

Supplementary Material

Effective synthesis of novel furan-fused pentacyclic triterpenoids via anionic 5-exo dig cyclization of 2-alkynyl-3-oxotriterpene acids

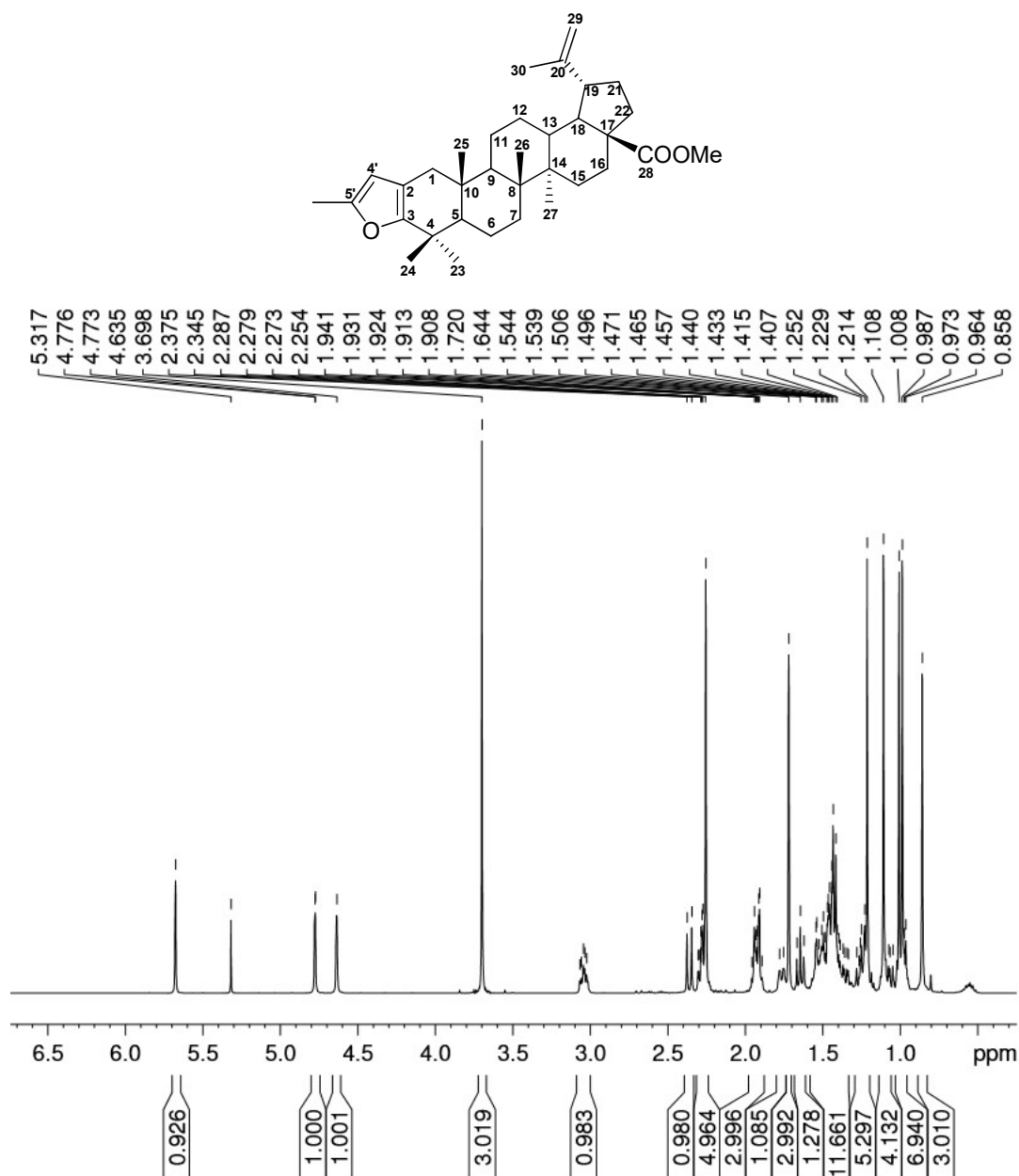
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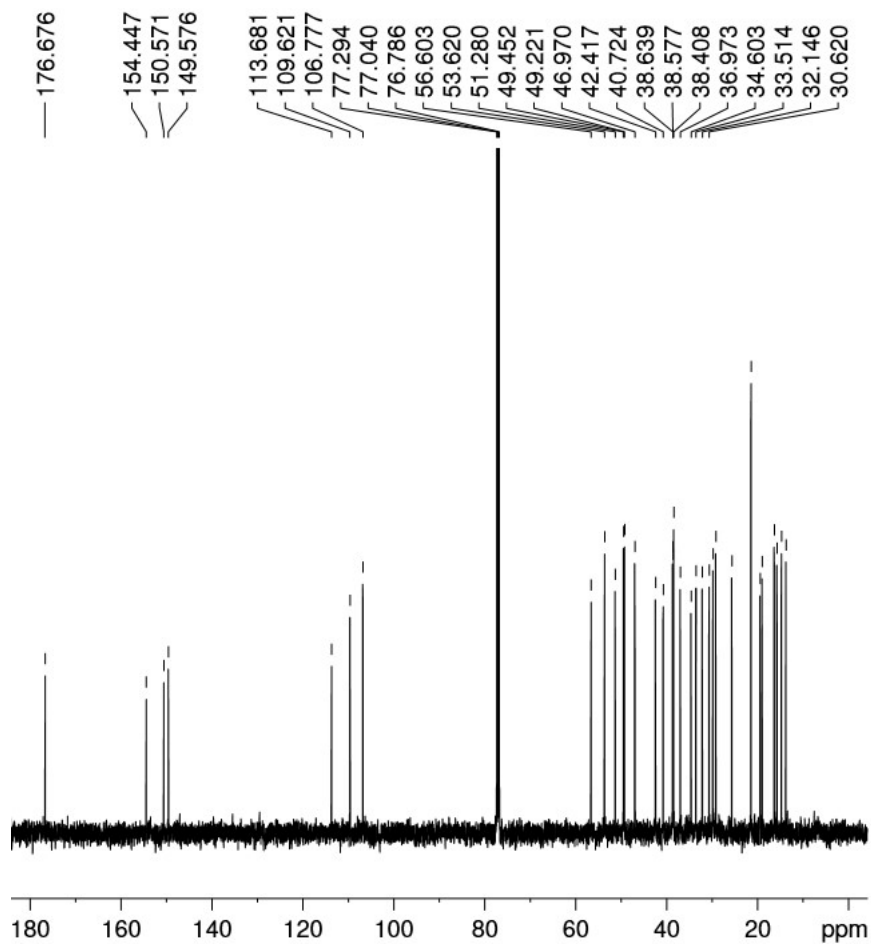
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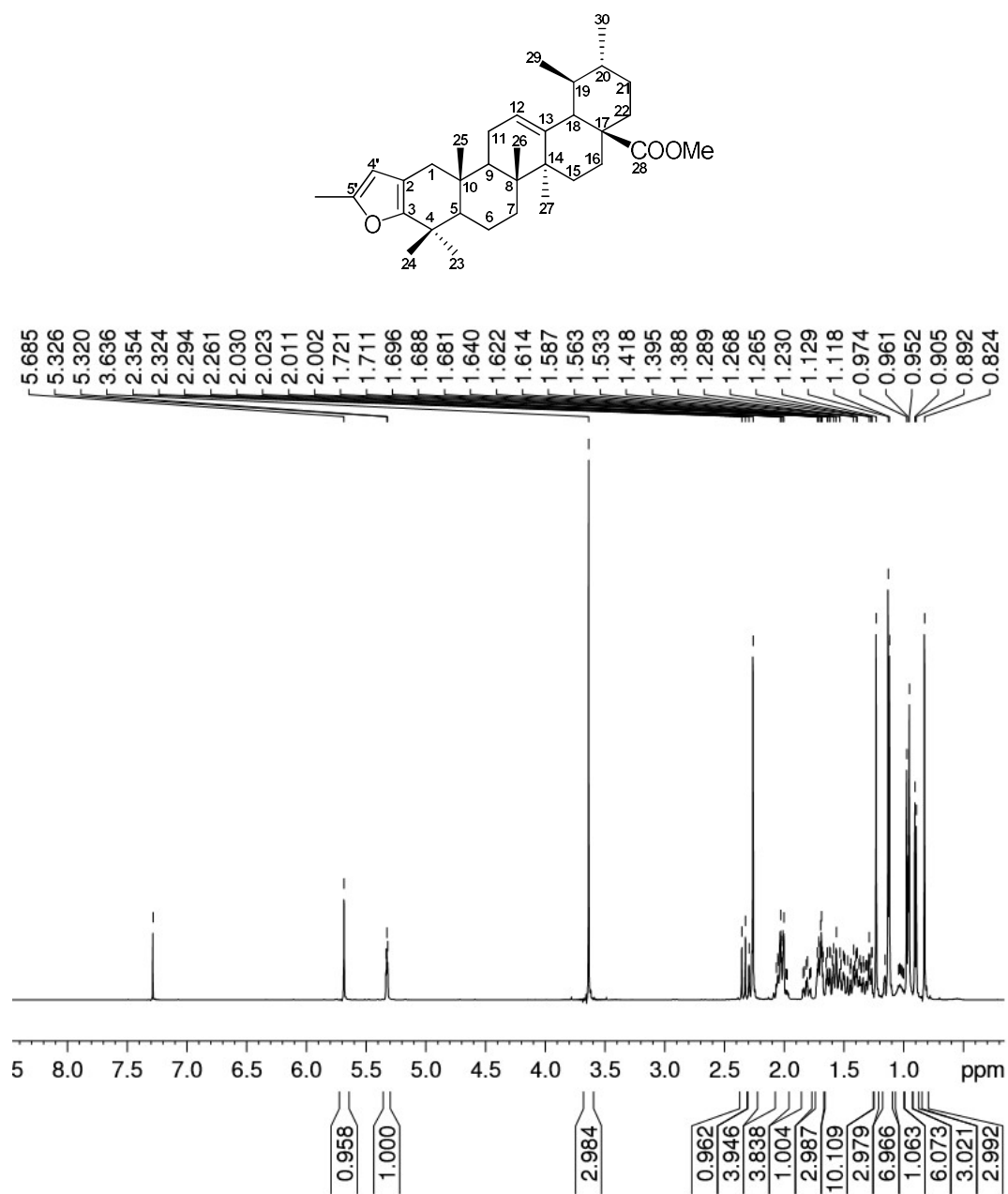
¹H NMR and ¹³C NMR data of new compounds

