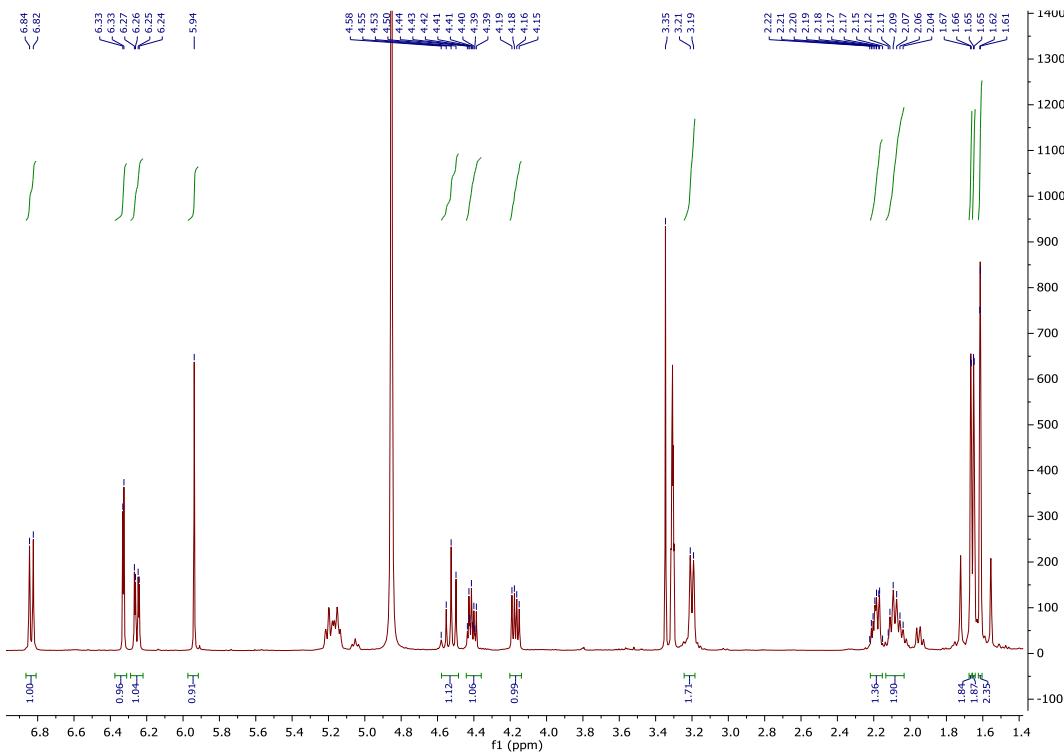


Figure S6_1: ^1H NMR spectrum (400 MHz, CD_3OD) of compound 6

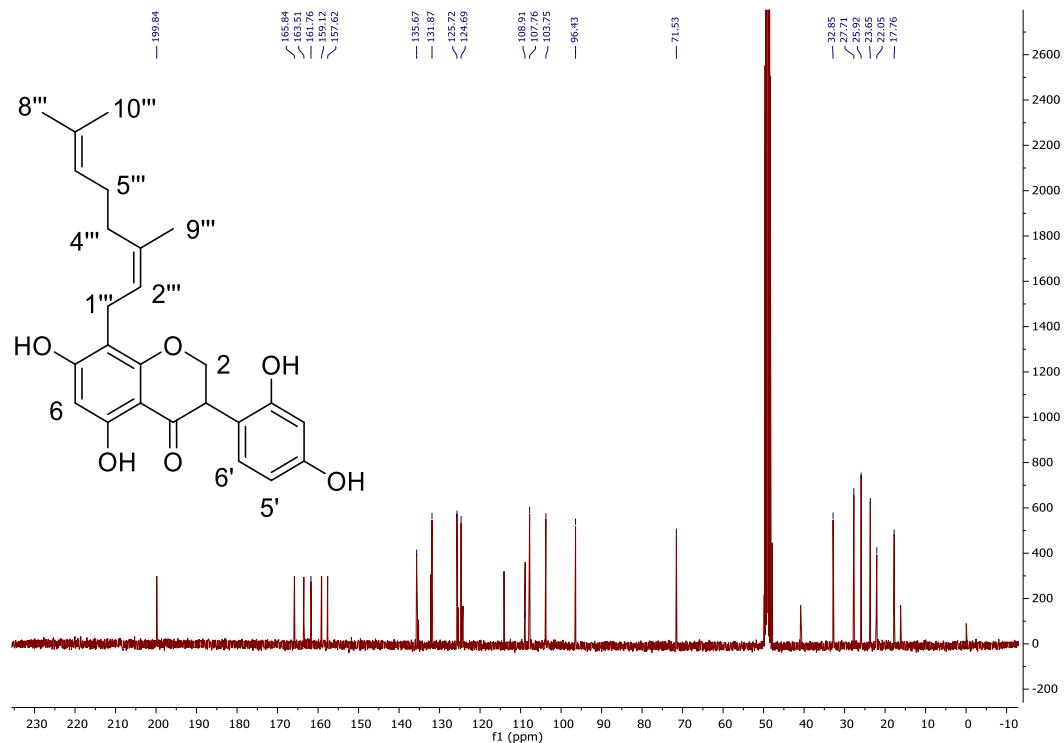


Figure S6_2: ^{13}C NMR spectrum (125 MHz, CD_3OD) of compound 6

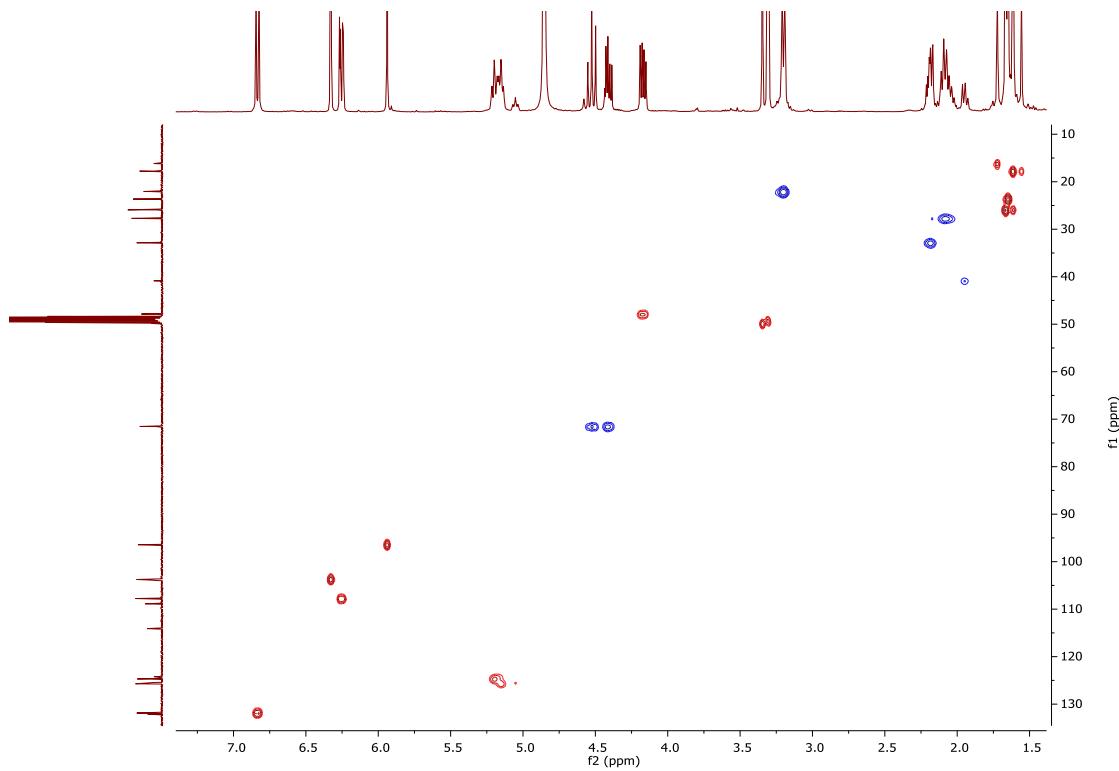


Figure S6_3: HSQCAD spectrum (125 MHz, CD₃OD) of compound **6**

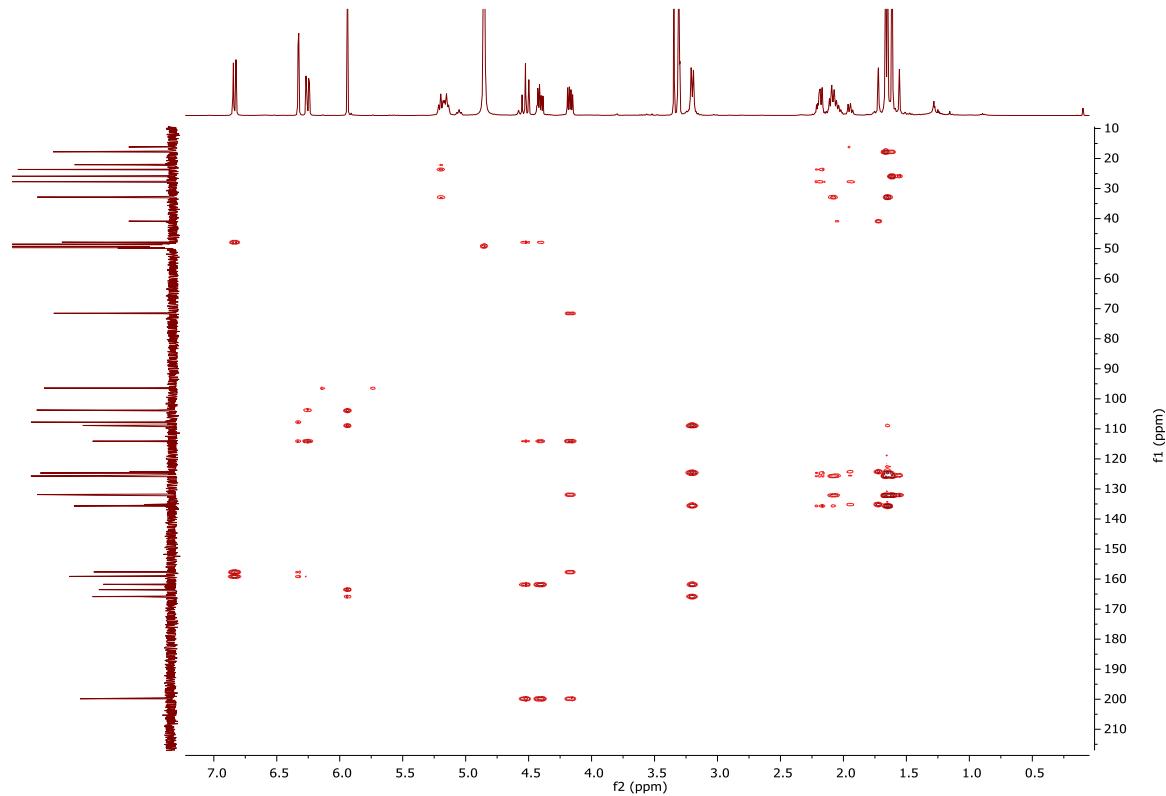


Figure S6_4: HMBC spectrum (125 MHz, CD₃OD) of compound **6**

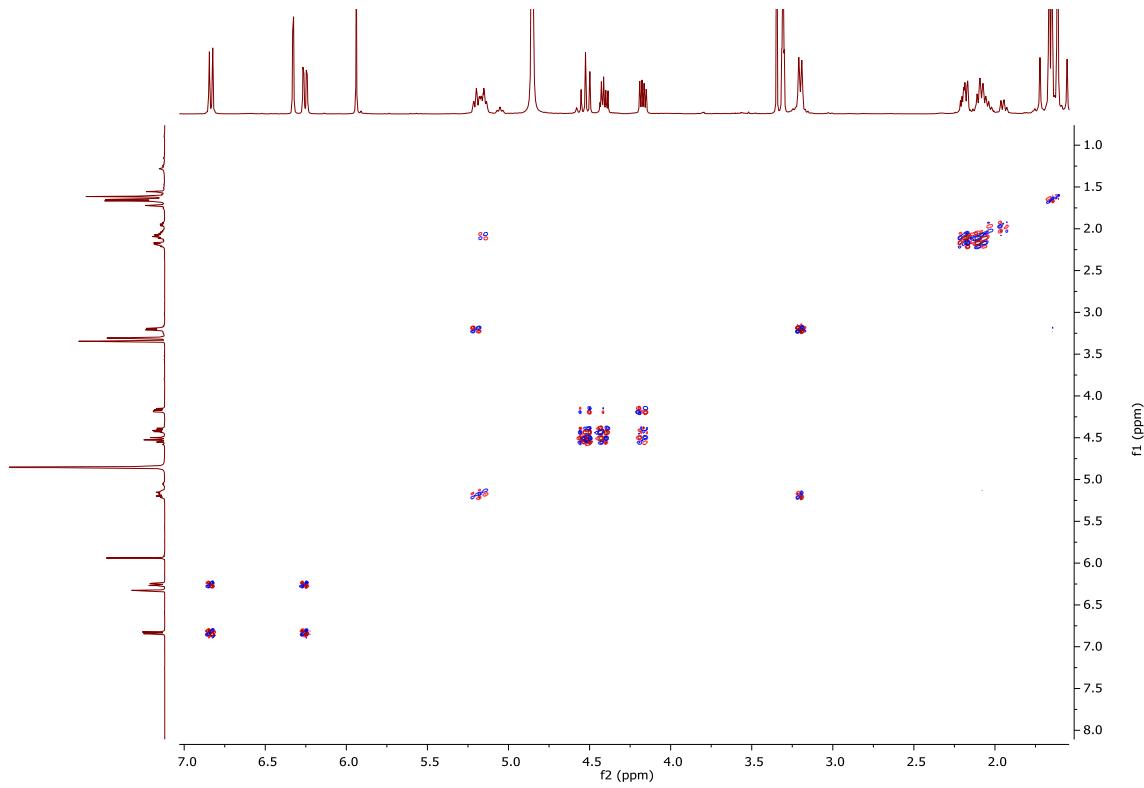


Figure S6_5: COSY spectrum (125 MHz, CD_3OD) of compound **6**

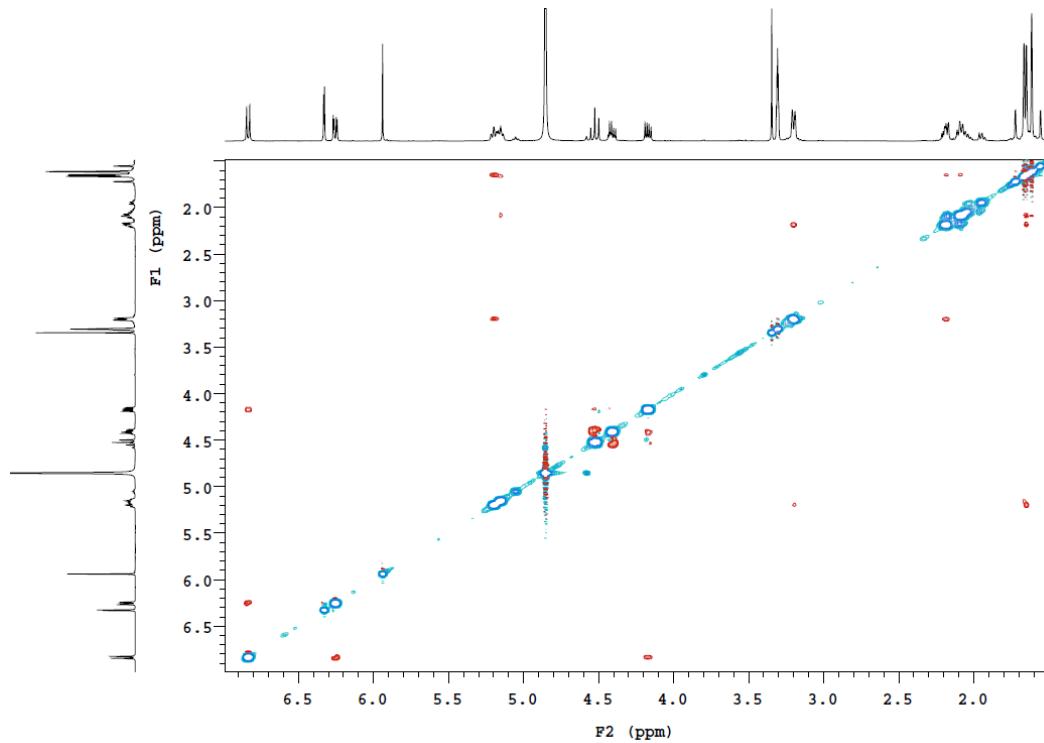


Figure S6_6: NOESY spectrum (125 MHz, CD_3OD) of compound **6**

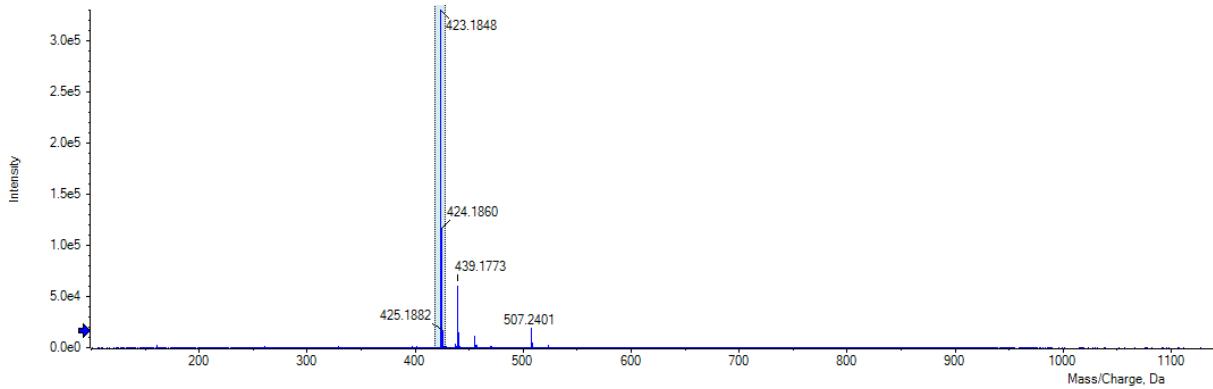


Figure S6_7: Negative ion ESI-HRMS spectrum of compound **6**

Table S6: NMR data of compound **6**

No	δ_{H} , mult (J in Hz)	δ_{C}	COSY	NOESY	HMBC	
2	A: 4.53, <i>t</i> (10.8) B: 4.41, <i>dd</i> (10.8, 5.5)	71.4	CH ₂	H2B, H3 H2A, H3	H2B H2A, H3	C4, C9, C3, C1' C4, C9, C3, C1'
3	4.17, <i>dd</i> (10.8, 5.5)	47.9	CH	H2A/H2B	H2A, H6'	C4, C2', C1', C6'
4		199.8	C=O			
5		163.5	C			
6	5.94, <i>s</i>	96.4	CH			C5, C7, C10, C8
7		165.8	C			
8		108.9	C			
9		161.8	C			
10		103.9	C			
1'		113.8	C			
2'		157.7	C			
3'	6.33, <i>d</i> (2.4)	103.8	CH			C2', C4'
4'		159.1	C			
5'	6.26, <i>dd</i> (8.3, 2.4)	107.8	CH	H6'	H6'	C4'
