Supplementary Material

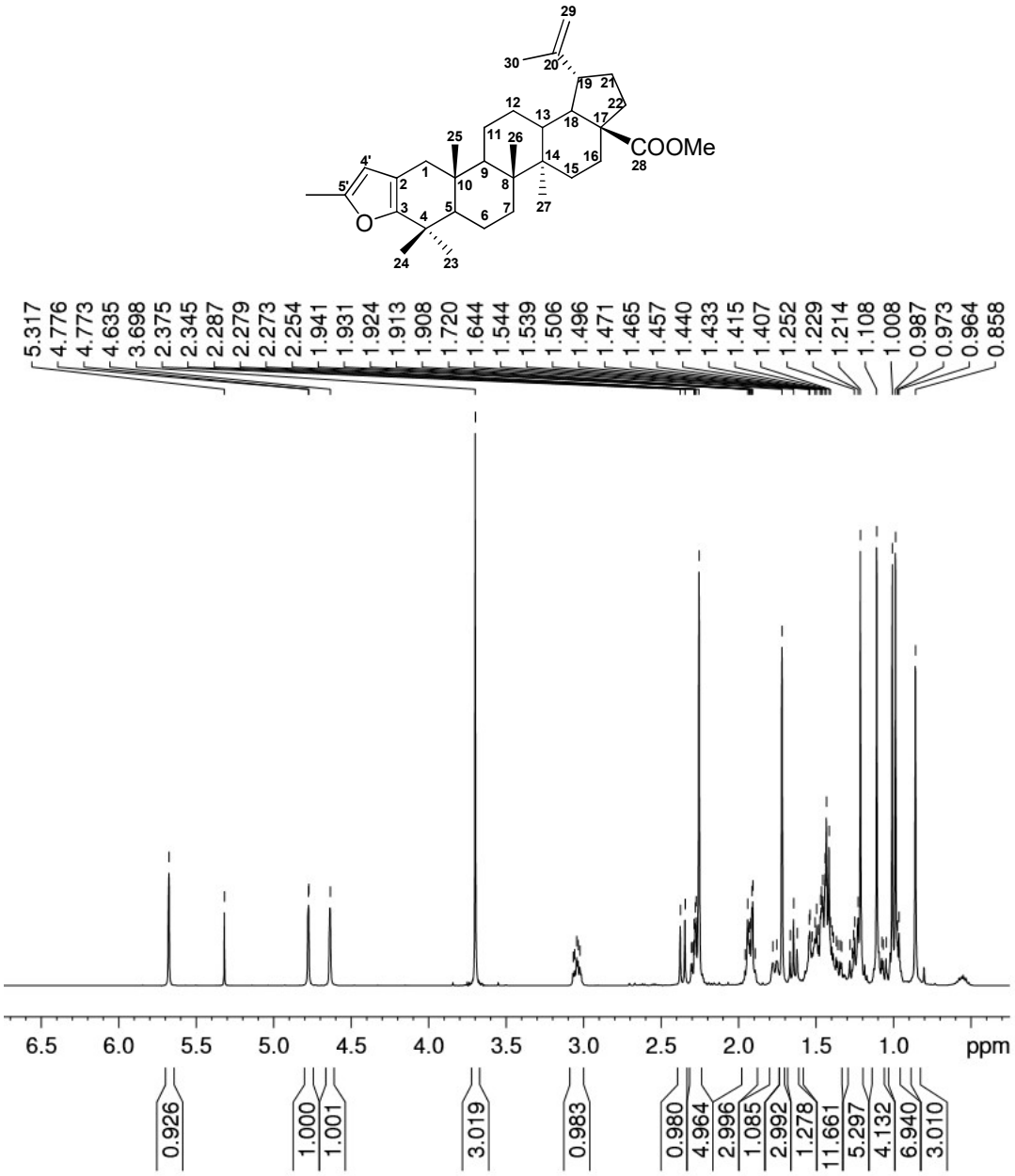
Effective synthesis of novel furan-fused pentacyclic triterpenoids via anionic 5-exo dig cyclization of 2-alkynyl-3-oxotriterpene acids

Rinat R. Gubaidullin, Darina S. Yarmukhametova, Darya A. Nedopekina, Rezeda R. Khalitova, and Anna Yu. Spivak*.

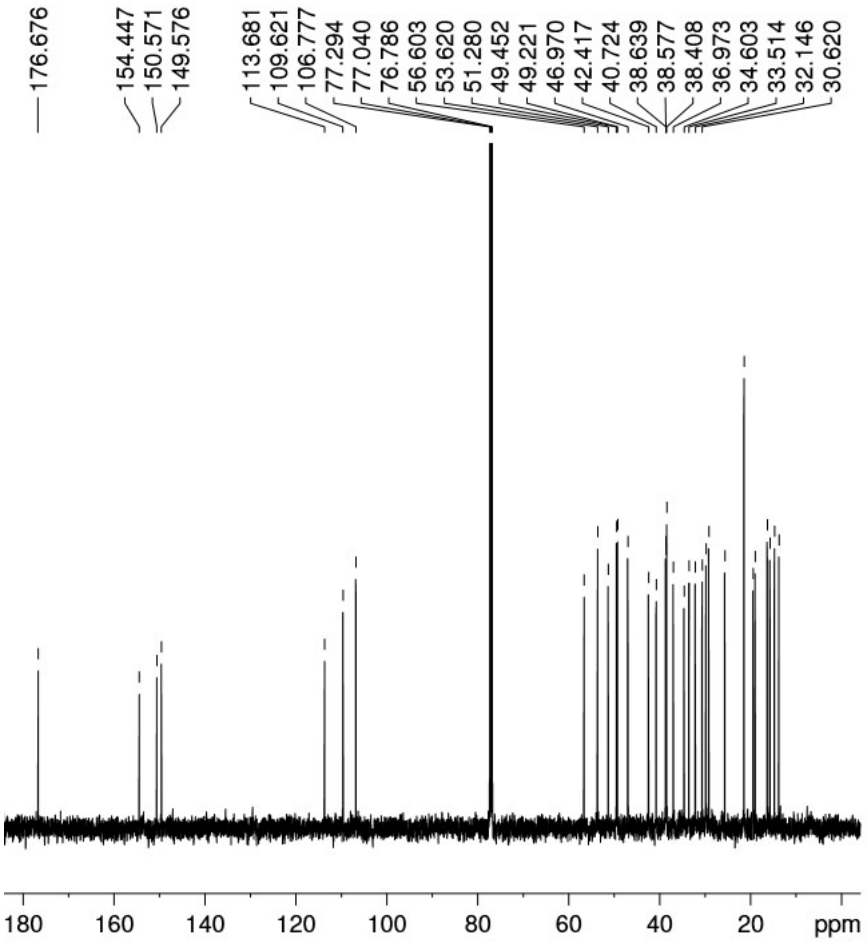
Institute of Petrochemistry and Catalysis, Russian Academy of Sciences, 141 Prospekt Oktyabrya, Ufa 450075, Russian Federation
Fax: +7 347 284 2750; E-mail: spivak.ink@gmail.com

^{1}H NMR and ^{13}C NMR data of new compounds

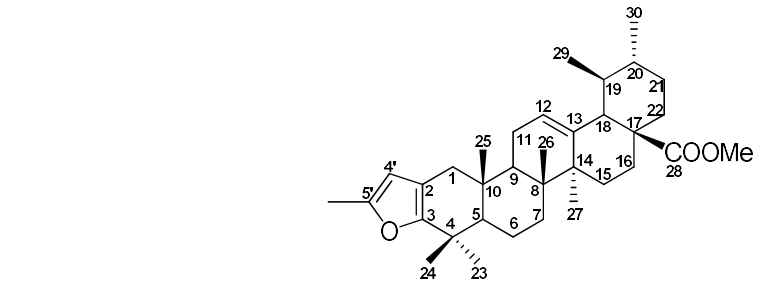
Methyl 5'-methylfurano[3,2-b]lup-20(29)-en-2-oate **11a** ^{1}H NMR spectra ($CDCl_3$)

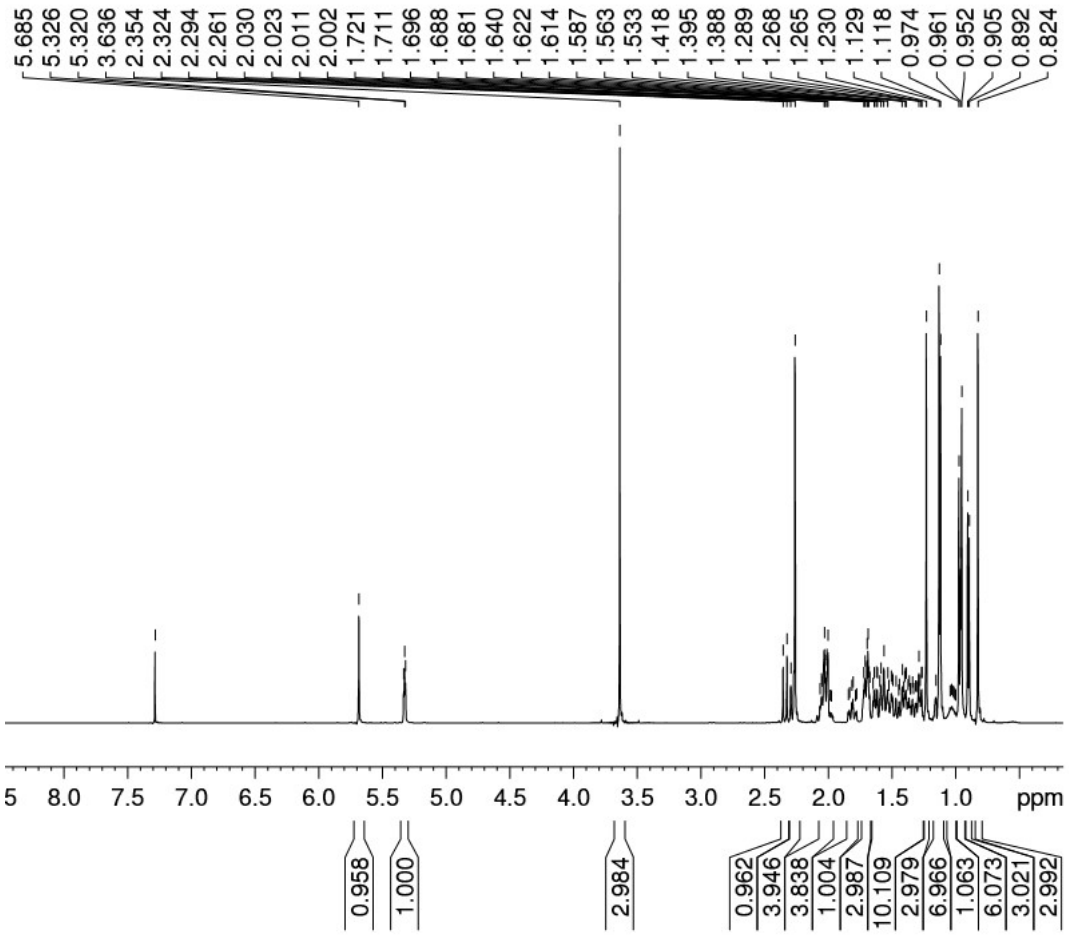


Methyl 5'-methylfurano[3,2-b]lup-20(29)-en-2-oate **11a** ^{13}C NMR spectra ($CDCl_3$)

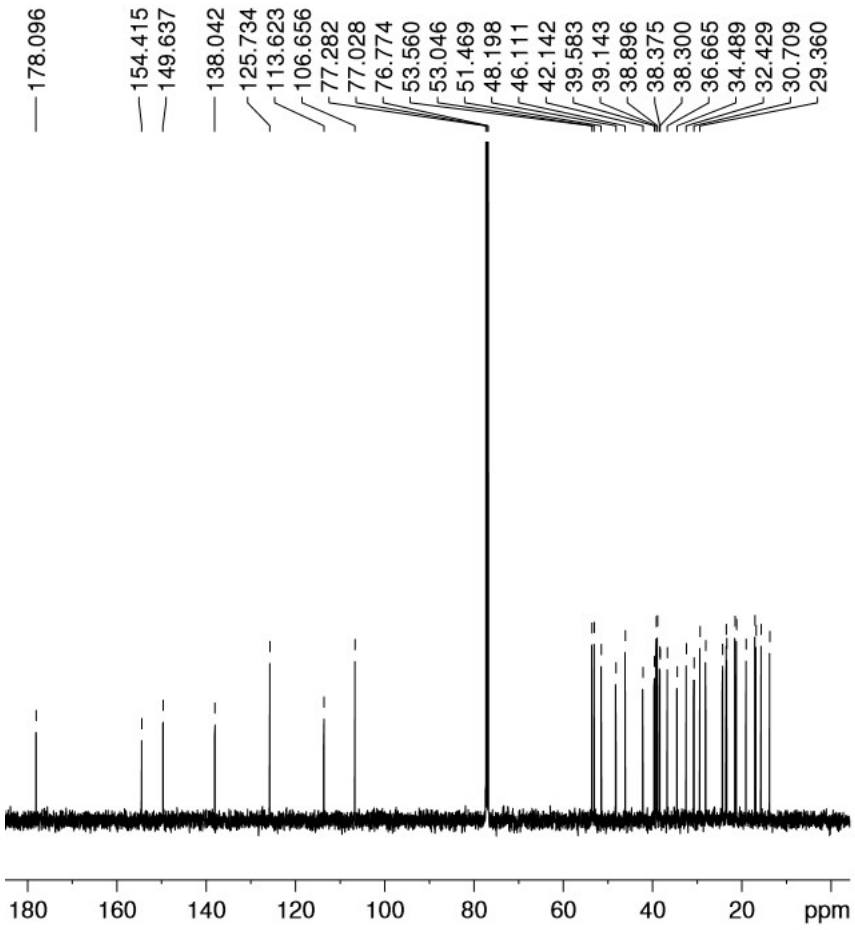


Methyl 5'-methylfurano[3,2-b]urs-12-en-28-oate **12a** ^{1}H NMR spectra ($CDCl_3$)