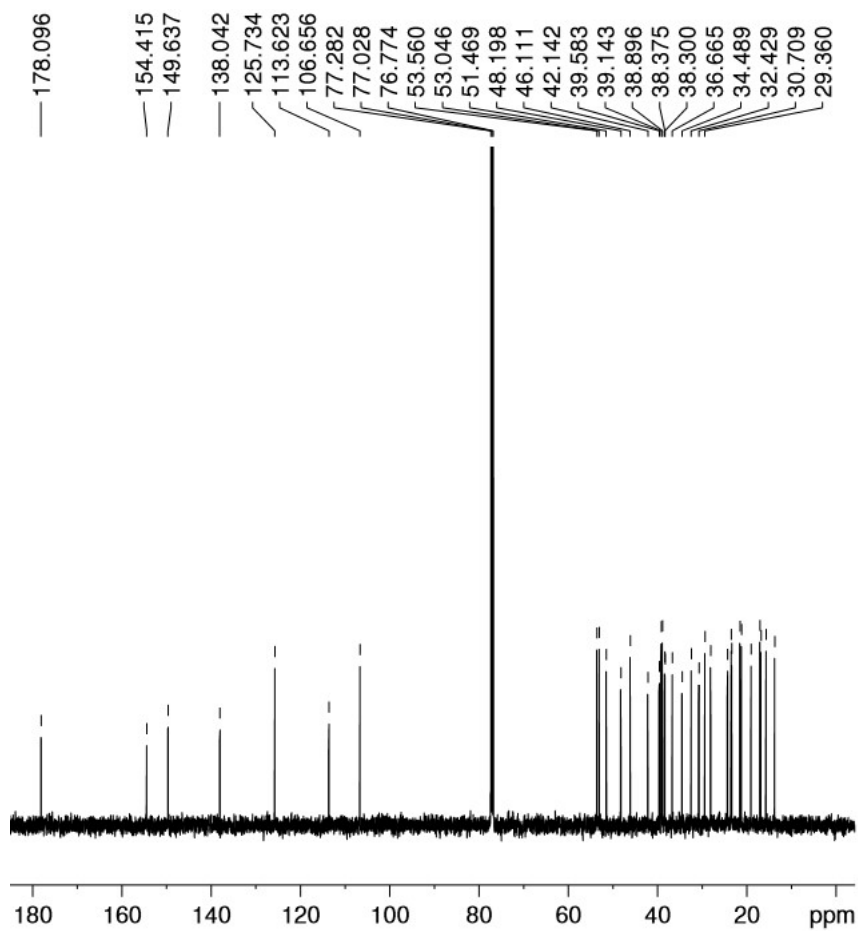
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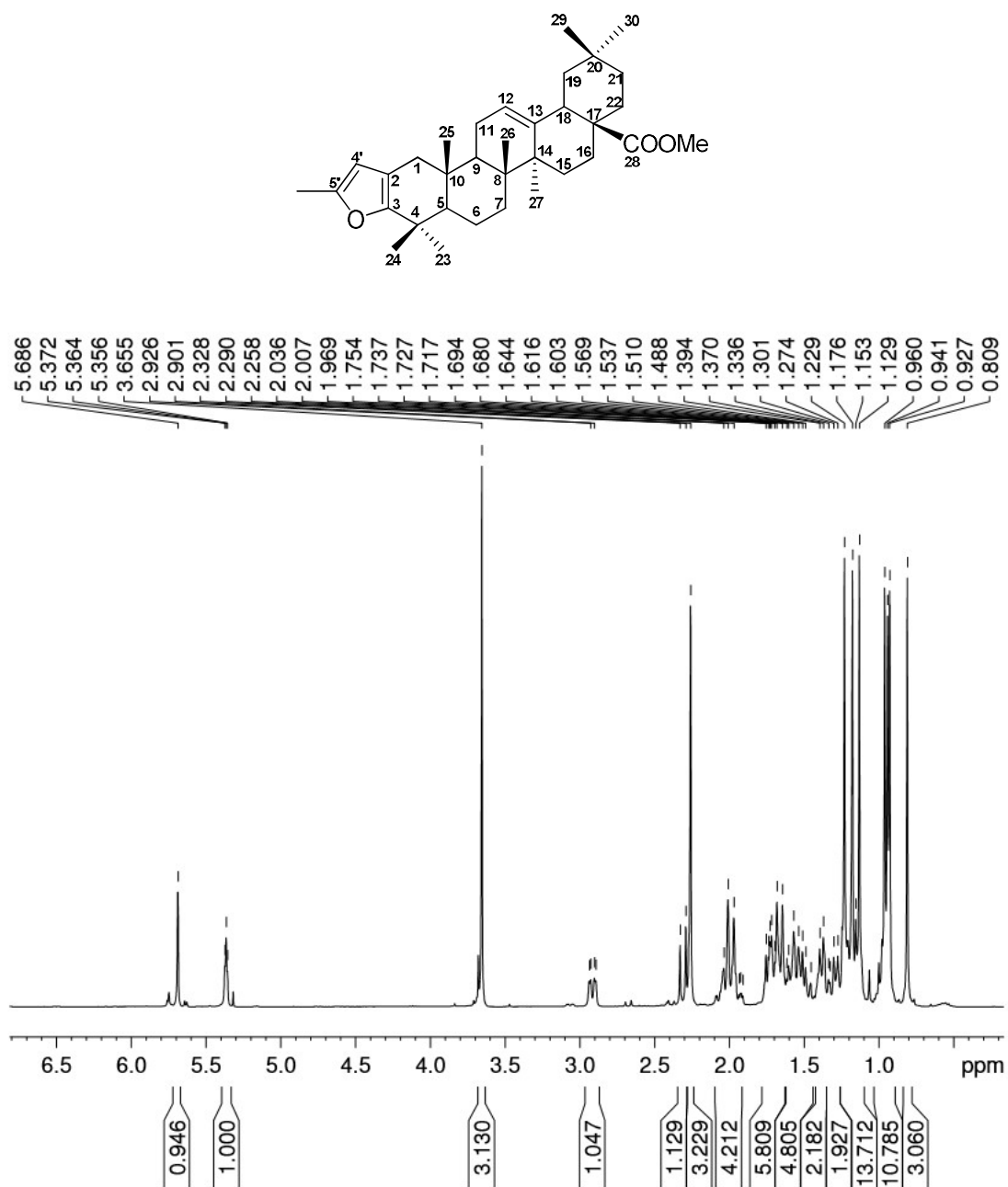
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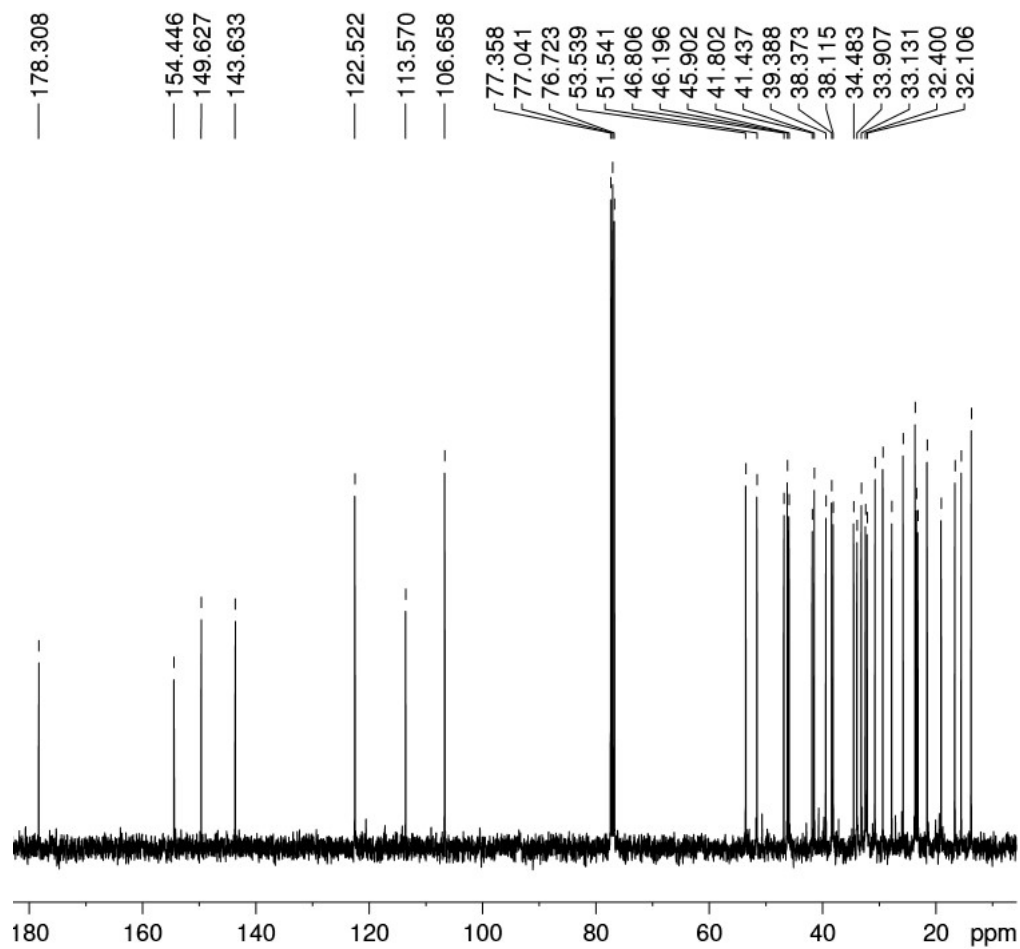
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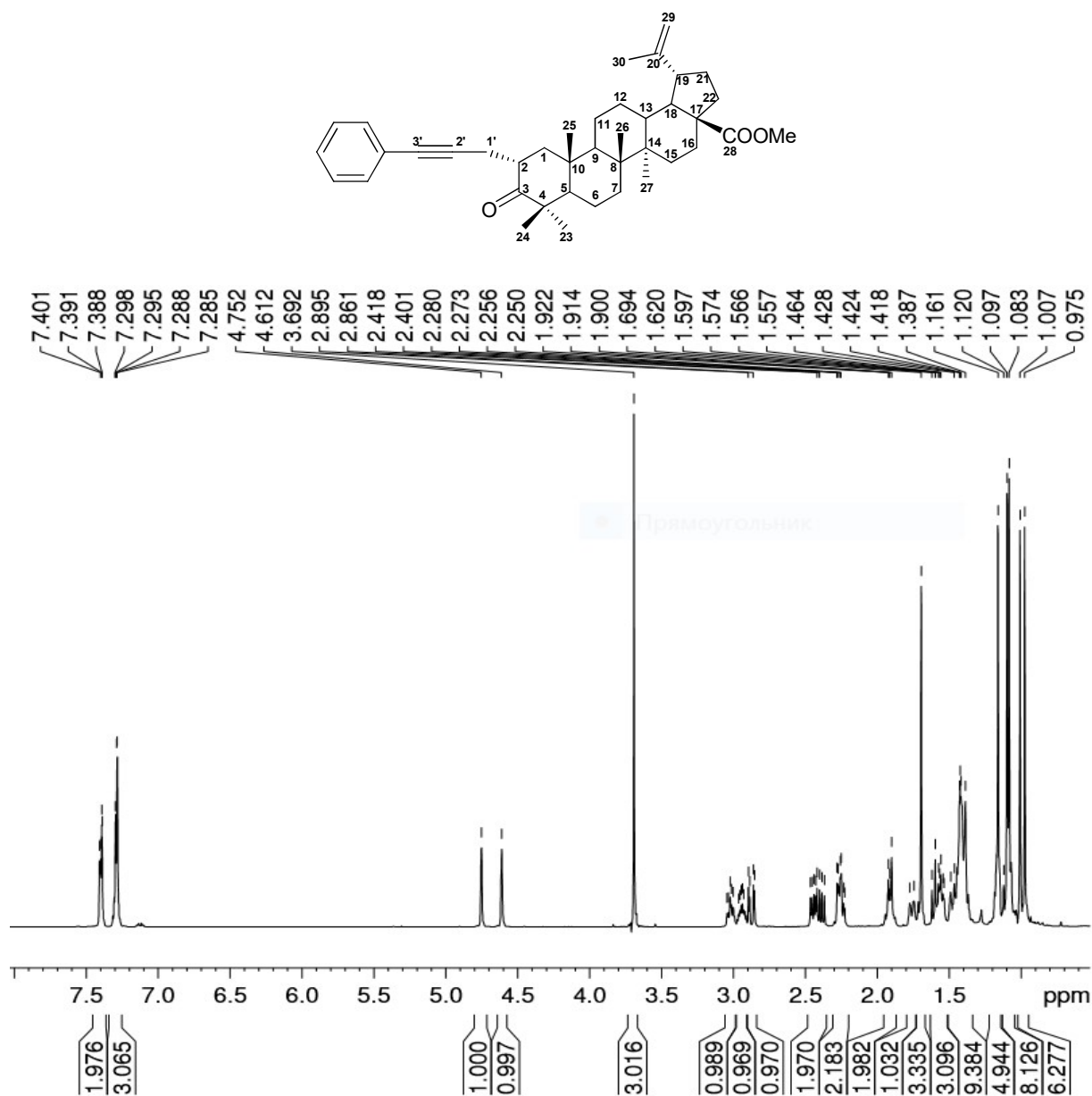
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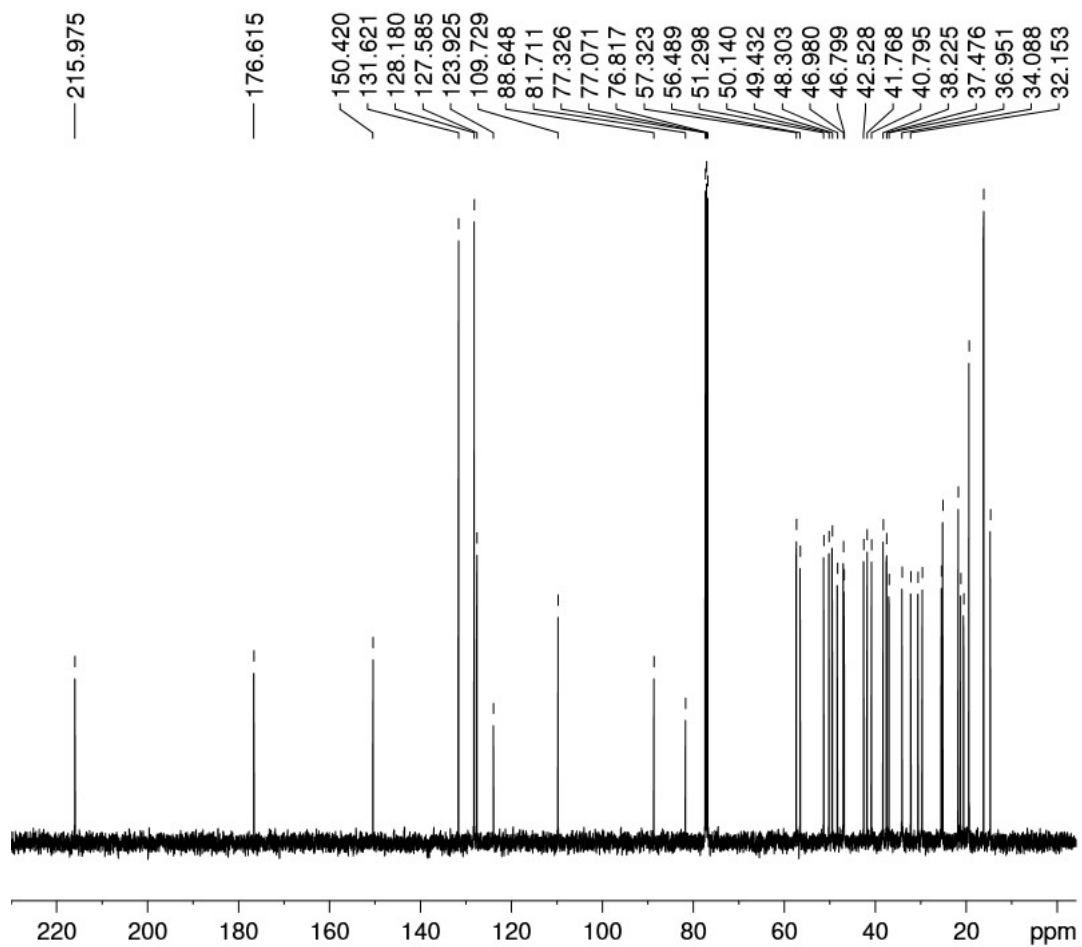
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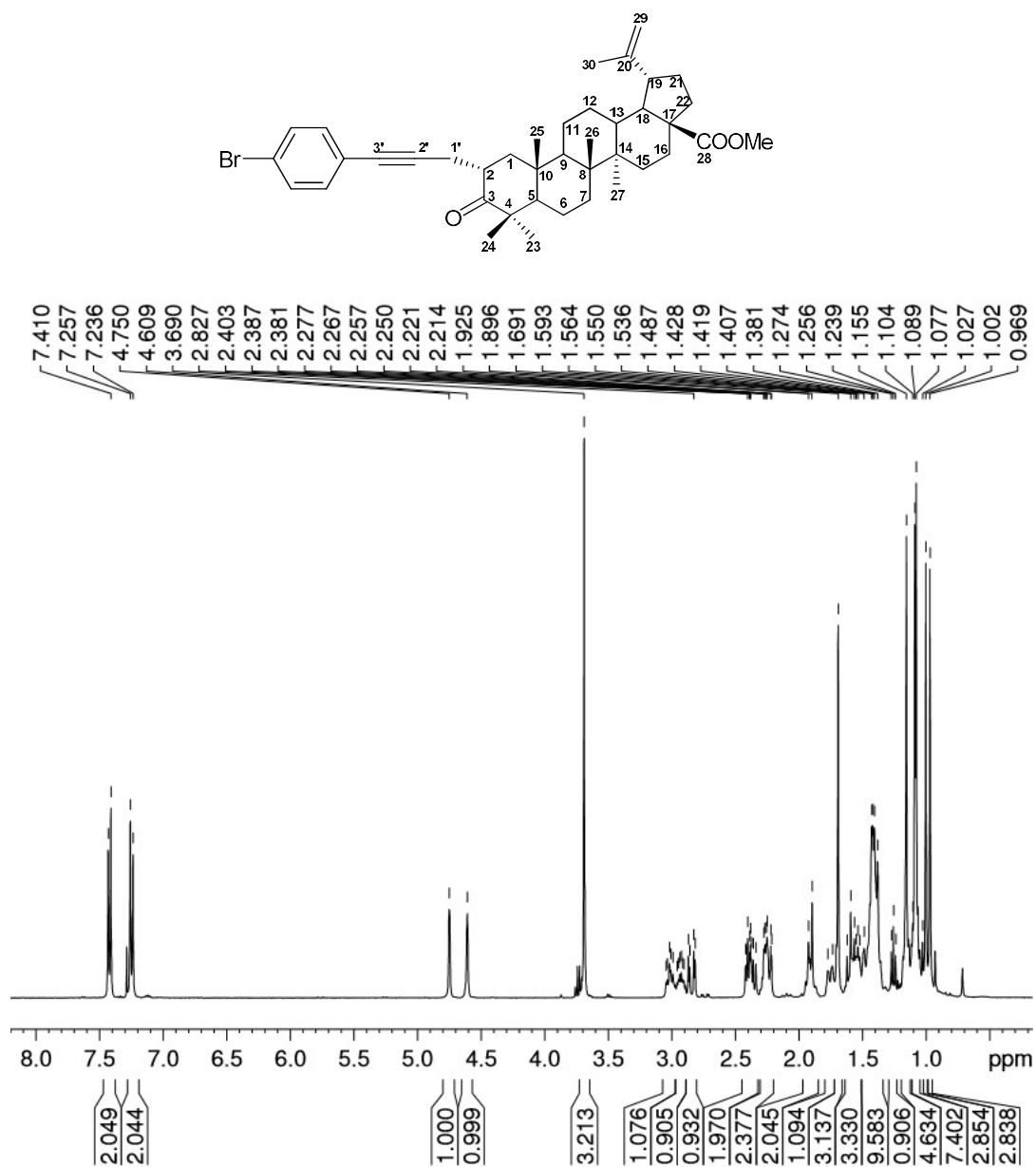
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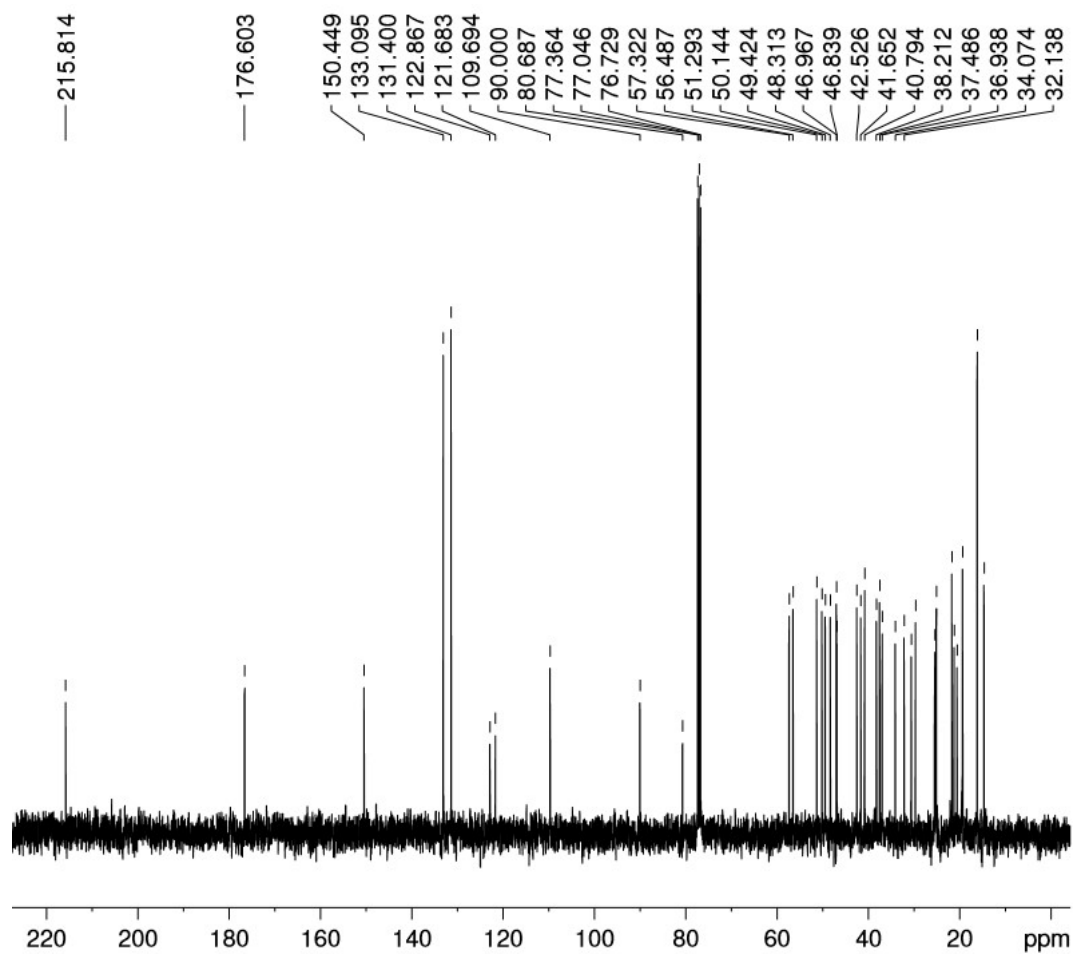
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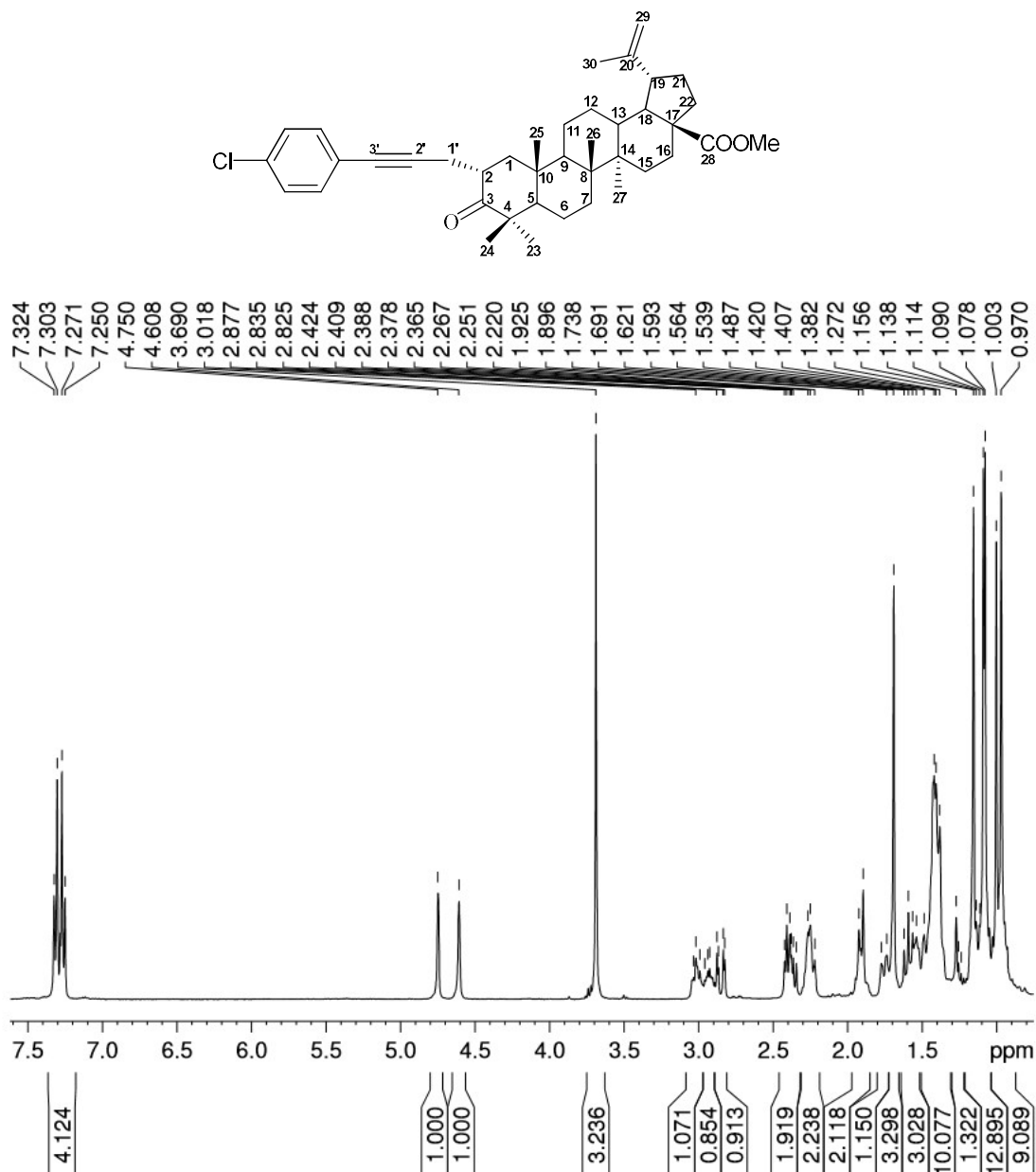
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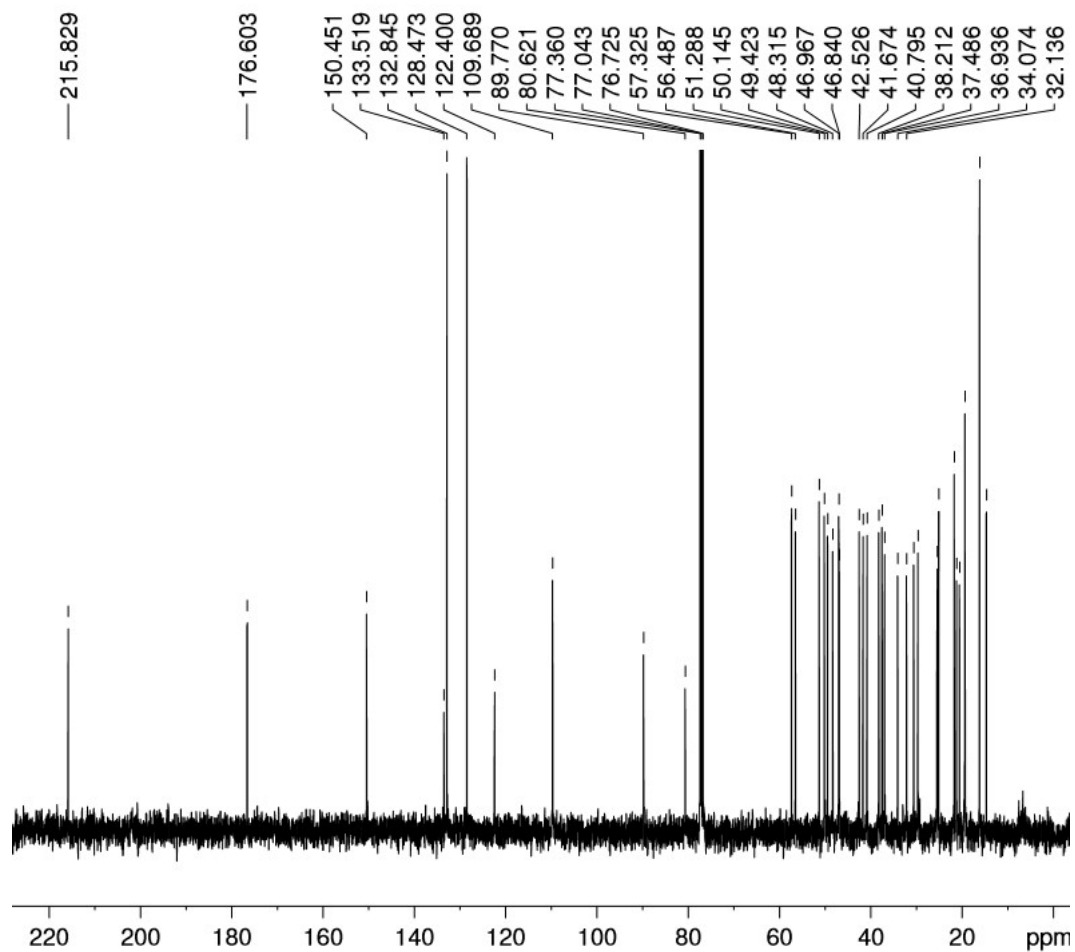
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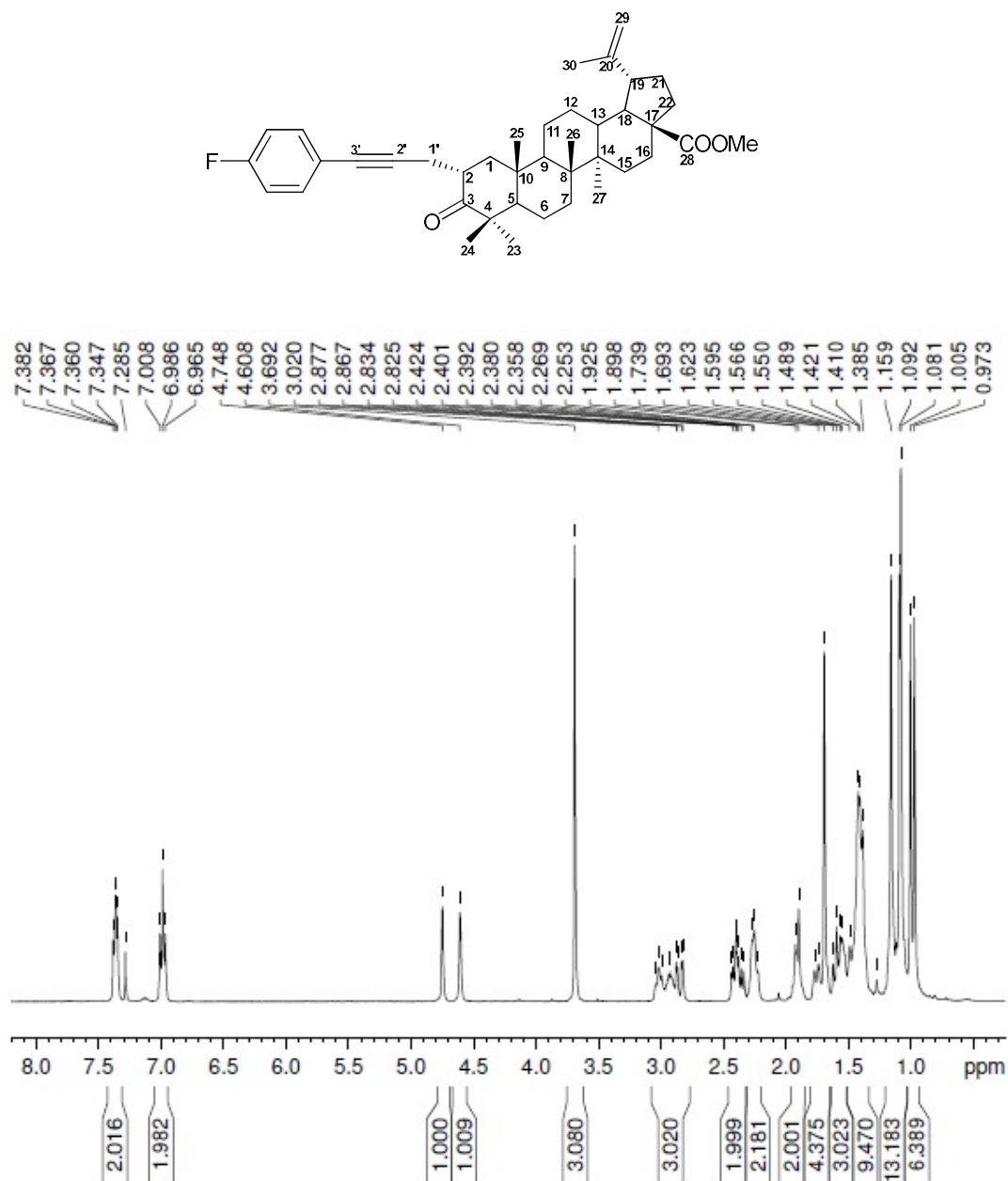
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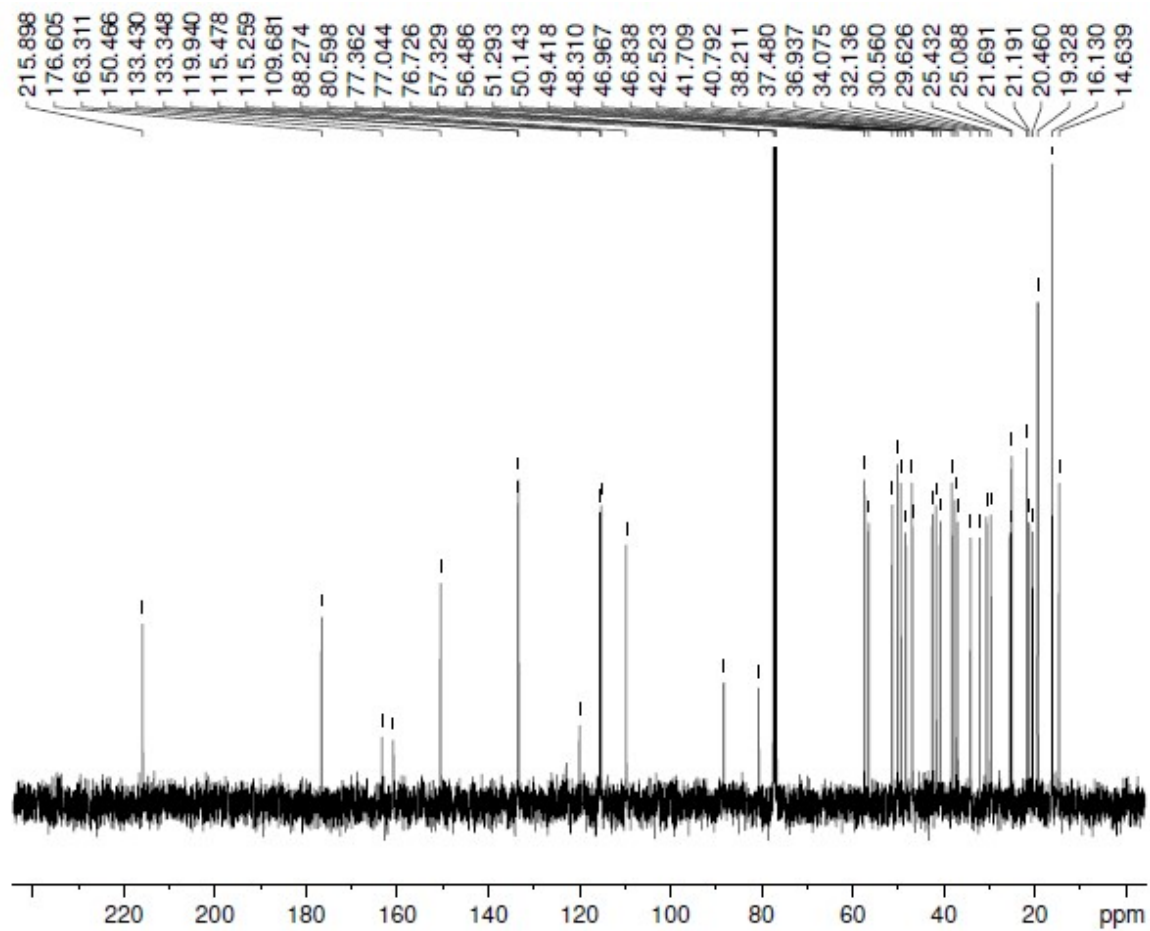
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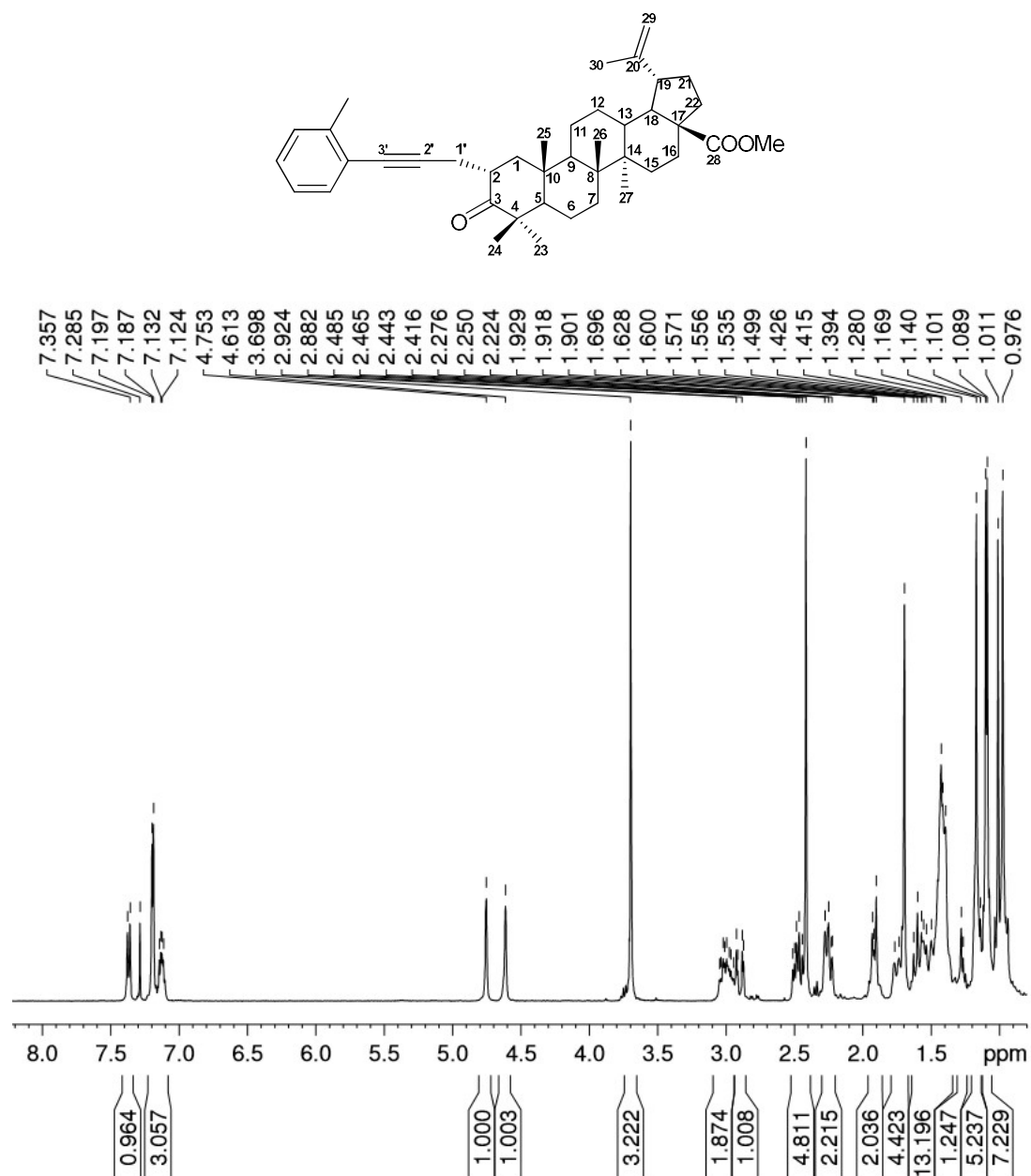
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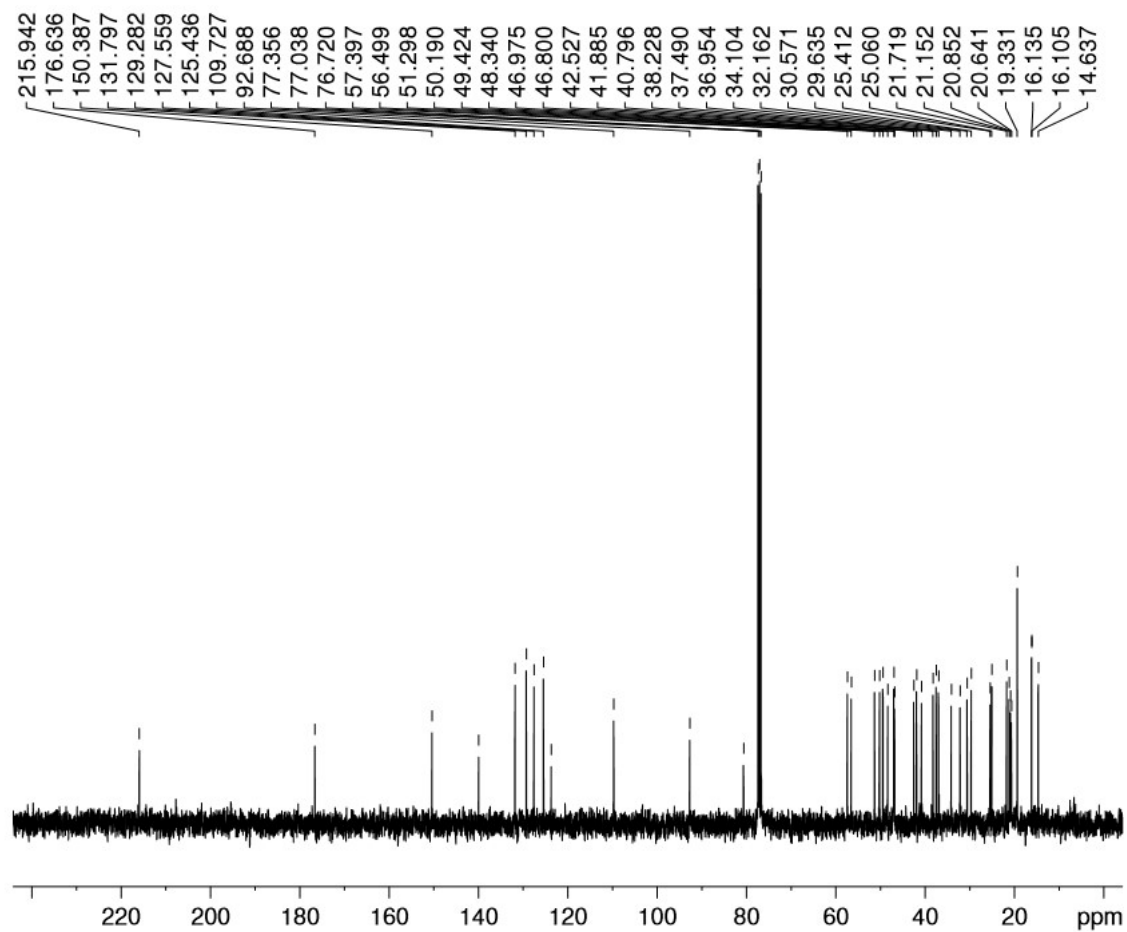
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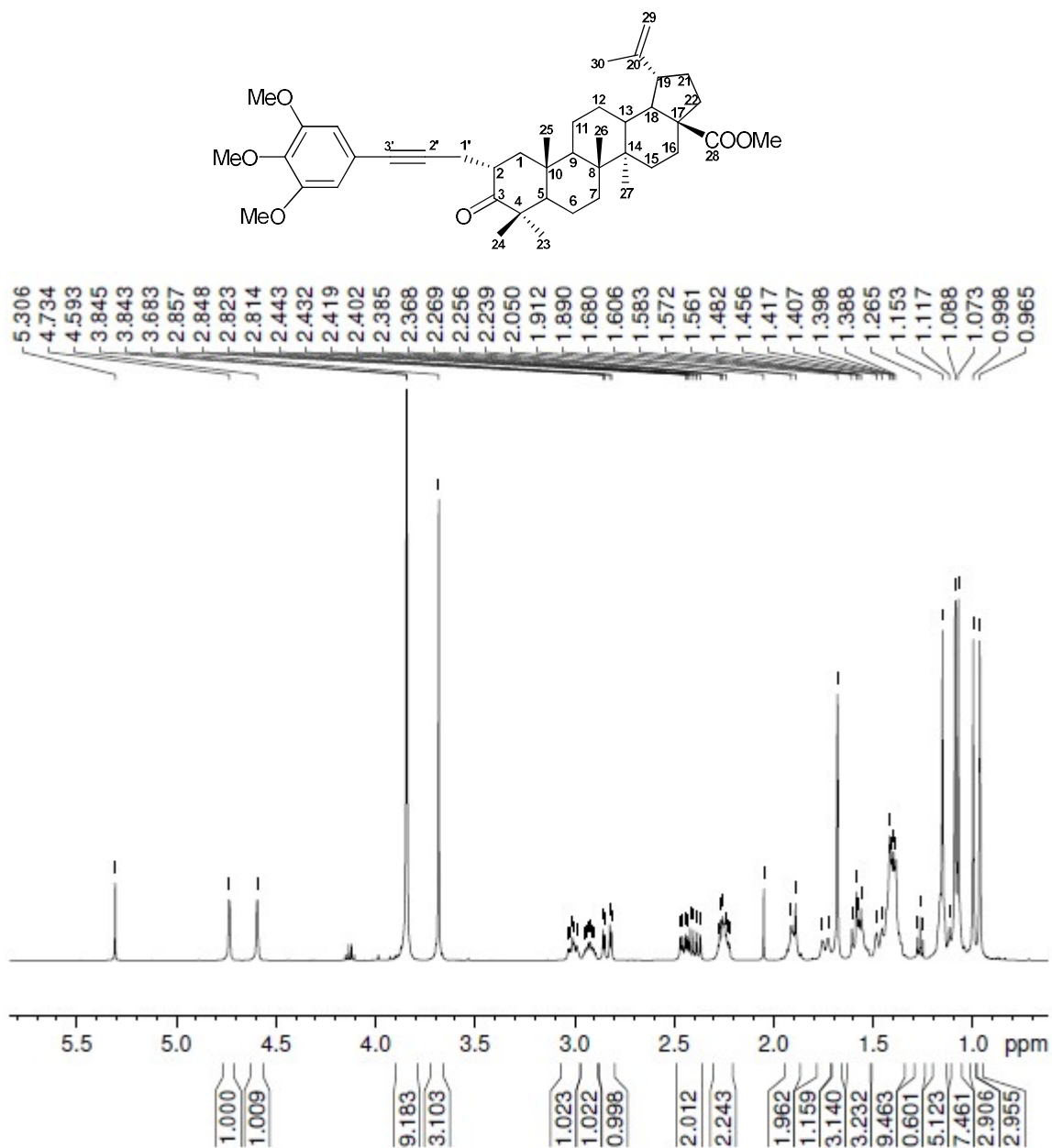
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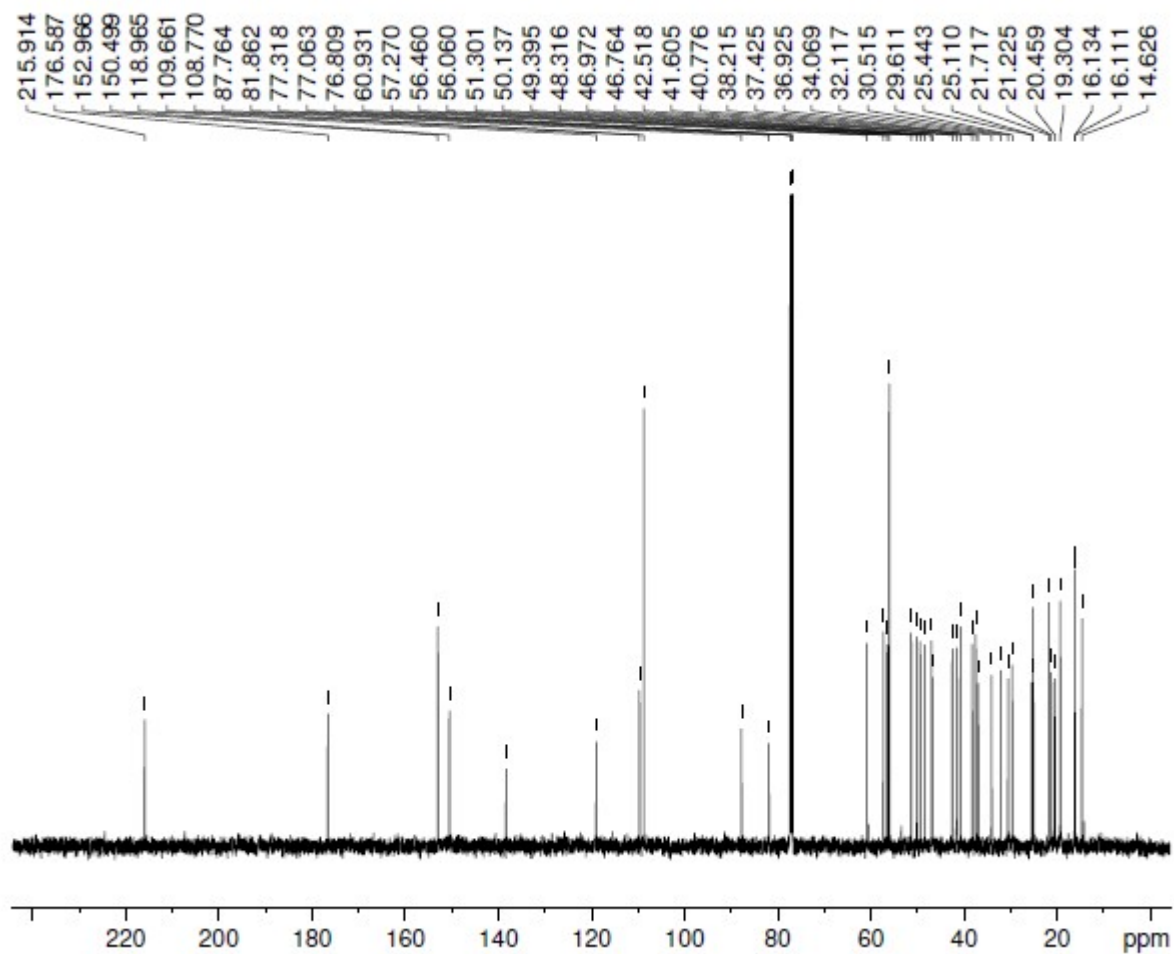
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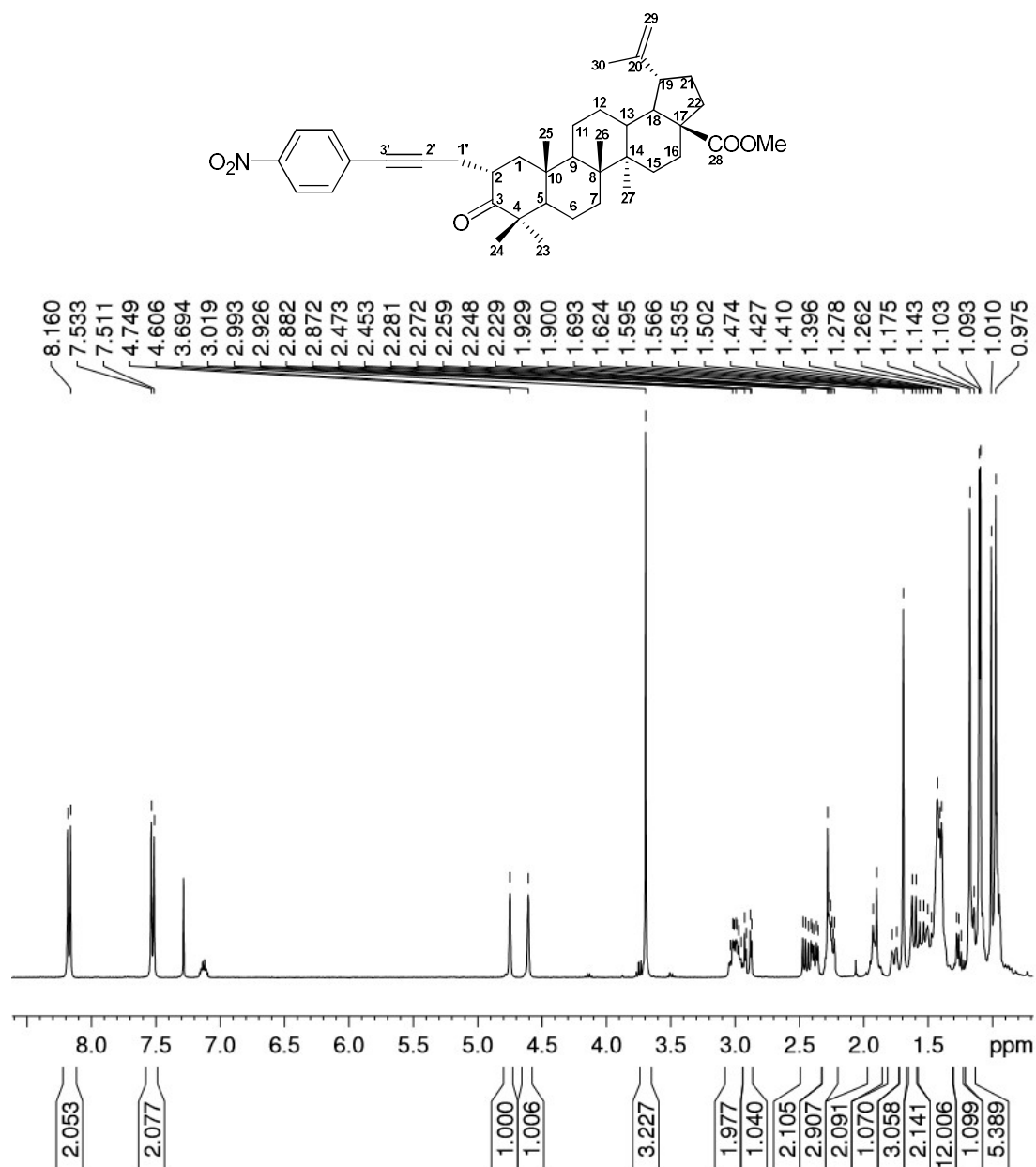
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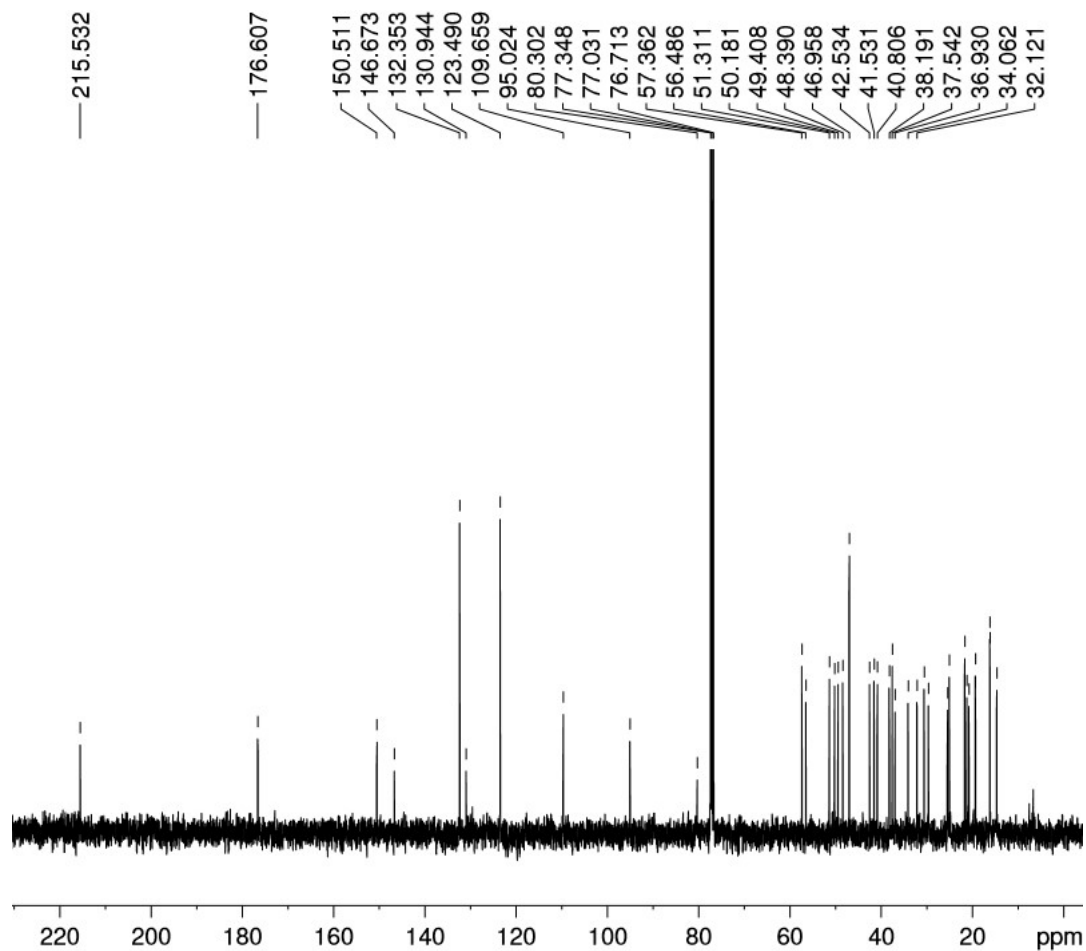
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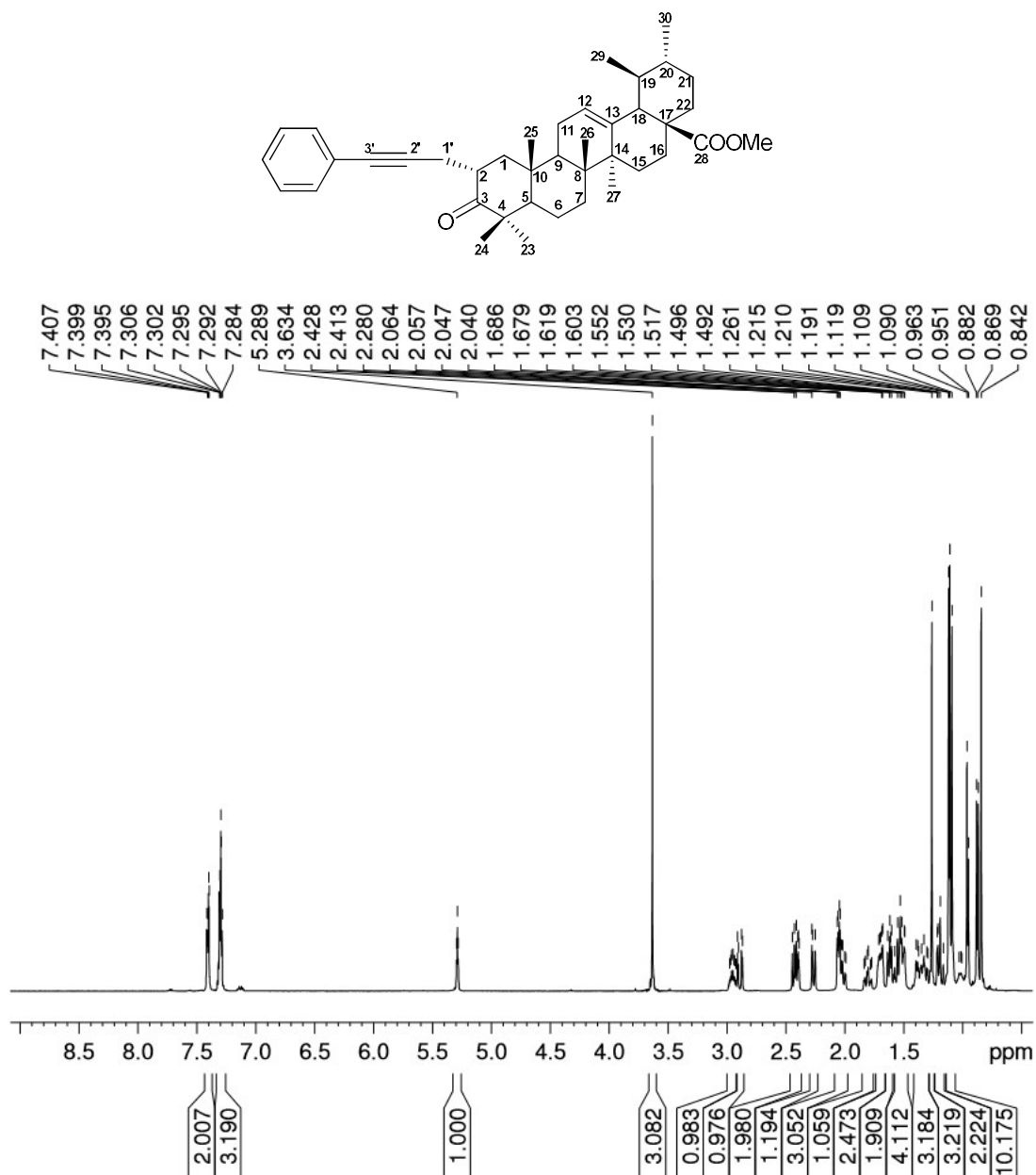
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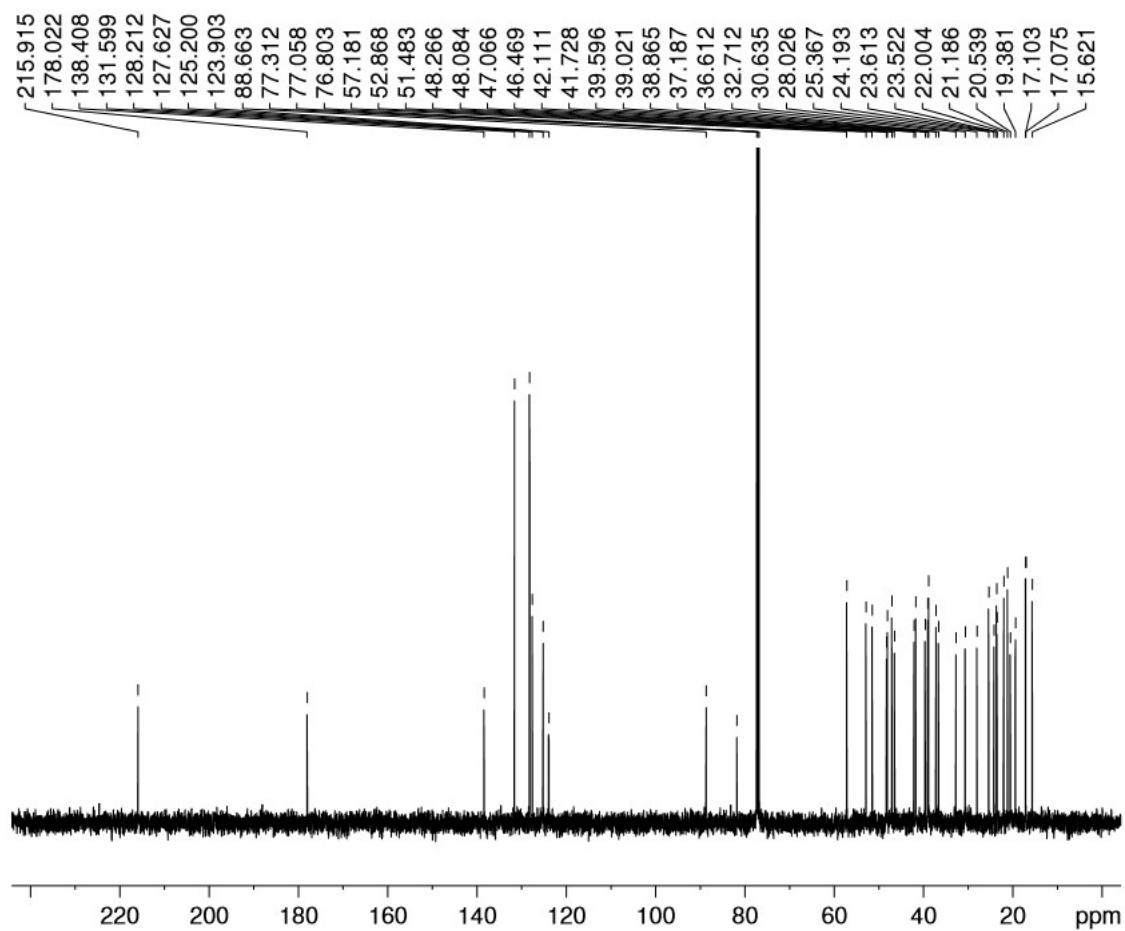
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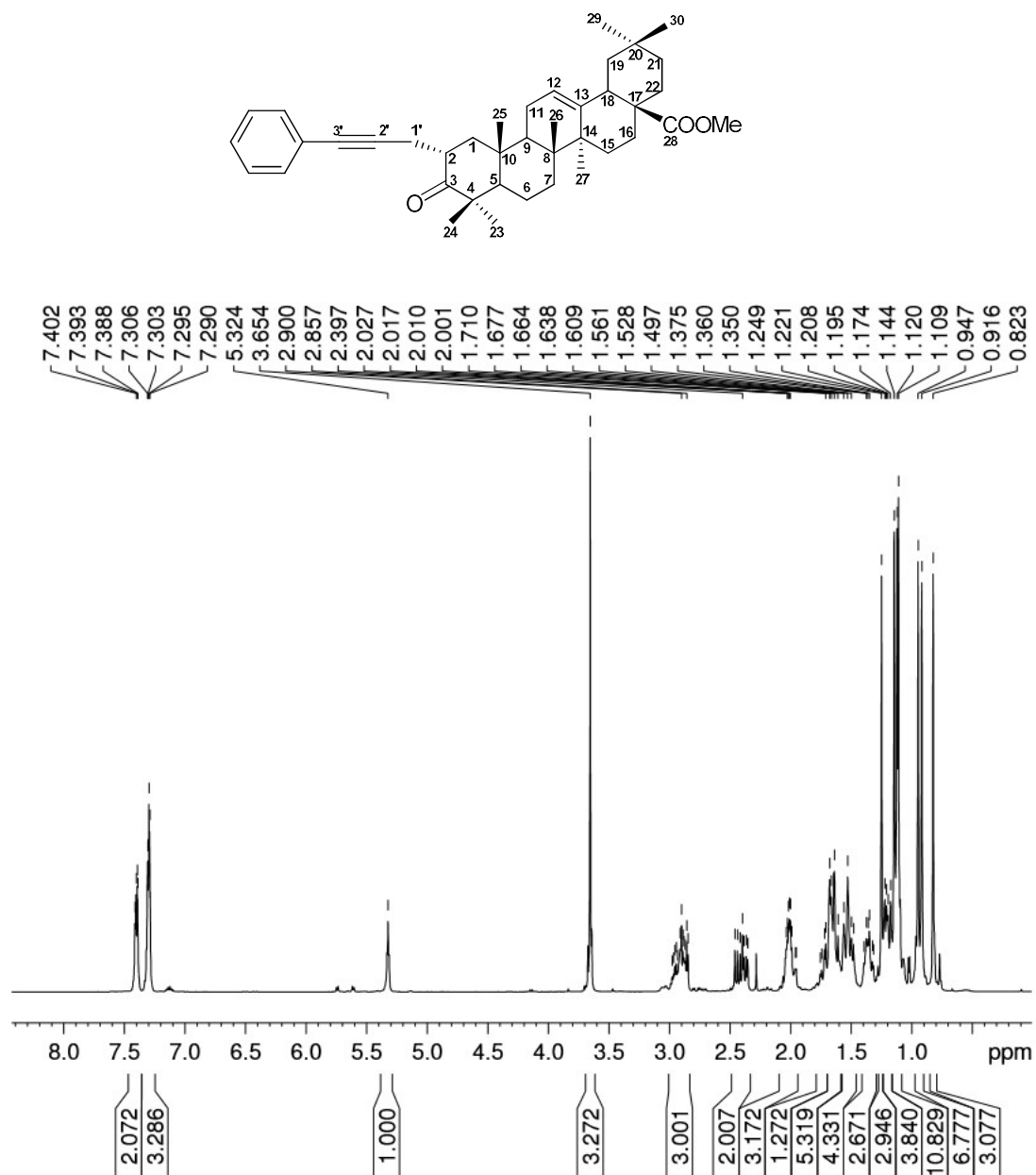


