

Identification of Antiadipogenic Constituents of the Rhizomes of *Anemarrhena asphodeloides*

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Running title: Phenolic compounds from *Anemarrhena asphodeloides*

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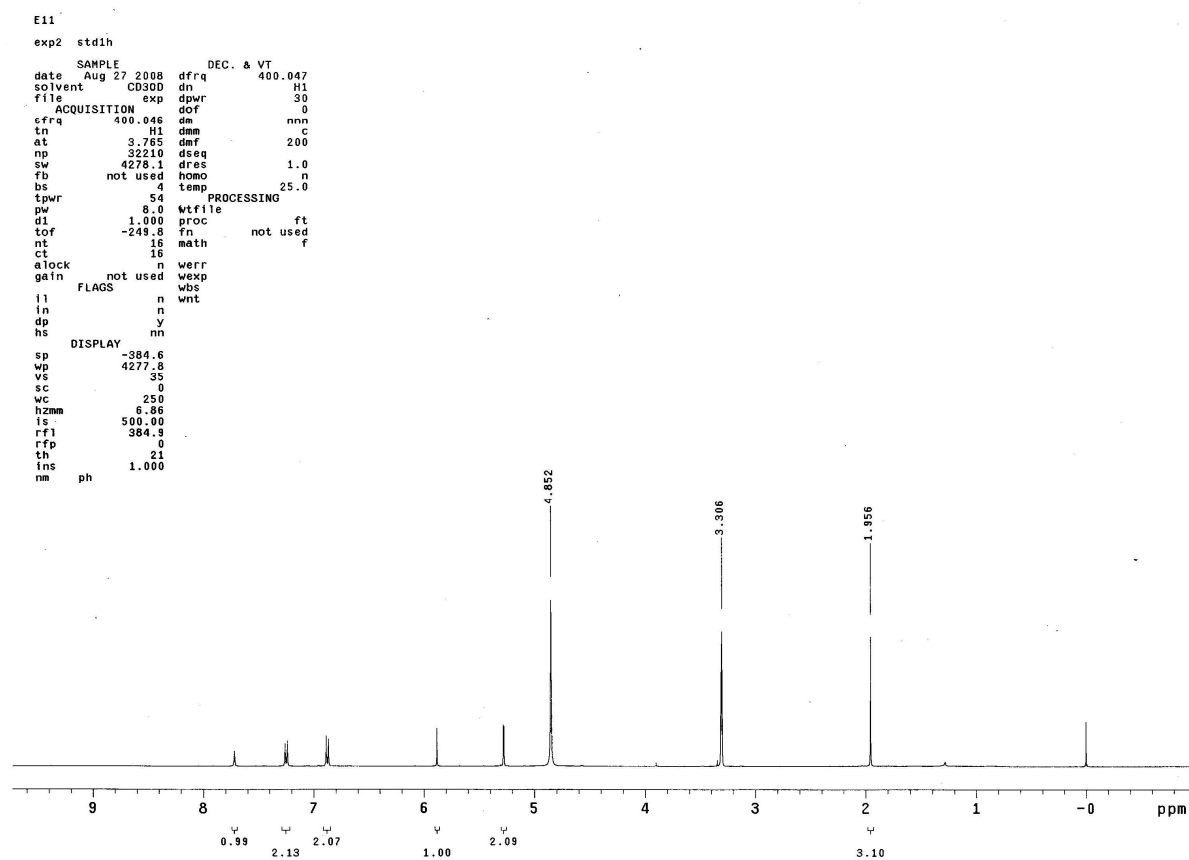
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[§] Dongguk University.

[⊥] Korea University.

^{||} Seoul National University.

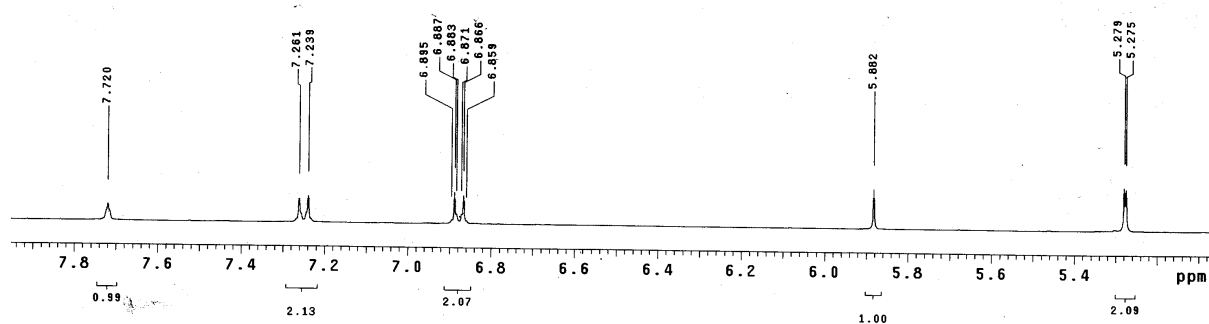
S1. ^1H NMR (400 MHz, CD_3OD) spectrum of the new compound **1**.



S1-1. Expanded ^1H NMR (400 MHz, CD_3OD) spectrum of the new compound **1**.

E11

Pulse Sequence: s2pu1

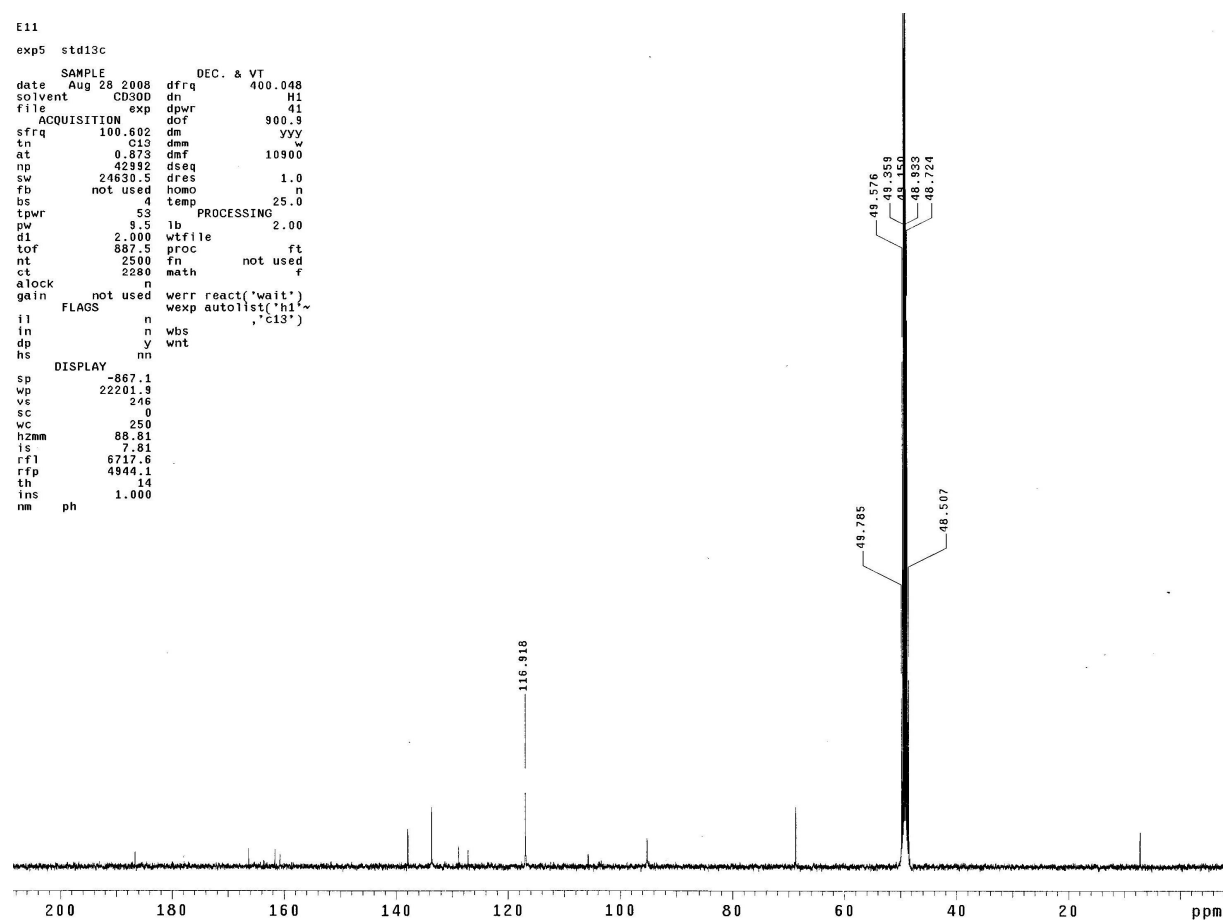


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at      0.873          dseq      10900
np      4292           dsew
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ws      not used       homo      n
bs      4              temp      25.0
tpwr    53             PROCESSING
pw      9.5            lb        2.00
d1      2.000          wfile
tof      887.5         proc      ft
nt      2500           fn        not used
ct      2280          math      f
alock    n
gain     not used     werr react('wait',
                     flags, 'h1',
                     n,
                     wbs,
                     dp,   y,   wnt,
                     hs,   nn)
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nm      ph