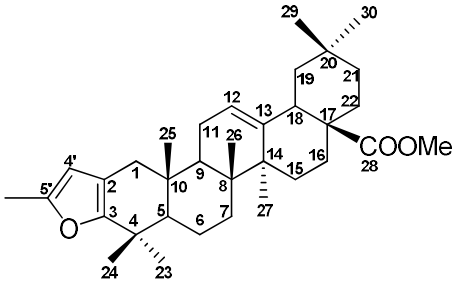


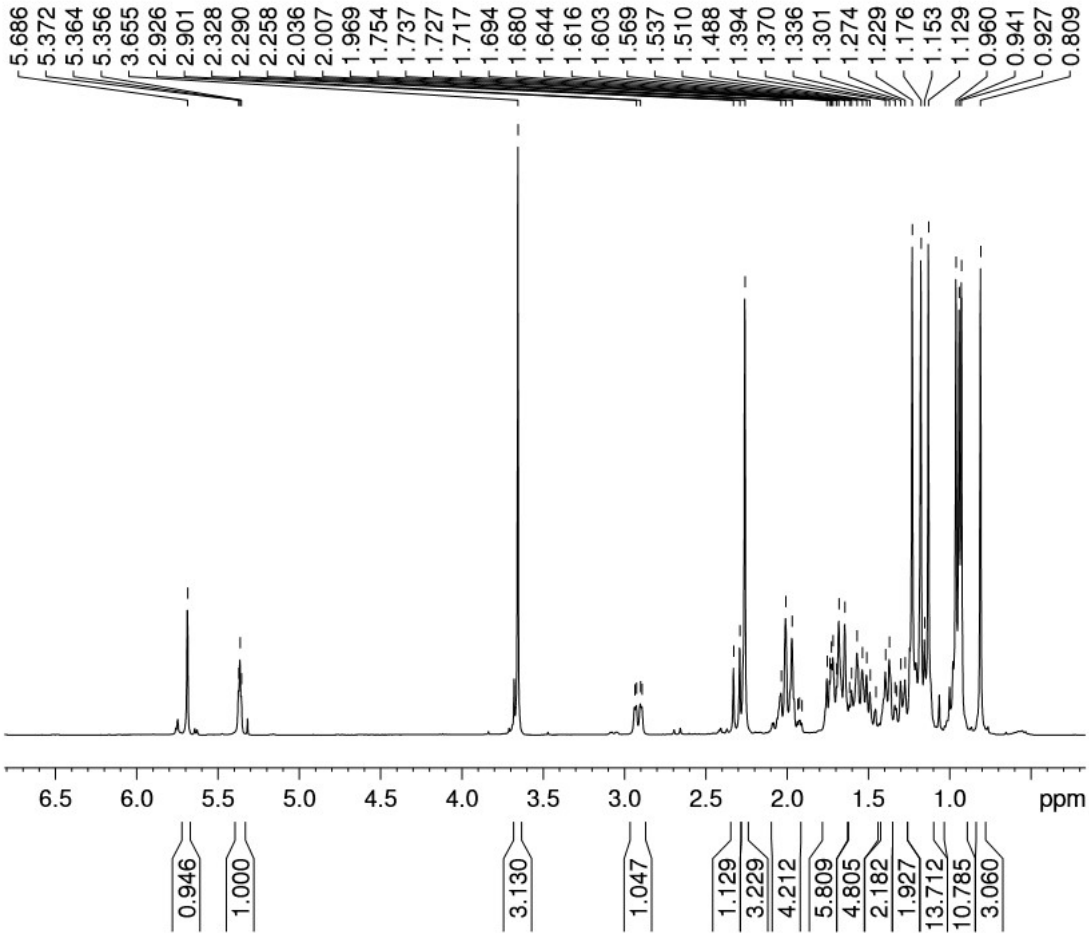


Methyl 5'-methylfurano[3,2-b]urs-12-en-28-oate **12a** ^{13}C NMR spectra ($CDCl_3$)

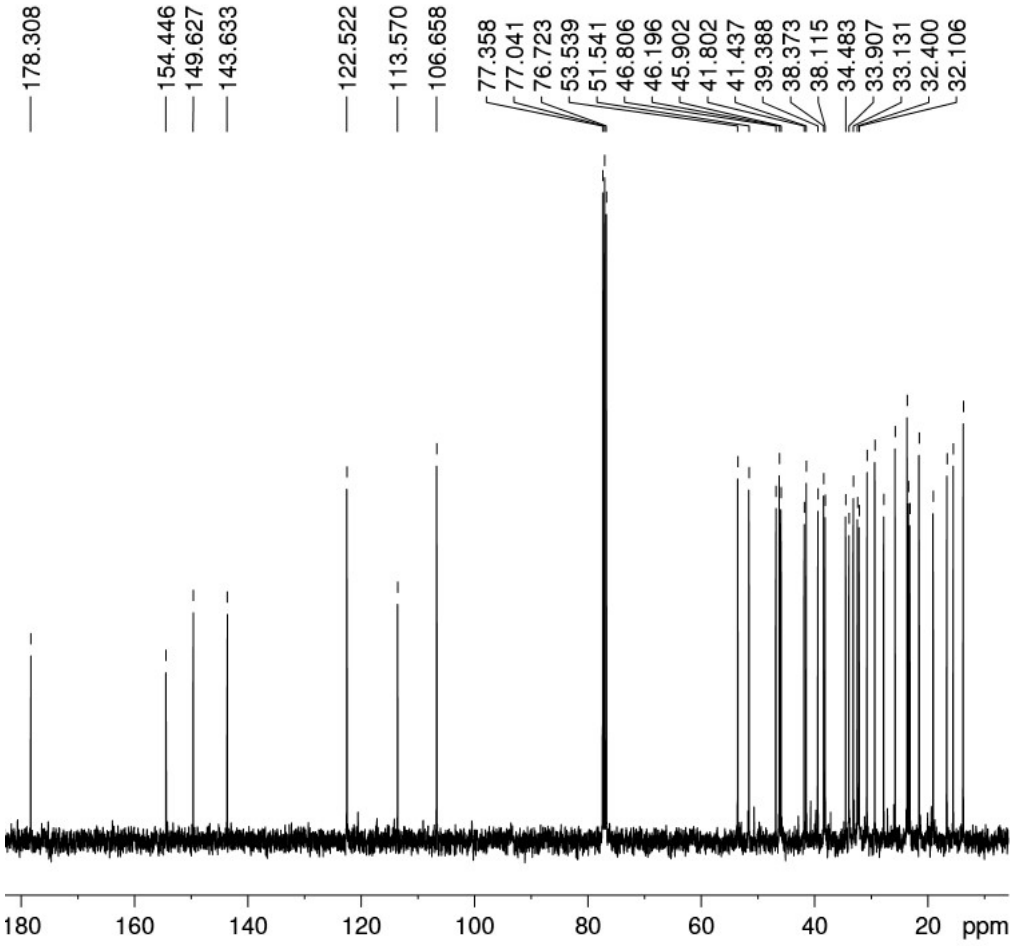


Methyl 5'-methylfurano[3,2-b]olean-12-en-28-oate **13a** ^{1}H NMR spectra ($CDCl_3$)

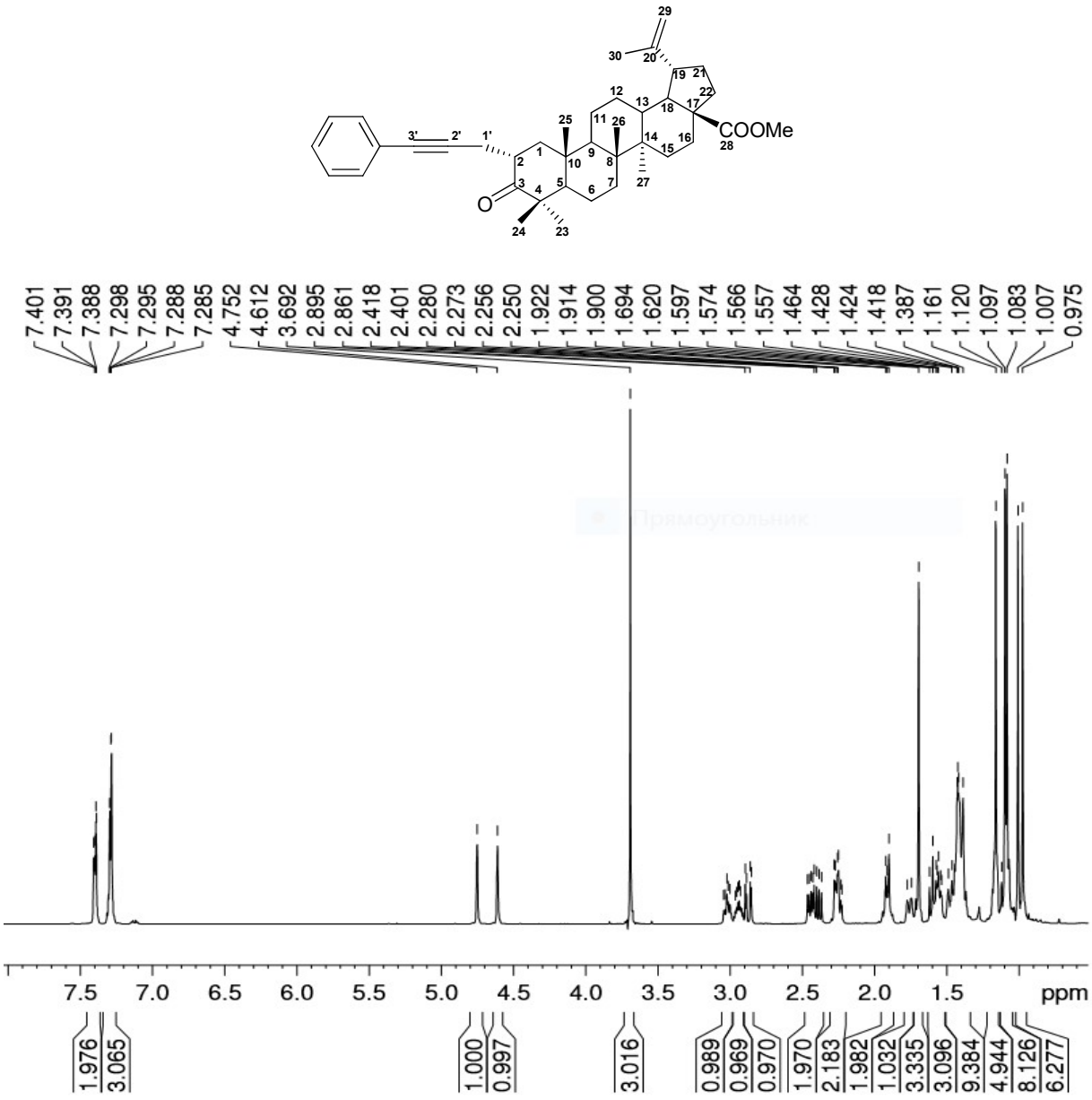




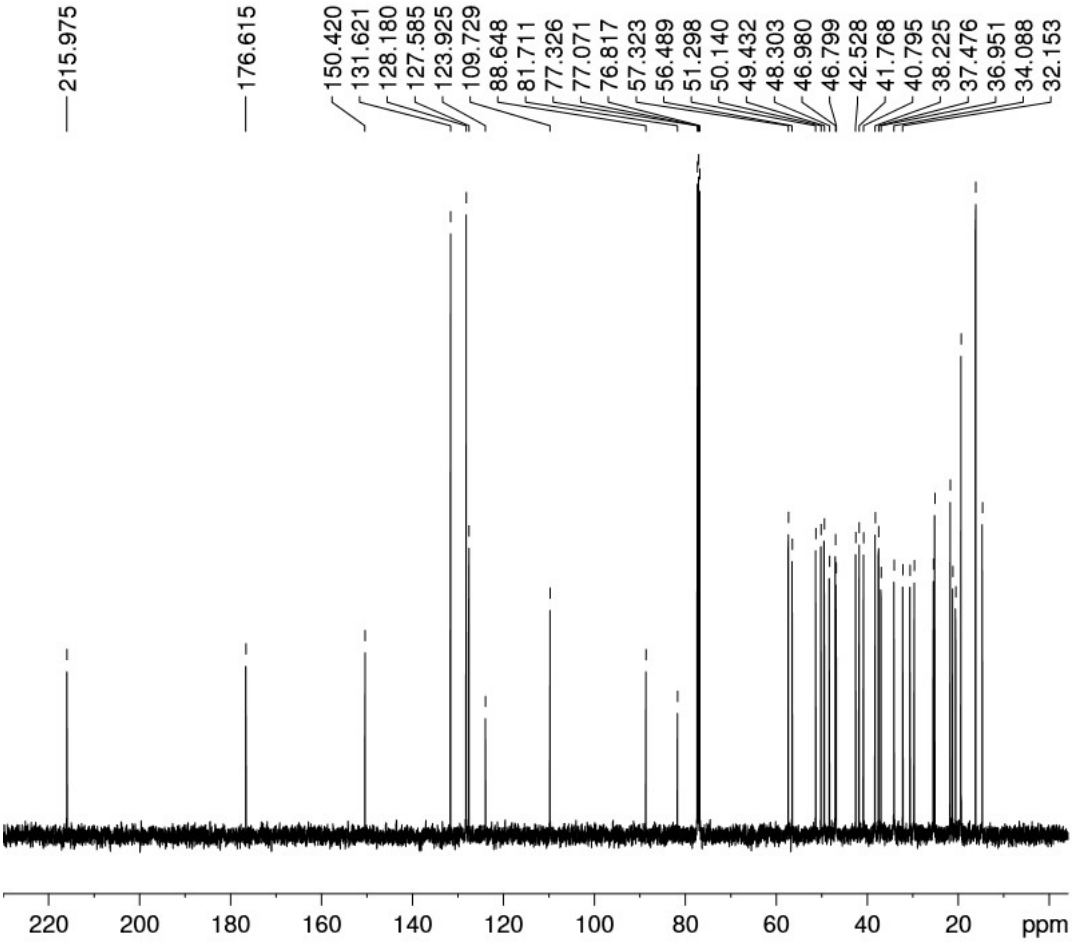
Methyl 5'-methylfurano[3,2-b]olean-12-en-28-oate **13a** ^{13}C NMR spectra ($CDCl_3$)