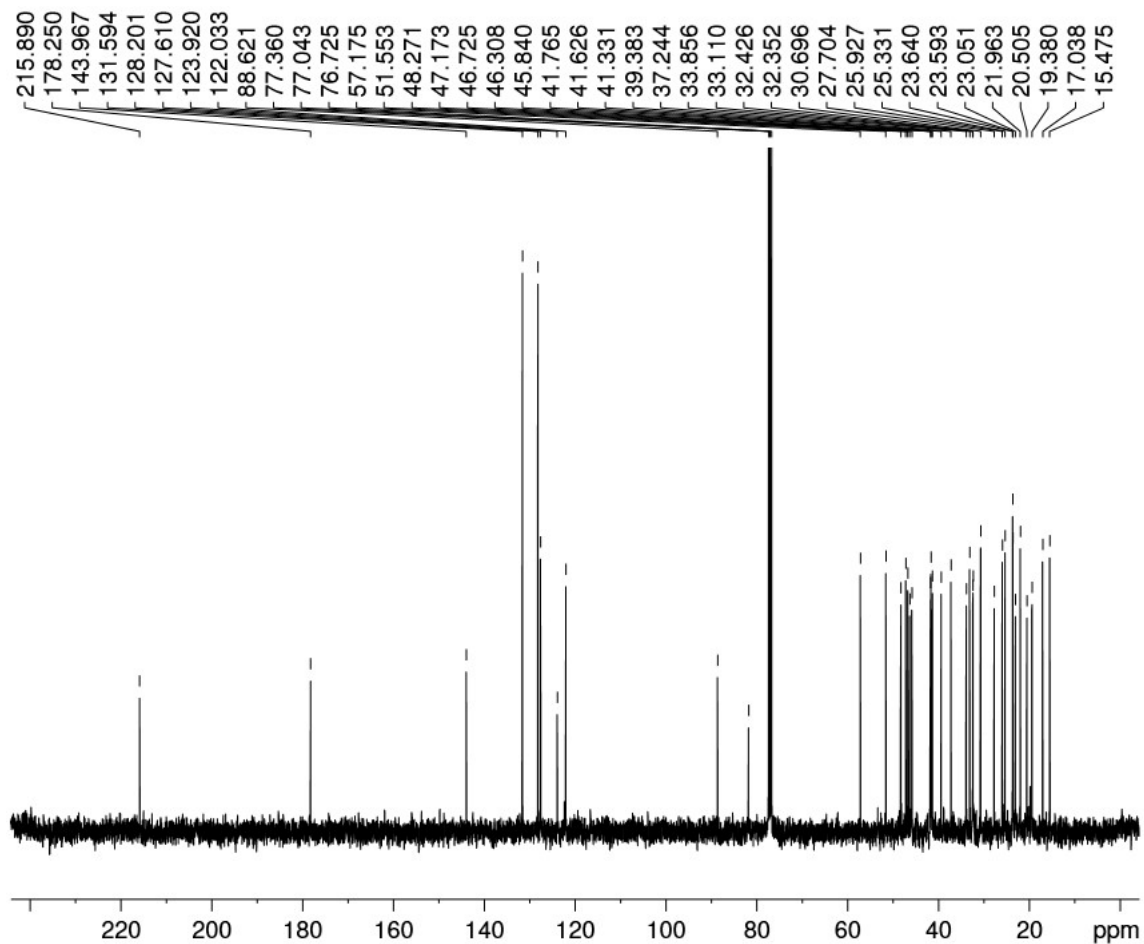
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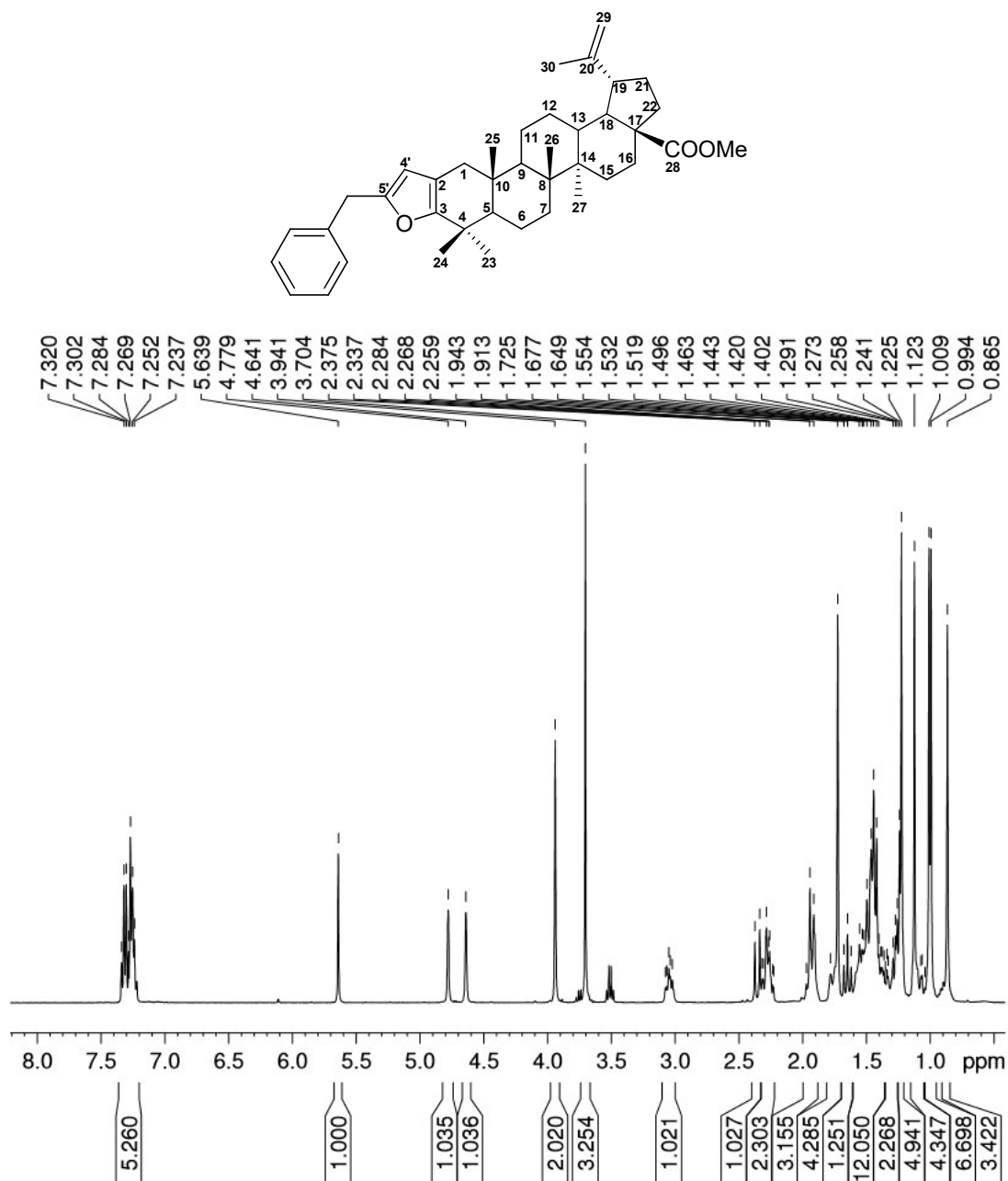
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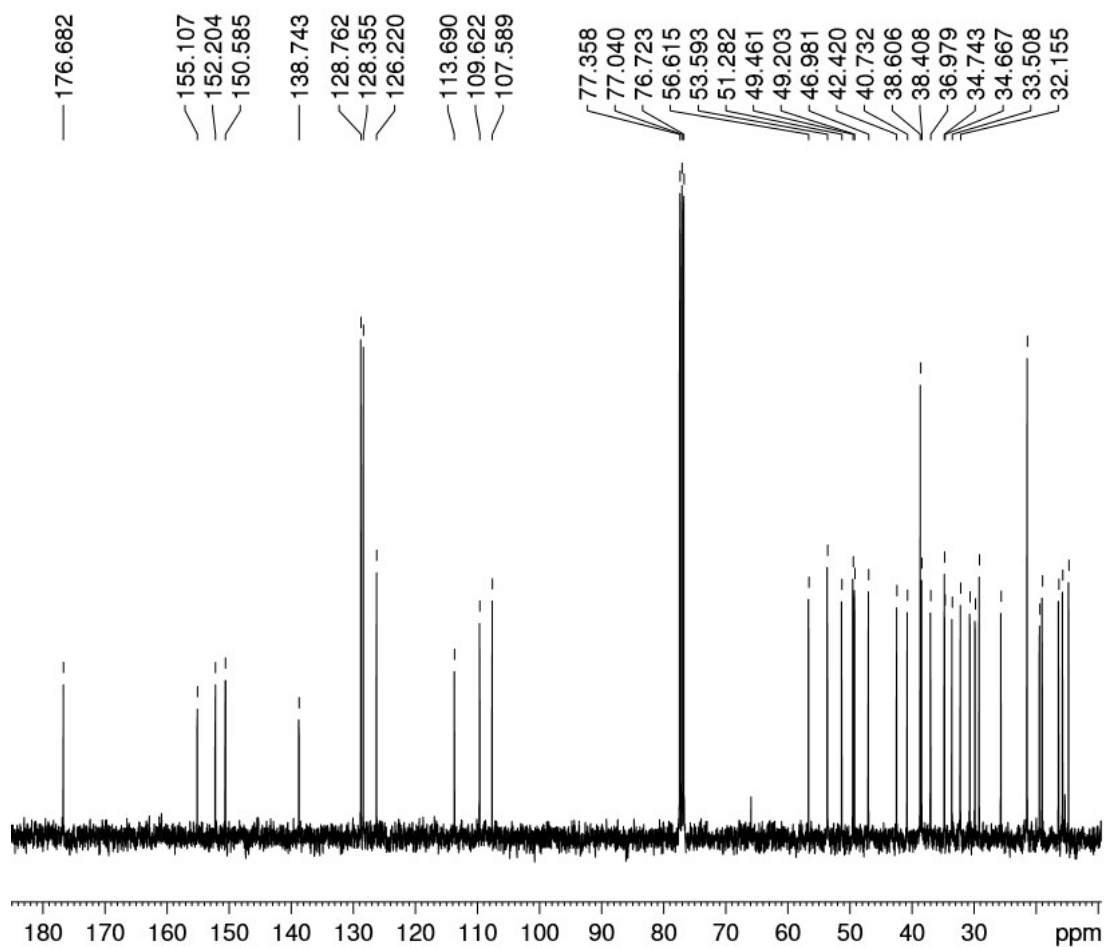
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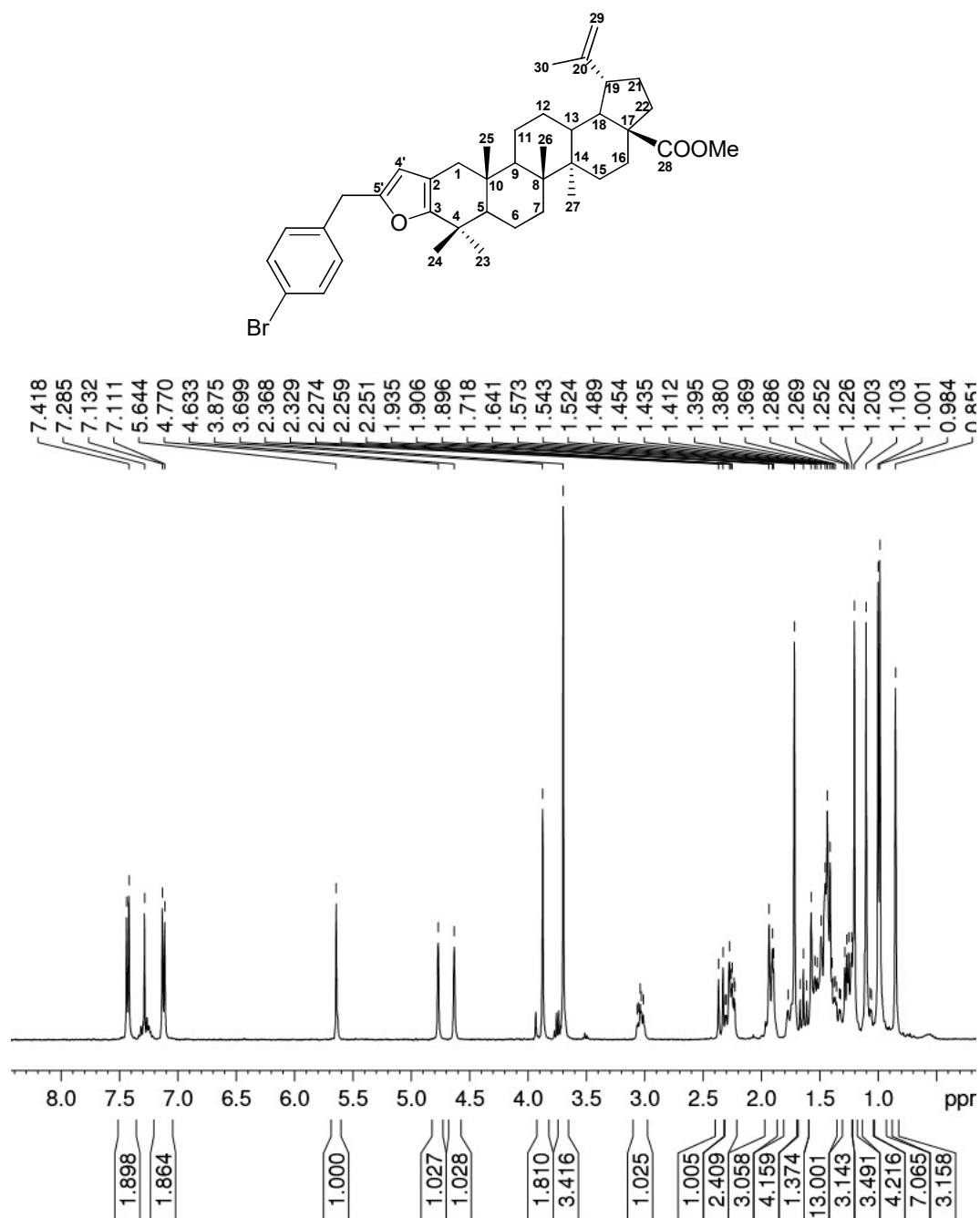
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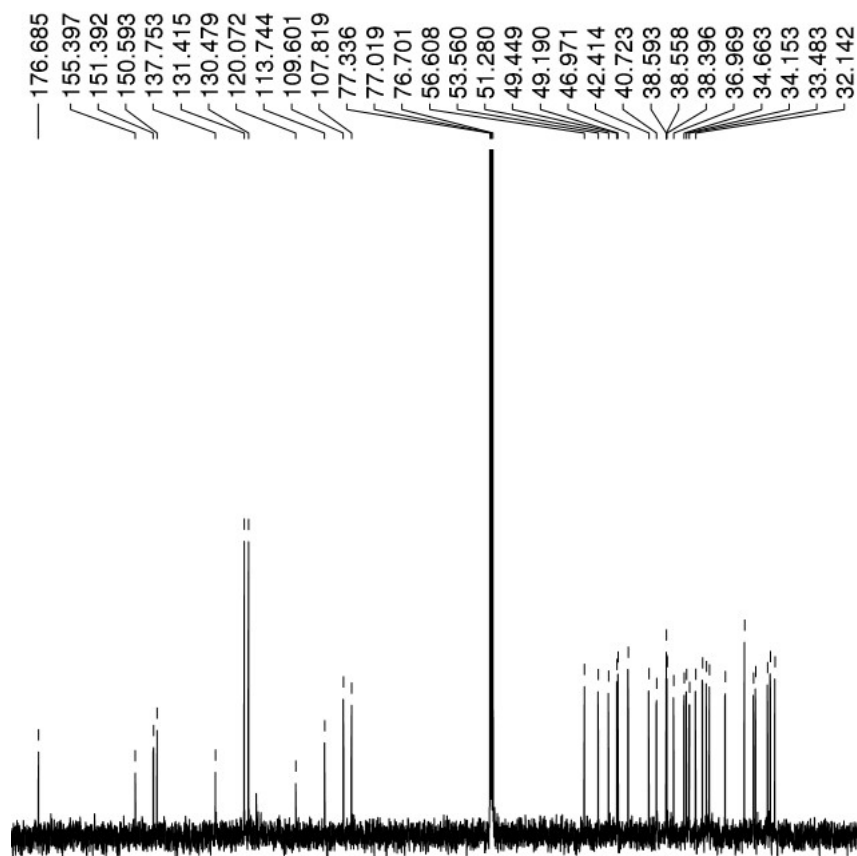
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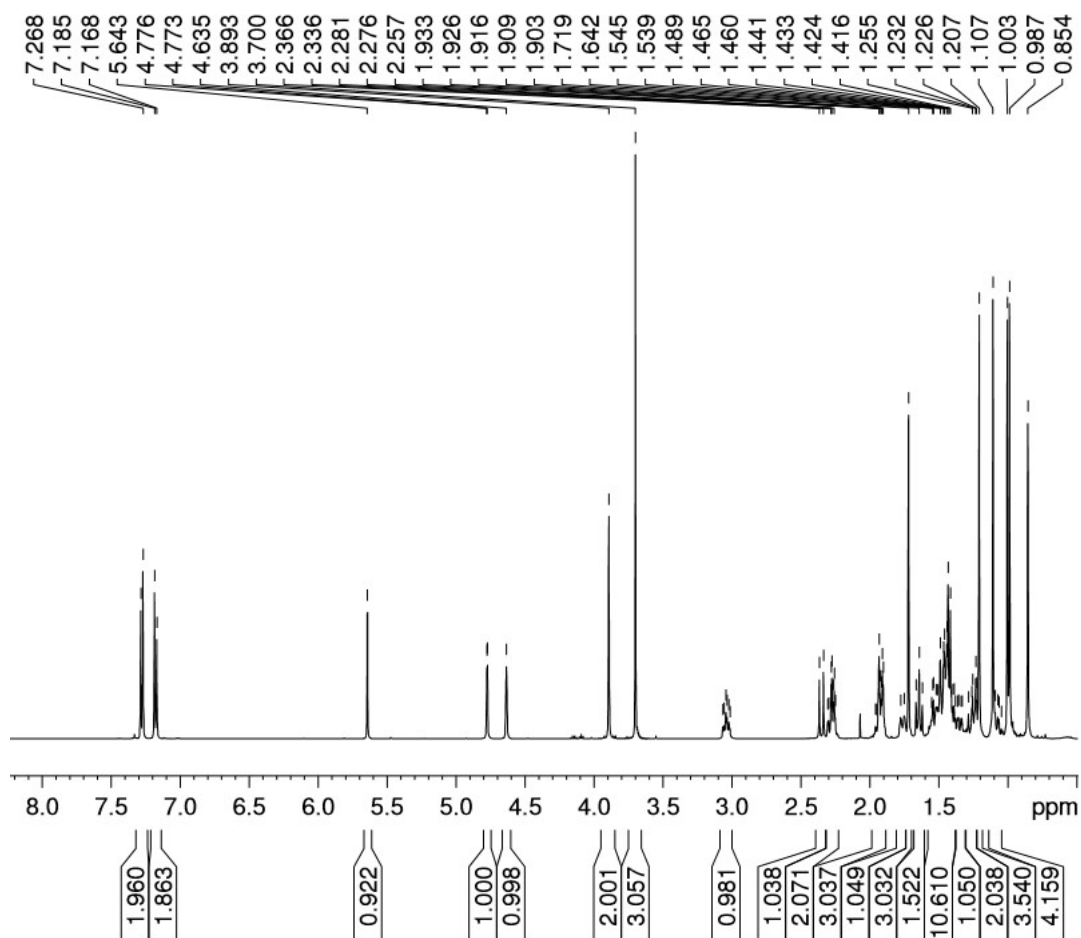
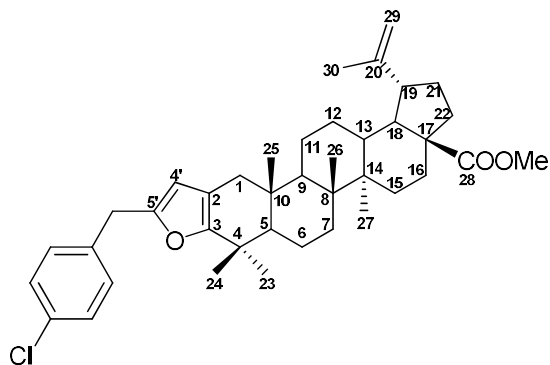
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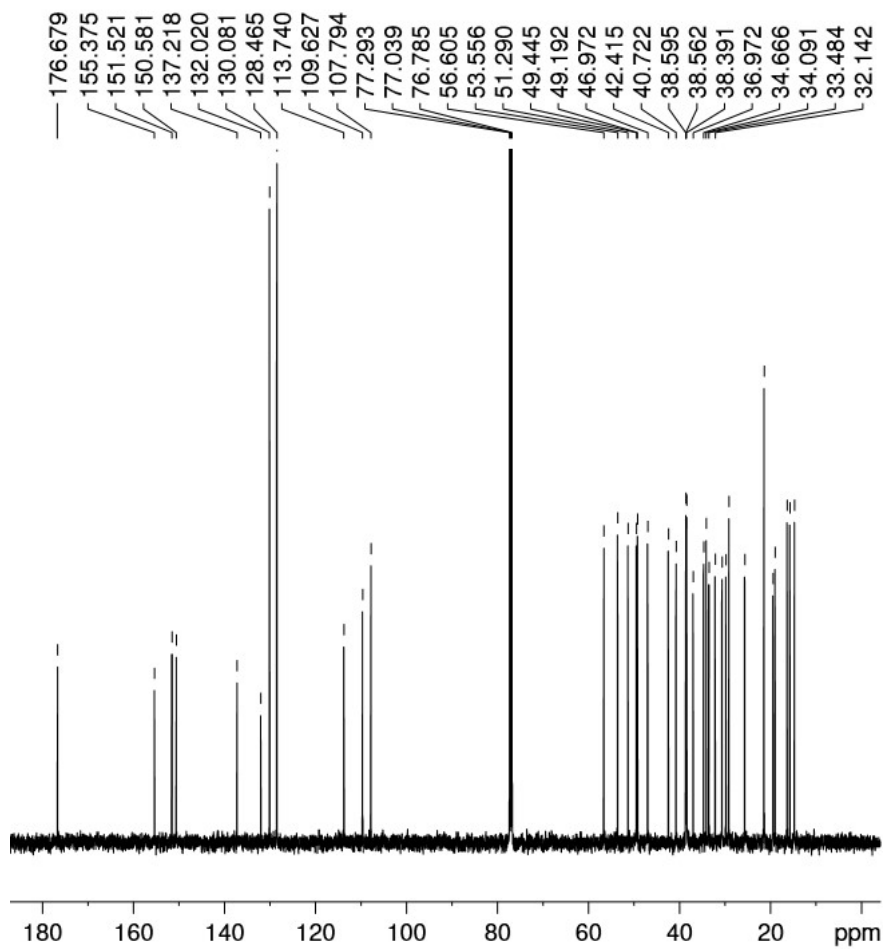
Methyl 5'-benzylfurano[3,2-b]lup-20(29)-en-28-oate **15a** ^1H NMR spectra (CDCl_3)

