Supporting information

3-Acetyl-11-keto-β-boswellic acid-based hybrids alleviate acetaminophen induced hepatotoxicity in HepG2 by regulation of inflammatory and oxidative stress pathways: An integrated approach.

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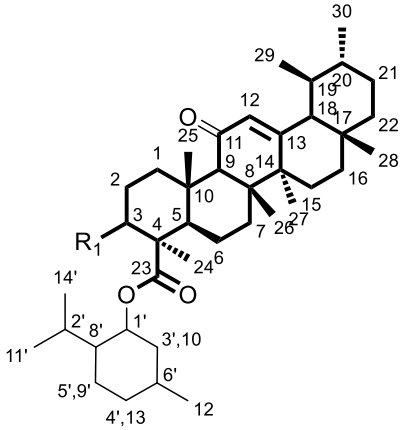
Table S1. NMR assignment of Compound 3a

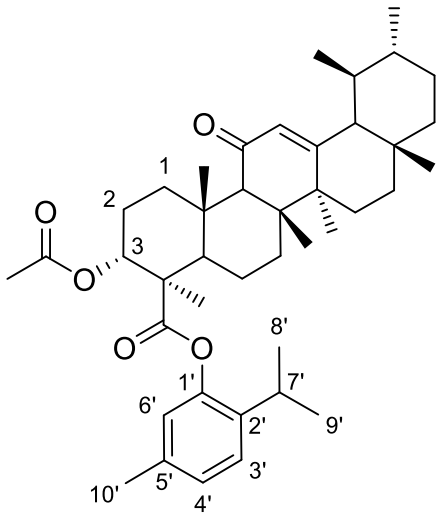


Parent compound			Hybrid compound		
Atom **C/H**	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)	DEPT	^{1}H (δ, ppm) (J,Hz)	\$^{13}$C (δ, ppm)
11	-	199.6	C	--	200.2
24	-	182.2	C	--	175.9
CH3CO	-	170.5	C	--	171.1
13	-	165.3	C	--	169.6
12	5.54 s	130.8	CH	5.56 (s, 1H)	128.5
3	5.28 t	73.6	CH	5.23 (s, 1H)	80.6
Menthol 1***(Kwan and Huang 2008)***	3.4 td, (j=10.4,4.3)	71.5	CH	4.61 (td, *J* = 11.3, 4.0 Hz, 1H)	74
9	2.39 s	60.7	CH	2.30 (s, 1H)	61.7
18	1.37 d (J=12.3)	59.4	CH	1.27 – 1.16 (m, 1H)	55
5	1.38 dd, (J=12,2)	50.8	CH	1.85 – 1.47 (m, 1H)	48.4
8’	1.1	50.12	CH	0.87 – 0.79 (m, 1H)	48.4
4	-	46.7	C	--	46.9
14	-	45.3	C	--	45.4
10’	0.95	45	CH	0.87 – 0.79 (m, 1H)s	43.97
3’	1.9	45	CH	1.85 – 1.47 (m, 1H)	43.97
8	-	43.9	C	--	43.25

22	1.29 m	41.3	CH2	1.05 – 0.88 (m, 2H)	41.08
19	1.52 m	39.7	CH	1.46 – 1.28 (m, 1H)	40.92
20	1.39 m	39.6	CH	1.46 – 1.28 (m, 1H)	38.8
10	-	37.6	C	--	38.05
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.73 (d, J = 13.5 Hz, 2H)	37.7
13’	0.84	34.52	CH	0.87 – 0.79 (m, 1H)	36.9
4’	1.66	34.5	CH	1.85 – 1.47 (m, 1H)	36.9
17	-	34.2	C	--	34.2
15	1.66 m	33.2	CH_2	1.85 – 1.47 (m, 2H)	32.72
6’	1.43	31.6	CH	1.85 – 1.47 (m, 1H)	31.8
7	1.43 m	31.3	CH_2	1.46 – 1.28 (m, 2H)	31.4
30	0.80 d (J=7.4)	29.3	CH3	0.76 – 0.65(m, 3H)	31.2
21	1.01 dd (J=11.8, 3)	27.9	CH2	1.05 – 0.88 (m, 2H)	28.6
16	1.88 m	27.6	CH_2	1.85 – 1.47 (m, 2H)	28.3
2’	2.17	25.8	CH	2.05 (d, J = 13.0 Hz, 1H)	28.05
23	1.21 s	24.3	CH3	1.16 – 1.04 (m, 3H)	26.44
2	1.56 m, 2.22 m	23.9	CH_2	1.46 – 1.28 (m, 2H)	26
9’	0.97	23.1	CH	0.87 – 0.79 (m, 1H)	23.58
5’	1.61	23.1	CH	1.85 – 1.47 (m, 1H)	23.58
12’	0.91	22.2	CH3	0.87 – 0.79 (m, 3H)	23.3
CH3CO	2.07 s	21.7	CH3	1.91 (t, J = 14.3 Hz, 3H)	23.12
28	0.93 s	21.5	CH3	0.87 – 0.79 (m, 3H)	22.03
11’	0.92	21	CH3	0.87 – 0.79 (m, 3H)	21.3

27	1.33 s	20.9	CH3	1.46 – 1.28 (m, 3H)	20.8
6	1.75 m	19.2	CH_2	1.85 – 1.47 (m, 2H)	18.7
26	1.17 s	18.8	CH3	1.16 – 1.04 (m, 3H)	17.4
29	0.78 d (J=6.3)	17.8	CH3	0.76 – 0.65 (m, 3H)	16.7
14’	0.8	16	CH3	0.76 – 0.65(m, 3H)	16.4
25	1.12 s	13.6	CH3	1.16 – 1.04 (m, 3H)	15.9
7’	1.35	--	--	--	--

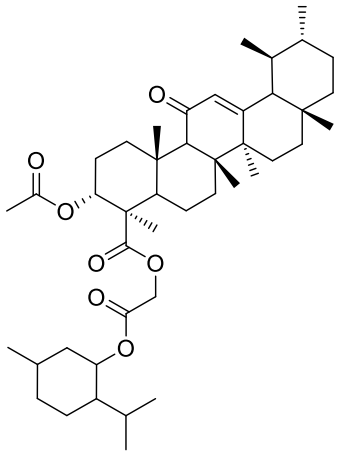
Table S2. NMR assignment of Compound 3b



Parent compound			Hybrid compound		
\Atom **C/H**	^1H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)	DEPT	^1H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)
OH-	9.99	-		--	--
25	1.12 s	13.6	CH3	1.21 – 1.09 (m, 3H)	14.2
29	0.78 d(J=6.3)	17.8	CH3	1.02 – 0.69 (m, 3H)	17.4
10’	2.2	18.7	CH3	2.1	18.4
26	1.17 s	18.8	CH3	1.21 – 1.09 (m, 3H)	19
6	1.75 m	19.2	CH_2	1.63 – 1.47 (m, 2H)	20.6
27	1.33 s	20.9	CH3	1.46 – 1.22 (m, 3H)	21.1
28	0.93 s	21.5	CH3	1.02 – 0.69 (m, 3H)	21.6
CH3CO	2.07 s	21.7	CH3	1.86 (s, 3H)	22.7

2	1.56 m, 2.22 m	23.9	CH_2	1.63 – 1.47 (m, 2H)	23.59
23	1.21 s	24.3	CH3	1.46 – 1.22 (m, 3H)	23.85
7’	3.3	25.5	CH	2.6 (dt, *J* = 13.5, 3.6 Hz, 1H)	23.85
8’,9’	1.05	26.1	CH3	1.02 – 0.69 (m, 6H)	26.6
16	1.88 m	27.6	CH_2	1.75 – 1.64 (m, 2H),	27.25
21	1.01 dd(J=11.8, 3)	27.9	CH2	1.21 – 1.09 (m, 2H)	27.46
30	0.80 d(J=7.4)	29.3	CH3	1.02 – 0.69 (m, 3H)	28.8
7	1.43 m	31.3	CH_2	1.46 – 1.22 (m, 2H)	32.7
15	1.66 m	33.2	CH_2	1.63 – 1.47 (m, 2H)	33.9
17	-	34.2	C	--	34.2
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.22 (s, 2H),	34.2
10	-	37.6	C	--	37.4
20	1.39 m	39.6	CH	1.46 – 1.22 (m, 1H)	39.2
19	1.52 m	39.7	CH	1.63 – 1.47 (m, 1H)	39.3
22	1.29 m	41.3	CH2	1.46 – 1.22 (m, 2H)	40.8
8	-	43.9	C	--	43.8
14	-	45.3	C	--	45.0
4	-	46.7	C	--	47.2
5	1.38 dd, (J=12,2)	50.8	CH	1.46 – 1.22 (m, 1H)	50.57
18	1.37 d (J=12.3)	59.4	CH	1.46 – 1.22 (m, 1H)	59.05
9	2.39 s	60.7	CH	2.44 (s, 1H)	60.15
3	5.28 t	73.6	CH	5.4(d, *J* = 3.0 Hz, 1H)	72.2
2’	5.4	116.9	CH	7.30 (d, *J* = 2.4 Hz, 1H)	121.6
4’	6.19	123.6	CH	7.36 (t, *J* = 7.7 Hz, 1H)	124.89
5’	7.08	126.3	CH	7.5 (t, *J* = 7.7 Hz, 1H)	128.7
12	5.54 s	130.8	CH	5.5 (s, 1H)	128.88
6‘	--	131.7	C	--	130.4
3’	-	138.4	C	--	143
1’	-	150.2	C	--	147
13	-	165.3	C	--	165
CH3CO	-	170.5	C	--	170
24	-	182.2	C	--	172.3
11	-	199.6	C	--	198.9

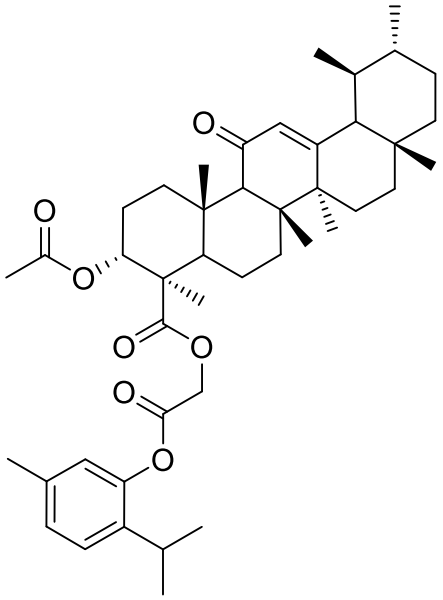
Table S3. NMR assignment of Compound 5a



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)	DEPT	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)
11	-	199.6	C	--	199.32
24	-	182.2	C	--	175.06
CH3CO	-	170.5	C	--	170.18
-CH2-CO MENTHOL	--	167.2	C	--	167.19
13	-	165.3	C	--	164.99
12	5.54 s	130.8	CH	5.48 (s, 1H)	130.51
3	5.28 t	73.6	CH	5.30 (d, *J* = 2.9 Hz, 1H)	75.63
Menthol 1***(Kwan and Huang 2008)***	3.4 td, (j=10.4,4.3)	71.5	CH	4.69 (dt, *J* = 10.9, 5.5 Hz, 1H)	73.23
9	2.39 s	60.7	CH	2.35 (s, 1H)	60.76
18	1.37 d (J=12.3)	59.4	CH	1.51 – 1.31 (m, 1H)	59.03
5	1.38 dd, (J=12,2)	50.8	CH	1.51 – 1.31 (m, 1H)	50.39
8’	1.1	50.12	CH	1.51 – 1.31 (m, 1H)	46.91
4	-	46.7	C	--	46.76
14	-	45.3	C	--	45.09
3’	1.9	45	CH	1.93 (d, *J* = 12.1 Hz, 1H)	43.77
10’	0.95	45	CH	0.88 (s, 1H)	43.77
8	-	43.9	C	--	40.92
22	1.29 m	41.3	CH2	1.31 – 1.11 (m, 2H)	40.74

19	1.52 m	39.7	CH	1.51 – 1.31 (m, 1H)	39.33
20	1.39 m	39.6	CH	1.51 – 1.31 (m, 1H)	39.29
10	-	37.6	C	--	37.30
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.47 (dt, *J* = 13.2, 3.6 Hz, 2H)	34.56
13’	0.84	34.52	CH	0.82 (t, *J* = 6.2 Hz, 1H)	34.12
4’	1.66	34.5	CH	1.89 – 1.70 (m, 1H)	34.12
17	-	34.2	C	--	33.98
15	1.66 m	33.2	CH_2	1.64 – 1.52 (m, 2H)	32.87
6’	1.43	31.6	CH	1.51 – 1.31 (m, 1H)	31.41
7	1.43 m	31.3	CH_2	1.51 – 1.31 (m, 2H)	30.92
30	0.80 d (J=7.4)	29.3	CH3	0.78 – 0.71 (m, 3H)	28.88
21	1.01 dd (J=11.8, 3)	27.9	CH2	1.01 (s, 2H)	27.53
16	1.88 m	27.6	CH_2	1.89 – 1.70 (m, 2H)	27.22
2’	2.17	25.8	CH	2.15 (ddd, *J* = 17.9, 9.5, 3.3 Hz, 1H)	26.11
23	1.21 s	24.3	CH3	1.31 – 1.11 (m, 3H)	23.85
2	1.56 m, 2.22 m	23.9	CH_2	1.64 – 1.52 (m, 2H)	23.54
5’	1.61	23.1	CH	1.51 – 1.31 (m, 1H)	23.30
9’	0.97	23.1	CH	1.31 – 1.11 (m, 1H)	23.30
12’	0.91	22.2	CH3	0.82 (t, *J* = 6.2 Hz, 3H)	21.98
CH3CO	2.07 s	21.7	CH3	2.03 (s, 3H)	21.38
28	0.93 s	21.5	CH3	0.88 (s, 3H)	21.17
11’	0.92	21	CH3	0.82 (t, *J* = 6.2 Hz, 3H)	20.76
27	1.33 s	20.9	CH3	1.31 – 1.11 (m, 3H)	20.56
6	1.75 m	19.2	CH_2	1.89 – 1.70 (m, 2H)	18.78
26	1.17 s	18.8	CH3	1.31 – 1.11 (m, 3H)	18.35
29	0.78 d (J=6.3)	17.8	CH3	0.68 (d, *J* = 6.8 Hz, 3H)	17.45
14’	0.8	16	CH3	0.78 – 0.71 (m, 3H)	16.22
25	1.12 s	13.6	CH3	1.01 (s, 3H)	13.38
7’	1.35	--	--	--	--
-CH2-CO	4.61-4.46 (2H, q, J=16.0, 16.2Hz	60.9	CH2	4.52 (q, *J* = 15.8 , 15.78 Hz, 2H)	60.29

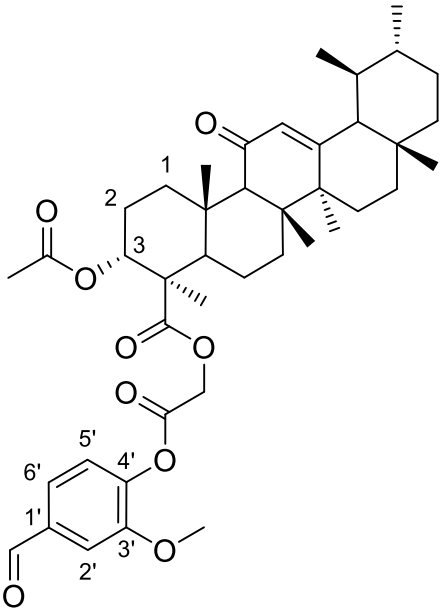
Table S4 NMR assignment of compound 5b



Parent compound			Hybrid compound		
Atom C/H	1H (δ, ppm) (J,Hz)	13C (δ, ppm)	DEPT	1H (δ, ppm) (J,Hz)	13C (δ, ppm)
11	-	199.6	C	--	199.4
24	-	182.2	C	--	175.15
CH3CO	-	170.5	C	--	170.26
CH2CO LINKER	-	166.5	C	--	166.56
13	-	165.3	C	--	165.17
1’	-	150.2	C	--	147.12
3’	-	138.4	C	--	137.03
6‘	--	131.7	C	--	136.8
12	5.54 s	130.8	CH	5.48 (s, 1H)	130.47
5’	7.08	126.3	CH	7.13 (d, J = 7.9 Hz, 1H)	127.62
4’	6.19	123.6	CH	6.96 (dd, J = 8.0, 1.7 Hz, 1H)	126.62
2’	5.4	116.9	CH	6.74 (d, J = 1.8 Hz, 1H)	122.38
3	5.28 t	73.6	CH	5.32 (d, J = 2.9 Hz, 1H)	73.2
9	2.39 s	60.7	CH	2.36 (s, 1H)	60.53
CH2-CO	4.90-4.73 (2H, q, J=16.0, 16.1 Hz,	60.7	CH2	4.82 (q, J = 17.5 Hz, 2H)	60.29
18	1.37 d (J=12.3)	59.4	CH	1.28 (s, 1H)	59.03

5	1.38 dd, (J=12,2)	50.8	CH	1.28 (s, 1H)	50.38
4	-	46.7	C	--	46.85
14	-	45.3	C	--	45.09
8	-	43.9	C	--	43.79
22	1.29 m	41.3	CH2	1.12 – 1.09 (s, 2H)	40.9
19	1.52 m	39.7	CH	1.49 – 1.35 (m, 1H)	39.34
20	1.39 m	39.6	CH	1.49 – 1.35 (m, 1H)	39.28
10	-	37.6	C	--	37.32
1	2.53 dd, (J=13.2,2)	35.0	CH2	2.48 (dt, J = 13.2, 3.6 Hz, 1H) 1.49 – 1.35(m, 1H)	34.51
17	-	34.2	C	--	33.98
15	1.66 m	33.2	CH2	1.49 – 1.35 (m, 2H)	32.87
7	1.43 m	31.3	CH2	1.49 – 1.35 (m, 2H)	30.92
30	0.80 d (J=7.4)	29.3	CH3	0.77 – 0.70 (m, 3H)	28.88
21	1.01 dd (J=11.8, 3)	27.9	CH2	0.97 – 0.85 (m, 2H)	27.52
16	1.88 m	27.6	CH2	1.94 – 1.76 (m, 2H)	27.23
8',9'	1.05	23.6-26.1	CH3	1.12 – 1.09 (m, 6H)	23.87-26.97
7'	3.38	25.5	CH	2.88 (dq, J = 16.1, 7.8 Hz, 1H)	23.56
23	1.21 s	24.3	CH3	1.21 – 1.15 (m, 3H)	23.13
2	1.56 m, 2.22 m	23.9	CH2	1.76 – 1.68 (m, 1H) 2.16 (t, J = 12.2 Hz, 1H)	23.11
CH3CO	2.07 s	21.7	CH3	2.02 (s, 3H)	21.37
28	0.93 s	21.5	CH3	0.97 – 0.85 (m, 3H)	21.17
27	1.33 s	20.9	CH3	1.28 (s, 3H)	20.82
6	1.75 m	19.2	CH2	1.60 (ddq, J = 15.5, 10.5, 3.8 Hz, 2H)	20.55
26	1.17 s	18.8	CH3	1.21 – 1.15 (m, 3H)	18.8
10'	2.2	18.7	CH3	2.24 (s, 3H)	18.34
29	0.78 d (J=6.3)	17.8	CH3	0.77 – 0.70 (m, 3H)	17.44
25	1.12 s	13.6	CH3	1.03 (s, 3H)	13.47
OH-	9.99	-		--	--

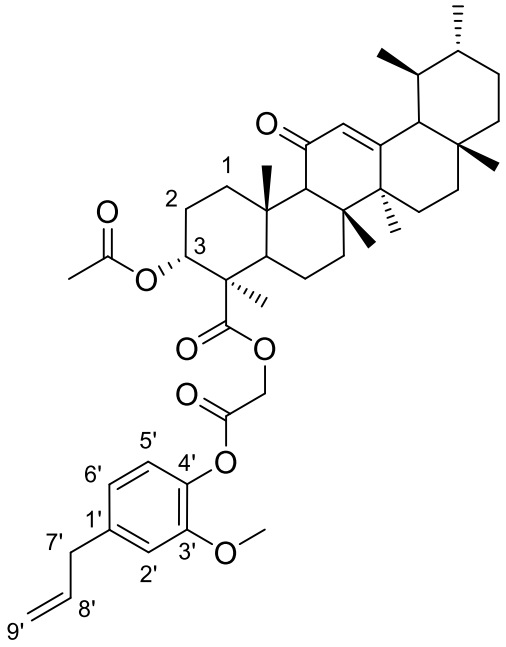
Table S5 NMR assignment of compound 5c



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)	DEPT	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)
11	-	199.6	C	--	199.56
C=O vanillin	10.11	191.2		9.84 (s, 1H)	191.1
24	-	182.2	C	--	175.02.
CH3CO	-	170.5	C	--	170.38
CH2CO LINKER	-	166.5	C	--	165.44
13	-	165.3	C	--	165.38
4’	--	152.14		--	151.79
3’	--	147.5		--	147.20
12	5.54 s	130.8	CH	5.58 (s, 1H)	130.41
1’	--	129.77		--	129.80
6’	6.9 d(J=7.5)	127.49	CH	7.06 (d, *J* = 8.5 Hz, 1H)	127.66
5’	7.2	114.75	CH	7.44 (d, *J* = 1.9 Hz, 1H)	114.43
2’	7.3 d(J=1.50)	109.14	CH	7.45 (d, *J* = 1.8 Hz, 1H)	108..81
3	5.28 t	73.6	CH	5.40 (dt, *J* = 12.3, 2.8 Hz, 1H)	73.2
9	2.39 s	60.7	CH	2.43 (d, *J* = 2.5 Hz, 1H)	60.28
CH2-CO	4.90-4.73 (2H, q, J=16.0, 16.1 Hz,	60.7	CH2	4.76 (d, *J* = 16.2 Hz, 1H) 4.61 (d, *J* = 16.2 Hz, 1H)	60.16
18	1.37 d (J=12.3)	59.4	CH	1.27 (t, *J* = 7.0 Hz, 1H)	59.02
-OCH3	3.84	56.2		3.98 (s, 3H)	56.14

vanillin					
5	1.38 dd, (J=12,2)	50.8	CH	1.27 (t, *J* = 7.0 Hz, 1H)	50.39
4	-	46.7	C	--	46.79
14	-	45.3	C	--	45.09
8	-	43.9	C	--	43.80
22	1.29 m	41.3	CH2	1.27 (t, *J* = 7.0 Hz, 2H)	40.9
19	1.52 m	39.7	CH	1.56 (d, *J* = 11.0 Hz, 1H)	39.33
20	1.39 m	39.6	CH	1.36 (s, 1H)	39.27
10	-	37.6	C	--	37.31
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.56 (dd, *J* = 13.2, 3.7 Hz, 1H) 1.53 – 1.38 (m, 1H)	34.50
17	-	34.2	C	--	33.98
15	1.66 m	33.2	CH_2	1.92 (dd, *J* = 9.3, 4.1 Hz, 2H)	32.86
7	1.43 m	31.3	CH_2	1.53 – 1.38 (m, 2H)	30.91
30	0.80 d (J=7.4)	29.3	CH3	0.86 – 0.79 (m, 3H)	28.89
21	1.01 dd (J=11.8, 3)	27.9	CH2	0.96 (s, 2H)	27.52
16	1.88 m	27.6	CH_2	2.23 (t, *J* = 15.7 Hz, 2H)	27.23
23	1.21 s	24.3	CH3	1.24 – 1.14 (m, 3H)	23.88
2	1.56 m, 2.22 m	23.9	CH_2	1.83 – 1.59 (m, 2H)	23.55
CH3CO	2.07 s	21.7	CH3	2.11 (d, *J* = 2.0 Hz, 3H)	21.38
28	0.93 s	21.5	CH3	0.96 (s, 3H)	21.16
27	1.33 s	20.9	CH3	1.36 (s, 3H)	20.5
6	1.75 m	19.2	CH_2	2.11 (d, *J* = 2.0 Hz, 2H)	18.7
26	1.17 s	18.8	CH3	1.24 – 1.14 (m, 3H)	18.3
29	0.78 d (J=6.3)	17.8	CH3	0.86 – 0.79 (m, 3H)	17.43
25	1.12 s	13.6	CH3	1.11 (d, *J* = 10.0 Hz, 3H)	13.44
OH-	8.71	-		--	--

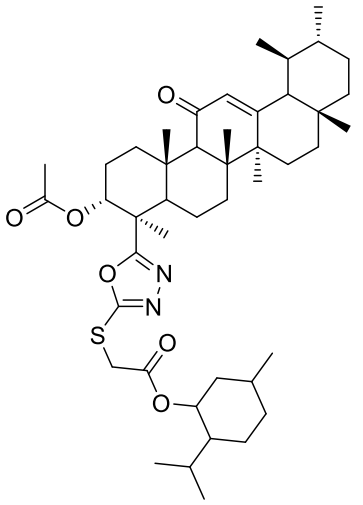
Table S6 NMR assignment of compound 5d



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H (δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ, ppm)
11	-	199.6	C	--	199.35
24	-	182.2	C	--	175.02
CH3CO	-	170.5	C	--	170.24
CH2CO LINKER	-	166.5	C	--	165.94
13	-	165.3	C	--	165.02
3’	--	146.6	C	--	150.64
4’	--	144.03	C	--	139.47
-CH= eugenol	5.9	137.9	CH	5.87 (ddt, *J* = 16.9, 10.2, 6.7 Hz, 1H)	137.19
1’	--	131.94	C	--	136.97
12	5.54 s	130.8	CH	5.47 (s, 1H)	130.51
5’	6.67	121.2	CH	6.73 – 6.65 (m, 1H)	122.33
6’	6.82	115.49	CH	6.89 (d, *J* = 7.9 Hz, 1H)	120.70
2’	6.66	114.46	CH	6.73 – 6.65 (m, 1H)	116.26
Eugenol-CH=CH2	5.06, 5.04	111.8	CH	5.06 – 4.99 (m, 2H)	112.79
3	5.28 t	73.6	CH	5.33 (d, *J* = 2.9 Hz, 1H)	73.24
9	2.39 s	60.7	CH	2.35 (s, 1H)	60.35

CH2-CO	4.90-4.73 (2H, q, J=16.0, 16.1 Hz,	60.7	CH2	4.90 (d, *J* = 16.0 Hz, 1H) 4.77 (d, *J* = 16.0 Hz, 1H)	60.30
18	1.37 d (J=12.3)	59.4	CH	1.37 – 1.18 (m, 1H)	59.03
-OCH3 Eugenol	3.8	55.8	CH3	3.73 (s, 3H)	55.86
5	1.38 dd, (J=12,2)	50.8	CH	1.37 – 1.18 (m, 1H)	50.39
4	-	46.7	C	--	46.84
14	-	45.3	C	--	45.09
8	-	43.9	C	--	43.78
22	1.29 m	41.3	CH2	1.16 (s, 2H)	40.92
CH2-CH= eugenol	3.29	39.9	CH2	3.29 (d, *J* = 6.8 Hz, 2H)	40.10
19	1.52 m	39.7	CH	1.39 (ddd, *J* = 12.1, 10.0, 7.2 Hz, 1H)	39.34
20	1.39 m	39.6	CH	1.37 – 1.18 (m, 1H)	39.29
10	-	37.6	C	--	37.33
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.47 (dt, *J* = 13.0, 3.5 Hz, 1H) 1.39 (ddd, J = 12.1, 10.0, 7.2 Hz, 1H)	34.54
17	-	34.2	C	--	33.99
15	1.66 m	33.2	CH_2	1.66 – 1.53 (m, 2H)	32.88
7	1.43 m	31.3	CH_2	1.39 (ddd, *J* = 12.1, 10.0, 7.2 Hz, 2H)	30.92
30	0.80 d (J=7.4)	29.3	CH3	0.81 – 0.70 (m, 3H)	28.87
21	1.01 dd (J=11.8, 3)	27.9	CH2	0.87 (s, 2H)	27.53
16	1.88 m	27.6	CH_2	1.93 – 1.68 (m, 2H)	27.23
23	1.21 s	24.3	CH3	1.37 – 1.18 (m, 3H)	23.87
2	1.56 m, 2.22 m	23.9	CH_2	2.18 (td, *J* = 14.2, 3.5 Hz, 1H) 1.51 – 1.44 (m, 1H)	23.56
CH3CO	2.07 s	21.7	CH3	2.02 (s, 3H)	21.39
28	0.93 s	21.5	CH3	0.87 (s, 3H)	21.17
27	1.33 s	20.9	CH3	1.37 – 1.18 (m, 3H)	20.56
6	1.75 m	19.2	CH_2	1.93 – 1.68 (m, 2H)	18.76
26	1.17 s	18.8	CH3	1.11 (s, 3H)	18.32
29	0.78 d (J=6.3)	17.8	CH3	0.81 – 0.70 (m, 3H)	17.45
25	1.12 s	13.6	CH3	1.03 (s, 3H)	13.45
OH-	5.6	-		--	--

Table S7 NMR assignment of compound 8a

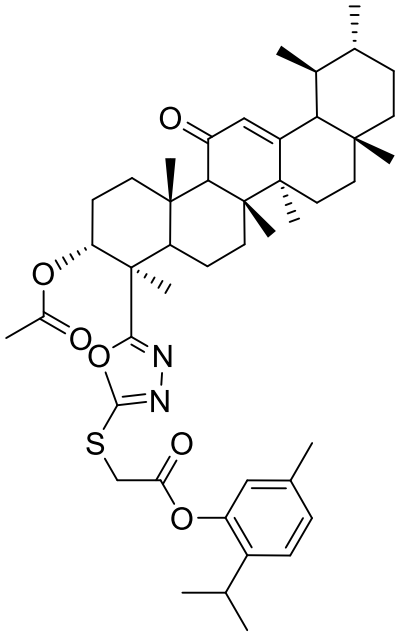


Parent compound			Hybrid compound		
Atom **C/H**	^{1}H (δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ, ppm)
11	-	199.6	C	--	199.32
24	-	182.2	C	--	--
CH3CO	-	170.5	C	--	172.16
-CH2-CO MENTHOL		167.2	C	--	167.19
13	-	165.3	C	--	165
12	5.54 s	130.8	CH	5.46 (s, 1H)	130.41
3	5.28 t	73.6	CH	4.34 (d, *J* = 2.9 Hz, 1H)	76.70
Menthol 1***(Kwan and Huang 2008)***	3.4 td, (j=10.4,4.3)	71.5	CH	4.68 (td, *J* = 10.9, 4.4 Hz, 1H)	70.62
-CH2-CO	4.61-4.46 (2H, q, J=16.0, 16.2Hz	60.9	CH2	3.98 (s, 2H)	60.34
9	2.39 s	60.7	CH	2.09 – 1.88 (m, 1H)	59.01
18	1.37 d (J=12.3)	59.4	CH	1.69 – 1.55 (m, 1H)	53.47
5	1.38 dd, (J=12,2)	50.8	CH	1.50 – 1.34 (m, 1H)	49.16
8’	1.1	50.12	CH	1.50 – 1.34 (m, 1H)	46.92
4	-	46.7	C	--	43.81
14	-	45.3	C	--	45.09

3’	1.9	45	CH	1.87 – 1.73 (m, 1H)	41.91
10’	0.95	45	CH	0.90 – 0.76 (m, 1H)	41.91
8	-	43.9	C	--	40.91
22	1.29 m	41.3	CH2	1.20 – 1.11 (m, 2H)	40.61
19	1.52 m	39.7	CH	1.50 – 1.34 (m, 1H)	39.28
20	1.39 m	39.6	CH	1.50 – 1.34 (m, 1H)	39.28
10	-	37.6	C	--	37.11
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.52 – 2.36 (m, 2H)	34.71
13’	0.84	34.52	CH	0.76 – 0.62 (m, 1H)	34.09
4’	1.66	34.5	CH	1.69 – 1.55 (m, 1H)	33.96
17	-	34.2	C	--	33.96
15	1.66 m	33.2	CH_2	1.69 – 1.55 (m, 2H)	33.70
6’	1.43	31.6	CH	1.50 – 1.34 (m, 1H)	32.71
7	1.43 m	31.3	CH_2	1.69 – 1.55 (m, 2H)	31.41
30	0.80 d (J=7.4)	29.3	CH3	0.76 – 0.62 (m, 3H)	30.91
21	1.01 dd (J=11.8, 3)	27.9	CH2	1.03 – 0.91 (m, 1H)	28.88
16	1.88 m	27.6	CH_2	1.87 – 1.73 (m, 2H)	27.49
2’	2.17	25.8	CH	2.09 – 1.88 (m, 1H)	27.17
23	1.21 s	24.3	CH3	1.34 – 1.21 (m, 3H)	26.17
2	1.56 m, 2.22 m	23.9	CH_2	1.69 – 1.55 (m, 2H)	26.03
5’	1.61	23.1	CH	1.50 – 1.34 (m, 1H)	25.39
9’	0.97	23.1	CH	1.03 – 0.91 (m, 1H)	23.29
12’	0.91	22.2	CH3	0.90 – 0.76 (m, 3H)	23.29

CH3CO	2.07 s	21.7	CH3	2.09 – 1.88 (m, 3H)	21.99
28	0.93 s	21.5	CH3	0.90 – 0.76 (m, 3H)	21.16
11’	0.92	21	CH3	0.90 – 0.76 (m, 3H)	20.79
27	1.33 s	20.9	CH3	1.34 – 1.21 (m, 3H)	20.58
6	1.75 m	19.2	CH_2	1.69 – 1.55 (m, 2H)	18.64
26	1.17 s	18.8	CH3	1.34 – 1.21 (m, 3H)	18.36
29	0.78 d (J=6.3)	17.8	CH3	0.76 – 0.62 (m, 3H)	17.46
14’	0.8	16	CH3	0.76 – 0.62 (m, 3H)	16.24
25	1.12 s	13.6	CH3	1.07 (s, 3H)	13.11
O-C=N oxadiazole	--	--	C	--	167
S-C=N oxadiazole	--	--	C	--	162.2
7’	1.35	--	--	--	--

