

Supplementary Materials

Acuminatol and Other Antioxidative Resveratrol Oligomers from the Stem Bark of *Shorea acuminata*

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Acuminatol and Other Antioxidative Resveratrol Oligomers from the Stem Bark of *Shorea acuminata*.

Figure 1. ¹H-NMR spectrum of compound 1.

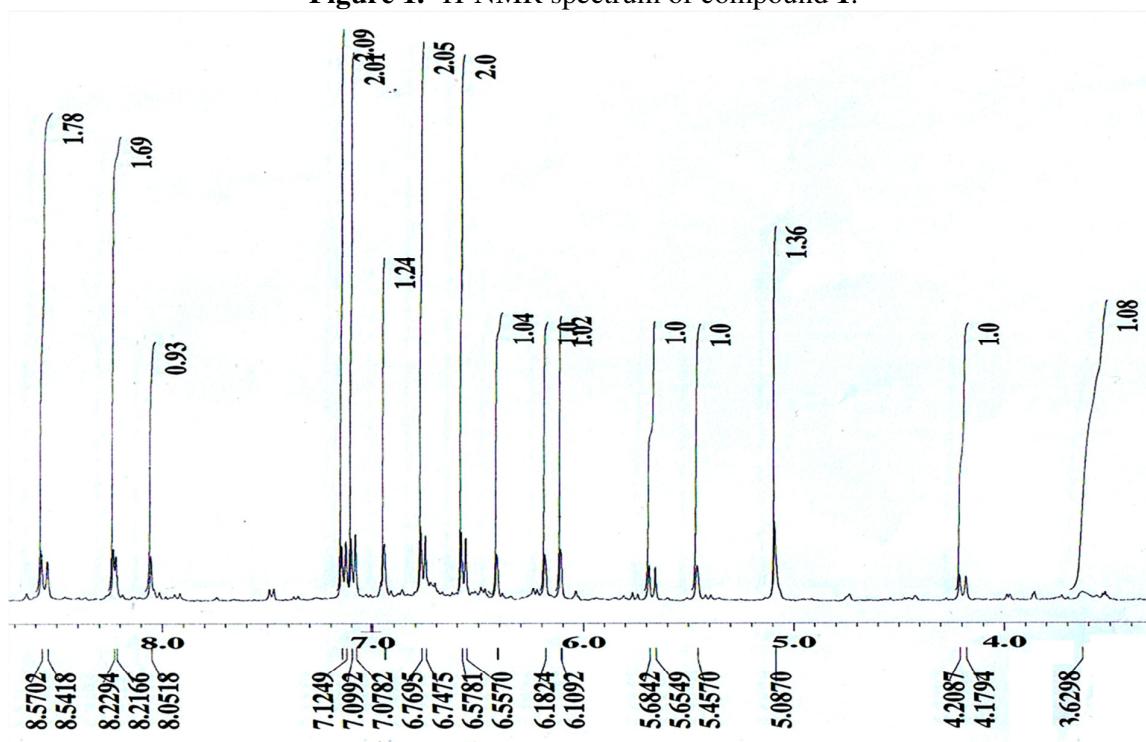


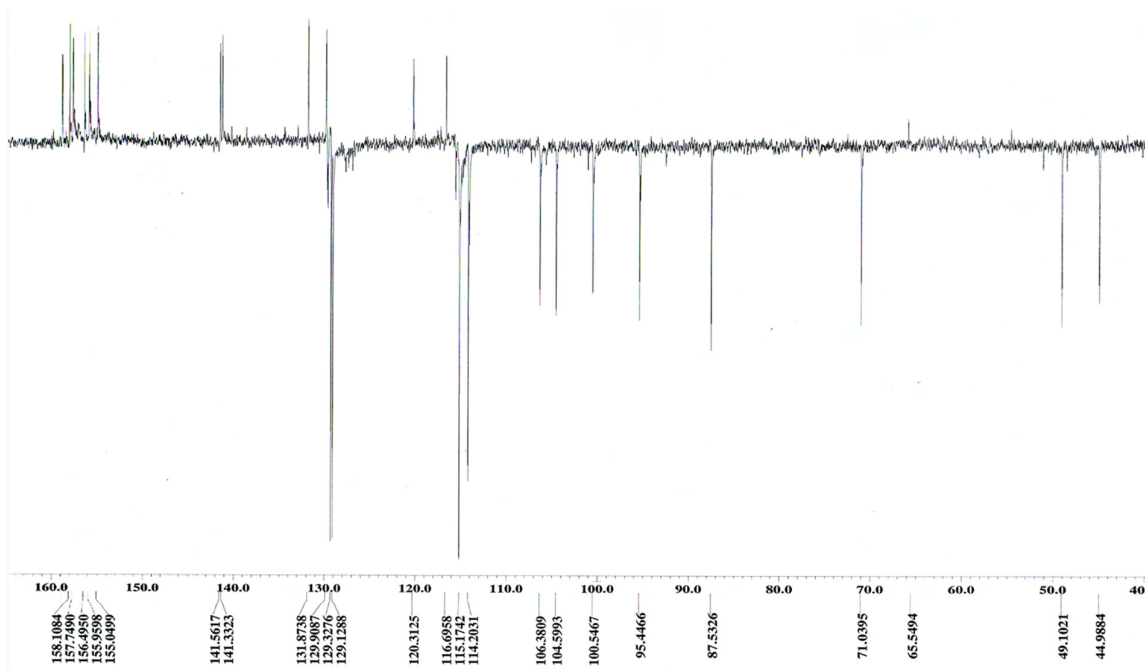
Figure 2. ^{13}C -APT NMR spectrum of compound 1.

Figure 3. HMQC spectrum of compound 1.

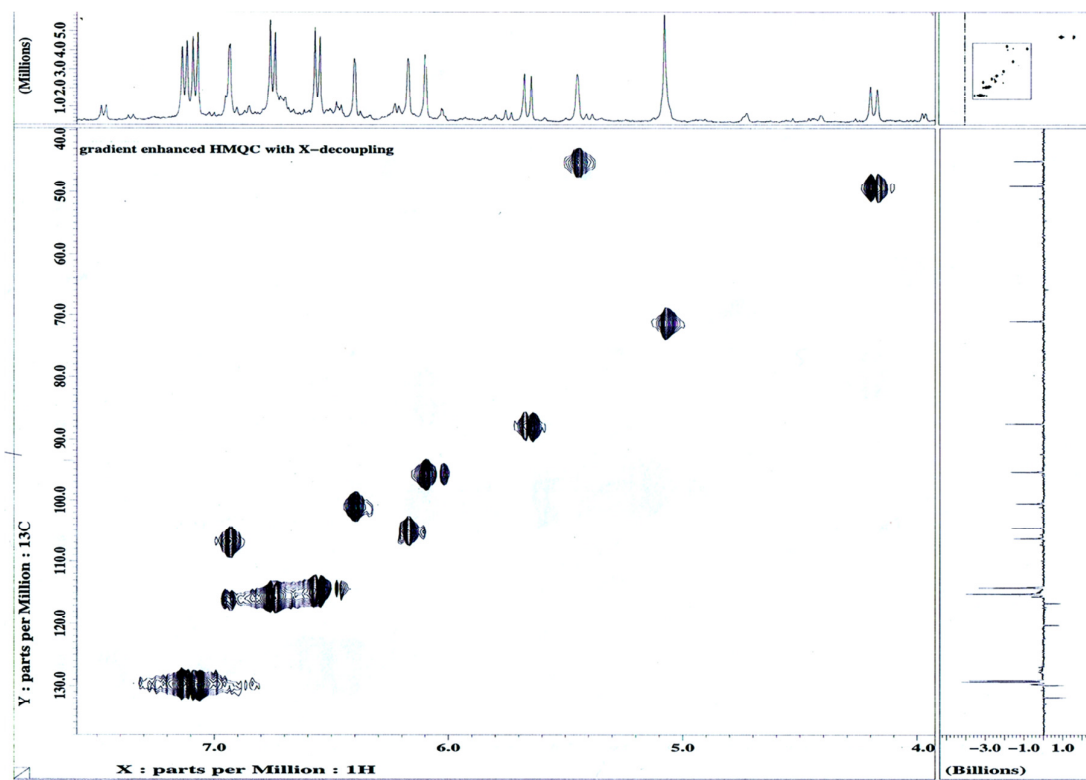


Figure 4. COSY spectrum of compound 1.