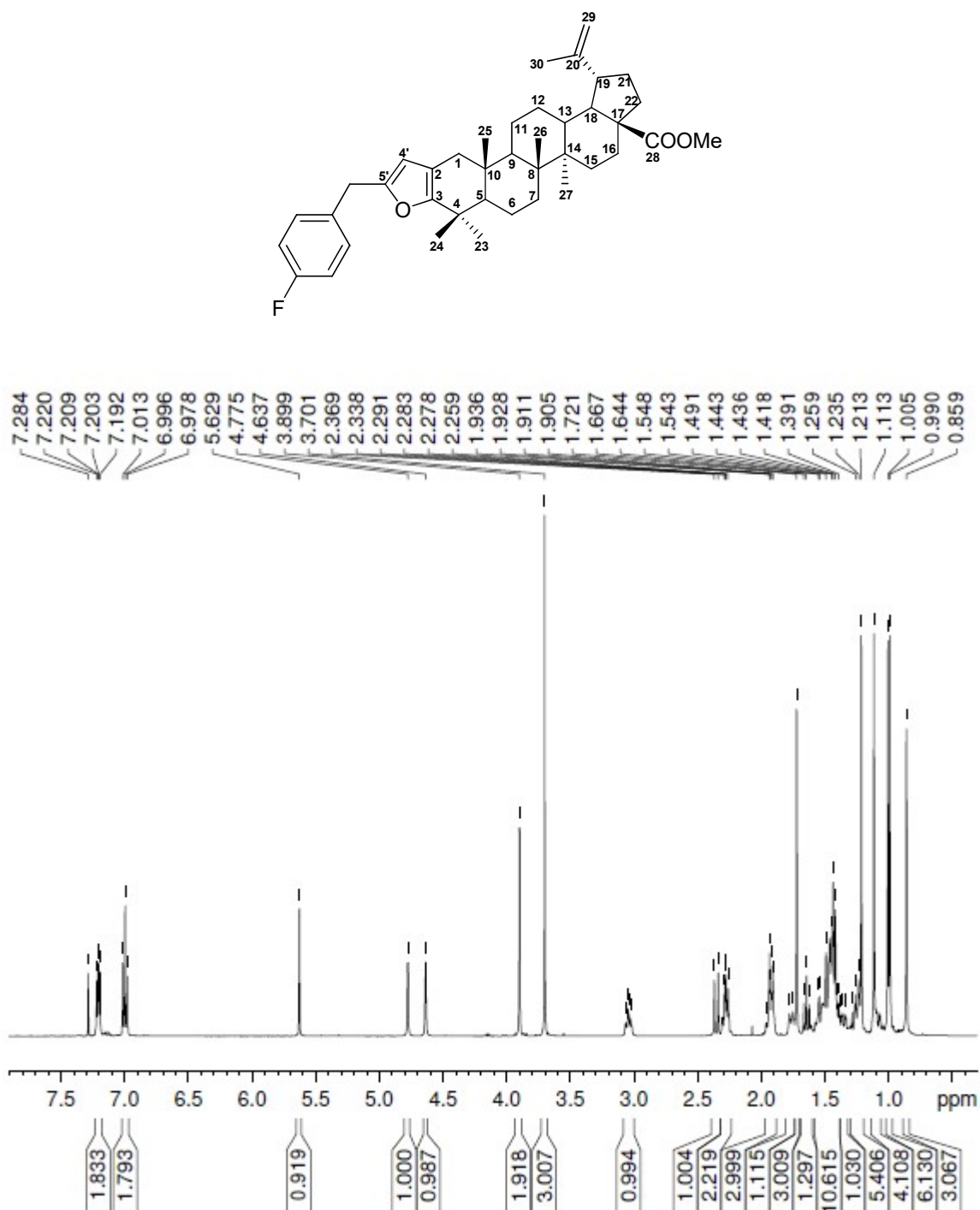
Methyl 5'-benzylfurano[3,2-b]lup-20(29)-en-28-oate **15a** ^{13}C NMR spectra (CDCl_3)

Methyl 5'-(4-bromobenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15b** ^1H NMR spectra (CDCl_3)

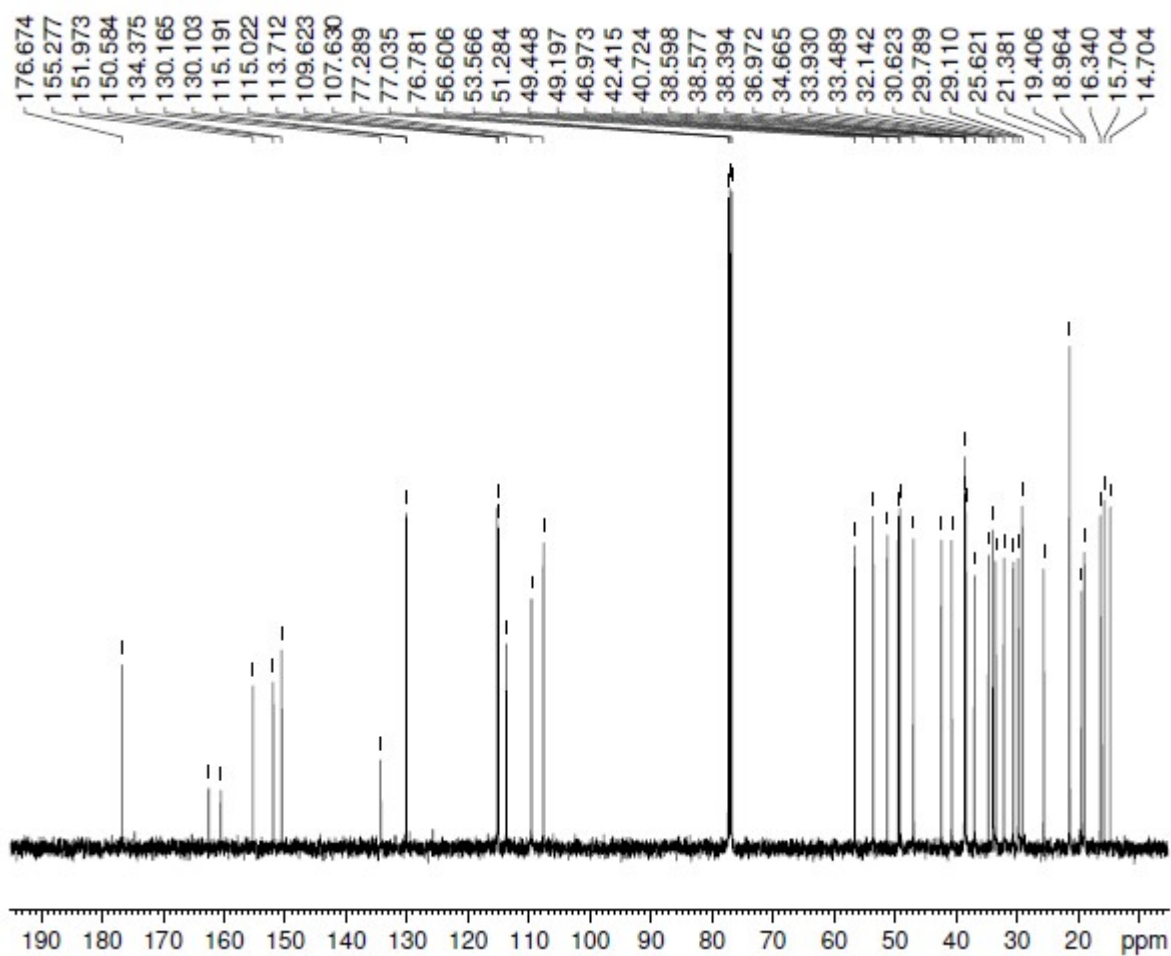
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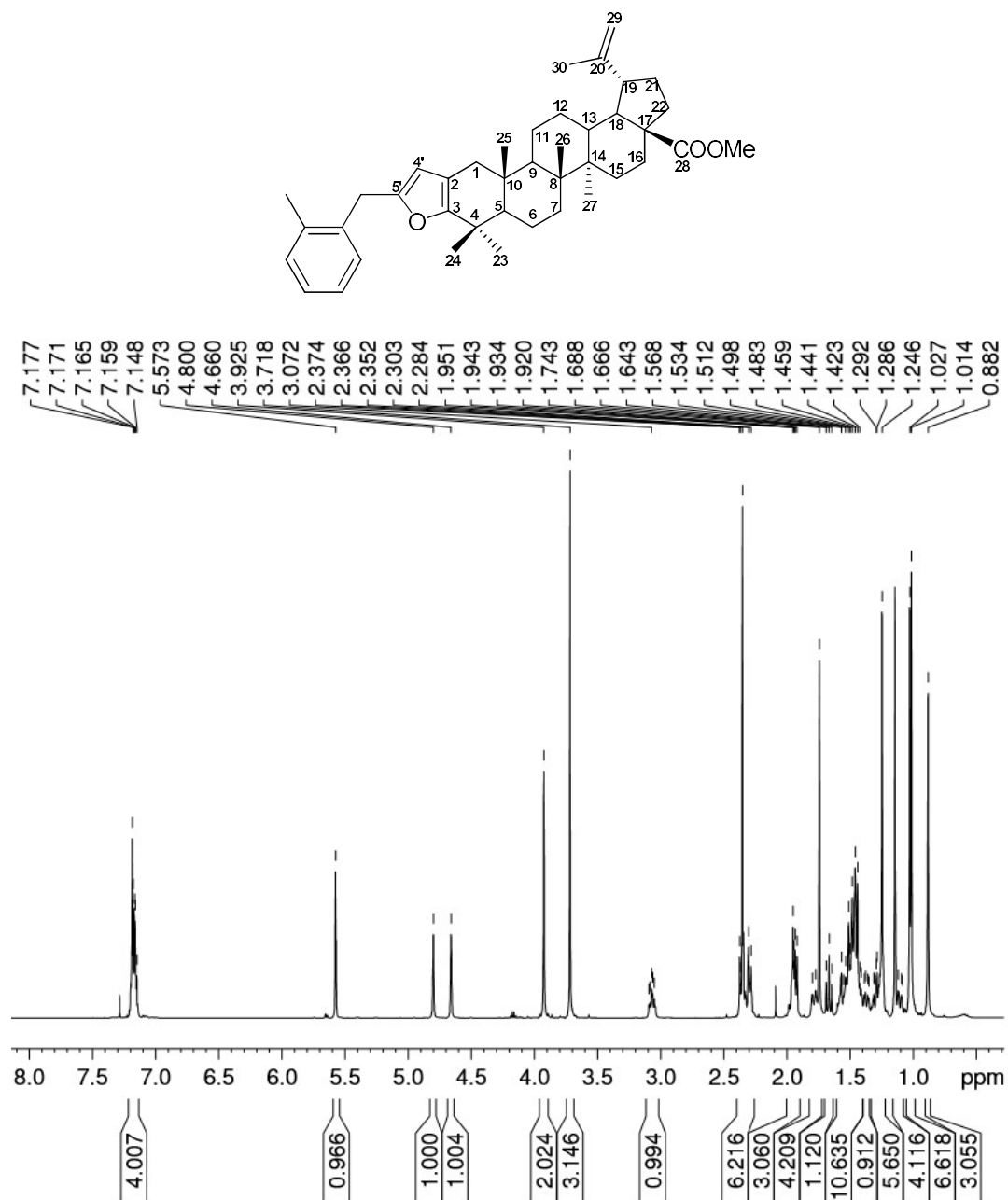
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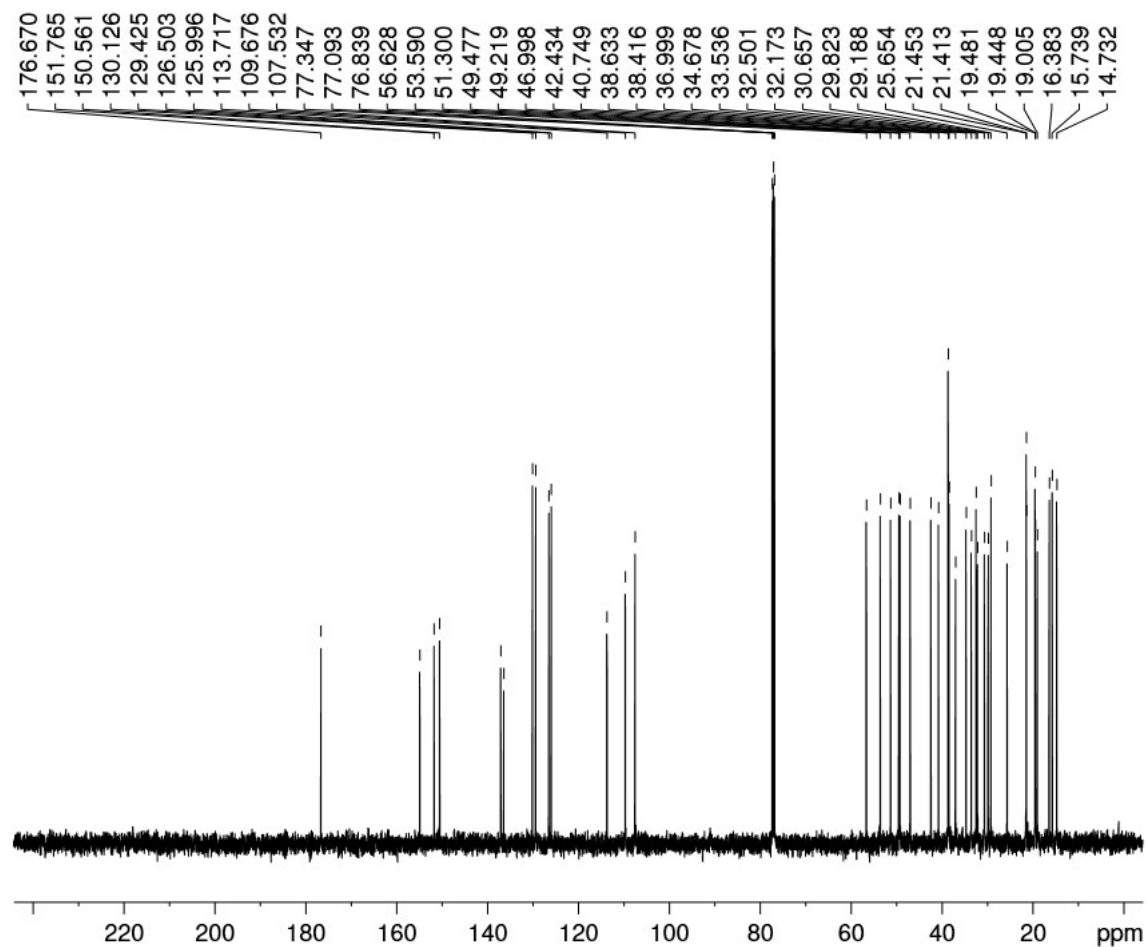
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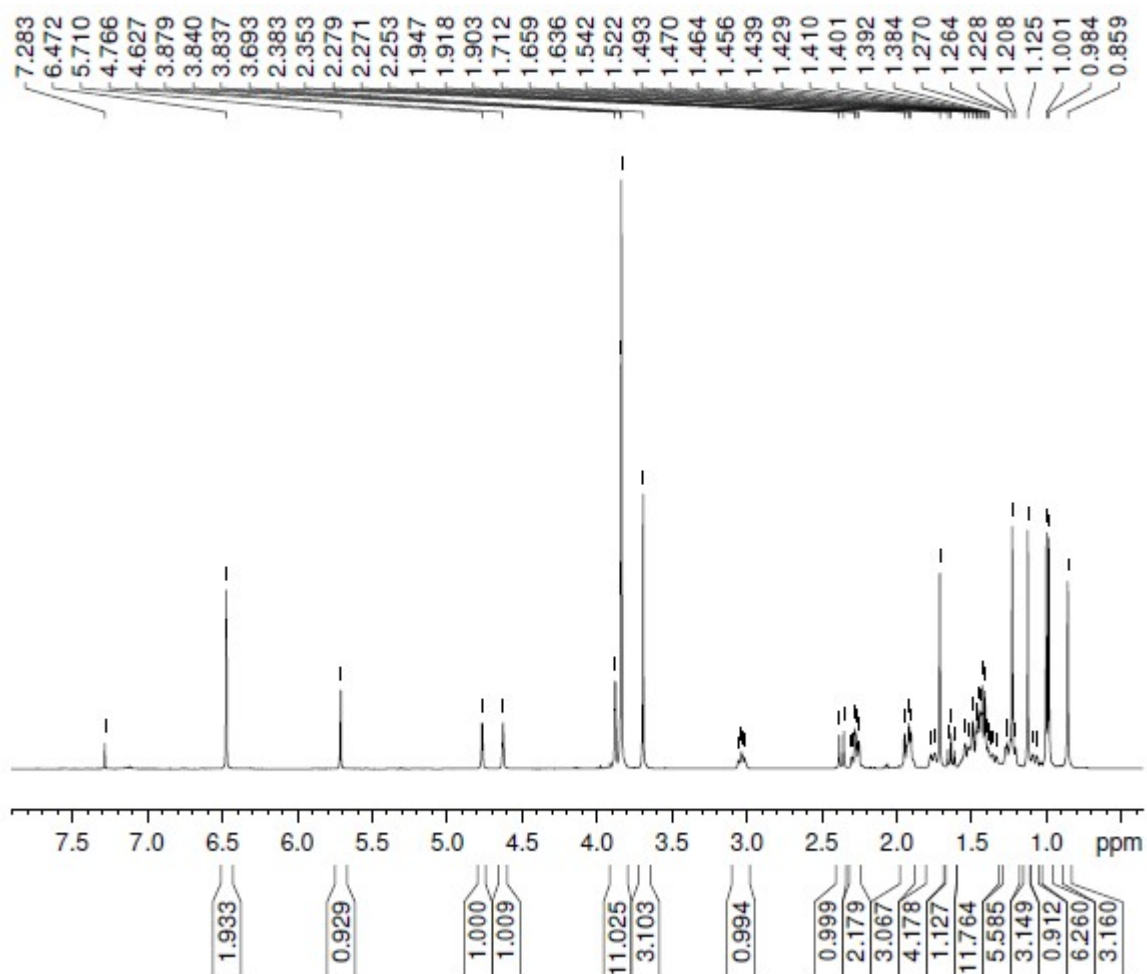
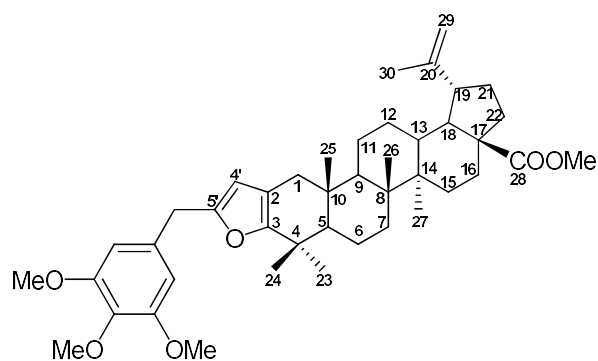
Methyl 5'-(4-fluorobenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15d** ^{13}C NMR spectra (CDCl_3)