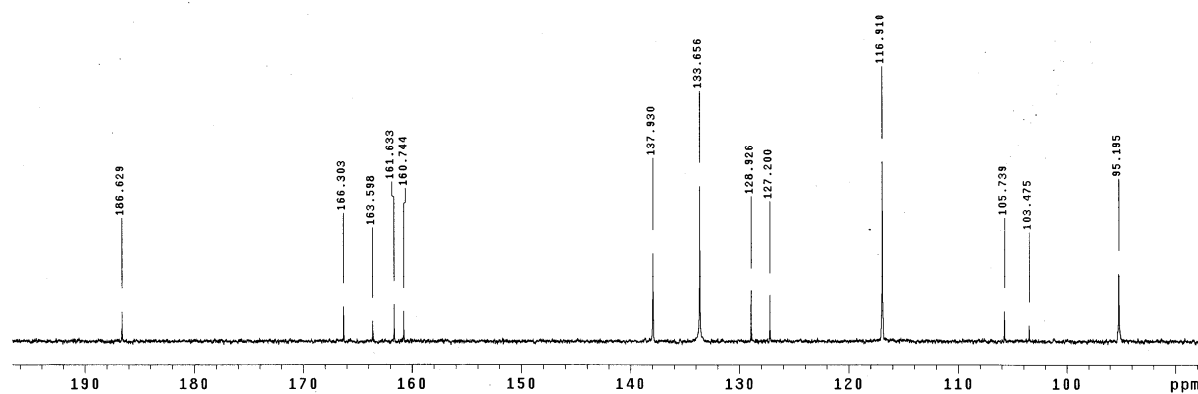
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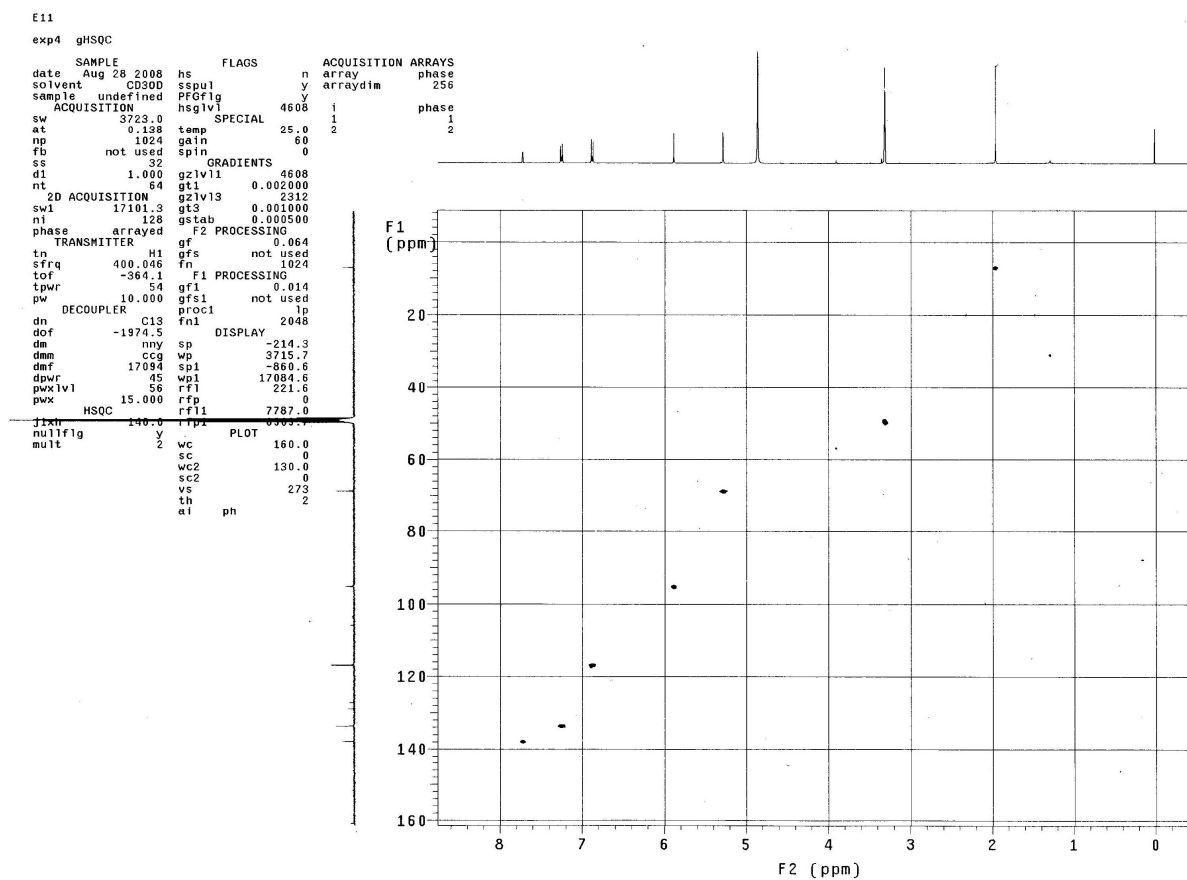
S2-1. Expanded ^{13}C NMR (100 MHz, CD_3OD) spectrum of the new compound **1**.

E11

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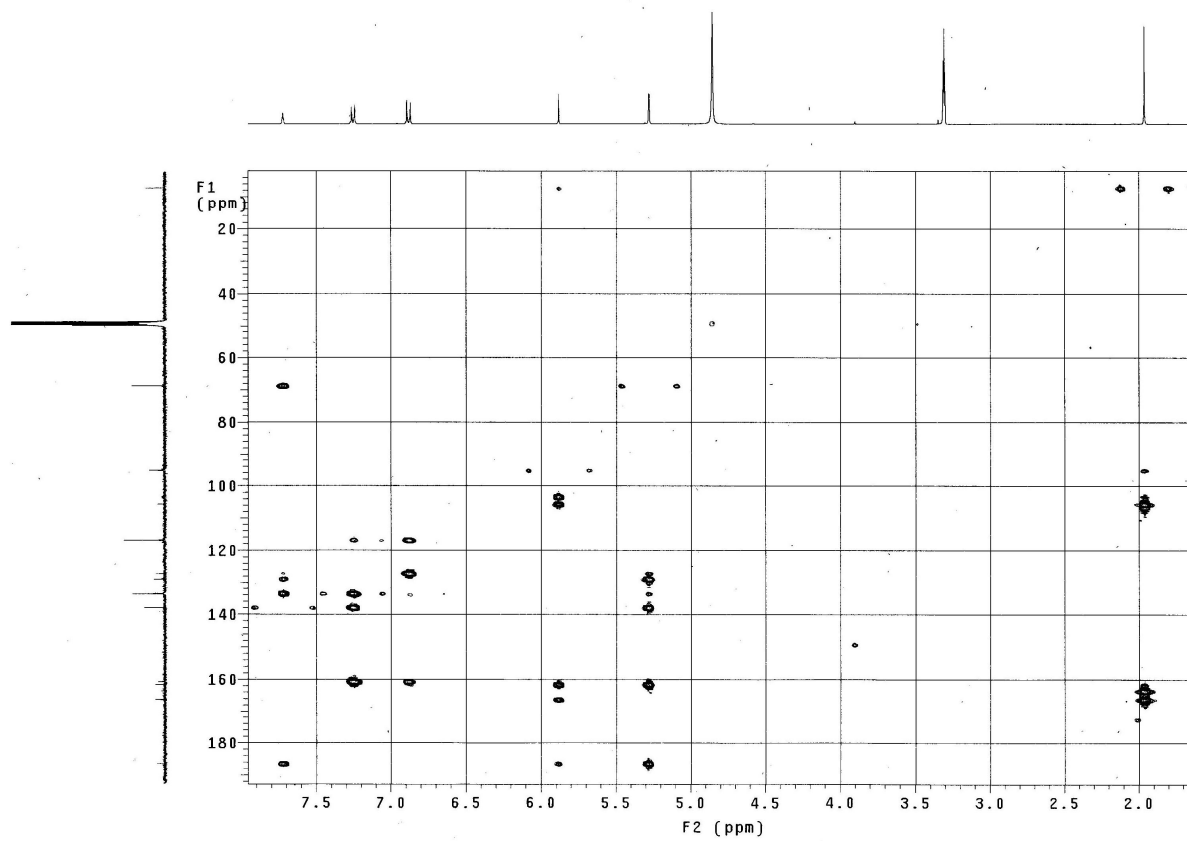
S3. HSQC spectrum (400 MHz, CD₃OD) of the new compound 1.