6'	6.83, <i>d</i> (8.3)	131.9	CH	H5'	H5', H3, H2A	C2', C4', C3
1''	3.21, <i>br d</i> (7.1)	22.1	CH ₂	H2''	H 2'', H4''	C7, C8, C9, C2'', C3''
2''	5.20, <i>br t</i> (7.1)	124.7	CH	H1'''	H 5''	C9'', C4''
3'''		135.6	C			
4'''	2.18, <i>m</i>	32.9	CH ₂	H5'''	H1''', H2'''	C9''', C5''', C3''', C2''', C6'''
5'''	2.08, <i>m</i>	27.7	CH ₂	H4'''	H6'''	C4''', C7''', C6''', C3'''
6'''	5.16, <i>m</i>	125.7	CH	H5'''	H5''', H8'''	C8''', C10'',
7'''		131.9	C			
8'''	1.67, <i>s</i>	25.9	CH ₃		H6'''	C10''', C6''', C7'''
9'''	1.65, <i>s</i>	23.7	CH ₃		H2''', H5'''	C4''', C2''', C3'''
10'''	1.61, <i>s</i>	17.7	CH ₃			C8''', C6''', C7'''
5-OH	12.21					

Kenusanone H (7), contains compound 6 as impurity

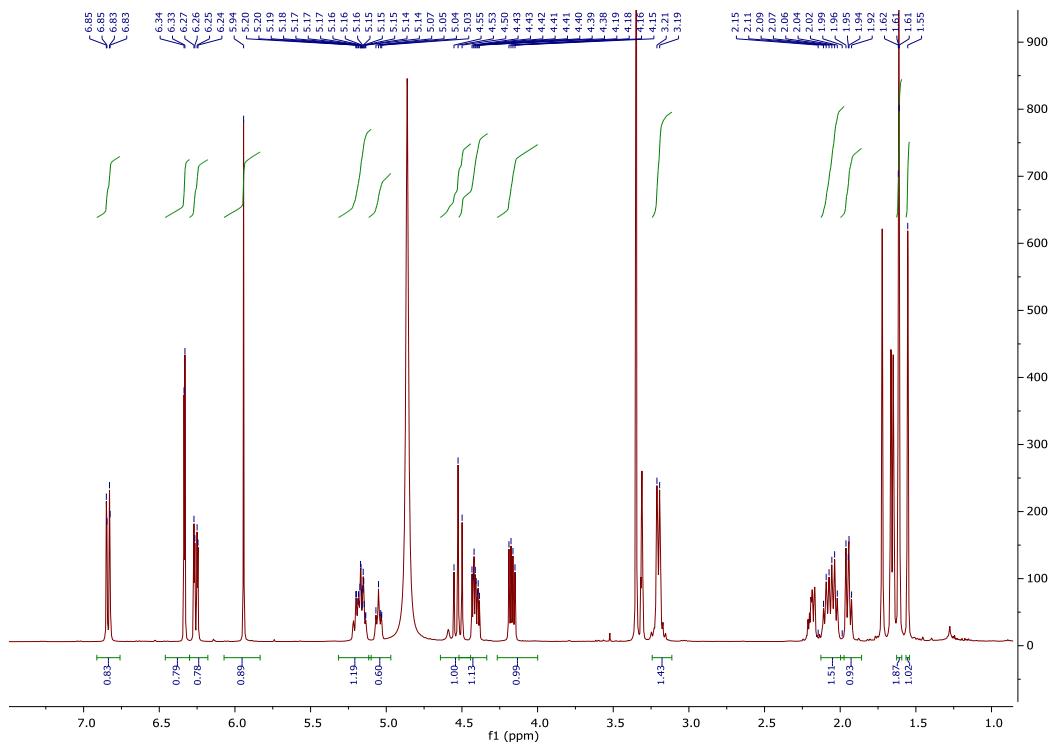


Figure S7_1: ^1H NMR spectrum (400 MHz, CD_3OD) of kenusanone H (7)

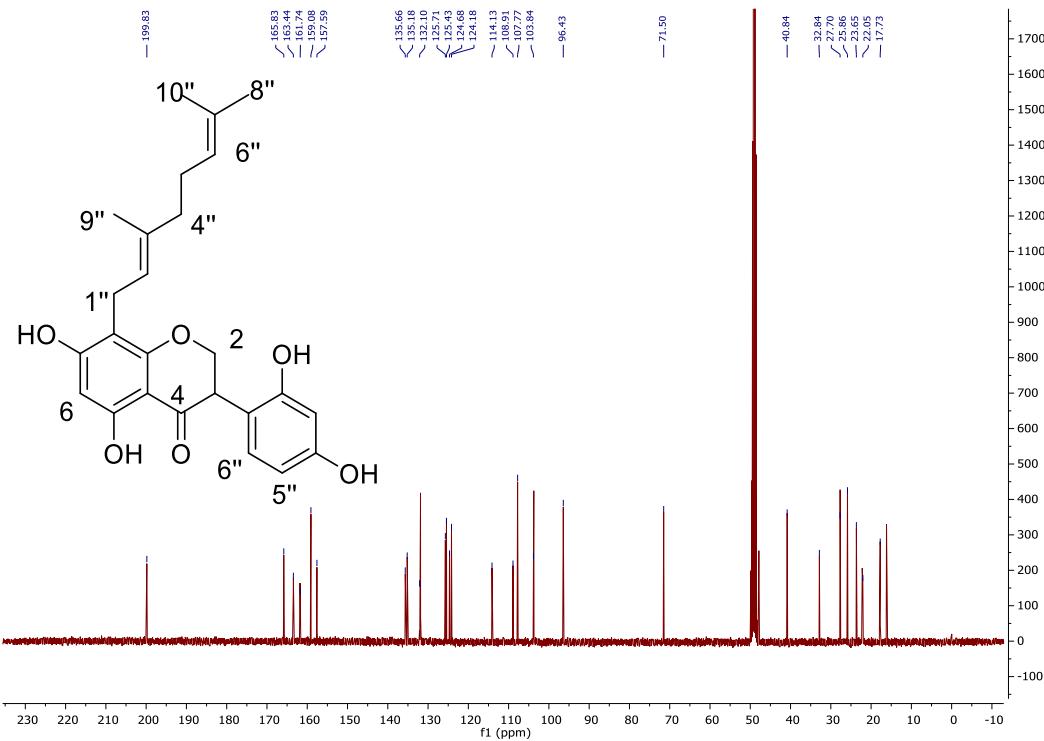


Figure S7_2: ^{13}C NMR spectrum (125 MHz, CD_3OD) of kenusanone H (7)

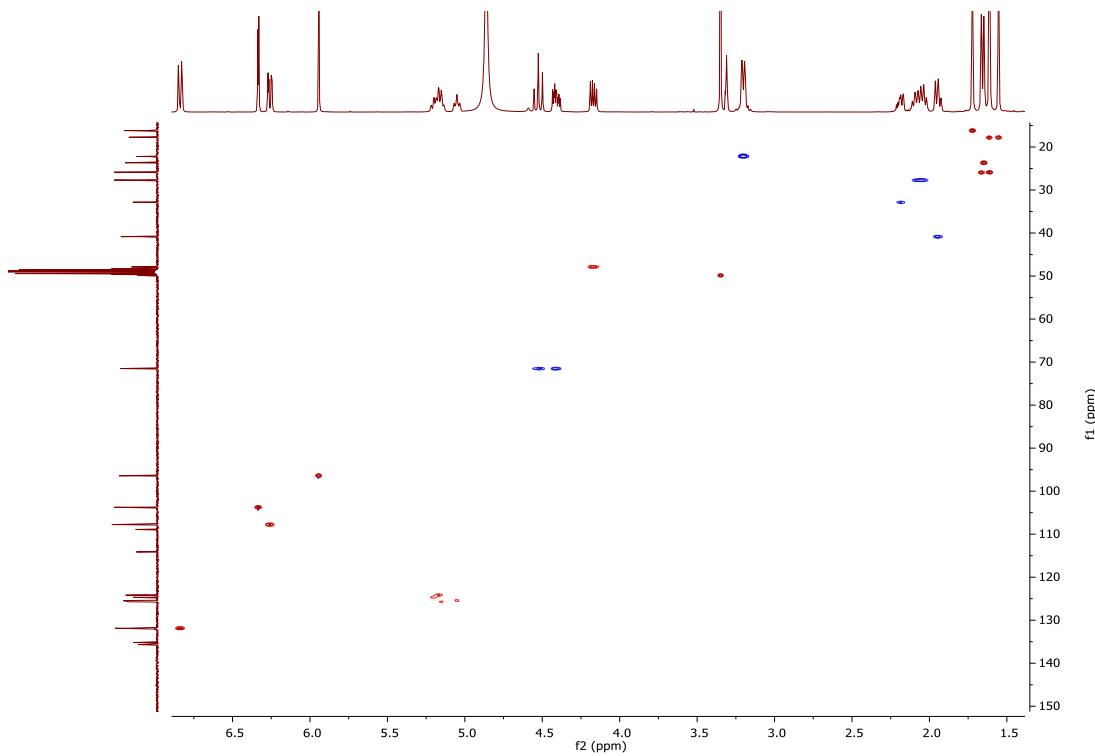


Figure S7_3: HSQCAD spectrum (125 MHz, CD₃OD) of kenusanone H (**7**)

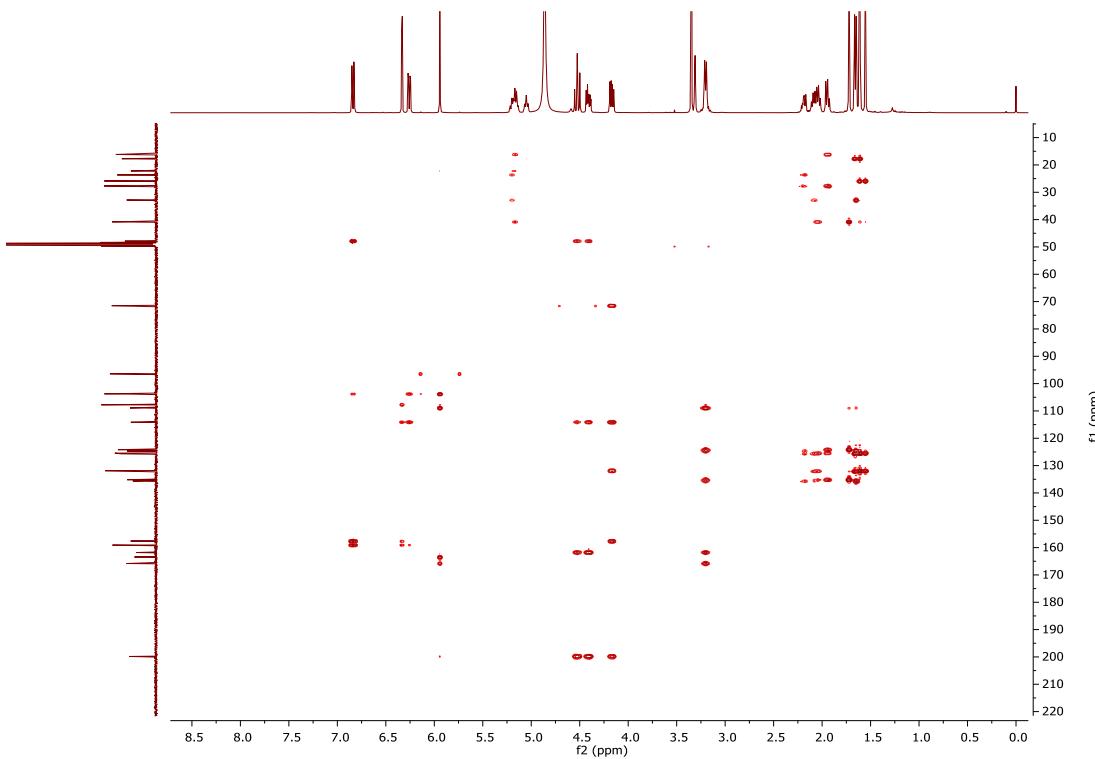


Figure S7_4: HMBC spectrum (125 MHz, CD₃OD) of kenusanone H (**7**)

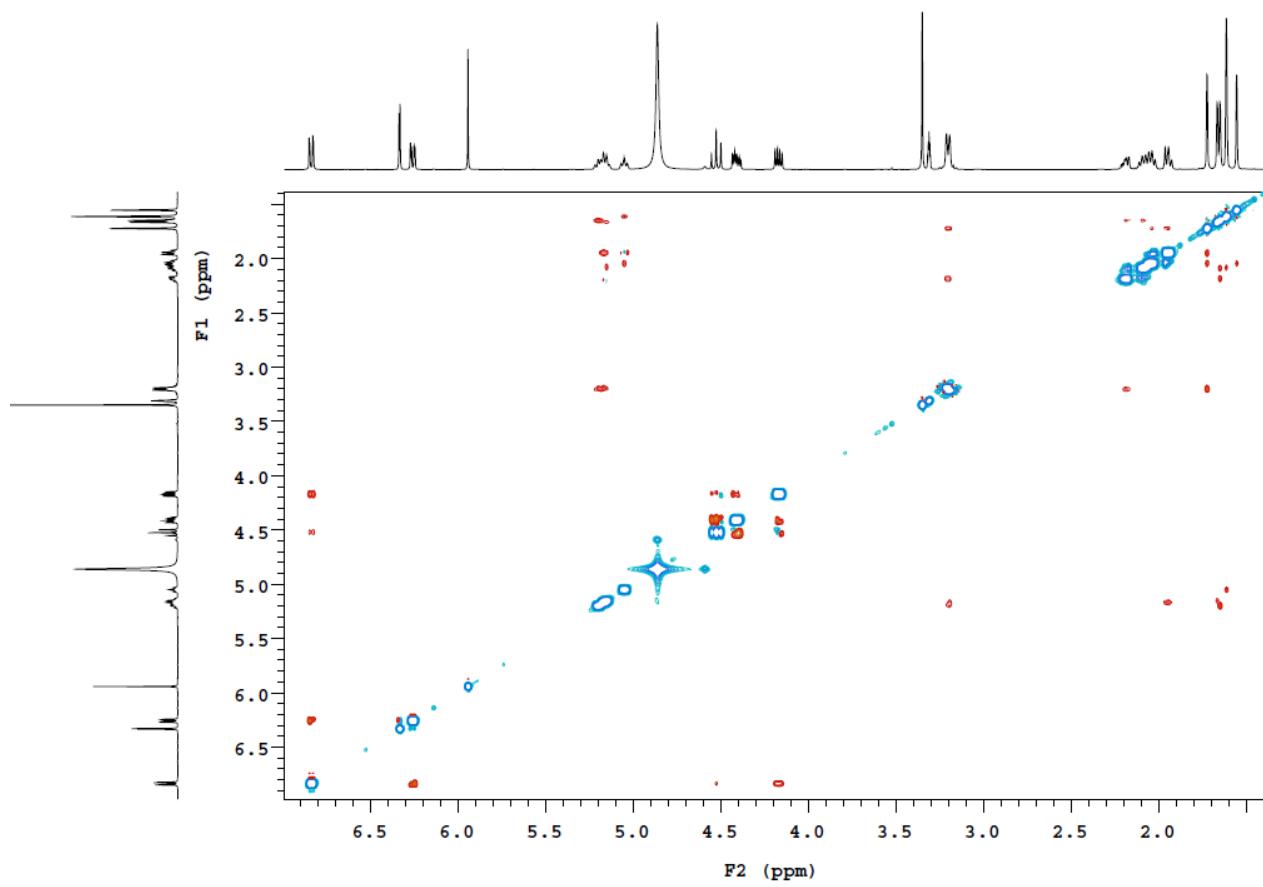


Figure S7_5: NOESY spectrum (125 MHz, CD_3OD) of kenusanone H (**7**)