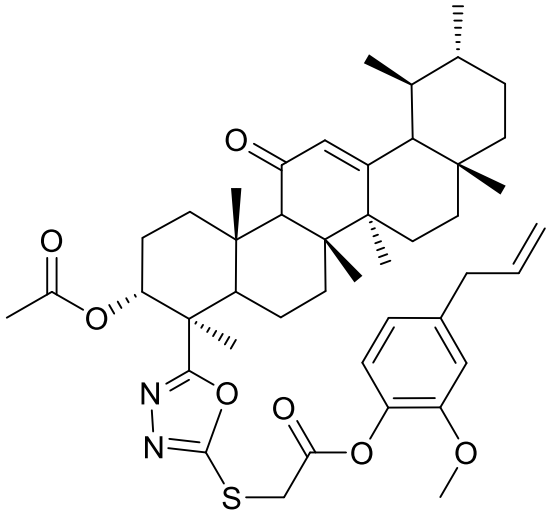
Table S8 NMR assignment of compound 8b



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)	DEPT	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)
11	-	199.6	C	--	199.23
24	-	182.2	C	--	
CH3CO	-	170.5	C	--	172.43
O-C=N		167			166.47
CH2CO LINKER	-	166.5	C	--	166.47
13	-	165.3	C	--	165.06
S-C=N		163			161.94
1’	-	150.2	C	--	147.64
3’	-	138.4	C	--	136.88
6‘	--	131.7	C	--	136.77
12	5.54 s	130.8	CH	5.55 (s, 1H)	130.42
5’	7.08	126.3	CH	7.21 (d, *J* = 7.9 Hz, 1H)	127.65
4’	6.19	123.6	CH	7.05 (dd, *J* = 7.9, 1.7 Hz, 1H)	126.56
2’	5.4	116.9	CH	6.86 (d, *J* = 1.8 Hz, 1H)	122.29
3	5.28 t	73.6	CH	5.32 (s, 1H)	70.65
9	2.39 s	60.7	CH	2.46 (s, 1H)	60.33
CH2-CO	4.90-4.73 (2H, q, J=16.0, 16.1 Hz,	60.7	CH2	4.33 (d, *J* = 4.1 Hz, 2H)	59

18	1.37 d (J=12.3)	59.4	CH	1.41 – 1.27 (m, 3H)	49.19
5	1.38 dd, (J=12,2)	50.8	CH	1.60 – 1.45 (m, 1H)	45.01
4	-	46.7	C	--	43.8
14	-	45.3	C	--	41.97
8	-	43.9	C	--	40.91
22	1.29 m	41.3	CH2	1.44 – 1.27 (m, 2H)	39.28
19	1.52 m	39.7	CH	1.60 – 1.45 (m, 1H)	39.28
20	1.39 m	39.6	CH	1.60 – 1.45 (m, 1H)	37.1
10	-	37.6	C	--	34.42
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.63 – 2.50 (m, 2H)	33.96
17	-	34.2	C	--	33.67
15	1.66 m	33.2	CH_2	1.93 – 1.65 (m, 2H)	32.68
7	1.43 m	31.3	CH_2	1.60 – 1.45 (m, 2H)	30.91
30	0.80 d (J=7.4)	29.3	CH3	0.84 – 0.80 (m, 3H)	28.86
21	1.01 dd (J=11.8, 3)	27.9	CH2	0.96 (s, 2H)	27.49
16	1.88 m	27.6	CH_2	1.93 – 1.65 (m, 2H)	27.17
8',9'	1.05	26	CH3	1.19 (d, *J* = 6.9 Hz, 6H)	27
7'	3.38	25.5	CH	3.00 (hept, J = 6.9 Hz, 1H)	26.06
23	1.21 s	24.3	CH3	1.44 – 1.27 (m, 3H)	25.41
2	1.56 m, 2.22 m	23.9	CH_2	1.93 – 1.65 (m, 2H)	23.11
CH3CO	2.07 s	21.7	CH3	1.93 – 1.65 (m, 3H)	23.08
28	0.93 s	21.5	CH3	0.96 (s, 3H)	21.16
27	1.33 s	20.9	CH3	1.44 – 1.27 (m, 3H)	20.83
6	1.75 m	19.2	CH_2	1.93 – 1.65 (m, 2H)	20.58
26	1.17 s	18.8	CH3	1.44 – 1.27 (m, 3H)	18.64
10'	2.2	18.7	CH3	2.32 (s, 3H)	18.32
29	0.78 d (J=6.3)	17.8	CH3	0.84 – 0.80 (m, 3H)	17.45
25	1.12 s	13.6	CH3	1.13 (s, 3H)	13.1
OH-	9.99	-		--	

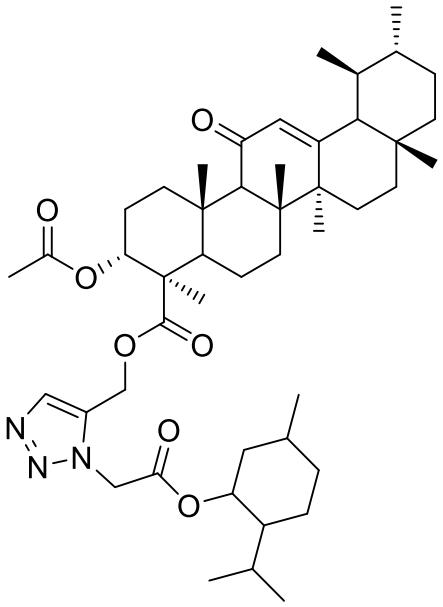
Table S9 NMR assignment of compound 8b



Parent compound		Hybrid compound			
Atom **C/H**	^{1}H (δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ, ppm)
3’	6.82	115.49	CH	6.99 (d, *J* = 7.9 Hz, 1H)	120.69
4’	6.67	121.2	CH	6.82 – 6.74 (m, 1H)	122.21
6’	6.66	114.46	CH	6.82 – 6.74 (m, 1H)	116.31
-CH= eugenol	5.9	137.9	CH	5.96 (ddt, *J* = 15.6, 10.4, 6.7 Hz, 1H)	137.66
12	5.54 s	130.8	CH	5.54 (s, 1H)	130.42
3	5.28 t	73.6	CH	5.32 (s, 1H)	70.66
Eugenol-CH=CH2	5.06, 5.04	111.8	CH2	5.18 – 5.07 (m, 2H)	112.73
CH2-CO	4.90-4.73 (2H, q, J=16.0, 16.1 Hz,	60.7	CH2	4.32 (d, *J* = 1.5 Hz, 2H)	59
-OCH3 Eugenol	3.8	55.8	CH3	3.81 (s, 3H)	53.47
CH2-CH= eugenol	3.29	39.9	CH2	3.38 (d, *J* = 6.7 Hz, 2H)	40.08
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.63 – 2.49 (m, 2H)	34.26
9	2.39 s	60.7	CH	2.46 (s, 1H)	60.34
2	1.56 m, 2.22 m	23.9	CH_2	2.11 (td, *J* = 13.7, 4.91H) 1.58 – 1.40 (m, 1H) Hz,	26.05
16	1.88 m	27.6	CH_2	1.86 (qd, *J* = 14.4, 8.2 Hz, 2H)	27.49
CH3CO	2.07 s	21.7	CH3	1.75 – 1.69 (m, 3H)	25.37

15	1.66 m	33.2	CH_2	1.75 – 1.69 (m, 2H)	33.68
6	1.75 m	19.2	CH_2	1.75 – 1.69 (m, 2H)	18.62
7	1.43 m	31.3	CH_2	1.58 – 1.40 (m, 2H)	32.68
19	1.52 m	39.7	CH	1.58 – 1.40 (m, 1H)	39.28
18	1.37 d (J=12.3)	59.4	CH	1.49 – 1.44 (m, 1H)	55.84
5	1.38 dd, (J=12,2)	50.8	CH	1.49 – 1.44 (m, 1H)	49.2
20	1.39 m	39.6	CH	1.49 – 1.44 (m, 1H)	39.28
23	1.21 s	24.3	CH3	1.40 – 1.15 (m, 3H)	27.16
27	1.33 s	20.9	CH3	1.40 – 1.15 (m, 3H)	20.58
22	1.29 m	41.3	CH2	1.40 – 1.15 (m, 2H)	40.91
26	1.17 s	18.8	CH3	1.11 (s, 3H)	18.3
25	1.12 s	13.6	CH3	1.04 – 0.95 (m, 3H)	13.08
21	1.01 dd (J=11.8, 3)	27.9	CH2	1.04 – 0.95 (m, 2H)	28.87
30	0.80 d (J=7.4)	29.3	CH3	0.84 – 0.78 (m, 3H)	30.91
28	0.93 s	21.5	CH3	0.84 – 0.78 (m, 3H)	21.16
29	0.78 d (J=6.3)	17.8	CH3	0.71 (s, 3H)	17.46
11	-	199.6	C	--	199.26
24	-	182.2	C	--	--
CH3CO	-	170.5	C	--	172.32
CH2CO LINKER	-	166.5	C	--	165.92
13	-	165.3	C	--	165.06
1’	--	146.6	C	--	150.55
2’	--	144.03	C	--	139.57
5’	--	131.94	C	--	136.91
4	-	46.7	C	--	45.01
14	-	45.3	C	--	43.8
8	-	43.9	C	--	41.95
10	-	37.6	C	--	37.1
17	-	34.2	C	--	33.96
OH-	5.6	-		--	
O-C=N	--	166			165.92
S-C=N	--	163			161.96

Table S10 NMR assignment of compound 14b

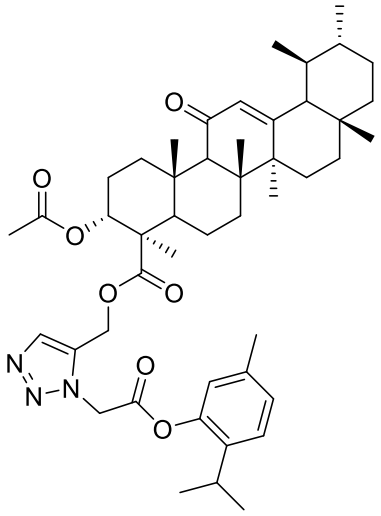


Parent compound			Hybrid compound		
Atom **C/H**	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)	DEPT	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)
11	-	199.6	C	--	199.33
24	-	182.2	C	--	175.63
CH3CO	-	170.5	C	--	170.23
-CH2-CO MENTHOL		167.2	C		165.53
13	-	165.3	C	--	165.09
CH=N triazole	8.0	142	CH	7.78 (s, 1H)	130.46
C=N triazole	--	124	C	--	125.66
12	5.54 s	130.8	CH	5.55 (s, 1H)	130.46
3	5.28 t	73.6	CH	5.35 – 5.23 (m, 1H)	77.2
Menthol 1***(Kwan and Huang 2008)***	3.4 td, (j=10.4,4.3)	71.5	CH	4.80 (td, *J* = 10.9, 4.4 Hz, 1H)	73.20

-CH2-CO	4.61-4.46 (2H, q, J=16.0, 16.2Hz	60.9	CH2	5.15 (d, *J* = 3.4 Hz, 2H)	60.23
9	2.39 s	60.7	CH	2.40 (s, 1H)	59.02
CH2-triazole	5.23	60	CH_2	5.35 – 5.23 (m, 2H)	58.50
18	1.37 d (J=12.3)	59.4	CH	1.35 (s, 1H)	57.38
5	1.38 dd, (J=12,2)	50.8	CH	1.35 (s, 1H)	51.08
8’	1.1	50.12	CH	1.34 – 1.14 (m, 1H)	50.46
4	-	46.7	C	--	46.83
14	-	45.3	C	--	46.71
3’	1.9	45	CH	2.24 – 1.99 (m, 1H)	45.04
10’	0.95	45	CH	0.97 – 0.89 (m, 1H)	45.04
8	-	43.9	C	--	43.76
22	1.29 m	41.3	CH2	1.34 – 1.14 (m, 2H)	40.91
19	1.52 m	39.7	CH	1.61 – 1.51 (m, 1H)	40.64
20	1.39 m	39.6	CH	1.35 (s, 1H)	39.32
10	-	37.6	C	--	39.28
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.56 – 2.48 (m, 1H) 1.71 – 1.61 (m, 1H)	37.23
13’	0.84	34.52	CH	0.97 – 0.89 (m, 1H)	34.54
4’	1.66	34.5	CH	1.93 – 1.76 (m, 1H)	33.98
17	-	34.2	C	--	32.77
15	1.66 m	33.2	CH_2	1.75 – 1.71 (m, 2H)	31.39
6’	1.43	31.6	CH	1.54 – 1.36 (m, 1H)	30.91
7	1.43 m	31.3	CH_2	1.54 – 1.36 (m, 2H)	28.85
30	0.80 d (J=7.4)	29.3	CH3	0.89 – 0.79 (m, 3H)	27.51
21	1.01 dd (J=11.8, 3)	27.9	CH2	0.97 – 0.89 (m, 2H)	27.22

16	1.88 m	27.6	CH_2	2.24 – 1.99 (m, 2H)	26.29
2’	2.17	25.8	CH	2.24 – 1.99 (m, 1H)	23.72
23	1.21 s	24.3	CH3	1.34 – 1.14 (m, 3H)	23.56
2	1.56 m, 2.22 m	23.9	CH_2	1.75 – 1.71 (m, 2H)	23.30
5’	1.61	23.1	CH	1.75 – 1.71 (m, 1H)	21.94
9’	0.97	23.1	CH	0.97 – 0.89 (m, 1H)	21.94
12’	0.91	22.2	CH3	0.97 – 0.89 (m, 3H)	21.37
CH3CO	2.07 s	21.7	CH3	2.24 – 1.99 (m, 3H)	21.16
28	0.93 s	21.5	CH3	0.97 – 0.89 (m, 3H)	20.73
11’	0.92	21	CH3	0.97 – 0.89 (m, 3H)	20.53
27	1.33 s	20.9	CH3	1.34 – 1.14 (m, 3H)	18.82
6	1.75 m	19.2	CH_2	1.75 – 1.71 (m, 2H)	18.45
26	1.17 s	18.8	CH3	1.34 – 1.14 (m, 3H)	18.29
29	0.78 d (J=6.3)	17.8	CH3	0.76 (d, J = 6.9 Hz, 3H)	17.43
14’	0.8	16	CH3	0.89 – 0.79 (m, 3H)	16.27
25	1.12 s	13.6	CH3	1.11 – 0.97 (m, 3H)	13.20
7’	1.35	--	--	--	--

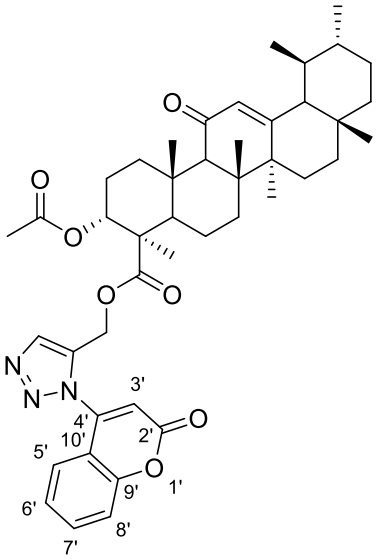
Table S11 NMR assignment of compound 14b



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)	DEPT	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)
OH-	9.99	-		--	--
CH=N triazole	8.0	142	CH	7.77 (s, 1H)	142.96
5’	7.08	126.3	CH	7.13 (d, *J* = 7.9 Hz, 1H)	127.92
4’	6.19	123.6	CH	6.98 (d, *J* = 8.0 Hz, 1H)	126.70
12	5.54 s	130.8	CH	5.45 (s, 1H)	130.45
2’	5.4	116.9	CH	6.77 (s, 1H)	122.14
3	5.28 t	73.6	CH	5.22 (d, *J* = 5.4 Hz, 3H)	73.19
CH2-triazole	5.23	60	CH_2	5.39 – 5.35 (m, 2H)	50.87
7’	3.38	25.5	CH	2.81 (p, *J* = 6.9 Hz, 1H)	23.72
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.41 (dd, *J* = 13.5, 3.4 Hz, 1H) 2.20 – 1.93 (m, 1H)	34.53
9	2.39 s	60.7	CH	2.35 – 2.22 (m, 1H)	60.21
10’	2.2	18.7	CH3	2.35 – 2.22 (m, 3H)	18.22,
CH3CO	2.07 s	21.7	CH3	2.20 – 1.93 (m, 3H)	21.38
16	1.88 m	27.6	CH_2	2.20 – 1.93 (m, 2H)	27.20
6	1.75 m	19.2	CH_2	1.83 – 1.31 (m, 2H)	20.53
15	1.66 m	33.2	CH_2	1.83 – 1.31 (m, 2H)	32.75

2	1.56 m, 2.22 m	23.9	CH_2	2.35 – 2.22 (m, 1H) 1.83 – 1.31 (m, 1H)	23.03
19	1.52 m	39.7	CH	1.83 – 1.31 (m, 1H)	39.32
7	1.43 m	31.3	CH_2	1.83 – 1.31 (m, 2H)	30.92
20	1.39 m	39.6	CH	1.30 – 1.22 (m, 1H)	39.29
5	1.38 dd, (J=12,2)	50.8	CH	1.30 – 1.22 (m, 1H)	50.45
18	1.37 d (J=12.3)	59.4	CH	1.30 – 1.22 (m, 1H)	57.44
27	1.33 s	20.9	CH3	1.19 – 1.01 (m, 3H)	20.83
22	1.29 m	41.3	CH2	1.30 – 1.22 (m, 2H)	40.9
23	1.21 s	24.3	CH3	1.19 – 1.01 (m, 3H)	23.55
26	1.17 s	18.8	CH3	1.19 – 1.02 (m, 3H)	18.8
25	1.12 s	13.6	CH3	0.95 – 0.85 (m, 3H)	13.20.
8',9'	1.05	23.6- 26.1	CH3	1.19 – 1.02 (m, 6H)	23.03-27.16
21	1.01 dd (J=11.8, 3)	27.9	CH2	0.95 – 0.85 (m, 2H)	27.51
28	0.93 s	21.5	CH3	0.83 (s, 3H)	21.17
30	0.80 d (J=7.4)	29.3	CH3	0.78 – 0.69 (m, 3H)	28.88
29	0.78 d (J=6.3)	17.8	CH3	0.78 – 0.69 (m, 3H)	17.44
11	-	199.6	C	--	199.3
24	-	182.2	C	--	175.63
CH3CO	-	170.5	C	--	170.24
CH2CO LINKER	-	166.5	C	--	165.07
13	-	165.3	C	--	164.86
1'	-	150.2	C	--	147.09
3'	-	138.4	C	--	136.95
6'	--	131.7	C	--	136.67
C=N triazole	--	124	C	--	125.61
CH2-CO	4.90-4.73 (2H, q, J=16.0, 16.1 Hz,	60.7	CH2	5.22 (q, *J* = 6.6 Hz, 3H)	59.03
4	-	46.7	C	--	46.71
14	-	45.3	C	--	45.01
8	-	43.9	C	--	43.75
10	-	37.6	C	--	37.21

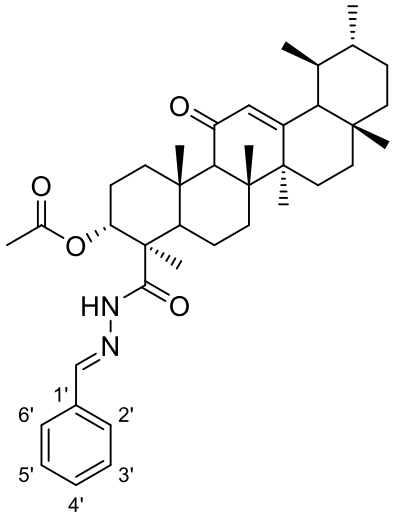
Table S12 NMR assignment of compound 14c



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)	DEPT	PMR	C13
11	-	199.6	C	-	199.21
24	-	182.2	C	-	175.6
$CH_3\underline{C}O$	-	170.5	C	-	170.25
2’	--	166.1	C	--	165.19
13	-	165.3	C	-	165.19
4’	--	162.32	C	--	159.8
9’	--	153.98	C	--	154.26
C=N	--	142		--	146.6
7’	7.65 (d, *J* = 7.8 Hz, 1H)	133.17	CH	7.62 (dd, *J* = 7.4 Hz, 1H)	133.76
12	5.54 s	130.8	CH	5.46 (s, 1H)	130.4
6’	7.38 7.34 (m, 1H)	124.39	CH	7.41 (d, *J* = 8.2 Hz, 1H)	125.29
CH=N	8	124	CH	8.05 (s, 1H)	125.19
5’	7.83 (d, *J* = 7.2 Hz, 1H)	123.66	CH	7.70 (dd, *J* = 8.2, 1.5 Hz, 1H)	**125.19**
8’	7.38 7.34 (m, 1H)	116.7	CH	7.30 (t, *J* = 7.7 Hz, 1H)	117.79

10’	--	116.27	C		114.29
3’	5.60 (s, 1H)	91.46	CH	6.50 (s, 1H)	110.34
3	5.28 t	73.6	CH	5.29 – 5.21 (m, 1H)	72.98
9	2.39 s	60.7	CH	2.33 (s, 1H)	60.14
CH2CO	5.3	60	CH2	5.31 (s, 2H)	59.02
18	1.37 d (J=12.3)	59.4	CH	1.38 – 1.19 (m, 1H)	57.03
5	1.38 dd, (J=12,2)	50.8	CH	1.38 – 1.19 (m, 1H)	50.48
4	-	46.7	C	-	46.81
14	-	45.3	C	-	45.03
8	-	43.9	C	-	43.77
22	1.29 m 1.46 m	41.3	CH_2	0.98 – 0.91 (m, 2H)	40.89
19	1.52 m	39.7	CH	1.57 – 1.38 (m, 1H)	39.32
20	1.39 m	39.6	CH	1.38 – 1.19 (m, 1H)	39.27
10	-	37.6	C		37.23
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.43 (dt, *J* = 13.4, 3.5 Hz, 2H)	34.46
17	-	34.2	C		33.97
15	1.66 m	33.2	CH_2	1.57 – 1.38 (m, 2H)	32.7
7	1.43 m	31.3	CH_2	1.38 – 1.19 (m, 2H)	30.90
30	0.80 d (J=7.4)	29.3	CH_3	0.89 – 0.82 (m, 3H)	28.86
21	1.01 dd (J=11.8, 3)	27.9	CH_2	0.77 – 0.69 (m, 2H)	27.49
16	1.88 m	27.6	CH_2	1.74 – 1.57 (m, 2H)	27.22
23	1.21 s	24.3	CH_3	1.19 – 1.06 (m, 3H)	23.81
2	1.56 m, 2.22 m	23.9	CH_2	2.31 – 2.01 (m, 2H)	23.59
$\underline{C}H_3CO$	2.07 s	21.7	CH_3	2.02 (s, 3H)	21.37
28	0.93 s	21.5	CH_3	0.89 – 0.82 (m, 3H)	21.16
27	1.33 s	20.9	CH_3	1.38 – 1.19 (m, 3H)	20.5
6	1.75 m	19.2	CH_2	1.57 – 1.38 (m, 2H)	18.8
26	1.17 s	18.8	CH_3	1.19 – 1.06 (m, 3H)	18.3
29	0.78 d (J=6.3)	17.8	CH_3	0.77 – 0.69 (m, 3H)	17.43
25	1.12 s	13.6	CH_3	1.19 – 1.06 (m, 3H)	13.3
4-OH	12.53	-	-	--	--

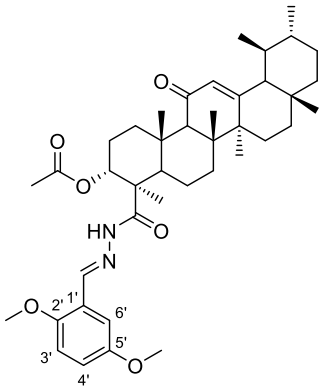
Table S13 NMR assignment of compound 16a



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)	DEPT	^{1}H (δ, ppm) (J,Hz)	^{13}C (δ, ppm)
11	-	199.6	C	--	199.23
CHO/CH=N	10.2	189.37	CH	8.54 (s, 1H)	143.45
24	-	182.2	C	-	162.75
$CH_3\underline{C}O$	-	170.5	C	-	173.16
13	--	165.3	C	--	164.94
2’	--	156.73	C	--	153.98
5’	--	153.69	C	--	152.92
12	5.54 s	130.8	CH	5.54 (s, 1H)	130.64
1’	--	125.03	C	-	130.64
4’	7.78	123.29	CH	7.56 (d, J = 3.1 Hz, 1H)	121.96
6’	6.4	113.38	CH	6.84 (d, J = 9.1 Hz, 1H)	119.71
3’	6.5	110.60	CH	6.93 (dd, J = 9.1, 3.1 Hz, 1H)	112.67
3	5.28 t	73.6	CH	4.24 (s, 1H)	70.51
9	2.39 s	60.7	CH	2.57 – 2.38 (m, 1H)	60.56
18	1.37 d (J=12.3)	59.4	CH	1.39 – 1.30 (m, 1H)	59.12
OCH3	3.8	56.17	CH_3	3.84 (s, 3H)	56.36
OCH3	3.8	56.16	CH_3	3.80 (s, 3H)	56.15
5	1.38 dd, (J=12,2)	50.8	CH	1.04 – 0.89(m, 1H)	49.04
4	-	46.7	C	-	47.48
14	-	45.3	C	-	45.16

8	-	43.9	C	-	43.94
22	1.29 m 1.46 m	41.3	CH_2	1.39 – 1.30 (m, 2H)	41.01
19	1.52 m	39.7	CH	1.93 – 1.71 (m, 1H)	39.42
20	1.39 m	39.6	CH	1.64 – 1.39 (m, 1H)	39.38
10	-	37.6	C		37.66
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.57 – 2.38 (m, 2H)	36.67
17	-	34.2	C	--	34.30
15	1.66 m	33.2	CH_2	1.64 – 1.39 (m, 2H)	34.09
7	1.43 m	31.3	CH_2	1.39 – 1.30 (m, 2H)	33.30
30	0.80 d (J=7.4)	29.3	CH_3	0.83 – 0.75 (m, 3H)	31.02
21	1.01 dd (J=11.8, 3)	27.9	CH_2	1.04 – 0.89 (s, 2H)	28.99
16	1.88 m	27.6	CH_2	1.64 – 1.39 (m, 2H)	27.61
23	1.21 s	24.3	CH_3	1.31 – 1.11 (m, 3H)	27.27
2	1.56 m, 2.22 m	23.9	CH_2	2.15 – 2.01 (m, 2H)	26.71
$\underline{C}H_3CO$	2.07 s	21.7	CH_3	1.93 – 1.71 (m, 3H)	24.80
28	0.93 s	21.5	CH_3	1.04 – 0.89 (s, 3H)	21.25
27	1.33 s	20.9	CH_3	1.39 – 1.30 (m, 3H)	20.62
6	1.75 m	19.2	CH_2	1.64 – 1.39 (m, 2H)	20.03
26	1.17 s	18.8	CH_3	1.31 – 1.11 (m, 3H)	18.48
29	0.78 d (J=6.3)	17.8	CH_3	0.83 – 0.75 (m, 3H)	17.55
25	1.12 s	13.6	CH_3	1.31 – 1.11 (m, 3H)	13.90
NH	11.25	--	NH	8.86 (s, 1H)	

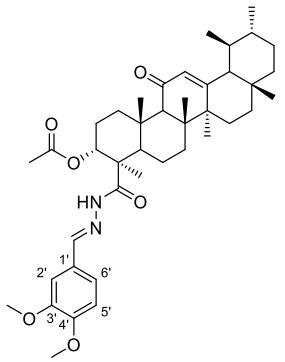
Table S14 NMR assignment of compound 16b



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H (δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ, ppm)
11	-	199.6	C	--	199.23
CHO/CH=N	10.2	189.37	CH	8.54 (s, 1H)	143.45
24	-	182.2	C	-	162.75
$CH_3\underline{C}O$	-	170.5	C	-	173.16
13	--	165.3	C	--	164.94
2’	--	156.73	C	--	153.98
5’	--	153.69	C	--	152.92
12	5.54 s	130.8	CH	5.54 (s, 1H)	130.64
1’	--	125.03	C	-	130.64
4’	7.78	123.29	CH	7.56 (d, *J* = 3.1 Hz, 1H)	121.96
6’	6.4	113.38	CH	6.84 (d, *J* = 9.1 Hz, 1H)	119.71
3’	6.5	110.60	CH	6.93 (dd, *J* = 9.1, 3.1 Hz, 1H)	112.67
3	5.28 t	73.6	CH	4.24 (s, 1H)	70.51
9	2.39 s	60.7	CH	2.57 – 2.38 (m, 1H)	60.56
18	1.37 d (J=12.3)	59.4	CH	1.39 – 1.30 (m, 1H)	59.12
OCH3	3.8	56.17	CH_3	3.84 (s, 3H)	56.36
OCH3	3.8	56.16	CH_3	3.80 (s, 3H)	56.15
5	1.38 dd, (J=12,2)	50.8	CH	1.04 – 0.89(m, 1H)	49.04
4	-	46.7	C	-	47.48
14	-	45.3	C	-	45.16
8	-	43.9	C	-	43.94
22	1.29 -1.46 m	41.3	CH_2	1.39 – 1.30 (m, 2H)	41.01
19	1.52 m	39.7	CH	1.93 – 1.71 (m, 1H)	39.42
20	1.39 m	39.6	CH	1.64 – 1.39 (m, 1H)	39.38
10	-	37.6	C		37.66
1	2.53 dd, (J=13.2,2)	35.0	CH_2	2.57 – 2.38 (m, 2H)	36.67

17	-	34.2	C	--	34.30
15	1.66 m	33.2	CH_2	1.64 – 1.39 (m, 2H)	34.09
7	1.43 m	31.3	CH_2	1.39 – 1.30 (m, 2H)	33.30
30	0.80 d(J=7.4)	29.3	CH_3	0.83 – 0.75 (m, 3H)	31.02
21	1.01 dd(J=11.8, 3)	27.9	CH_2	1.04 – 0.89 (s, 2H)	28.99
16	1.88 m	27.6	CH_2	1.64 – 1.39 (m, 2H)	27.61
23	1.21 s	24.3	CH_3	1.31 – 1.11 (m, 3H)	27.27
2	1.56 - 2.22 m	23.9	CH_2	2.15 – 2.01 (m, 2H)	26.71
$\underline{C}H_3CO$	2.07 s	21.7	CH_3	1.93 – 1.71 (m, 3H)	24.80
28	0.93 s	21.5	CH_3	1.04 – 0.89 (s, 3H)	21.25
27	1.33 s	20.9	CH_3	1.39 – 1.30 (m, 3H)	20.62
6	1.75 m	19.2	CH_2	1.64 – 1.39 (m, 2H)	20.03
26	1.17 s	18.8	CH_3	1.31 – 1.11 (m, 3H)	18.48
29	0.78 d(J=6.3)	17.8	CH_3	0.83 – 0.75 (m, 3H)	17.55
25	1.12 s	13.6	CH_3	1.31 – 1.11 (m, 3H)	13.90
NH	11.25	--	NH	8.86 (s, 1H)	

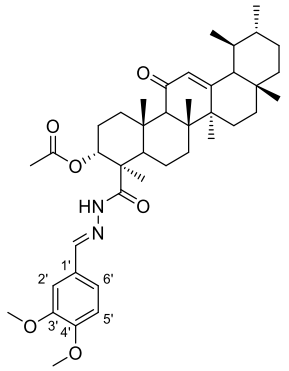
Table S15 NMR assignment of compound 16b



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ, ppm)
11	-	199.6	C	--	199.14
CHO/CH=N	10.2	189.37	CH	8.54 (s, 1H)	148.05
24	-	182.2	C	-	164.88
$CH_3\underline{C}O$	-	170.5	C	-	173.12
13	--	165.3	C	--	164.88
4’	--	154.61	CH	--	151.25
3’	--	149.73	CH	--	149.40
12	5.54 s	130.8	CH	5.48 (s, 1H)	130.35
1’	--	130.27		-	126.65
2’	7.41	110.62	CH	7.02 (dd, *J* = 8.3, 1.9 Hz, 1H)	110.46
6’	7.47	126.59	CH	7.38 (d, *J* = 1.9 Hz, 1H)	122.70

5’	6.99	109.29	CH	6.78 (d, *J* = 8.3 Hz, 1H)	108.26
3	5.28 t	73.6	CH	4.17 (s, 1H)	70.42
9	2.39 s	60.7	CH	2.50 – 2.36 (m, 1H)	60.45
18	1.37 d(J=12.3)	59.4	CH	1.33 – 1.28 (m, 1H)	59.01
OCH3	3.8	56.17	CH_3	3.86 (s, 3H)	56.10
OCH3	3.8	56.16	CH_3	3.83 (s, 3H)	55.93
5	1.38 dd, (J=12.2)	50.8	CH	0.97 – 0.85 (m, 1H)	48.91
4	-	46.7	C	-	47.40
14	-	45.3	C	-	45.05
8	-	43.9	C	-	43.84
22	1.29 -1.46 m	41.3	CH_2	1.26 – 1.17 (m, 2H)	40.90
19	1.52 m	39.7	CH	1.55 – 1.38 (m, 1H)	39.32
20	1.39 m	39.6	CH	1.33 – 1.28 (m, 1H)	39.27
10	-	37.6	C		37.57
1	2.53,dd,(J=13.2,2)	35.0	CH_2	2.50 – 2.36 (m, 2H)	34.23
17	-	34.2	C	--	33.9
15	1.66 m	33.2	CH_2	1.55 – 1.38 (m, 2H)	33.99
7	1.43 m	31.3	CH_2	1.33 – 1.28 (m, 2H)	33.22
30	0.80 d(J=7.4)	29.3	CH_3	0.77 – 0.69 (m, 3H)	30.91
21	1.01 dd(J=11.8, 3)	27.9	CH_2	0.97 – 0.85 (s, 2H)	28.88
16	1.88 m	27.6	CH_2	1.87 – 1.67 (m, 2H)	27.50
23	1.21 s	24.3	CH_3	1.20 – 1.10 (m, 3H)	27.17
2	1.56 -2.22 m	23.9	CH_2	2.09 – 1.96 (m, 2H)	26.59
$\underline{C}H_3CO$	2.07 s	21.7	CH_3	1.87 – 1.67 (m, 3H)	24.78
28	0.93 s	21.5	CH_3	0.97 – 0.85 (s, 3H)	21.15
27	1.33 s	20.9	CH_3	1.26 – 1.17 (m, 3H)	20.51
6	1.75 m	19.2	CH_2	1.55 – 1.38 (m, 2H)	19.93
26	1.17 s	18.8	CH_3	1.20 – 1.10 (m, 3H)	18.37
29	0.78 d(J=6.3)	17.8	CH_3	0.77 – 0.69 (m, 3H)	17.45
25	1.12 s	13.6	CH_3	1.20 – 1.10 (m, 3H)	13.82
NH	11.25	--	NH	8.86 (s, 1H)	

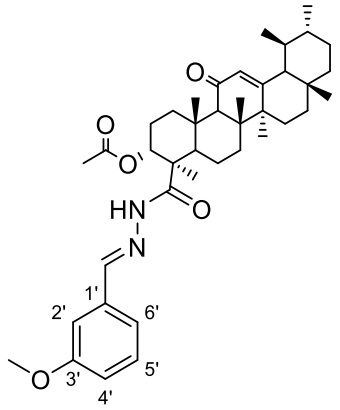
Table S16 NMR assignment of compound 16c