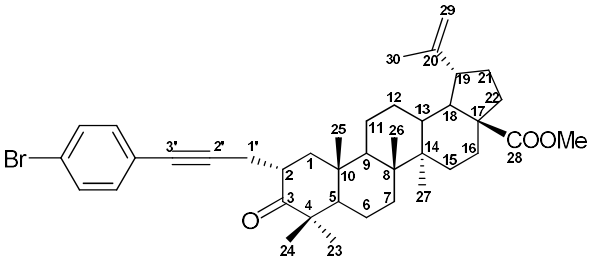
Methyl-2α-phenylpropynyl-3-oxolup-20(29)-en-28-oate **14a** ^{1}H NMR spectra ($CDCl_3$)

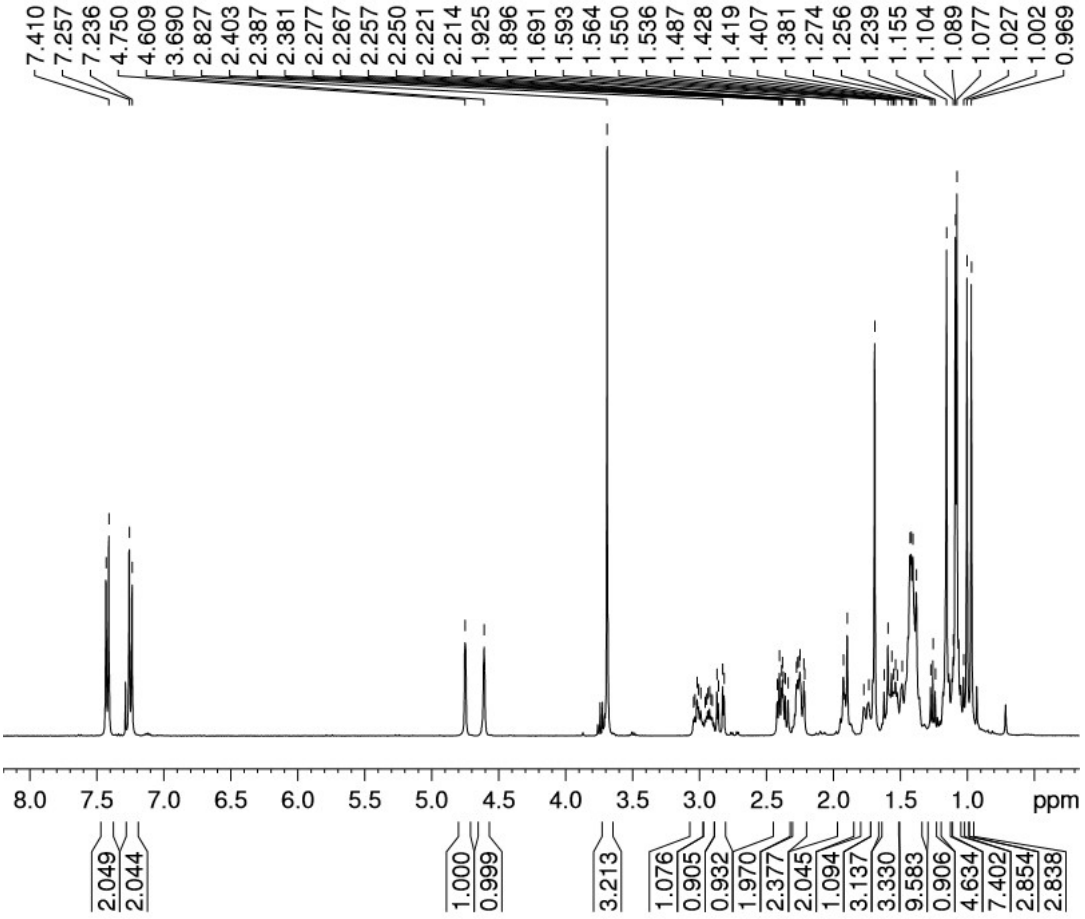


Methyl-2α-phenylpropynyl-3-oxolup-20(29)-en-28-oate **14a** ^{13}C NMR spectra ($CDCl_3$)

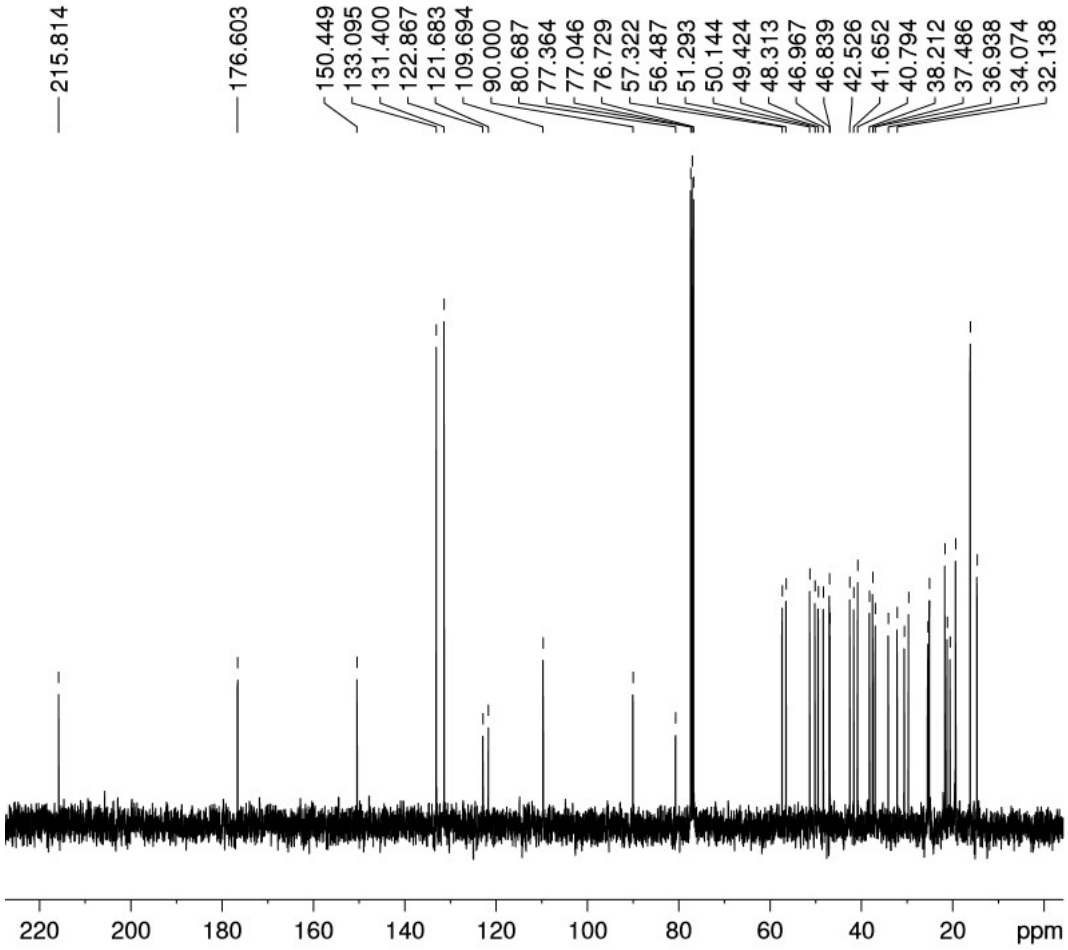


Methyl-2α-(4-bromophenylpropynyl)-3-oxolup-20(29)en-28-oate **14b** ^{1}H NMR spectra ($CDCl_3$)

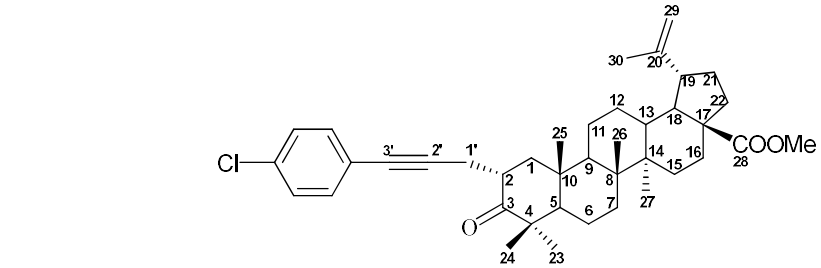


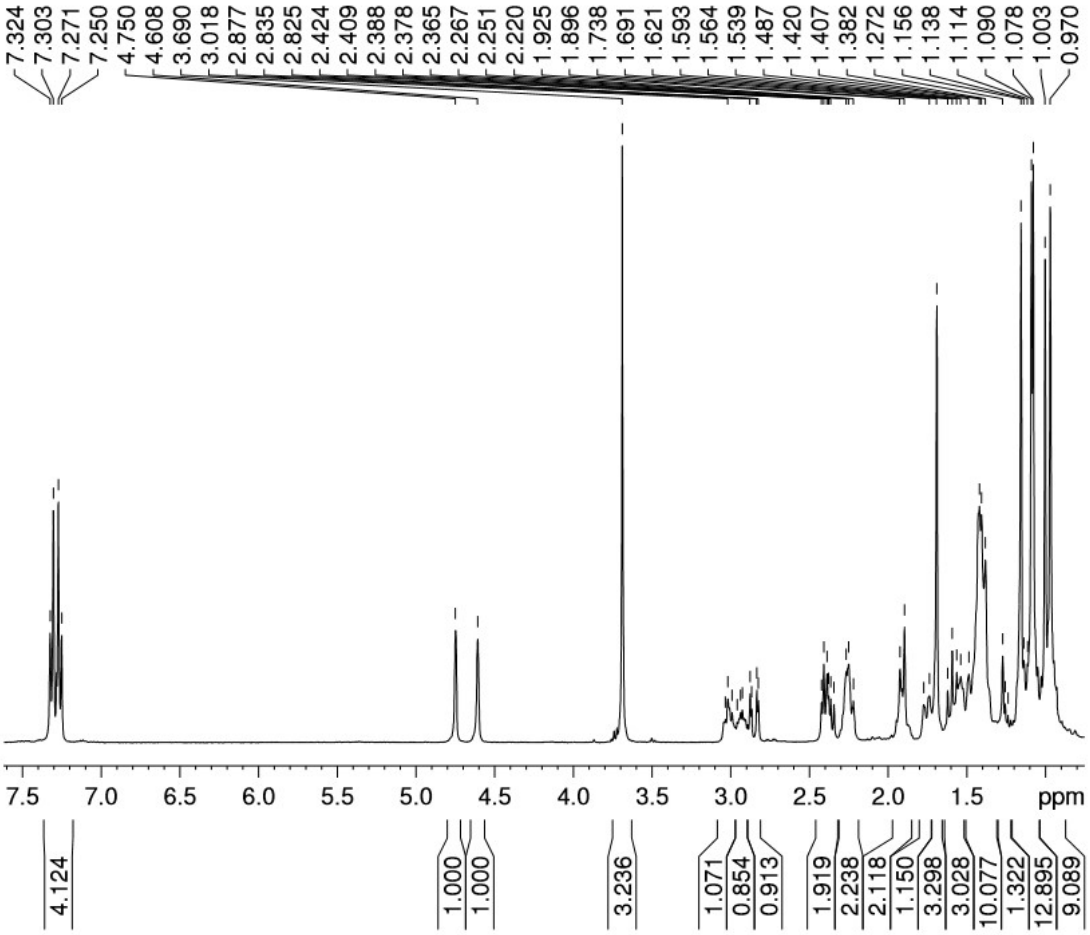


Methyl-2α-(4-bromophenylpropynyl)-3-oxolup-20(29)en-28-oate **14b** ^{13}C NMR spectra ($CDCl_3$)

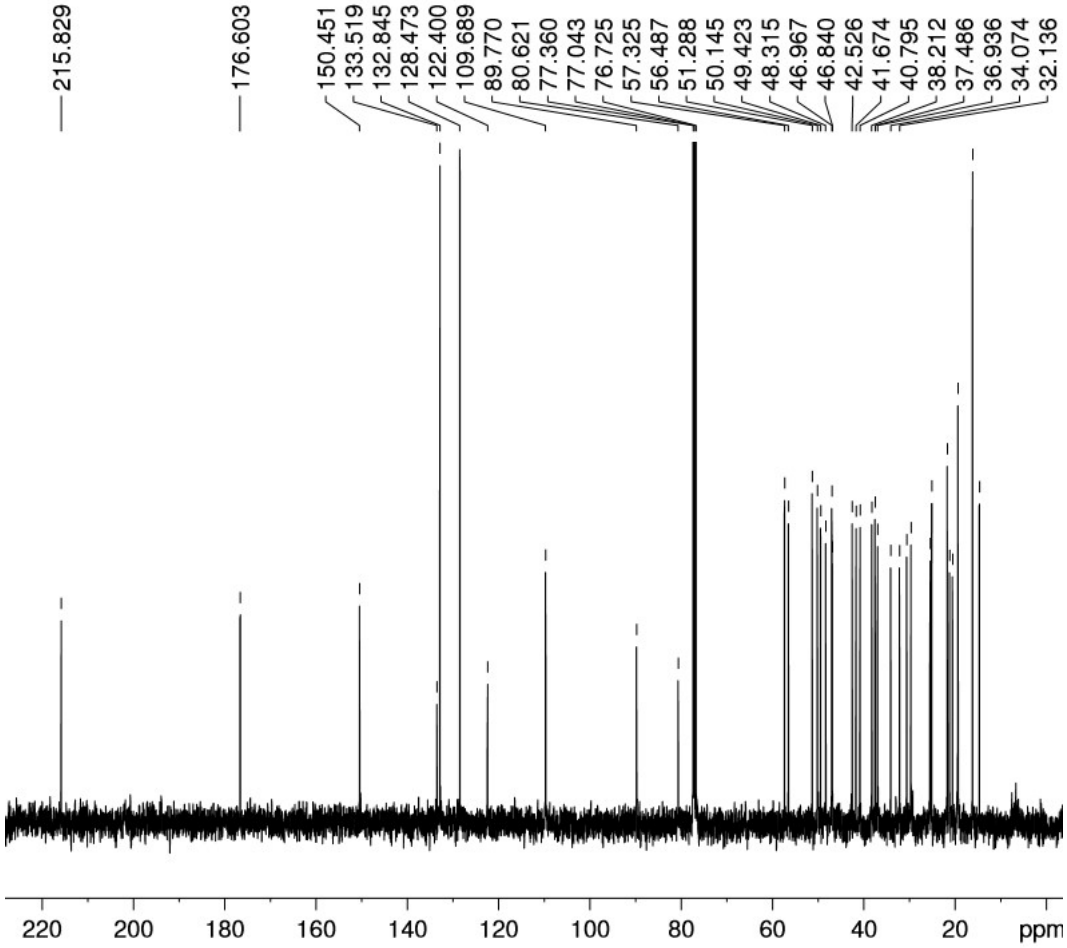


Methyl-2α-(4-chlorophenylpropynyl)-3-oxolup-20(29)en-28-oate **14c** ^{1}H NMR spectra ($CDCl_3$)