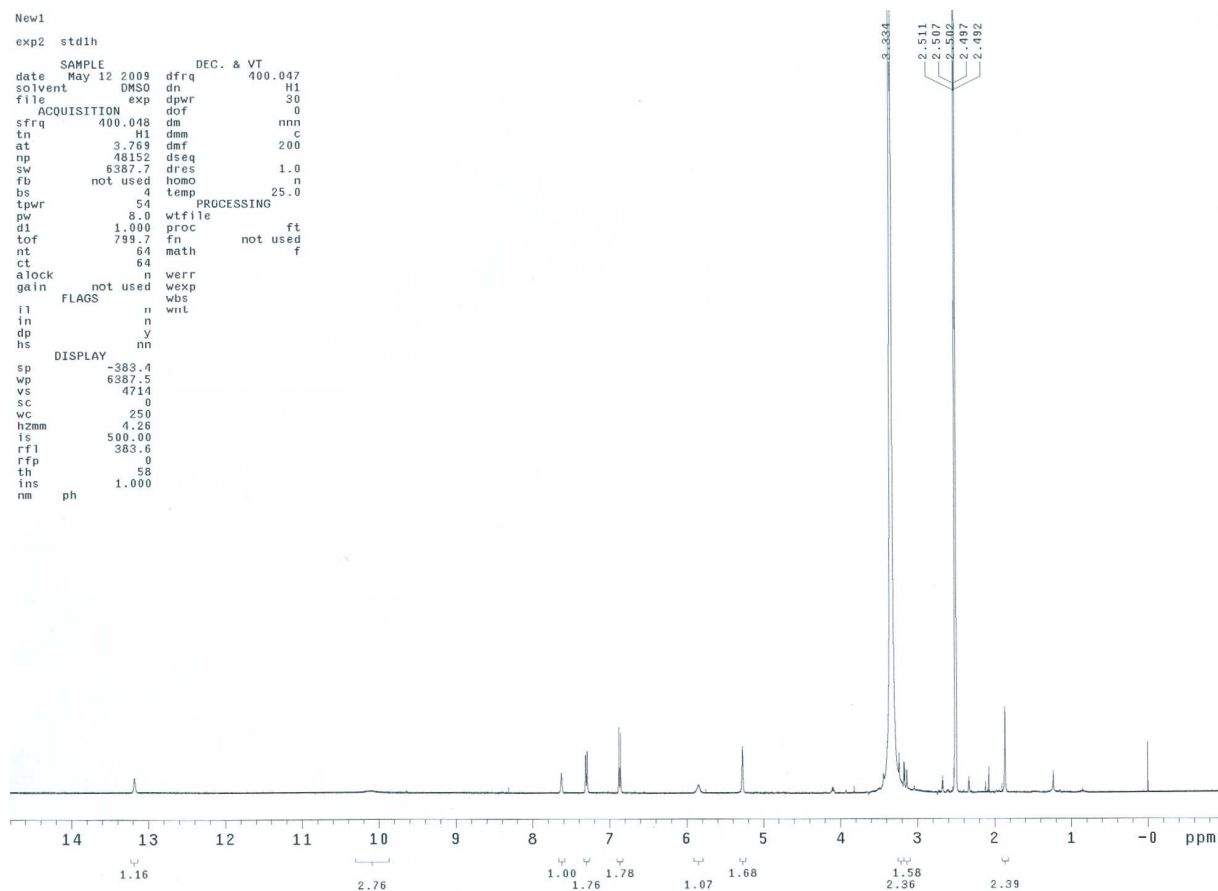
S4. HMBC spectrum (400 MHz, CD₃OD) of the new compound **1**.

F11

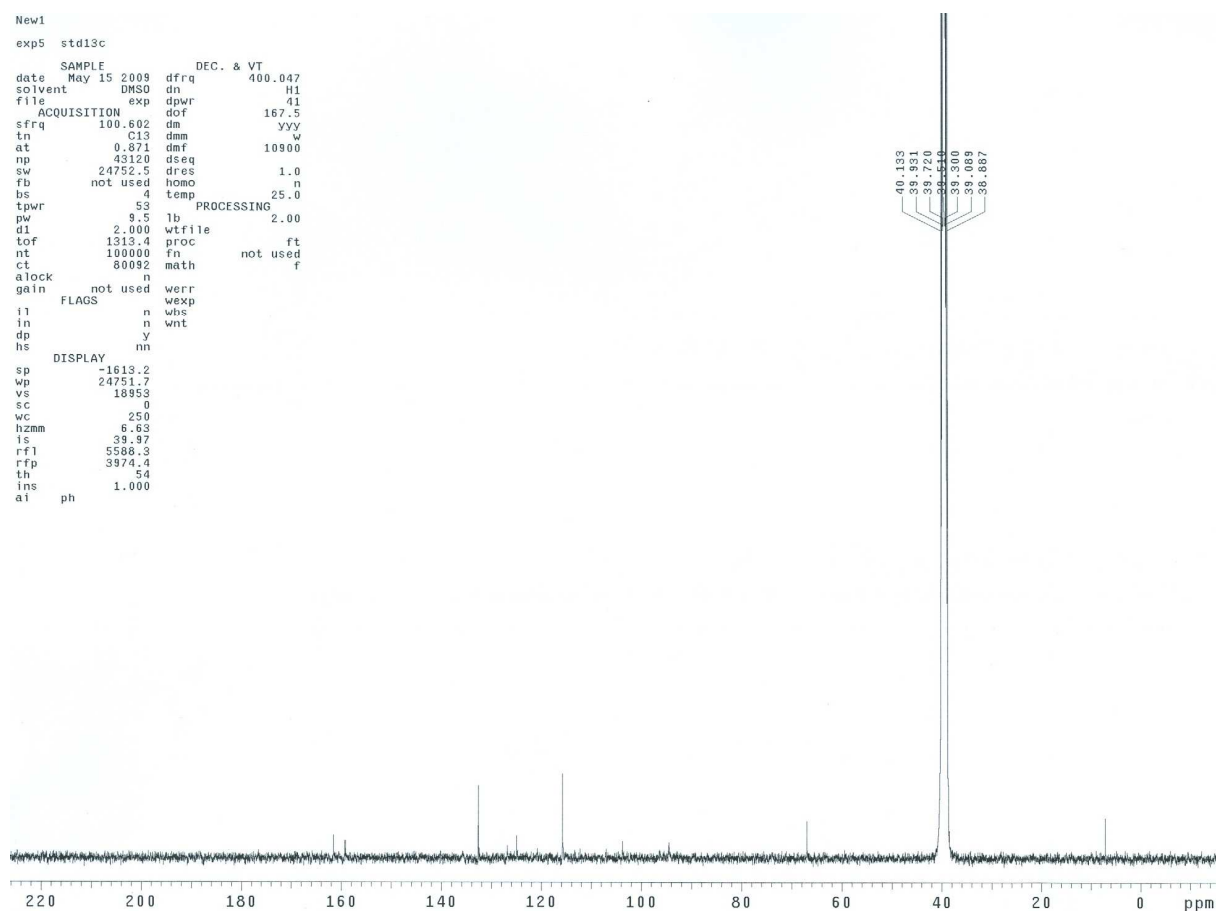
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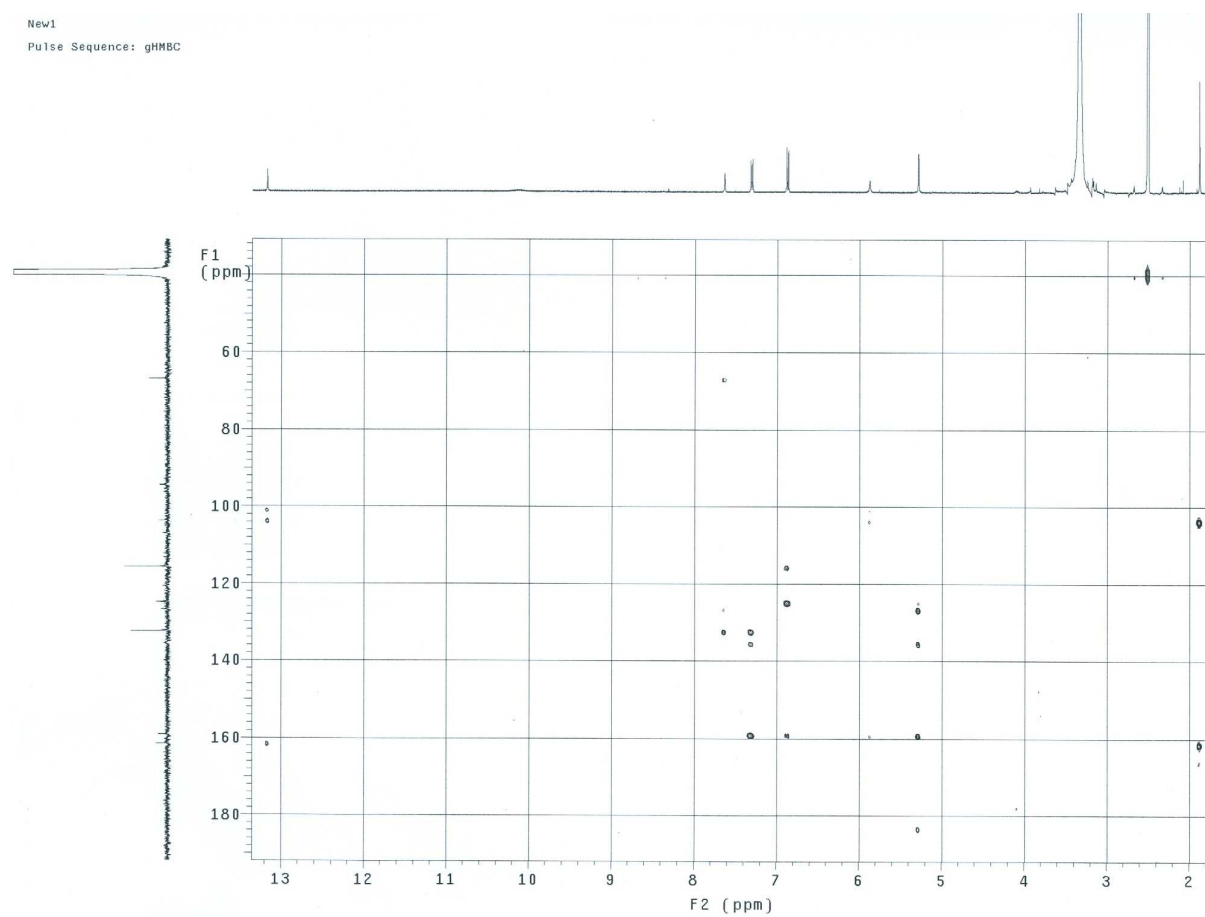
S5. ^1H NMR (400 MHz, DMSO- d_6) spectrum of the new compound **1**.