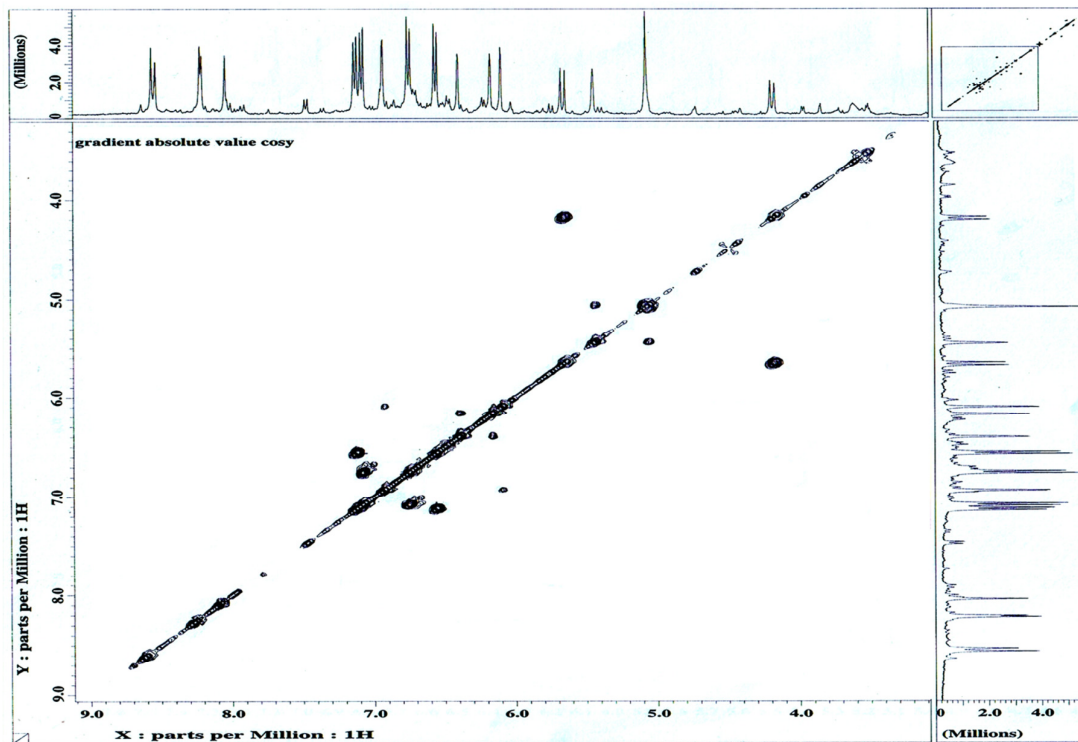


Figure 5. NOESY spectrum of compound 1.

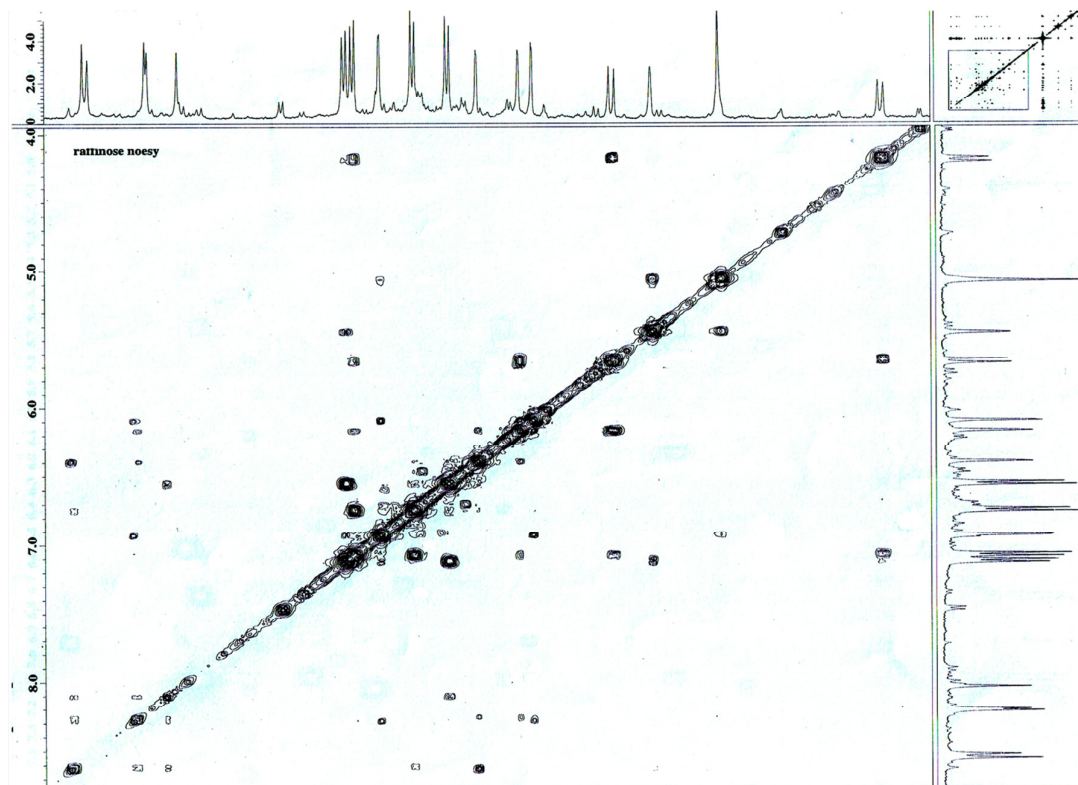


Figure 6. HMBC spectrum of compound 1.