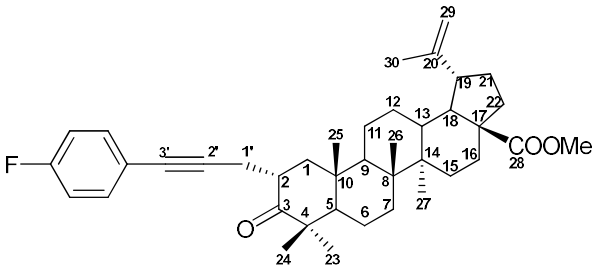


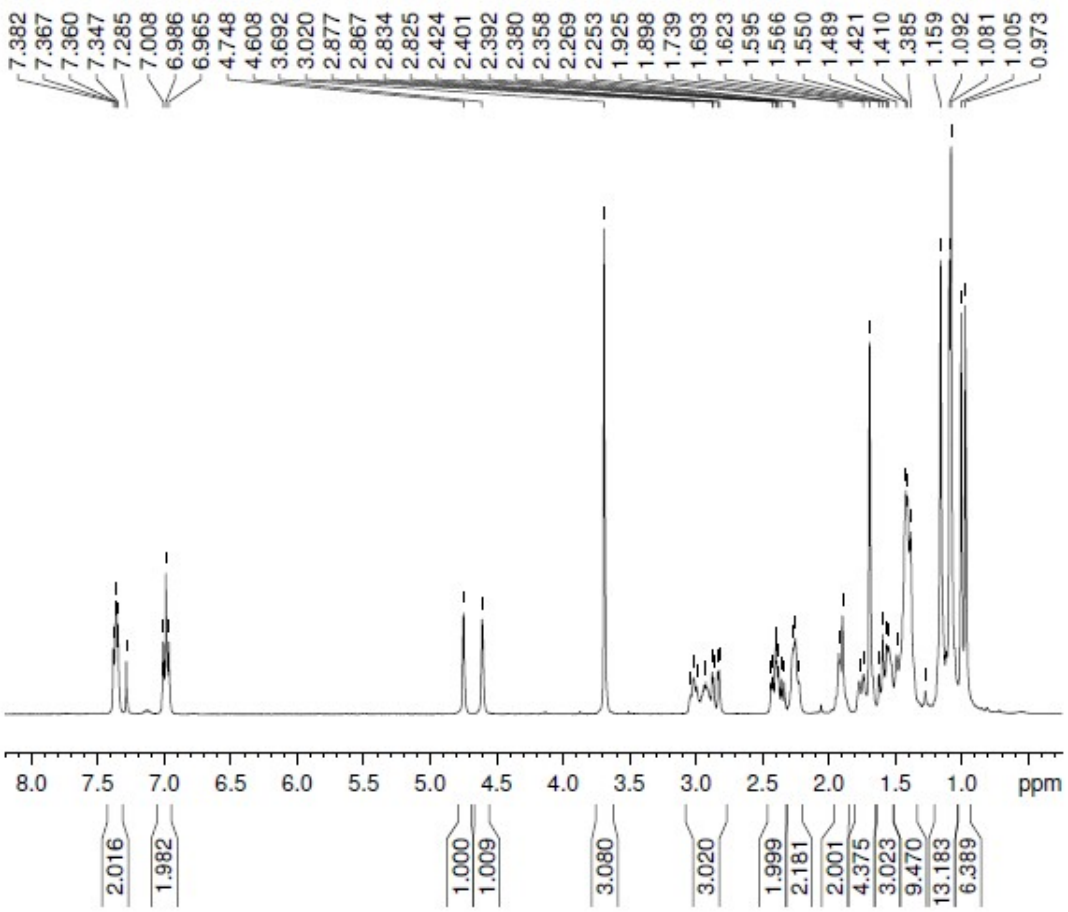


Methyl-2α-(4-chlorophenylpropynyl)-3-oxolup-20(29)en-28-oate **14c** ^{13}C NMR spectra ($CDCl_3$)

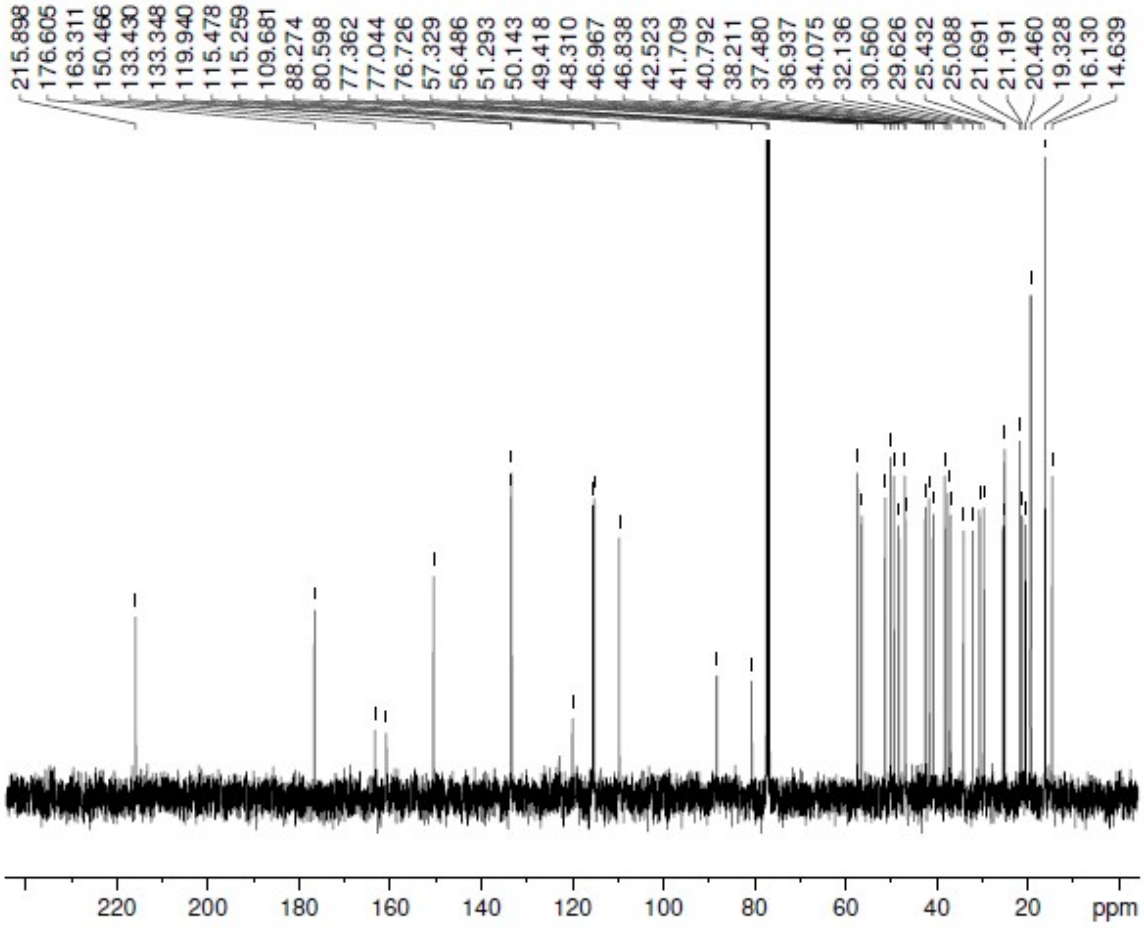


Methyl-2α-(4-fluorophenylpropynyl)-3-oxolup-20(29)en-28-oate **14d** ^{1}H NMR spectra ($CDCl_3$)

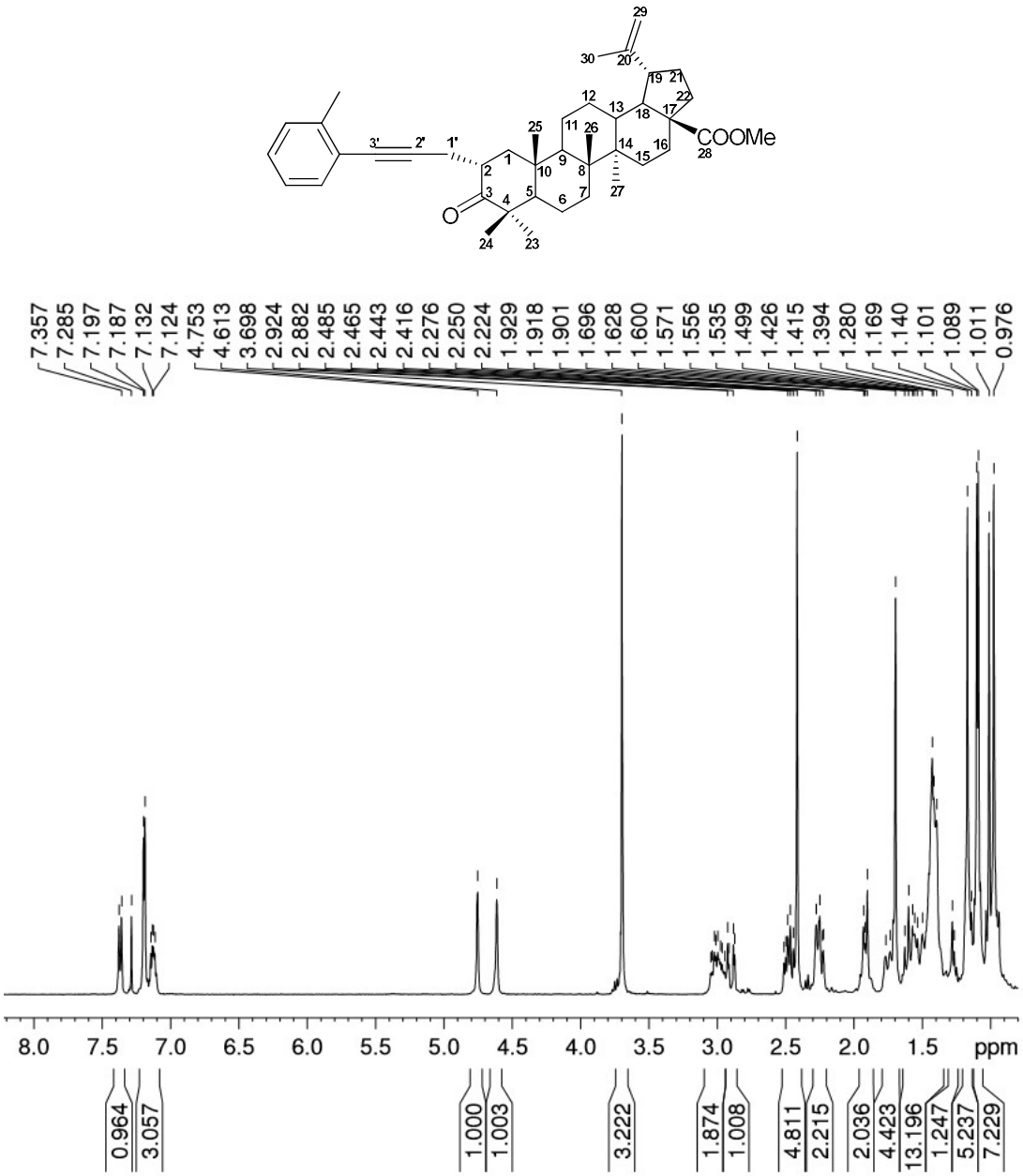




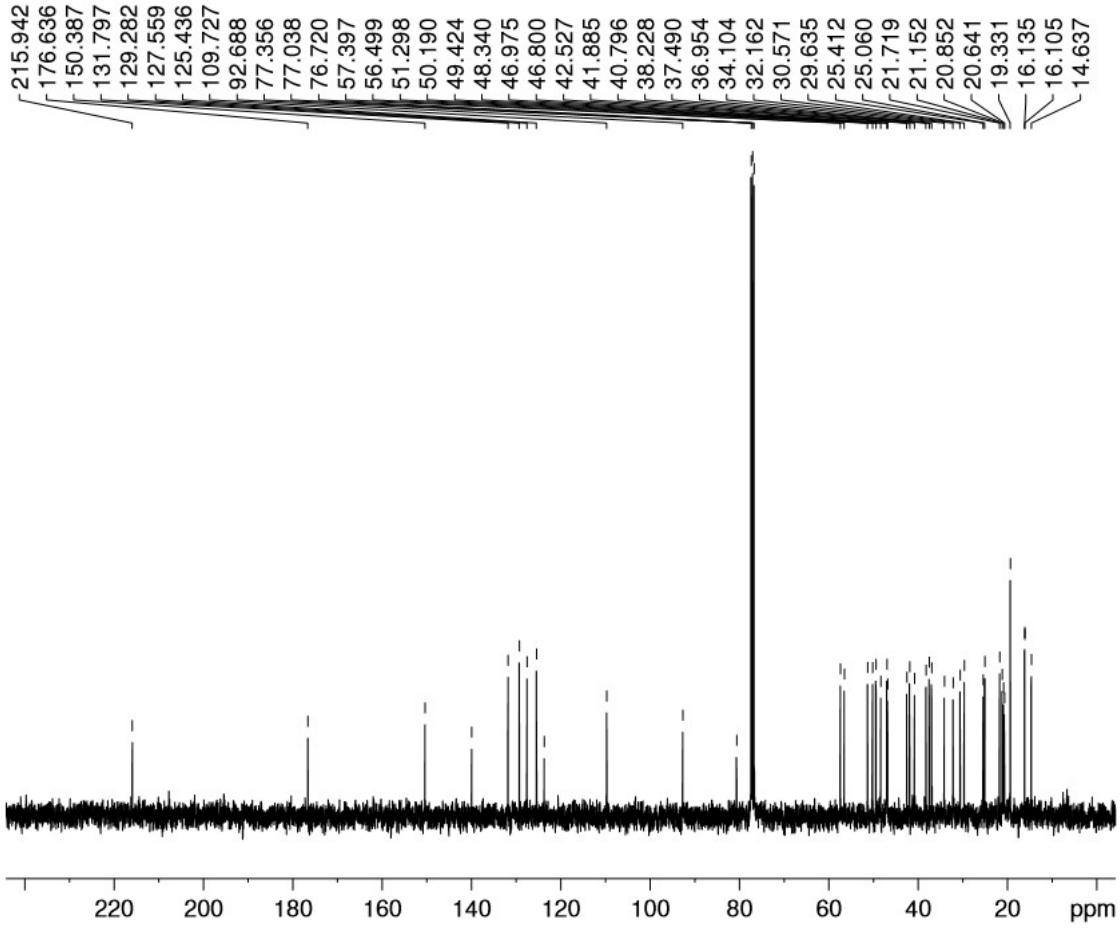
Methyl-2α-(4-fluorophenylpropynyl)-3-oxolup-20(29)en-28-oate **14d** ^{13}C NMR spectra ($CDCl_3$)