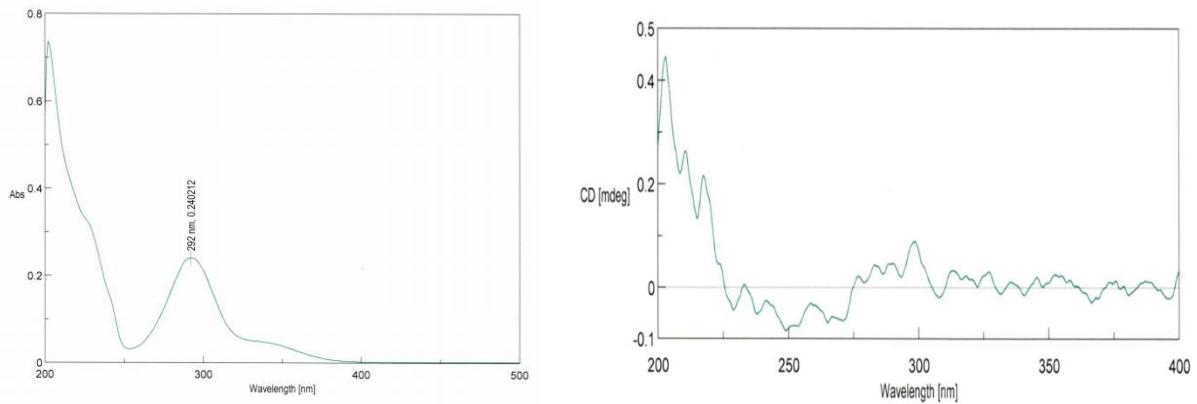


Figure S7_6: UV and CD data of kenusanone H (**7**) racemate

Table S7: NMR data of kenusanone H (**7**)

No	δ_{H} , mult (J in Hz)	δ_{C}	COSY	NOSY	HMBC
2	A: 4.53, <i>t</i> (10.7) B: 4.41, <i>dd</i> (10.9, 5.4)	71.5	H2B, H3 H2A, H3	H2B, H6' H2A, H3	C4, C1' C4, C1'
3	4.17, <i>dd</i> (10.5, 5.4)	47.9	H2A, H2	H2A, H6'	C4, C2', C2
4		199.8			
5		163.5			
6	5.94, <i>s</i>	96.4			C4, C5, C7, C10
7		165.8			
8		108.9			
9		161.8			
10		103.8			
1'		114.1			
2'		157.6			
3'	6.33, <i>d</i> (2.4)	103.8			C2', C4', C1', C5'
4'		159.1			
5'	6.26, <i>dd</i> (8.3, 2.4)	107.8	H6'	H6'	C1', C3'
6'	6.84, <i>d</i> (8.3)	131.9	H5'	H5', H3, H2A	C3, C2', C4'
1'''	3.20, <i>d</i> (7.1)	22.2	H2'''	H9''', H2'''	C9, C8, C7
2'''	5.17, <i>m</i>	124.2	H1'''	H1'''	C4''', C9'''
3'''		135.2			
4'''	1.94, <i>m</i>	40.8	H5'''		C9''', C5''', C2''', C3''', C6'''
5'''	2.05, <i>m</i>	27.6	H6''', H4'''		C7''', C4''', C8'''
6'''	5.05, <i>m</i>	125.4	H5'''		C8'', C10''
7'''		132.1			
8'''	1.61, <i>s</i>	25.9			C7''', C6'''
9'''	1.72, <i>s</i>	16.2		H1'''	C4''', C2''', C3'''
10'''	1.56, <i>s</i>	17.7			C7''', C6''', C8'''
5-OH	12.22, <i>s</i>				

(3*R*)-Kenusanone F (8), $[\alpha]_D^{25} -112.5$ (c 0.260, MeOH)

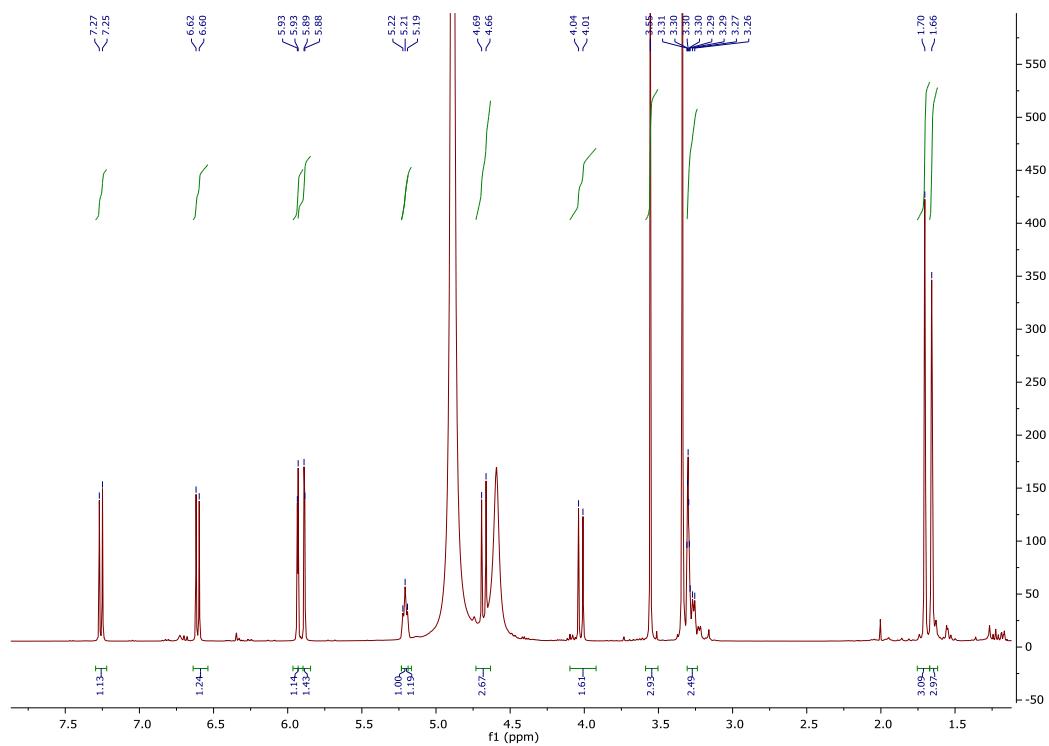


Figure S8_1: ^1H NMR spectrum (400 MHz, CD_3OD) of kenusanone F (8)

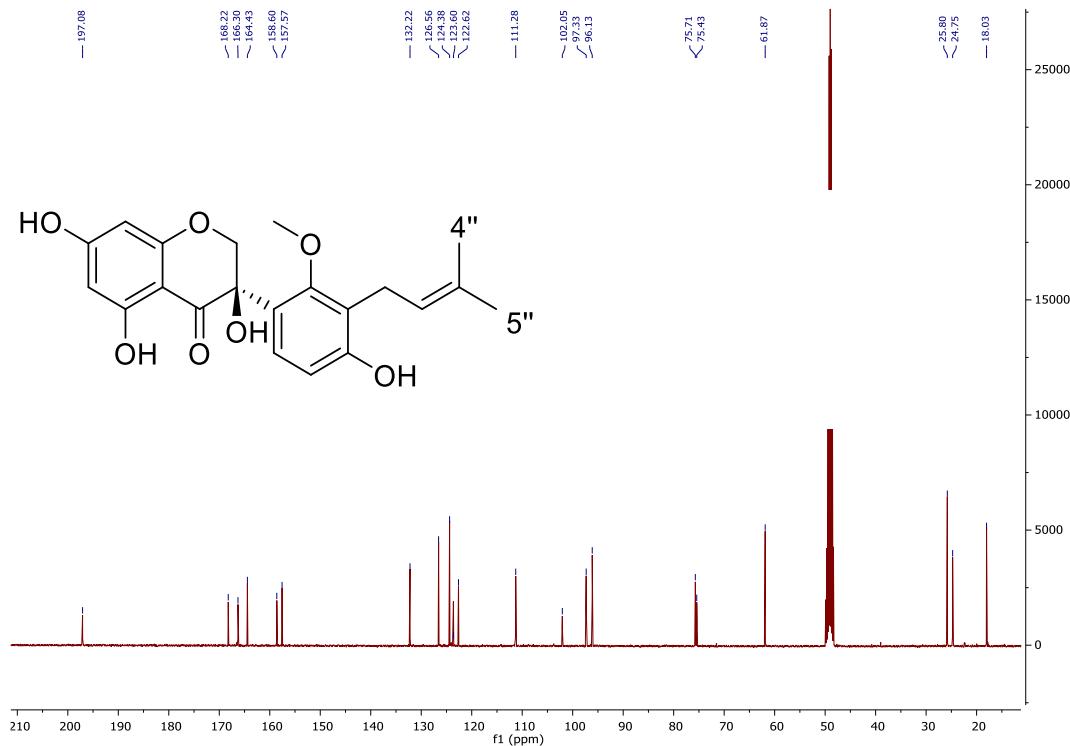


Figure S8_2: ^{13}C NMR spectrum (125 MHz, CD_3OD) of kenusanone F (8)

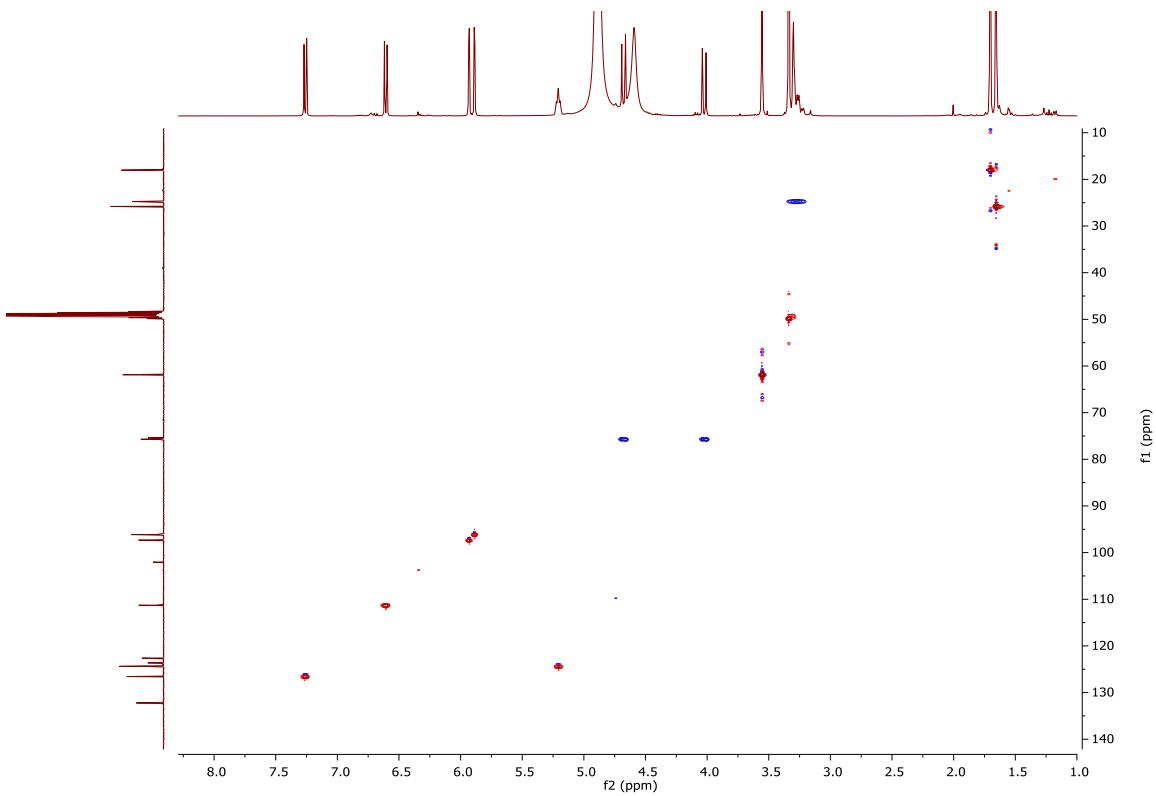


Figure S8_3: HSQCAD spectrum (125 MHz, CD₃OD) of kenusanone F (**8**)

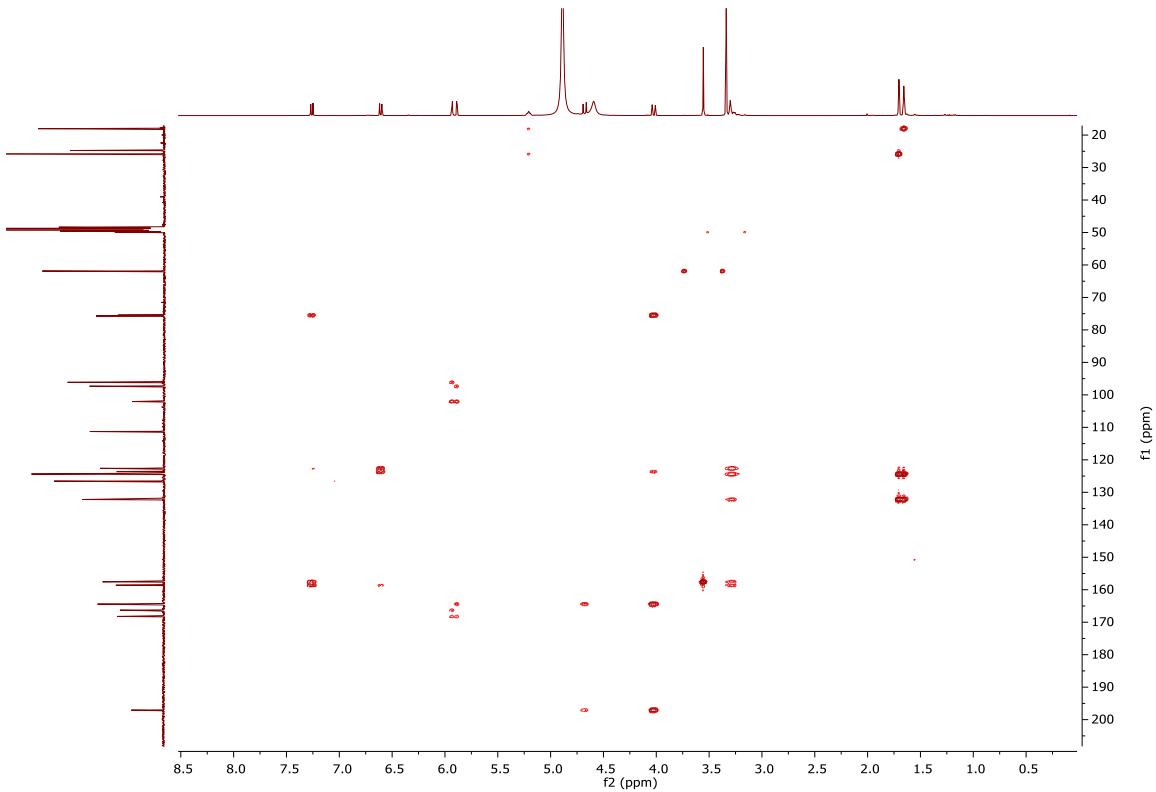


Figure S8_4: HMBC spectrum (125 MHz, CD₃OD) of kenusanone F (**8**)

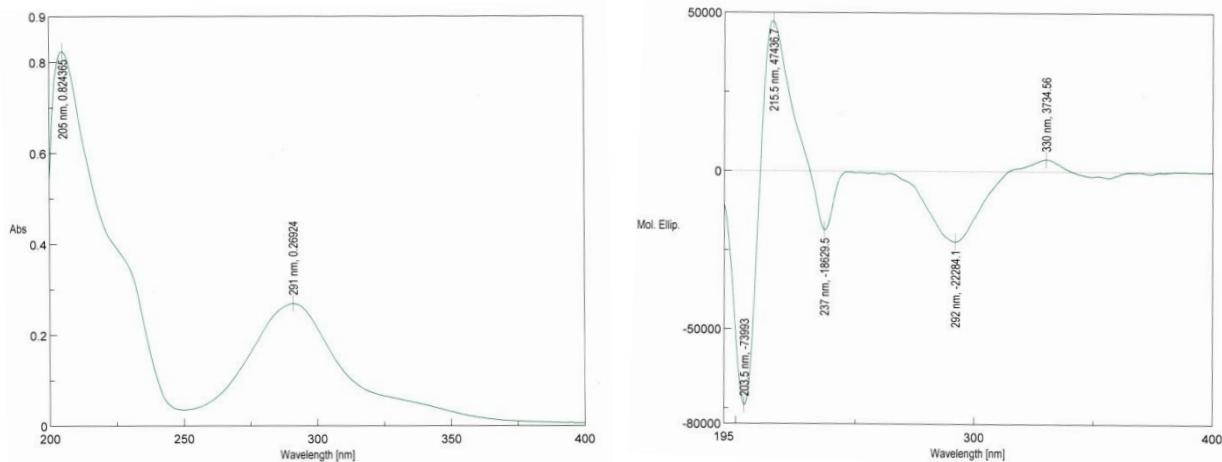


Figure S8_5: UV and CD data of (3R)-kenusanone F (**8**)

Table S8: NMR data of kenusanone F (**8**)

No	δ_{H} , mult (J in Hz)	δ_{C}	COSY	HMBC
2	A: 4.68, d (11.9) B: 4.02, d, (11.9)	75.7 75.4	H2B H2A	C9, C4 C3, C1', C9, C4
3		197.1		
4		166.3		
6	5.93, d (2.2)	97.3	H8	C8, C10, C5, C7
7		168.2		
8	5.89, d (2.2)	96.1	H6	C6, C10, C9, C7
9		164.4		
10		102.0		
1'		123.6		
2'		157.6		
3'		122.6		
4'		158.6		
5'	6.61, d (8.5)	111.3	H6'	C3', C1', C4'
6'	7.26, d (8.5)	126.6	H5'	C3, C2', C4'
1''	A: 3.32, dd (from COSY) B: 3.24, dd (15.4/6.1)	24.8	H2''	C3', C2'', C3'', C2', C4'
2''	5.21, br t (6.6)	124.4	H1''	
3''		132.2		
4''	1.66, s	25.8		C5'', C2'', C3''
5''	1.70, s	18.1		C4'', C2'', C3''
2'-OCH ₃	3.55, s	61.9		C2'
5-OH	12.07, s			