S6. ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of the new compound **1**.

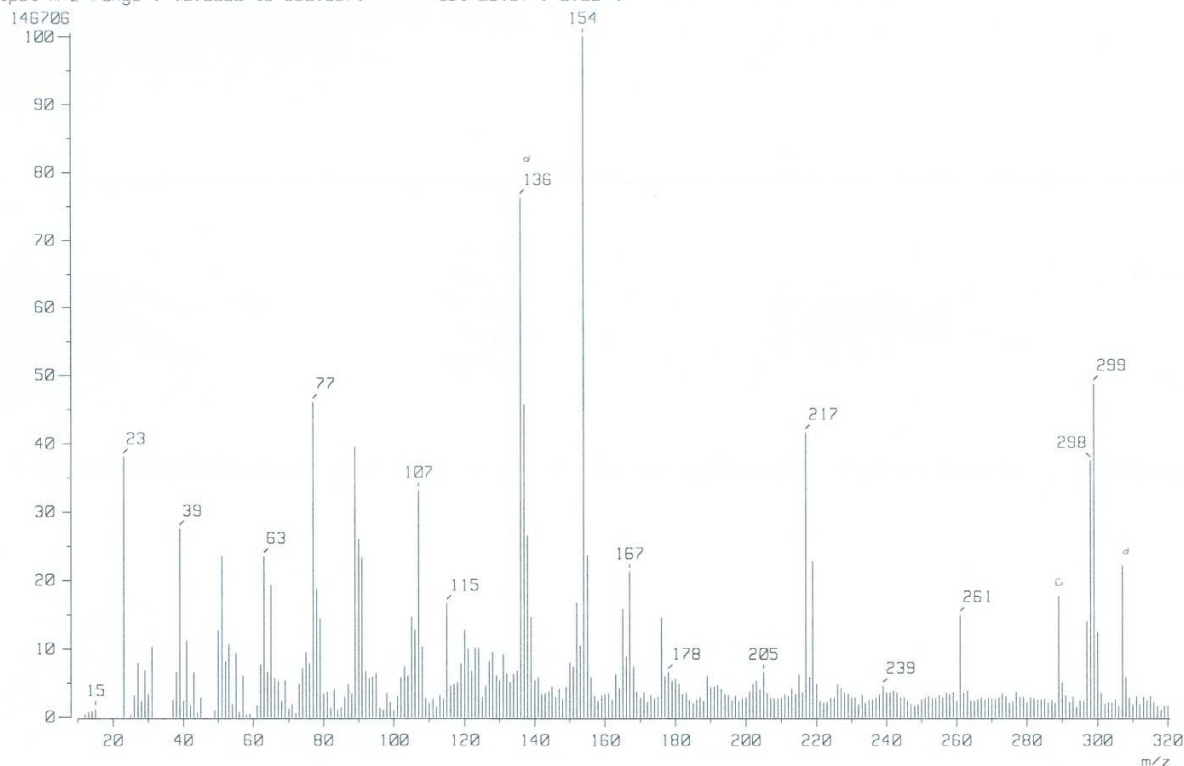


S7. HMBC spectrum (400 MHz, DMSO- d_6) of the new compound **1**.



S8. HRFABMS spectrum of the new compound 1.

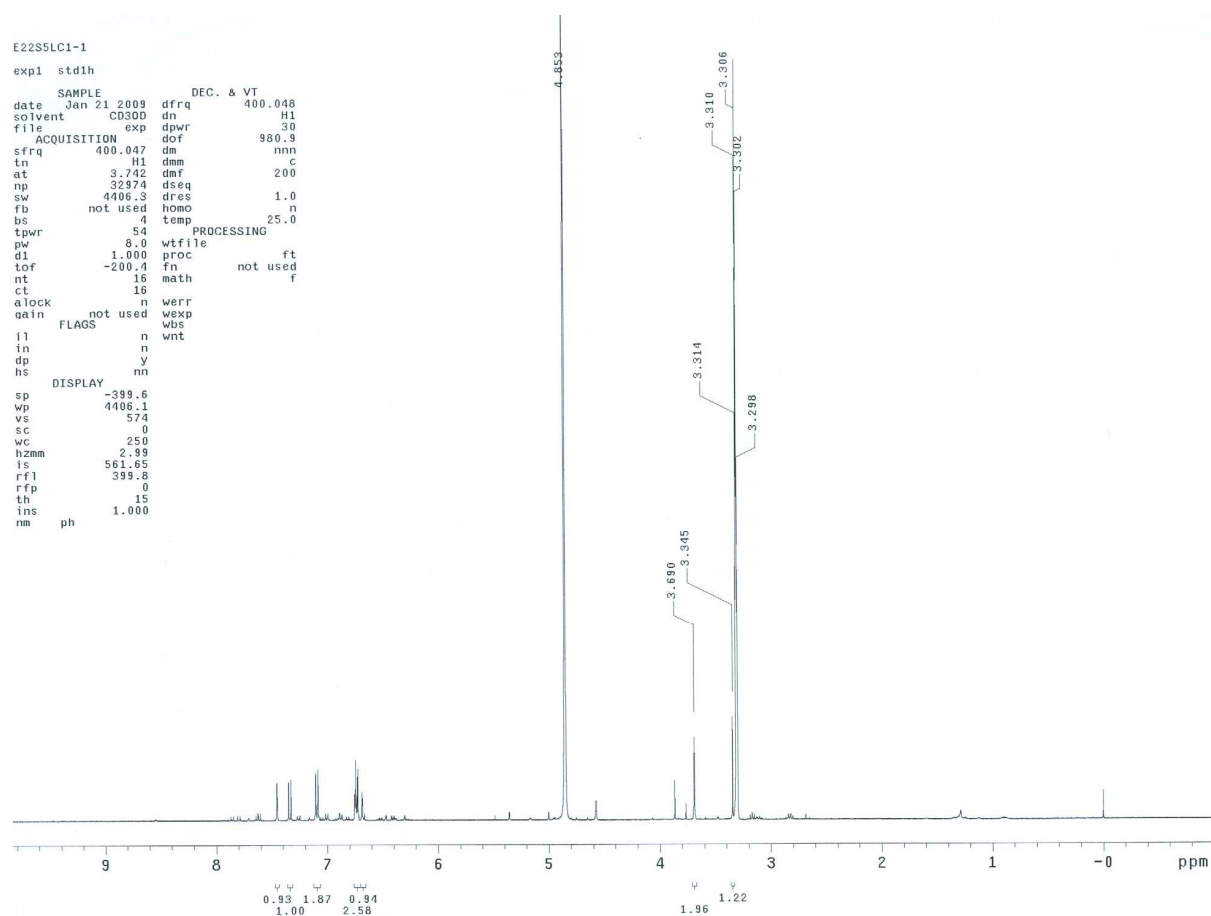
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 Sample: E11R16
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 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 0.20 min Scan# : (1,3)
 BP : m/z 154.0000 Int. : 13.92
 Output m/z range : 10.0000 to 320.6271 Cut Level : 0.00 %