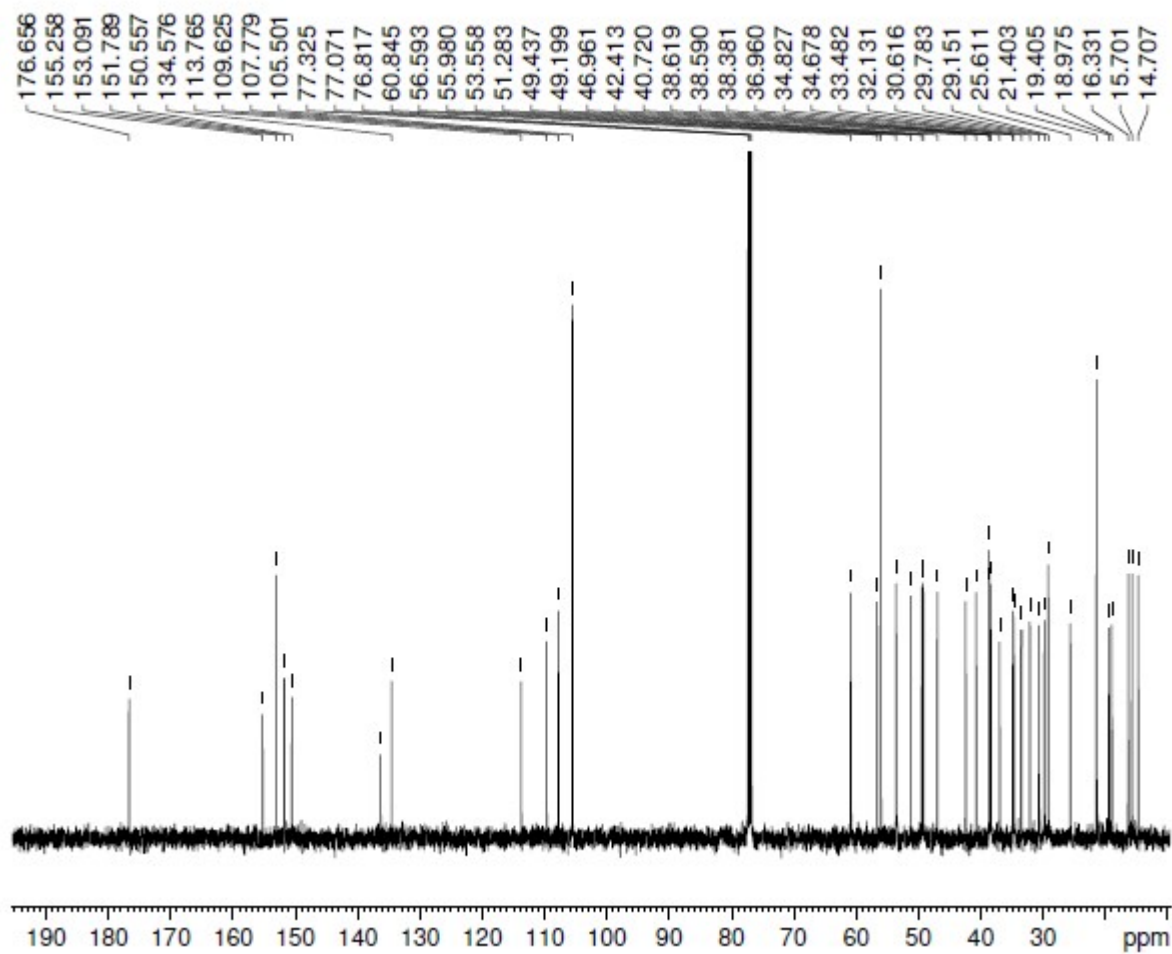
Methyl 5'-(2-methylbenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15e** ^1H NMR spectra (CDCl_3)

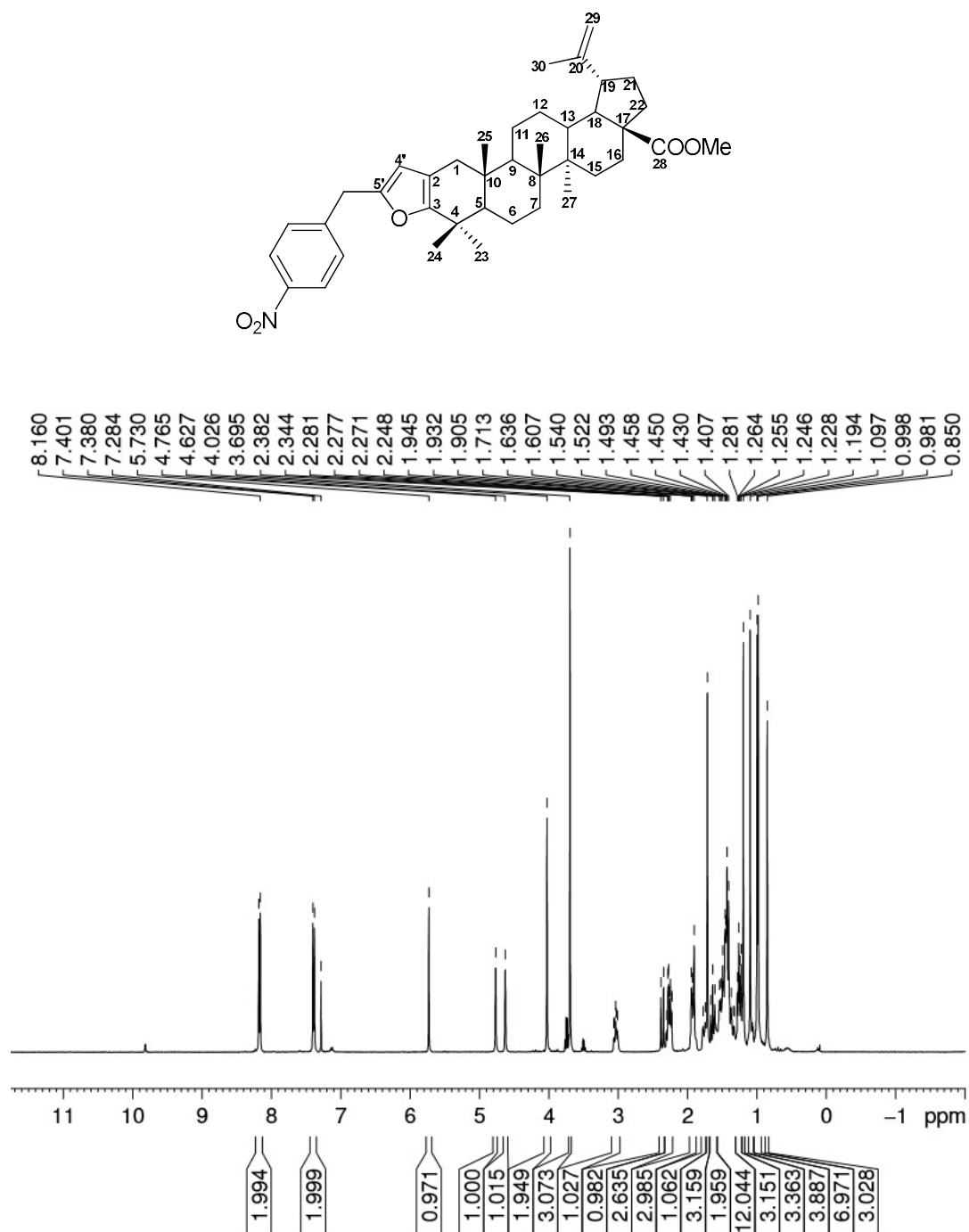
Methyl 5'-(2-methylbenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15e** ^{13}C NMR spectra (CDCl_3)

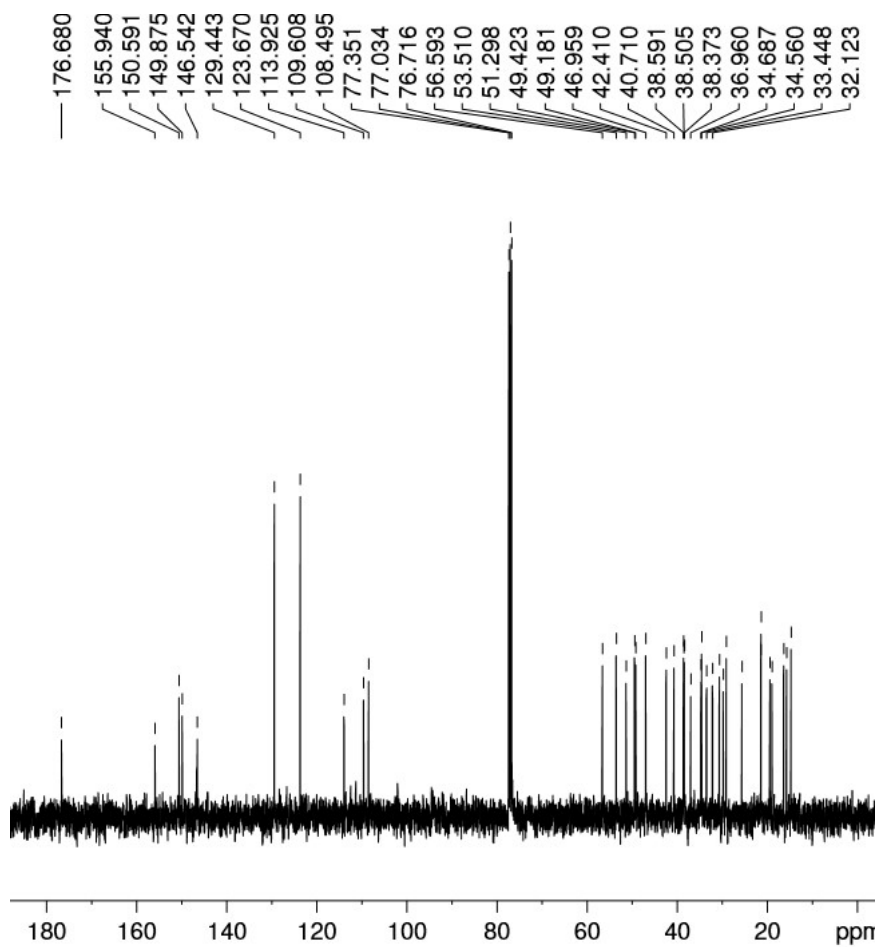
Methyl 5'-(3,4,5-trimethoxybenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15f** ^1H NMR spectra (CDCl_3)

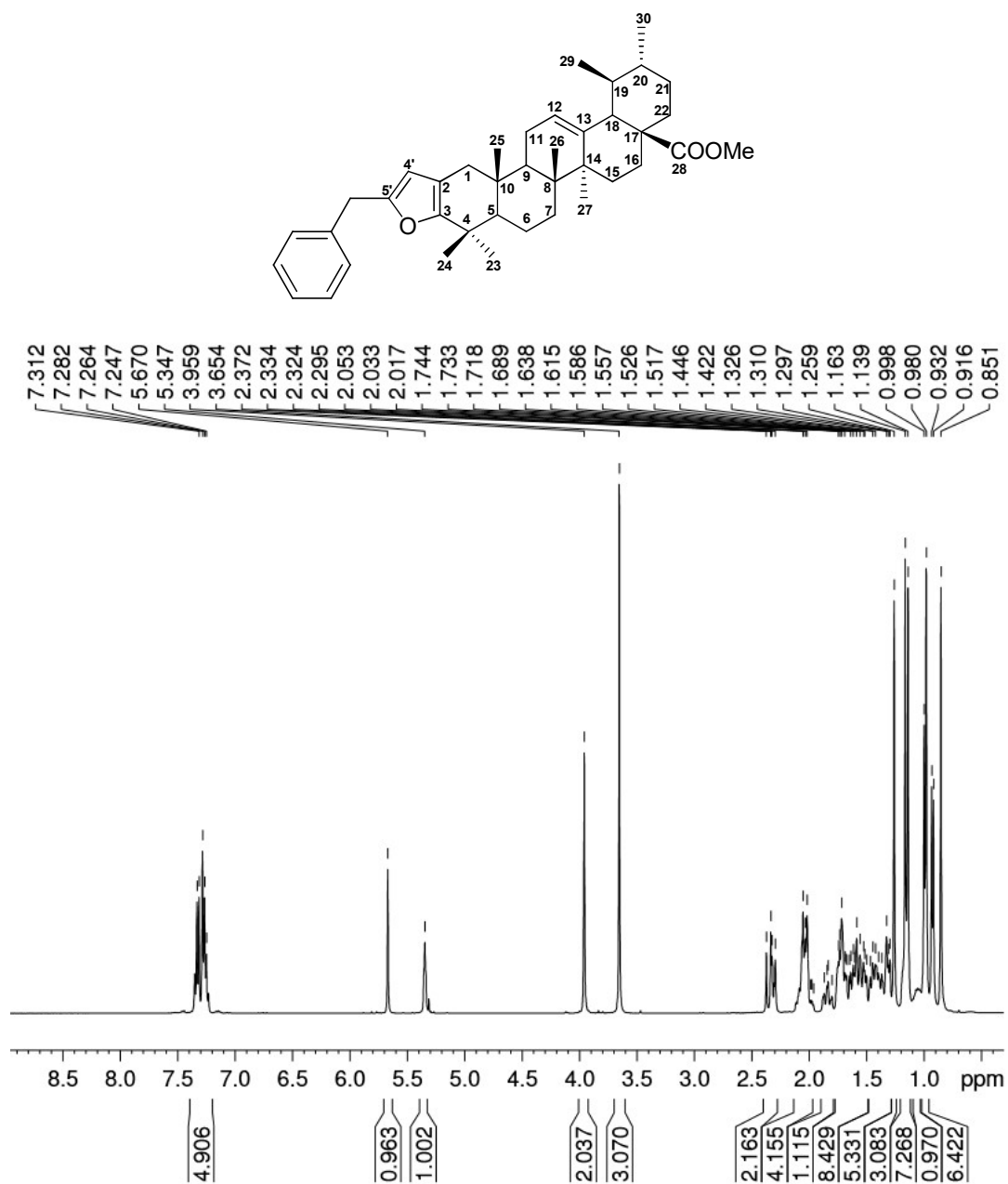


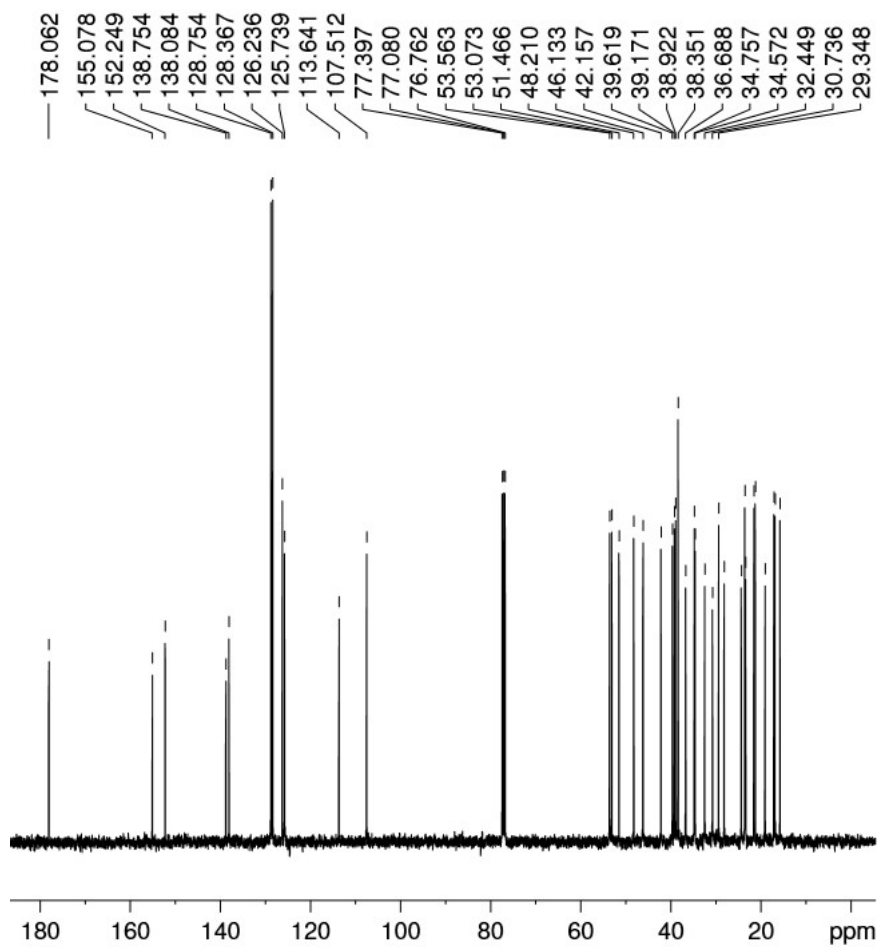
Methyl 5'-(3,4,5-trimethoxybenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15f** ^{13}C NMR spectra (CDCl_3)

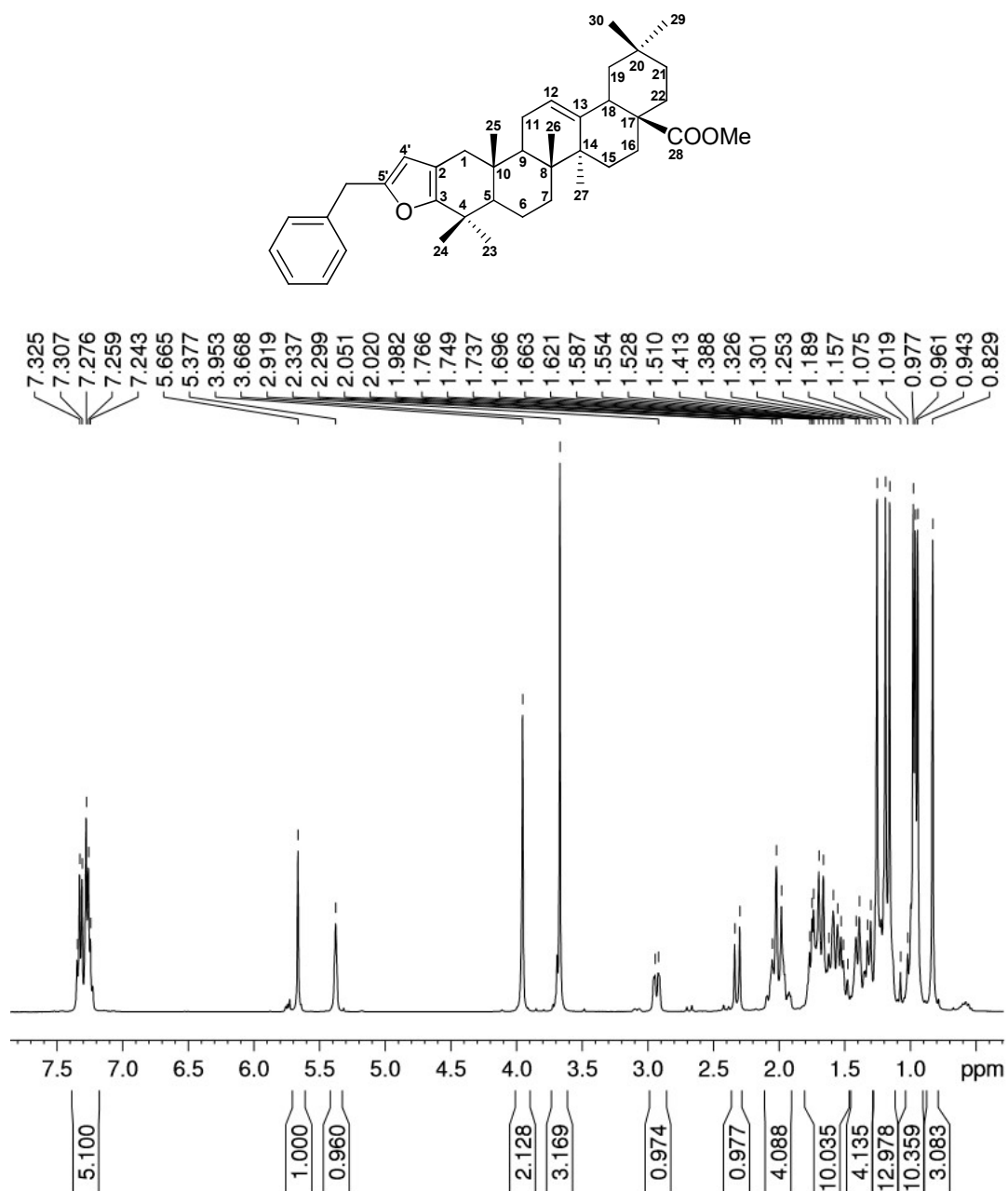


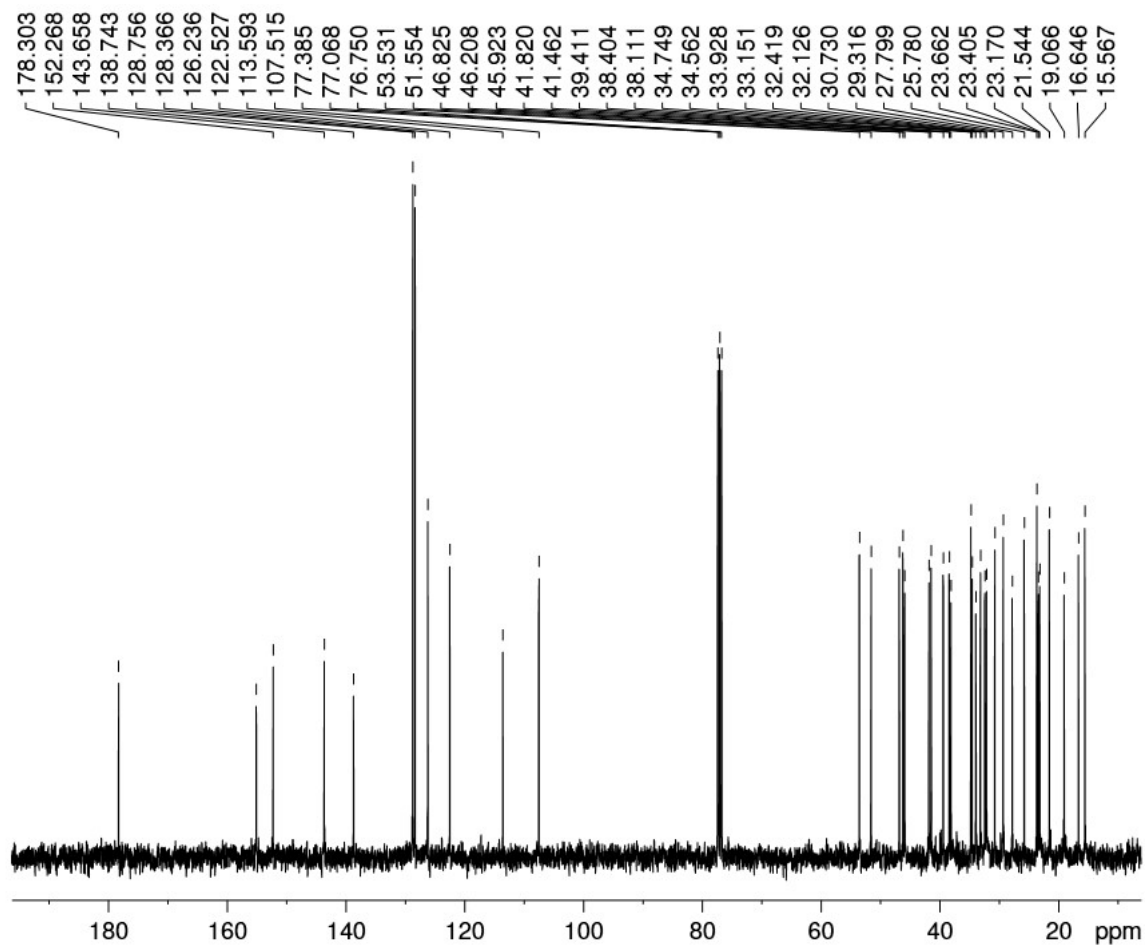
Methyl 5'-(4-nitrobenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15g** ^1H NMR spectra (CDCl_3)

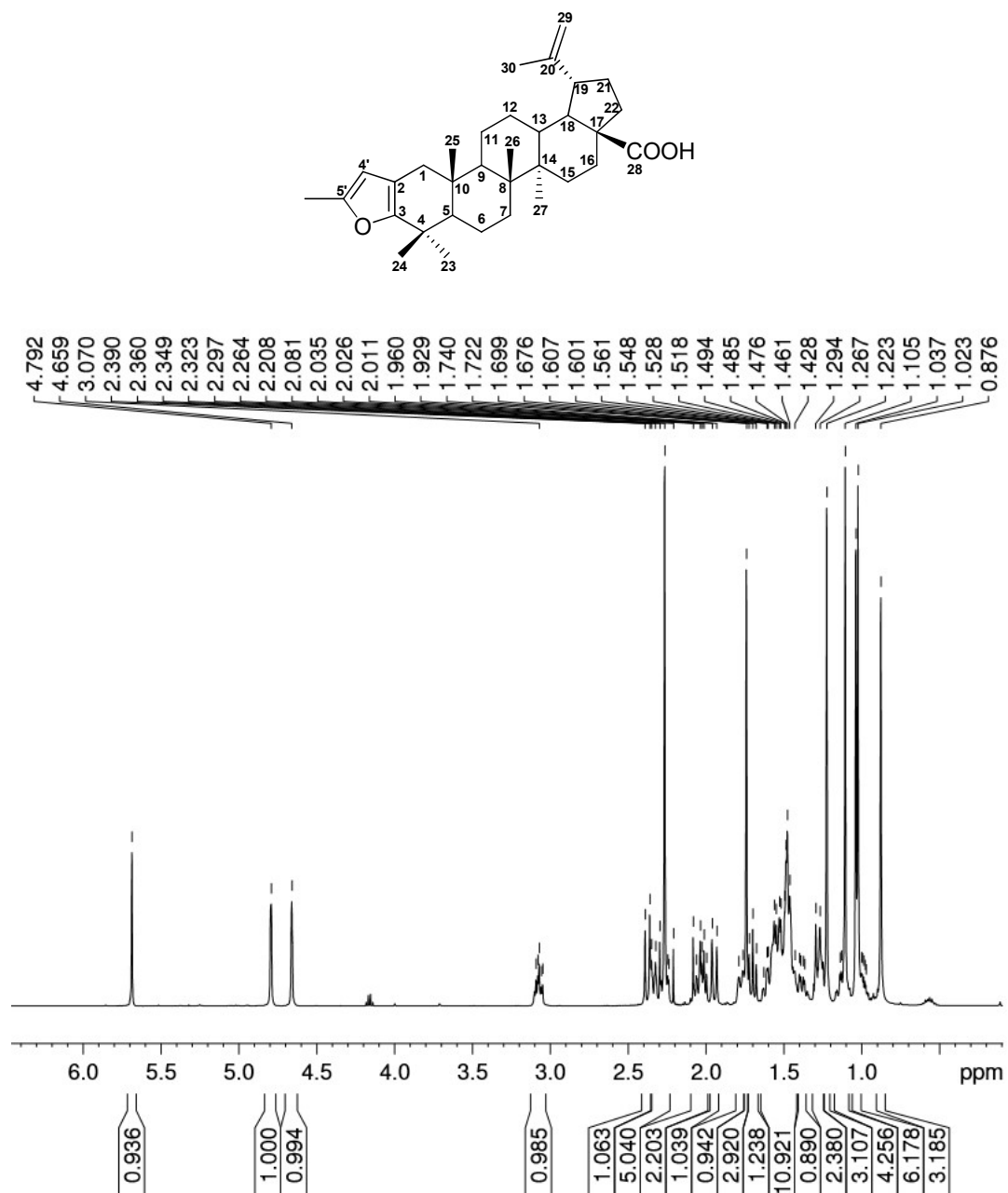
Methyl 5'-(4-nitrobenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15g** ^{13}C NMR spectra (CDCl_3)