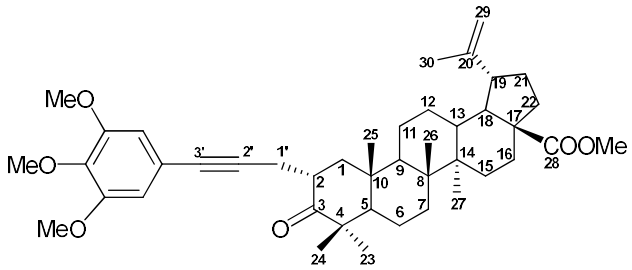
Methyl-2α-(2-methylphenylpropynyl)-3-oxolup-20(29)en-28-oate **14e** ^{1}H NMR spectra ($CDCl_3$)

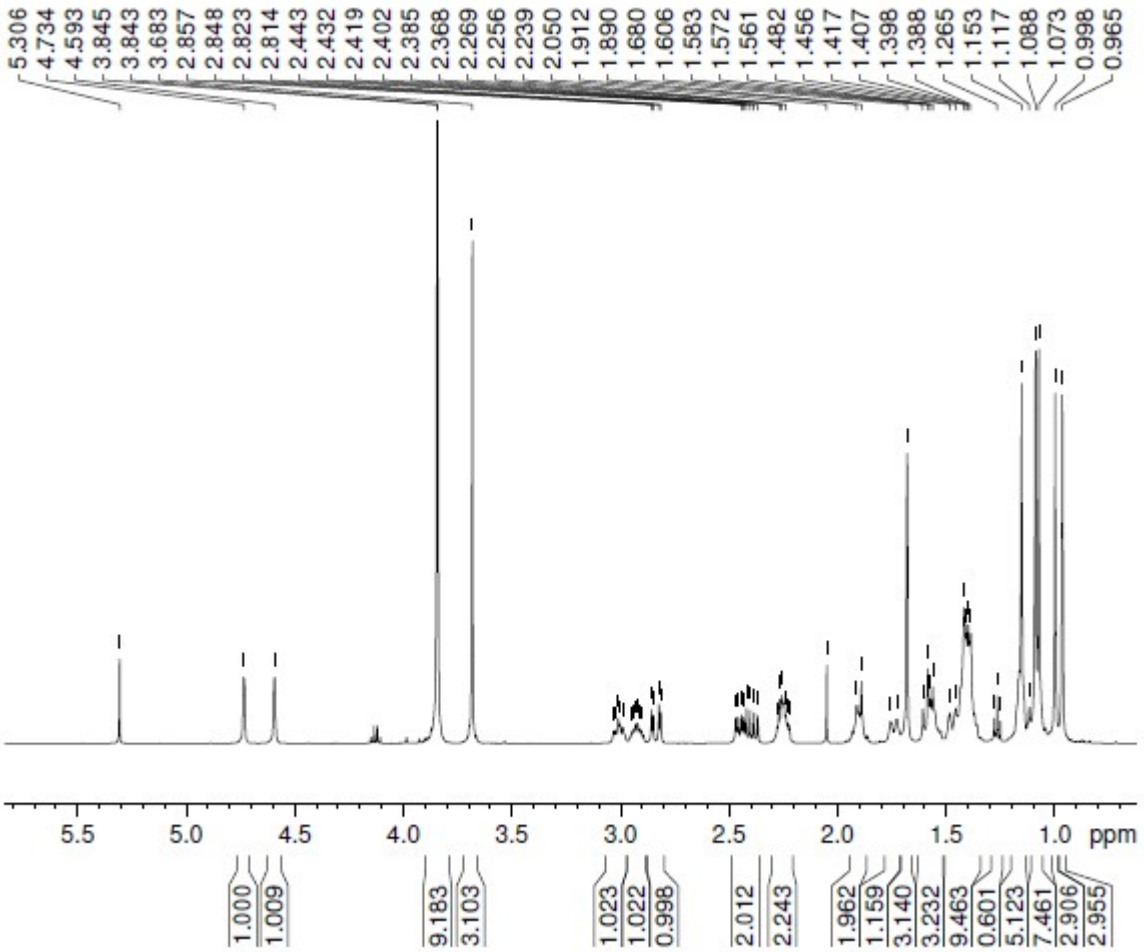


Methyl-2α-(2-methylphenylpropynyl)-3-oxolup-20(29)en-28-oate **14e** ^{13}C NMR spectra ($CDCl_3$)

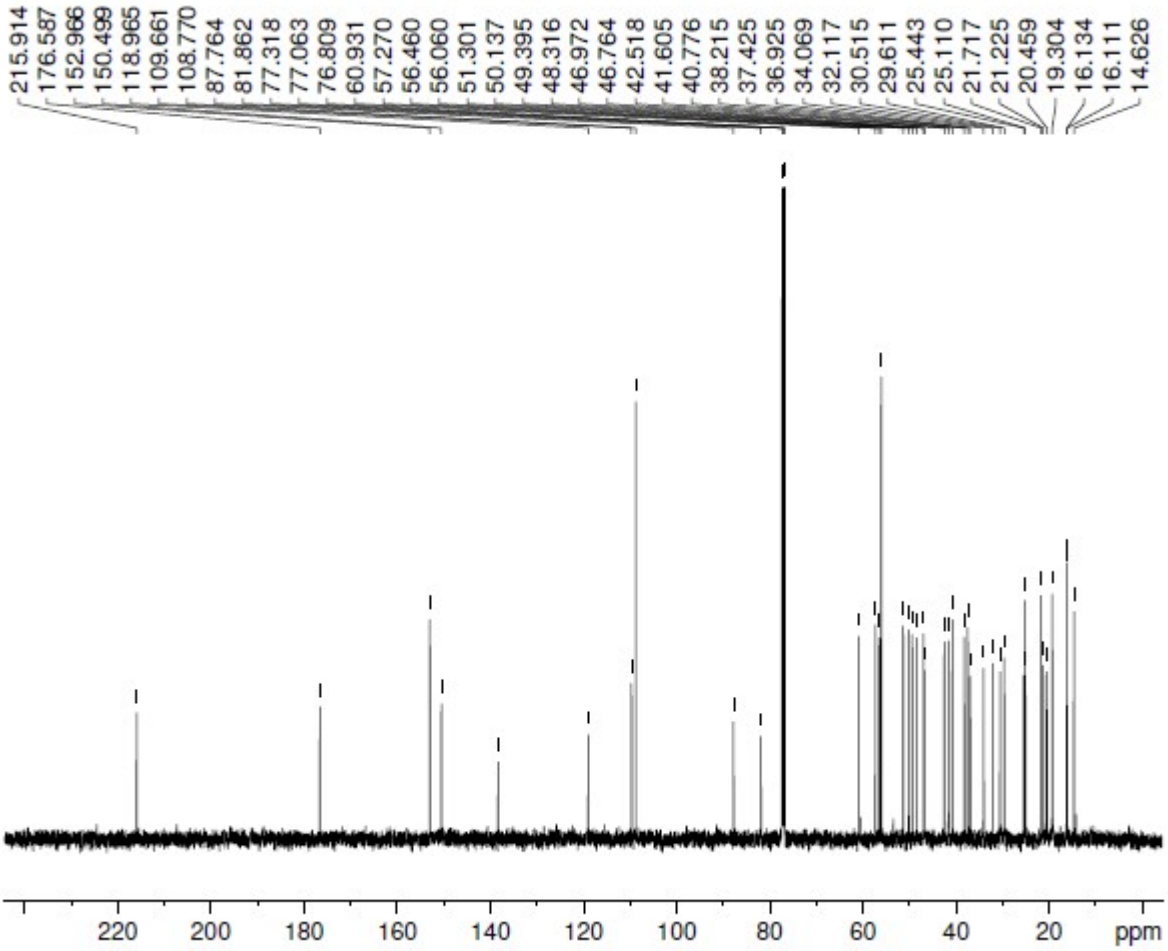


Methyl-2α-(3,4,5-trimethoxyphenylpropynyl)-3-oxolup-20(29)en-28-oate **14f** ^{1}H NMR spectra ($CDCl_3$)