(3*R*)-Tomentosanol B (9), $[\alpha]_D^{25} -126.7$ (c 0.300, MeOH)

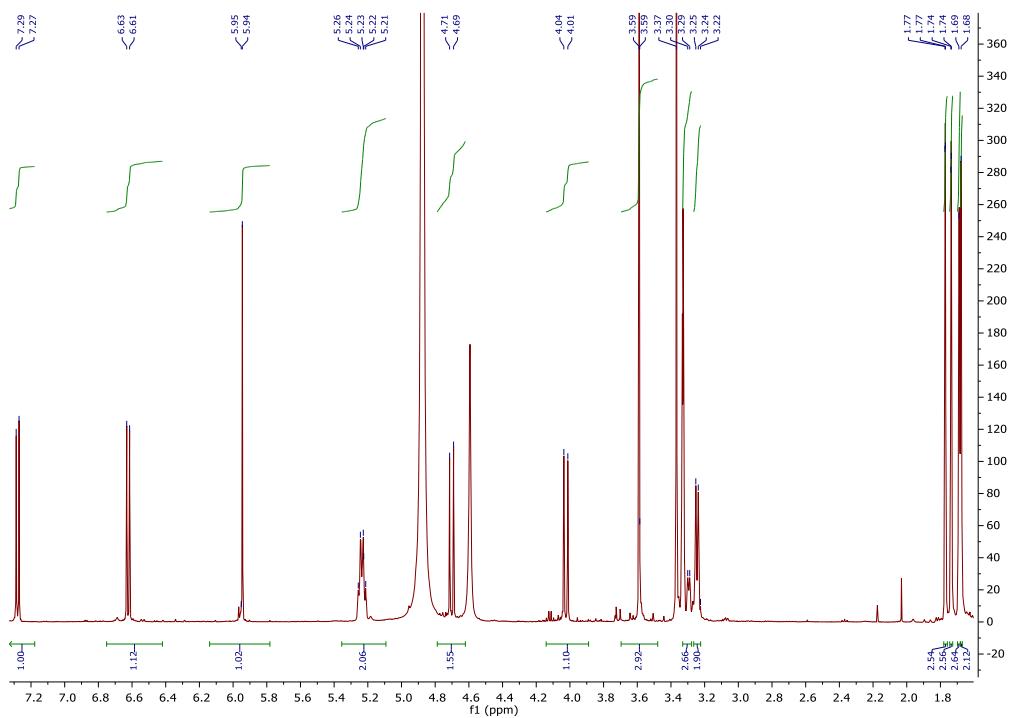


Figure S9_1: ^1H NMR spectrum (500 MHz, CD_3OD) of tomentosanol B (9)

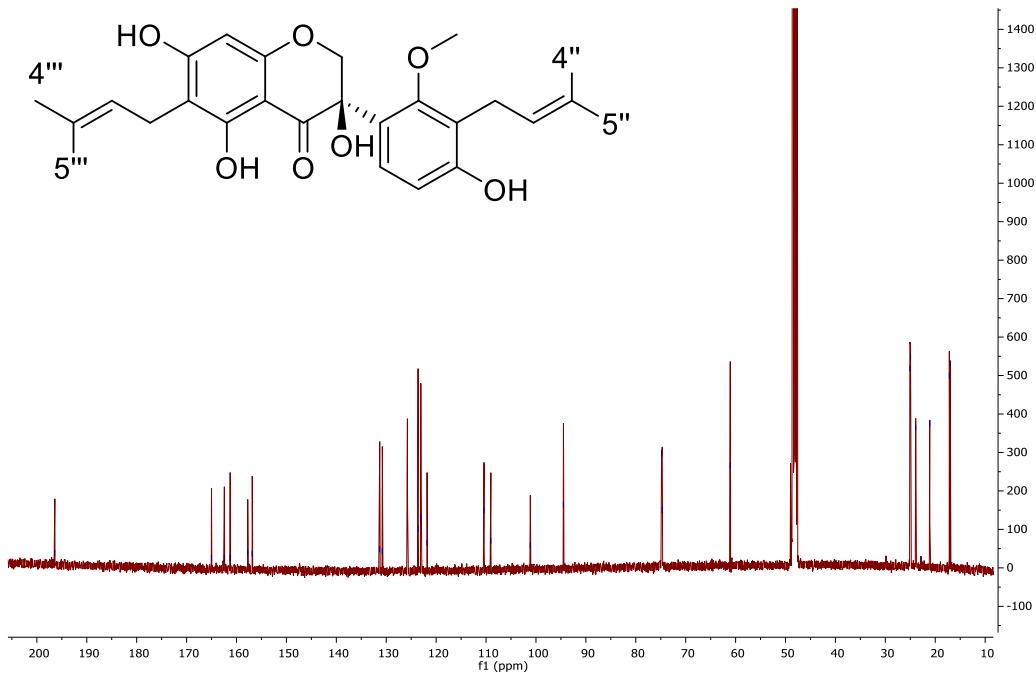


Figure S9_2: ^{13}C NMR spectrum (125 MHz, CD_3OD) of tomentosanol B (9)

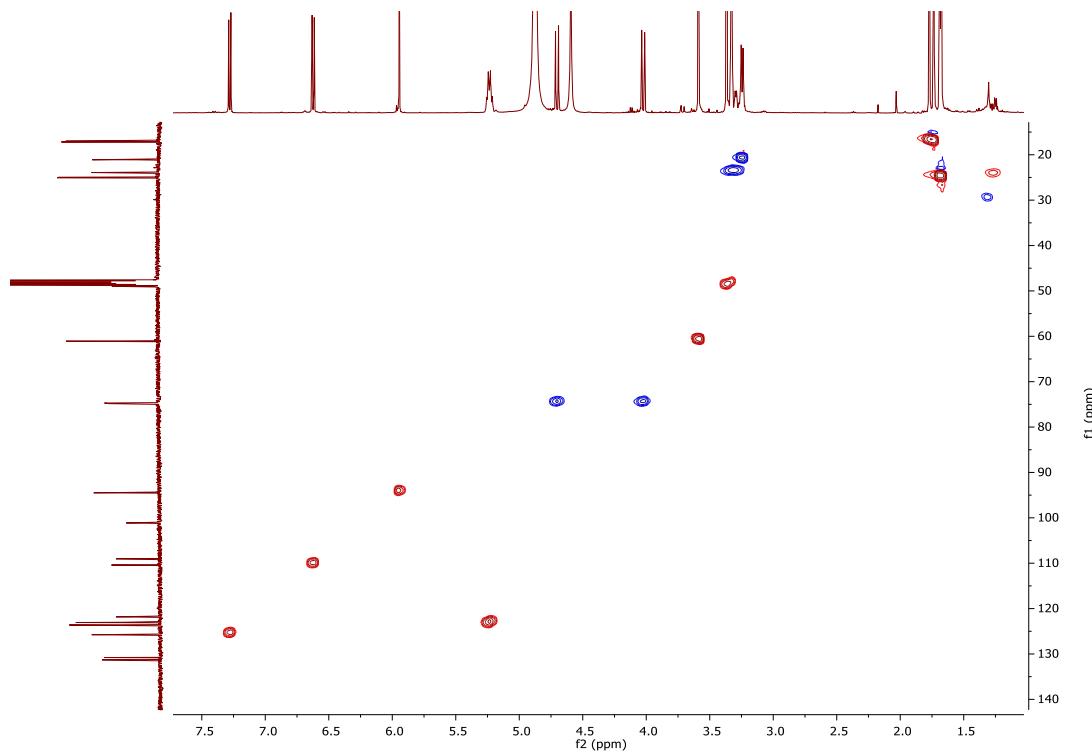


Figure S9_3: HSQCAD spectrum (125 MHz, CD₃OD) of tomentosanol B (**9**)

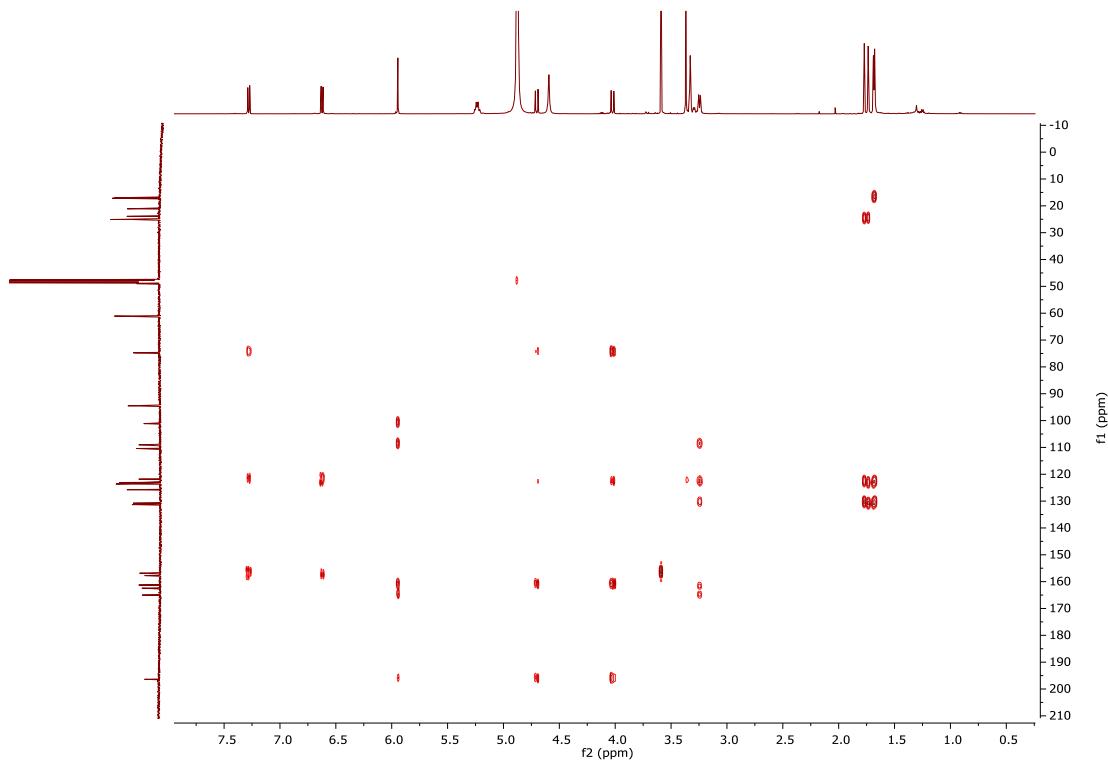


Figure S9_4: HMBC spectrum (125 MHz, CD₃OD) of tomentosanol B (**9**)

CDU_001_neg #1-27 RT: 0.00-0.10 AV: 27 NL: 9.58E7
T: FTMS -p ESI Full ms [110.00-2000.00]

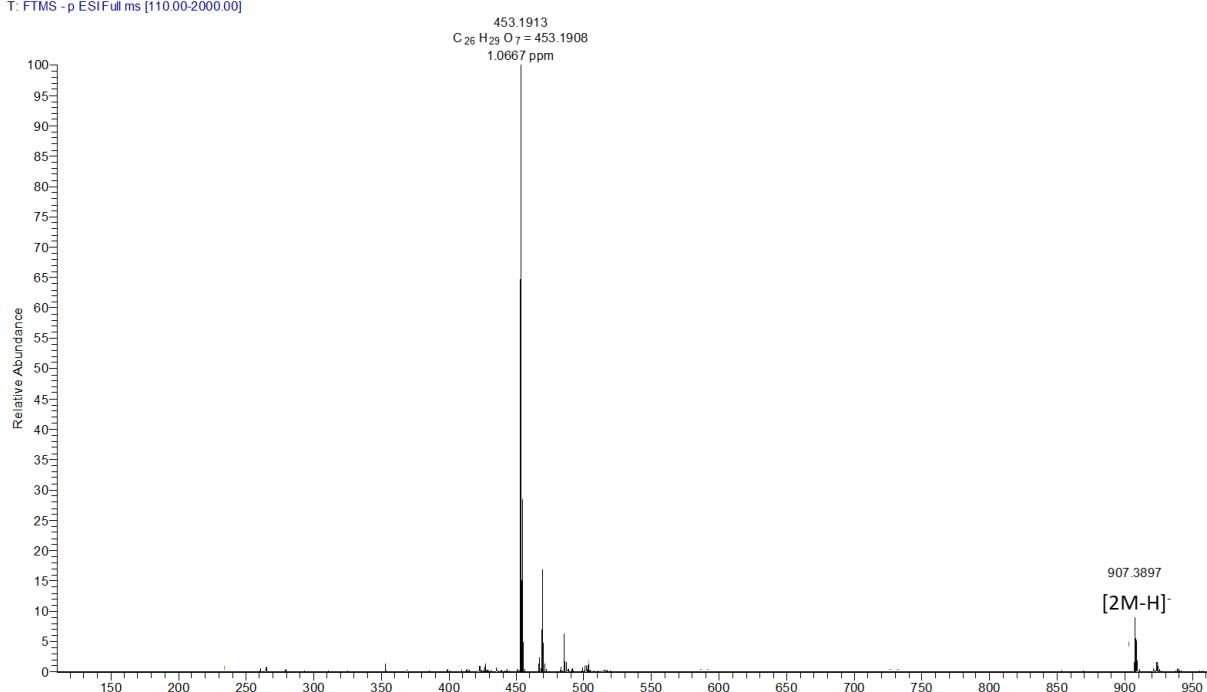


Figure S9_5: Negative ion ESI-HRMS spectrum of tomentosanol B (**9**)

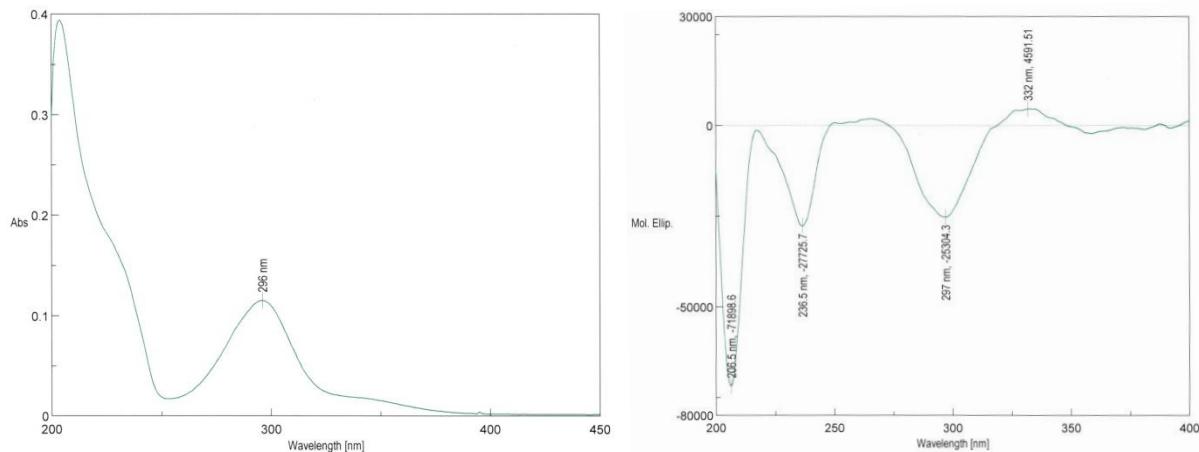


Figure S9_6: UV and CD data of (3*R*)-tomentosanol B (**9**)

Table S9: NMR of tomentosanol B (**9**)

No	$\delta_{\text{H}},^*$ mult (J in Hz)	δ_{C}	COSY	HMBC
2	A: 4.68, d (11.8) B: 4.01, d (11.8)	75.6 CH CH	H2B H2A	C9, C3, C4 C3, C4, C9, C1'
3		75.7	C	
4		197.3	C	
5		163.3	C	
6		109.9	C	
7		165.9	C	
8	5.93, s	95.4	CH	C6, C10, C9, C7, C4
9		162.1	C	
10		102.0	C	
1'		122.7	C	
2'		157.7	C	
3'		124.5	C	
4'		158.6	C	
5'	6.60, d (8.5)	111.3	CH	H6' C1', C6'
6'	7.26, d (8.5)	126.6	CH	H5' C5', C1', C2'
1''	A: 3.33, m B: 3.26, dd (15.2/5.8)	24.8	CH ₂	H2''
2''	5.23, m	124.0	CH	H1''
3''		132.2	C	
4''	1.67, s	25.9	CH ₃	C2'', C3'', C5''
5''	1.75, s	17.9	CH ₃	C2'', C3'', C4''
1'''	3.23, br d (7.3)	22.0	CH ₂	H2''' C5, C6, C3''', C2'''
2'''	5.24, m	123.9	CH	H1'''
3'''		131.6	C	
4'''	1.68, s	25.8	CH ₃	C2'', C3'', C5'''
5'''	1.72, s	18.0	CH ₃	C2'', C3'', C4'''
2'-OCH ₃	3.57, s	61.9		C2'
5-OH	12.30, s			

*referenced to methanol-d4 solvent signal

Sophoraisoflavanone A (10)