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ, ppm)
11	-	199.6	C	--	199.05
CHO/CH=N	10.2	190.95	CH	8.27 (s, 1H)	148.12
24	-	182.2	C	-	164.85
$CH_3\underline{C}O$	-	170.5	C	-	173.12
13	--	165.3	C	--	164.88
5’	--	153.72	CH	--	153.66
3’	--	153.72	CH	--	153.45
4’	--	143.72	CH	--	140.10
1’	--	131.84		-	130.54
12	5.54 s	130.8	CH	5.57 (s, 1H)	129.18
2’	7.13	106.81	CH	6.98 (s, 1H)	106.72
6’	7.13	106	CH	6.98 (s, 1H)	104.70
3	5.28 t	73.6	CH	4.25 (s, 1H)	70.47
OCH3	3.93	60.93	CH_3	3.97 – 3.87 (m, 3H)	60.98
9	2.39 s	60.7	CH	2.60 – 2.42 (m, 1H)	60.42
18	1.37 d(J=12.3)	59.4	CH	1.29 – 1.14(m, 1H)	59.02
OCH3	3.93	57.27	CH_3	3.97 – 3.87 (m, 3H)	58.50
OCH3	3.93	57.27	CH_3	3.97 – 3.87 (m, 3H)	56.31
5	1.38 dd,(J=12,2)	50.8	CH	1.41 – 1.29 (m, 1H)	48.87
4	-	46.7	C	-	47.47
14	-	45.3	C	-	45.04
8	-	43.9	C	-	43.84
22	1.29 -1.46 m	41.3	CH_2	1.41 – 1.29 (m, 2H)	40.90
19	1.52 m	39.7	CH	1.95 – 1.73 (m, 1H)	39.33
20	1.39 m	39.6	CH	1.41 – 1.29 (m, 1H)	39.27
10	-	37.6	C		37.57
1	2.53dd,(J=13.2,2)	35.0	CH_2	2.60 – 2.42 (m, 2H)	34.20
17	-	34.2	C	--	34.00

15	1.66 m	33.2	CH_2	1.41 – 1.29 (m, 2H)	34.00
7	1.43 m	31.3	CH_2	1.41 – 1.29 (m, 2H)	33.24
30	0.80 d(J=7.4)	29.3	CH_3	0.86 – 0.78 (m, 3H)	30.91
21	1.0 dd(J=11.8, 3)	27.9	CH_2	1.05 – 0.94 (s, 2H)	28.89
16	1.88 m	27.6	CH_2	1.95 – 1.73 (m, 2H)	27.50
23	1.21 s	24.3	CH_3	1.29 – 1.14 (m, 3H)	27.18
2	1.56 -2.22 m	23.9	CH_2	2.11 (tt, *J* = 9.9, 4.8 Hz, 2H)	26.57
CH_3CO	2.07 s	21.7	CH_3	1.95 – 1.73 (m, 3H)	24.77
28	0.93 s	21.5	CH_3	1.05 – 0.94 (s, 3H)	21.15
27	1.33 s	20.9	CH_3	1.41 – 1.29 (m, 3H)	20.51
6	1.75 m	19.2	CH_2	1.48 (dt, *J* = 13.7, 8.0 Hz, 2H)	19.99
26	1.17 s	18.8	CH_3	1.29 – 1.14 (m, 3H)	18.45
29	0.78 d(J=6.3)	17.8	CH_3	0.86 – 0.78 (m, 3H)	17.45
25	1.12 s	13.6	CH_3	1.29 – 1.14 (m, 3H)	13.82
NH	11.25	--	NH	8.60 (s, 1H)	

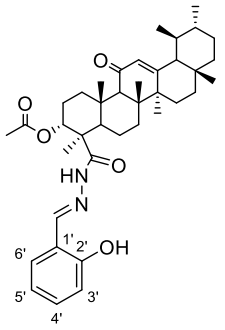
Table S17 NMR assignment of compound 16d



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ, ppm)
11	-	199.6	C	--	199.22
CHO/CH=N	10.2	190.95	CH	8.17 (s, 1H)	147.95
24	-	182.2	C	-	164.98
CH_3CO	-	170.5	C	-	173.40
13	--	165.3	C	--	164.98
3’	--	160.15	CH	--	159.99
1’	--	137.79	C	-	135.19
12	5.54 s	130.8	CH	5.48 (s, 1H)	130.64
5’	7.44	130.05	CH	7.29 – 7.21 (m, 1H)	129.75
6’	7.44	123.57	CH	7.29 – 7.21 (m, 1H)	121.12

4’	7.18	121.25	CH	6.87 (dd, *J* = 8.2, 2.6 Hz, 1H)	117.55
2’	7.37	112.05	CH	7.15 (d, *J* = 7.5 Hz, 1H)	111.02
3	5.28 t	73.6	CH	4.17 (s, 1H)	70.53
9	2.39 s	60.7	CH	2.50 – 2.35 (m, 1H)	60.55
18	1.37 d(J=12.3)	59.4	CH	1.34 – 1.21 (m, 1H)	59.13
OCH3	3.85	55.48	CH_3	3.76 (s, 3H)	55.58
5	1.38 dd(J=12,2)	50.8	CH	1.34 – 1.21 (m, 1H)	49.02
4	-	46.7	C	-	47.57
14	-	45.3	C	-	45.16
8	-	43.9	C	-	43.95
22	1.29 m 1.46 m	41.3	CH_2	1.34 – 1.21 (m, 1H) 1.20 – 1.15 (m, 1H)	41.01
19	1.52 m	39.7	CH	1.34 – 1.21 (m, 1H)	39.43
20	1.39 m	39.6	CH	1.34 – 1.21 (m, 1H)	39.38
10	-	37.6	C		37.68
1	2.53dd,(J=13.2,2)	35.0	CH_2	2.50 – 2.35 (m, 2H)	34.32
17	-	34.2	C	--	34.10
15	1.66 m	33.2	CH_2	1.57 – 1.35 (m, 2H)	34.00
7	1.43 m	31.3	CH_2	1.57 – 1.35 (m, 2H)	33.32
30	0.80 d(J=7.4)	29.3	CH_3	0.77 – 0.69 (m, 3H)	31.02
21	1.01dd(J=11.8, 3)	27.9	CH_2	0.98 – 0.85 (m, 2H)	28.99
16	1.88 m	27.6	CH_2	1.86 – 1.65 (m, 2H)	27.61
23	1.21 s	24.3	CH_3	1.15 – 1.08 (m, 9H)	27.28
2	1.56-,2.22 m	23.9	CH_2	2.50 – 2.35 (m, 1H) 2.08 – 1.95 (m, 1H)	26.68
$\underline{C}H_3CO$	2.07 s	21.7	CH_3	1.86 – 1.65 (m, 3H)	24.80
28	0.93 s	21.5	CH_3	0.98 – 0.85 (m, 3H)	21.26
27	1.33 s	20.9	CH_3	1.34 – 1.21 (m, 3H)	20.60
6	1.75 m	19.2	CH_2	1.57 – 1.35 (m, 2H)	20.05
26	1.17 s	18.8	CH_3	1.15 – 1.08 (m, 9H)	18.47
29	0.78 d(J=6.3)	17.8	CH_3	0.77 – 0.69 (m, 3H)	17.56
25	1.12 s	13.6	CH_3	1.15 – 1.08 (m, 9H)	17.56
NH	11.25	--	NH	8.59 (s, 1H)	

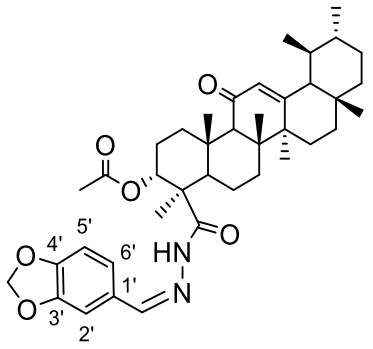
Table S18 NMR assignment of compound 16f



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^{1}H(δ,ppm)(J,Hz)	^{13}C(δ, ppm)
11	-	199.6	C	--	199.11
CHO/CH=N	10.2	196.5	CH	8.41 (s, 1H)	150.90
24	-	182.2	C	-	165.00
$CH_3\underline{C}O$	-	170.5	C	-	172.89
13	--	165.3	C	--	165.00
2’	--	162	CH		158.50
4’	6.69	136.68	CH	6.92 (dd, *J* = 8.5, 4.1 Hz, 1H)	131.84
6’	6.45	133.69	CH	6.82 (t, *J* = 7.4 Hz, 1H)	130.86
12	5.54 s	130.8	CH	5.49 (s, 1H)	130.50
1’	--	120.926	C	-	119.33
5’	6.7	119.43	CH	7.13 (d, *J* = 7.5 Hz, 1H)	117.49
3’	6.9	117.69	CH	7.23 (d, *J* = 7.6 Hz, 1H)	117.24
3	5.28 t	73.6	CH	4.14 (s, 1H)	70.32
9	2.39 s	60.7	CH	2.50 – 2.29 (m, 1H)	60.44
18	1.37 d(J=12.3)	59.4	CH	1.28 – 1.11 (m, 1H)	59.03
5	1.38 dd,(J=12,2)	50.8	CH	1.38 – 1.29 (m, 1H)	48.88
4	-	46.7	C	-	47.51
14	-	45.3	C	-	45.05
8	-	43.9	C	-	43.86
22	1.29-1.46 m	41.3	CH_2	1.38 – 1.29 (m, 2H)	40.90
19	1.52 m	39.7	CH	1.38 – 1.29 (m, 1H)	39.32
20	1.39 m	39.6	CH	1.38 – 1.29 (m, 1H)	39.27
10	-	37.6	C		37.54
1	2.53dd,(J=13.2,2)	35.0	CH_2	2.50 – 2.29 (m, 2H)	34.18
17	-	34.2	C	--	34.00
15	1.66 m	33.2	CH_2	1.59 – 1.38 (m, 2H)	34.00
7	1.43 m	31.3	CH_2	1.59 – 1.38 (m, 2H)	33.18
30	0.80 d (J=7.4)	29.3	CH_3	0.77 – 0.69 (m, 3H)	30.91
21	1.01dd(J=11.8, 3)	27.9	CH_2	0.98 – 0.85 (m, 2H)	28.9

16	1.88 m	27.6	CH_2	1.87 – 1.68 (m, 2H)	27.49
23	1.21 s	24.3	CH_3	1.28 – 1.11 (m, 3H)	27.18
2	1.56 -2.22 m	23.9	CH_2	2.03 (td, *J* = 13.5, 4.5 Hz, 2H)	26.55
$\underline{C}H_3CO$	2.07 s	21.7	CH_3	1.87 – 1.68 (m, 3H)	24.58
28	0.93 s	21.5	CH_3	0.98 – 0.85 (m, 3H)	21.15
27	1.33 s	20.9	CH_3	1.28 – 1.11 (m, 3H)	20.51
6	1.75 m	19.2	CH_2	1.59 – 1.38 (m, 2H)	19.94
26	1.17 s	18.8	CH_3	1.28 – 1.11 (m, 3H)	18.38
29	0.78 d(J=6.3)	17.8	CH_3	0.77 – 0.69 (m, 3H)	17.45
25	1.12 s	13.6	CH_3	1.08 (s, 3H)	13.76
NH	11.25	--	NH	8.56 (s, 1H)	
OH	9.1	--	--	--	--

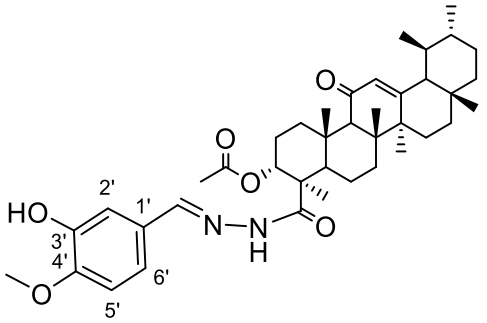
Table S19 NMR assignment of compound 16g



Parent compound			Hybrid compound		
Atom **C/H**	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^{1}H(δ,ppm)(J,Hz)	^{13}C(δ, ppm)
NH	11.25	--	NH	8.50 (s, 1H)	
CHO/CH=N	10.2	190	CH	8.09 (s, 1H)	147.62
6’	7.23	108.3	CH	7.32 (d, *J* = 1.6 Hz, 1H)	108.16
2’	7.2	106.9	CH	6.98 (dd, *J* = 8.0, 1.7 Hz, 1H)	106.16
5’	6.92	128.6	CH	6.72 (d, *J* = 8.0 Hz, 1H)	123.82
O-CH2-O	6.06	102.1	CH2	5.92 (s, 2H)	101.52
12	5.54 s	130.8	CH	5.48 (s, 1H)	128.25
3	5.28 t	73.6	CH	4.15 (d, *J* = 2.9 Hz, 1H)	70.42
1	2.53 dd,(J=13.2,2)	35.0	CH_2	2.49 – 2.32 (m, 2H)	34.23
9	2.39 s	60.7	CH	2.49 – 2.32 (m, 1H)	60.45
$\underline{C}H_3CO$	2.07 s	21.7	CH_3	1.86 – 1.68 (m, 3H)	24.72
16	1.88 m	27.6	CH_2	1.86 – 1.68 (m, 2H)	27.50
6	1.75 m	19.2	CH_2	1.57 – 1.37 (m, 2H)	19.91

15	1.66 m	33.2	CH_2	1.57 – 1.37 (m, 2H)	33.99
2	1.56-2.22 m	23.9	CH_2	2.09 – 1.96 (m, 1H) 1.86 – 1.68 (m, 1H)	26.58
19	1.52 m	39.7	CH	1.35 – 1.28 (m, 1H)	39.32
7	1.43 m	31.3	CH_2	1.57 – 1.37 (m, 2H)	33.21
20	1.39 m	39.6	CH	1.35 – 1.28 (m, 1H)	39.27
5	1.38 dd,(J=12,2)	50.8	CH	1.35 – 1.28 (m, 1H)	48.91
18	1.37 d(J=12.3)	59.4	CH	1.35 – 1.28 (m, 1H)	59.02
27	1.33 s	20.9	CH_3	1.27 – 1.15 (m, 3H)	20.51
22	1.29 -1.46 m	41.3	CH_2	1.35 – 1.28 (m, 1H) 0.99 – 0.90 (m, 1H)	40.91
23	1.21 s	24.3	CH_3	1.27 – 1.15 (m, 3H)	27.17
26	1.17 s	18.8	CH_3	1.14 – 1.09 (m, 3H)	18.36
25	1.12 s	13.6	CH_3	1.14 – 1.09 (m, 3H)	13.79
21	1.01dd(J=11.8, 3)	27.9	CH_2	0.90 – 0.85 (m, 2H)	28.88
28	0.93 s	21.5	CH_3	0.90 – 0.85 (m, 3H)	21.15
30	0.80 d(J=7.4)	29.3	CH_3	0.77 – 0.69 (m, 3H)	30.91
29	0.78 d(J=6.3)	17.8	CH_3	0.77 – 0.69 (m, 3H)	17.45
11	-	199.6	C	--	199.15
24	-	182.2	C	--	164.86
$CH_3\underline{C}O$	-	170.5	C	--	173.14
13	--	165.3	C	--	164.86
4’	--	153.1	C	--	149.75
3’	--	148.7	C	--	148.34
1’	--	131.9	C	-	130.54
4	-	46.7	C	-	47.40
14	-	45.3	C	-	45.05
8	-	43.9	C	-	43.84
10	-	37.6	C		37.56
17	-	34.2	C	--	33.99

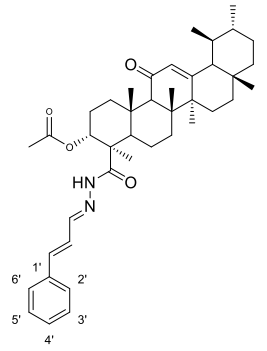
Table S20 NMR assignment of compound 16h



Atom **C/H**	Parent compound			Hybrid compound	
	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^{1}H(δ,ppm)(J,Hz)	^{13}C(δ, ppm)
NH	11.25	--	NH	8.87 (s, 1H)	
CHO/CH=N	10.2	196.5	CH	8.00 (s, 1H)	147.94
OH	9.1	--	--	--	--
2’	7.44	108.7	CH	7.28 (d, *J* = 2.0 Hz, 1H)	110.64
6’	7.41	127.5	CH	7.02 (dd, *J* = 8.4, 2.0 Hz, 1H)	`121.05
5’	6.9	114.3	CH	6.71 (d, *J* = 8.4 Hz, 1H)	112.94
12	5.54 s	130.8	CH	5.47 (s, 1H)	130.47
3	5.28 t	73.6	CH	4.19 (s, 1H)	70.25
OCH3	3.96	56.24	CH3	3.79 (s, 3H)	55.91
1	2.53dd,(J=13.2,2)	35.0	CH_2	2.49 – 2.29 (m, 2H)	34.25
9	2.39 s	60.7	CH	2.07 – 1.95 (m, 1H)	60.47
$\underline{C}H_3CO$	2.07 s	21.7	CH_3	2.49 – 2.29 (m, 3H)	24.65
16	1.88 m	27.6	CH_2	1.58 – 1.31 (m, 2H)	27.50
6	1.75 m	19.2	CH_2	1.58 – 1.31 (m, 2H)	19.79
15	1.66 m	33.2	CH_2	1.58 – 1.31 (m, 2H)	33.99
2	1.56 -2.22 m	23.9	CH_2	1.74 – 1.61 (m, 1H) 1.58 – 1.31 (m, 2H)	26.56
19	1.52 m	39.7	CH	1.31 – 1.27 (m, 1H)	39.30
7	1.43 m	31.3	CH_2	1.58 – 1.31 (m, 2H)	33.17
20	1.39 m	39.6	CH	1.31 – 1.27 (m, 1H)	39.27
5	1.38 dd,(J=12,2)	50.8	CH	1.31 – 1.27 (m, 1H)	49.03
18	1.37 d(J=12.3)	59.4	CH	1.31 – 1.27 (m, 1H)	59.03
27	1.33 s	20.9	CH_3	1.26 – 1.12 (m, 3H)	20.50
22	1.29 m 1.46 m	41.3	CH_2	1.26 – 1.12 (m, 1H) 1.12 – 1.07 (m, 1H)	40.91
23	1.21 s	24.3	CH_3	1.26 – 1.12 (m, 3H)	27.17
26	1.17 s	18.8	CH_3	1.12 – 1.07 (m, 3H)	18.35
25	1.12 s	13.6	CH_3	1.12 – 1.07 (m, 3H)	13.92
21	1.01dd(J=11.8, 3)	27.9	CH_2	0.89 – 0.85 (m, 2H)	28.88

28	0.93 s	21.5	CH_3	0.89 – 0.85 (m, 3H)	21.15
30	0.80 d(J=7.4)	29.3	CH_3	0.75 – 0.65 (m, 3H)	30.91
29	0.78 d(J=6.3)	17.8	CH_3	0.75 – 0.65 (m, 3H)	17.45
11	-	199.6	C	--	199.46
24	-	182.2	C	-	165.14
$CH_3\underline{C}O$	-	170.5	C	-	173.53
13	--	165.3	C	--	165.14
4’	--	151.6	CH	6.92 (dd, J = 8.5, 4.1 Hz, 1H)	149.14
3’	-	147.1	CH	7.23 (d, J = 7.6 Hz, 1H)	146.09
1’	--	129.8		-	127.00
4	-	46.7	C	-	47.44
14	-	45.3	C	-	45.08
8	-	43.9	C	-	43.84
10	-	37.6	C		37.54
17	-	34.2	C	--	33.99

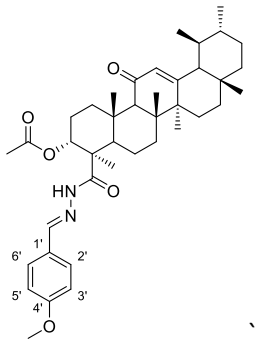
Table S21 NMR assignment of compound 16i



Atom **C/H**	Parent compound		Hybrid compound		
	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^{1}H(δ,ppm)(J,Hz)	^{13}C(δ, ppm)
11	-	199.6	C	--	199.46
CHO/CH=N	10.2	193.36	CH	7.96 (d, *J* = 8.8 Hz, 1H)	149.36
24	-	182.2	C	-	164.87
$CH_3\underline{C}O$	-	170.5	C	-	173.19
13	--	165.3	C	--	164.87
Ph-CH	7.48	152.46		6.99 (dd, *J* = 16.1, 8.7 Hz, 1H)	152.94
1’	--	134.12		-	135.68
CH=CH	6.6	131.17		6.84 (d, *J* = 15.9 Hz, 1H)	131.34
12	5.54 s	130.8	CH	5.49 (s, 1H)	130.54
5’	6.6	129.07	CH	7.29 (t, *J* = 7.0 Hz, 1H)	129.30
3’	6.6	129.07	CH	7.29 (t, *J* = 7.0 Hz, 2H)	129.15
4’	6.6	128.62	CH	7.28 – 7.20 (m, 1H)	128.92
2’	7.64-7.33	128.46	CH	7.47 – 7.34 (m, 1H)	128.54
6’	7.64-7.33	127.5	CH	7.47 – 7.34 (m, 1H)	127.23
3	5.28 t	73.6	CH	4.17 (s, 1H)	70.36
9	2.39 s	60.7	CH	2.50 – 2.32 (m, 1H)	60.45
18	1.37 d(J=12.3)	59.4	CH	1.20 – 1.05 (m, 1H)	59.02
5	1.38 dd,(J=12,2)	50.8	CH	1.34 – 1.20 (m, 1H)	48.89
4	-	46.7	C	-	47.34
14	-	45.3	C	-	45.04
8	-	43.9	C	-	43.84
22	1.29 -1.46 m	41.3	CH_2	1.34 – 1.20 (m, 2H)	40.91
19	1.52 m	39.7	CH	1.58 – 1.35 (m, 1H)	39.33
20	1.39 m	39.6	CH	1.34 – 1.20 (m, 1H)	39.28
10	-	37.6	C		37.55
1	2.53dd,(J=13.2,2)	35.0	CH_2	2.50 – 2.32 (m, 2H)	34.18
17	-	34.2	C	--	33.99
15	1.66 m	33.2	CH_2	1.58 – 1.35 (m, 2H)	33.99

7	1.43 m	31.3	CH_2	1.58 – 1.35 (m, 2H)	33.20
30	0.80 d(J=7.4)	29.3	CH_3	0.77 – 0.69 (m, 3H)	30.91
21	1.01dd(J=11.8, 3)	27.9	CH_2	0.90 – 0.85 (m, 2H)	28.88
16	1.88 m	27.6	CH_2	1.87 – 1.64 (m, 2H)	27.50
23	1.21 s	24.3	CH_3	1.34 – 1.20 (m, 3H)	27.17
2	1.56 -2.22 m	23.9	CH_2	2.50 – 2.32 (m, 1H) 1.87 – 1.64 (m, 1H)	26.58
$\underline{C}H_3CO$	2.07 s	21.7	CH_3	2.09 – 1.96 (m, 3H)	24.54
28	0.93 s	21.5	CH_3	0.90 – 0.85 (m, 3H)	21.15
27	1.33 s	20.9	CH_3	1.34 – 1.20 (m, 3H)	20.51
6	1.75 m	19.2	CH_2	1.87 – 1.64 (m, 2H)	19.90
26	1.17 s	18.8	CH_3	1.20 – 1.05 (m, 3H)	18.38
29	0.78 d(J=6.3)	17.8	CH_3	0.77 – 0.69 (m, 3H)	17.45
25	1.12 s	13.6	CH_3	1.20 – 1.05 (m, 3H)	13.72
NH	11.25	--	NH	8.69 (s, 1H)	
OH	9.1	--	--	--	--

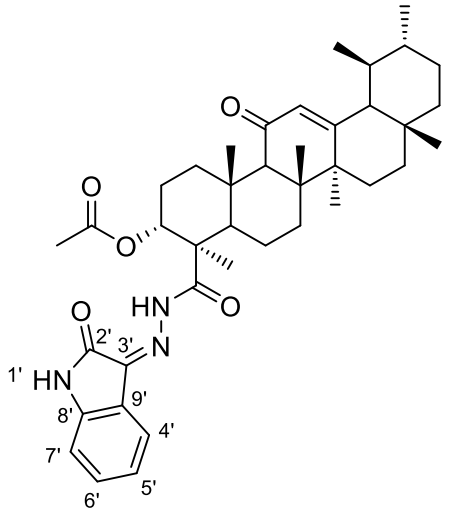
Table S22 NMR assignment of compound 16j



Atom **C/H**	Parent compound		Hybrid compound		
	^1H(δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^1H(δ,ppm)(J,Hz)	^{13}C (δ,ppm)
NH	11.25	--	NH	8.47 (s, 1H)	--
CHO/CH=N	10.2	190.7	CH	8.11 (s, 1H)	147.75

2’	7.8	131.93	CH	7.61 (d, J = 8.3 Hz, 1H)	132.04
6’	7.8	131.93	CH	7.61 (d, J = 8.3 Hz, 1H)	130.56
5’	6.98	114.33	CH	6.83 (d, J = 8.3 Hz, 1H)	114.34
3’	6.98	114.33	CH	6.83 (d, J = 8.3 Hz, 1H)	114.17
12	5.54 s	130.8	CH	5.48 (s, 1H)	129.28
3	5.28 t	73.6	CH	4.17 (s, 1H)	70.48
OCH3	3.85	56	CH_3	3.76 (s, 3H)	55.39
1	2.53dd,(J=13.2,2)	35.0	CH_2	2.51 – 2.34 (m, 2H)	34.23
9	2.39 s	60.7	CH	2.51 – 2.34 (m, 1H)	60.45
$\underline{C}H_3CO$	2.07 s	21.7	CH_3	1.88 – 1.69 (m, 3H)	24.75
16	1.88 m	27.6	CH_2	2.02 (ddd, J = 16.9, 11.0, 4.2 Hz, 2H)	27.51
6	1.75 m	19.2	CH_2	1.88 – 1.69 (m, 2H)	19.94
15	1.66 m	33.2	CH_2	1.56 – 1.42 (m, 2H)	33.99
2	1.56-2.22 m	23.9	CH_2	1.88 – 1.69 (m, 1H) 1.56 – 1.42 (m, 1H)	26.59
19	1.52 m	39.7	CH	1.32 – 1.28 (m, 1H)	39.3
7	1.43 m	31.3	CH_2	1.56 – 1.42 (m, 2H)	33.22
20	1.39 m	39.6	CH	1.32 – 1.28 (m, 1H)	39.28
5	1.38 dd,(J=12,2)	50.8	CH	1.32 – 1.28 (m, 1H)	48.91
18	1.37 d(J=12.3)	59.4	CH	1.32 – 1.28 (m, 1H)	59.02
27	1.33 s	20.9	CH_3	1.28 – 1.24 (m, 3H)	20.52
22	1.29 -1.46 m	41.3	CH_2	1.28 – 1.24 (m, 1H) 0.98 – 0.92 (m, 1H)	40.91
23	1.21 s	24.3	CH_3	1.24 – 1.15 (m, 3H)	27.18
26	1.17 s	18.8	CH_3	1.14 – 1.09 (m, 3H)	18.37
25	1.12 s	13.6	CH_3	1.14 – 1.09 (m, 3H)	13.78
21	1.01dd(J=11.8, 3)	27.9	CH_2	0.90 – 0.83 (m, 2H)	28.89
28	0.93 s	21.5	CH_3	0.90 – 0.83 (m, 3H)	21.15
30	0.80 d(J=7.4)	29.3	CH_3	0.77 – 0.69 (m, 3H)	30.92
29	0.78 d(J=6.3)	17.8	CH_3	0.77 – 0.69 (m, 3H)	17.45
11	-	199.6	C	--	199.13
24	-	182.2	C	-	164.82
$CH_3\underline{C}O$	-	170.5	C	-	173.33
13	-	165.3	C	-	164.79
4’	--	164.6	CH	7.33 – 7.27 (m, 1H)	161.50
1’	--	129.97	C	--	126.27
4	-	46.7	C	-	47.35
14	-	45.3	C	-	45.05
8	-	43.9	C	-	43.84
10	-	37.6	C	-	37.58
17	-	34.2	C	-	33.99

Table S23 NMR assignment of compound 18



Atom **C/H**	Parent compound		Hybrid compound		
	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ,ppm)	DEPT	^{1}H(δ,ppm)(J,Hz)	^{13}C (δ,ppm)
11	-	199.6	C	--	199.28
C=O/C=N	--	184.3	C	--	140.31
24	-	182.2	C	--	164.96
$CH_3\underline{C}O$	-	170.5	C	--	174.58
13	-	165.3	C	--	164.96
2’	--	159.26	C	--	162.56
8’	--	150.64	C	--	131.41
12	5.54 s	130.8	CH	5.57 (s, 1H)	130.54
4’	7.50	124.59	CH	7.35 (t, *J* = 7.7 Hz, 1H)	123.63
5’	7.07	122.68	CH	7.13 (t, *J* = 7.6 Hz, 1H)	122.29
6’	7.58	117.73	CH	7.82 (d, *J* = 7.6 Hz, 1H)	120.57
9’	--	117.73	C		120.57
7’	6.9	112.12	CH	6.91 (d, *J* = 7.8 Hz, 1H)	110.61
3	5.28 t	73.6	CH	4.29 (s, 1H)	70.51
9	2.39 s	60.7	CH	2.62 – 2.46 (m, 1H)	60.47
18	1.37 d(J=12.3)	59.4	CH	1.70 – 1.53 (m, 1H)	59.03
5	1.38 dd,(J=12,2)	50.8	CH	1.70 – 1.53 (m, 1H)	48.86
4	-	46.7	C	-	48.18
14	-	45.3	C	-	45.06
8	-	43.9	C	-	43.83
22	1.29 m 1.46 m	41.3	CH_2	1.37 – 1.24 (m, 1H) 1.51 – 1.36 (m, 1H)	 40.93
19	1.52 m	39.7	CH	1.70 – 1.53 (m, 1H)	39.29
20	1.39 m	39.6	CH	1.70 – 1.53 (m, 1H)	39.29
10	-	37.6	C	-	37.59
1	2.53dd,(J=13.2,2)	35.0	CH_2	2.62 – 2.46 (m, 2H)	34.11

17	-	34.2	C	-	33.99
15	1.66 m	33.2	CH_2	1.70 – 1.53 (m, 2H)	33.99
7	1.43 m	31.3	CH_2	1.70 – 1.53 (m, 2H)	30.92
30	0.80 d(J=7.4)	29.3	CH_3	0.90 – 0.77 (m, 3H)	30.92
21	1.01dd(J=11.8, 3)	27.9	CH_2	1.07 – 0.94 (m, 2H)	28.87
16	1.88 m	27.6	CH_2	1.99 – 1.74 (m, 2H)	27.53
23	1.21 s	24.3	CH_3	1.37 – 1.24 (m, 3H)	27.13
2	1.56-2.22 m	23.9	CH_2	2.11 (td, *J* = 13.7, 4.8 Hz, 1H)1.70 – 1.53 (m, 1H)	26.58
$\underline{C}H_3CO$	2.07 s	21.7	CH_3	1.70 – 1.53 (m, 3H)	24.56
28	0.93 s	21.5	CH_3	1.07 – 0.94 (m, 3H)	21.15
27	1.33 s	20.9	CH_3	1.51 – 1.36 (m, 3H)	20.53
6	1.75 m	19.2	CH_2	1.70 – 1.53 (m, 2H)	19.43
26	1.17 s	18.8	CH_3	1.25 – 1.14 (m, 3H)	18.27
29	0.78 d(J=6.3)	17.8	CH_3	0.90 – 0.77 (m, 3H)	17.46
25	1.12 s	13.6	CH_3	1.25 – 1.14 (m, 3H)	13.79
NH ISATIN	11.023	--	--	13.15 (s, 1H)	
NH-HYDRAZIDE	11		--	7.80 (s, 1H)	

Table S24. Gene distribution and correlation to KEGG enrichment and different biological process (BP), molecular functions(MF)

ID	Gene symbol	number of related KEGG	Numbers related BP	Numbers related MF
19	PIK3R1	46/56	61/445	24/103
1	GRB2	36/56	28/445	17/103
5	EGFR	35/56	70/445	22/103
16	MET	17/56	56/445	7/103
24	STAT1	12/56	46/445	14/103
13	CYP2C9	8/56	30/445	14/103
9	GSTM1	7/56	22/445	2/103
17	CYP2C8	7/56	25/445	15/103
15	HMOX1	6/56	93/445	9/103
20	CCL5	6/56	68/445	18/103
18	EPHA2	5/56	79/445	9/103
10	CCNA2	3/56	22/445	2/103
2	RARB	2/56	7/445	2/103
21	HSD11B1	2/56	1/445	1/103
26	AR	2/56	57/445	11/103
3	TPH1	1/56	14/445	4/103
22	ALAD	1/56	35/445	0/103
4	SERPINA1	0/56	3/445	0/103
6	NR1H4	0/56	71/445	12/103
7	PARP1	0/56	81/445	7/103
8	HPRT1	0/56	29/445	1/103
11	ALB	0/56	7/445	6/103
12	SEC14L2	0/56	13/445	2/103
14	GPI	0/56	41/445	3/103
23	NR3C1	0/56	33/445	7/103
25	LGALS3	0/56	50/445	8/103

TableS25. Primer design and sequence for qPCR analysis

Gene	Primer sequence	Description
TNF-α	5’TGGAACTGGCAGAAGAGGCACT 3’	Forward
	5’AGAGGCTGAGACATAGGCACCG 3’	Reverse
GAPDH	5’-ACTCCACTCACGGCAAATTC-3’	Forward
	R- 5’-GTCATGAGCCCTTCCACAAT-3’	Reverse