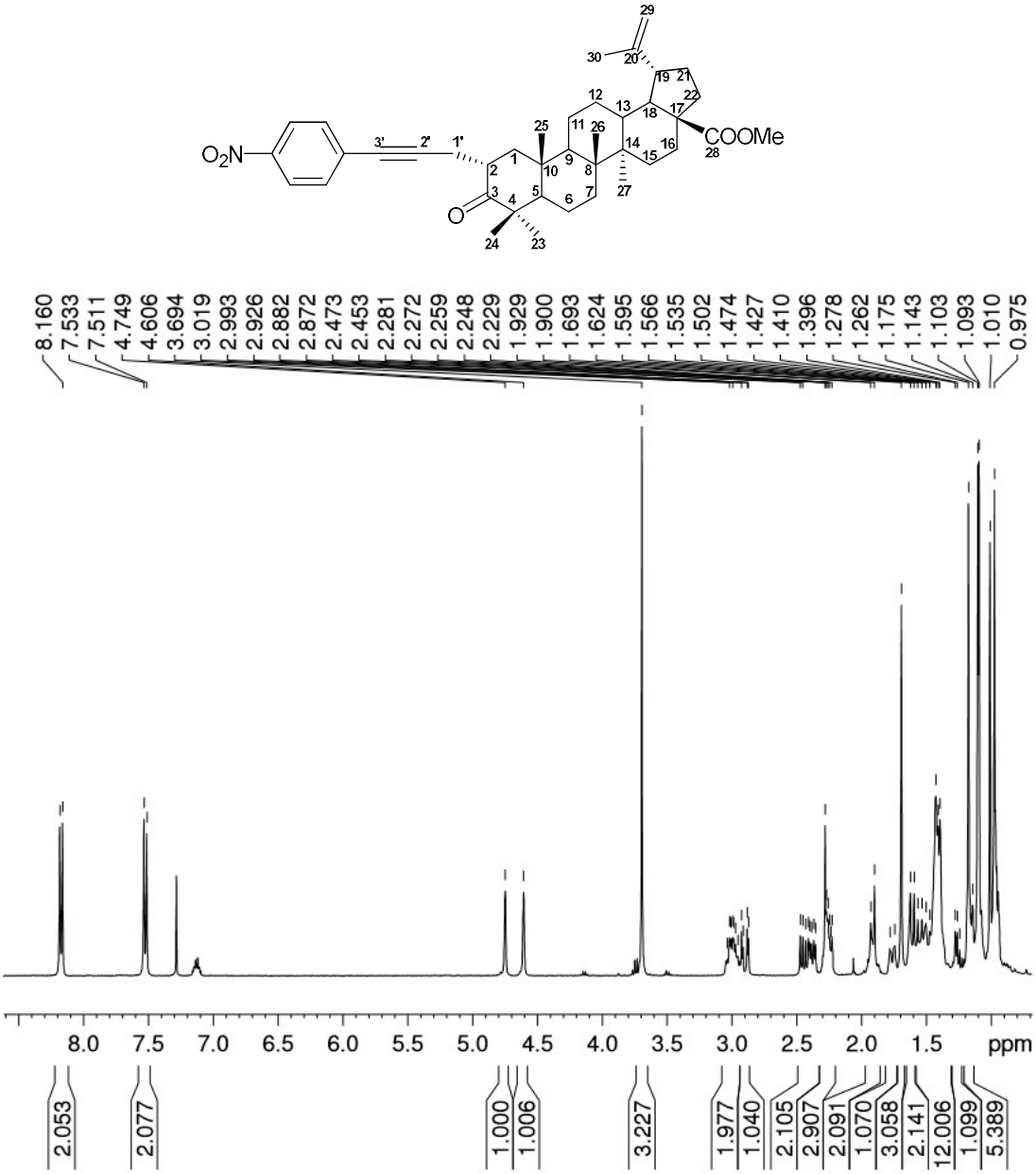




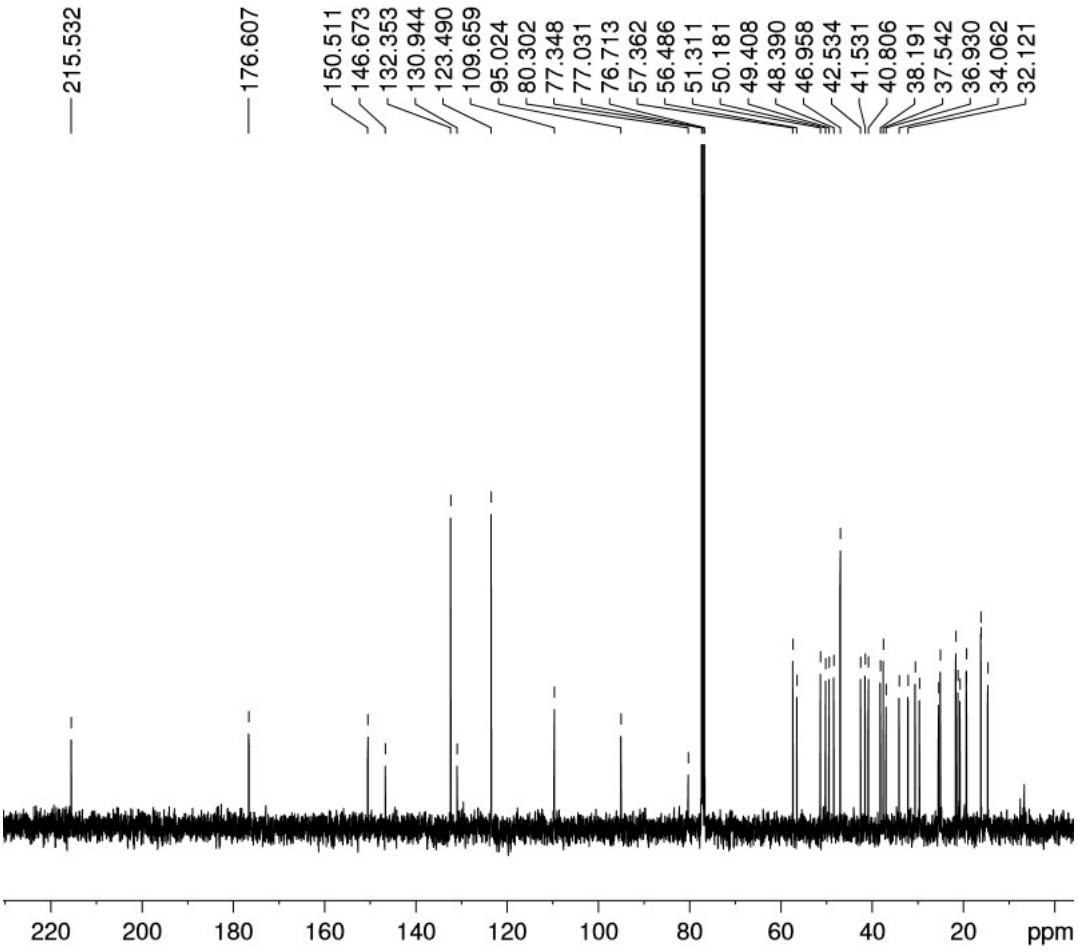
Methyl-2α-(3,4,5-trimethoxyphenylpropynyl)-3-oxolup-20(29)en-28-oate **14f** ^{13}C NMR spectra ($CDCl_3$)



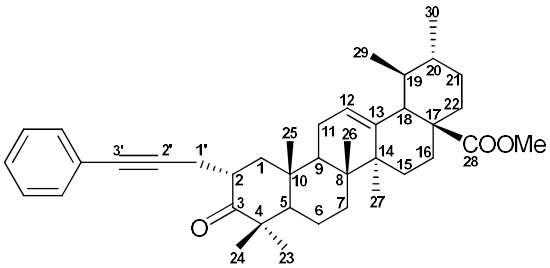
Methyl-2α-(4-nitrophenylpropynyl)-3-oxolup-20(29)en-28-oate **14g** ^{1}H NMR spectra ($CDCl_3$)

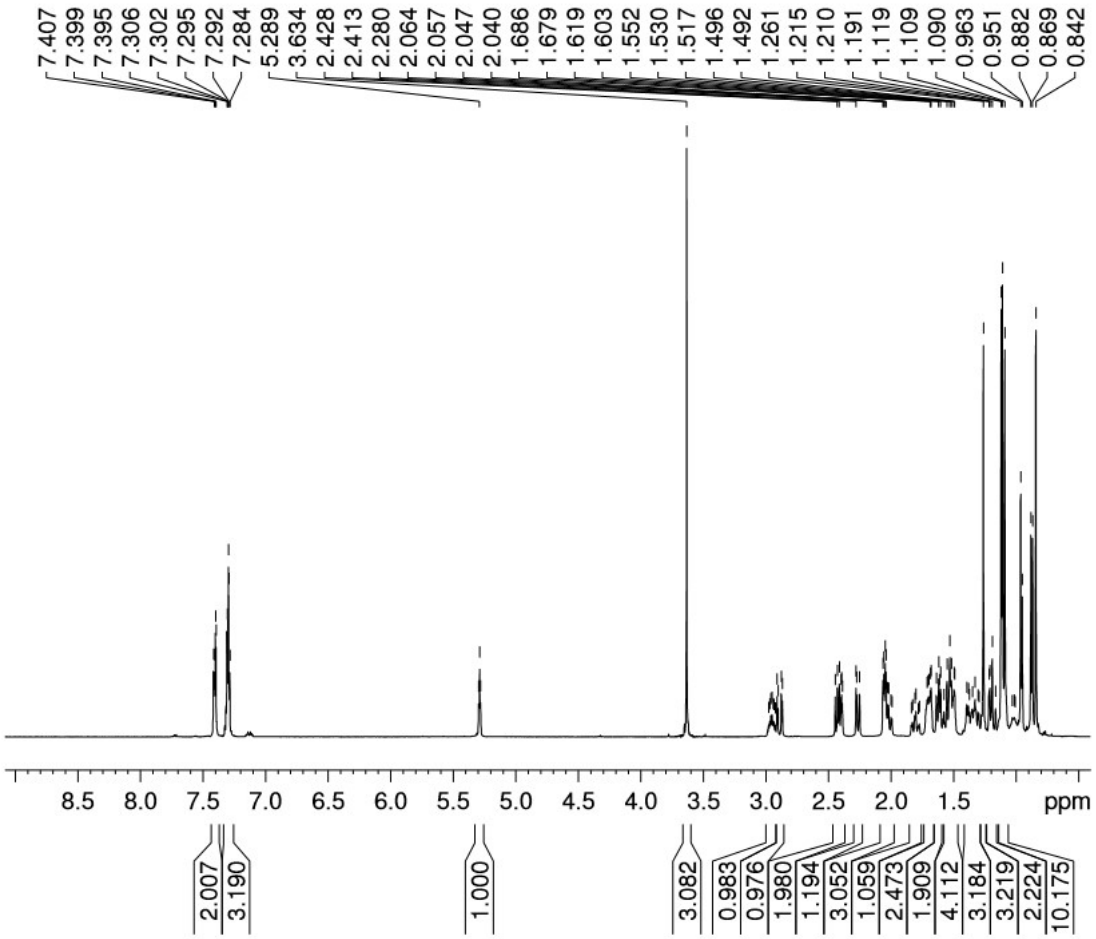


Methyl-2α-(4-nitrophenylpropynyl)-3-oxolup-20(29)en-28-oate **14g** ^{13}C NMR spectra ($CDCl_3$)

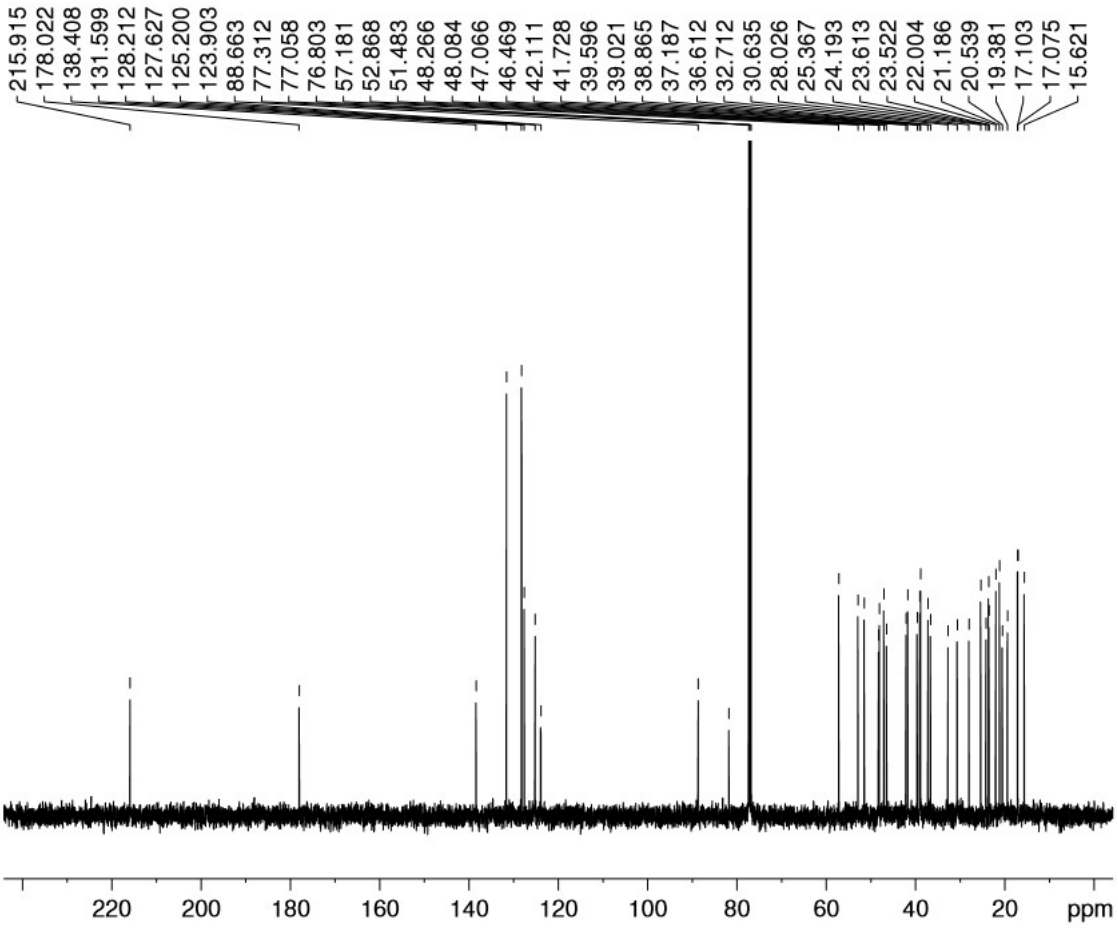


Methyl-2α-phenylpropynyl-3-oxours-12en-28-oate **17** ^{1}H NMR spectra ($CDCl_3$)

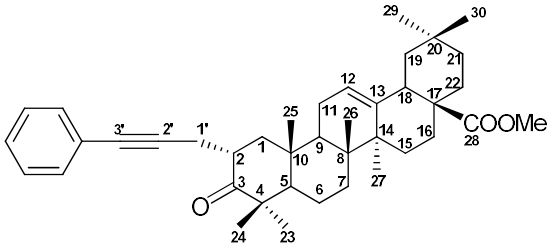


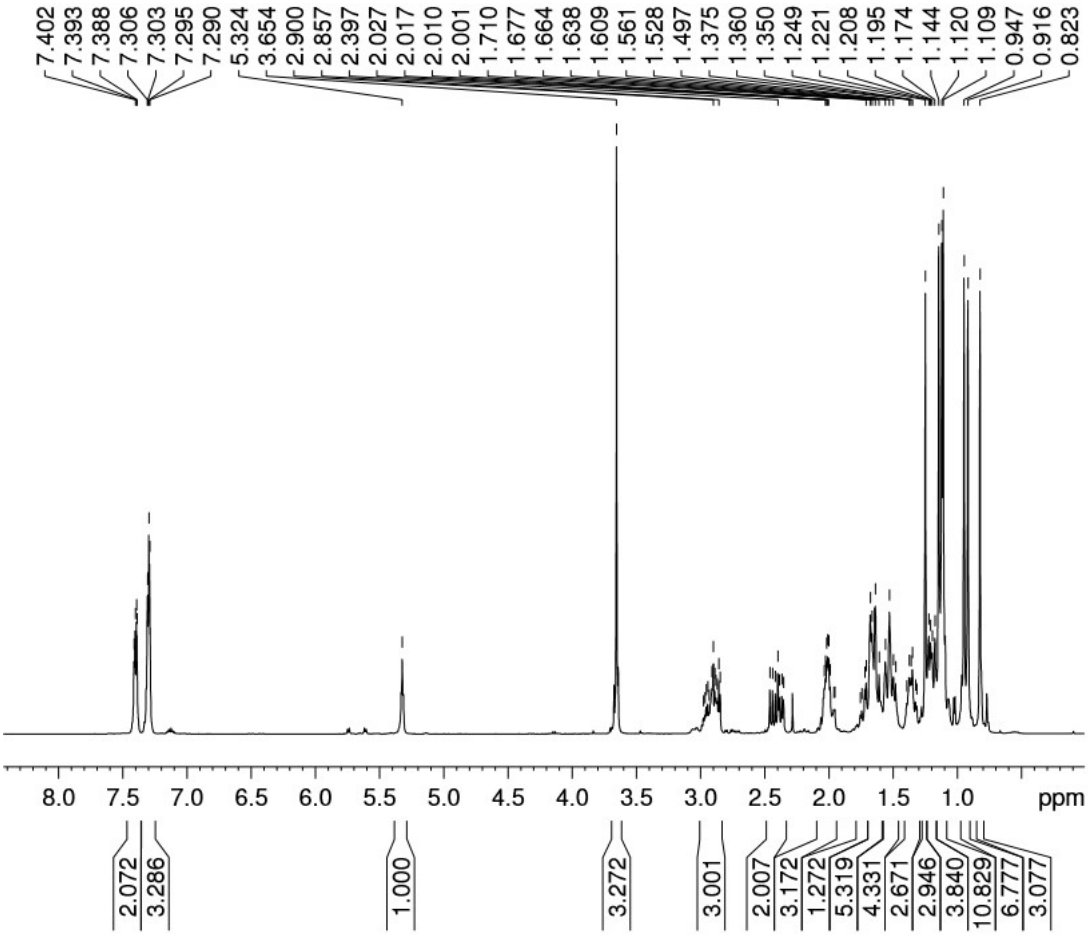


Methyl-2α-phenylpropynyl-3-oxours-12en-28-oate **17** ^{13}C NMR spectra ($CDCl_3$)