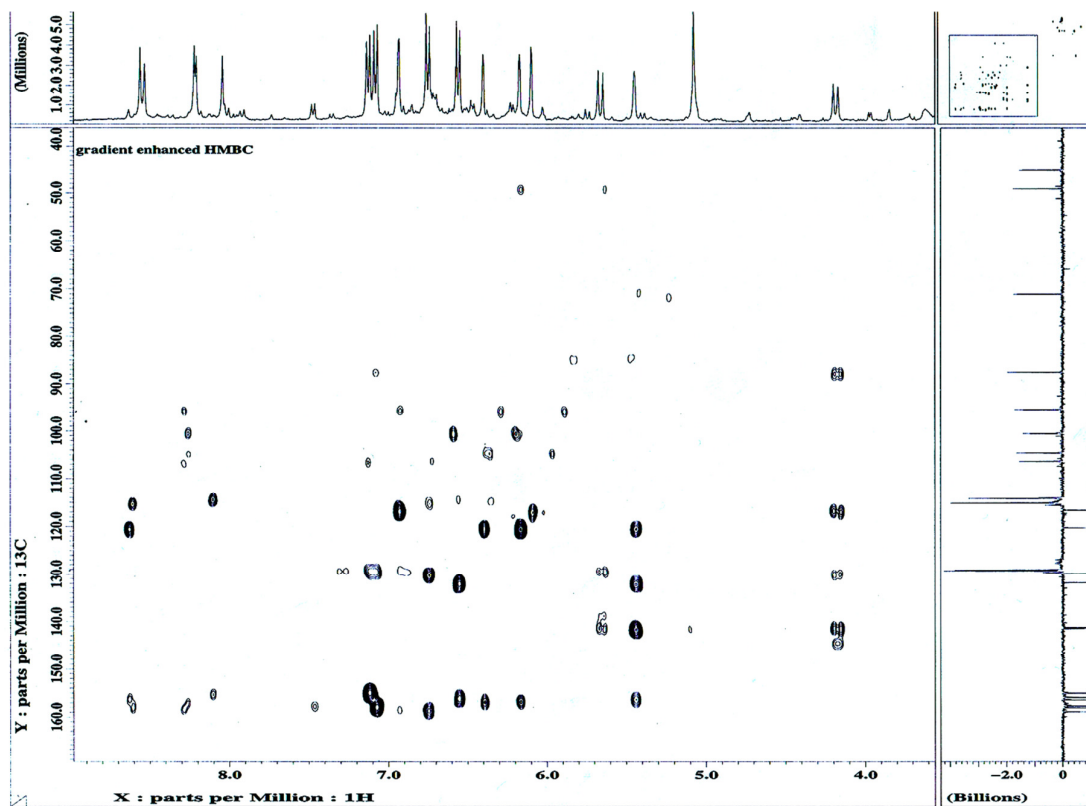


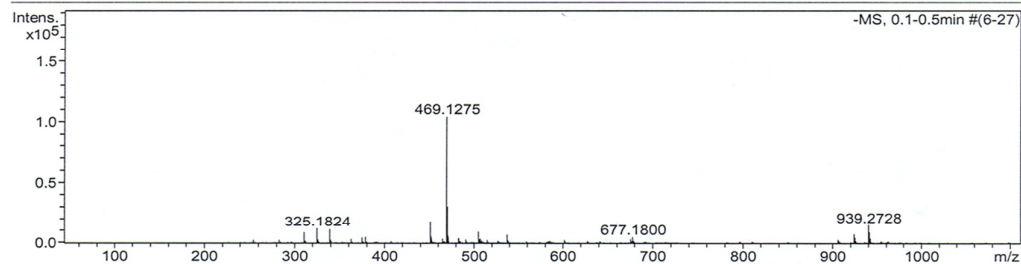
Figure 7. Mass spectrum of compound 1.

Mass Spectrum Molecular Formula Report

Analysis Info		Acquisition Date	11/10/2011 11:34:13 AM
Analysis Name	D:\Data\sample 2011\norhayati\101121.d	Operator	Alefee
Method	direct infuse -ve.m	Instrument / Ser#	micrOTOF-Q 86
Sample Name	SAK 151742462		
Comment	10.11.2011		

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1100 m/z	Set Collision Cell RF	450.0 Vpp	Set Divert Valve	Waste

Generate Molecular Formula Parameter					
Formula, min.	C20	Tolerance	10 mDa	Charge	-1
Formula, max.	N0	Minimum	0	Maximum	0
Measured m/z	469.128	Electron Configuration	both	Maximum	3
Check Valence	no	Minimum	0		
Nitrogen Rule	no				
Filter H/C Ratio	no				
Estimate Carbon	yes				



Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 21 H 25 O 12	0.033	469.1351	16.24	15.99	7.62	9.50	ok	even
C 28 H 21 O 7	0.008	469.1293	3.72	3.46	1.74	18.50	ok	even
C 35 H 17 O 2	0.046	469.1234	-8.80	-8.94	-4.13	27.50	ok	even

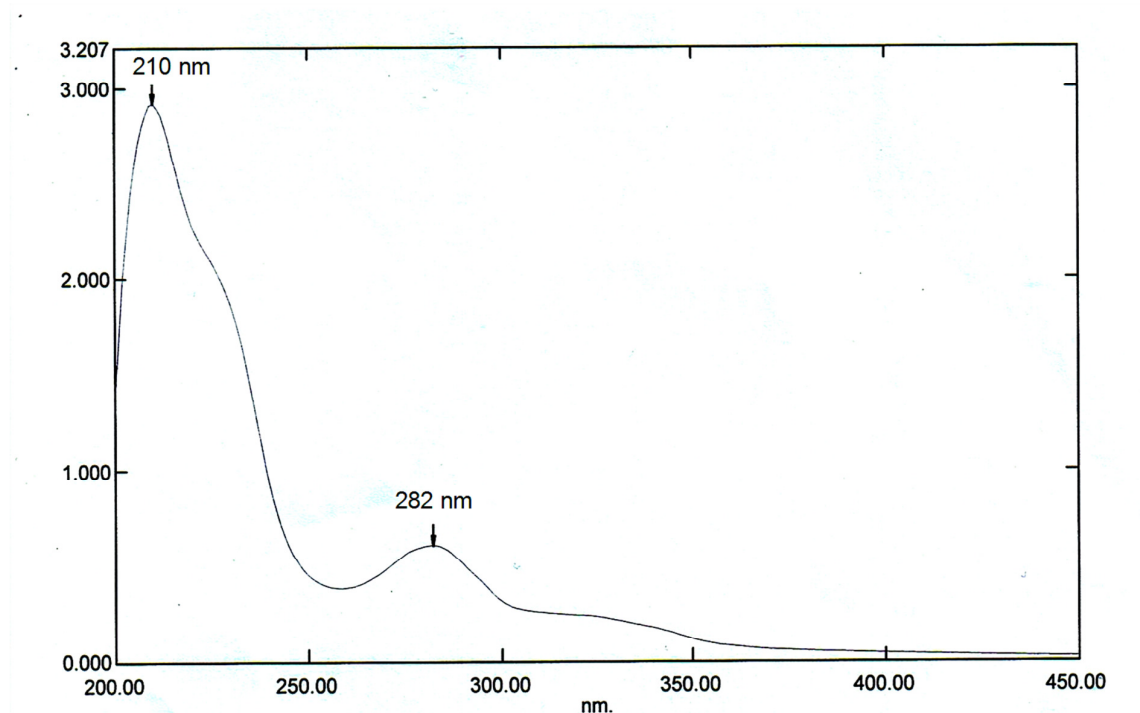
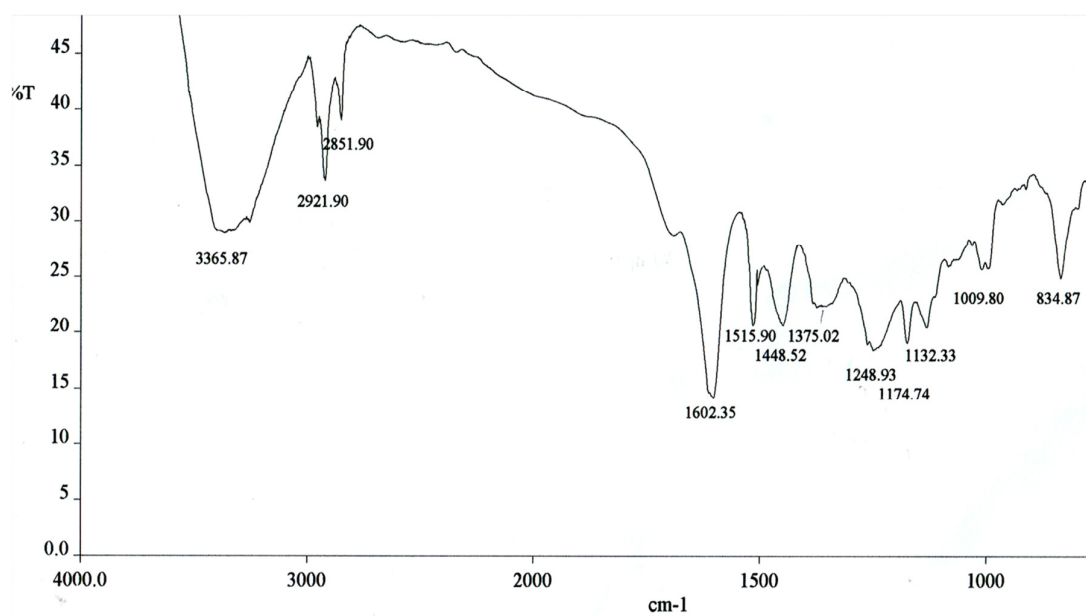
Figure 8. UV spectrum of compound 1.**Figure 9.** IR spectrum of compound 1