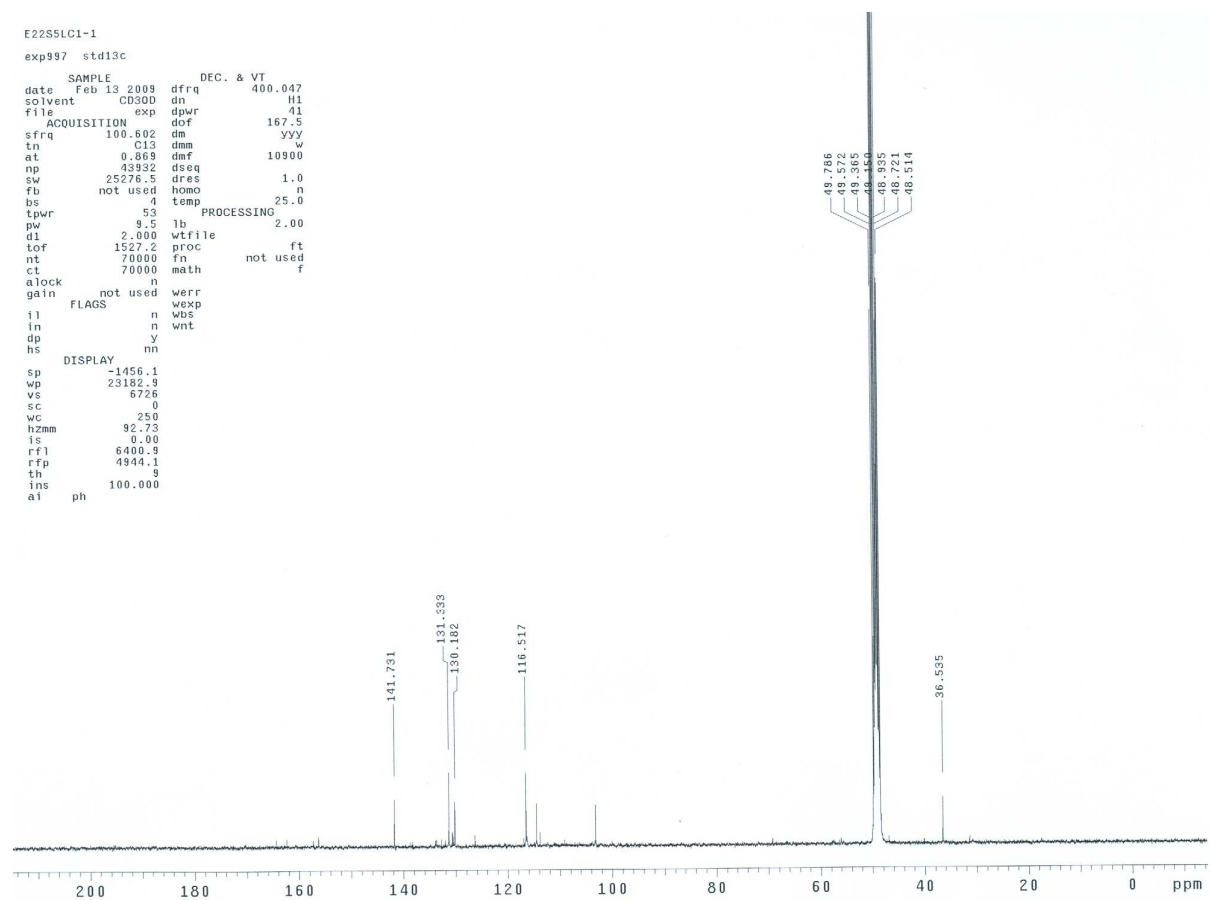
[Elemental Composition]
 Data : FAB-MS-J392 Date : 19-Sep-108 13:32
 Sample: E11R16
 Note : m-NBA
 Inlet : Direct Ion Mode : FAB+
 RT : 3.21 min Scan#: (270,280)
 Elements : C 100/0, H 100/0, O 10/0
 Mass Tolerance : 10ppm, 10mmu if m/z < 1000, 20mmu if m/z > 2000
 Unsaturation (U.S.) : 0.0 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
299.0922	100.0	+20.4 / +6.1	19.5	C 24 H 11
		✓+0.7 / +0.2	10.5	C 17 H 15 O 5
		-18.9 / -5.7	1.5	C 10 H 19 O 10

S9. ^1H NMR (400 MHz, CD_3OD) spectrum of the new compound **2**.



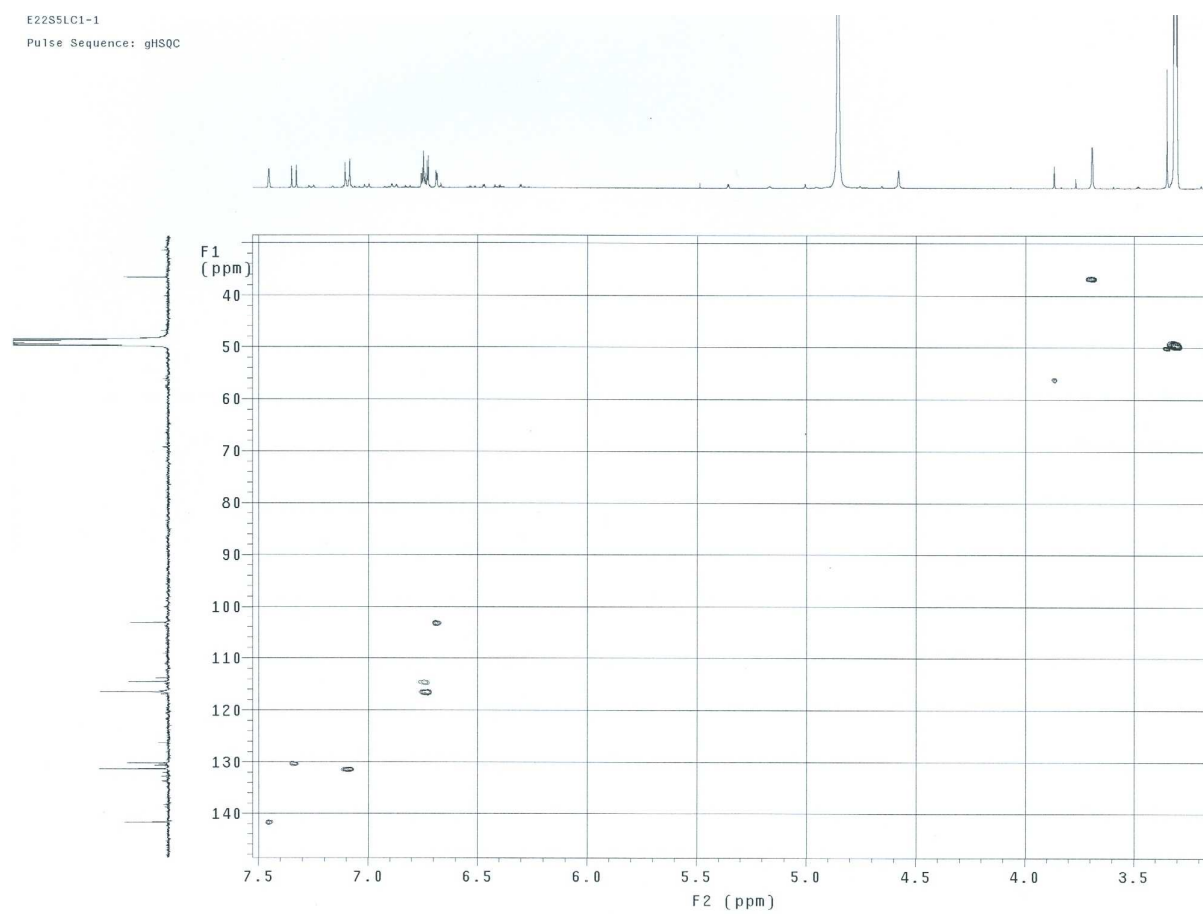
S10. ^{13}C NMR (100 MHz, CD_3OD) spectrum of the new compound 2.



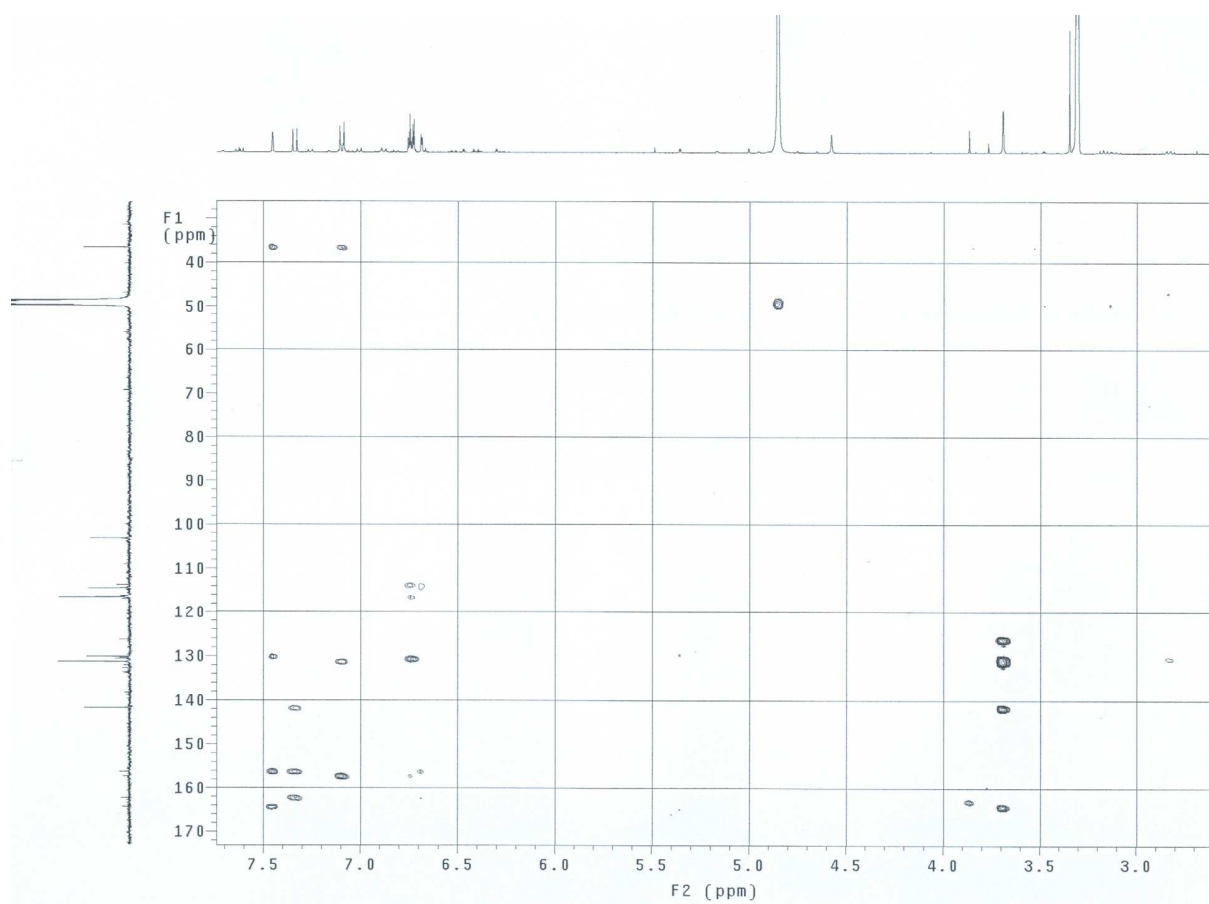
S11. HSQC spectrum (400 MHz, CD₃OD) of the new compound **2**.