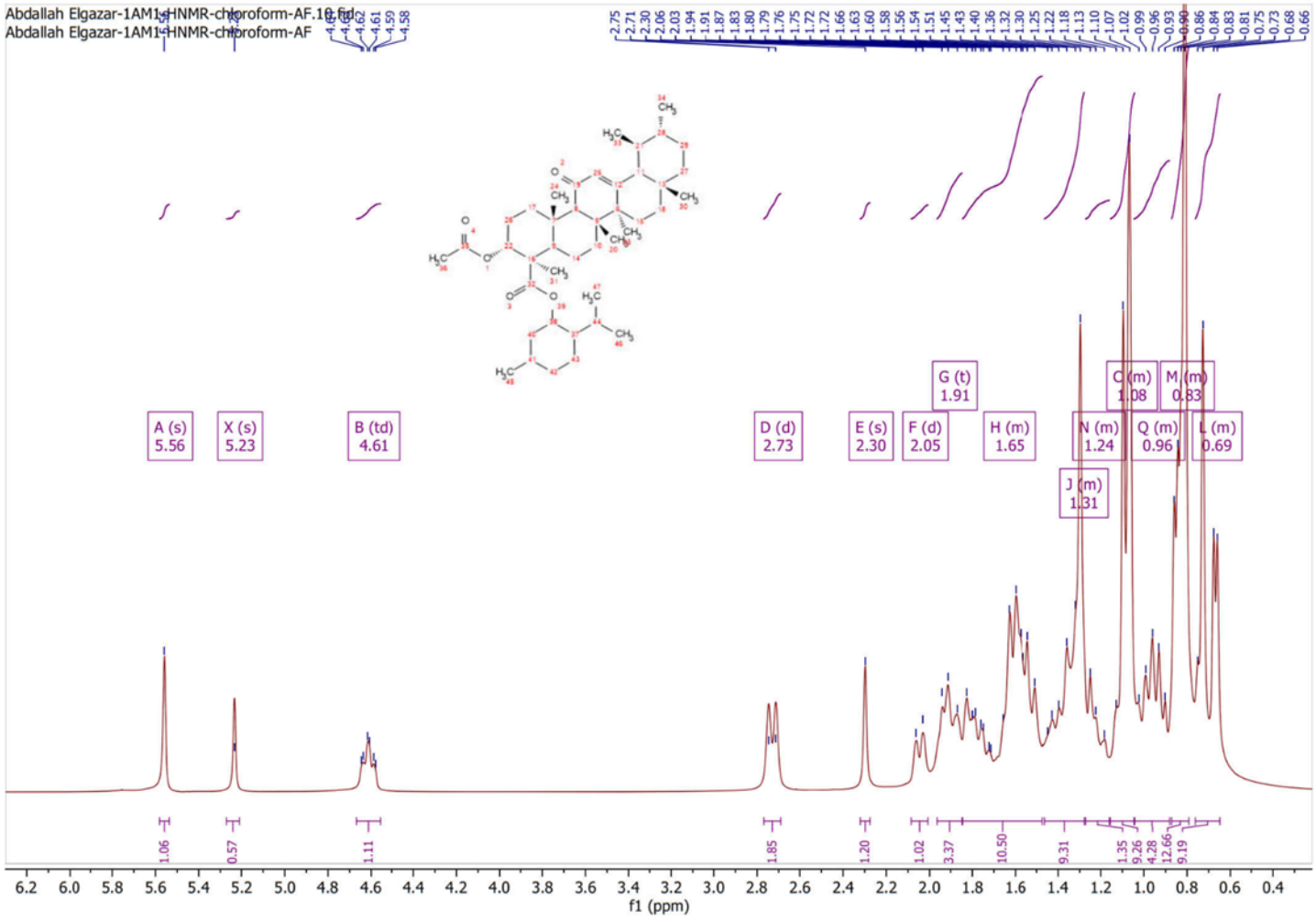


Figure S1. ^{1}H N.M.R spectrum of compound 3a

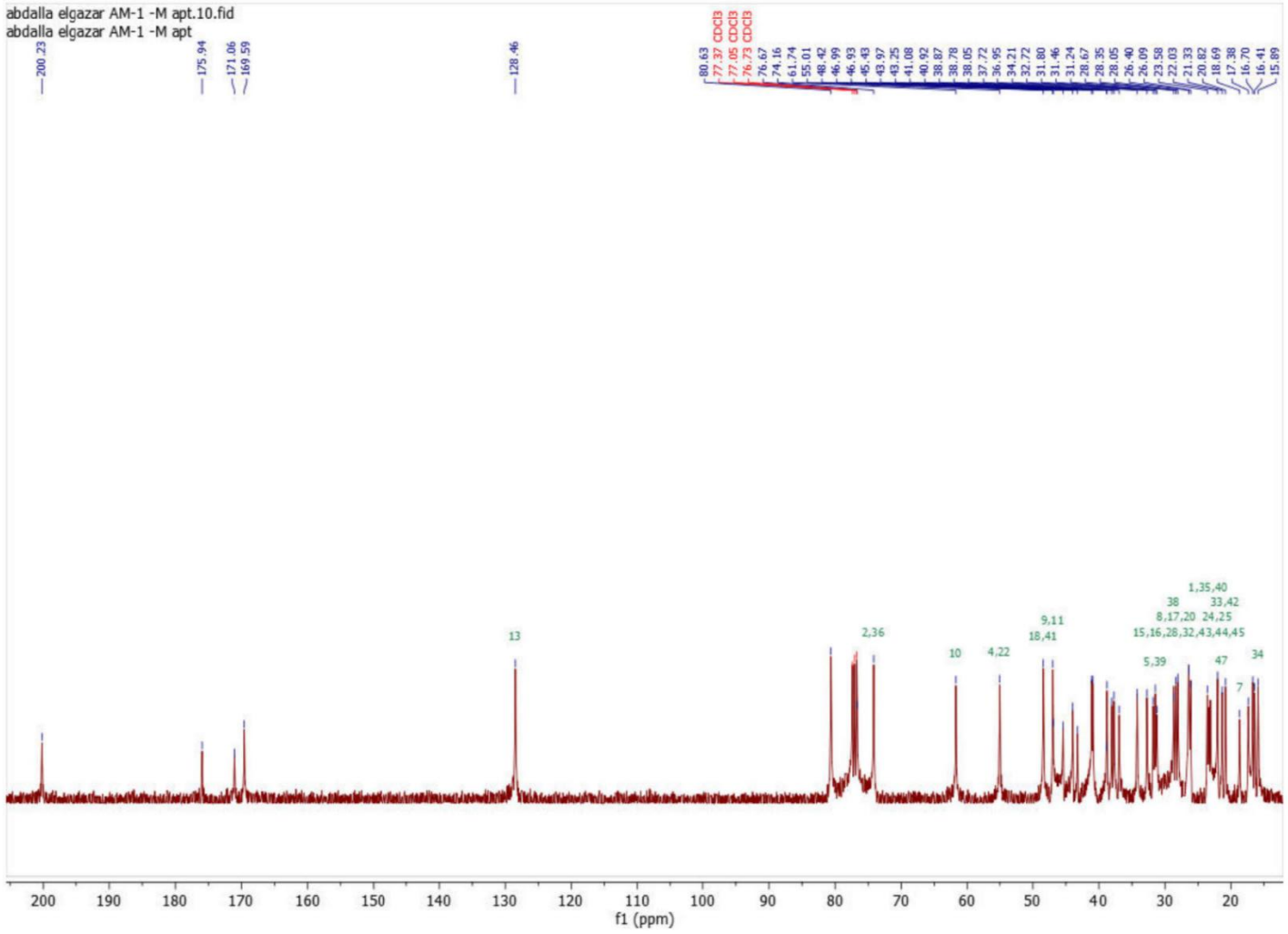


Figure S2. ^{13}C N.M.R spectrum of compound 3a

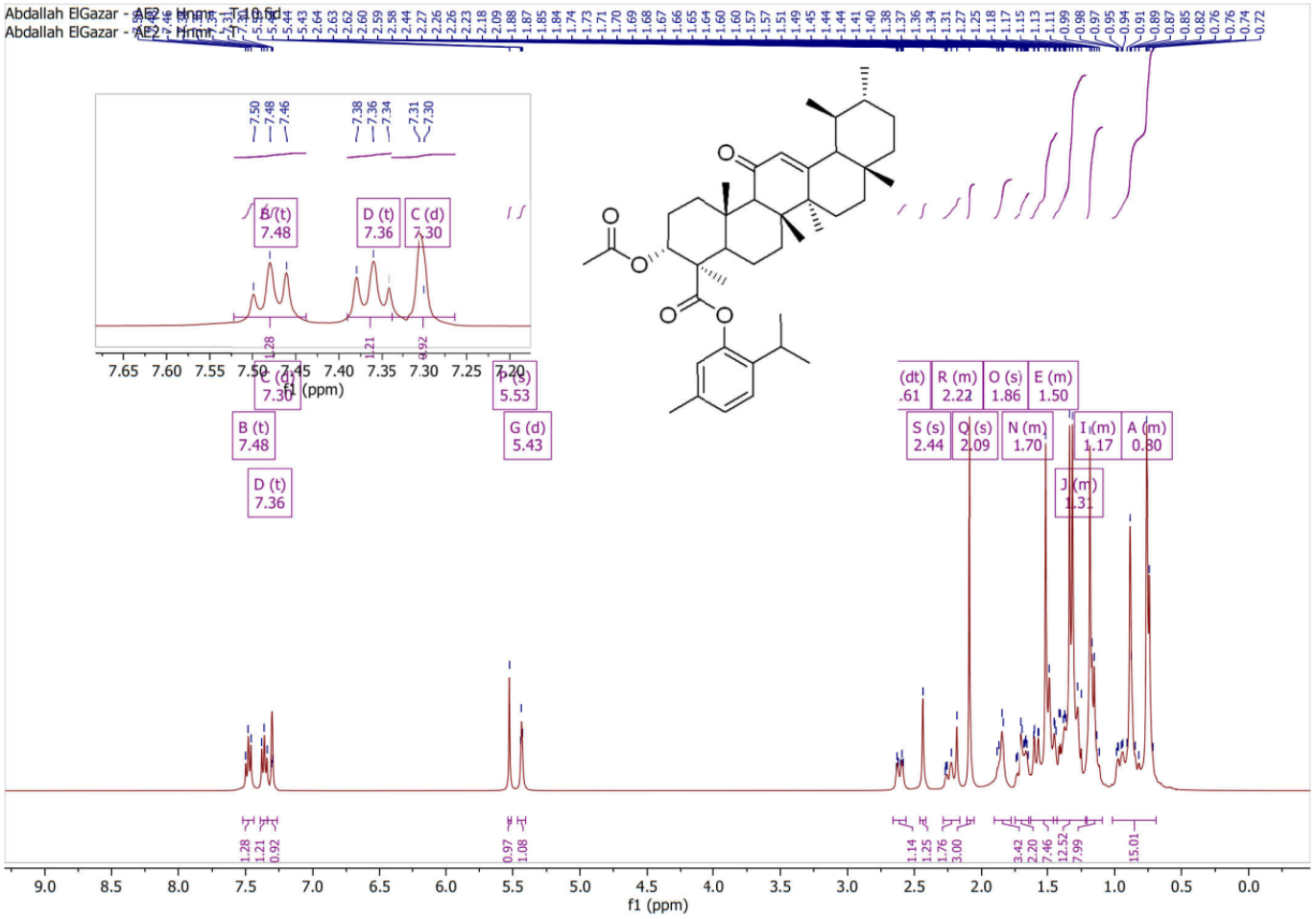


Figure S3 ^{1}H N.M.R spectrum of compound 3b

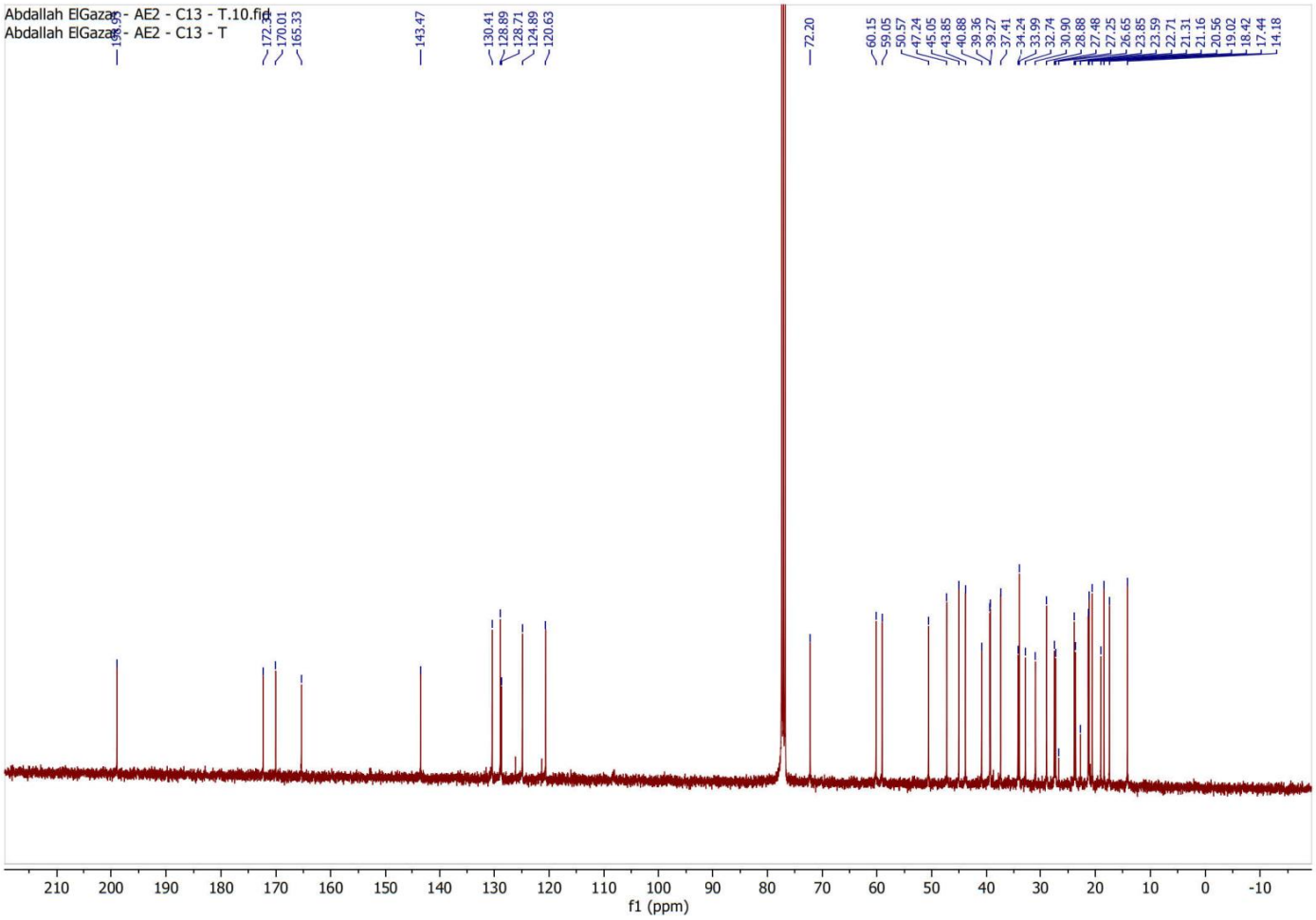


Figure S4. ^{13}C N.M.R spectrum of compound 3b

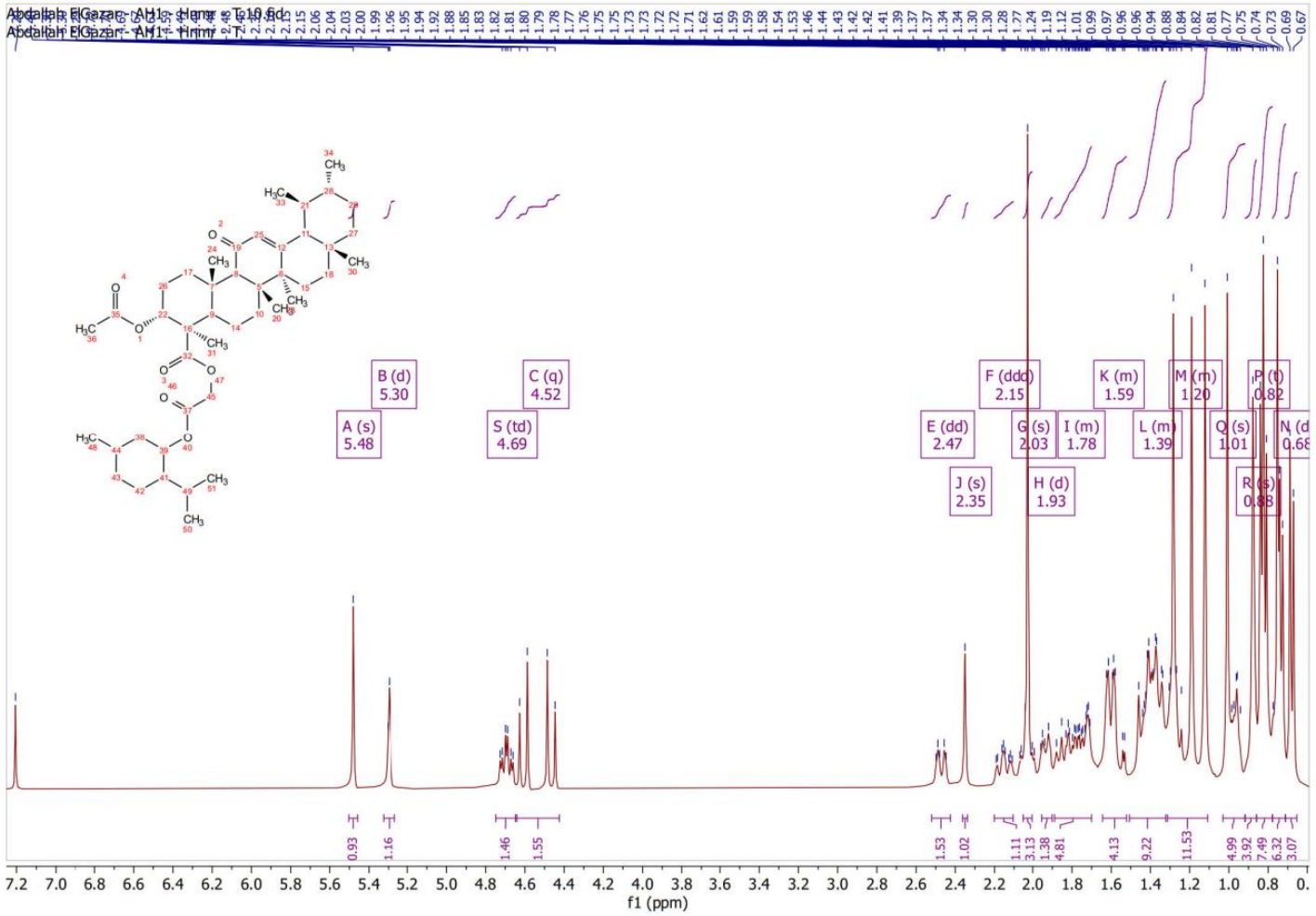


Figure S5 ^{1}H N.M.R spectrum of compound 5a

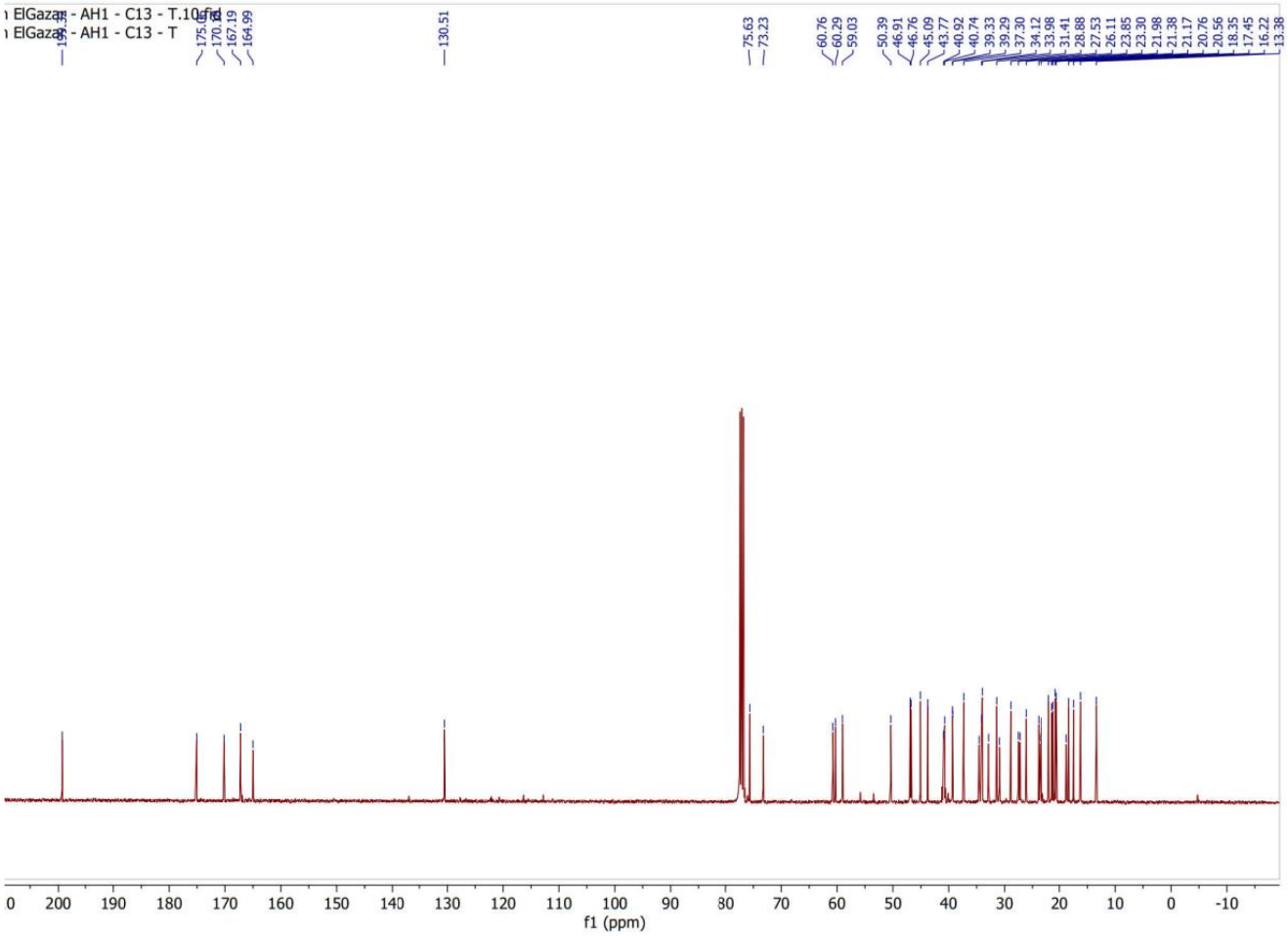


Figure S6. ^{13}C N.M.R spectrum of compound 5a

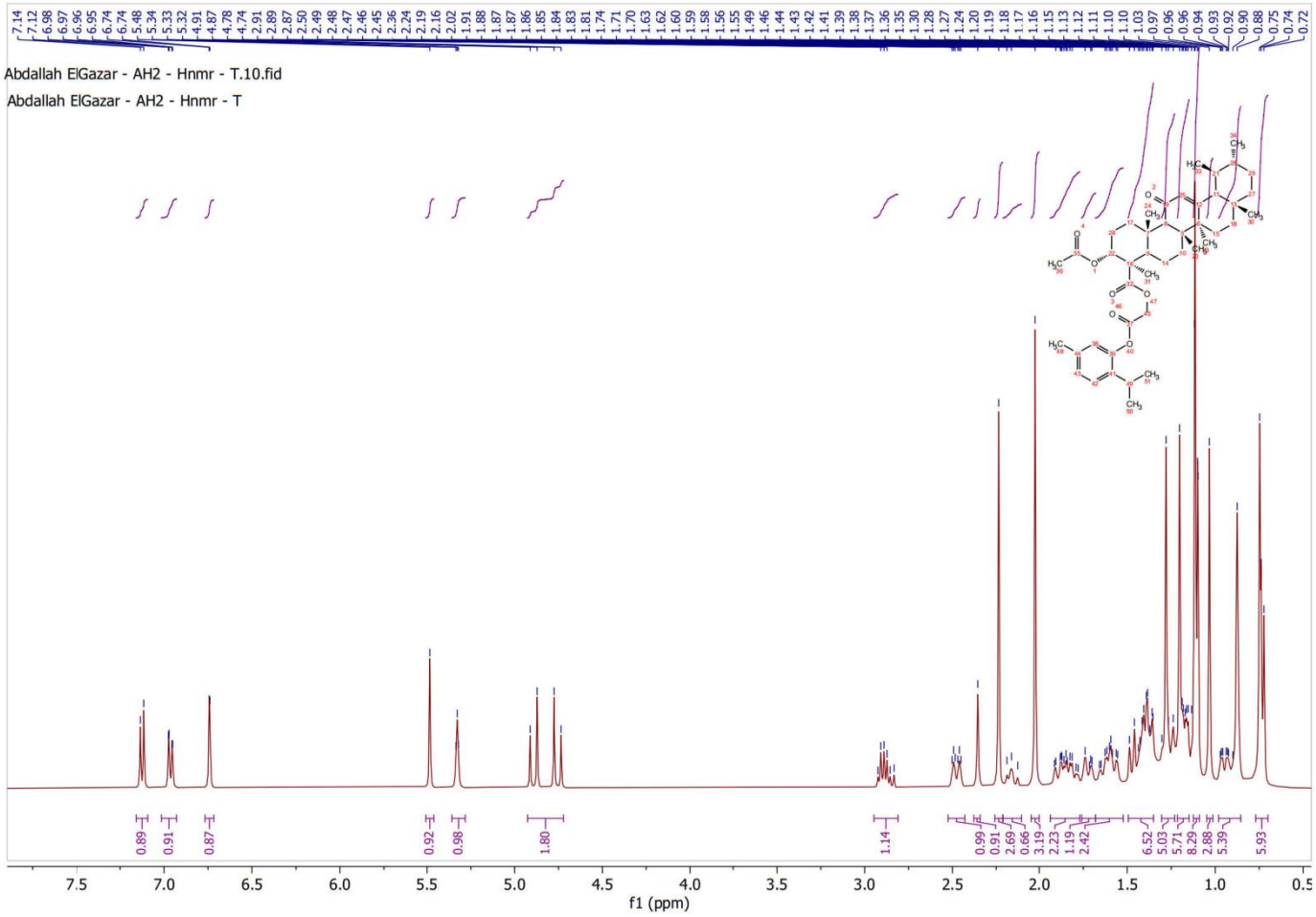


Figure S7. ^{1}H N.M.R spectrum of compound 5b

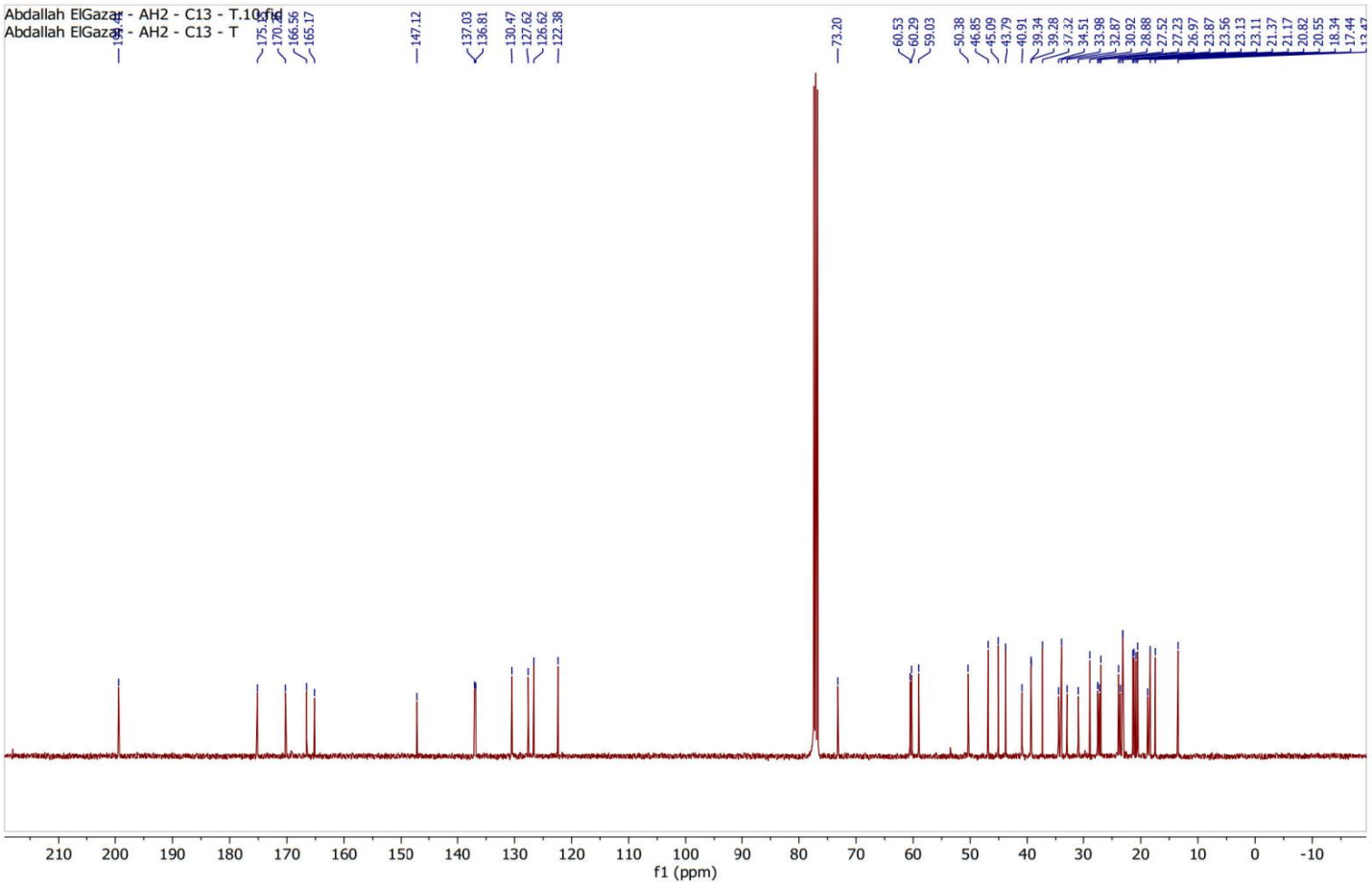


Figure S8. ^{13}C N.M.R spectrum of compound 5b

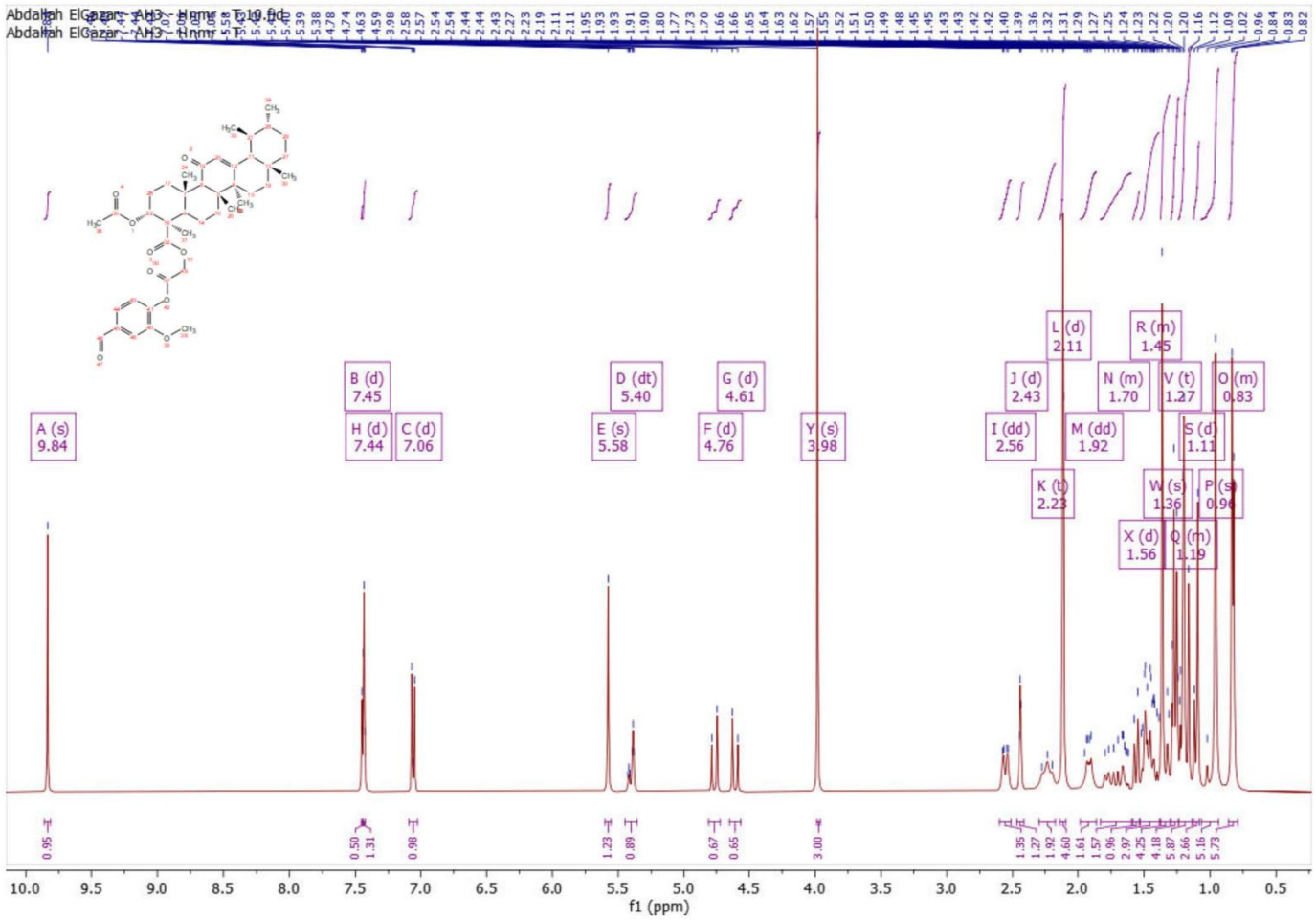


Figure S9. ^{1}H N.M.R spectrum of compound 5c

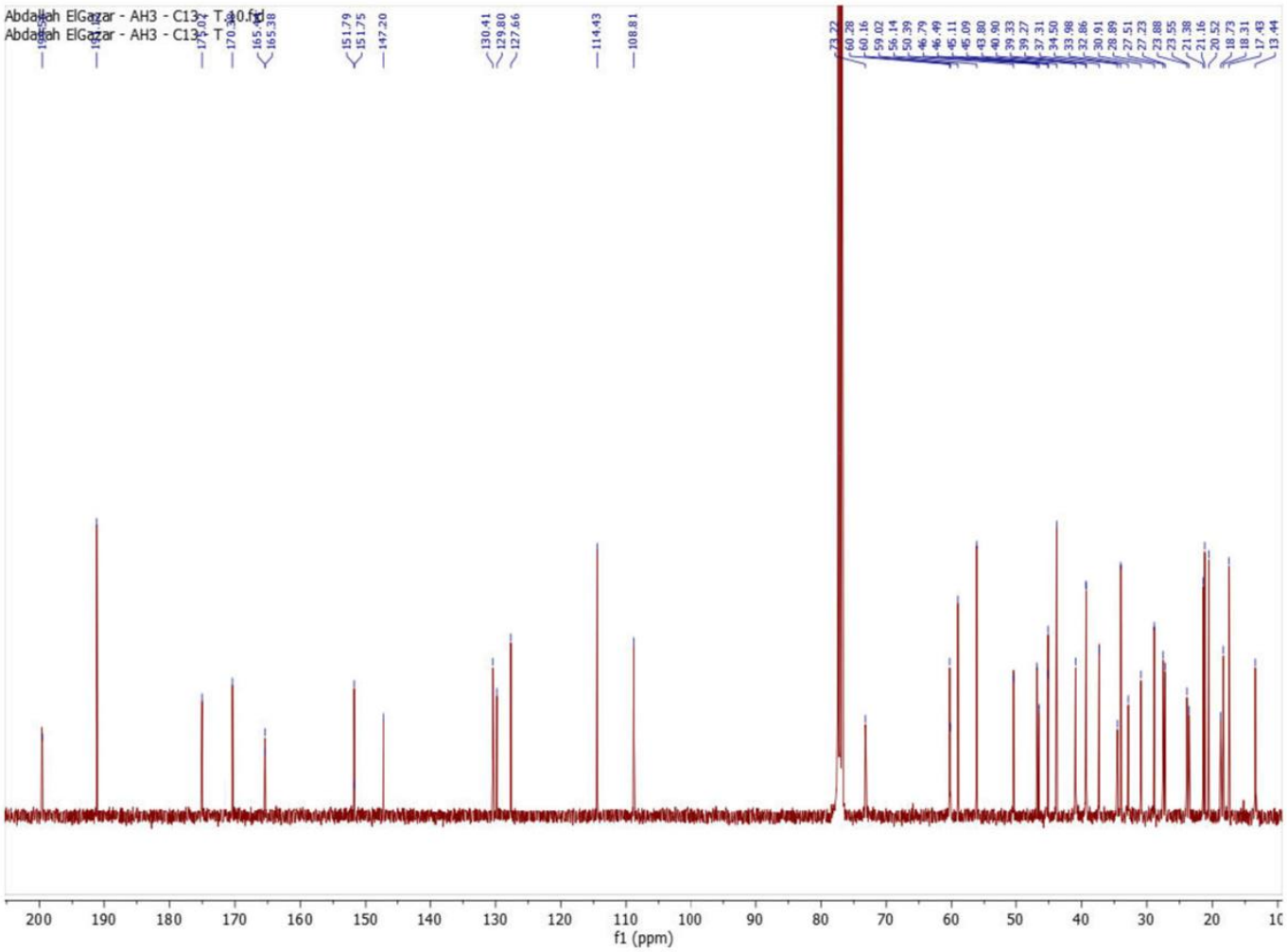