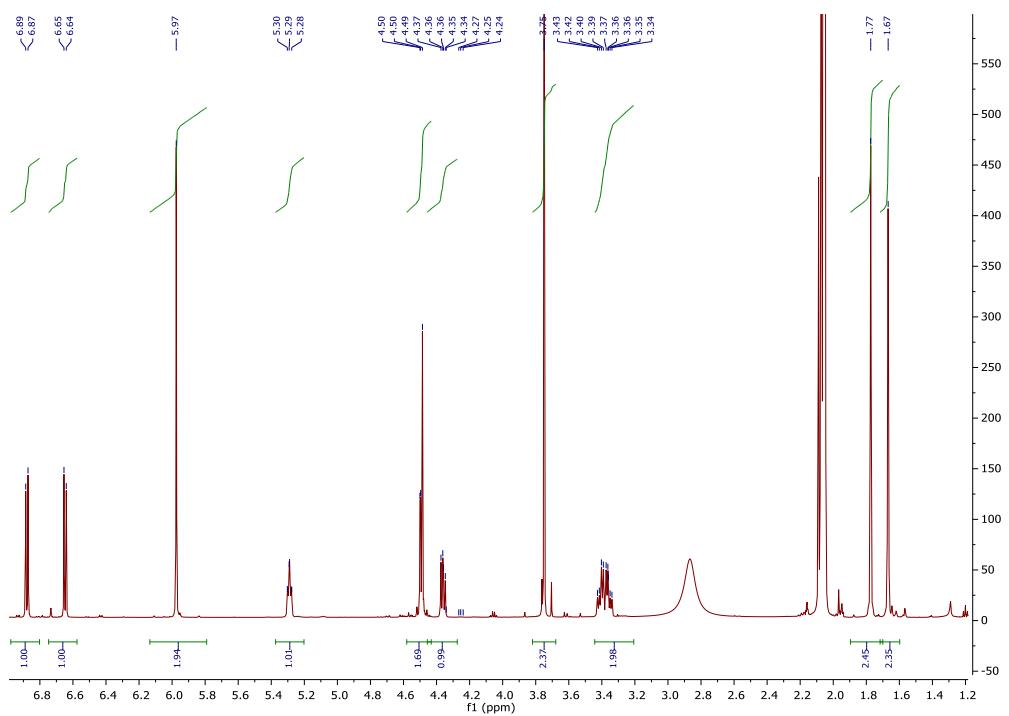


Figure S10_1: ¹H NMR (125 MHz, acetone-d₆) of sophoraisoflavanone A (10)

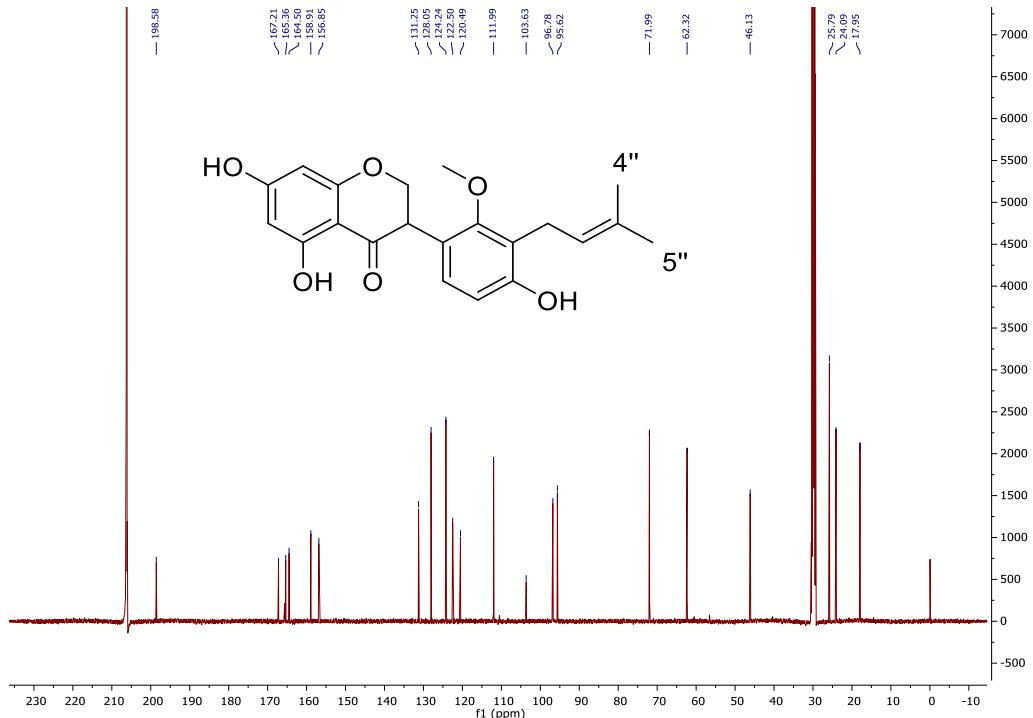


Figure S10_2: ¹³C NMR spectrum (125 MHz, acetone-d₆) of sophoraisoflavanone A (10)

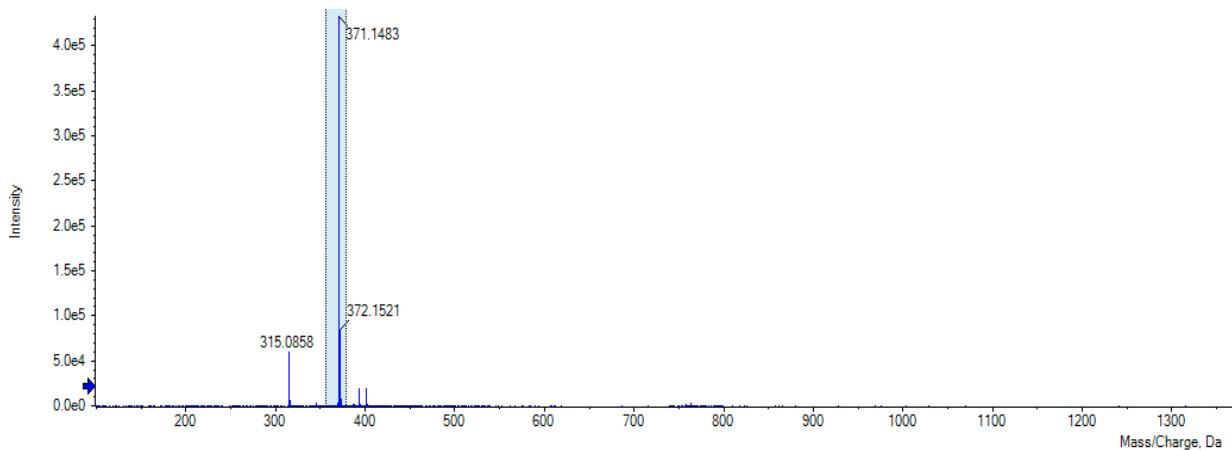


Figure S10_3: Positive ion ESI-HRMS of sophoraisoflavanone A (**10**)

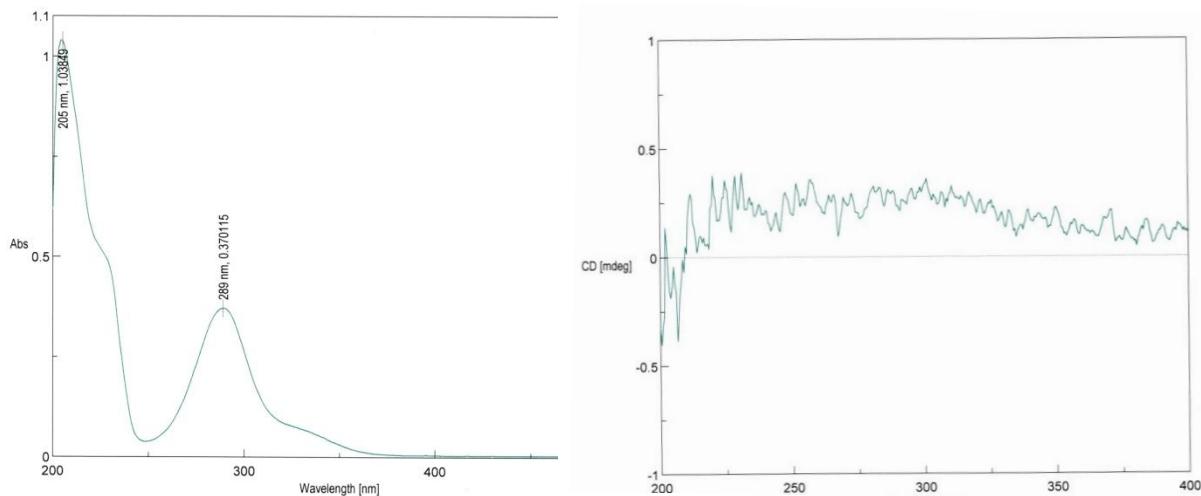


Figure S10_4: UV and CD data of sophoraisoflavanone A (**10**) racemate

Table S10: NMR data of sophoraisoflavanone A (**10**)

No	10		Kinoshita et al., 1990	Iinuma et al., 1992	
	δ_{H} , mult (J in Hz)	δ_{C}	δ_{C}	δ_{H}	δ_{C}
2	A: 4.495, d (8.8) B: 4.492, d (6.8)	72.0	72.0	4.50	72.1
3	4.36, dd (8.9, 6.8)	46.1	46.2	4.47	46.0
4		198.6	198.2		197.8
5		165.4	165.5		165.9
6	5.97, br s	96.8	97.0	5.97	97.8
7		167.2	167.2		170.7
8	5.97, br s	95.6	95.7	5.97	96.6
9		164.5	164.3		164.4
10		103.6	103.7		103.0
1'		122.5	122.5		124.6*
2'		156.8	156.8		157.1
3'		120.5	120.5		121.0
4'		158.9	158.8		159.0
5'	6.64, d (8.4)	112.0	112.1	6.64	112.3
6'	6.88, d (8.4)	128.0	127.9	6.88	128.2
1''	A: 3.41, dd (14.4/6.8) B: 3.35, dd (14.4/6.5)	24.1	24.3	3.38	24.3
2''	5.29, br t (6.8 Hz)	124.2	124.2	5.29	122.6*
3''		131.2	131.2		131.3
4''	1.67, br s	25.8	25.9	1.67	24.3
5''	1.77, br s	18.0	18.1	1.77	18.2
2'-OCH ₃	3.75, s	62.3	62.4	3.75	62.5
5-OH	12.30			12.30	

*assignment may be exchanged

References

Kinoshita, T., Ichinose, K., Takahashi, C., Wu, J.-B., Sankawa, U., 1990. Chemical studies on *Sophora tomentosa*: The isolation of a new class of isoflavanoid. Chem. Pharm. Bull. 38 (10), 2756-2759.
<https://doi.org/10.1248/cpb.38.2756>.

Iinuma, M., Ohyama, M., Tanaka, T., Mizuno, M., Soon-Keun, H., 1992. Three 2',4',6'-trioxygenated flavanones in roots of *Echinosophora koreensis*. Phytochemistry 31 (2), 665–669. [https://doi.org/10.1016/0031-9422\(92\)90056-V](https://doi.org/10.1016/0031-9422(92)90056-V).

Methyl dalbergin (**11**)

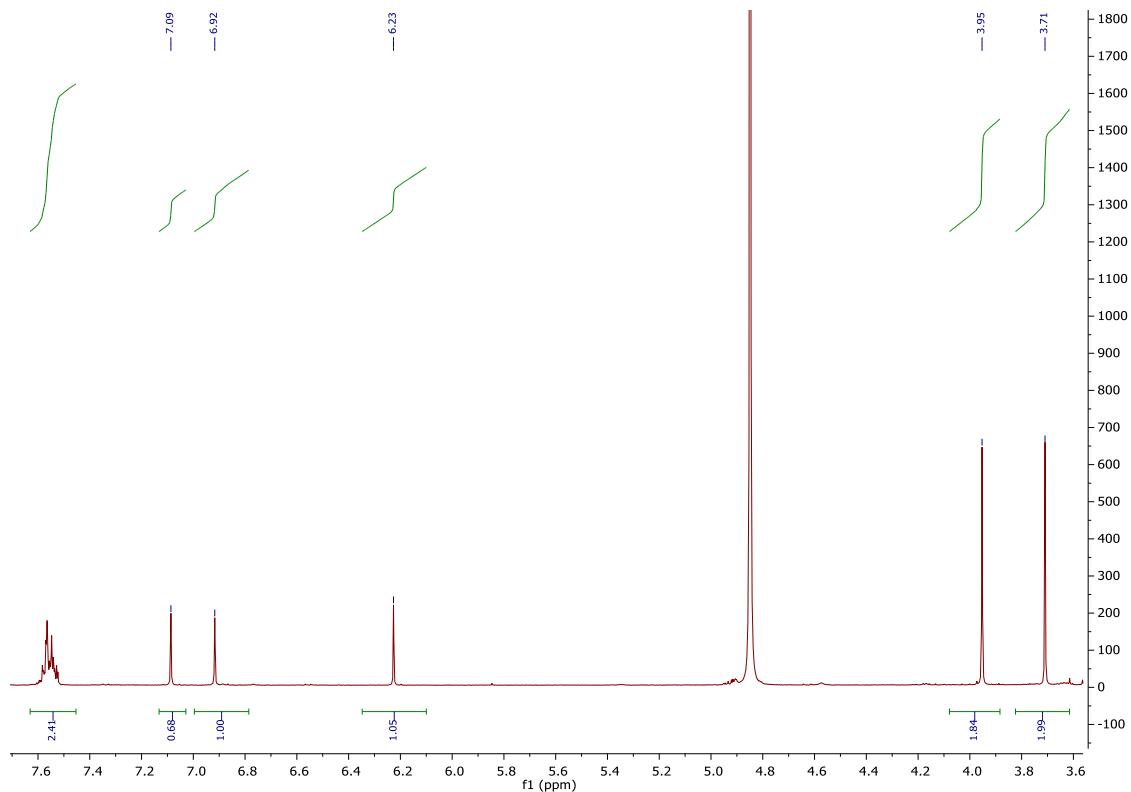


Figure S11_1: ^1H NMR spectrum (400 MHz, CD_3OD) of methyl dalbergin (**11**)

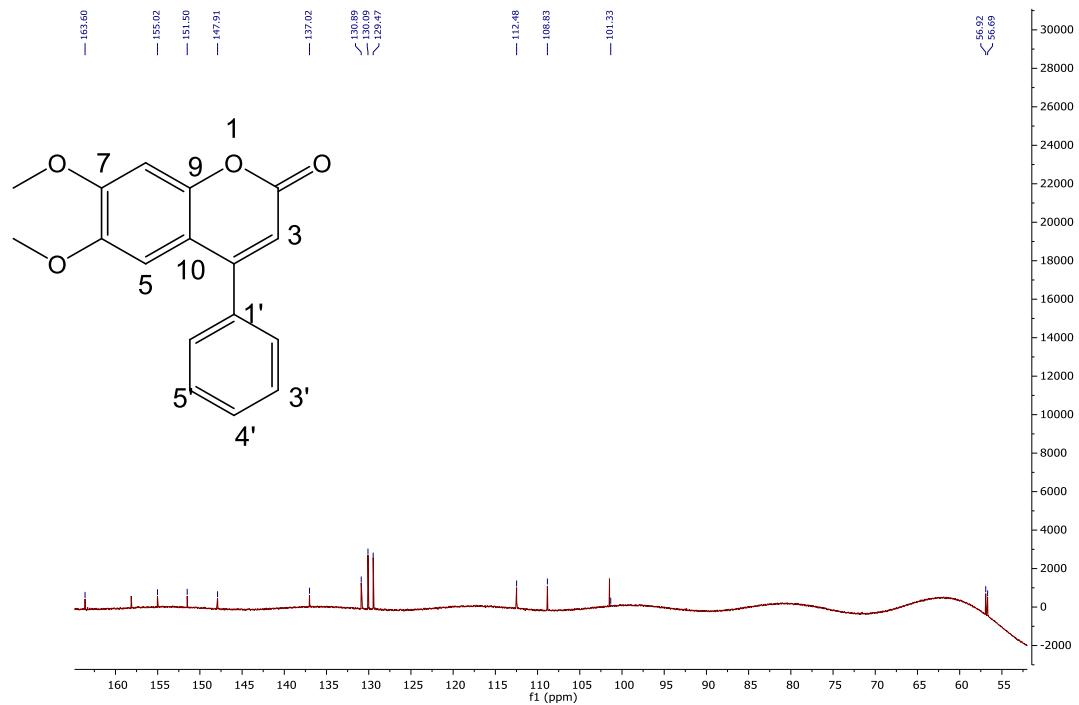


Figure S11_2: ^{13}C NMR spectrum (125 MHz, CD_3OD) of methyl dalbergin (**11**)