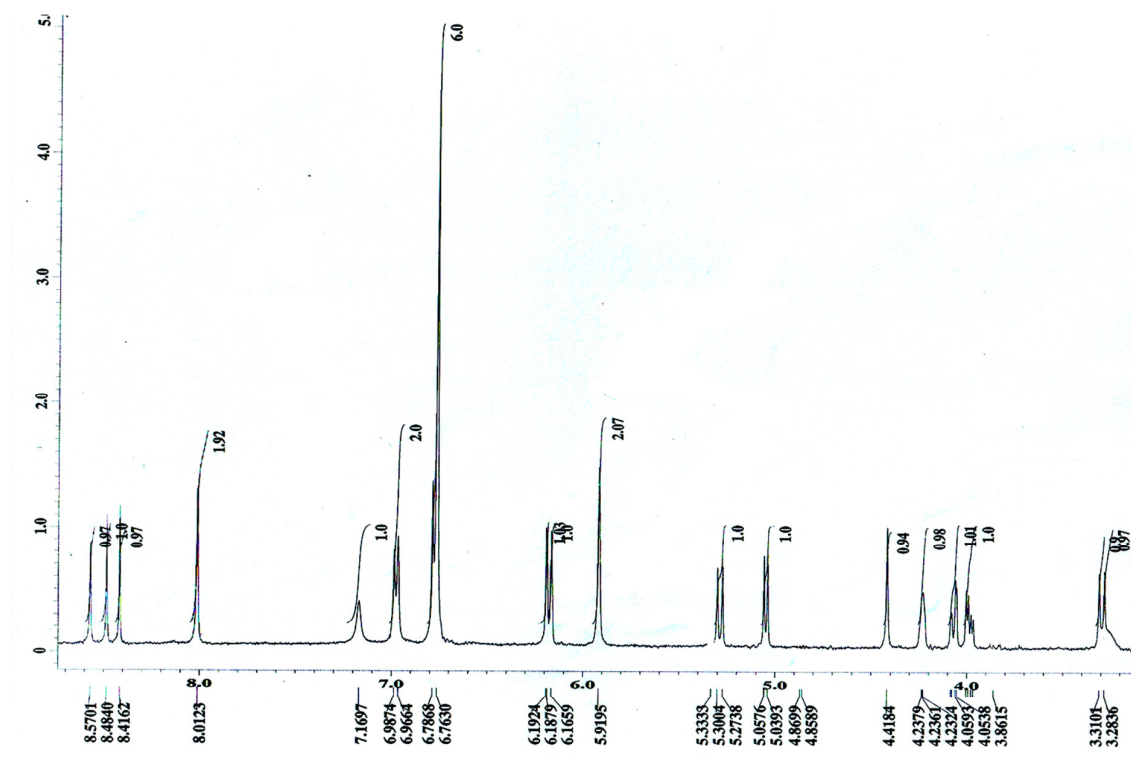
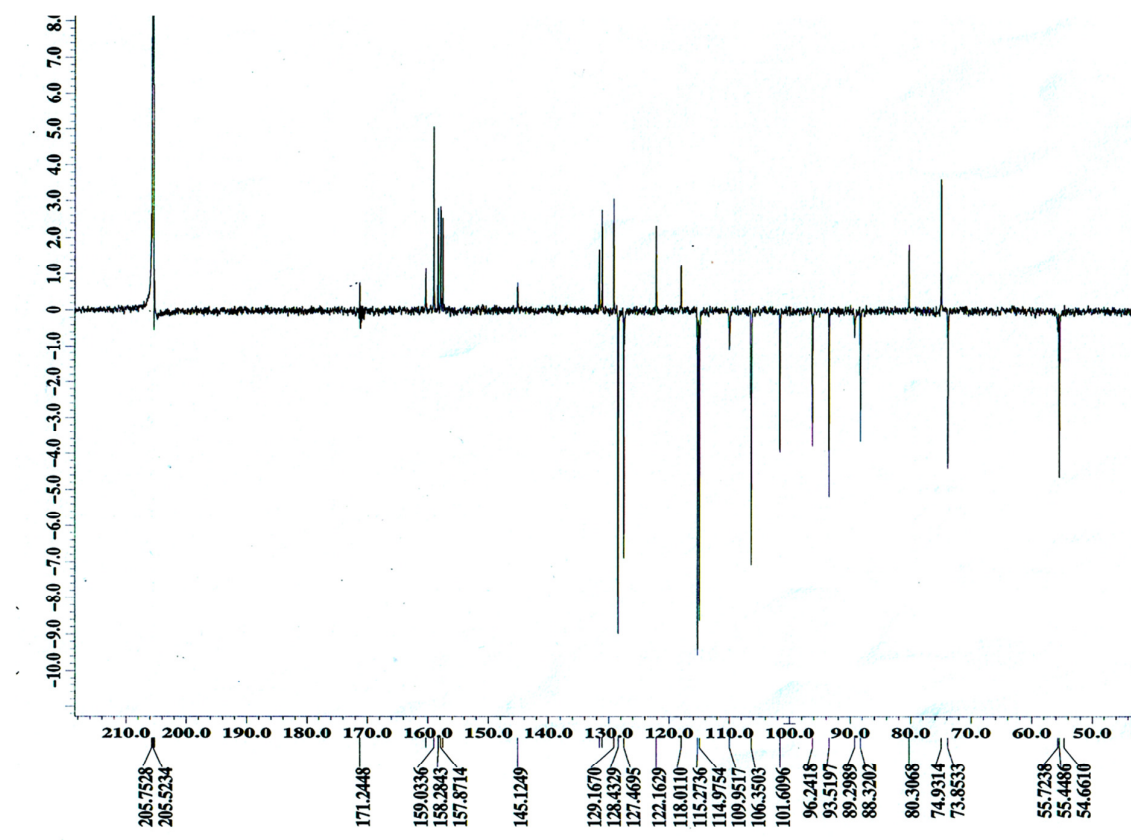
Figure 10. ^1H NMR spectrum of compound 2.Figure 11. ^{13}C -APT NMR spectrum of compound 2.

Table 1. ^{13}C -NMR and ^1H -NMR (100 MHz and 400 MHz, acetone- d_6) spectral data of **2**.

Position	δ_{C}	δ_{H}
1a	131.1	-
2a/6a	128.3	6.78 (m)
3a/5a	115.3	6.78 (m)
4a	157.5	-
7a	93.6	5.05 (d, 7.7)
8a	55.4	3.30 (d, 10.6)
9a	145.1	-
10a/14a	106.3	5.92 (d, 2.9)
11a/13a	158.9	-
12a	101.7	6.17 (t, 1.08, 1.84)
1b	129.1	-
2b/6b	127.4	6.98 (d, 8.4)
3b/5b	114.9	6.78 (m)
4b	158.2	-
7b	89.2	5.29 (d, 10.6)
8b	55.4	3.30 (d, 10.6)
9b	131.6	-
10b	124.6	-
11b	160.3	-
12b	96.3	6.19 (d, 2.2)
13b	157.8	-
14b	110.0	7.13 (br s)
1'	172.6	-
2'	80.3	-
3'	122.1	-
4'	88.3	4.44 (br s)
5'	73.9	4.24 (m)
6'	74.9	3.99 (dd, 10.6, 4.8), 4.07 (dd, 9.2, 1.8)