Figure S10. ^{13}C N.M.R spectrum of compound 5c

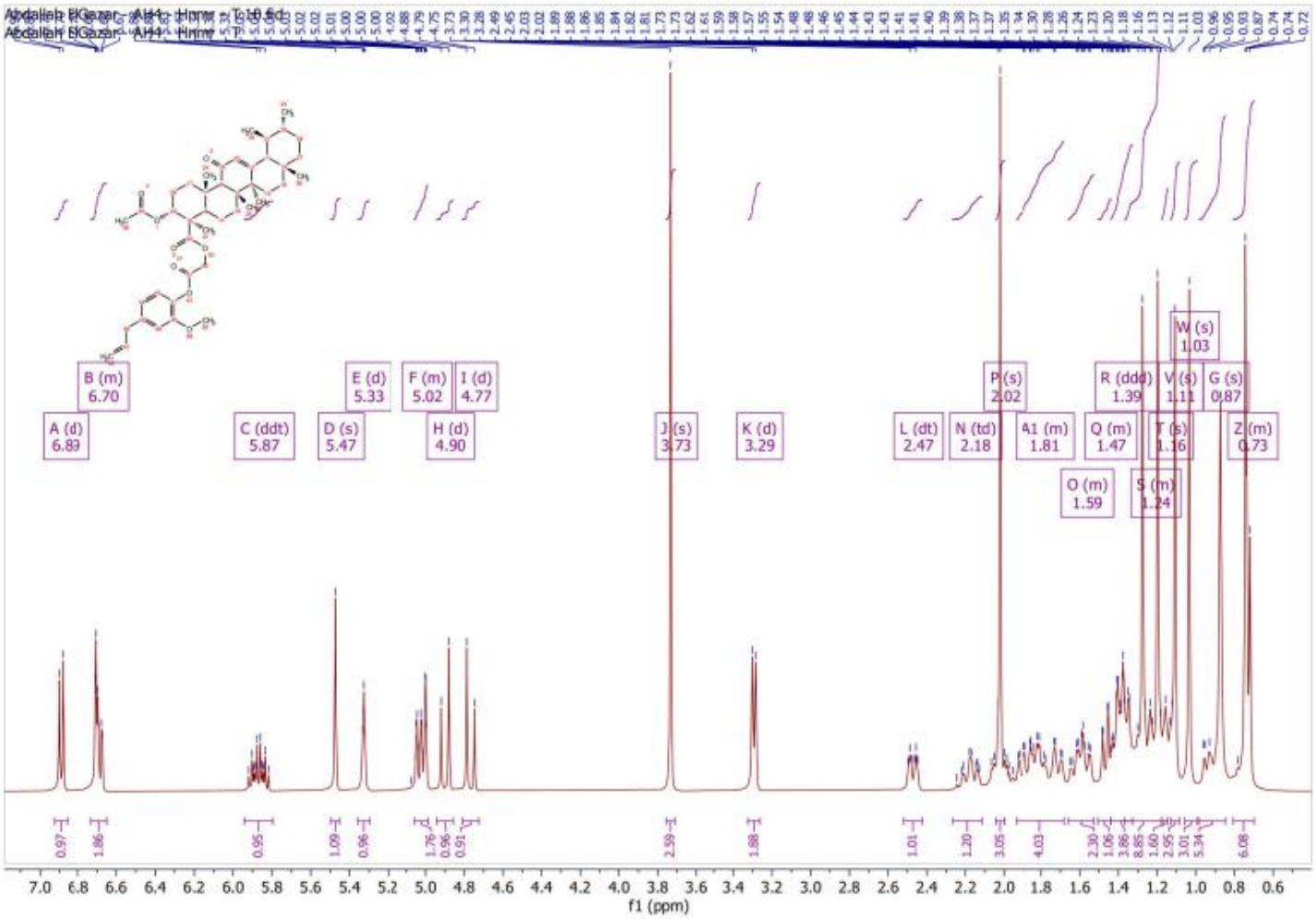


Figure S11. ^{1}H N.M.R spectrum of compound 5d

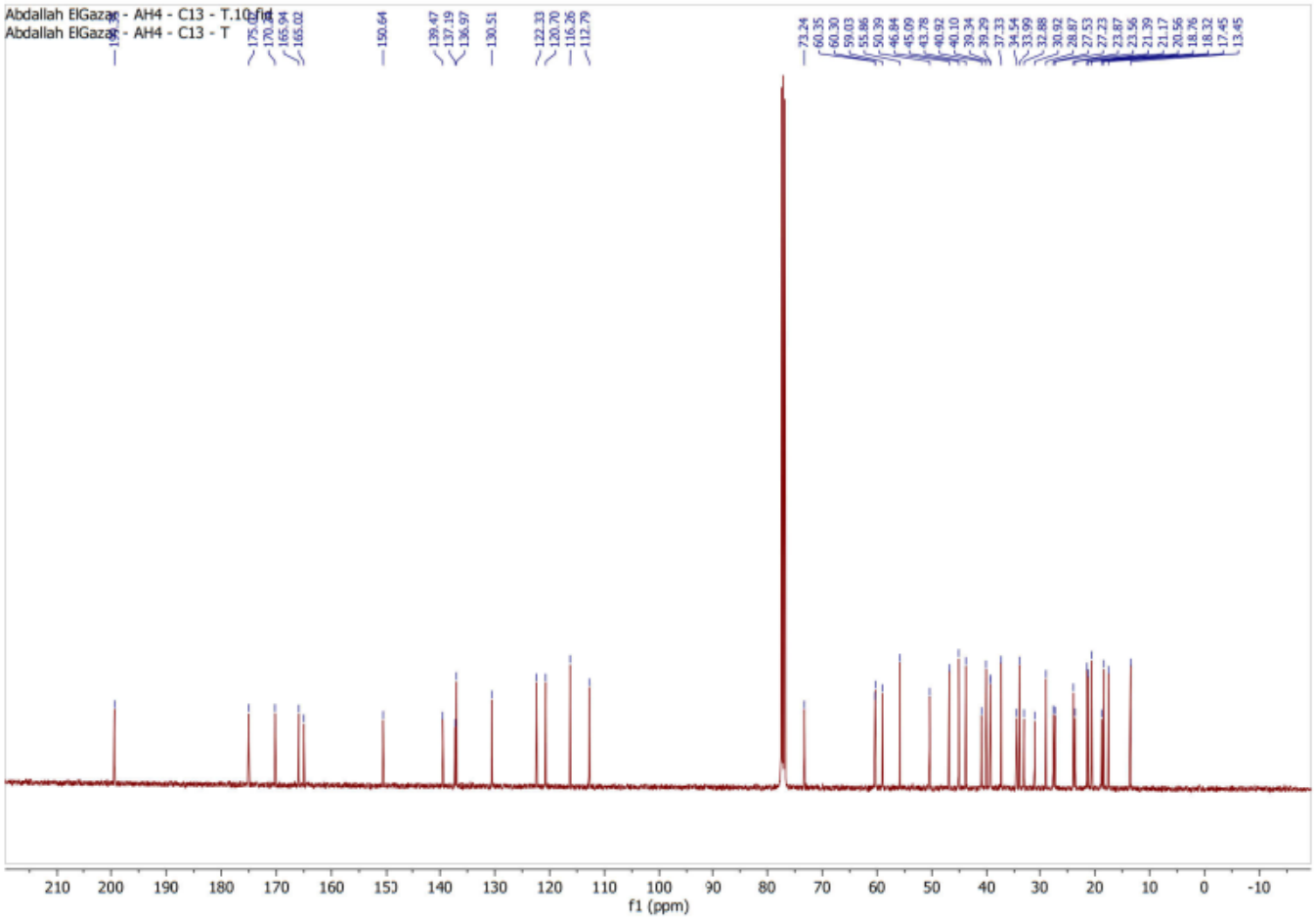


Figure S12. ^{13}C N.M.R spectrum of compound 5d

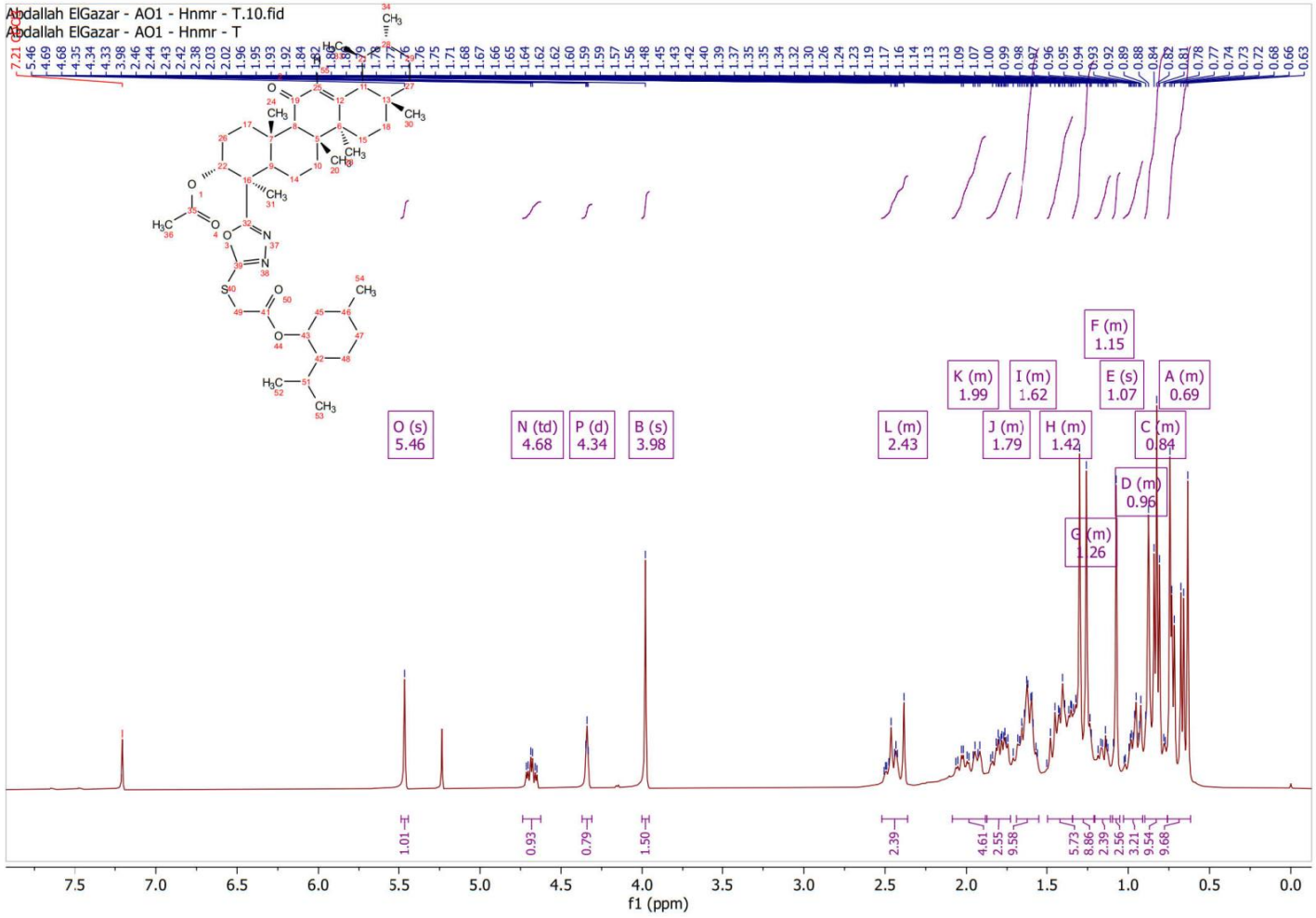


Figure S13. ^{1}H N.M.R spectrum of compound 8a

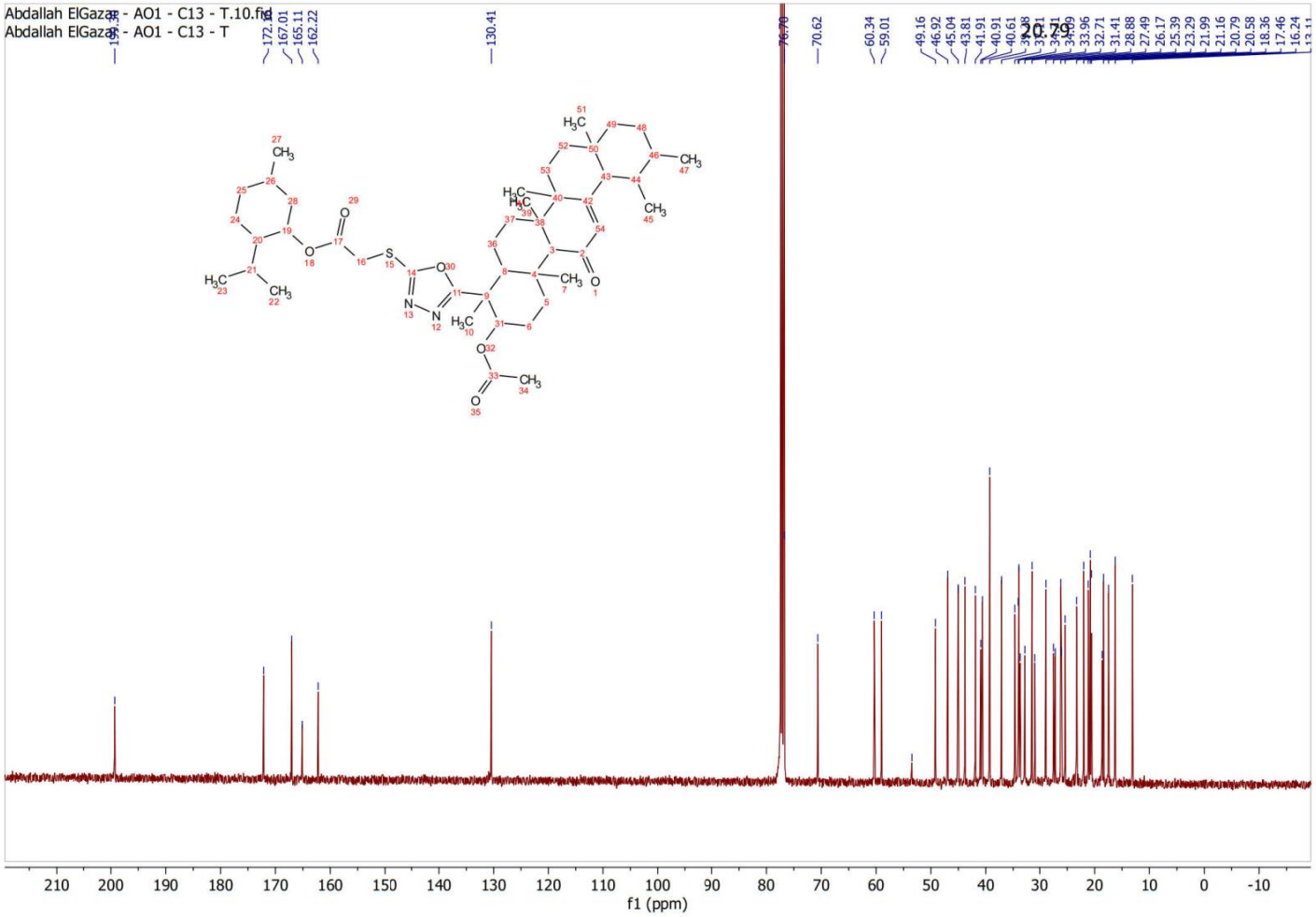


Figure S14. ^{13}c N.M.R spectrum of compound 8a

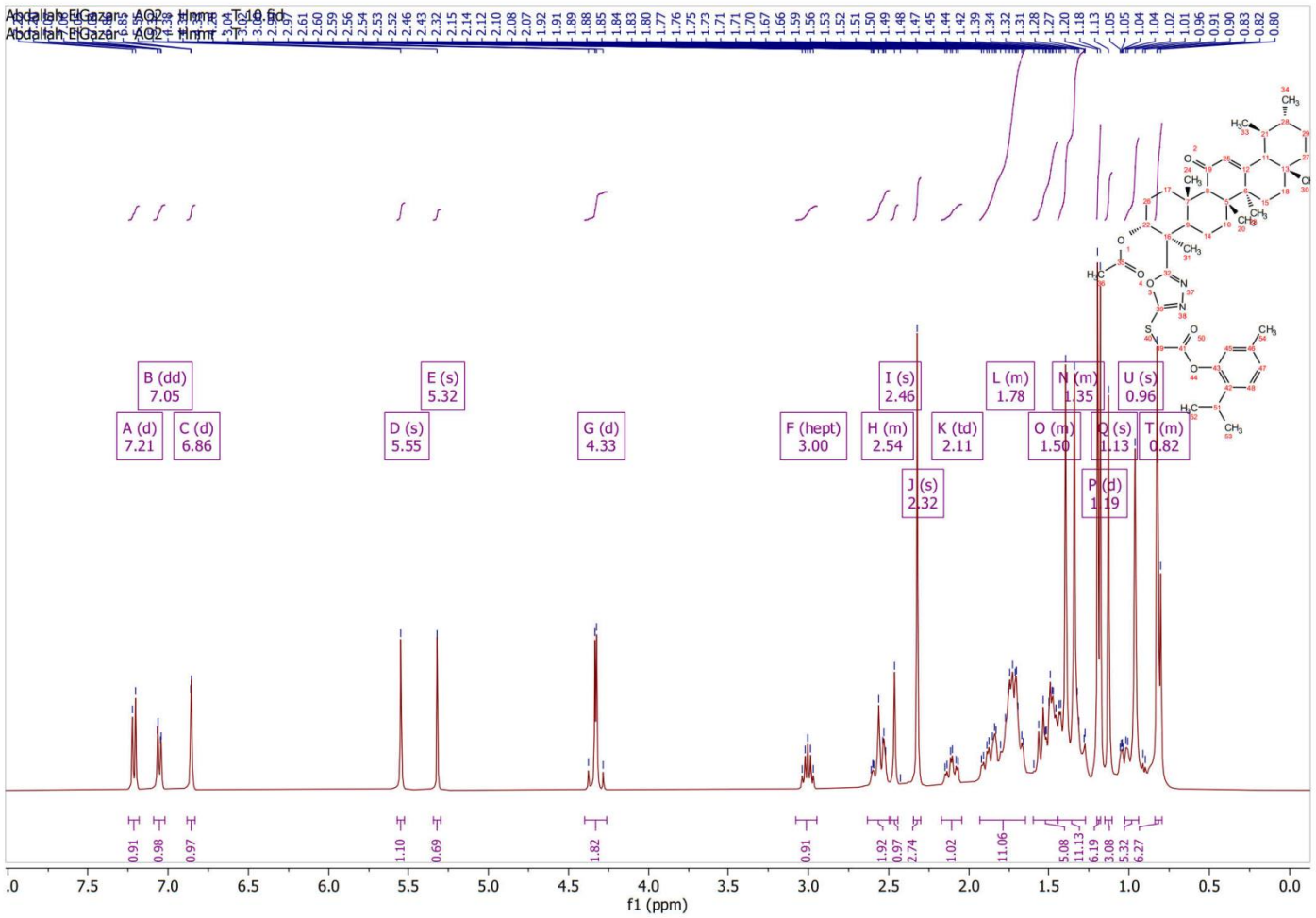


Figure S15. ^{1}H N.M.R spectrum of compound 8b

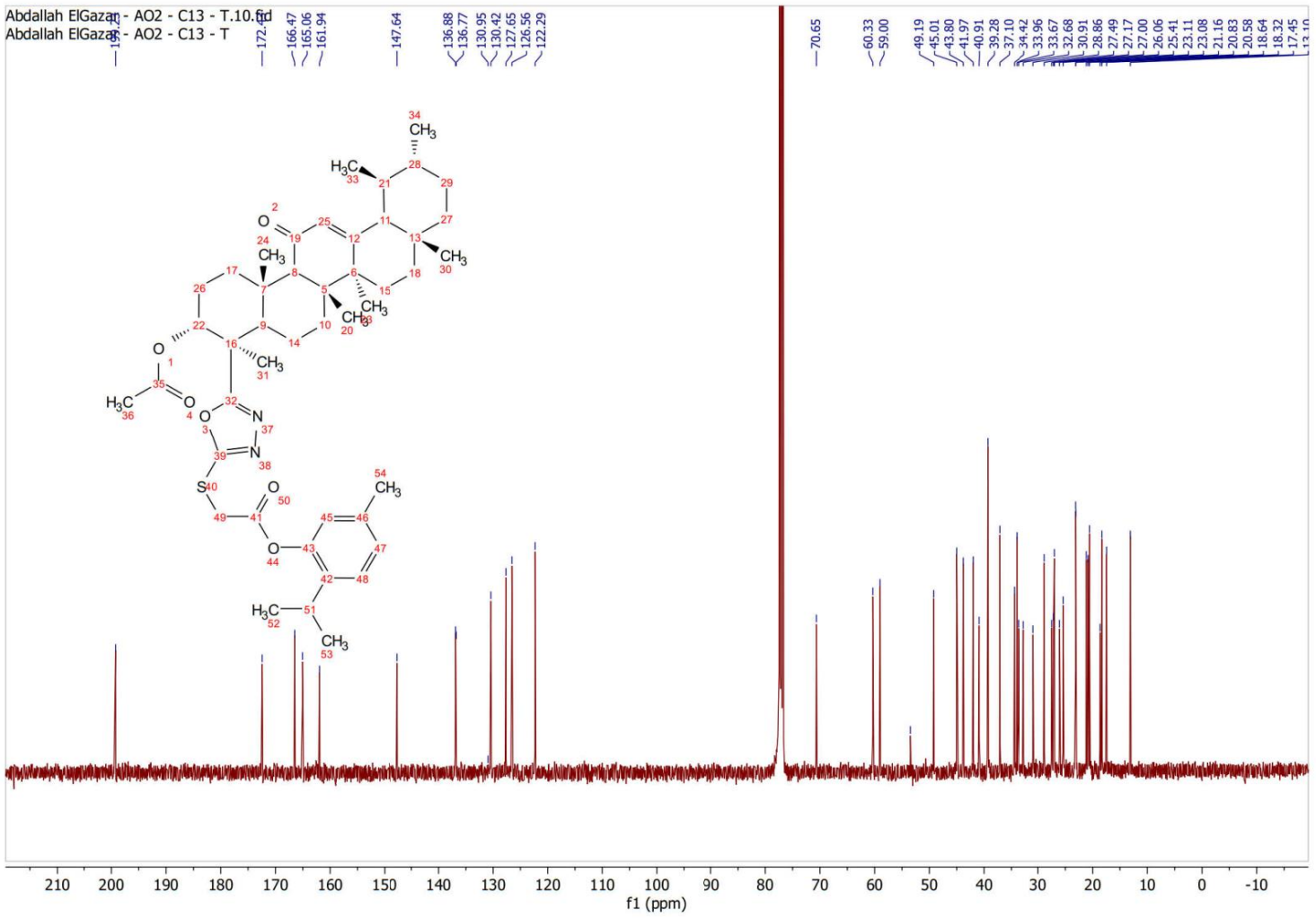


Figure S16. ^{13}c N.M.R spectrum of compound 8b

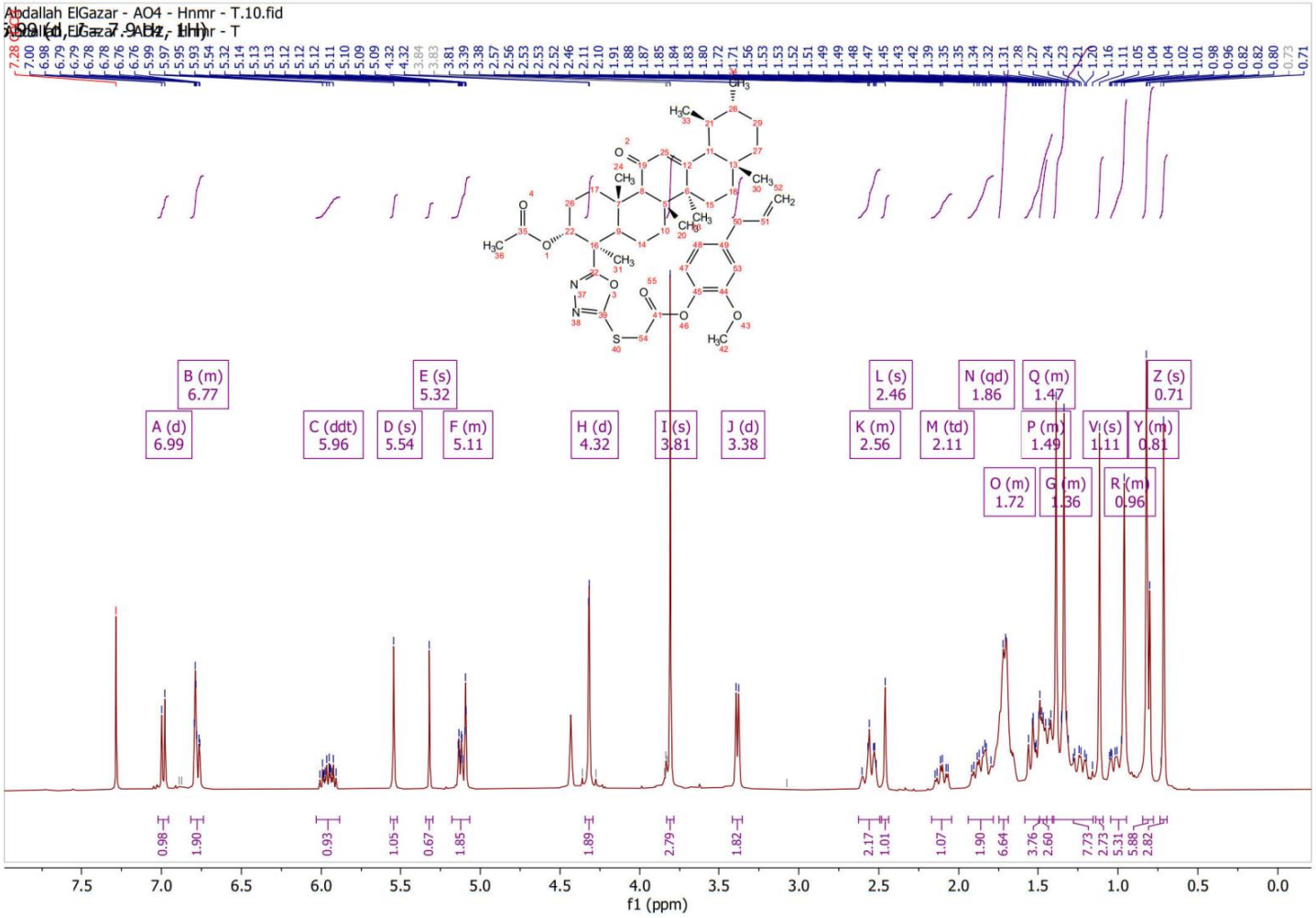


Figure S17. ^{1}H N.M.R spectrum of compound 8c

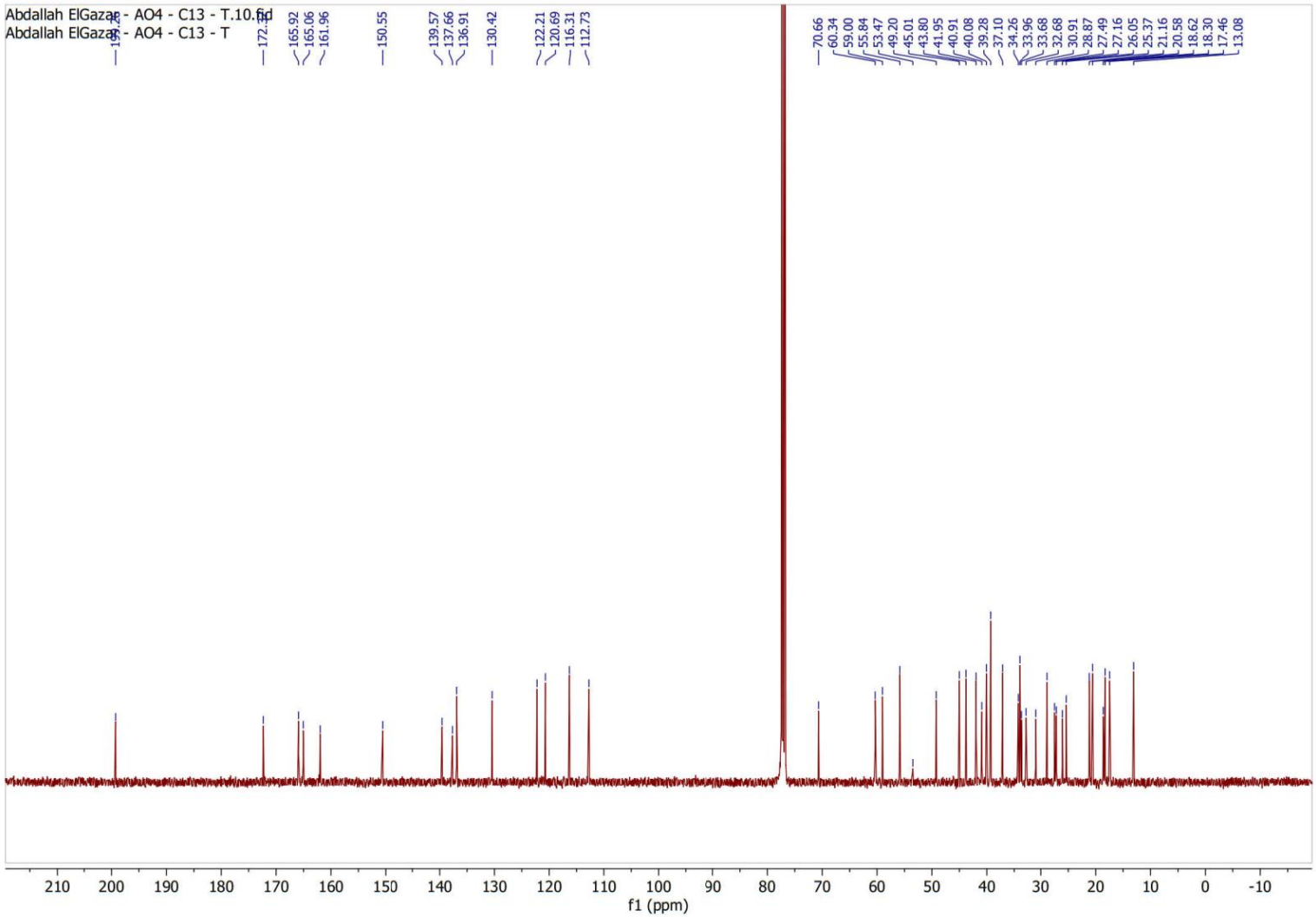


Figure S18. ^{13}C N.M.R spectrum of compound 8c

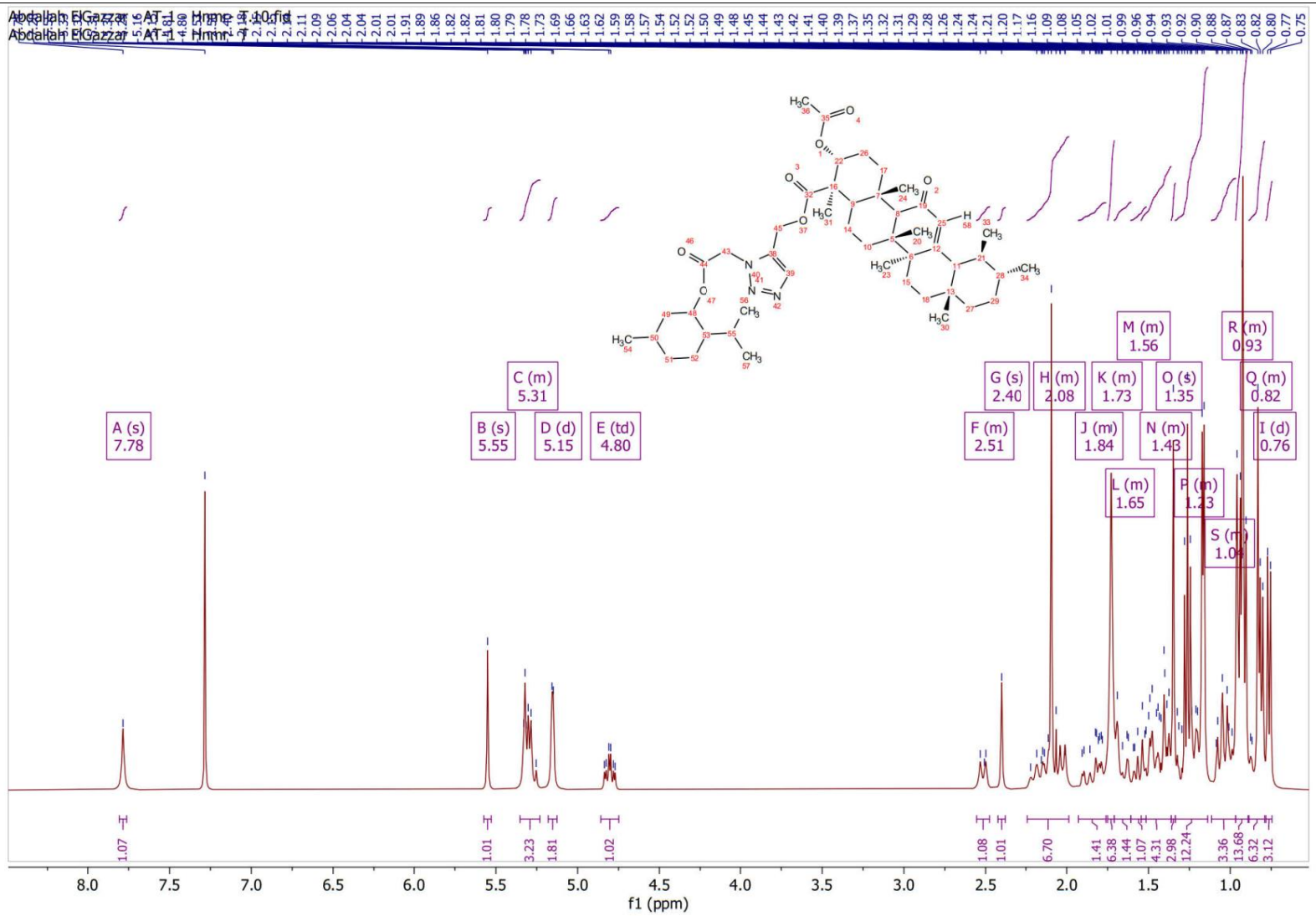