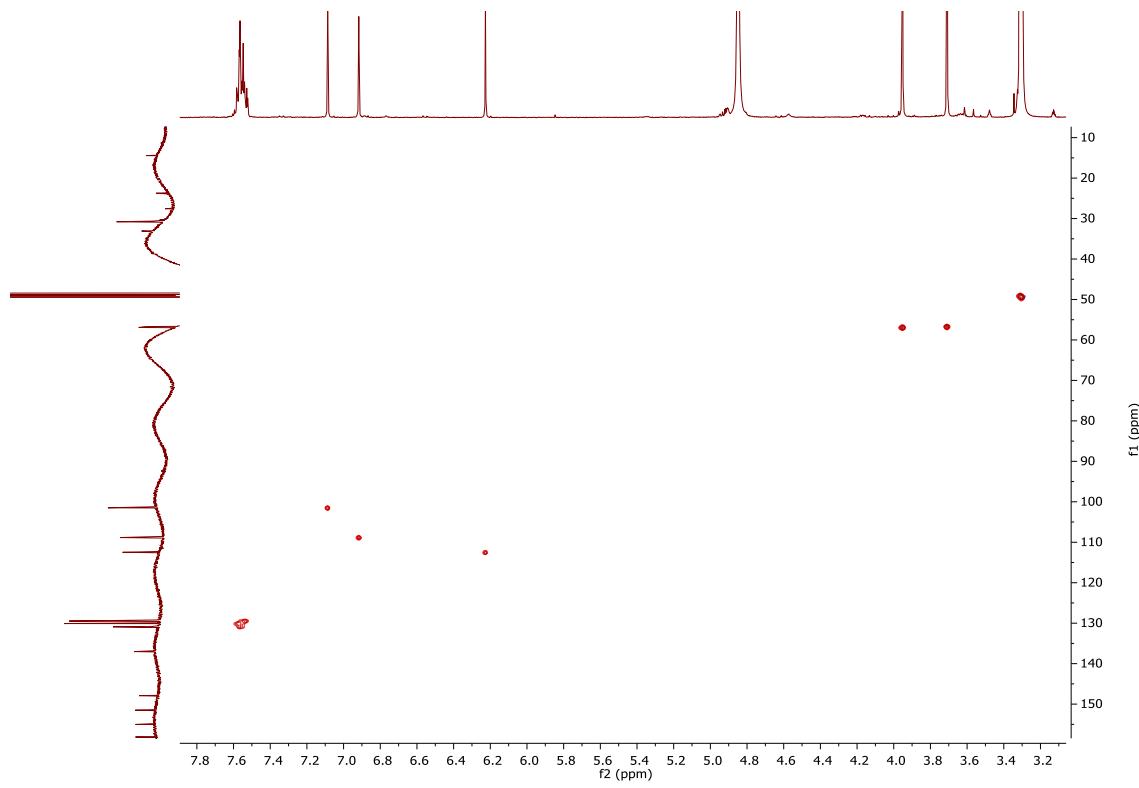


Figure S11_3: HSQCAD spectrum (125 MHz, CD₃OD) of methyl dalbergin (**11**)

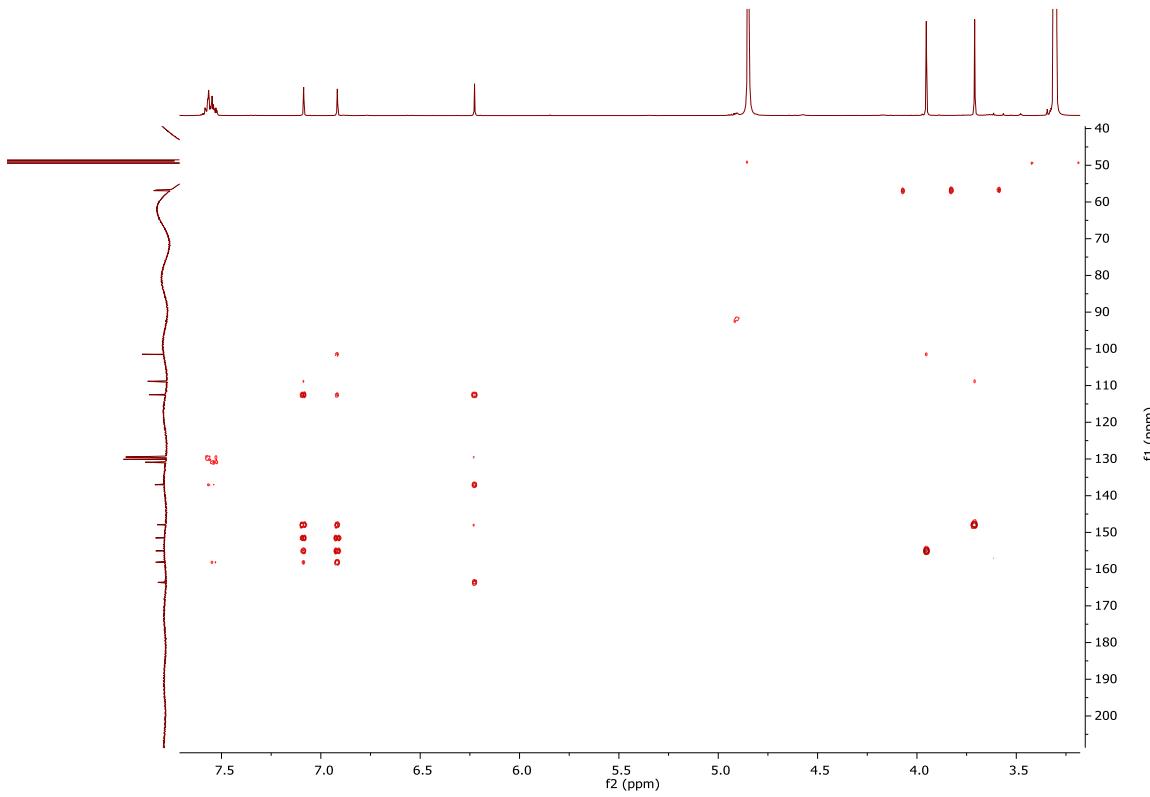


Figure S11_4: HMBC spectrum (125 MHz, CD₃OD) of methyl dalbergin (**11**)

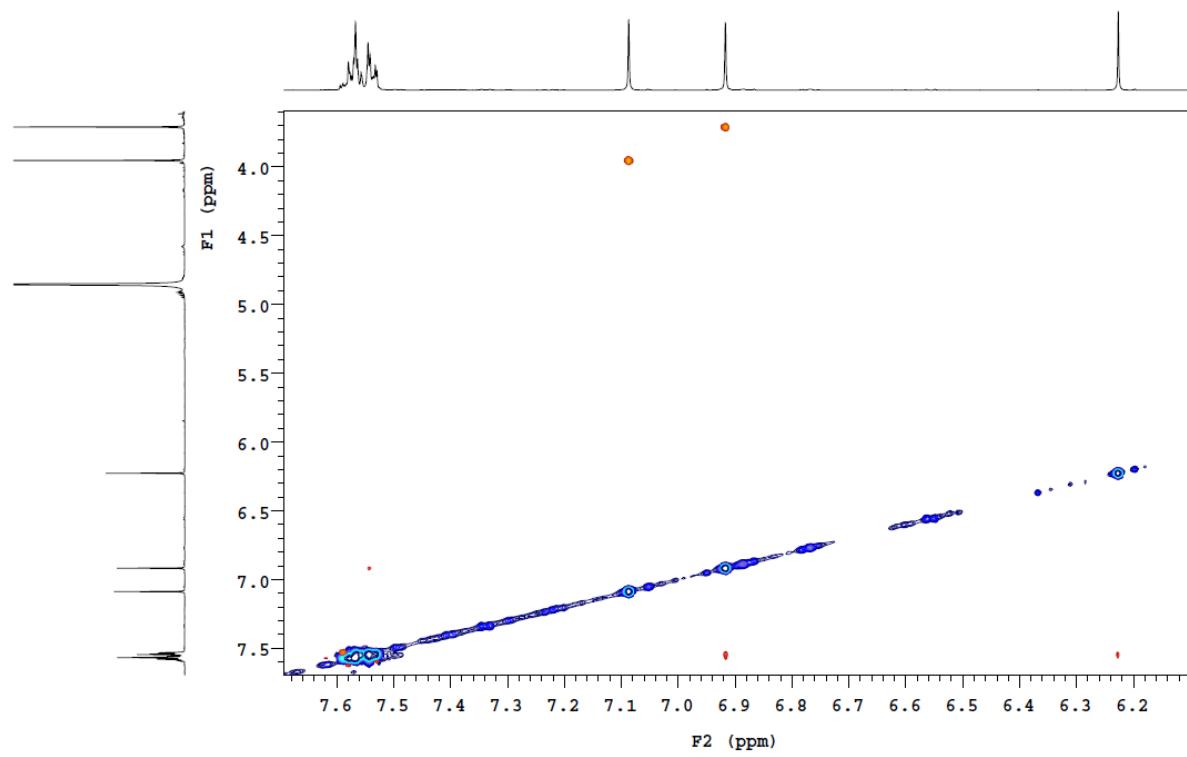


Figure S11_5: ROESY spectrum (125 MHz, CD₃OD) of methyl dalbergin (**11**)

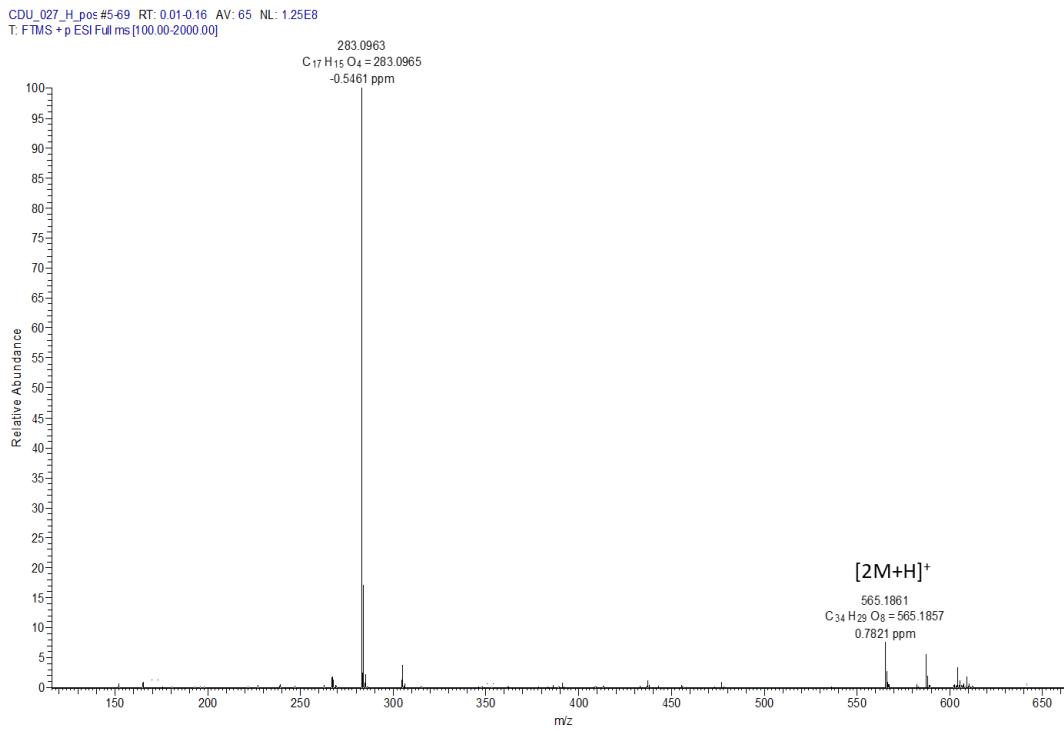


Figure S11_6: Positive ESI-HRMS spectrum of methyl dalbergin (**11**)

Table S11: NMR data (400 MHz, CD₃OD) of methyl dalbergin (**11**)

No	δ_{H} , <i>mult</i> (<i>J</i> in Hz)	δ_{C}	HMBC	ROESY
2		163.6		
3	6.23, <i>s</i>	112.5	C2, C1', C10	H2'/6'
4		151.5		
5	6.92, <i>s</i>	108.8	C10, C7, C9	6-OCH ₃ , H 2'/6'
6		147.9		
7		155.0		
8	7.10, <i>s</i>	101.4	C4, C7, C10	7-OCH ₃
9		158.5		
10		112.5		
1'		137.0		
2'/6'	7.54, <i>m</i>	129.5		H3, H5
3'/5'	7.57, <i>m</i>	130.1		
4'	7.57, <i>m</i>	130.9		
6-OCH ₃	3.71, <i>s</i>	56.7	C6, C5	H5
7-OCH ₃	3.96, <i>s</i>	56.9	C7, C8	H8

Dalbergin (12)

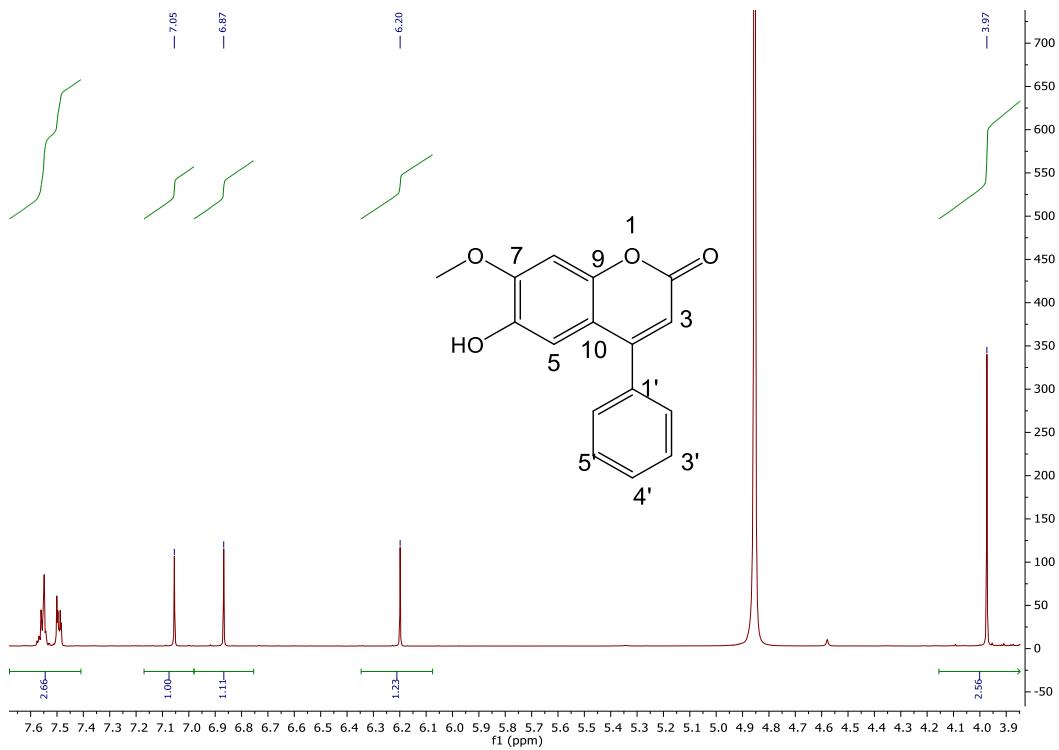


Figure S12_1: ¹H NMR spectrum (400 MHz, CD₃OD) of dalbergin (12)

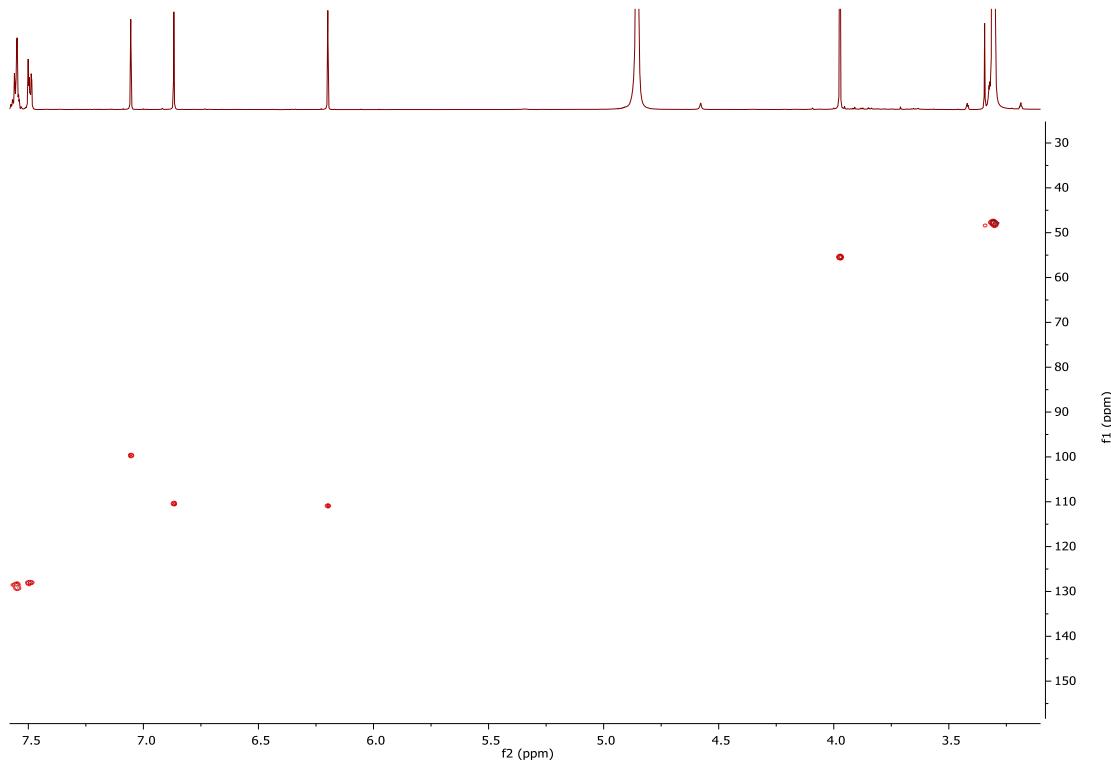


Figure S12_2: HSQC spectrum (400 MHz, CD₃OD) of dalbergin (12)