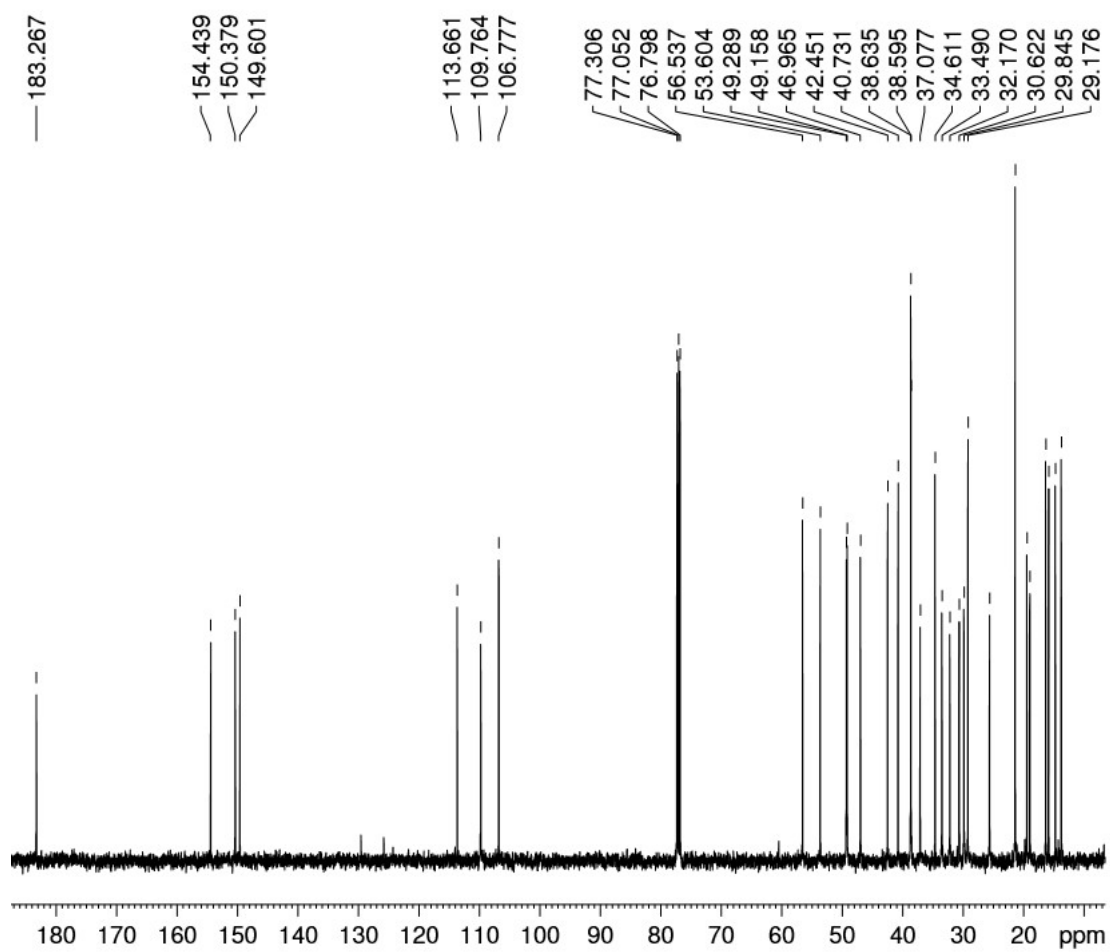
Methyl 5'-benzylfurano[3,2-b]urs-12-en-28-oate **18a** ^1H NMR spectra (CDCl_3)

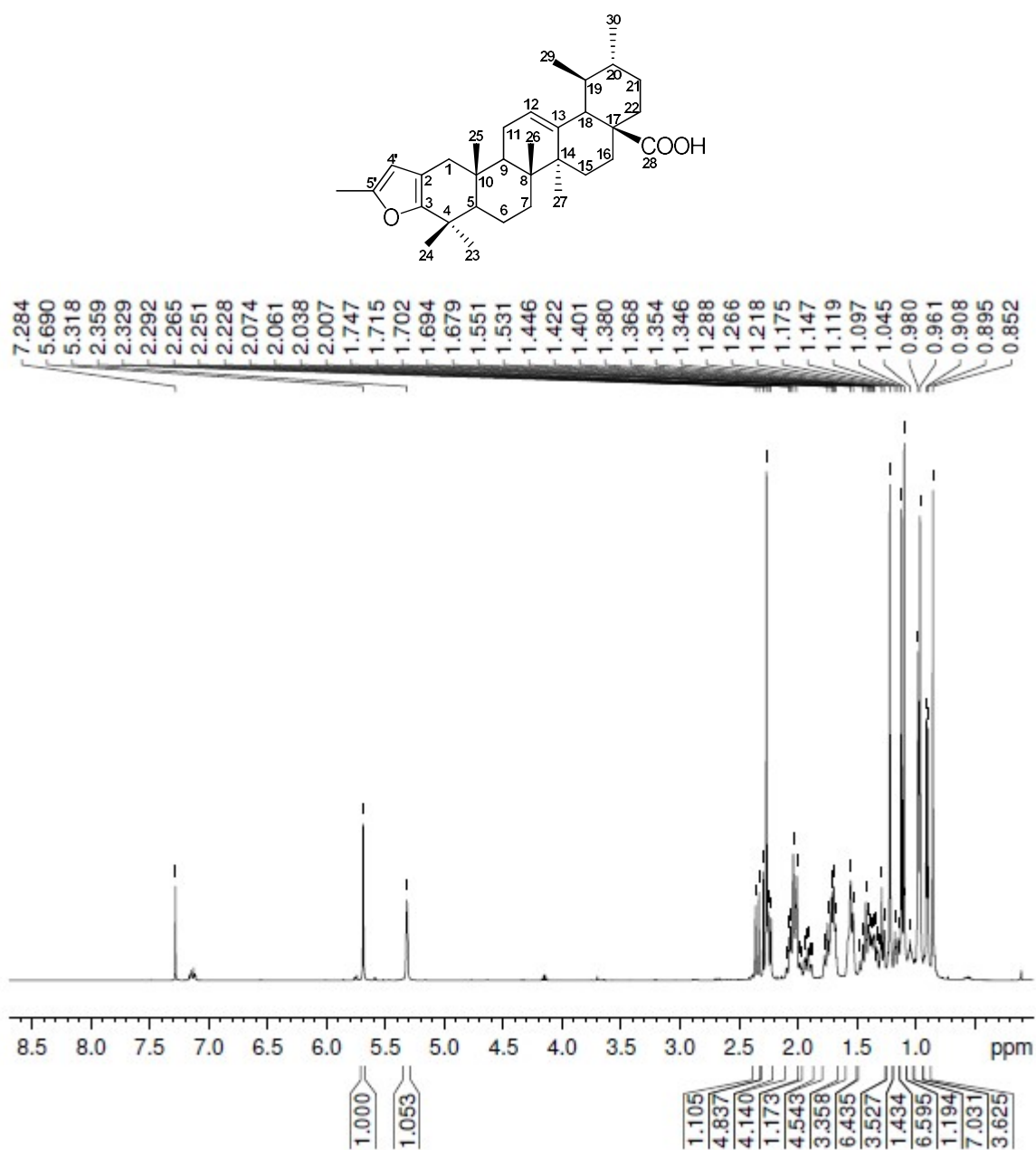
Methyl 5'-benzylfurano[3,2-b]urs-12-en-28-oate **18a** ^{13}C NMR spectra (CDCl_3)

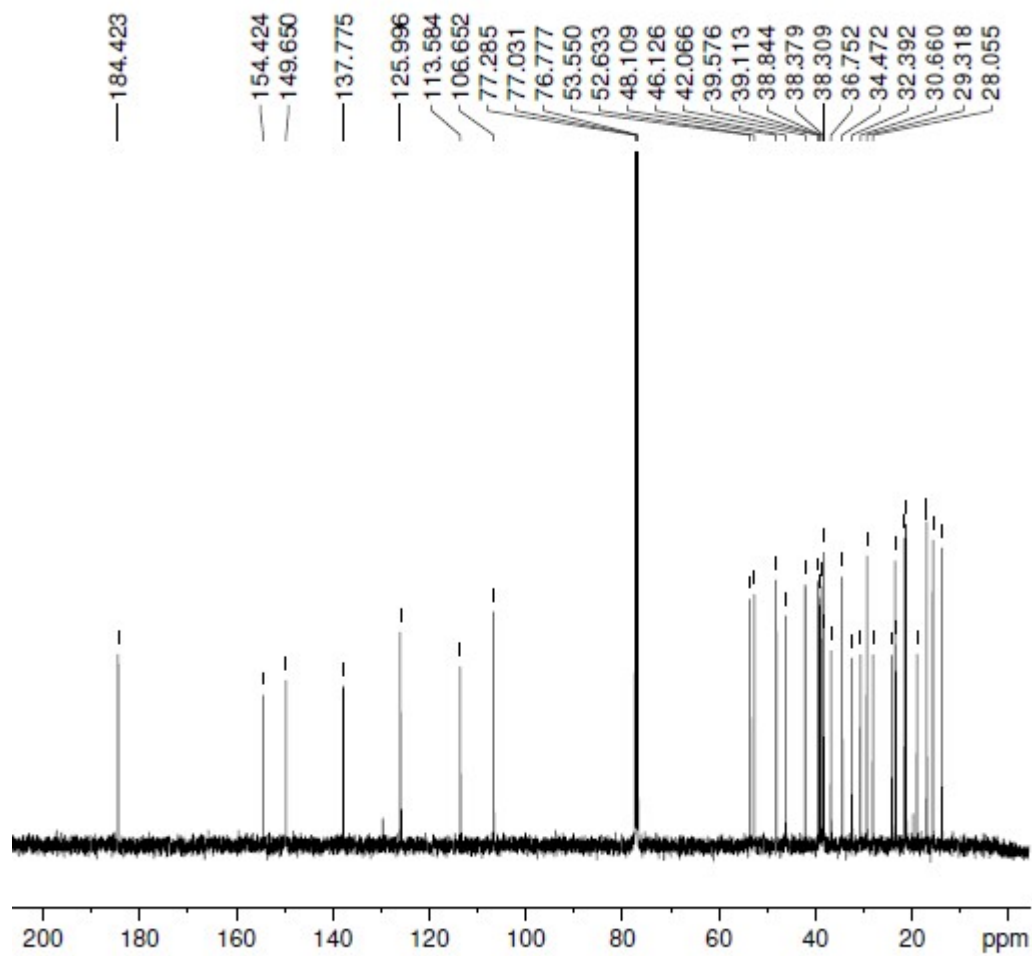
Methyl 5'-benzylfurano[3,2-b]olean-12-en-28-oate **20a** ^1H NMR spectra (CDCl_3)

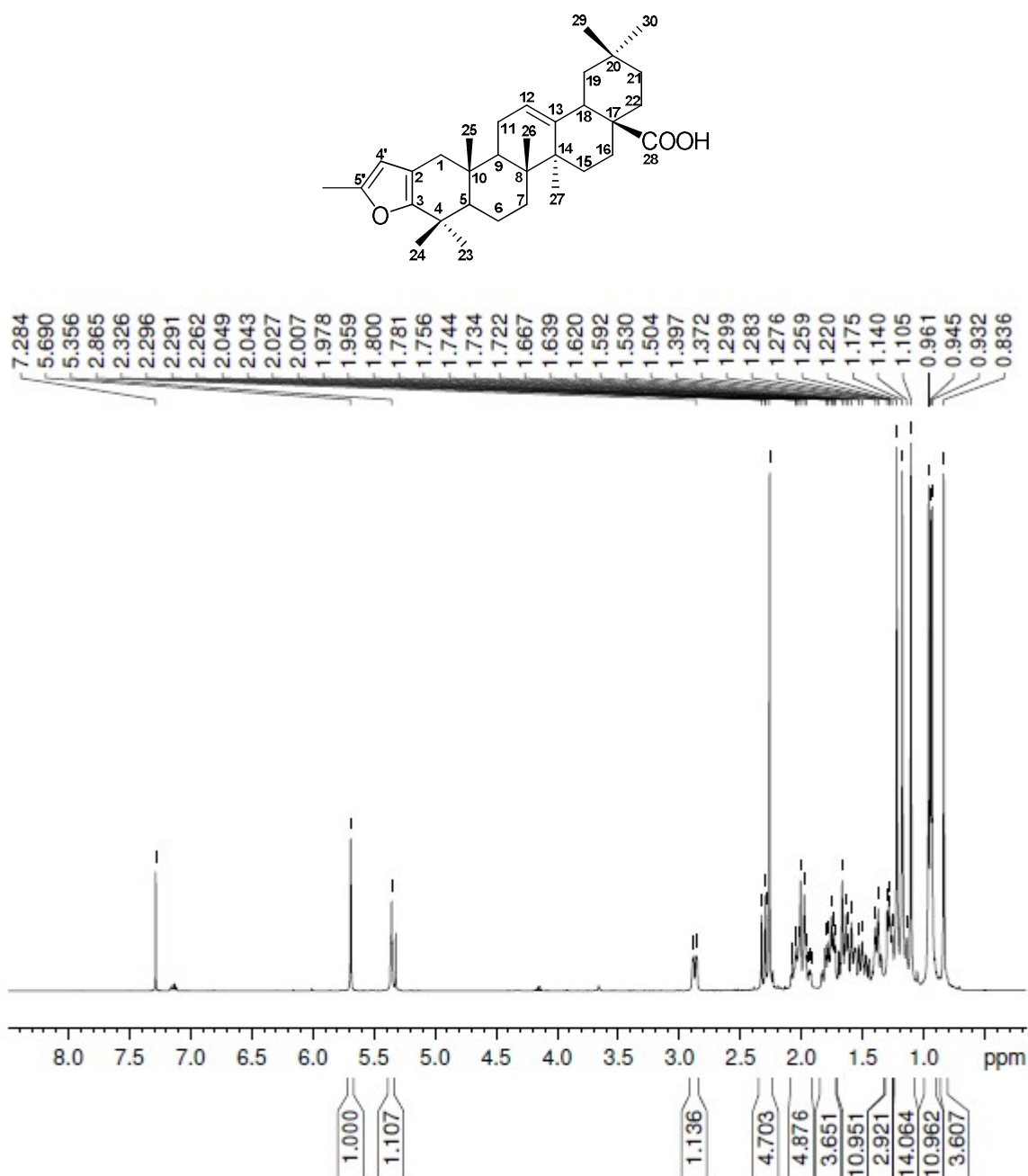
Methyl 5'-benzylfurano[3,2-b]olean-12-en-28-oate **20a** ^{13}C NMR spectra (CDCl_3)

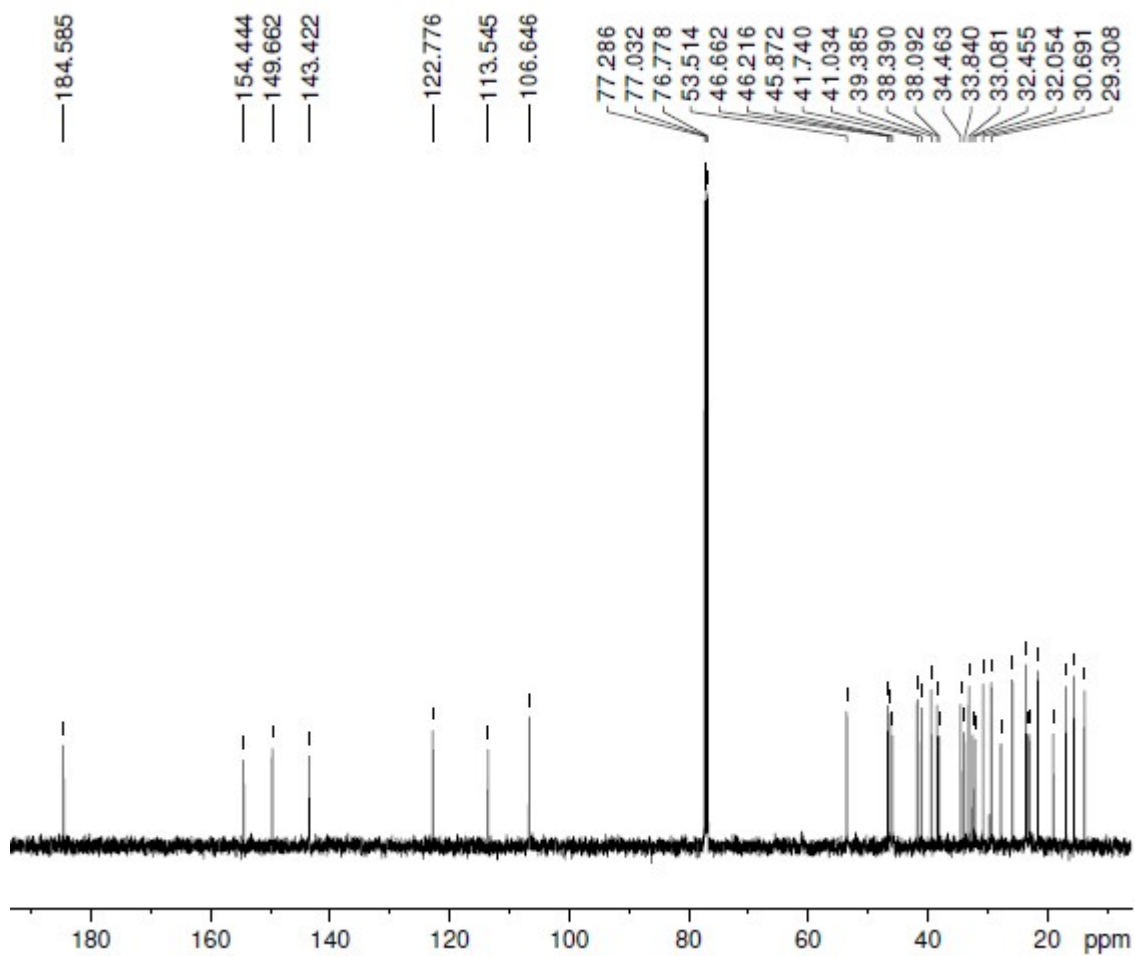
5'-Methylfurano[3,2-b]lup-20(29)-en-28-oic acid **11b** ^1H NMR spectra (CDCl_3)

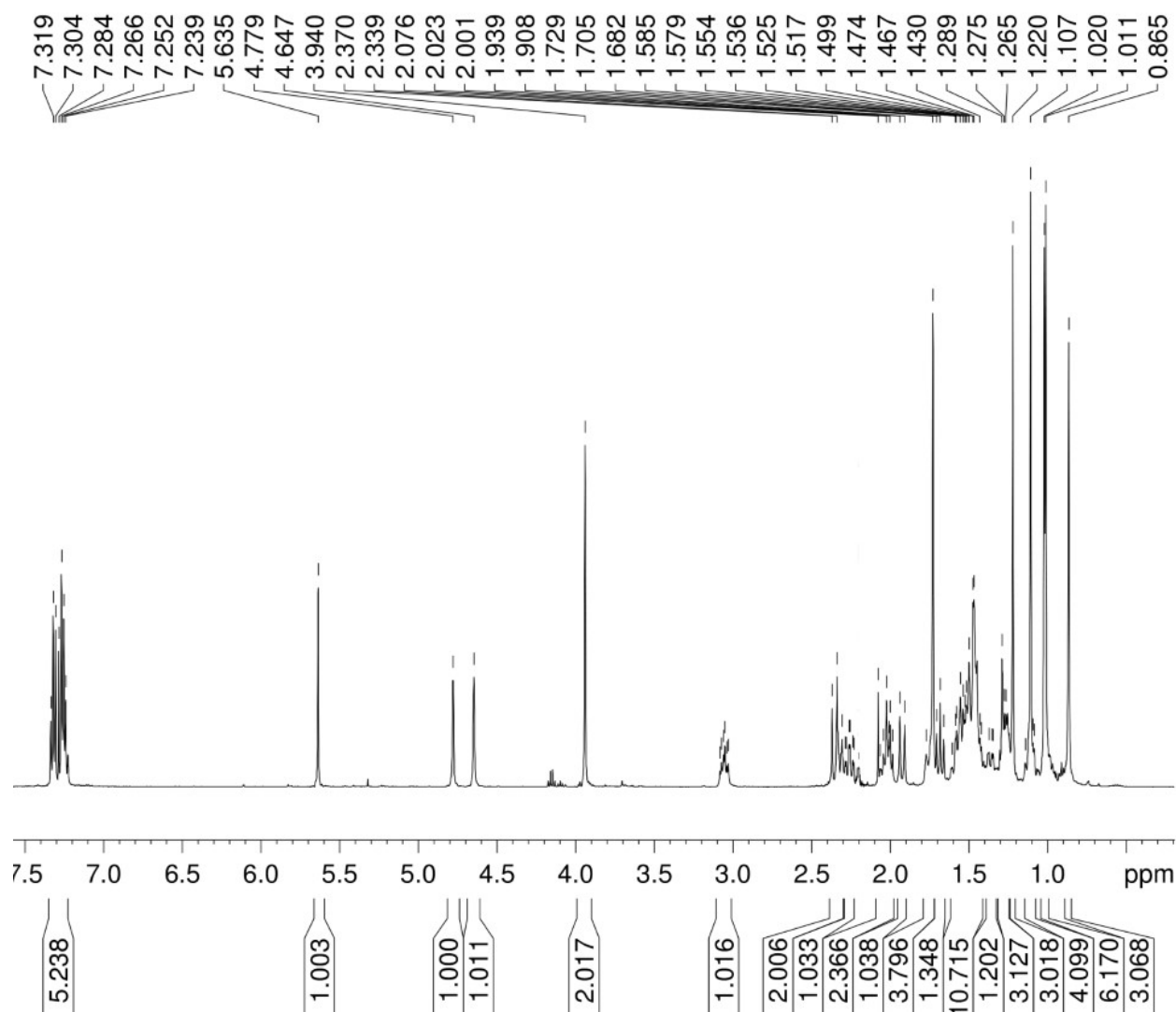
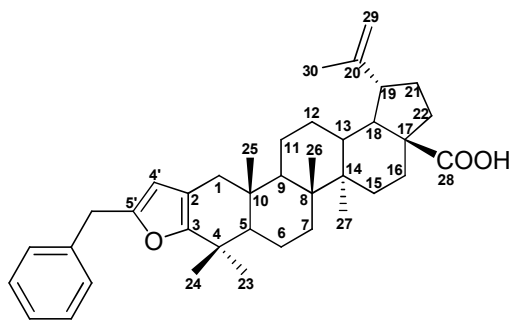
5'-Methylfurano[3,2-b]lup-20(29)-en-28-oic acid **11b** ^{13}C NMR spectra (CDCl_3)

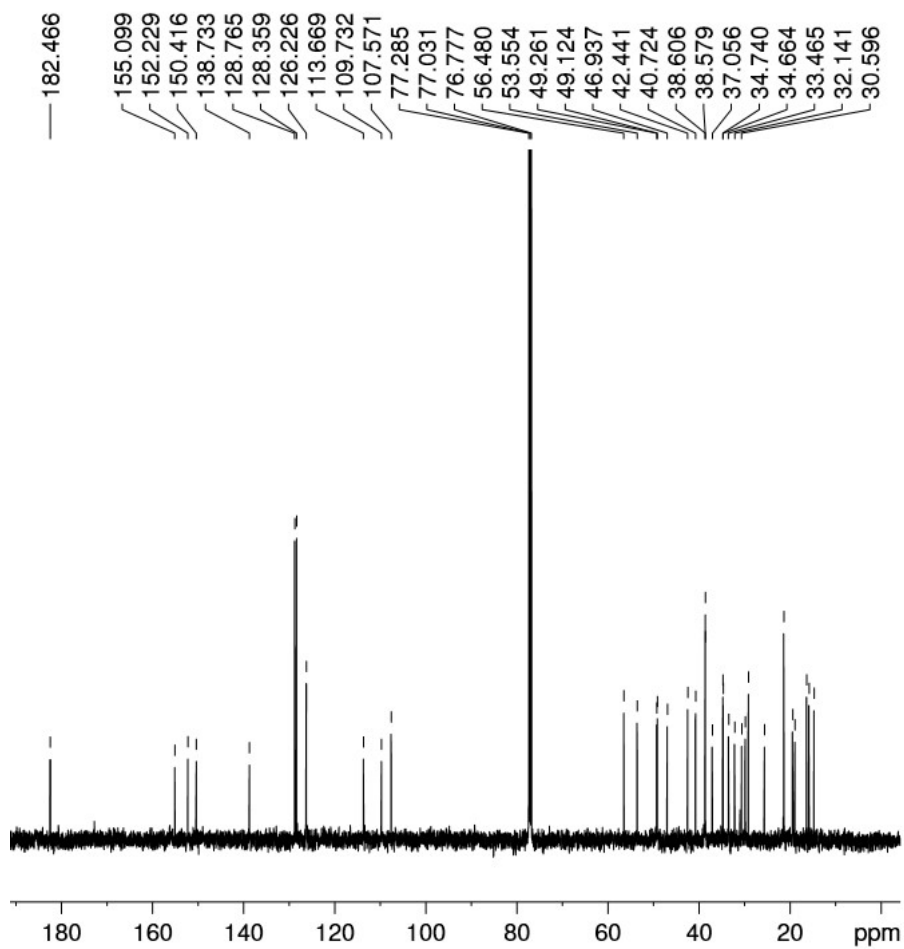
5'-Methylfurano[3,2-b]urs-12-en-28-oic acid **12b** ^1H NMR spectra (CDCl_3)

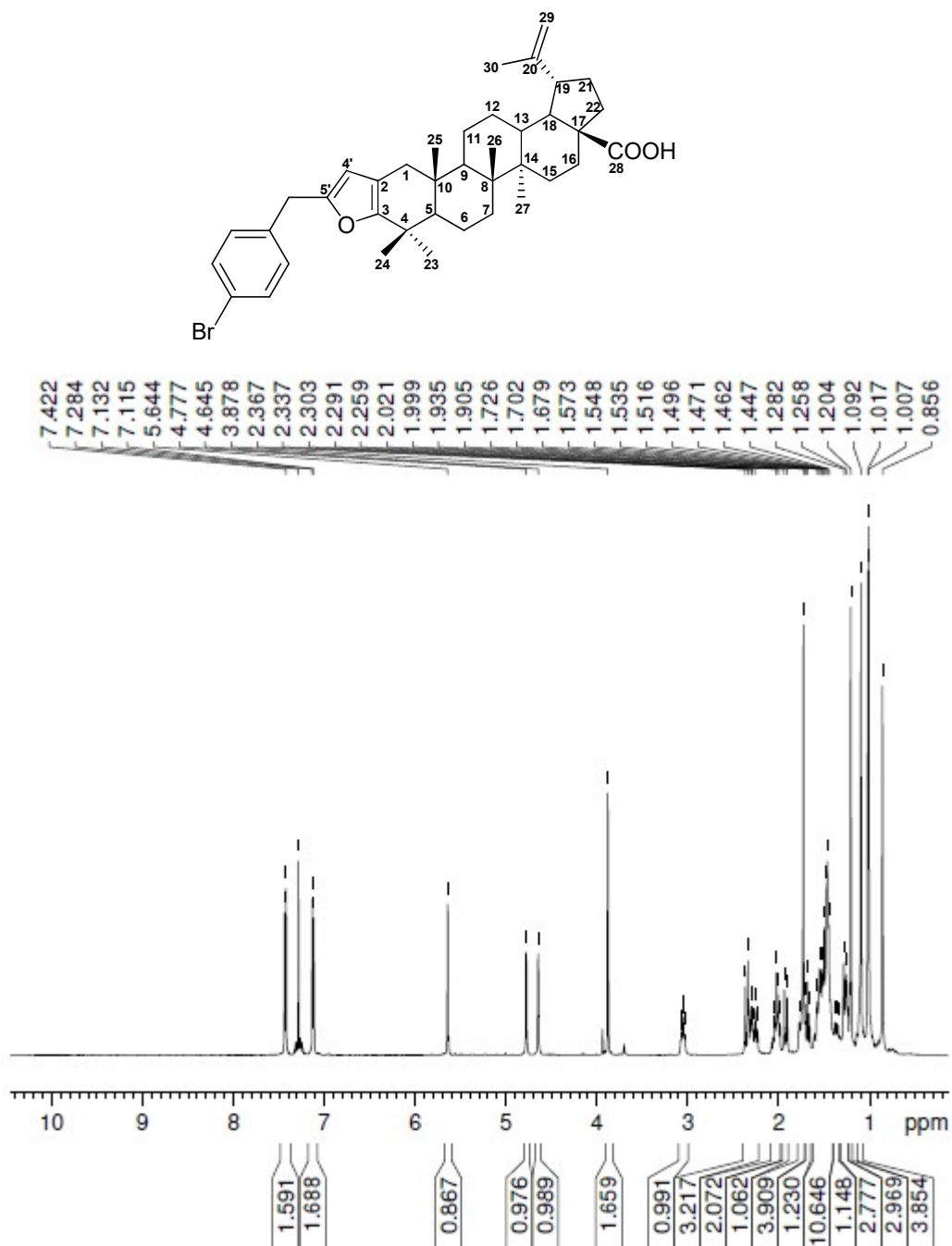
5^l-Methylfurano[3,2-b]urs-12-en-28-oic acid **12b** ¹³C NMR spectra (CDCl₃)