Figure S19. ^{1}H N.M.R spectrum of compound 14a

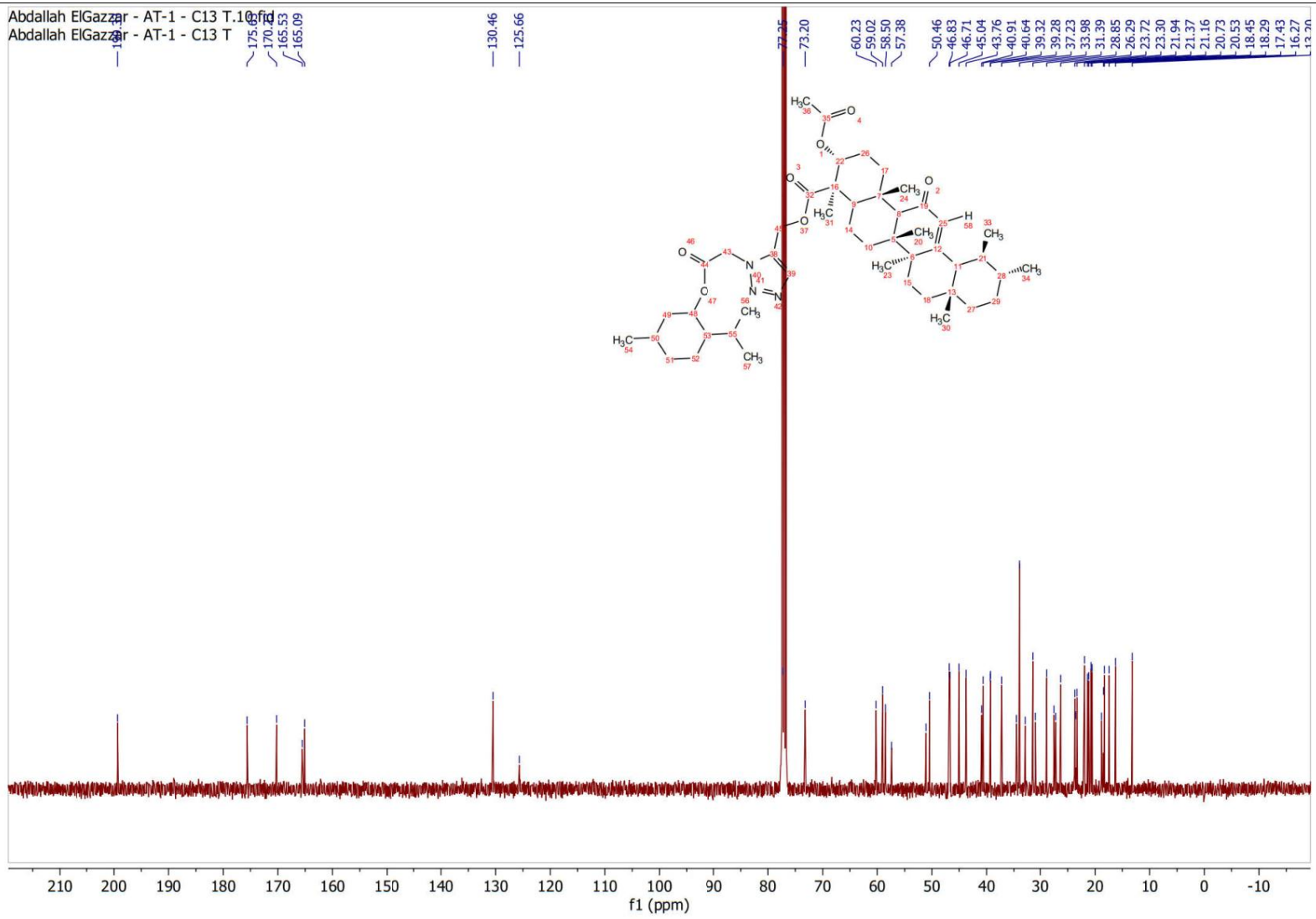


Figure S20. ^{13}C N.M.R spectrum of compound 14a

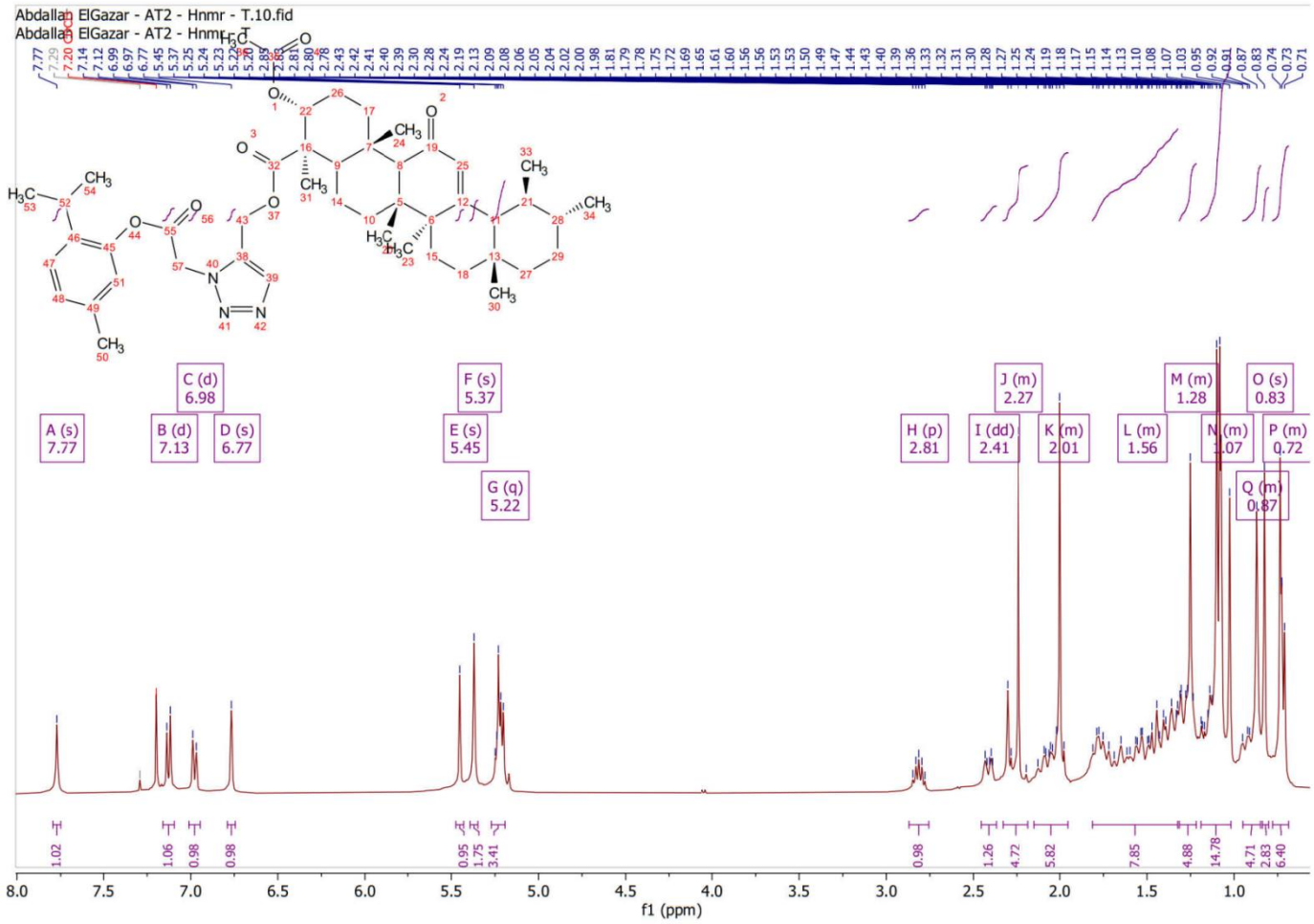


Figure S21. ^{1}HN.M.R spectrum of compound 14b

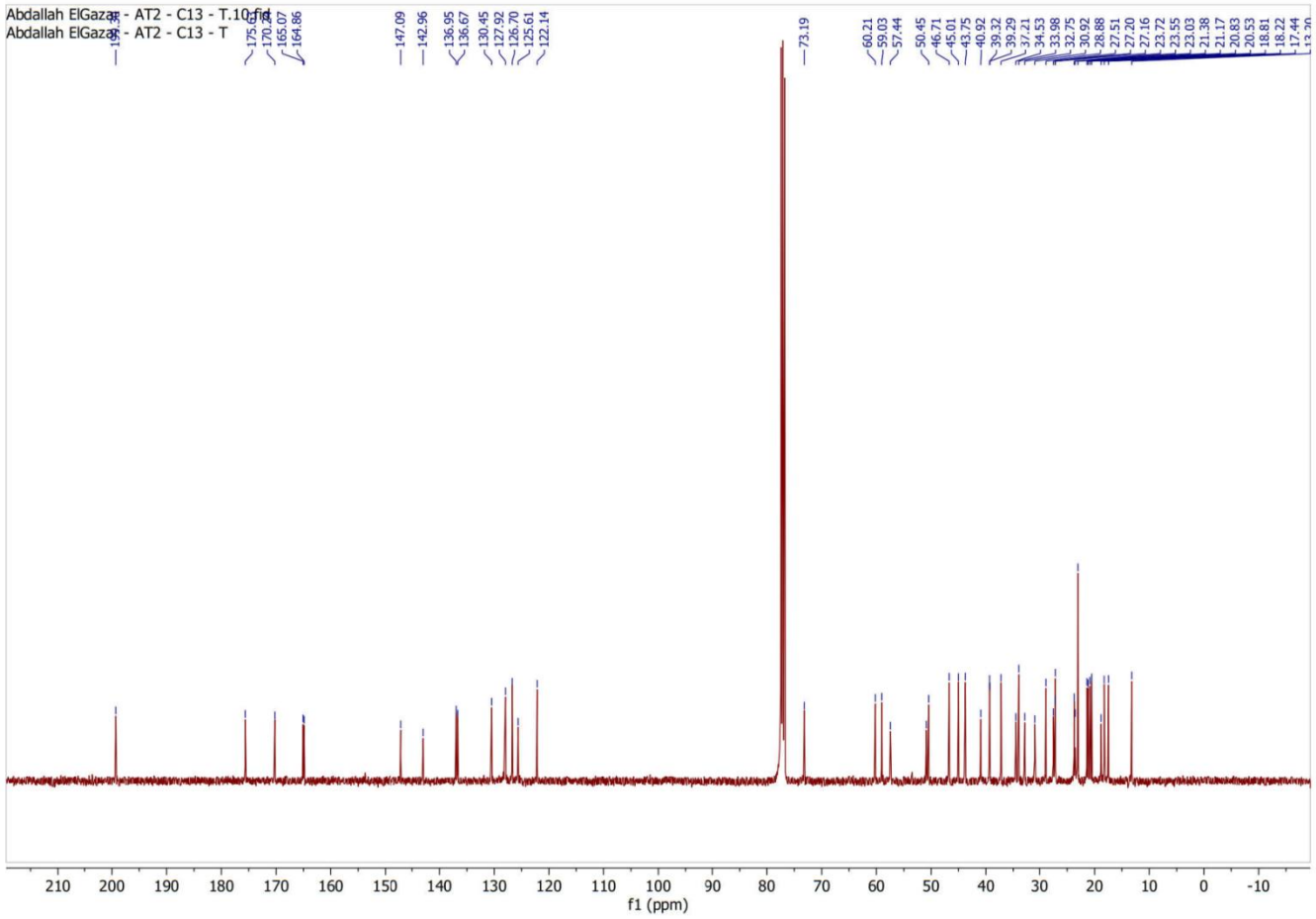


Figure S22. ^{13}C N.M.R spectrum of compound 14b

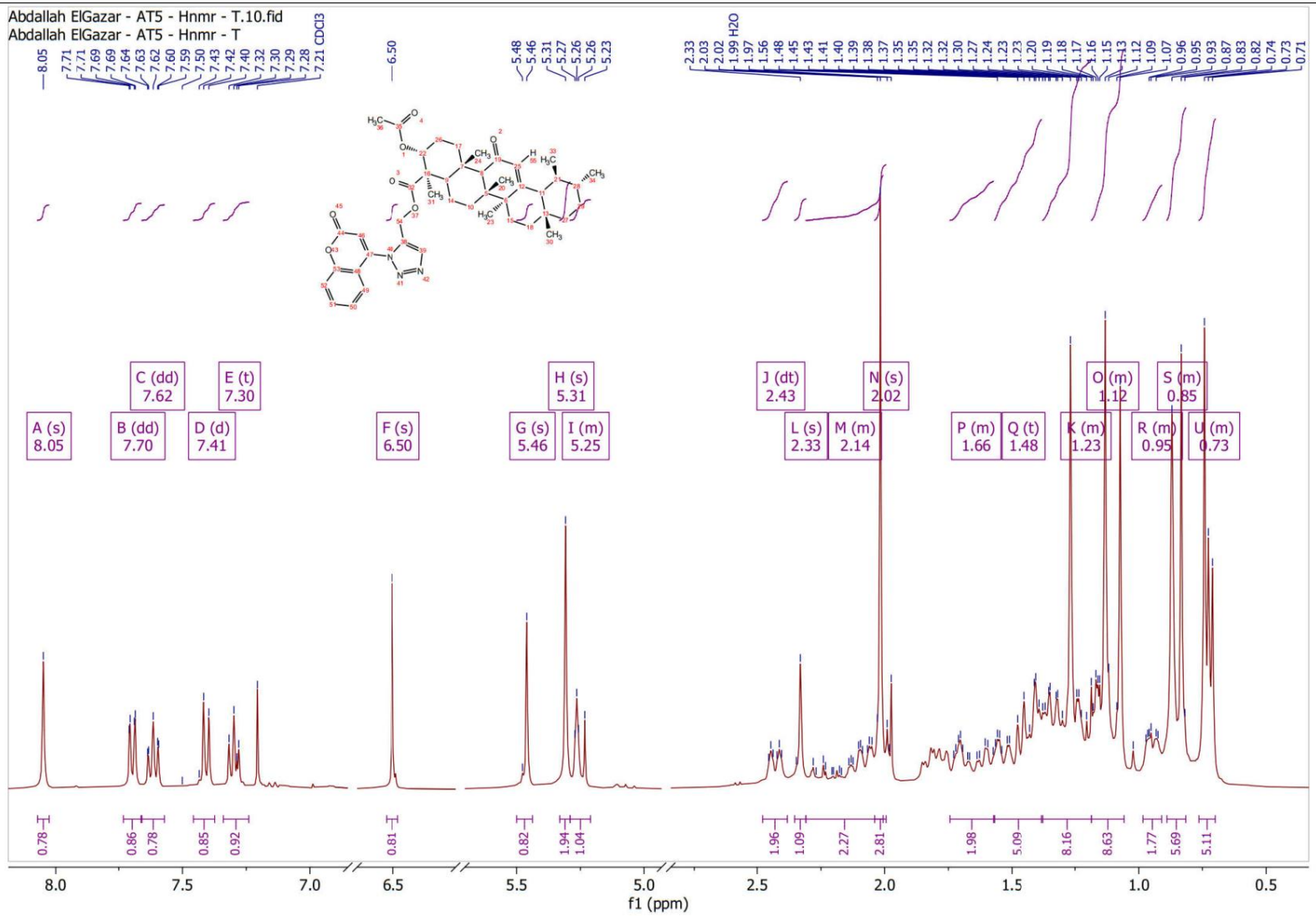


Figure S23. ^{1}H N.M.R spectrum of compound 14c

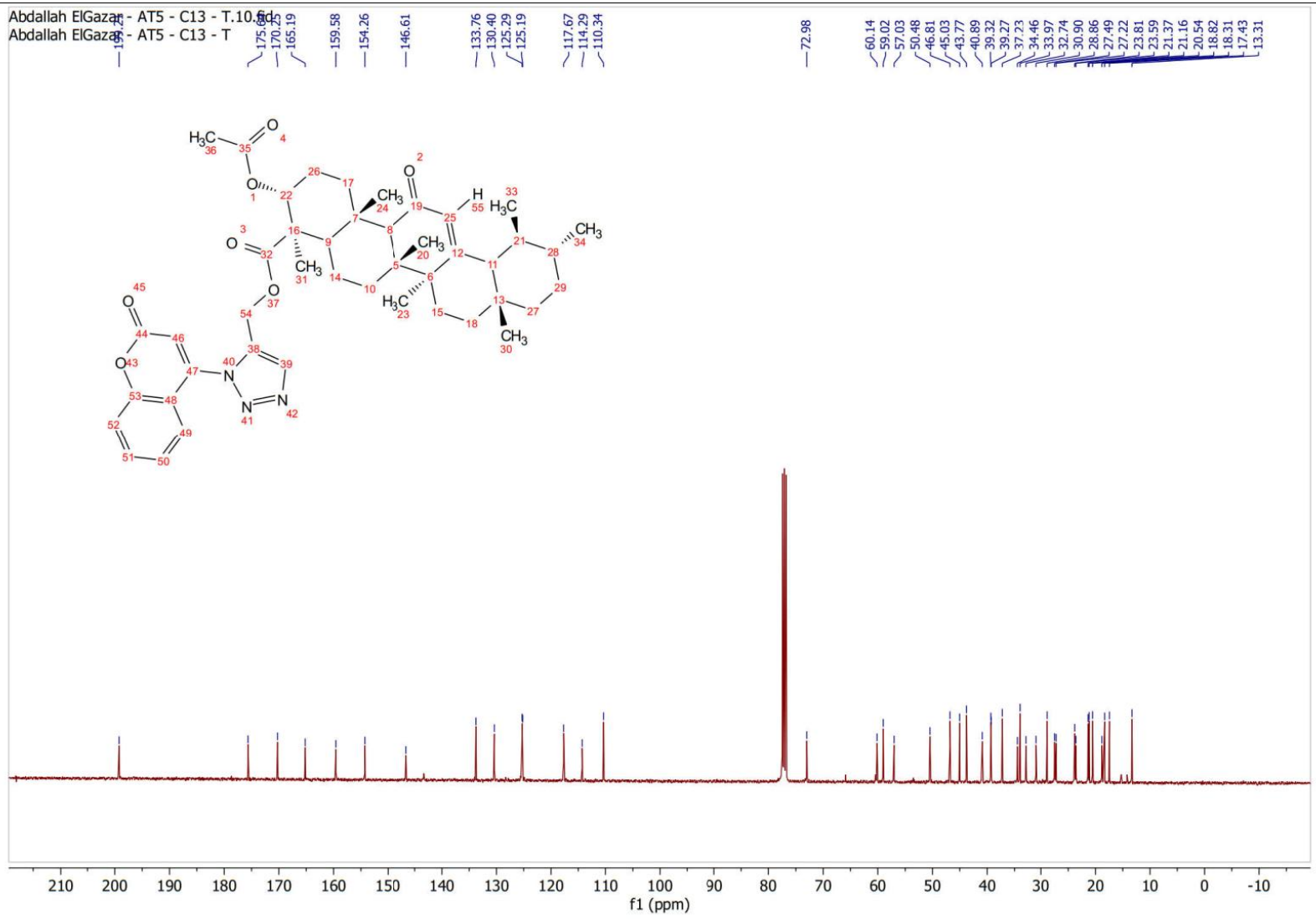


Figure S24. ^{13}C N.M.R spectrum of compound 14c

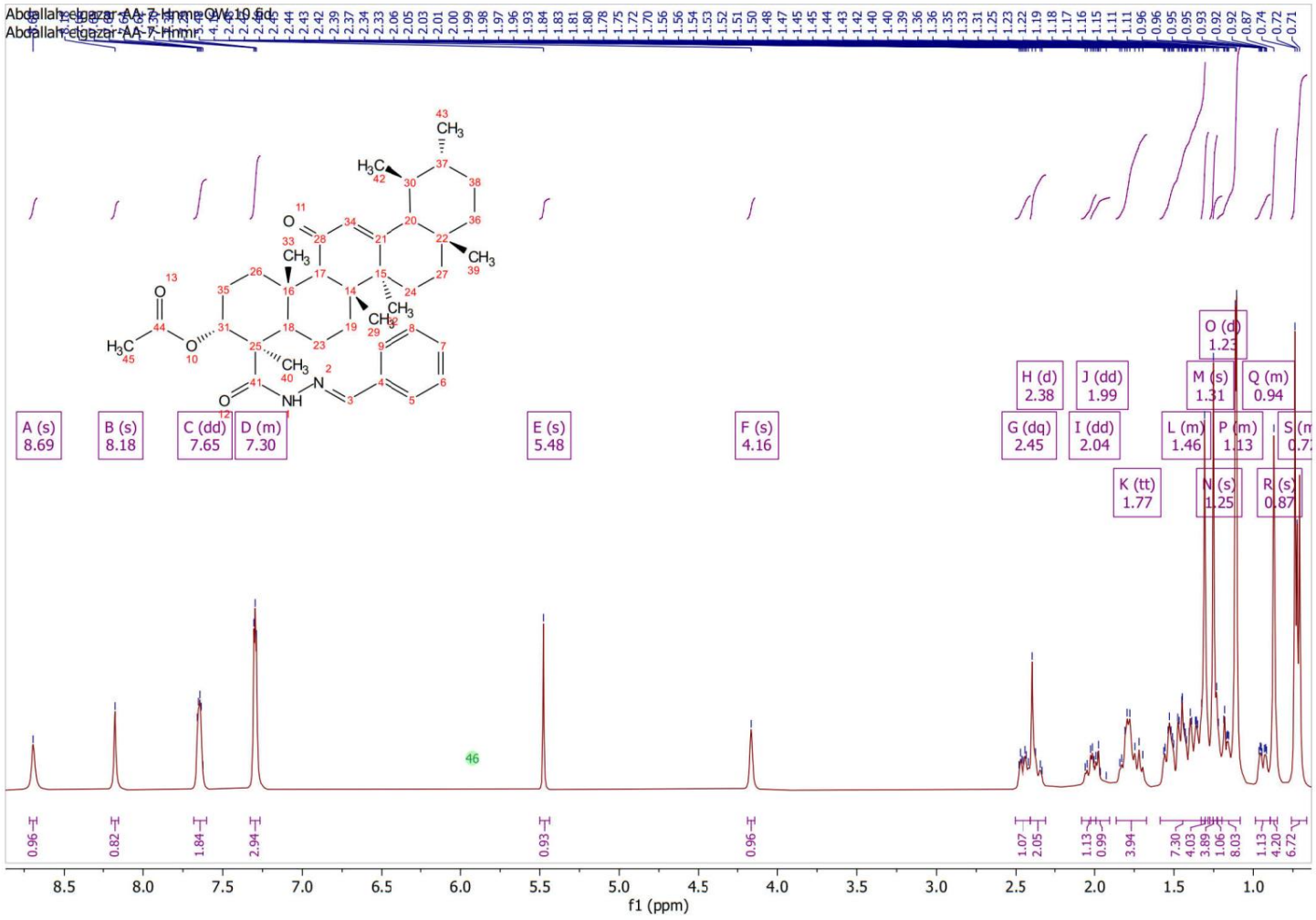


Figure S25. ^{1}H N.M.R spectrum of compound 16a

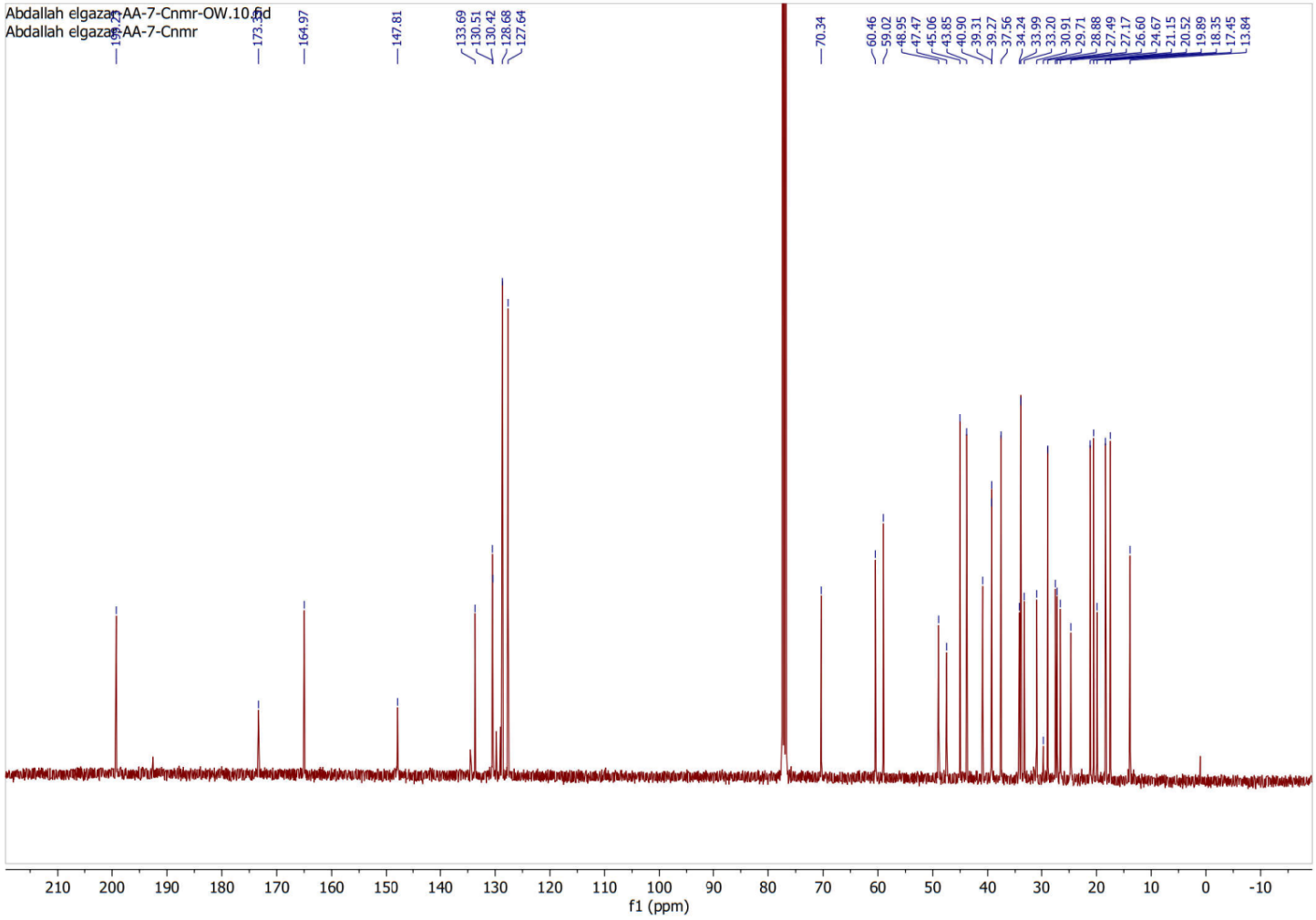


Figure S26. ^{13}C N.M.R spectrum of compound 16a

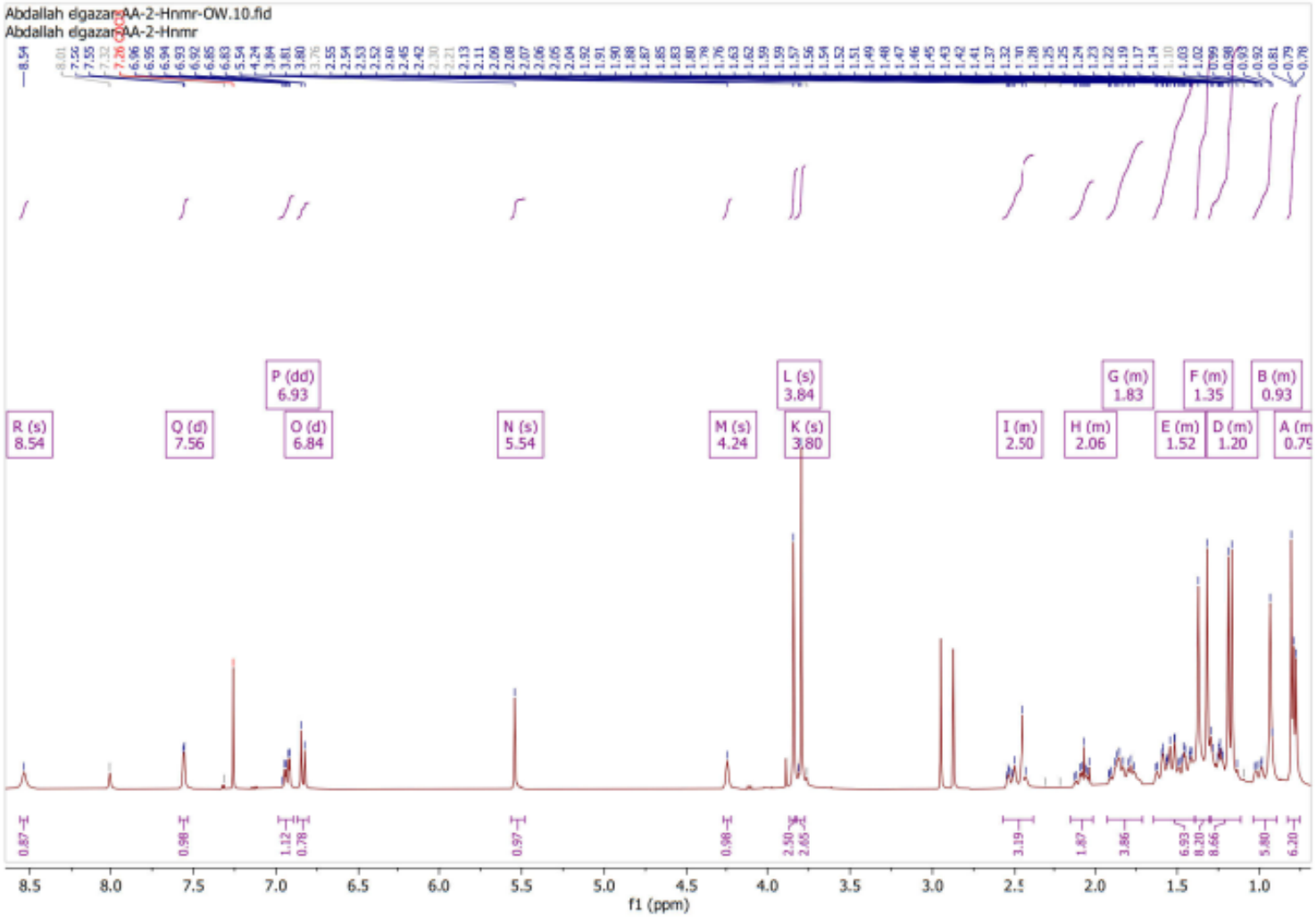


Figure S27. ^{1}H N.M.R spectrum of compound 16b

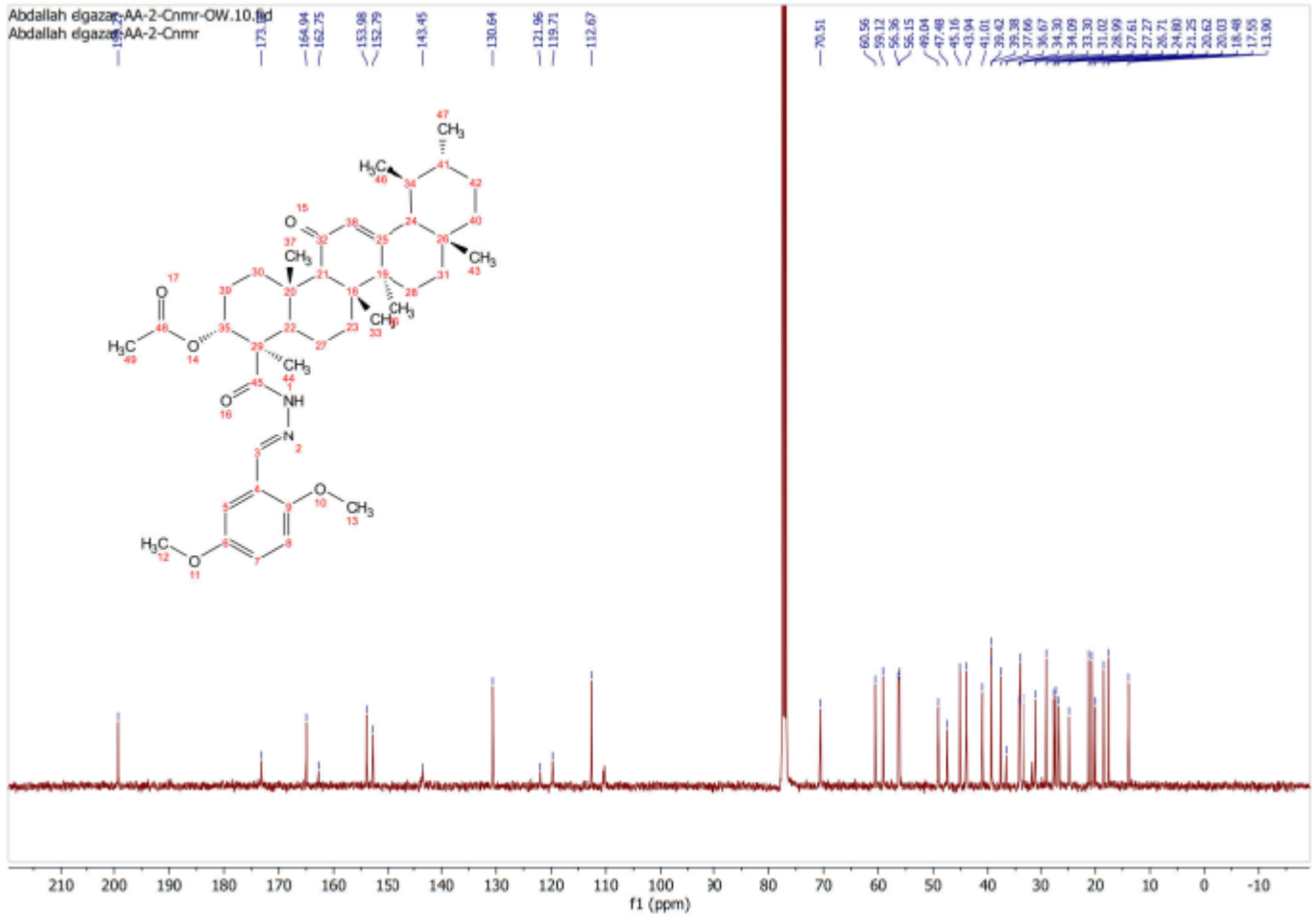