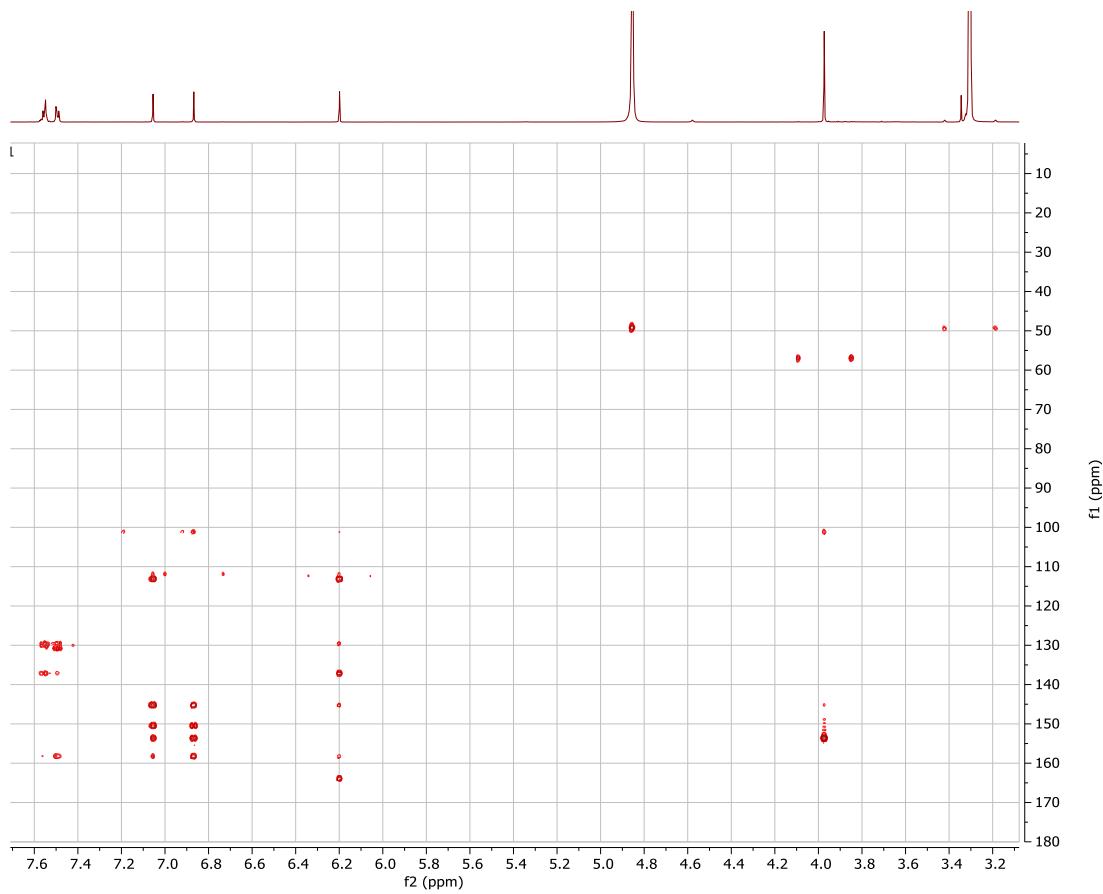


Figure S12_3: HMBC spectrum (400 MHz, CD₃OD) of dalbergin (**12**)

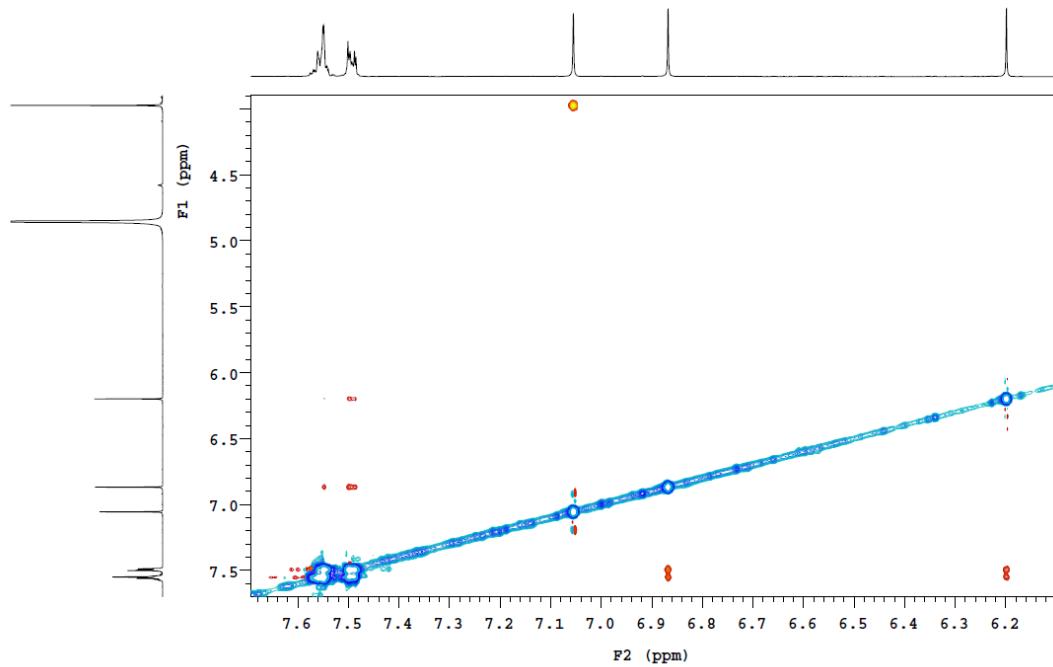


Figure S12_4: ROESY spectrum (400 MHz, CD₃OD) of dalbergin (**12**)

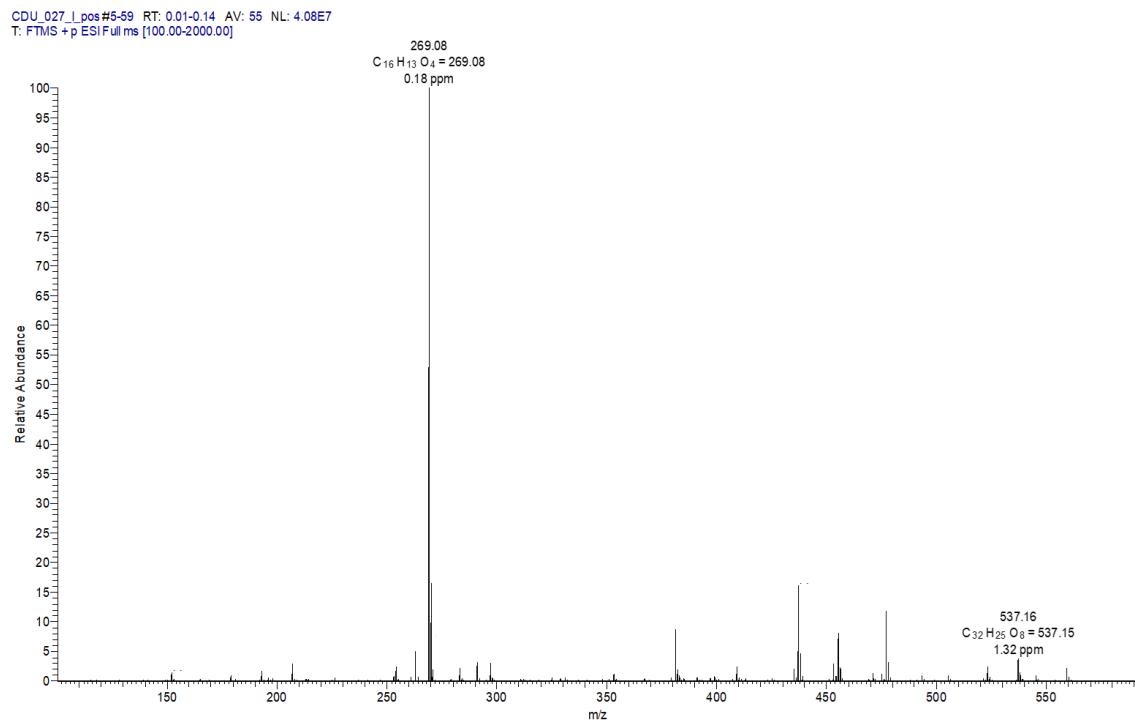


Figure S12_5: Positive ESI-HRMS spectrum of dalbergin (**12**)

Table S12: NMR data (400 MHz, CD₃OD) of dalbergin (**12**)

No	δ_{H} , mult	δ_{C}	HMBC	ROESY	δ_{C} (Chan et al. 1997)*
2		163.9			160.85
3	6.20, s	112.4	C10, C2, C1', C4, C6, C2'/6' (H 3'/5')	H2'/6', (H 3'/5')	111.70
4		158.2			155.55
5	6.87, s	111.9	C6, C7, C4, C10, C9, C4	H2'/6'	110.75
6		145.2			143.96
7		153.6			152.35
8	7.06, s	101.2	C6, C7, C9, C10, C4	7-OCH ₃	100.91
9		150.4			148.83
10		113.1			111.32
1'		137.1			135.72
2'/6'	7.50, m	129.5	C4', C2'/6'	H5, H3	128.71
3'/5'	7.55, m	130.0	C1', C2'/6',		129.24
4'	7.55, m	130.8	C3'/5'		129.95
7-OCH ₃	3.97, s	56.9	C7, C8	H8	56.67

*Chan, S.C., Chang, Y.S., Wang, J.P., Chen, S.C., Kuo, S.C., 1998. Three new flavonoids and antiallergic, anti-inflammatory constituents from the heartwood of *Dalbergia odorifera*. Planta Med. 64 (2), 153–158.

<https://doi.org/10.1055/s-2006-957394>.

Melanine (13)

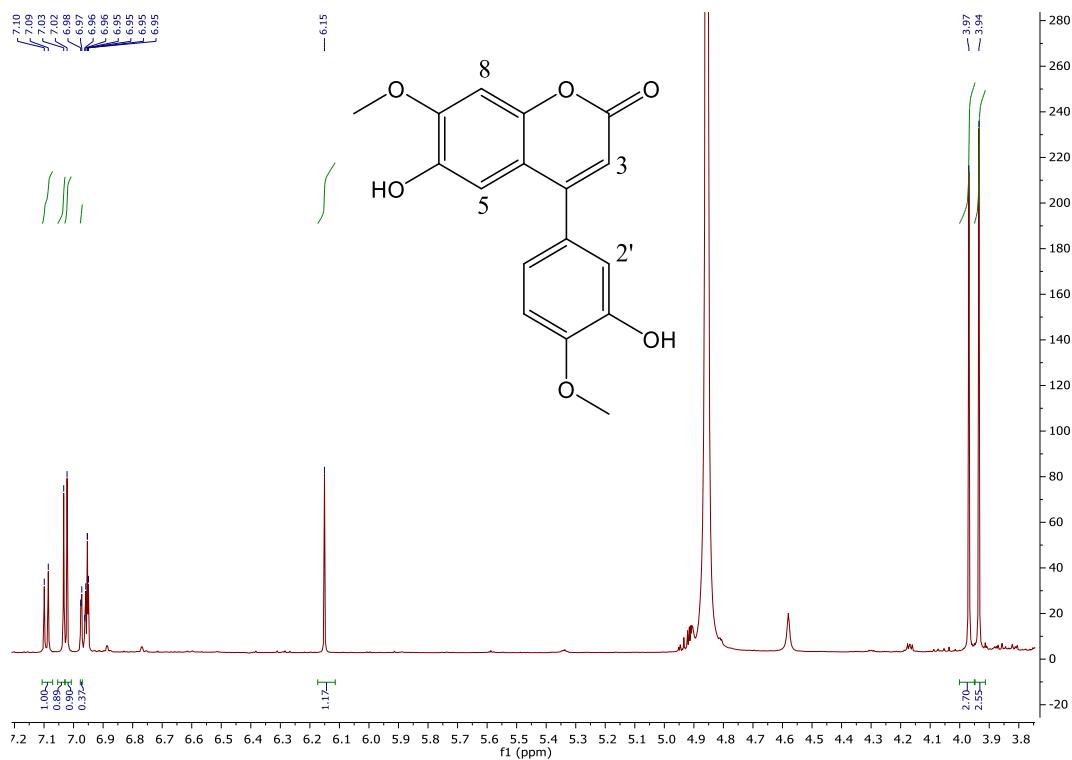


Figure S13_1: ^1H NMR spectrum (400 MHz, CD_3OD) of melannein (**13**)

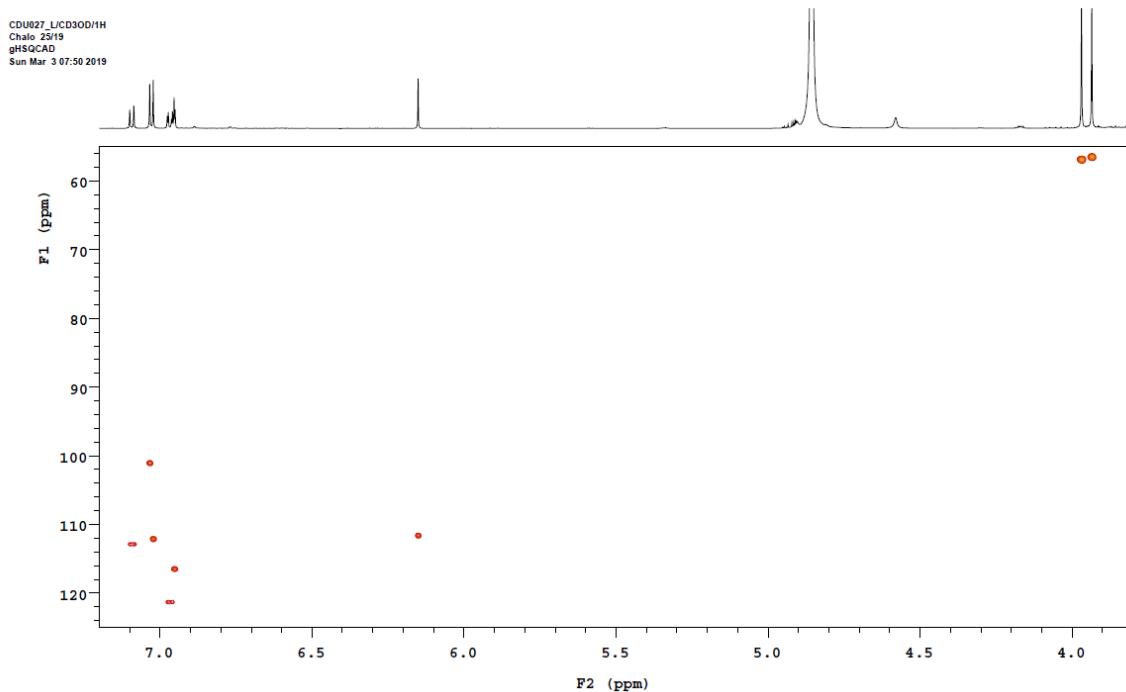


Figure S13_2: HSQCAD spectrum (125 MHz, CD₃OD) of melannein (**13**)

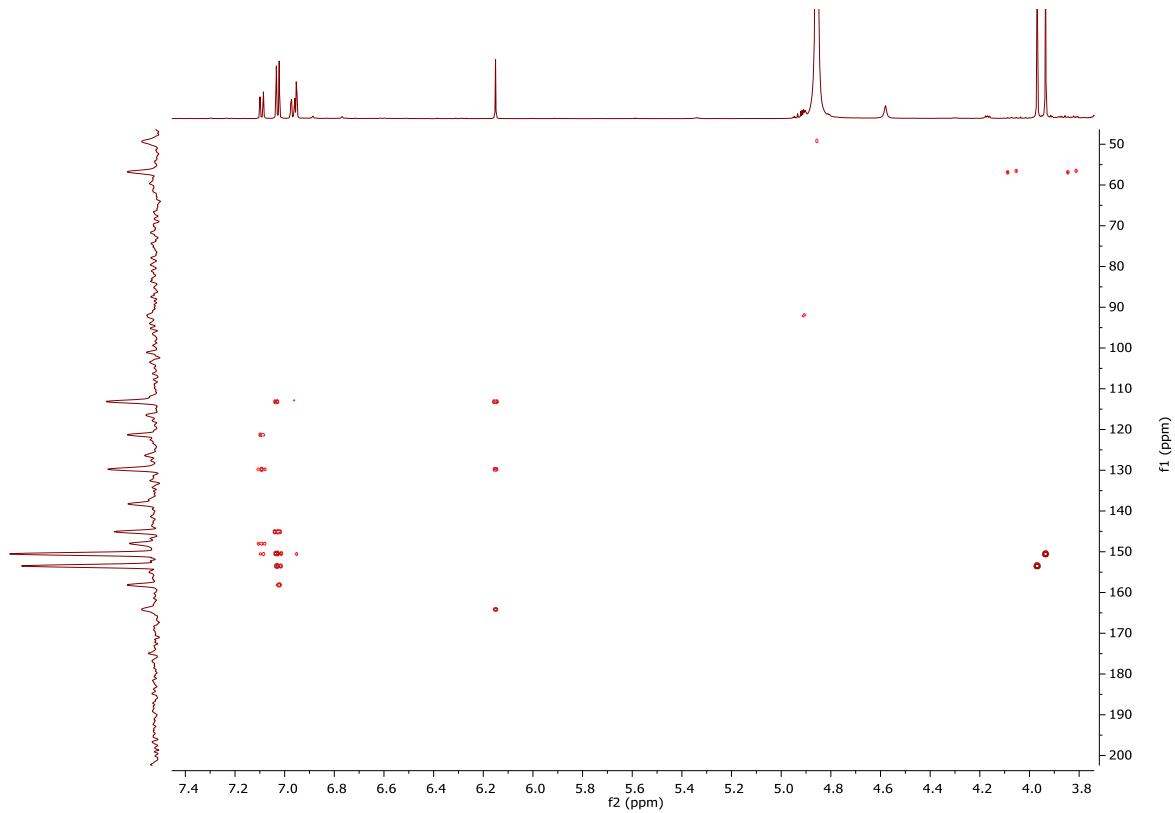


Figure S13_3: HMBC spectrum (125 MHz, CD_3OD) of melannein (**13**)