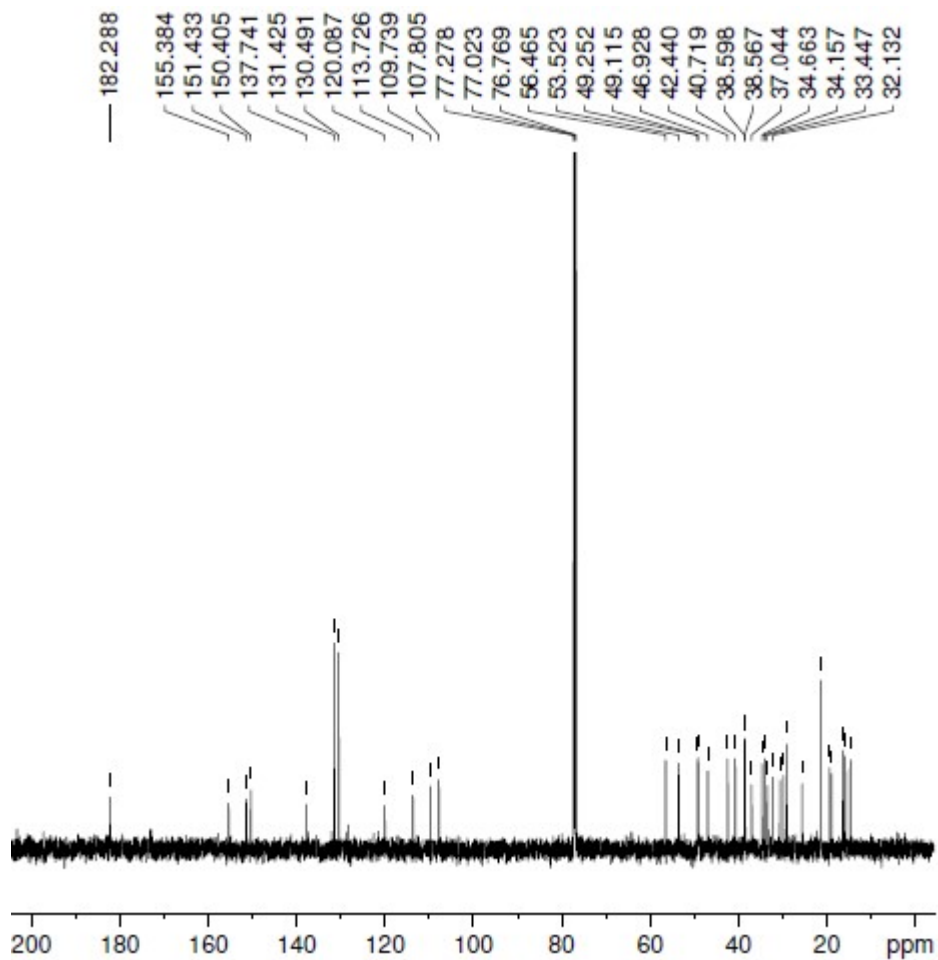
5'-Methylfurano[3,2-b]olean-12-en-28-oic acid **13b** ^1H NMR spectra (CDCl_3)

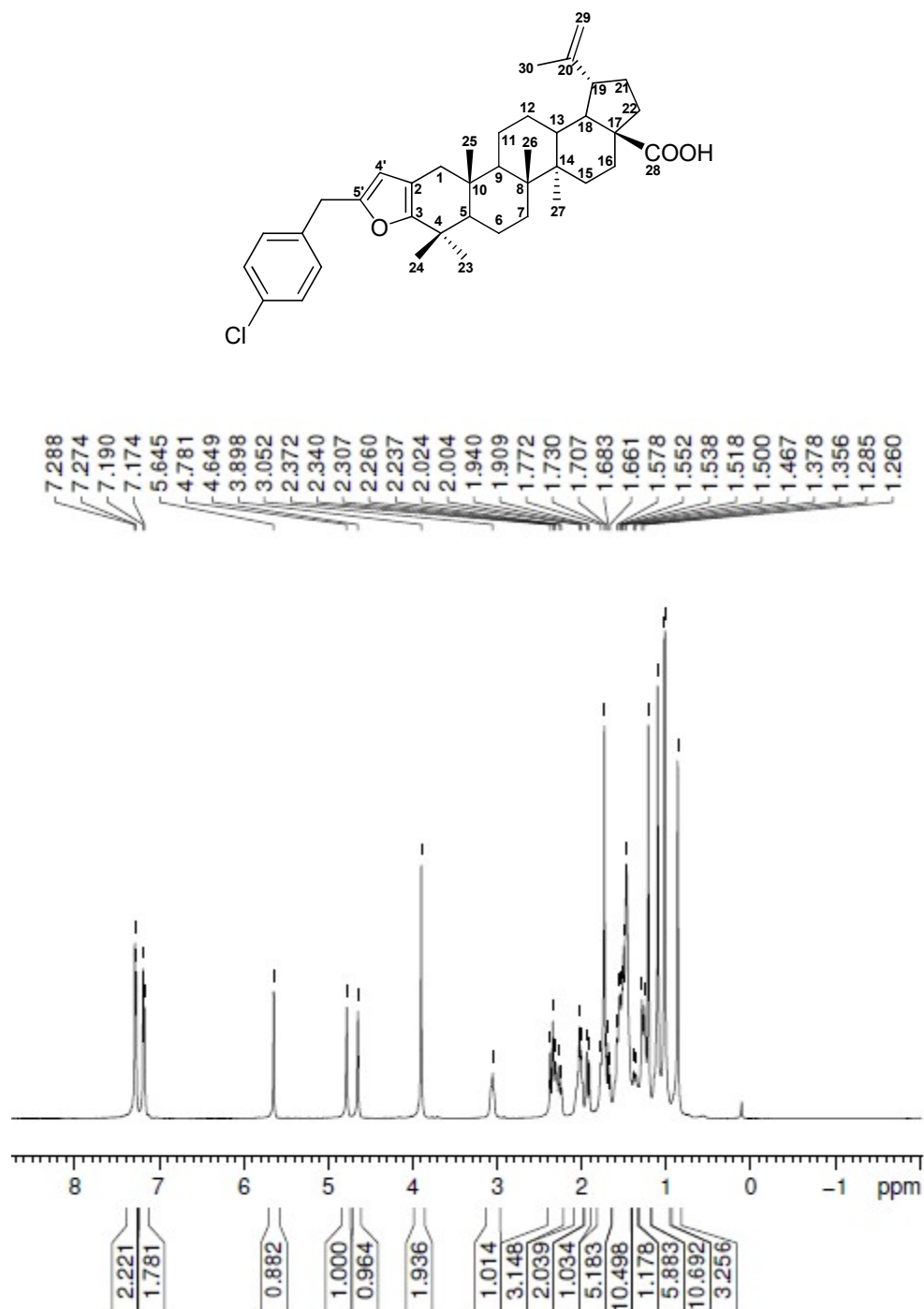
5^l-Methylfurano[3,2-b]olean-12-en-28-oic acid **13b** ¹³C NMR spectra (CDCl₃)

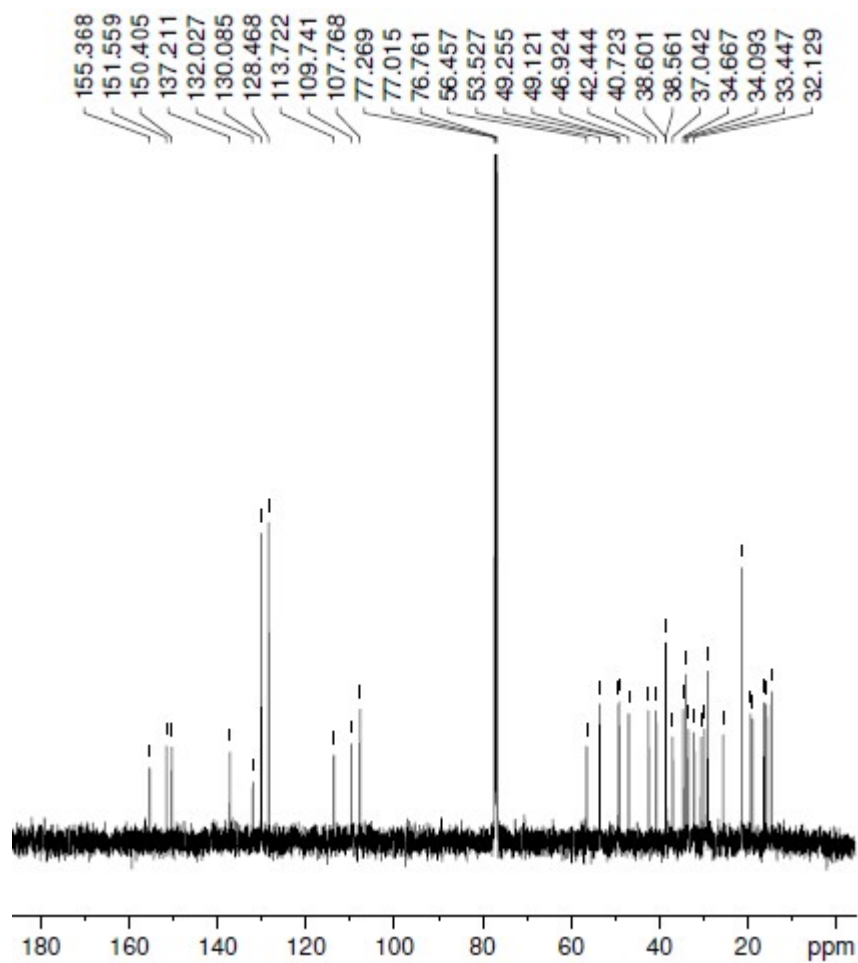
5'-Benzylfurano[3,2-b]lup-20(29)-en-28-oic acid **16a** ^1H NMR spectra (CDCl_3)

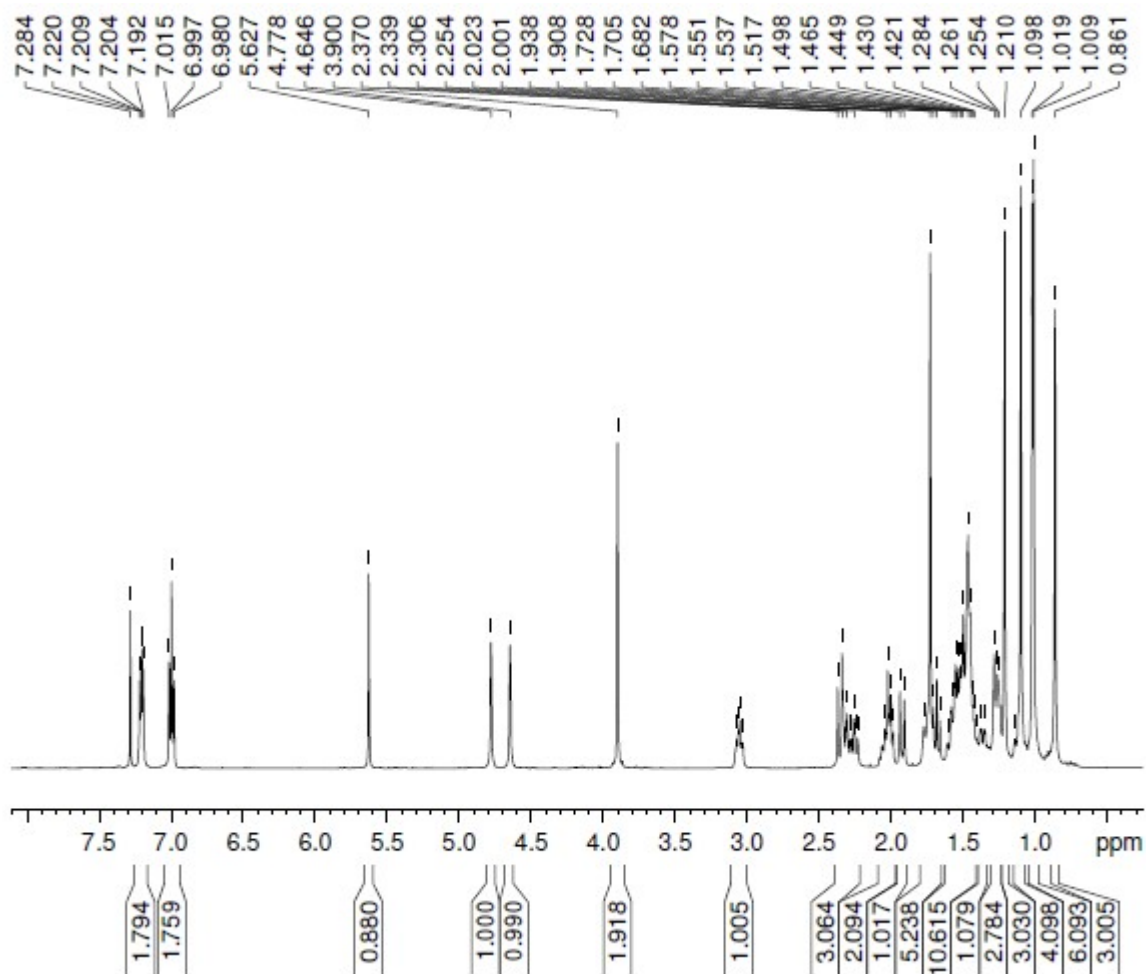
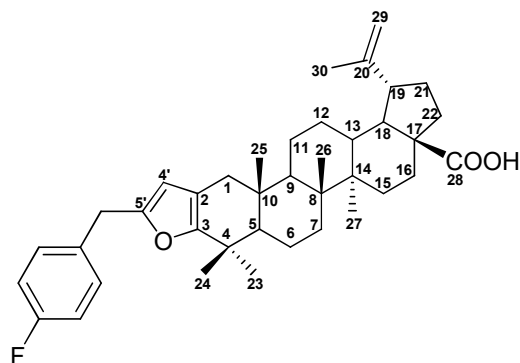
5'-Benzylfurano[3,2-b]lup-20(29)-en-28-oic acid **16a** ^{13}C NMR spectra (CDCl_3)

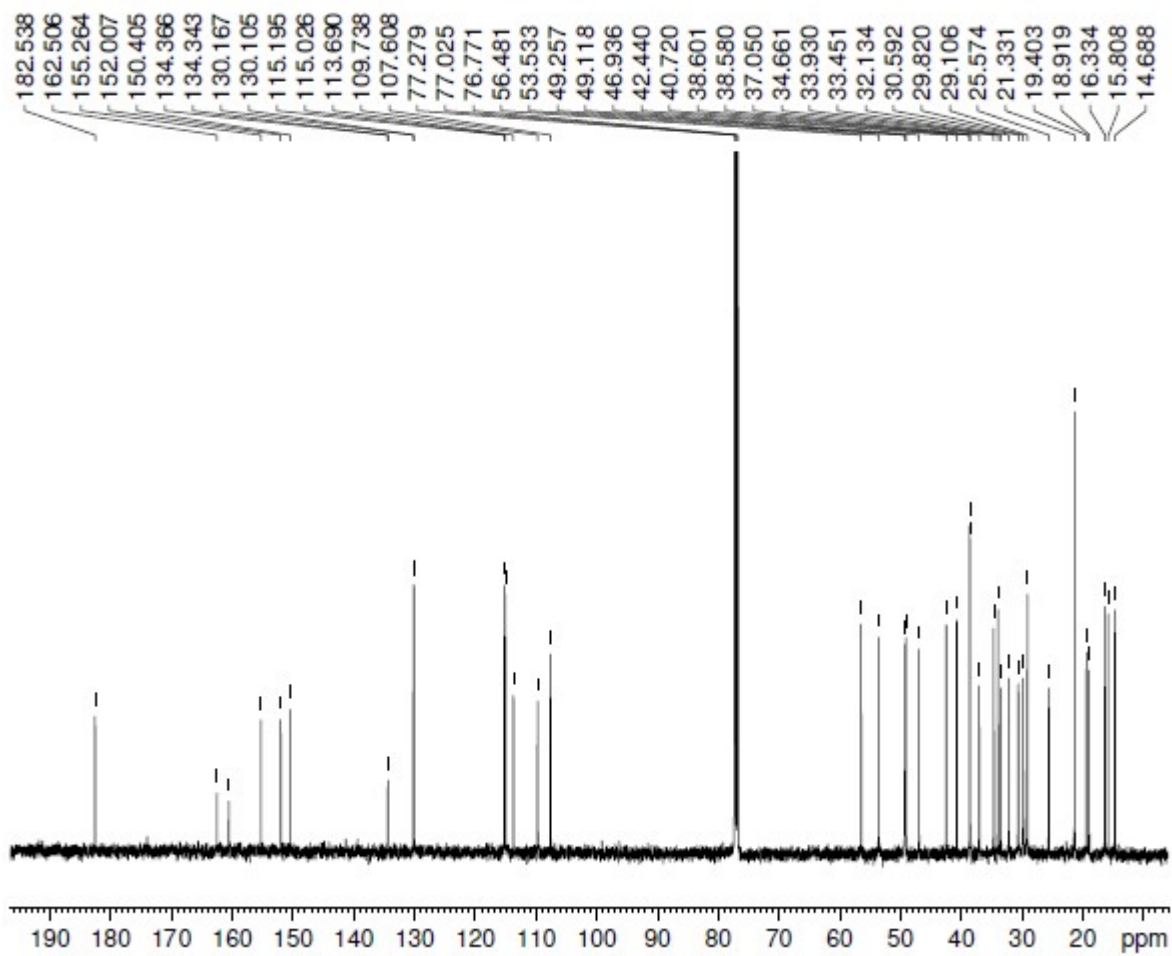
5'-(4-Brombenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16b** ^1H NMR spectra (CDCl_3)

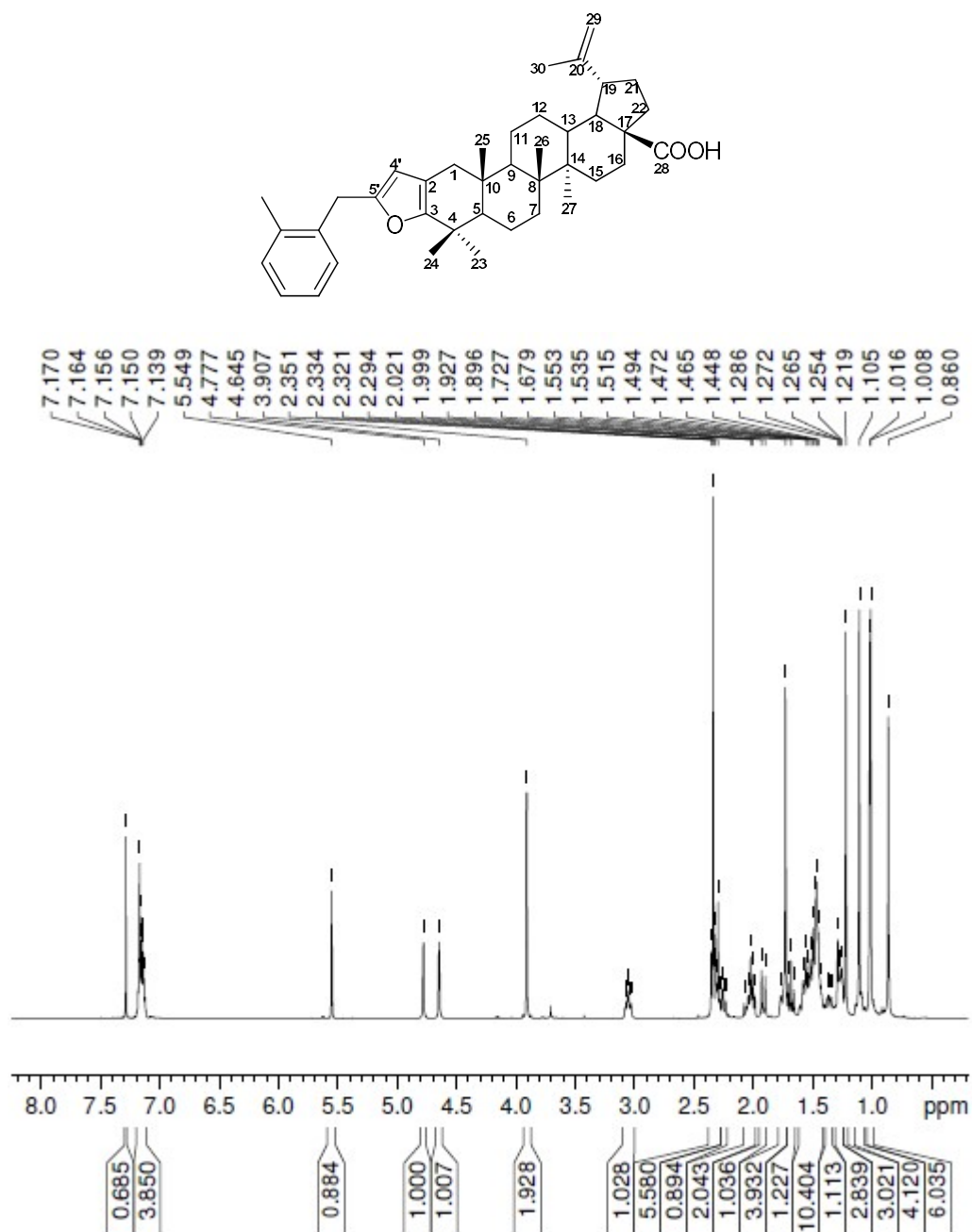
5'-(4-Brombenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16b** ^{13}C NMR spectra (CDCl_3)

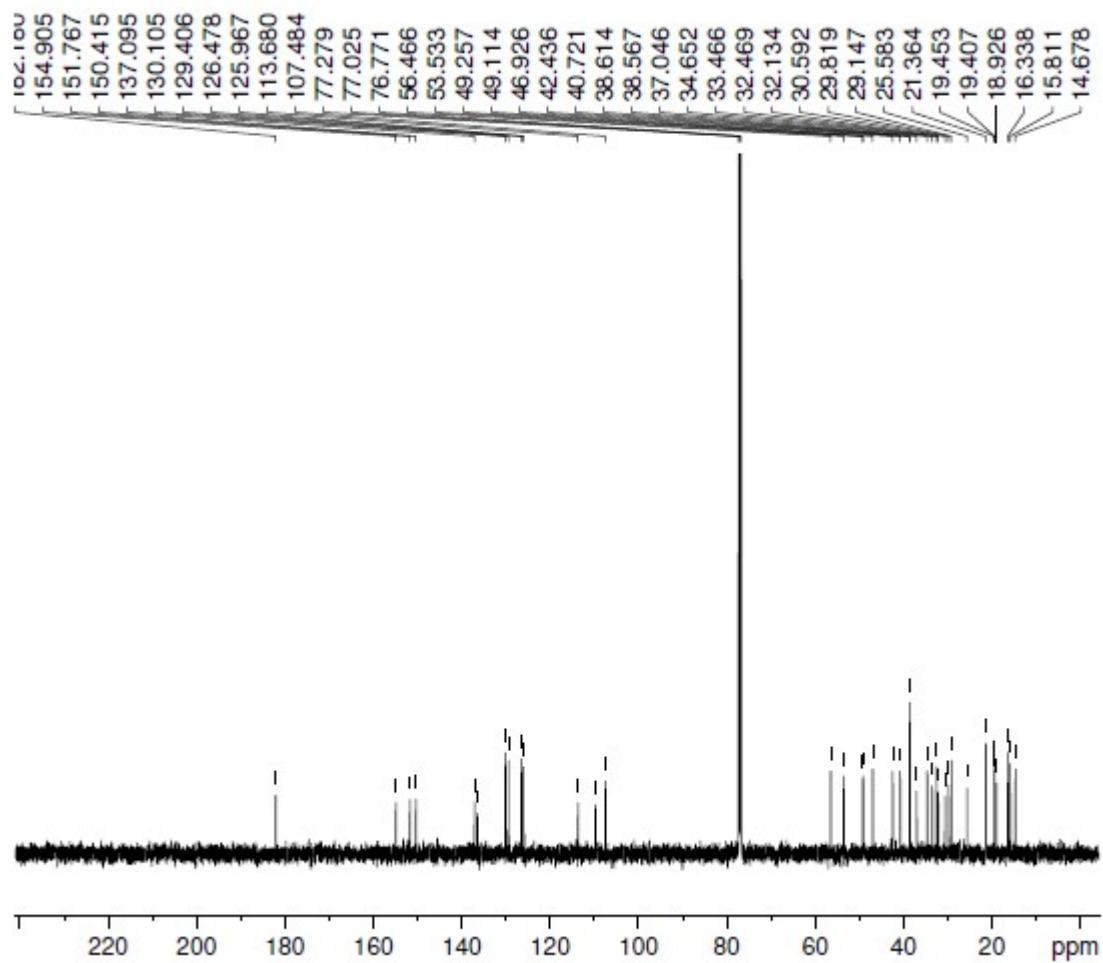
5'-(4-Chlorobenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16c** ^1H NMR spectra (CDCl_3)

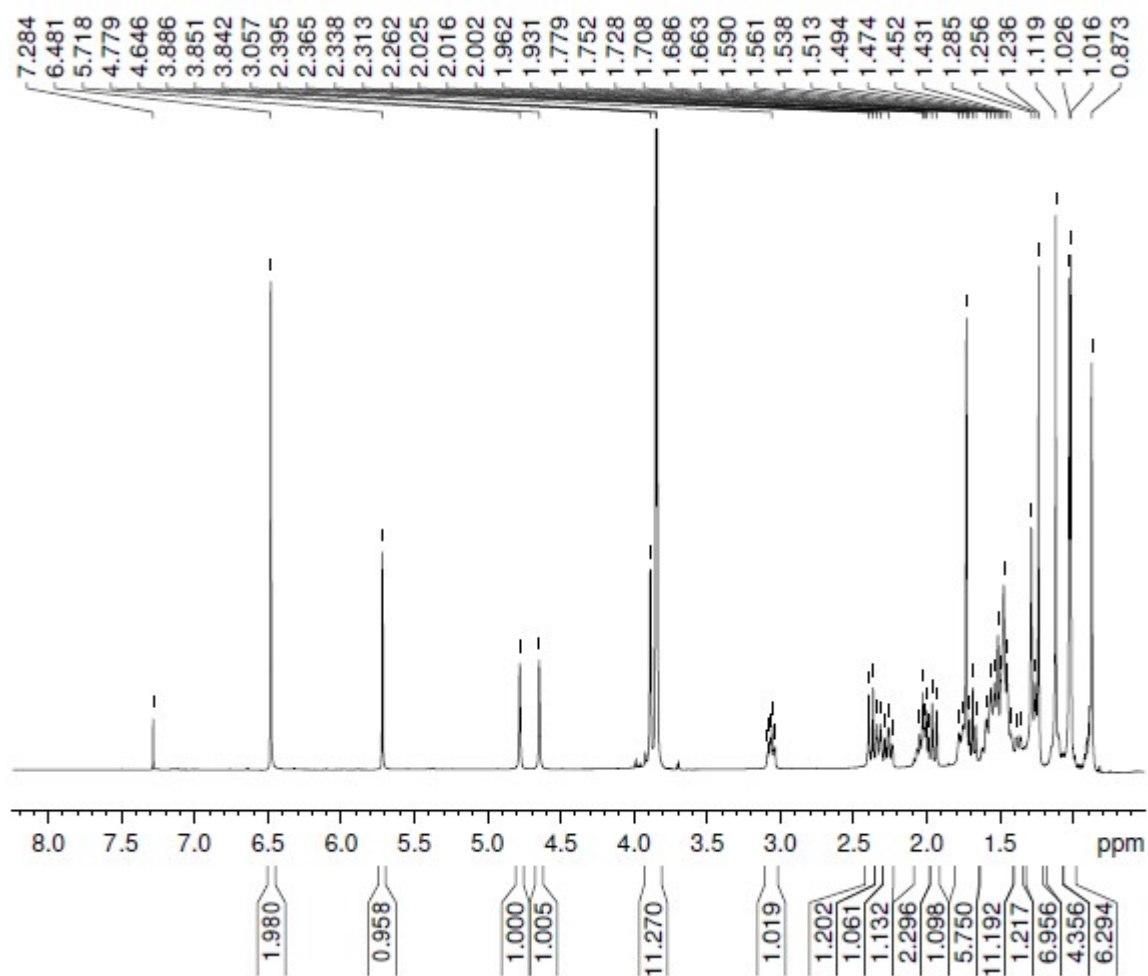
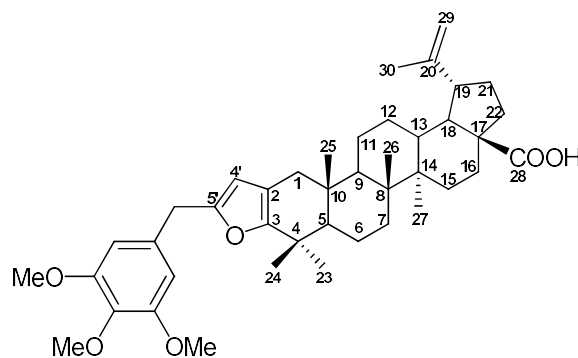
5'-(4-Chlorobenzyl)furano[3,2-b]lup-20,29-en-28-oic acid **16c** ^{13}C NMR spectra (CDCl_3)

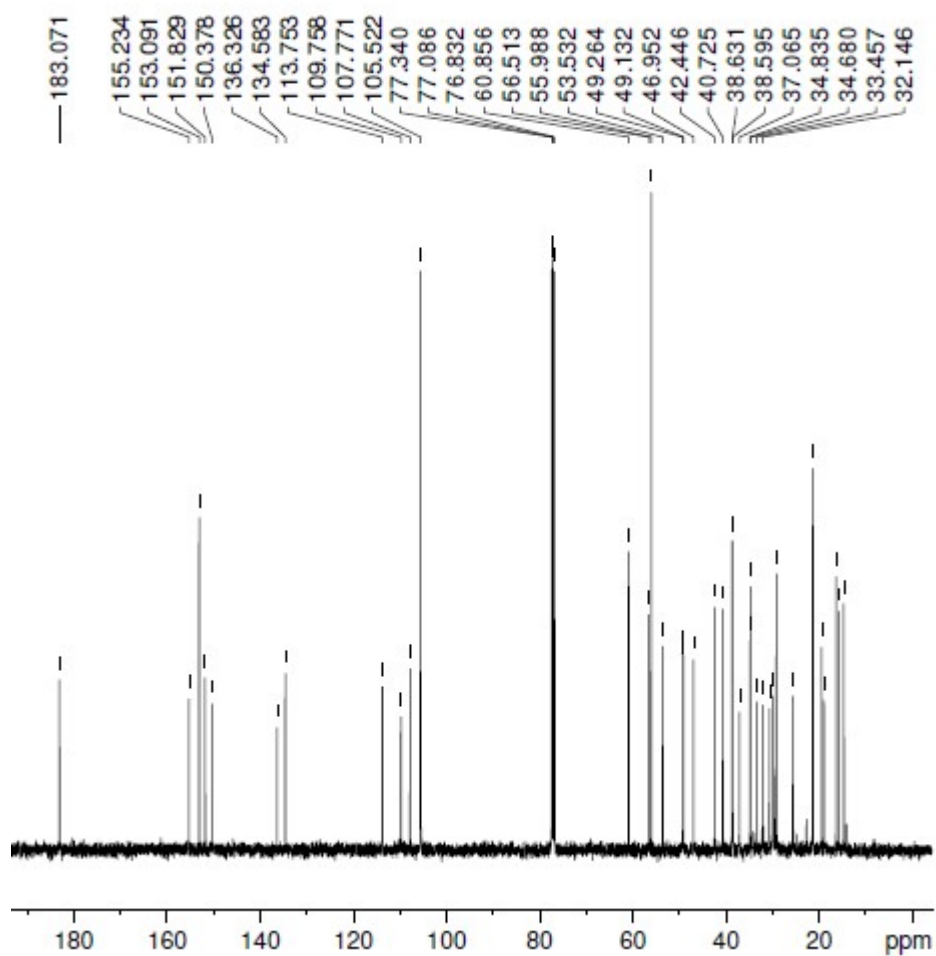
5'-(4-Fluorobenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16d** ^1H NMR spectra (CDCl_3)