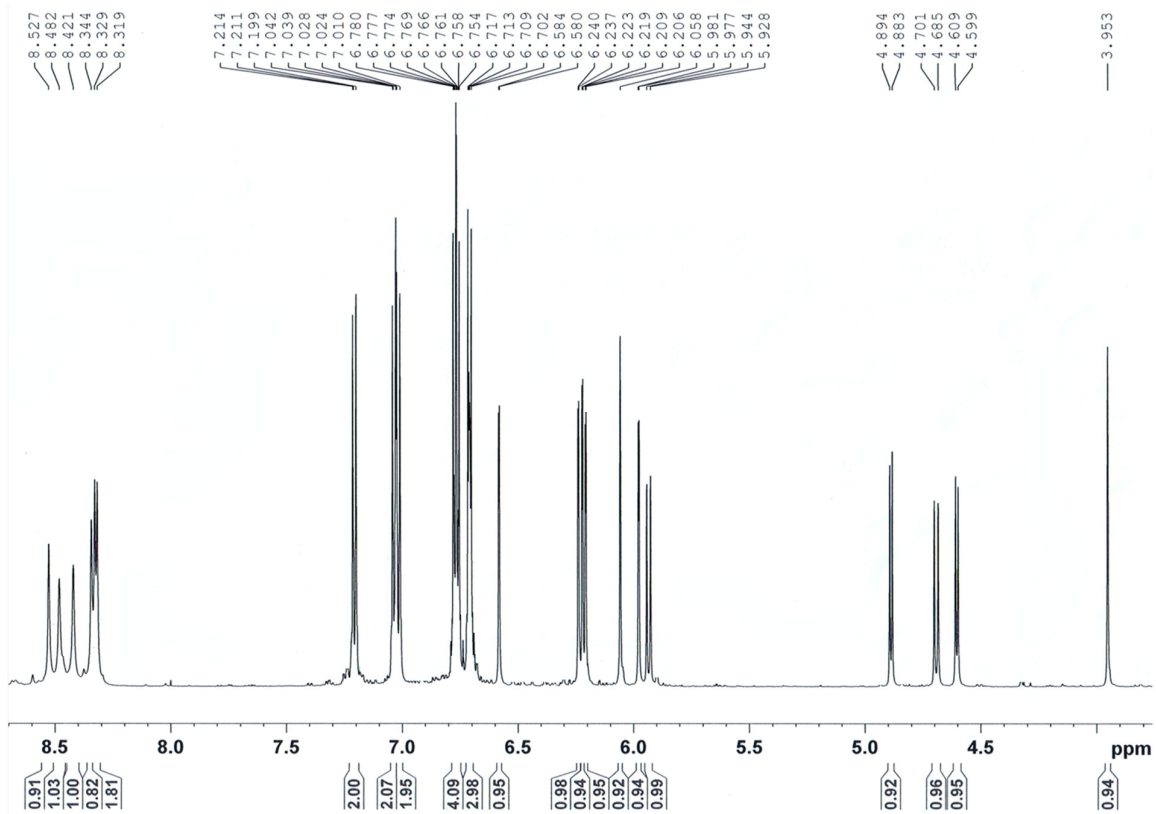
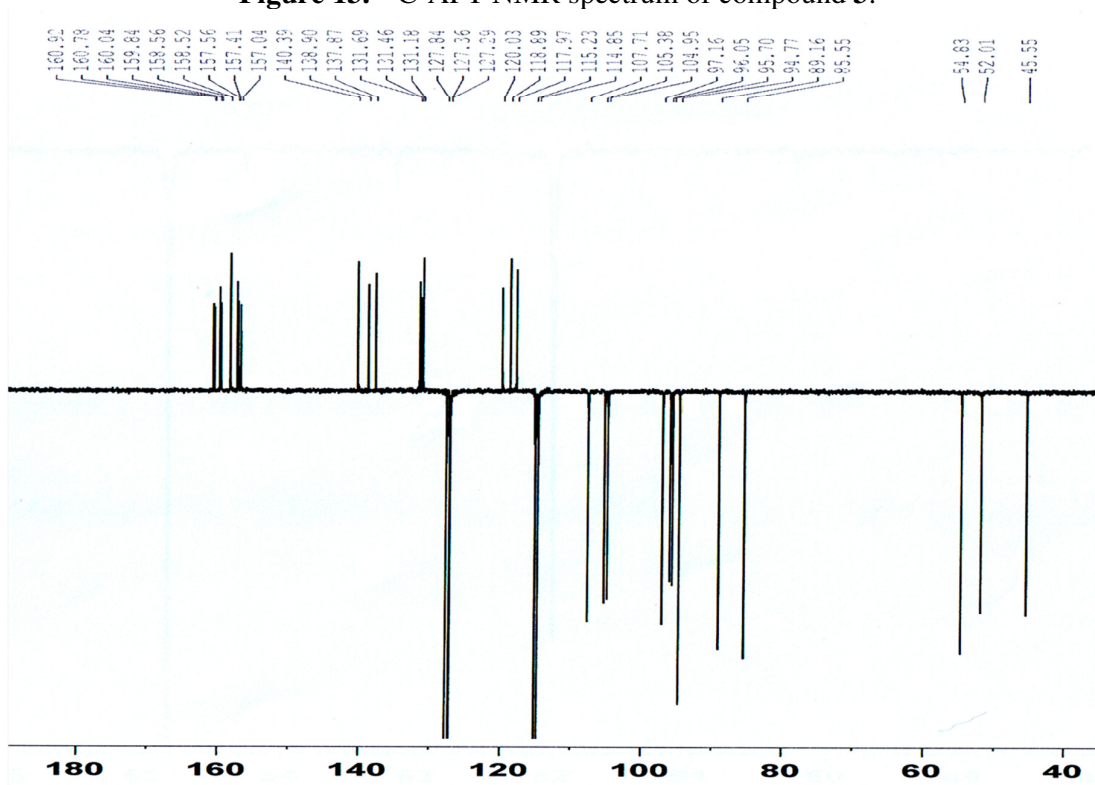
Figure 12. $^1\text{H-NMR}$ spectrum of compound 3.Figure 13. $^{13}\text{C-APT}$ NMR spectrum of compound 3.

Table 2. ^{13}C -NMR and ^1H -NMR (150 MHz and 600 MHz, acetone- d_6) spectral data of **3**.

Position	δ_{C}	δ_{H}
1a	131.2	
2a/6a	127.3	7.21 (d, 9.0)
3a/5a	115.2	6.77 (d, 8.4)
4a	157.0	-
7a	89.2	5.94 (d, 9.6)
8a	52.0	4.69 (d, 9.6)
9a	137.8	-
10a	118.9	-
11a	159.8	-
12a	95.7	6.24 (d, 1.8)
13a	160.9	-
14a	104.9	6.58 (d, 2.4)
1b	131.7	-
2b/6b	127.8	7.04 (d, 8.4)
3b/5b	115.2	6.76 (d, 9.0)
4b	157.6	-
7b	94.8	4.89 (d, 6.6)
8b	54.8	4.60 (d, 6.0)
9b	138.9	-
10b	118.0	-
11b	158.5	-
12b	96.0	6.21 (d, 1.8)
13b	160.0	-
14b	107.7	5.98 (d, 2.4)
1c	131.5	
2c/6c	127.4	7.02 (d, 8.4)
3c/5c	114.8	6.71 (d, 9.0)
4c	157.4	-
7c	85.5	6.06 (s)
8c	45.6	3.95 (s)
9c	140.4	-
10c	120.0	-
11c	158.6	-
12c	97.2	6.22 (d, 2.4)
13c	160.8	-
14c	105.4	6.71 (d, 2.4)
4a,4b,4c,13a,13b,13c (OH)		8.32, 8.33, 8.34, 8.42, 8.48, 8.53 (s)