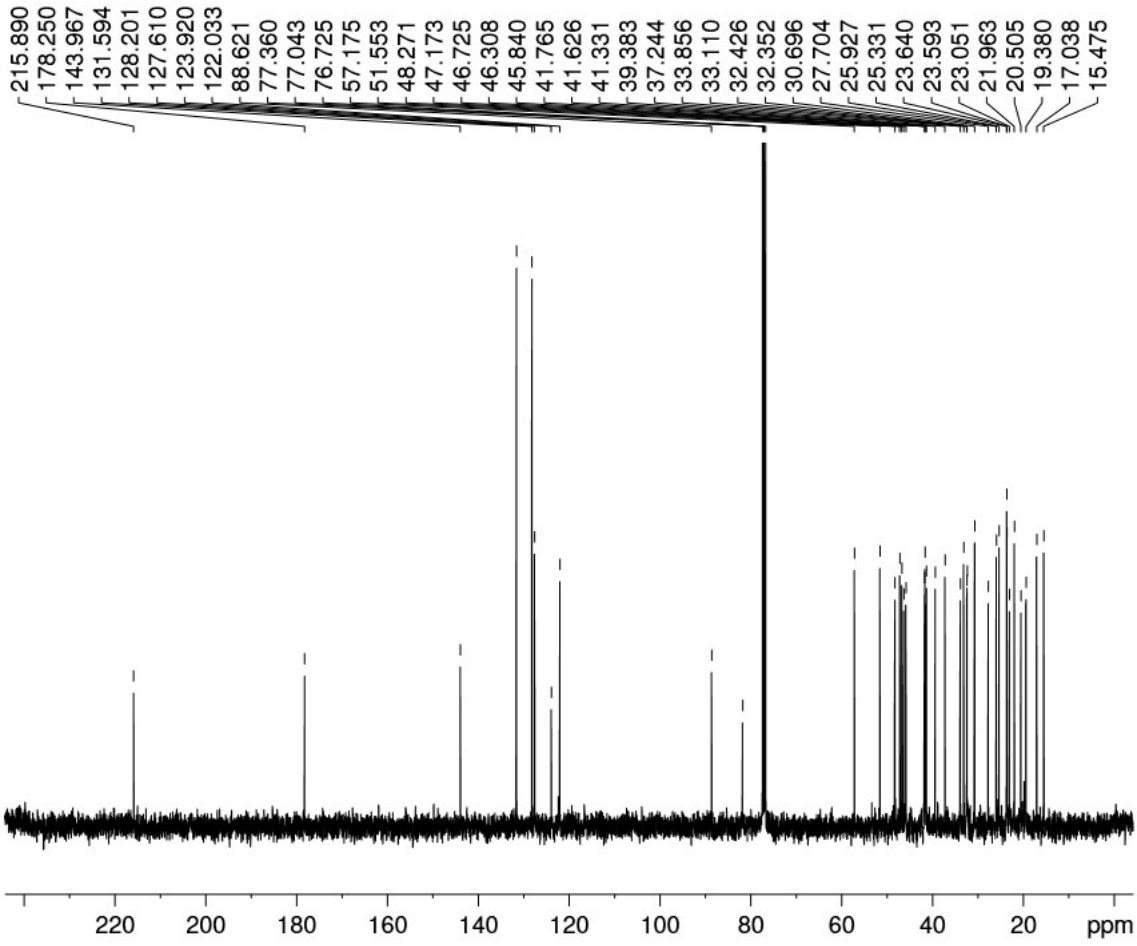


Methyl-2α-phenylpropynyl-3-oxoolean-12en-28-oate **19** ^{1}H NMR spectra ($CDCl_3$)

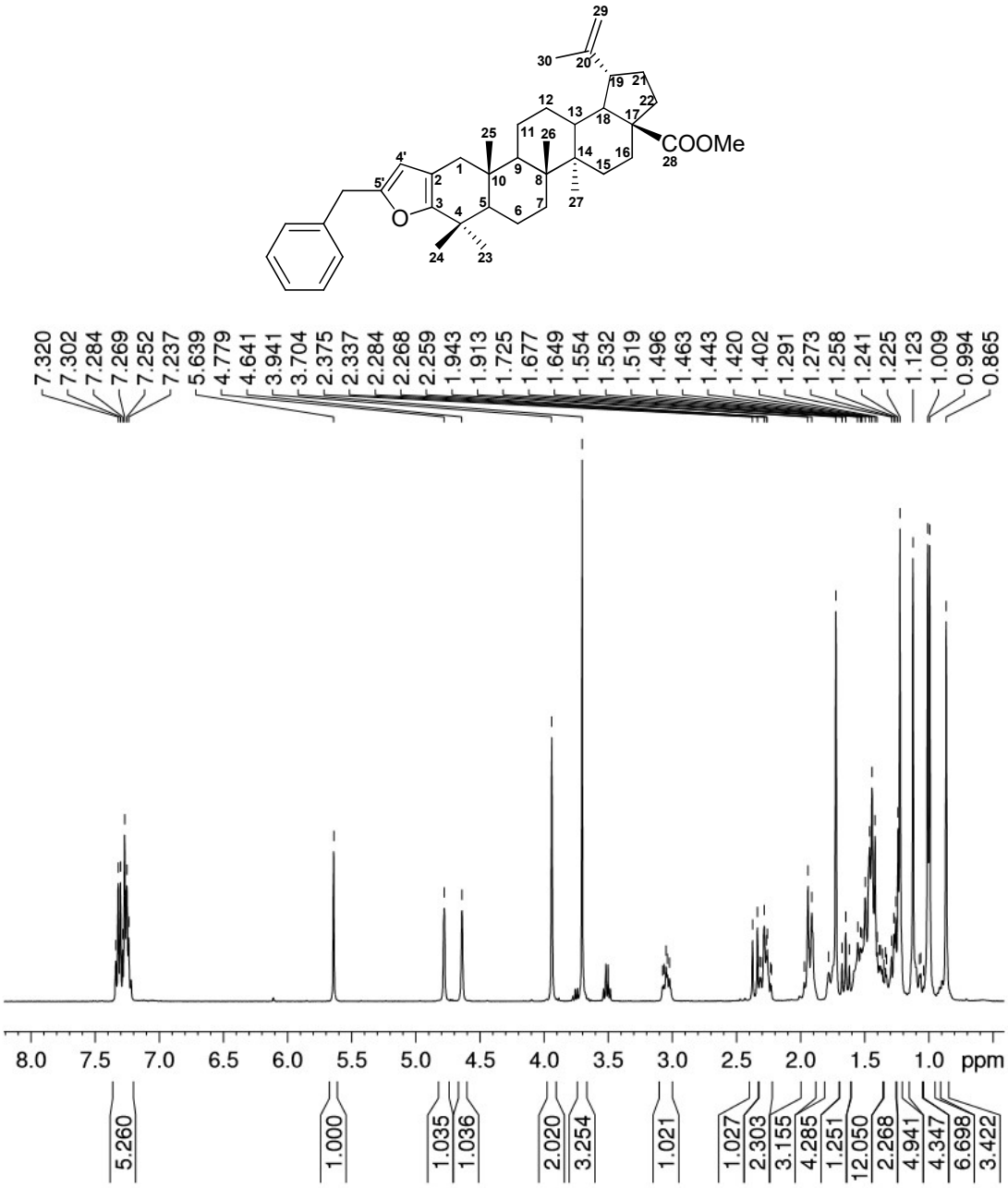




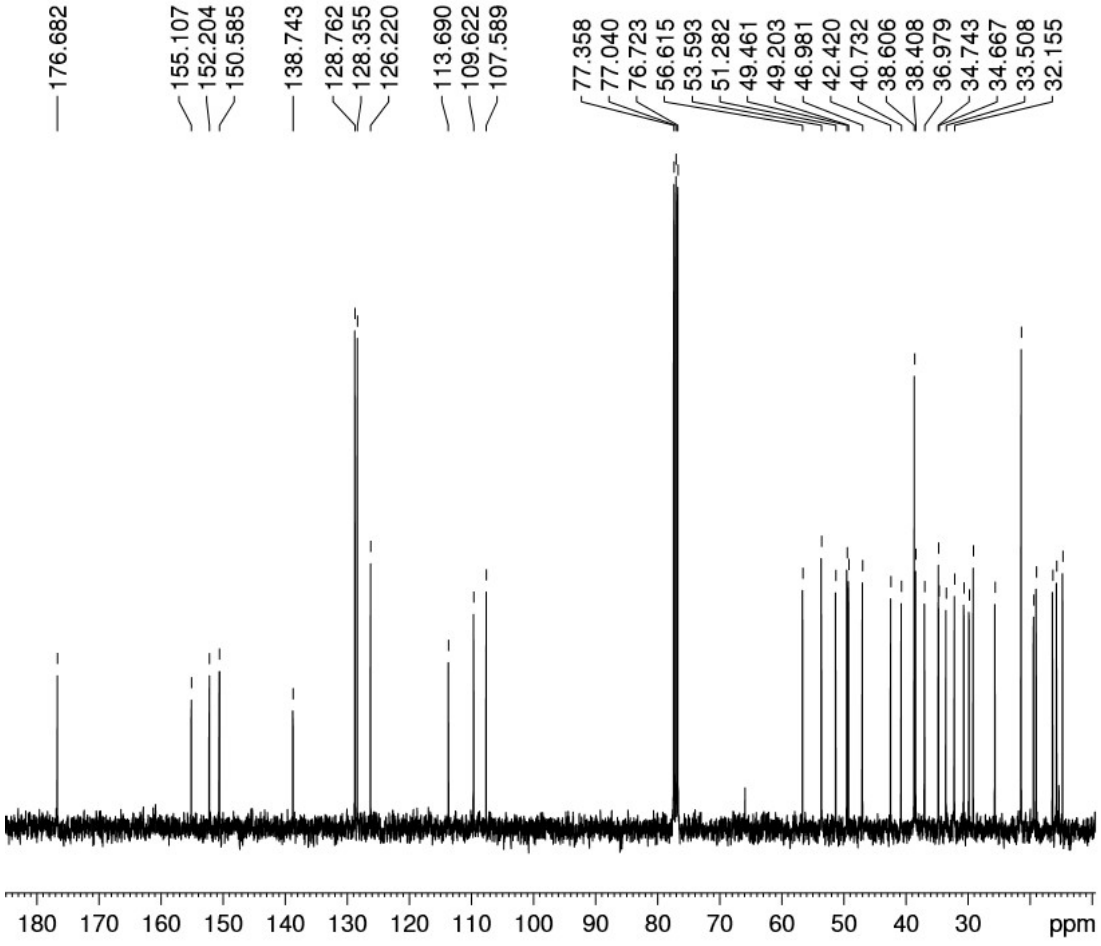
Methyl-2α-phenylpropynyl-3-oxoolean-12en-28-oate **19** ^{13}C NMR spectra ($CDCl_3$)



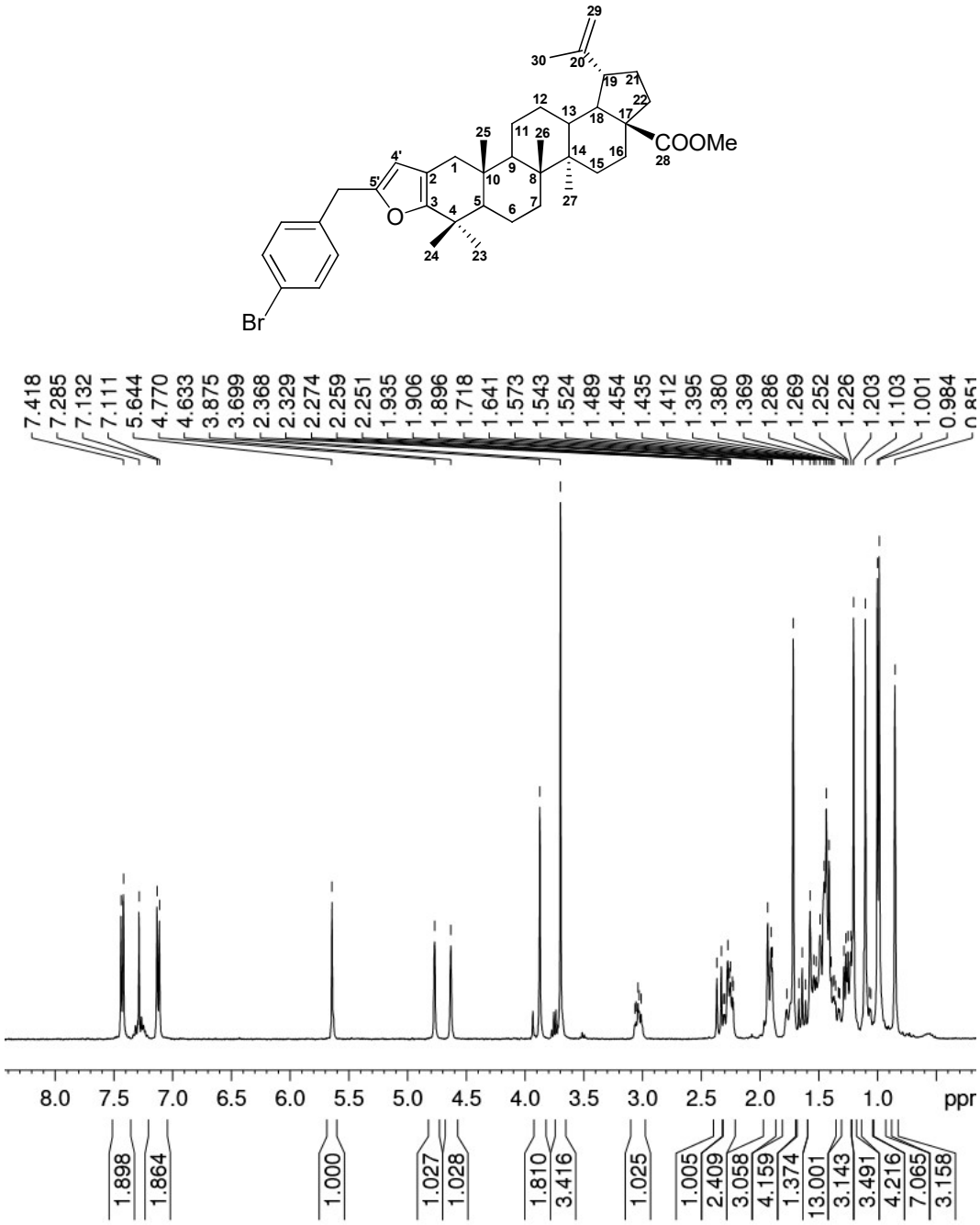
Methyl 5'-benzylfurano[3,2-b]lup-20(29)-en-28-oate **15a** ^{1}H NMR spectra ($CDCl_3$)