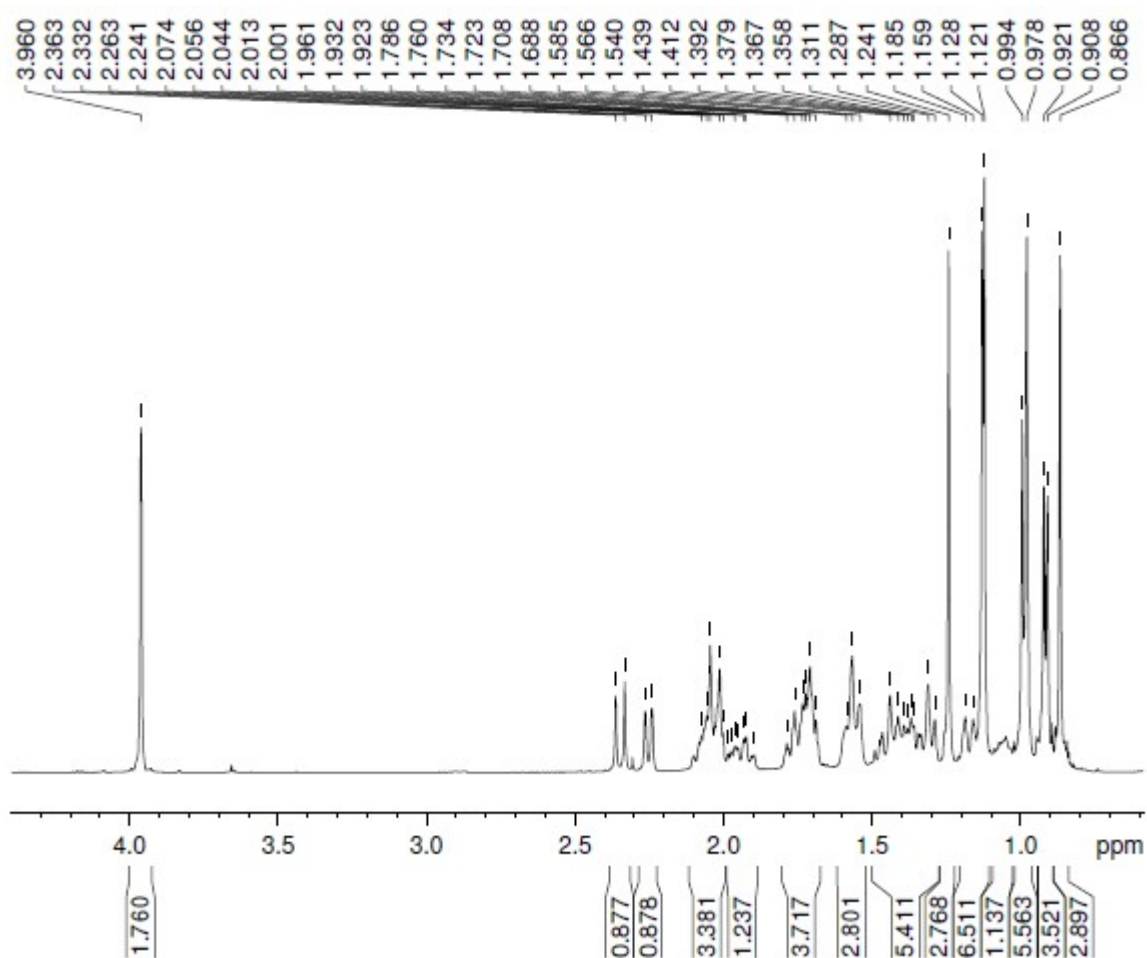
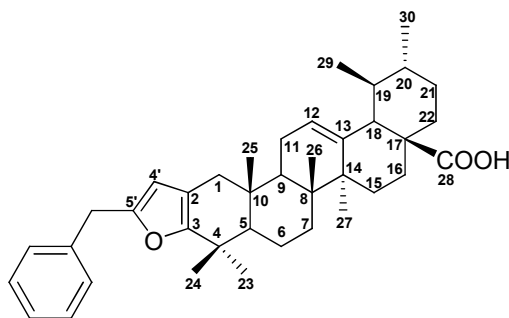
5'-(4-Fluorobenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16d** ^{13}C NMR spectra (CDCl_3)

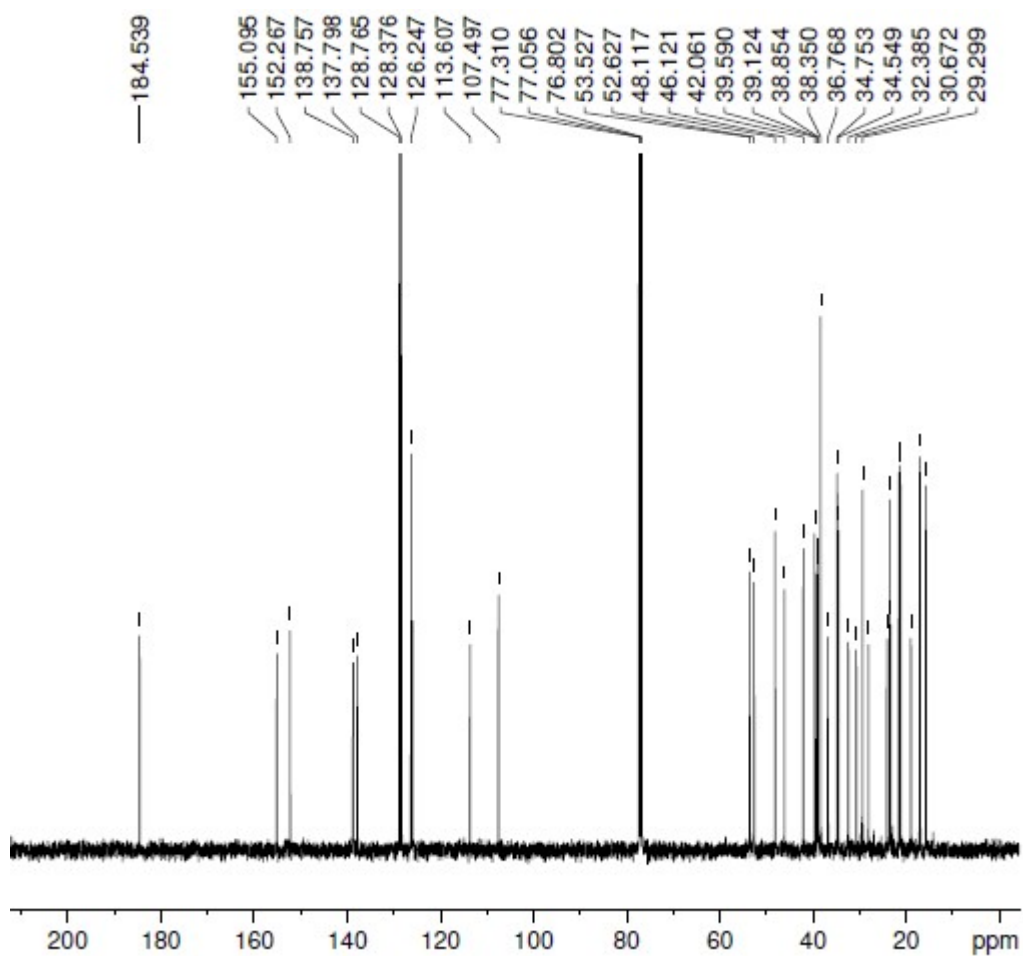
5'-(4-Methylbenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16e** ^1H NMR spectra (CDCl_3)

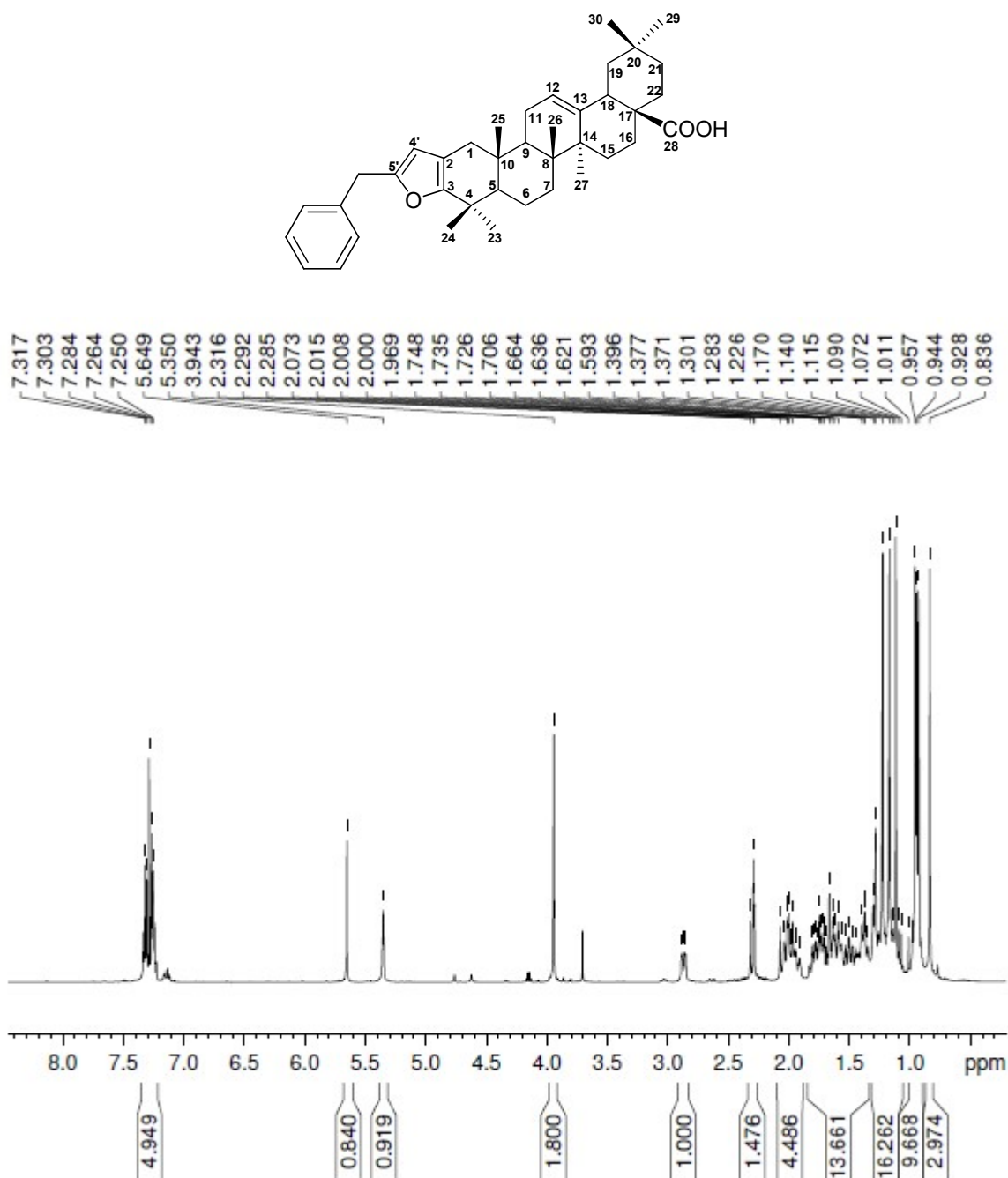
5'-(4-Methylbenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16e** ^{13}C NMR spectra (CDCl_3)

5'-(3,4,5-Trimethoxybenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16f** ^1H NMR spectra (CDCl_3)

5'-(3,4,5-Trimethoxybenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16f** ^{13}C NMR spectra (CDCl_3)

5'-Benzylfurano[3,2-b]urs-12-en-28-oic acid **18b** ^1H NMR spectra (CDCl_3)

5'-Benzylfurano[3,2-b]urs-12-en-28-oic acid **18b** ^{13}C NMR spectra (CDCl_3)

5'-Benzylfurano[3,2-b]olean-12-en-28-oic acid **20b** ^1H NMR spectra (CDCl_3)

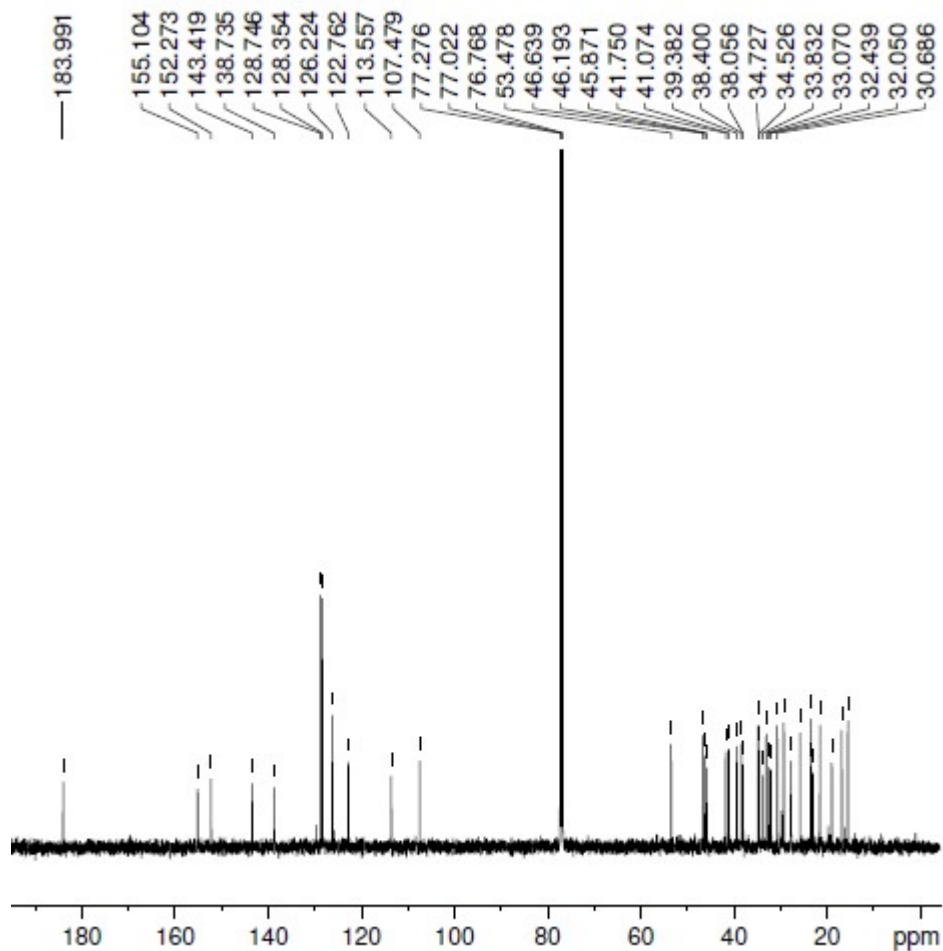
5'-Benzylfurano[3,2-b]olean-12-en-28-oic acid **20b** ^{13}C NMR spectra (CDCl_3)

Table 1. ^{13}C NMR spectra of compounds 14a-g, 17 and 19

Atom or group	14a	14b	14c	14d	14e	14f	14g	17	19
1	46.79	46.83	46.84	46.83	46.80	46.76	46.95	46.47	46.30
2	41.76	41.65	41.67	41.71	41.88	41.60	41.53	41.72	41.33
3	215.98	215.81	215.83	215.90	215.94	215.92	215.53	215.91	215.89
4	48.30	48.31	48.31	48.31	48.34	48.31	48.39	48.08	48.27
5	57.32	57.32	57.32	57.32	57.39	57.27	57.36	57.18	57.17
6	19.33	19.34	19.33	19.32	19.33	19.30	19.30	19.38	19.37
7	34.08	34.07	34.07	34.07	34.10	34.06	34.06	32.71	32.42
8	40.79	40.79	40.79	40.79	40.79	40.77	40.80	39.59	39.38
9	50.14	50.14	50.14	50.14	50.19	50.13	50.18	47.06	47.17
10	37.47	37.48	37.48	37.48	37.49	37.42	37.54	37.18	37.24
11	21.19	21.19	21.19	21.19	21.15	21.22	21.20	23.52	23.59
12	25.43	25.42	25.43	25.43	25.41	25.44	25.42	125.20	122.03
13	38.22	38.21	38.21	38.21	38.22	38.21	38.19	138.41	143.97
14	42.52	42.52	42.52	42.52	42.52	42.51	42.53	42.11	41.76
15	29.63	29.62	29.62	29.62	29.63	29.61	29.62	28.02	27.70
16	32.15	32.13	32.13	32.13	32.16	32.11	32.12	24.19	23.05
17	56.48	56.48	56.48	56.48	56.50	56.46	56.48	48.26	46.72
18	49.43	49.42	49.42	49.41	49.42	49.39	49.40	52.86	41.62
19	46.98	46.96	46.96	46.96	46.97	46.97	46.95	39.02	45.84
20	150.42	150.45	150.45	150.46	150.39	150.50	150.51	38.86	30.69
21	30.56	30.56	30.56	30.56	30.57	30.51	30.55	30.63	32.35
22	36.95	36.93	36.93	36.93	36.95	36.92	36.93	36.61	33.85
23	25.11	25.08	25.08	25.08	25.05	25.11	25.04	25.36	25.92
24	16.13	16.13	16.12	16.12	16.10	16.13	16.17	22.00	21.96
25	21.71	21.68	21.68	21.69	21.71	21.71	21.66	15.62	15.47
26	16.13	16.13	16.12	16.12	16.10	16.11	16.17	17.10	17.03
27	14.65	14.64	14.63	14.63	14.63	14.62	14.63	23.61	25.33
28	176.61	176.60	176.60	176.60	176.63	176.59	176.61	178.02	178.25
29	109.73	109.69	109.69	109.68	109.72	109.66	109.66	17.10	23.64
30	19.33	19.34	19.33	19.32	19.33	19.30	19.30	21.18	33.11
COOMe	51.29	51.29	51.28	51.29	51.29	51.30	51.31	51.48	51.55
1'	20.53	20.56	20.53	20.46	20.85	20.45	20.72	20.54	20.50
2'	81.71	80.68	80.62	80.59	80.61	81.86	80.30	81.78	81.78
3'	88.65	90.00	89.77	88.27	92.69	87.76	95.02	88.66	88.62
Ph	123.92 128.18 131.62 127.58	122.87 131.40 133.09 121.68	122.40 128.47 132.84 133.52	119.94 133.39 (d, $^1J_{\text{C,F}} = 8$) 115.37 (d, $^1J_{\text{C,F}} = 22$) 162.34 (d, $^1J_{\text{C,F}} = 247$)	121.68 131.79 139.95 123.69 129.28 125.43	118.96 108.77 152.96 138.31	130.94 132.35 130.94 146.67	123.90 131.60 127.63 128.21	123.92 131.59 128.20 127.61
Me-C ₆ H ₄	-	-	-	-	20.64	-	-	-	-
(O-Me) ₂ O-Me	-	-	-	-	-	56.06 60.93	-	-	-

Table 2. ^{13}C NMR spectra of compounds 11a-13a, 15a-g, 18a and 20a

Atom or group	11a	12a	13a	15a	15b	15c	15d	15e	15f	15g	18a	20a
1	38.64	38.37	38.11	38.60	38.59	38.59	38.59	38.63	38.59	38.59	38.35	38.11
2	113.68	113.62	113.57	113.69	113.74	113.74	113.71	113.71	113.76	113.92	113.64	113.59
3	154.45	154.41	154.45	155.11	155.40	155.37	155.28	154.91	155.26	155.94	155.08	155.12
4	34.60	34.48	34.48	34.74	34.66	34.66	34.66	34.67	34.82	34.68	34.75	34.74
5	53.62	53.56	53.53	53.59	53.56	53.55	53.57	53.59	53.55	53.51	53.56	53.53
6	18.98	19.02	19.05	18.97	18.95	18.96	18.96	19.00	18.97	18.93	19.04	19.06
7	33.51	32.42	32.39	33.50	33.14	33.48	33.49	33.53	33.48	33.44	32.44	32.41
8	40.72	39.58	39.38	40.73	40.72	40.72	40.72	40.74	40.72	40.71	39.61	39.41
9	49.22	49.11	46.19	49.20	49.19	49.19	49.20	49.21	49.20	49.18	46.13	46.20
10	38.57	38.29	38.37	38.60	38.59	38.56	38.59	38.63	38.61	38.50	38.35	38.40
11	21.39	24.29	23.40	21.39	21.36	21.37	21.37	21.41	21.40	21.35	23.37	23.40
12	25.63	125.73	122.52	25.63	25.61	25.61	25.62	25.65	25.61	25.59	124.58	122.53
13	38.40	138.04	143.63	38.40	38.39	38.39	38.39	38.41	38.38	38.37	138.08	143.66
14	42.41	42.14	41.43	42.42	42.41	42.41	42.41	42.43	42.41	42.41	42.15	41.46
15	29.79	28.08	27.77	29.13	29.78	29.78	29.79	29.82	29.78	29.77	28.12	27.79
16	32.15	23.36	23.14	32.15	32.14	32.14	32.14	32.50	32.13	32.12	24.32	23.71
17	56.60	48.19	46.80	56.61	56.50	56.50	56.60	56.62	56.59	56.59	48.21	46.82
18	49.45	53.04	41.80	49.46	49.44	49.44	49.45	49.47	49.43	49.42	53.07	41.82
19	46.97	39.14	45.90	46.98	46.97	46.97	46.97	46.99	46.96	46.95	39.17	45.92
20	150.57	38.89	30.71	150.58	150.59	150.58	150.58	150.56	150.56	149.87	38.92	30.73
21	30.62	30.70	32.10	30.63	30.62	30.62	30.62	30.65	30.61	30.60	30.73	32.12
22	36.97	36.66	33.90	36.97	36.96	36.97	36.97	36.99	36.96	36.96	36.68	33.92
23	29.16	29.36	29.33	29.13	29.10	29.10	29.10	29.18	29.15	29.07	29.34	29.31
24	21.39	21.50	21.52	21.39	21.36	21.37	21.37	21.45	21.40	21.35	21.53	21.54
25	16.30	16.80	15.50	16.34	16.32	16.33	16.33	16.38	16.33	16.32	16.82	15.56
26	14.72	17.04	16.61	14.71	14.69	14.70	14.70	14.73	14.70	14.68	17.09	16.64
27	15.70	23.49	25.77	15.70	15.69	15.70	15.70	15.73	15.70	15.69	23.52	25.77
28	176.67	178.10	178.31	176.68	176.68	176.68	176.67	176.67	176.66	176.68	178.06	178.30
29	109.62	15.67	23.63	109.62	109.60	109.62	109.62	109.67	109.62	109.61	15.74	23.66
30	19.40	21.18	33.13	19.41	19.39	19.40	19.40	19.49	19.40	19.39	21.21	33.15
COOMe	51.27	51.47	51.54	51.28	51.28	51.29	51.27	51.30	51.28	51.29	51.46	51.55
4'	106.78	106.65	106.66	107.59	107.82	107.79	107.63	107.53	107.78	108.49	107.51	107.51
5'	149.58	149.64	149.63	152.20	151.39	151.52	151.97	151.76	151.79	150.59	152.25	152.27
Me-5'	13.72	13.72	13.72	-	-	-	-	-	-	-	-	-
CH ₂ -5'	-	-	-	34.66	34.15	34.09	33.93	32.17	33.67	34.56	34.57	34.56
Ph	-	-	-	138.74 128.76 128.35 126.22	137.75 131.41 130.48 128.75	137.22 130.08 128.46 132.02	134.38 130.13 (d, $^1J_{\text{C,F}} = 8$) 115.10 (d, $^1J_{\text{C,F}} = 21$) 162.53 (d, $^1J_{\text{C,F}} = 242$)	136.43 130.12 137.10 125.99 129.42 126.50	134.57 105.50 153.09 136.32	146.54 129.44 123.67 146.54	138.75 128.75 128.37 126.23	138.74 128.75 128.36 126.23
Me-C ₆ H ₄	-	-	-	-	-	-	-	19.44	-	-	-	-
(O-Me) ₂ O-Me	-	-	-	-	-	-	-	-	55.98 60.84	-	-	-

Table 3. ^{13}C NMR spectra of compounds 11b-13b, 16a-f, 18b and 20b

Atom or group	11b	12b	13b	16a	16b	16c	16d	16e	16f	18b	20b
1	38.64	38.37	38.09	38.57	38.59	38.60	38.60	38.60	38.59	38.35	38.08
2	113.66	113.58	113.54	113.67	113.73	113.72	113.69	113.68	113.75	113.61	113.58
3	154.44	154.42	154.45	155.10	155.38	155.36	155.26	154.90	155.23	155.09	155.12
4	34.61	34.47	34.46	34.74	34.66	34.66	34.66	34.65	34.83	34.75	34.75
5	53.60	53.55	53.51	53.55	53.52	53.52	53.53	53.53	53.53	53.52	53.50
6	18.94	18.93	18.96	18.92	18.92	18.92	18.91	18.93	18.93	18.94	18.99
7	33.49	32.39	32.45	33.46	33.44	33.44	33.45	33.47	33.45	32.38	32.45
8	40.73	39.57	39.38	40.72	40.72	40.72	40.72	40.72	40.72	39.59	39.41
9	49.16	46.12	46.22	49.12	49.11	49.12	49.11	49.11	49.13	46.12	46.22
10	38.59	38.30	38.39	38.57	38.56	38.60	38.60	38.61	38.63	38.35	38.43
11	21.36	24.10	23.38	21.34	21.33	21.33	21.33	21.37	21.36	23.33	23.38
12	25.60	125.99	122.77	25.58	25.57	25.57	25.57	25.58	25.57	125.99	122.78
13	38.62	137.77	143.42	38.57	38.56	38.56	38.57	38.56	38.59	137.80	143.44
14	42.45	42.06	41.03	42.44	42.44	42.44	42.43	42.44	42.44	42.06	41.06
15	29.84	28.05	27.74	29.82	29.81	29.81	29.82	29.81	29.83	28.07	27.76
16	32.16	23.34	22.95	32.14	32.13	32.13	32.13	32.46	32.14	24.11	22.95
17	56.53	48.10	46.66	56.48	56.46	56.46	56.48	56.46	56.51	48.11	46.67
18	49.29	52.63	41.74	49.26	49.25	49.25	49.25	49.25	49.26	52.62	41.74
19	46.96	39.11	45.87	46.93	46.93	46.92	46.93	46.92	46.95	39.12	45.88
20	150.38	38.84	30.69	150.42	150.40	150.40	150.40	150.41	150.38	38.85	30.71
21	30.62	30.66	32.05	30.59	30.58	30.58	30.59	30.59	30.61	30.67	32.06
22	37.07	36.75	33.84	37.05	37.04	37.04	37.06	37.04	37.06	36.76	33.85
23	29.17	29.31	21.53	29.12	29.10	29.10	29.10	29.14	29.15	29.29	21.53
24	21.36	21.52	29.30	21.34	21.33	21.33	21.33	21.36	21.36	21.52	29.29
25	16.31	16.96	15.49	16.33	16.33	16.33	16.33	16.33	16.33	16.98	15.56
26	14.72	16.99	16.86	14.69	14.68	14.68	14.68	14.67	14.70	17.03	16.86
27	15.82	23.50	25.78	15.81	15.80	15.80	15.80	15.81	15.82	23.51	25.81
28	183.26	184.42	184.58	182.47	182.29	182.30	182.54	182.18	183.07	184.54	184.82
29	109.76	15.66	23.57	109.73	109.74	109.74	109.74	109.73	109.76	15.72	23.60
30	19.42	21.18	33.08	19.40	19.40	19.40	19.40	19.41	19.41	21.20	33.11
4'	106.78	106.65	106.65	107.57	107.80	107.77	107.61	107.48	107.77	107.50	107.51
5'	149.60	149.65	149.66	152.23	151.43	151.55	152.01	151.76	151.83	152.27	152.29
Me-5'	13.73	13.73	13.73	-	-	-	-	-	-	-	-
CH ₂ -5'	-	-	-	34.66	34.15	34.09	33.93	32.13	33.68	34.54	34.55
Ph	-	-	-	138.73 128.76 128.36 126.22	137.74 131.43 130.49 120.08	137.21 130.08 128.46 132.02	134.35 (d, ¹ J _{C,F} = 3,25) 130.13 (d, ¹ J _{C,F} = 8) 115.10 (d, ¹ J _{C,F} = 21) 161.53 (d, ¹ J _{C,F} = 242)	136.45 137.09 130.10 129.41 125.96 126.47	134.58 105.52 153.09 136.32	138.76 128.76 128.37 126.25	138.75 128.76 128.38 126.25
Me-C ₆ H ₄	-	-	-	-	-	-	-	19.45	-	-	-
(O-Me) ₂ O-Me	-	-	-	-	-	-	-	-	55.98 60.85	-	-