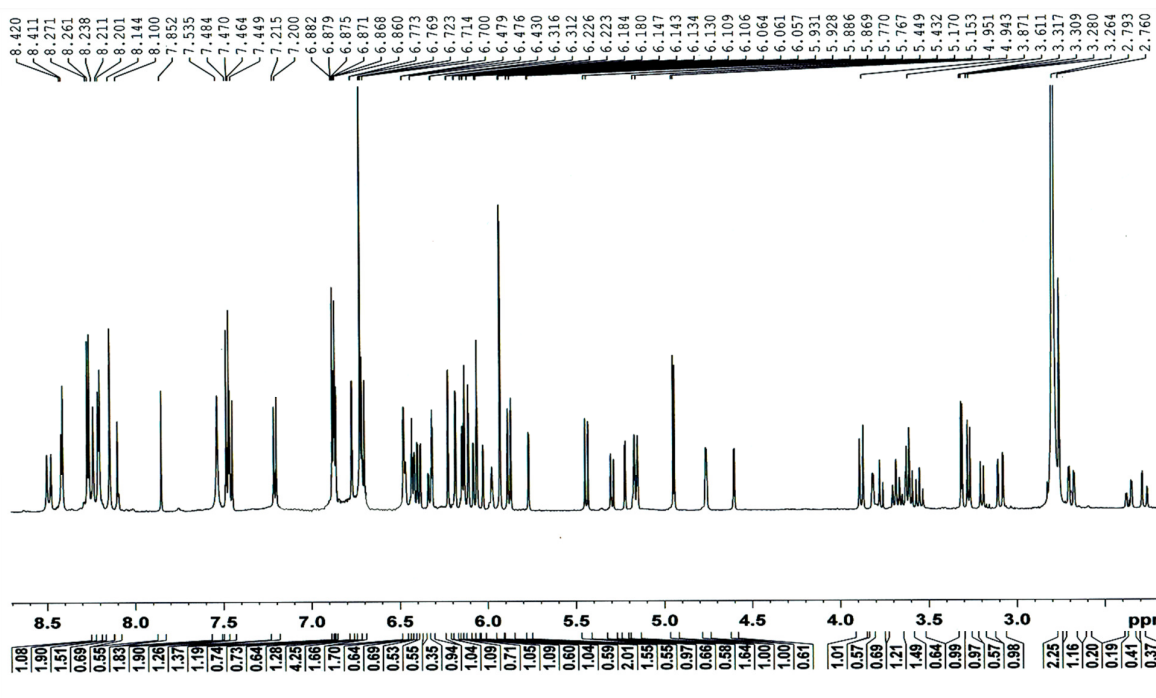
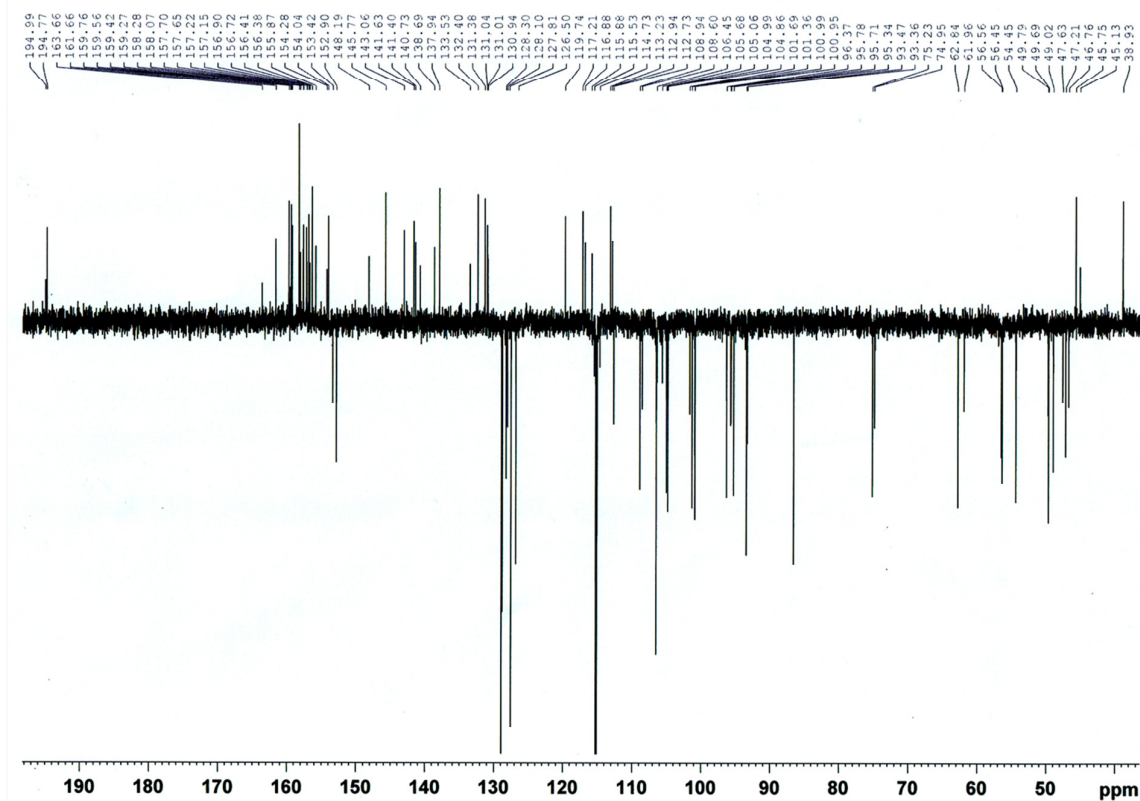
Figure 14. $^1\text{H-NMR}$ spectrum of compound 4.Figure 15. $^{13}\text{C-APT}$ NMR spectrum of compound 4.

Table 3. ^{13}C -NMR and ^1H -NMR (150 MHz and 600 MHz, acetone- d_6) spectral data of **4**.

Position	4a		4b	
	δ_{C}	δ_{H}	δ_{C}	δ_{H}
1a	131.04	-	130.94	-
2a, 6a	128.96	7.48 (d, 8.6)	128.83	7.46 (d, 4.6)
3a, 5a	115.30	6.88 (d, 8.4)	115.30	6.87 (d, 9.0)
4a	157.65	-	157.70	-
7a	86.63	5.88 (d, 10.2)	86.63	5.88 (d, 10.2)
8a	49.69	5.16 (br d, 10.2)	49.79	5.16 (br d, 10.2)
9a	141.63	-	141.40	-
10a	113.23	-	112.94	-
11a	154.04	-	154.28	-
12a	100.95	6.18 (d, 2.4)	100.99	6.08 (d, 2.4)
13a	156.90	-	156.72	-
14a	105.06	6.48 (d, 1.8)	104.99	6.42 (br, s)
1b	45.75	-	45.13	-
2b	75.23	4.77 (m)	74.95	3.81 (m)
3b	38.93	2.69 (dd, 16.8, 3.0) 3.09 (dd, 17.4, 1.8)	38.93	2.36 (dd, 17.4, 3.6) 2.27 (dd, 17.4, 1.8)
4b	194.77	-	194.99	-
5b	128.30	5.44 (d, 10.2)	128.10	5.29 (d, 10.2)
6b	152.90	6.39 (dd, 10.2, 2.4)	153.42	6.33 (dd, 10.2, 2.4)
7b	47.21	3.88 (d, 12.0)	47.63	3.73 (d, 11.4)
8b	49.02	3.68 (t, 11.4, 12.0)	46.76	3.61 (t, 9.0, 11.4)
9b	137.94	-	138.69	-
10b	117.21	-	116.88	-
11b	159.42	-	159.56	-
12b	96.37	6.13 (d, 2.4)	95.78	6.14 (d, 2.4)
13b	156.38	-	157.65	-
14b	108.94	6.11 (d, 1.8)	108.60	6.02 (d, 1.8)
1c	131.38	-	131.01	-
2c/6c	NI	NI	NI	NI
3c/5c	NI	NI	NI	NI
4c	156.41	-	155.87	-
7c	62.84	3.27 (d, 9.6)	56.56	3.19 (d, 10.8)
8c	56.45	3.61 (t, 9.0, 11.4)	61.96	3.55 (t, 11.4)
9c	143.06	-	140.73	-
10c	119.74	-	115.88	-
11c	161.66	-	163.66	-
12c	95.34	6.22 (d, 1.8)	95.71	6.31 (d, 2.4)
13c	159.27	-	158.07	-
14c	104.86	6.77 (d, 2.4)	112.73	5.77 (d, 2.4)
1d	132.40	-	133.53	-
2d, 6d	127.57	6.72 (s)	126.88	7.21 (d, 9.0)
3d, 5d	115.12	6.72 (s)	115.30	6.71 (d, 8.4)
4d	157.22/157.15	-	157.15	-
7d	93.47	4.95 (d, 4.8)	93.36	5.22 (d, 2.4)

Table 3. Cont.