F22S5LC1-1

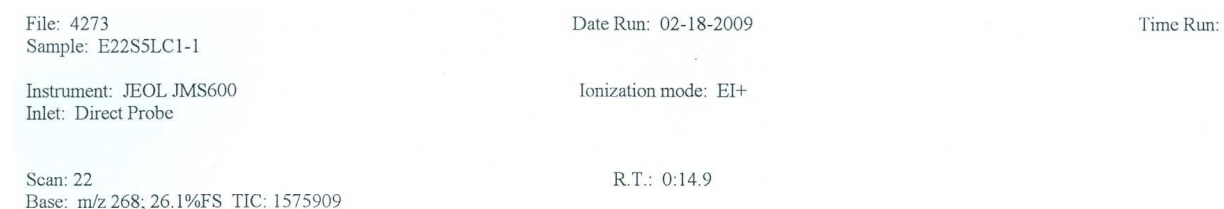
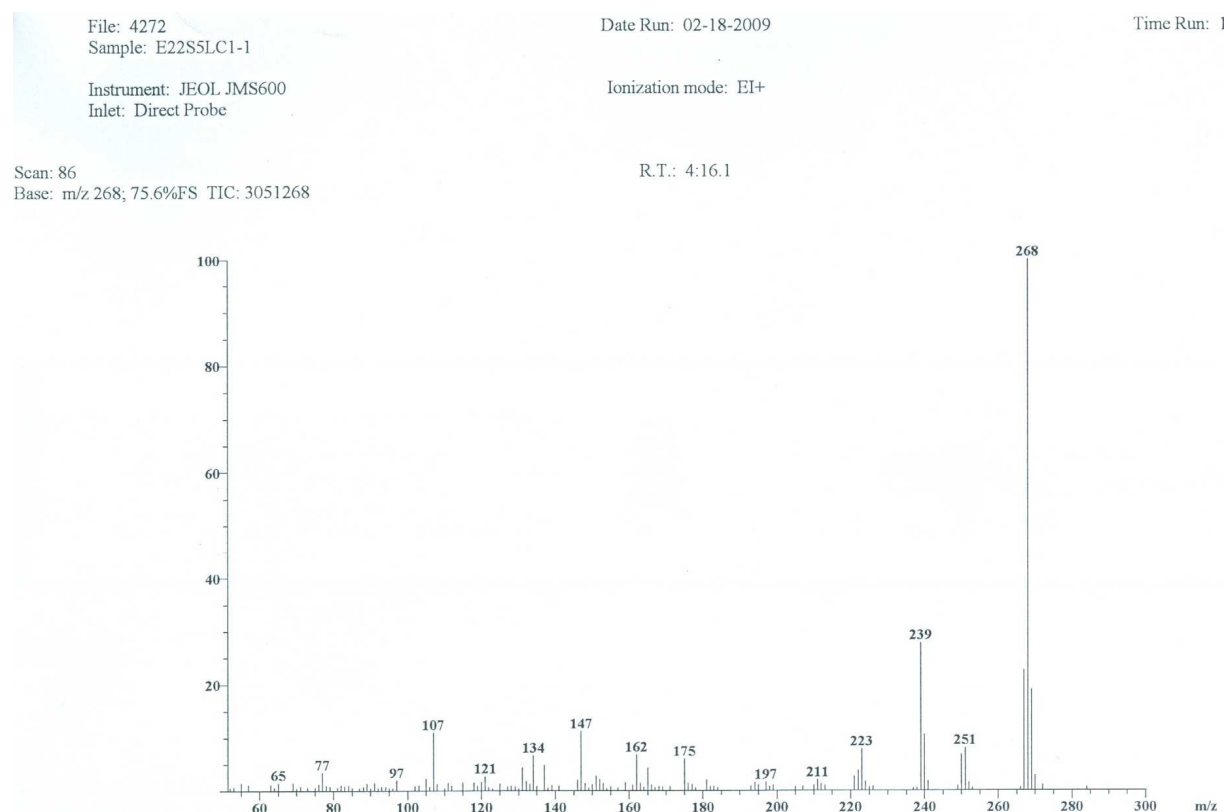
Pulse Sequence: gHSQC



S12. HMBC spectrum (400 MHz, CD₃OD) of the new compound **2**.



S13. HREIMS spectrum of the new compound 2.