Figure S28. ^{13}C N.M.R spectrum of compound 16b

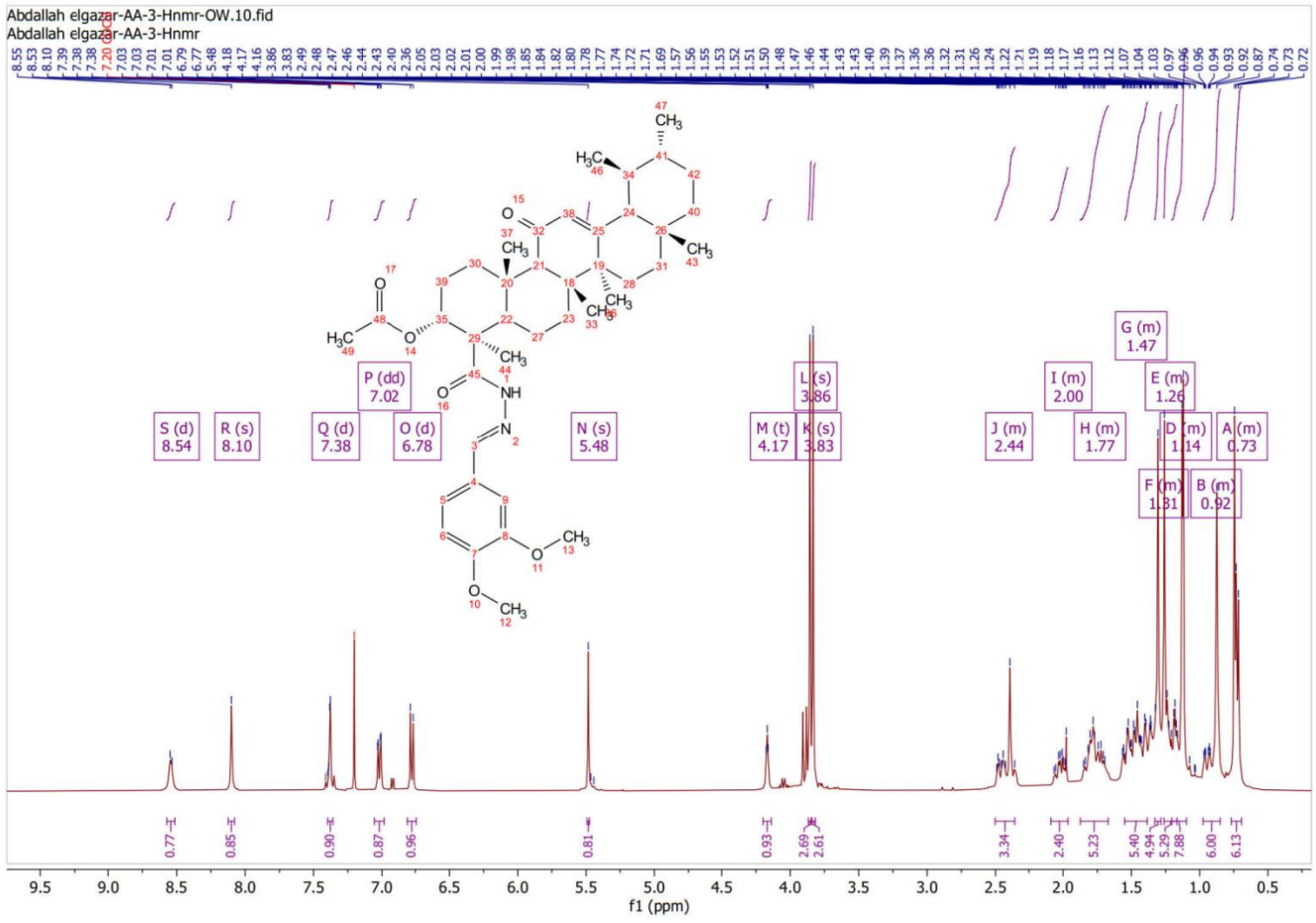


Figure S29. ^{1}H N.M.R spectrum of compound 16c

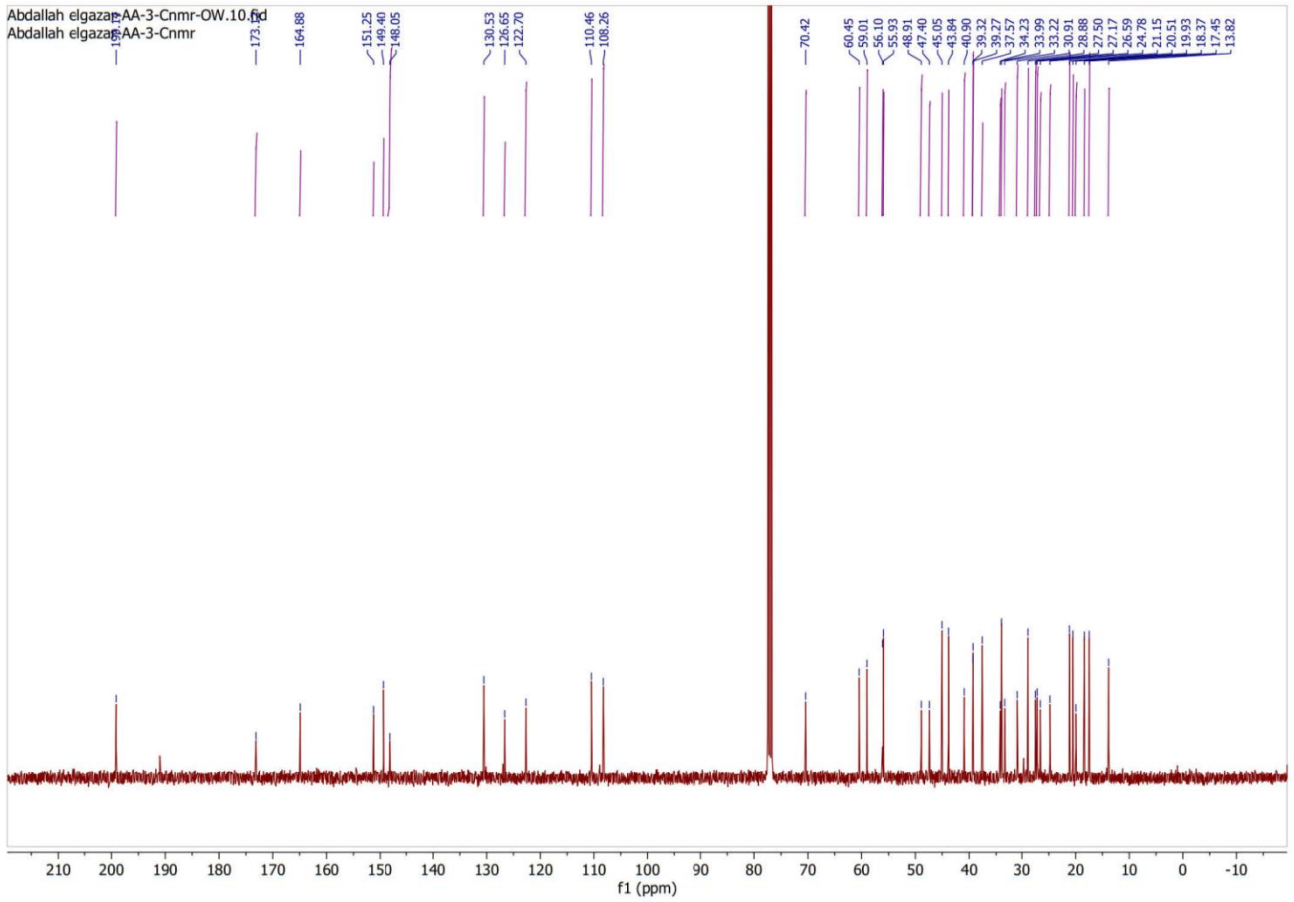


Figure S30. ^{13}C N.M.R spectrum of compound 16c

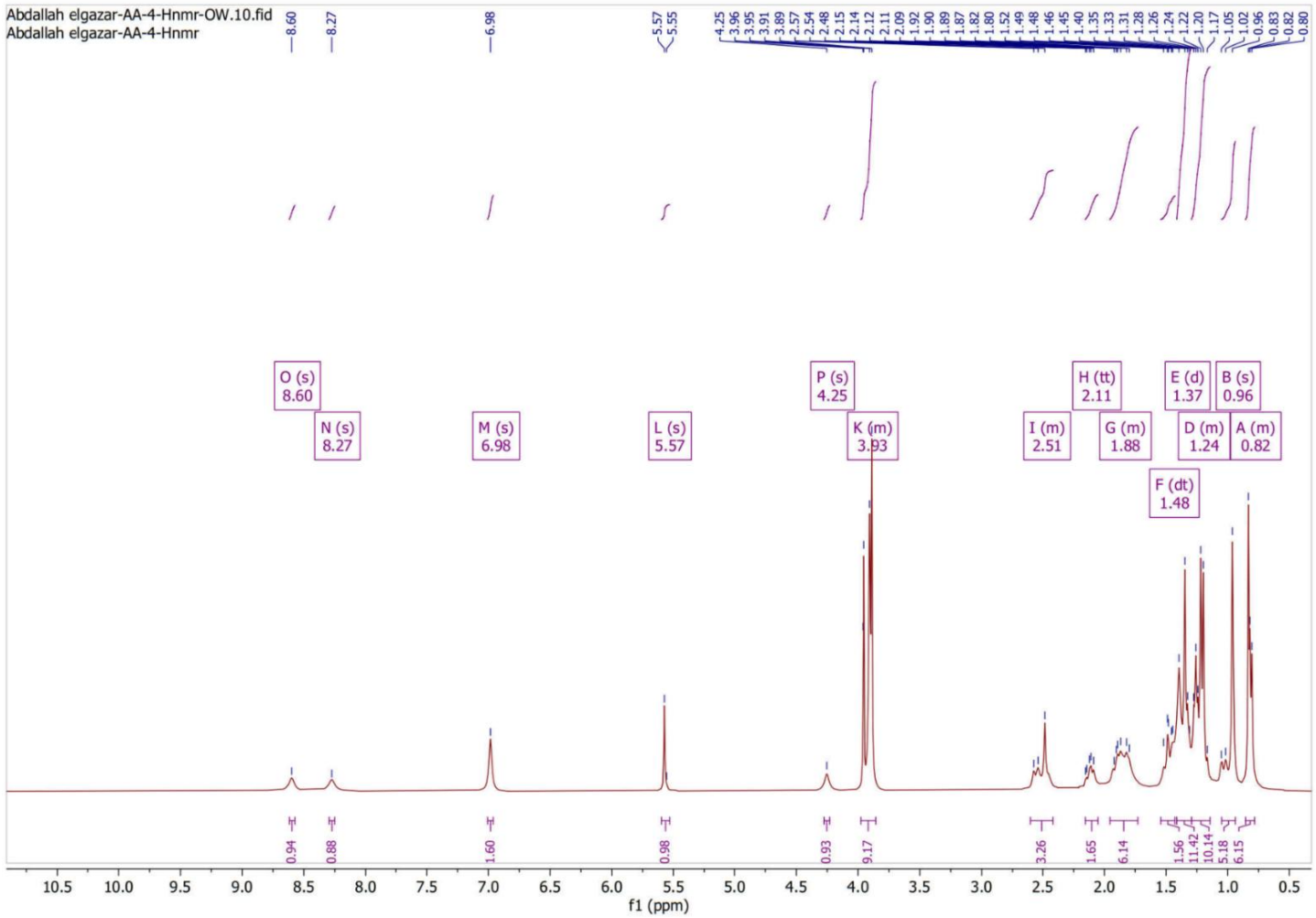


Figure S31 . ^{1}H N.M.R spectrum of compound 16d

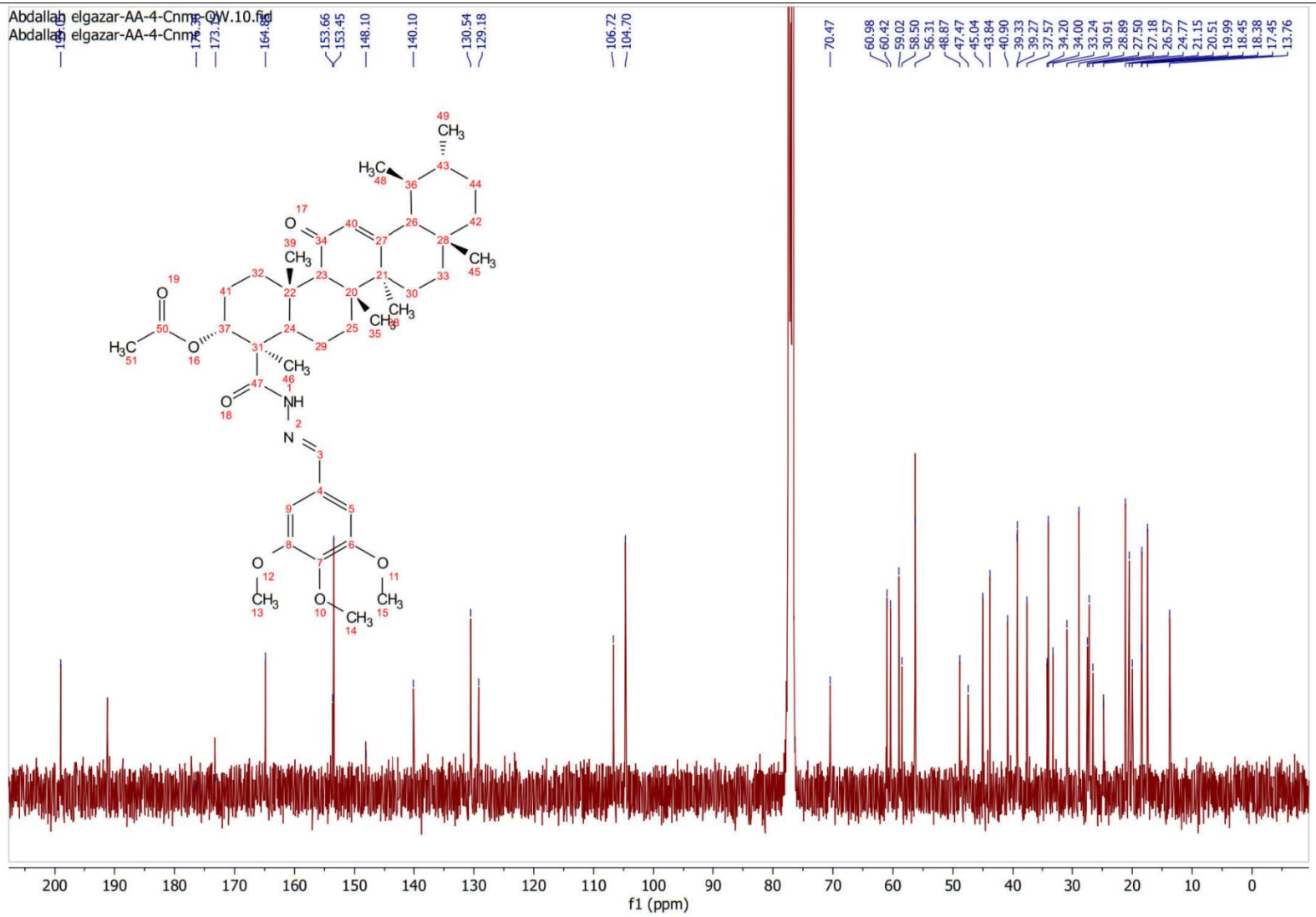


Figure S32. ^{13}C N.M.R spectrum of compound 16d

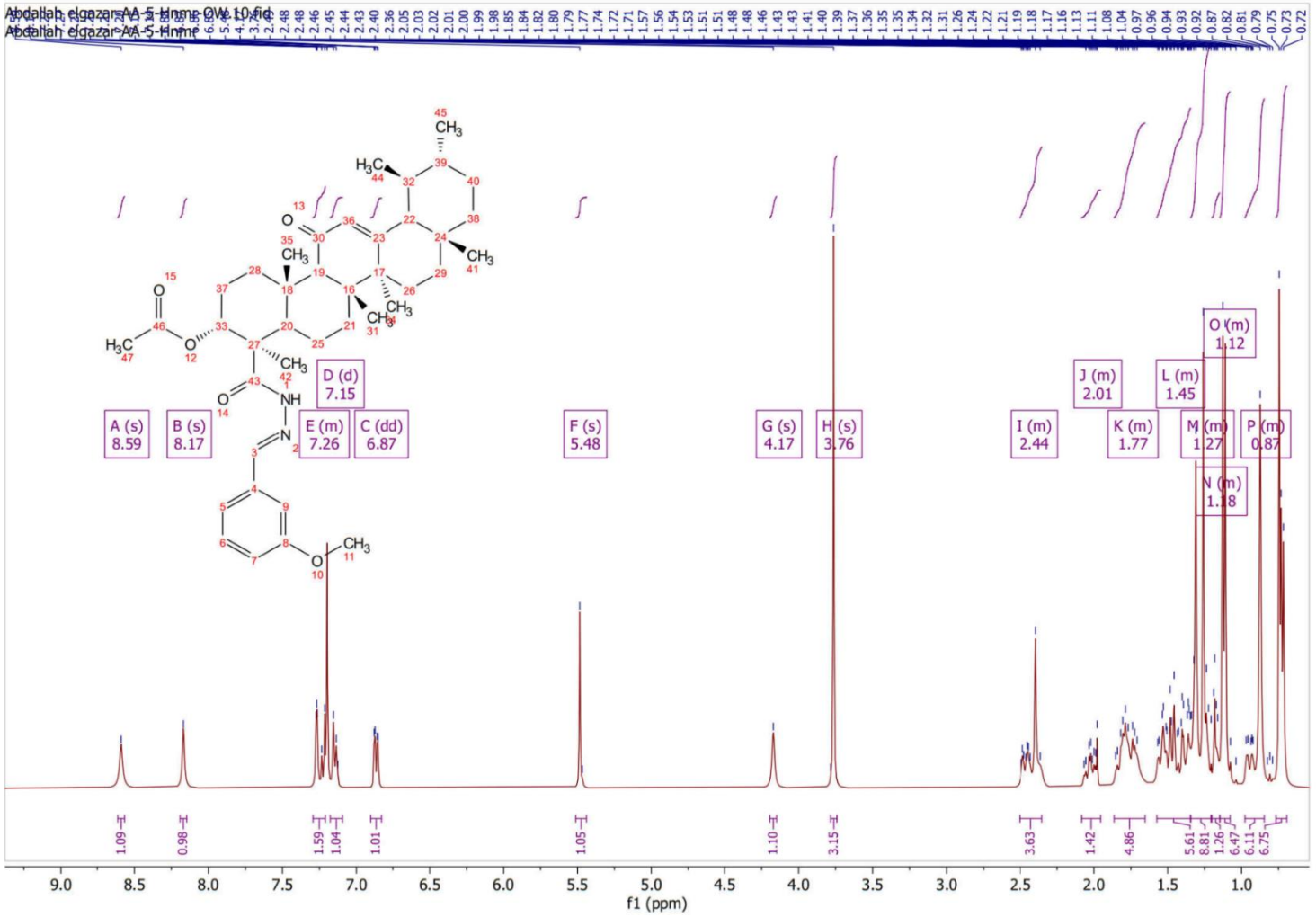


Figure S33. ^{1}H N.M.R spectrum of compound 16e

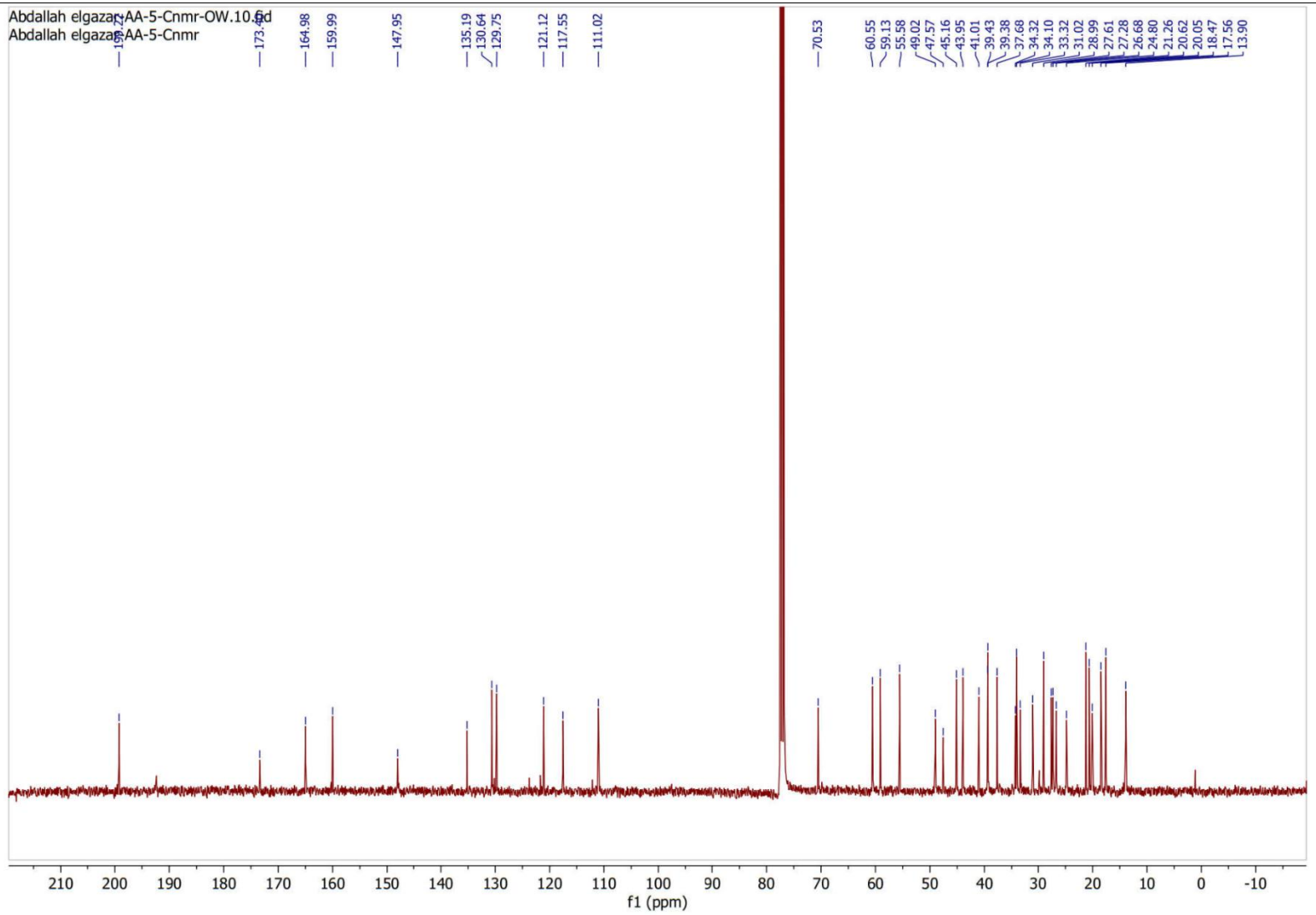


Figure S34. ^{13}c N.M.R spectrum of compound 16e

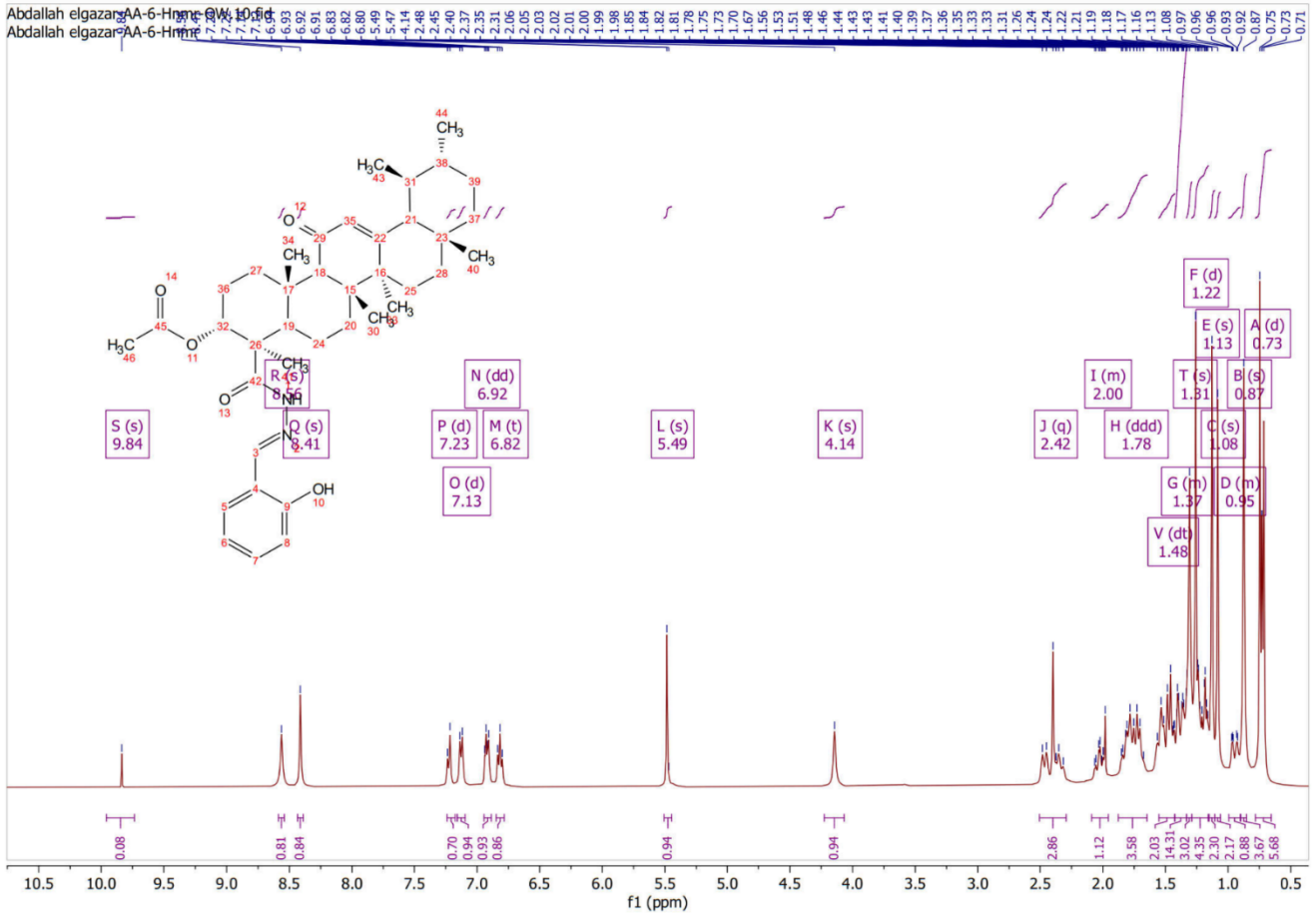


Figure S35 . ^{1}H N.M.R spectrum of compound 16f

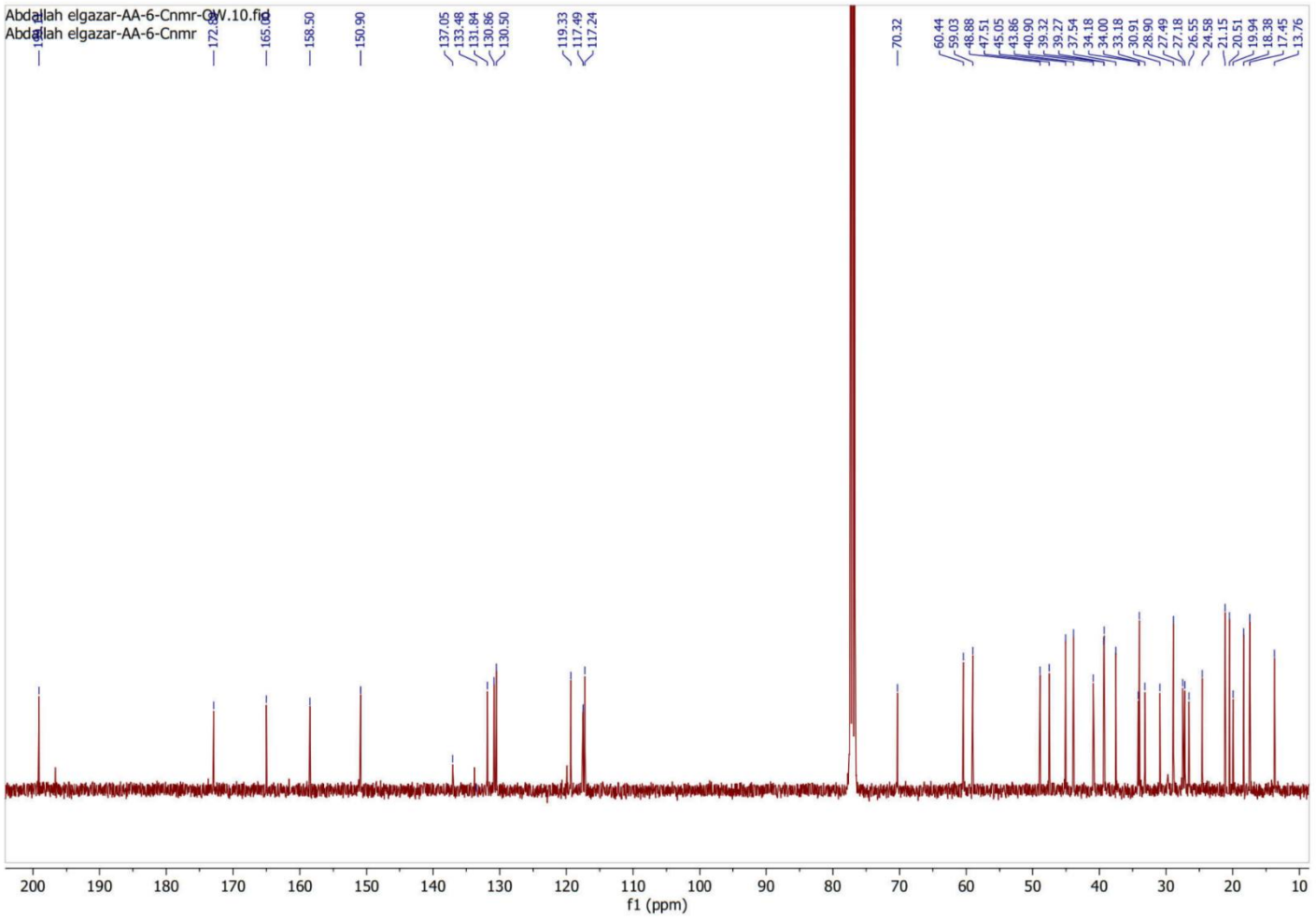


Figure S36. ^{13}c N.M.R spectrum of compound 16f

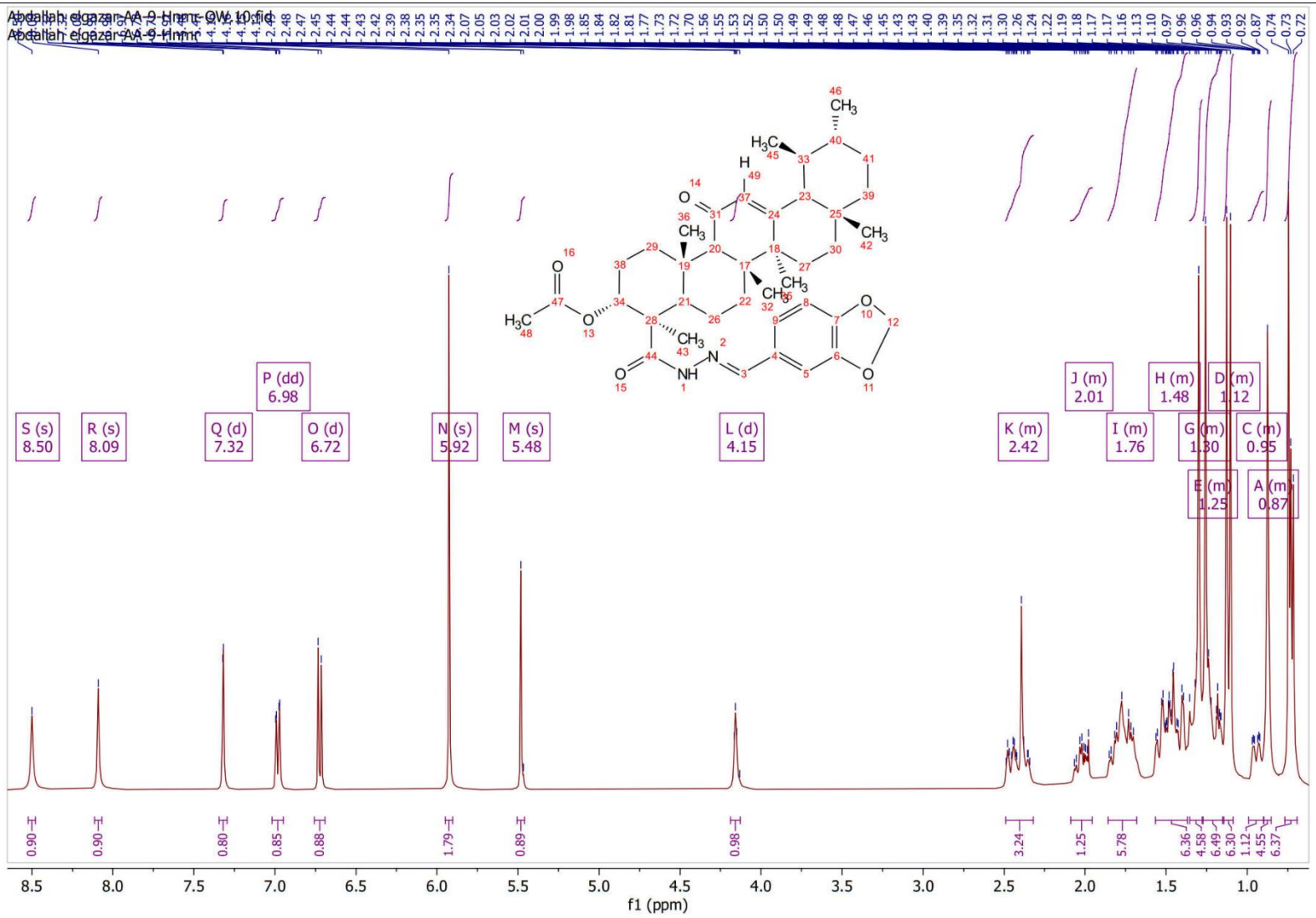


Figure S37. ^{1}H N.M.R spectrum of compound 16g