Position	4a		4b	
	δ_C	δ_H	δ_C	δ_H
8d	54.45	3.31 (d, 4.8)	56.56	4.60 (d, 2.4)
9d	145.77	-	148.19	-
10d	106.55	5.93 (d, 1.8)	105.68	5.98 (br s)
11d	158.28	-	159.76	-
12d	101.36	6.06 (t, 1.8, 2.4)	101.69	6.43 (t, 1.8, 2.4)
13d	158.28	-	159.76	-
14d	106.55	5.93 (d, 1.8)	106.45	6.47 (br, s)

^{4a}, ^{4b}, represent for major and minor conformer; NI: not identified.

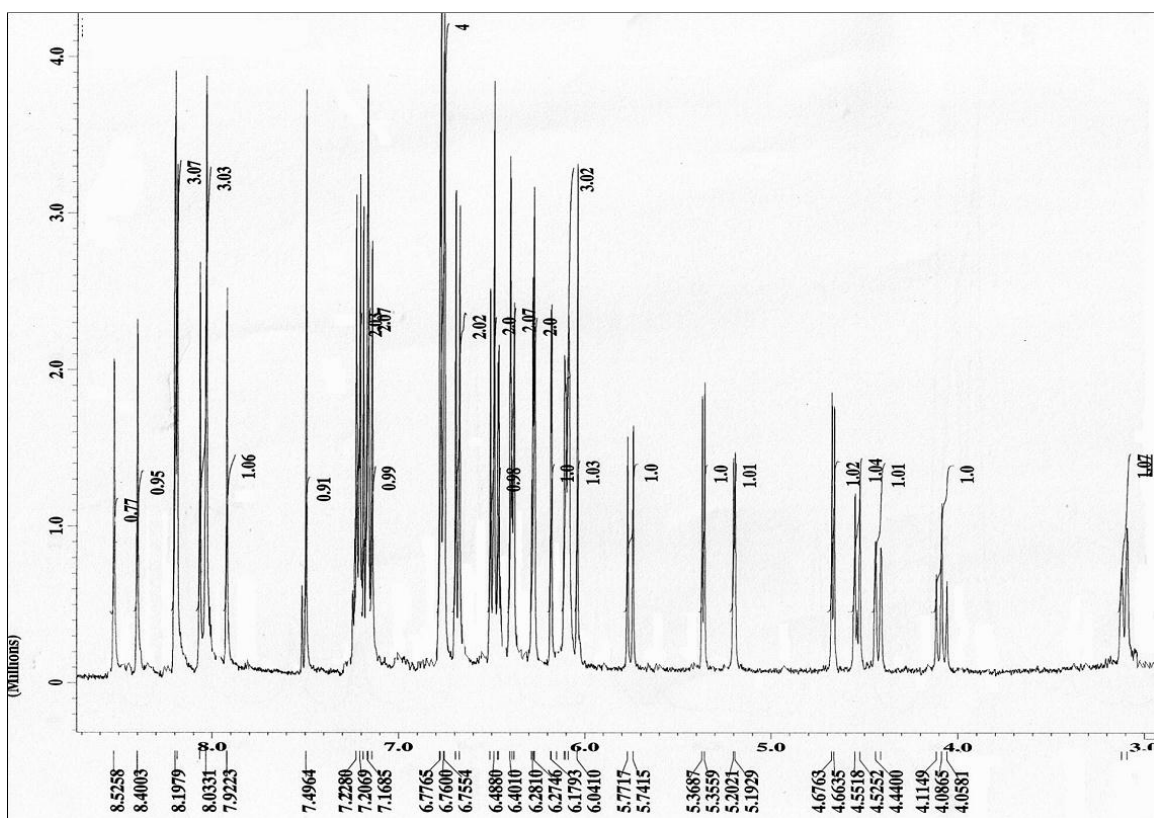
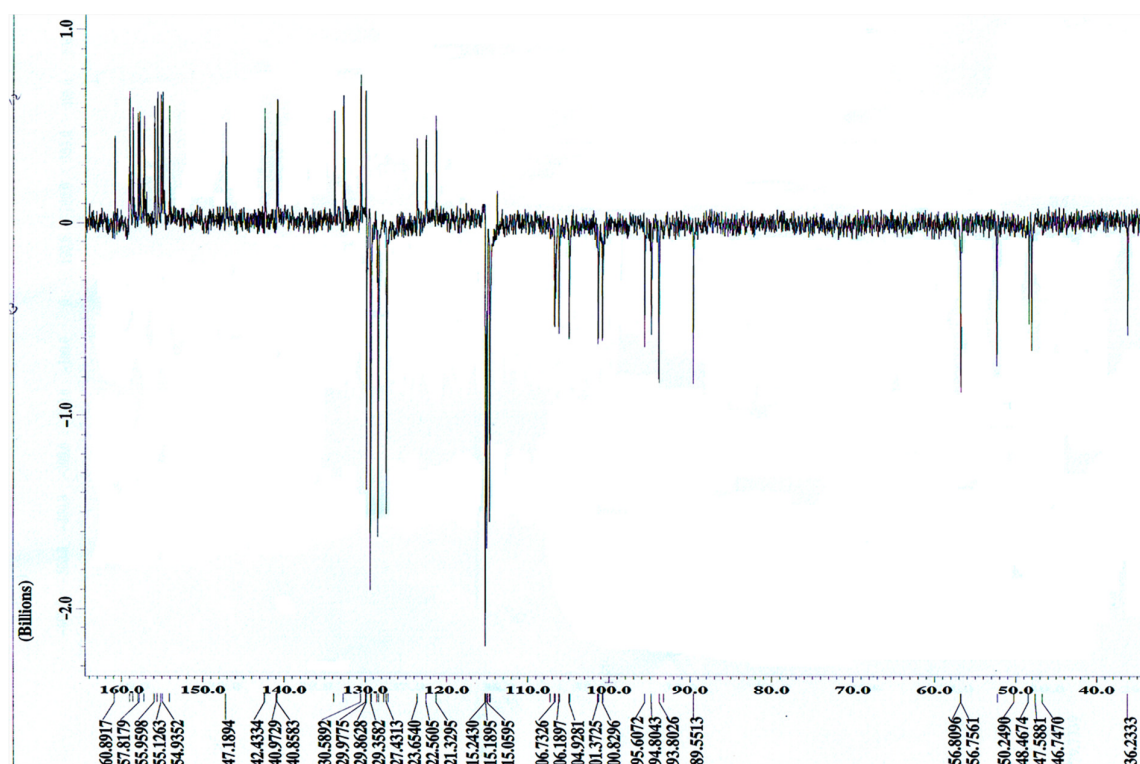
Figure 16. ¹H-NMR spectrum of compound 5.

Figure 17. ^{13}C -APT NMR spectrum of compound 5.Table 4. ^{13}C -NMR and ^1H -NMR (100 MHz and 400 MHz, acetone- d_6) spectral data of 5.

Position	δ_{C}	δ_{H}
1a	130.0	-
2a/6a	129.4	7.21 (d, 8.4)
3a/5a	115.2	6.77 (d, 8.4)
4a	157.8	-
7a	89.6	5.76 (d, 12.1)
8a	48.1	4.43 (d, 11.0)
9a	141.0	-
10a	123.7	-
11a	154.9	-
12a	100.8	6.28 (d, 2.2)
13a	156.0	-
14a	104.9	6.11(d, 2.6)
1b	132.7	-
2b/6b	130.0	7.15 (d, 8.4)
3b/5b	114.7	6.69 (d, 8.4)
4b	155.1	-
7b	36.2	5.20 (d, 3.7)
8b	52.3	3.11 (br d, 11.3)
9b	142.4	-
10b	114.9	-
11b	158.0	-

Table 4. Cont.