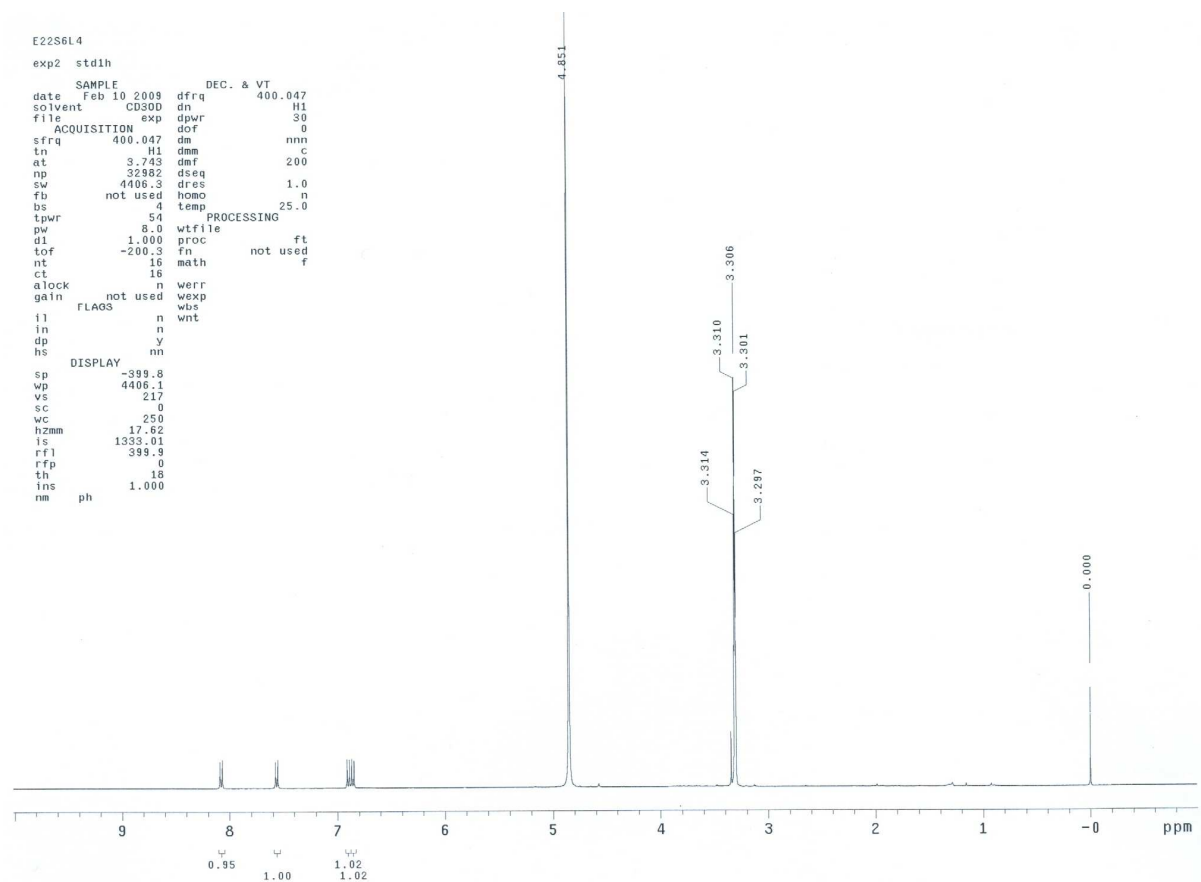


Selected Isotopes : C₀₋₅₀H₀₋₁₀₀O₀₋₁₀

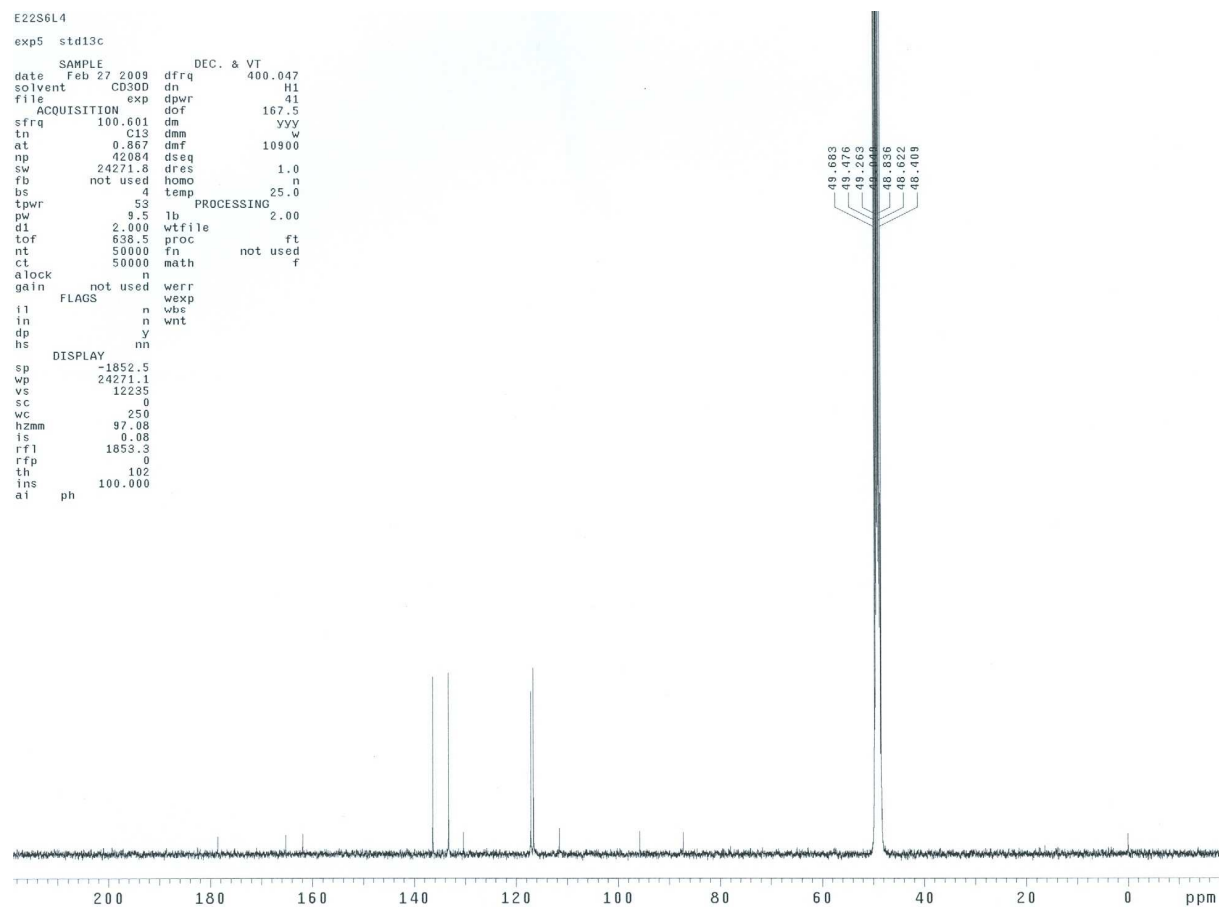
Error Limit : 20 ppm

<u>Measured Mass</u>	<u>% Base</u>	<u>Formula</u>	<u>Calculated Mass</u>	<u>Error</u>
268.0738	100.0%	C ₁₆ H ₁₂ O ₄	268.0735	-1.0

S14. ^1H NMR (400 MHz, CD_3OD) spectrum of the new compound **3**.



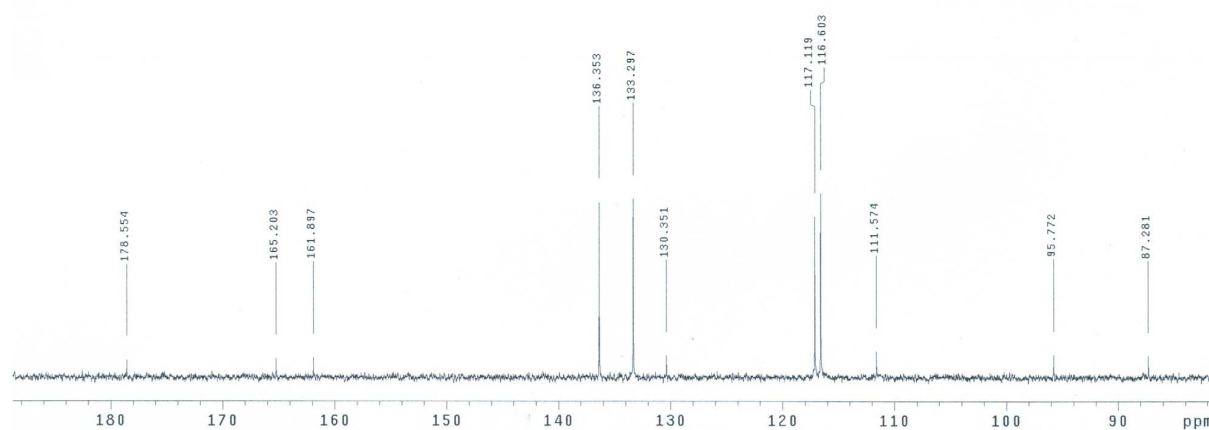
S15. ^{13}C NMR (100 MHz, CD_3OD) spectrum of the new compound **3**.



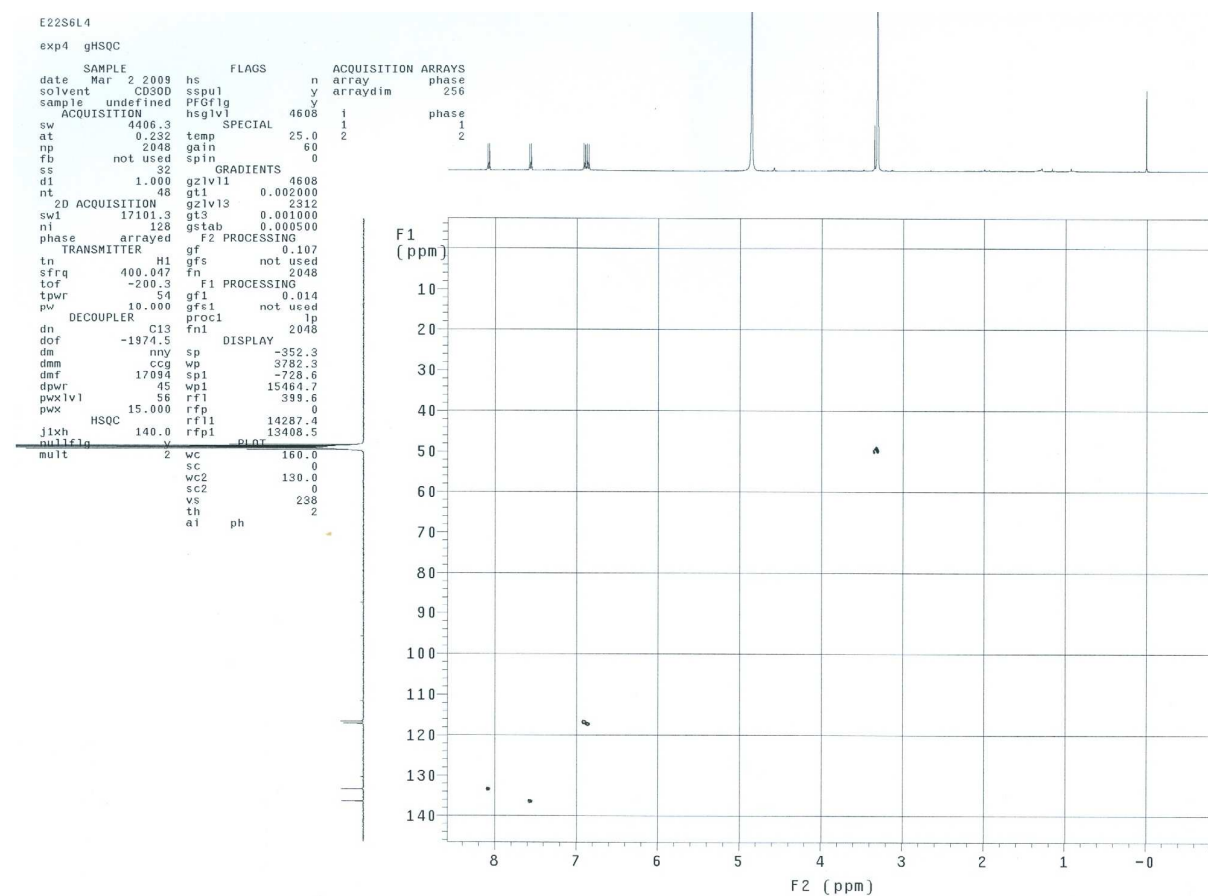
S16. Expanded ^{13}C NMR (100 MHz, CD_3OD) spectrum of the new compound **3**.