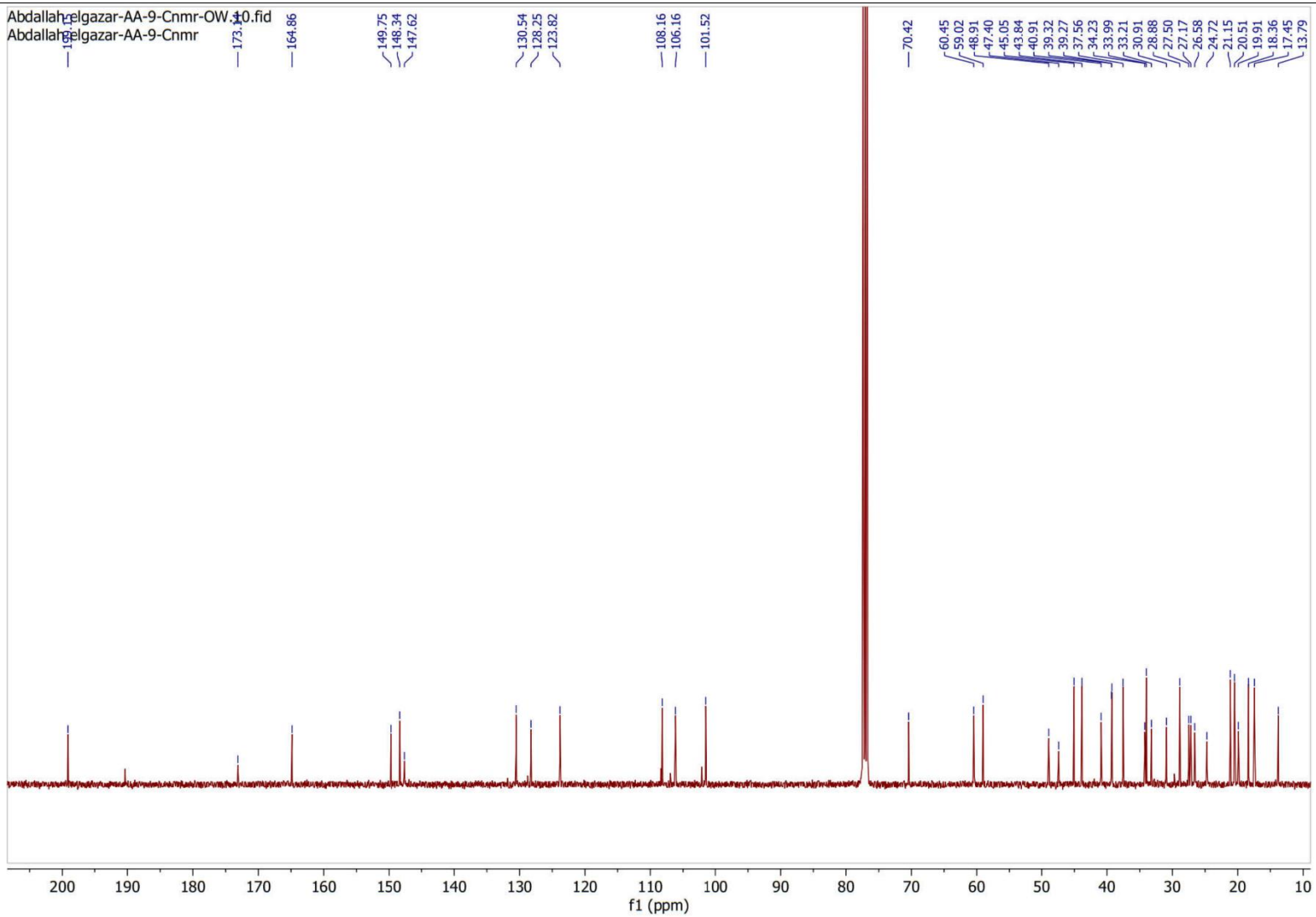


Figure S38. ^{13}c N.M.R spectrum of compound 16g

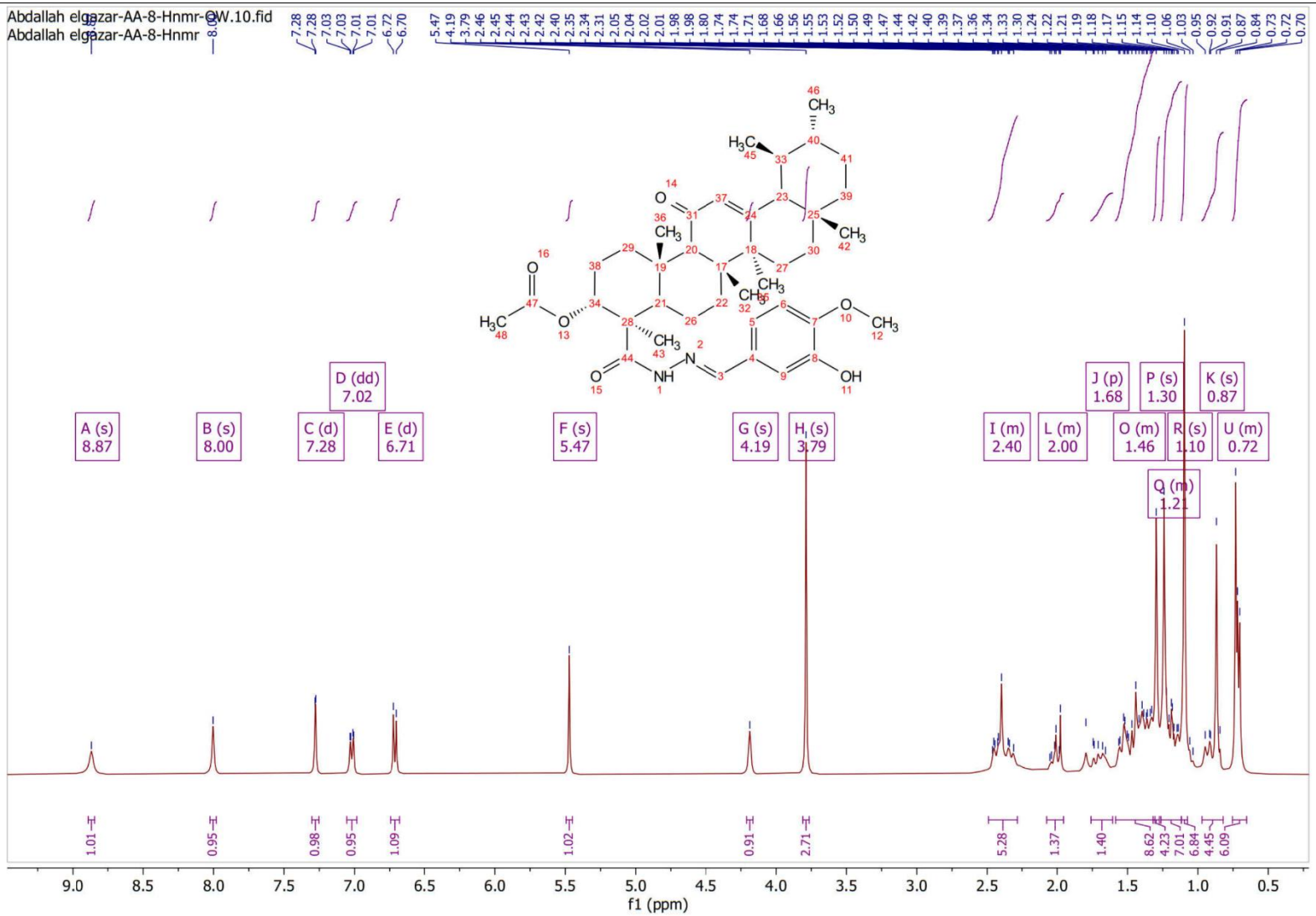


Figure S39. ^{1}HN.M.R spectrum of compound 16h

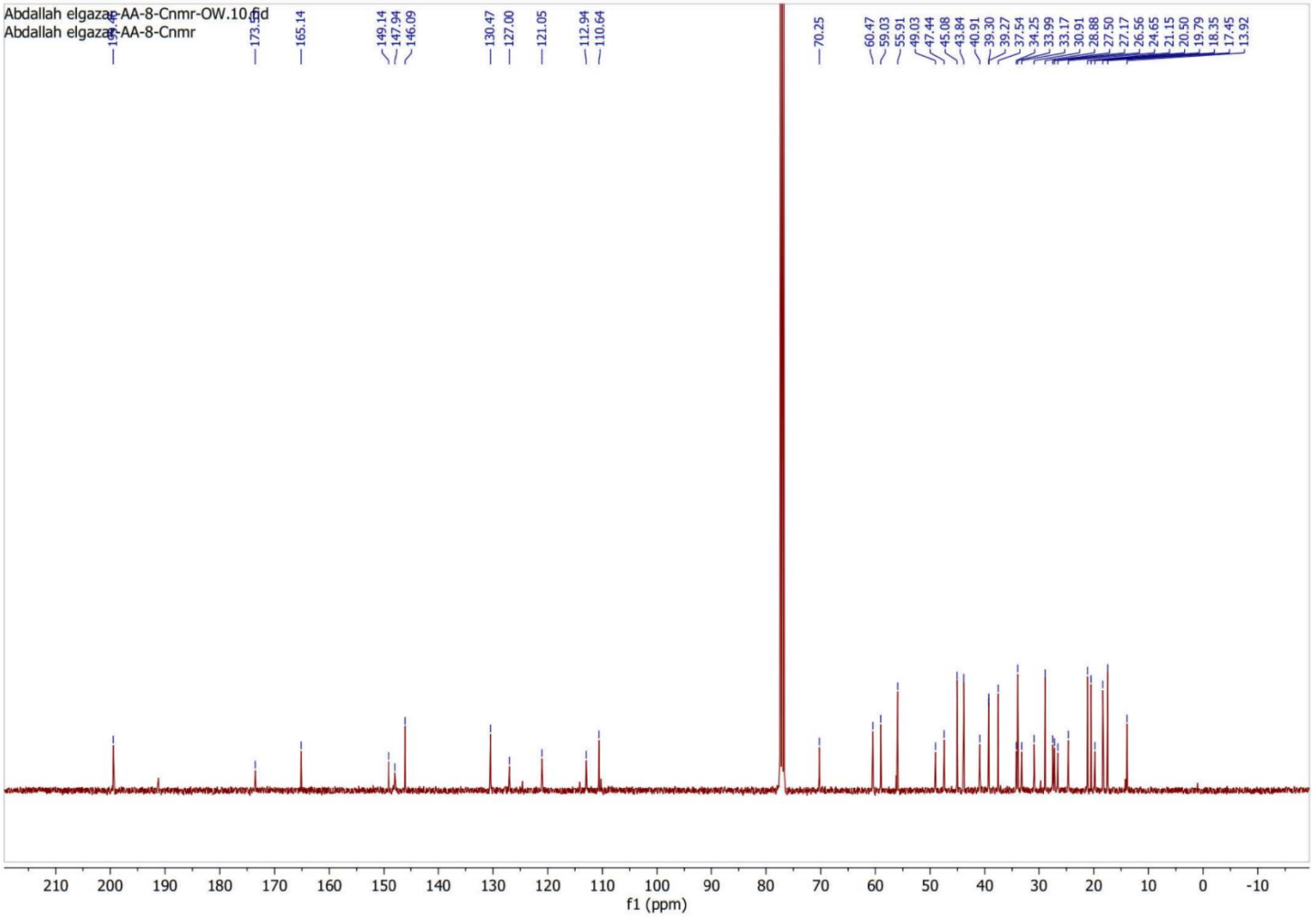


Figure S40. ^{13}C N.M.R spectrum of compound 16h

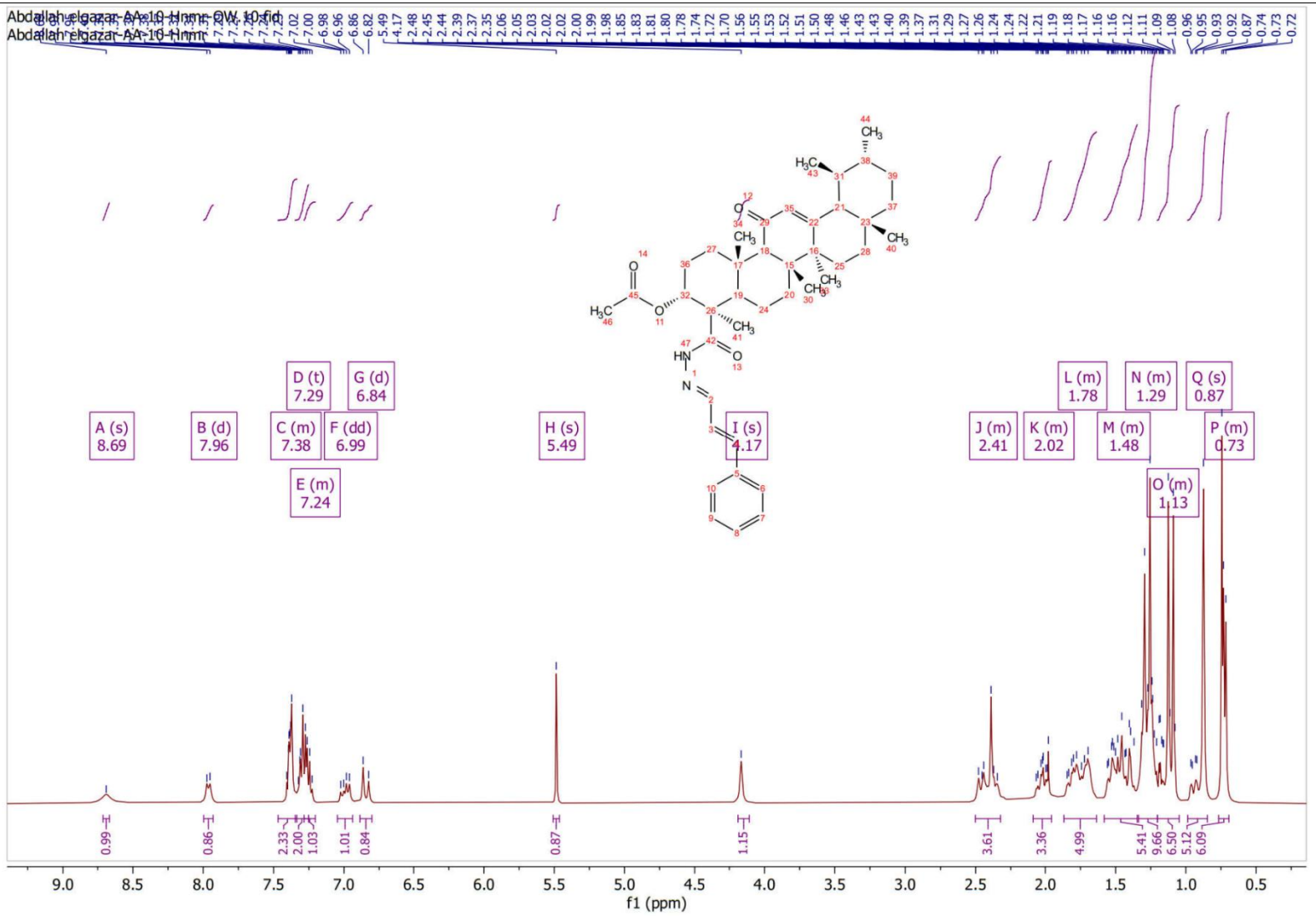


Figure S41. ^{1}H N.M.R spectrum of compound 16i

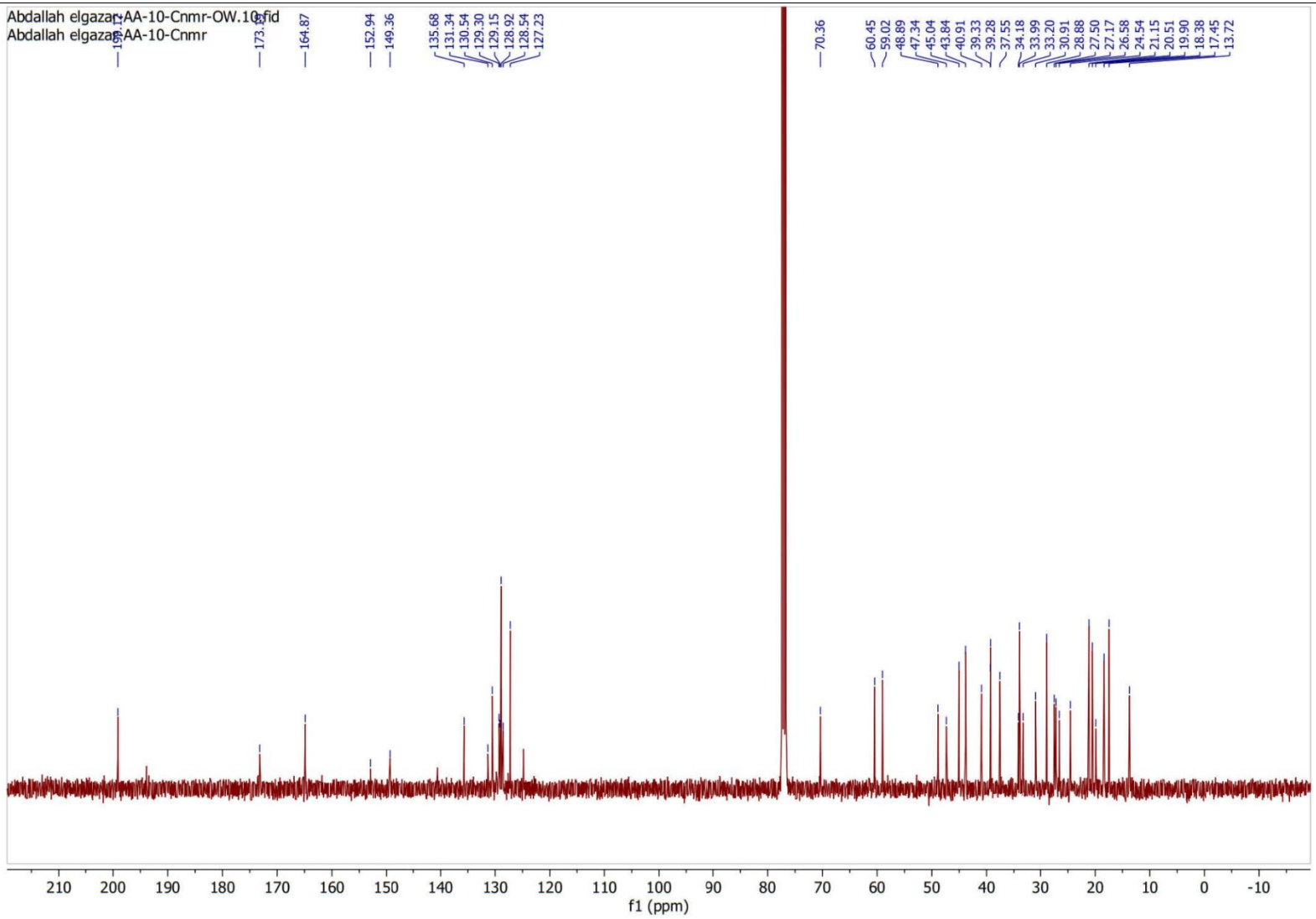


Figure S42. ^{13}C N.M.R spectrum of compound 16i

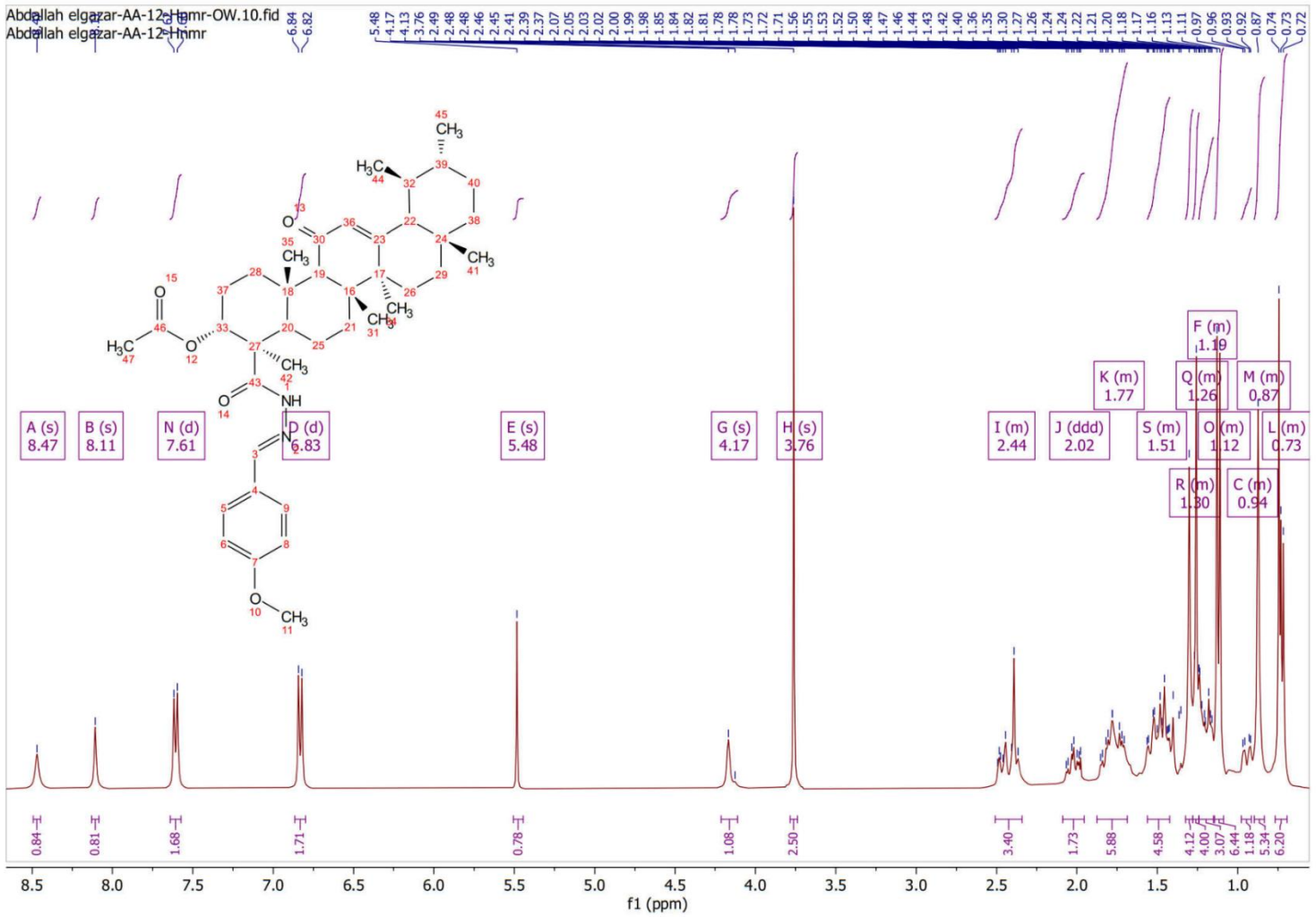


Figure S43. ^{1}H N.M.R spectrum of compound 16j

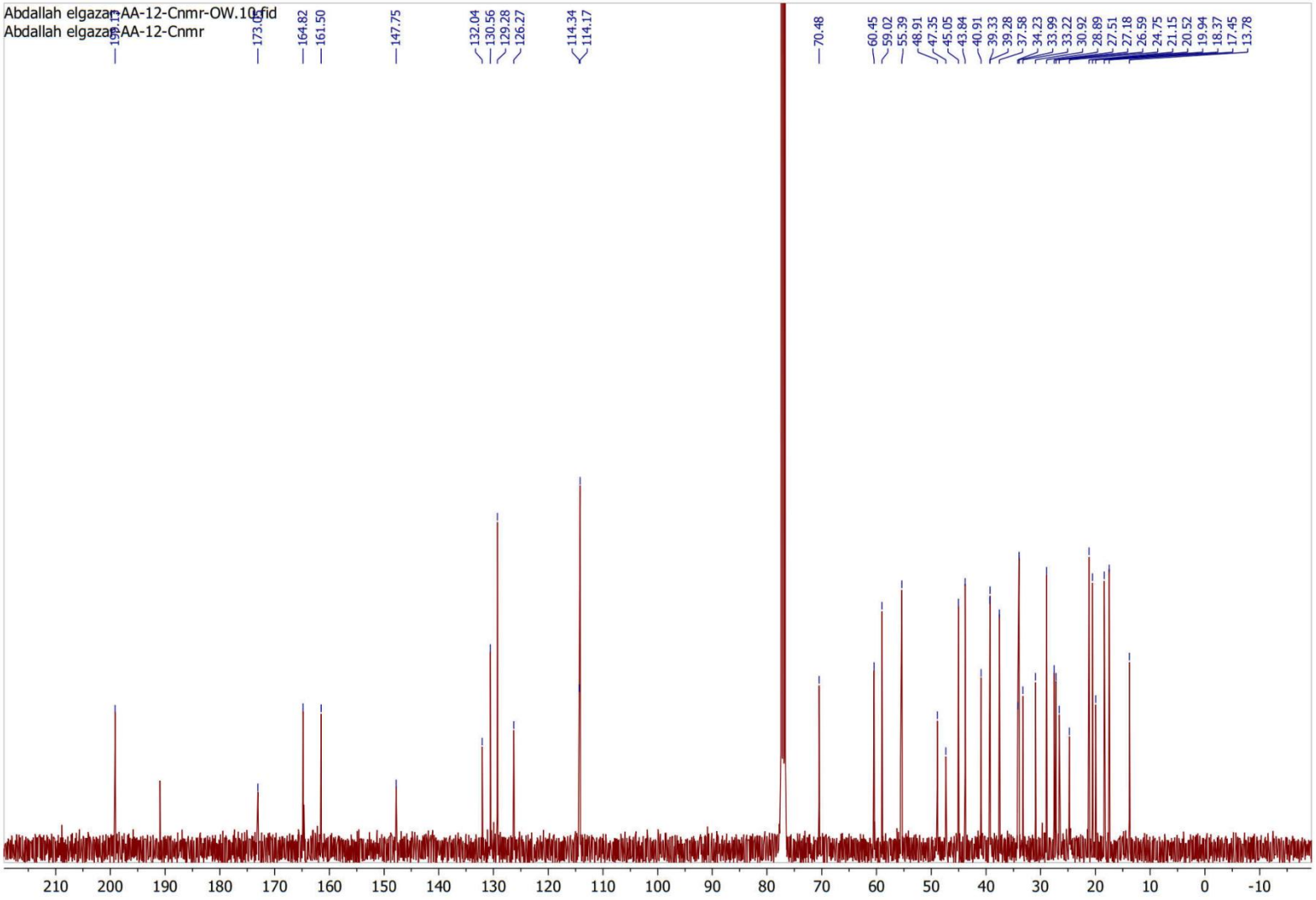


Figure S44.^{13}c N.M.R spectrum of compound 16j

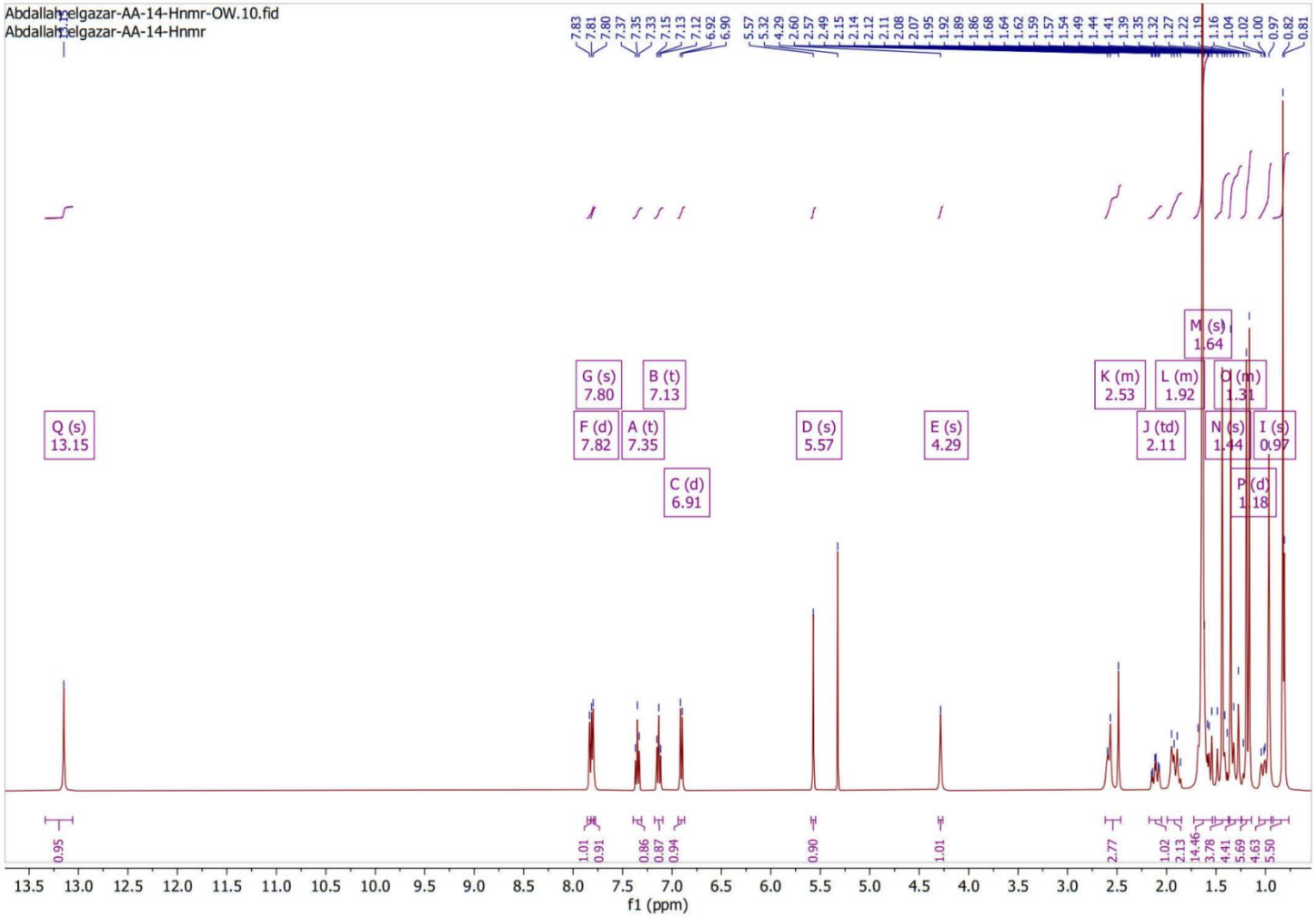


Figure S45. ^{1}H N.M.R spectrum of compound 18

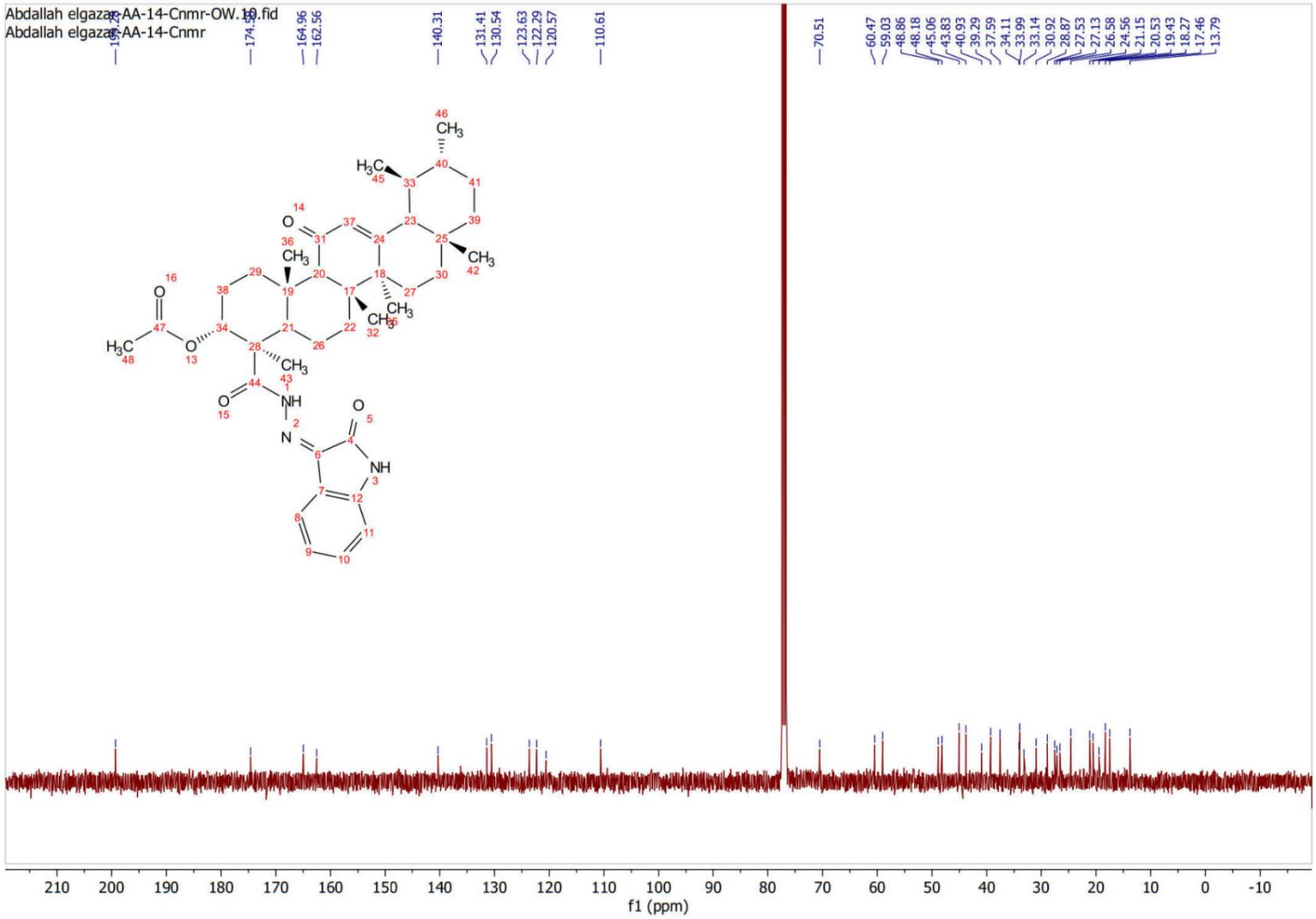


Figure S46. ^{13}C N.M.R spectrum of compound 18