Position	δ_C	δ_H
12b	95.6	6.04 (s)
13b	154.1	-
14b	121.3	-
1c	130.6	-
2c/6c	128.4	6.39 (d, 8.4)
3c/5c	115.1	6.50 (d, 8.4)
4c	155.6	-
7c	56.8	4.09 (t, 11.4)
8c	48.5	4.54 (d, 10.6)
9c	140.9	-
10c	122.6	-
11c	160.9	-
12c	94.8	6.18 (d, 2.2)
13c	158.6	-
14c	106.2	6.47 (d, 2.2)
1d	133.9	-
2d/6d	127.4	7.18 (d, 8.8)
3d/5d	115.1	6.77 (d, 8.4)
4d	157.2	-
7d	93.8	5.36 (d, 5.1)
8d	56.8	4.67 (d, 5.1)
9d	147.2	-
10d/14d	106.7	6.09 (br s)
11d/13d	159.0	-
12d	101.4	6.27 (t, 2.2)

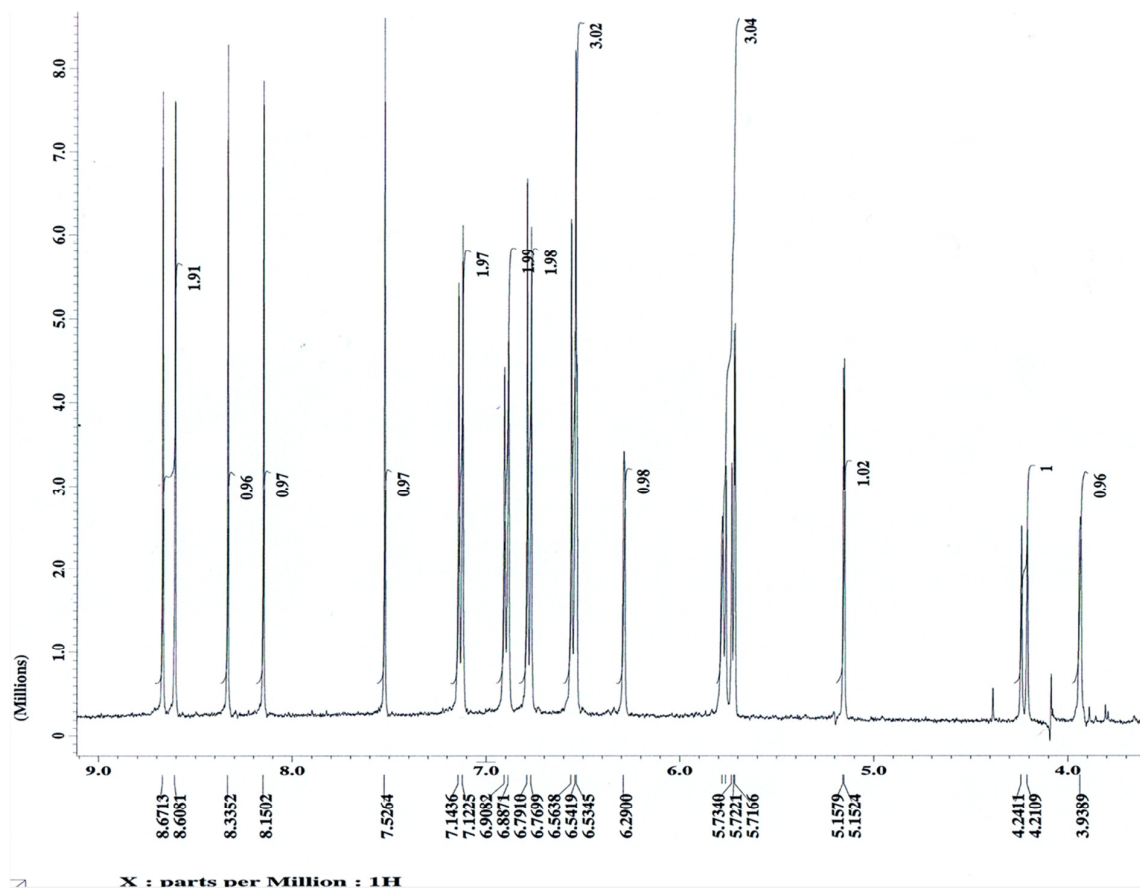
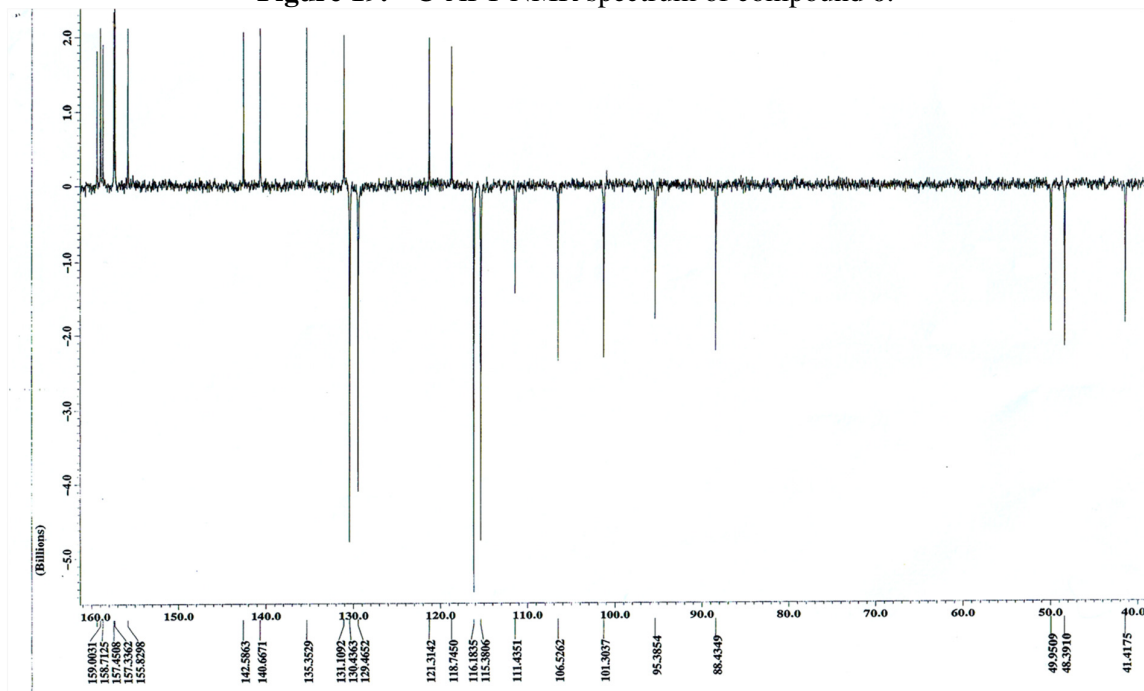
Figure 18. ^1H NMR spectrum of compound 6.Figure 19. ^{13}C -APT NMR spectrum of compound 6.

Table 5. ^{13}C -NMR and ^1H -NMR (100 MHz and 400 MHz, acetone- d_6) spectral data of **6**.

Position	δ_{C}	δ_{H}
1a	131.1	-
2a/6a	130.4	7.12 (d, 8.4)
3a/5a	115.4	6.77 (d, 8.4)
4a	158.7	-
7a	88.4	5.74 (d, 12.1)
8a	49.9	4.22 (d, 12.1)
9a	142.6	-
10a	121.3	-
11a	159.0	-
12a	101.3	6.53 (br s)
13a	157.4	-
14a	106.5	6.28 (br s)
1b	135.4	-
2b/6b	129.5	6.89 (d, 8.1)
3b/5b	116.2	6.54 (d, 8.8)
4b	155.8	-
7b	41.4	5.77 (br s)
8b	48.4	3.93 (s)
9b	140.7	-
10b	118.7	-
11b	159.5	-
12b	95.4	5.71 (d, 2.2)
13b	157.3	-
14b	111.4	5.15(d, 2.2)