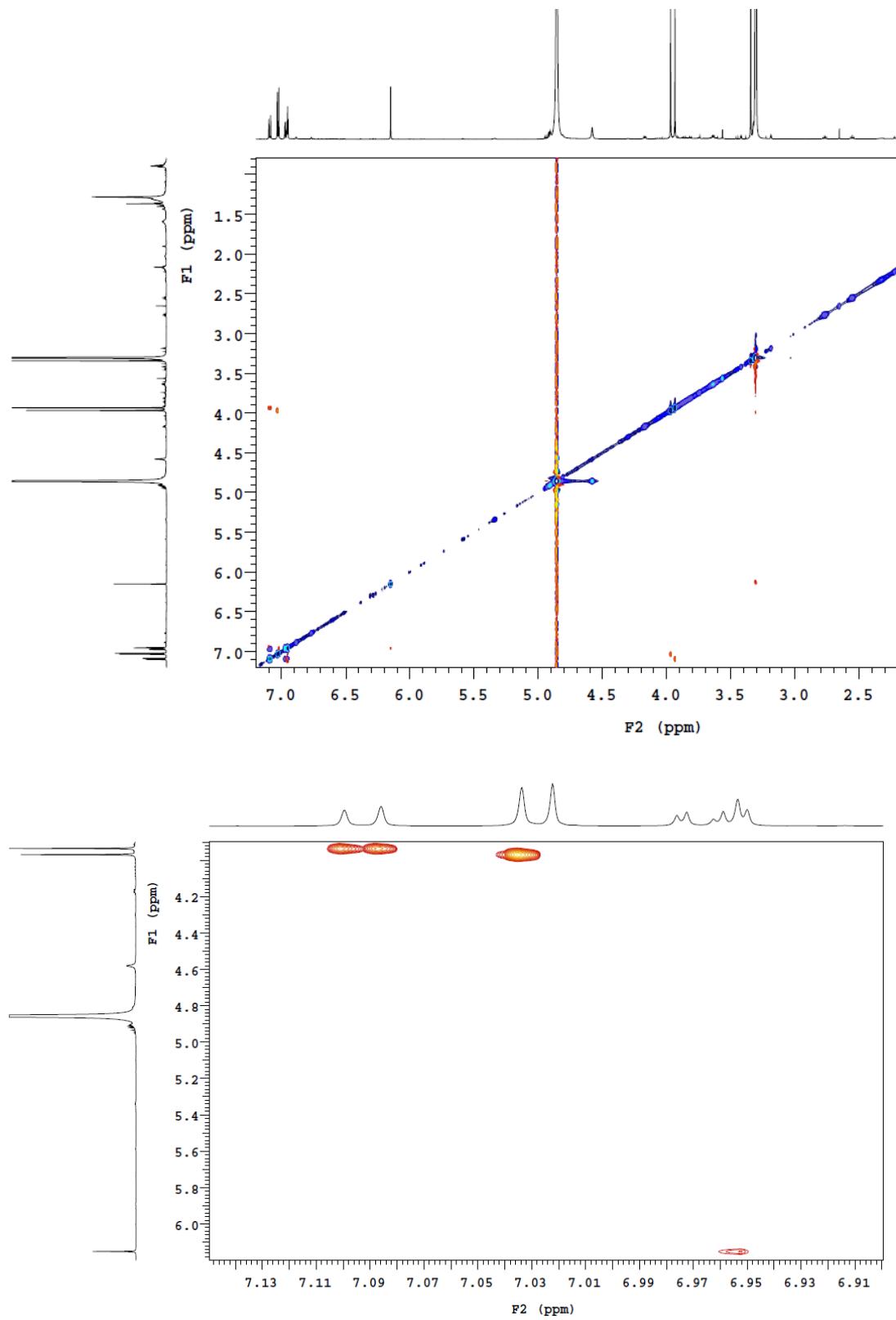


Figure S13_4: ROESY spectrum (125 MHz, CD_3OD) of melannein (**13**)

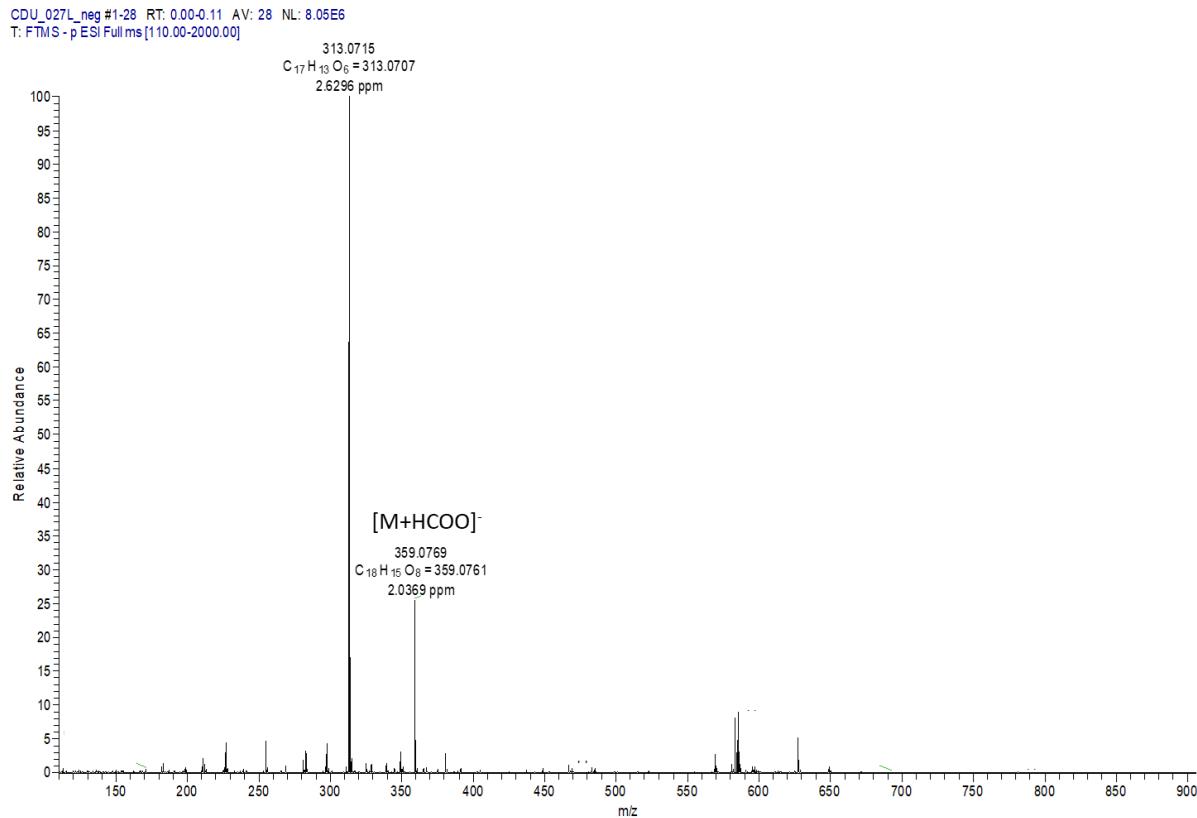


Table S13: NMR data (400 MHz, CD₃OD) of melannein (**13**)

No	δ_H , mult (J in Hz)	δ_C	HMBC	ROESY
2		164.2		
3	6.15, s	111.6	C10, C2, C1'	H6'
4		158.2		
5	7.02, s	112.1	C4, C6, C7	
6		145.1		
7		153.5		
8	7.03, s	101.2	C10, C6, C9, C7	7-OCH ₃
9		150.5		
10		113.2		
1'		129.8		
2'	6.97, d (2.2)	121.4	C4'	
3'		148.0		
4'		150.6		
5'	7.09, d (8.6)	113.0	C1', C2', C3', C4'	H6', 4'-OCH ₃
6'	6.95, dd (8.6, 2.2)	116.5	C4'	H3, H5'
7-OCH ₃	3.97, s	56.9	C7	H8
4'-OCH ₃	3.94, s	56.5	C4'	H5'

3',4'-Dihydroxy-*trans*-cinnamic acid octacosylester (14)

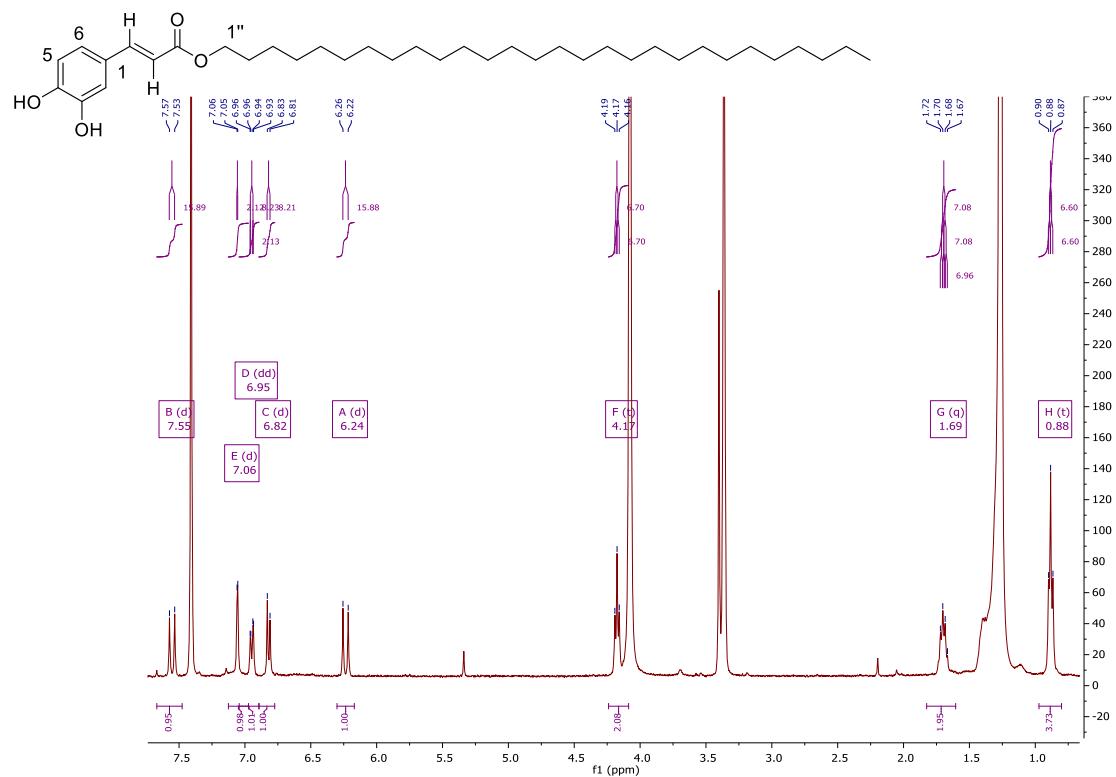


Figure S14_1: ^1H NMR spectrum (400 MHz, CDCl_3 and few drops CD_3OD) of compound **14**

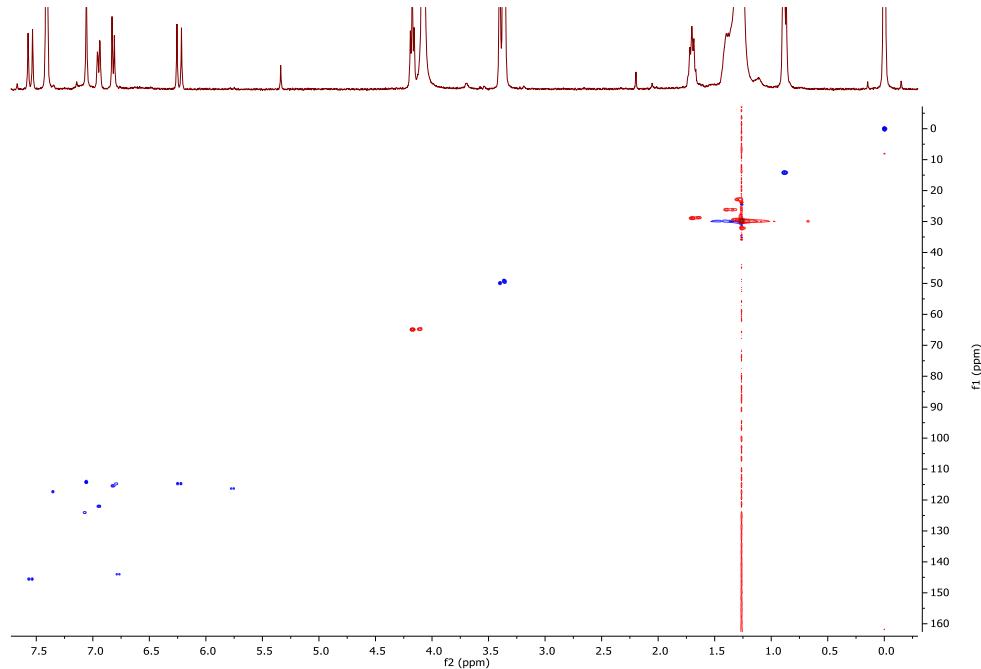


Figure S14_2: HSQCAD spectrum (400 MHz, CDCl_3 and few drops CD_3OD) of compound **14**

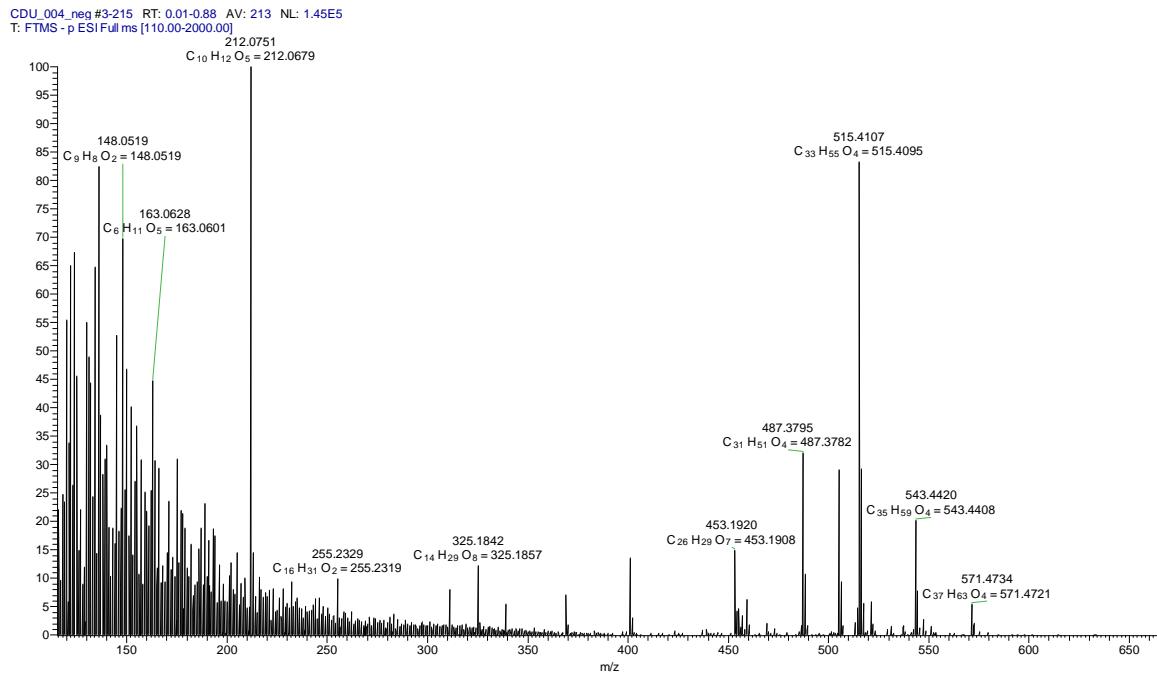


Figure S14_3: Negative ion ESI-HRMS spectrum of compound **14**

Table S14: NMR data of compound **14**

No	δ_H , mult (J in Hz)	δ_C (HSQC)
1		
2	7.06, d (2.1)	114.2 CH
3		
4		
5	6.82, d (8.2)	115.4 CH
6	6.95, dd (8.2, 2.1)	122.0 CH
1'	7.55, d (15.9)	145.5 CH
2'	6.24, d (15.9)	114.7 CH
3'		
1''	4.17, t (6.7)	65.0 CH ₂
2''	1.69, m	28.9 CH ₂
3''	1.39	26.1 CH ₂
4''	1.30	29.3 CH ₂
5''-20''	1.26	29.9 CH ₂
21''	1.26	29.9 CH ₂
22''	1.26	32.1 CH ₂
23''	1.26	23.9 CH ₂
24''	0.88, t (6.6)	14.2 CH ₃

Table S15: Cytotoxic activities of crude extract of *D. melanoxyton* against human cancer cell lines determined by MTT (cell viability) and CV (cell growth) assays. Values show survival [%].

	PC-3				HT-29			
	MTT		CV		MTT		CV	
Crude extract	50 µg/ml 1 ± 37	0.05 µg/ml 96 ± 4	50 µg/ml 1 ± 18	0.05 µg/ml 104 ± 4	50 µg/ml 0 ± 25	0.05 µg/ml 98 ± 4	50 µg/ml 0 ± 5	0.05 µg/ml 98 ± 2
Positive control*		0 ± 29		-1 ± 7		0 ± 40		0 ± 7
Negative control		100 ± 4		100 ± 7		100 ± 5		100 ± 3

* Digitonin, 125 µg/ml

Table S16: Antifungal activity of compounds from *D. melanoxyton* against human pathogens determined by agar diffusion assay (inhibition zone [mm]) and microdilution (MIC [µg/ml])

compounds (1mg/ml)	<i>S. salmonicolor</i> 549 H4	<i>C. albicans</i> H8	<i>P. notatum</i> JP36 P1	<i>A. fumigatus</i> ATCC204305
	[mm]	[mm]	[mm]	[µg/ml]
1	0	11P	12P	n.t.
2	17	0	11P	n.t.
7	0/A	12	14	32
9	0	0/A	15(p)	>128
10	17	12p	15	>128
Ampho B ^a	19p	21	18p	n.t.
DMSO ^b	13P	0	12P	>128

^aAmphotericin B, positive control tested at concentration of 10 µg/ml

^bnegative control