E22S6L4

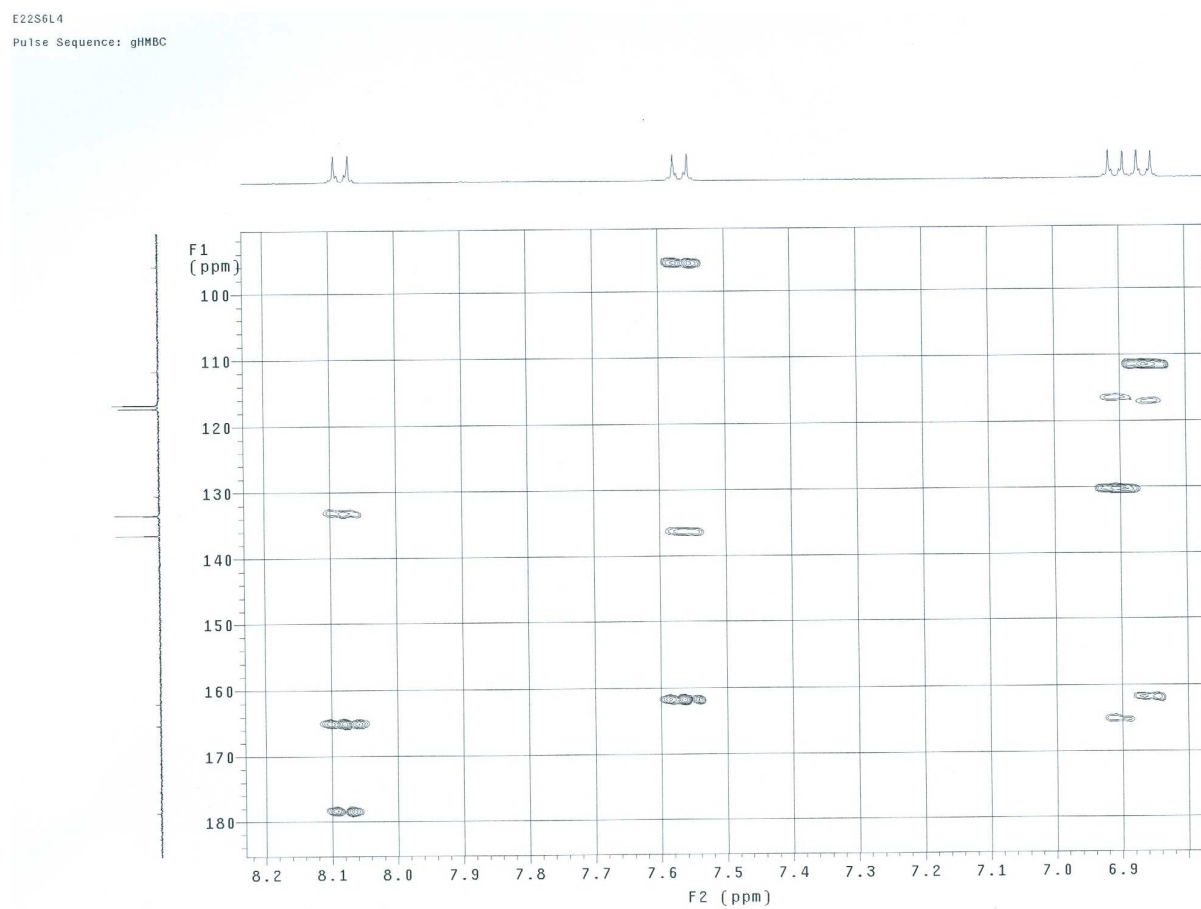
Pulse Sequence: s2pu1



S17. HSQC spectrum (400 MHz, CD₃OD) of the new compound **3**.



S18. HMBC spectrum (400 MHz, CD₃OD) of the new compound **3**.

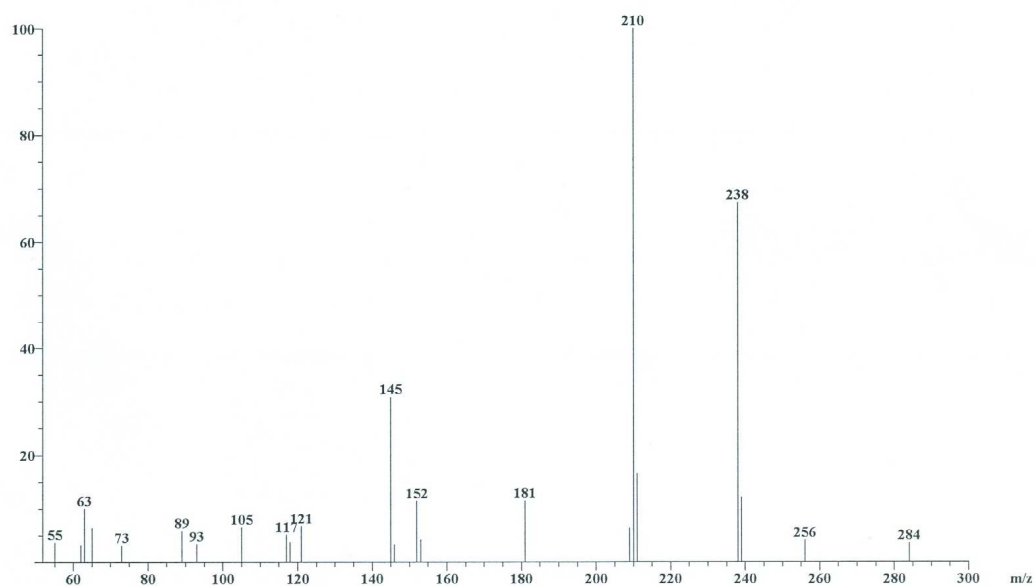


S19. HREIMS spectrum of the new compound **3**.

File: 4302	Date Run: 03-04-2009	Time Run:
Sample: E22SUL4		
Instrument: JEOL JMS600	Ionization mode: EI+	
Inlet: Direct Probe		

Scan: 49
Base: m/z 210; 10.5%FS TIC: 360859

R.T.: 2:25.1



File: 4303	Date Run: 03-04-2009	Time Run: 1
Sample: E22SUL4		
Instrument: JEOL JMS600	Ionization mode: EI+	
Inlet: Direct Probe		

Scan: 129
Base: m/z 238; 26.6%FS TIC: 4001921

R.T.: 2:09.4

Selected Isotopes : C ₀₋₅₀ H ₀₋₁₀₀ O ₀₋₁₀			Error Limit : 20 ppm	
<u>Measured Mass</u>	<u>% Base</u>	<u>Formula</u>	<u>Calculated Mass</u>	<u>Error</u>
238.0630	100.0%	C ₁₅ H ₁₀ O ₃	238.0630	-0.1

Table 1. ^1H and ^{13}C NMR Spectroscopic Data for (*E*)-4'-Demethyl-6-methyleucomin (**1**), Anemarcoumarin A (**2**), and Anemarchalconyn (**3**)

position	1^a		2^a		3^a	
	δ_{C} , mult.	δ_{H} , (<i>J</i> in Hz)	δ_{C} , mult.	δ_{H} , (<i>J</i> in Hz)	δ_{C} , mult.	δ_{H} , (<i>J</i> in Hz)
1					178.5, qC	
2	68.6, CH ₂	5.27, d (1.6)	164.3, qC		87.2, qC	
3	128.9, qC		126.2, qC		95.7, qC	
4	186.6, qC		141.7, CH	7.45, s		
4a	103.4, qC		113.8, qC			
5	163.5, qC		130.1, CH	7.32, d (8.4)		
6	105.7, qC		114.5, CH	6.75, dd (8.4, 2.0)		
7	166.3, qC		162.3, qC			
8	95.1, CH	5.88, s	103.1, CH	6.68, d (2.0)		
8a	161.6, qC		156.2, qC			
1'	127.2, qC		130.6, qC		130.3, qC	
2'	133.6, CH	7.23, d (8.4)	131.3, CH	7.10, d (8.8)	133.2, CH	8.07, d (8.8)
3'	116.9, CH	6.87, d (8.4)	116.5, CH	6.73, d (8.8)	116.6, CH	6.90, d (8.8)
4'	160.7, qC		157.3, qC		165.2, qC	
5'	116.9, CH	6.87, d (8.4)	116.5, CH	6.73, d (8.8)	116.6, CH	6.90, d (8.8)
6'	133.6, CH	7.23, d (8.4)	131.3, CH	7.10, d (8.8)	133.2, CH	8.07, d (8.8)
7'	137.9, CH	7.72, s	36.5, CH ₂	3.69, s		
1''					111.5, qC	
2''					136.3, CH	7.55, d (8.8)
3''					117.1, CH	6.85, d (8.8)
4''					161.8, qC	
5''					117.1, CH	6.85, d (8.8)
6''					136.3, CH	7.55, d (8.8)
CH ₃ -6	7.1, CH ₃	1.95, s				

^a Spectrum recorded at ^1H (400 MHz) and ^{13}C NMR (100 MHz) in CD₃OD.