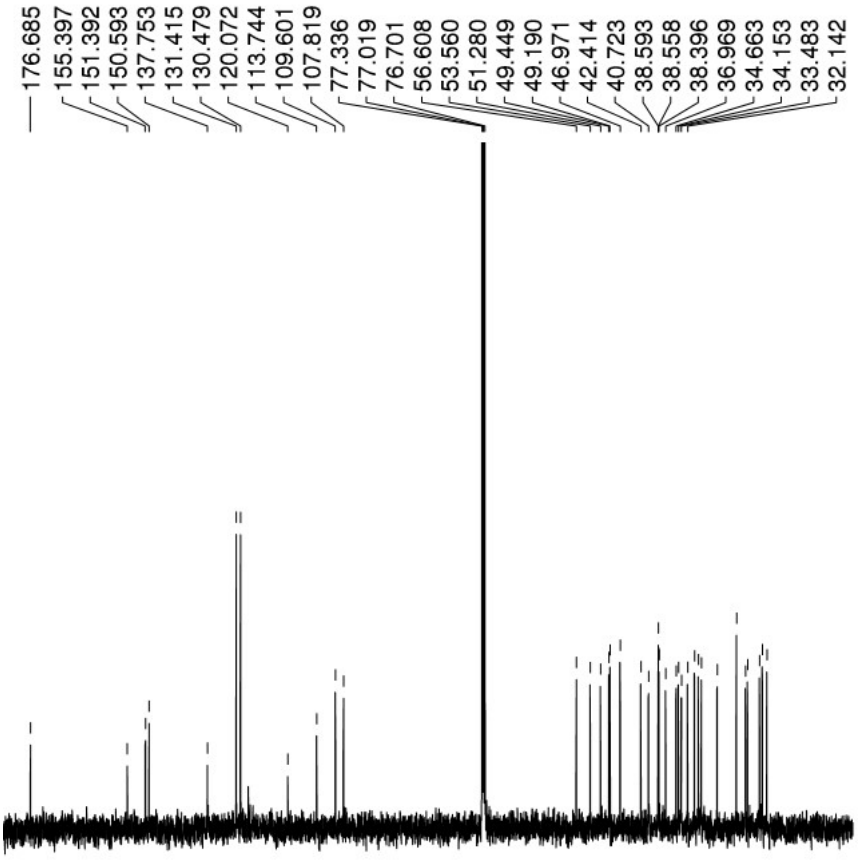
Methyl 5'-benzylfurano[3,2-b]lup-20(29)-en-28-oate **15a** ^{13}C NMR spectra ($CDCl_3$)



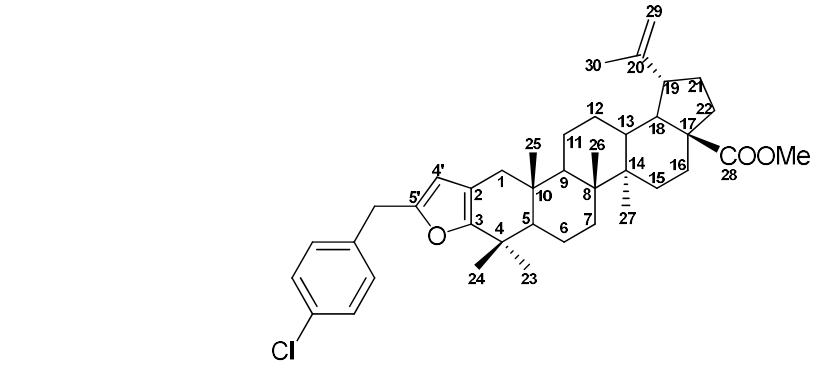
Methyl 5'-(4-bromobenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15b** ^{1}H NMR spectra ($CDCl_3$)

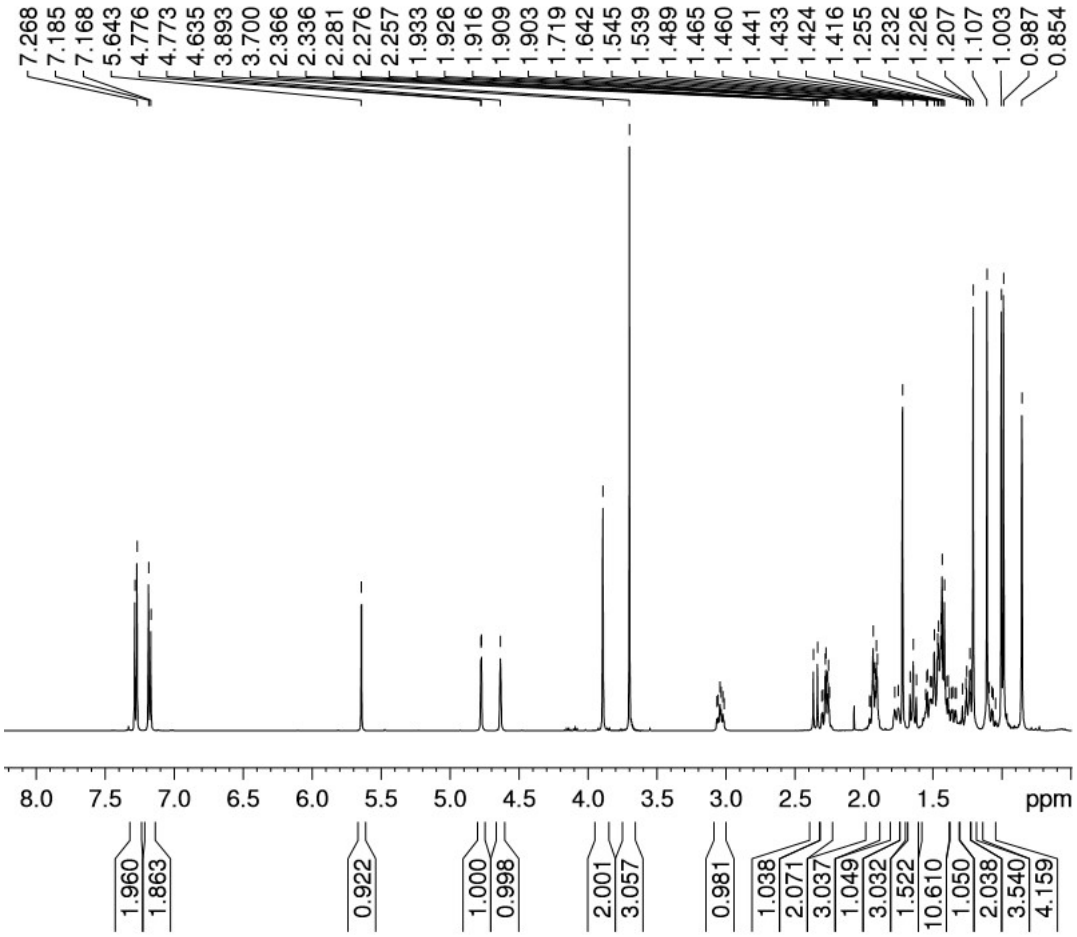


Methyl 5'-(4-bromobenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15b** ^{13}C NMR spectra ($CDCl_3$)

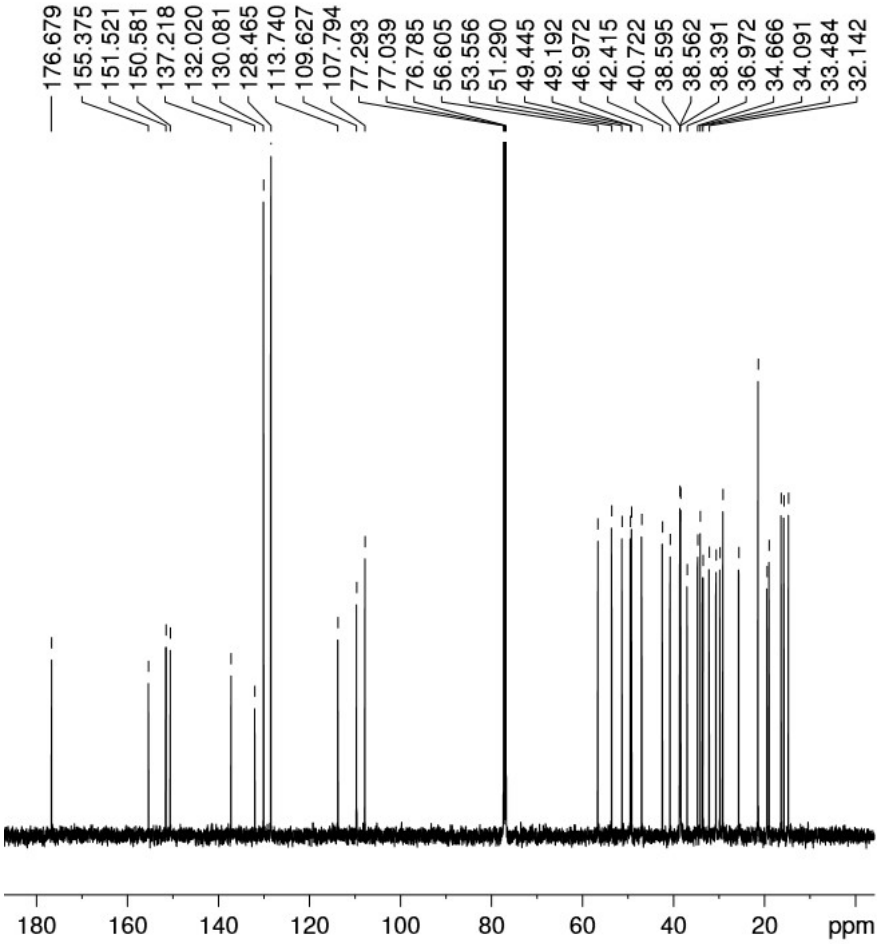


Methyl 5'-(4-chlorobenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15c** ^{1}H NMR spectra ($CDCl_3$)

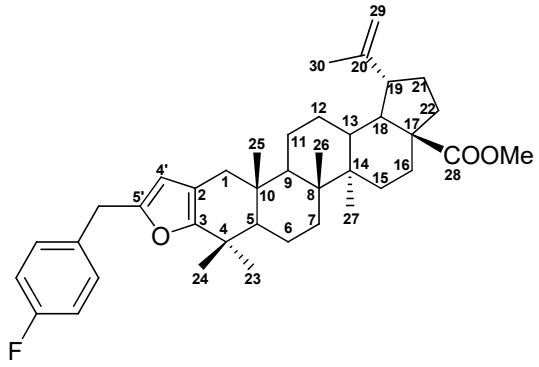


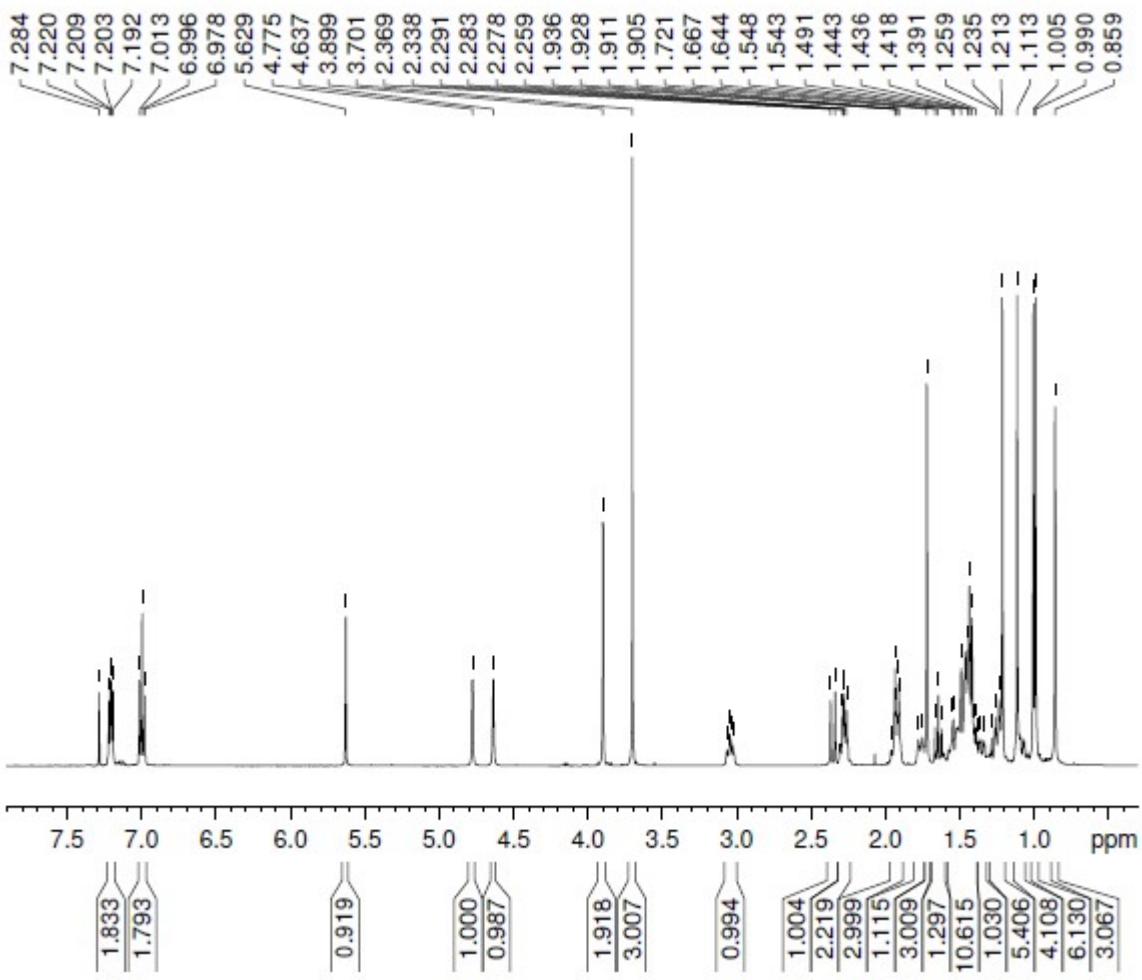


Methyl 5'-(4-chlorobenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15c** ^{13}C NMR spectra ($CDCl_3$)

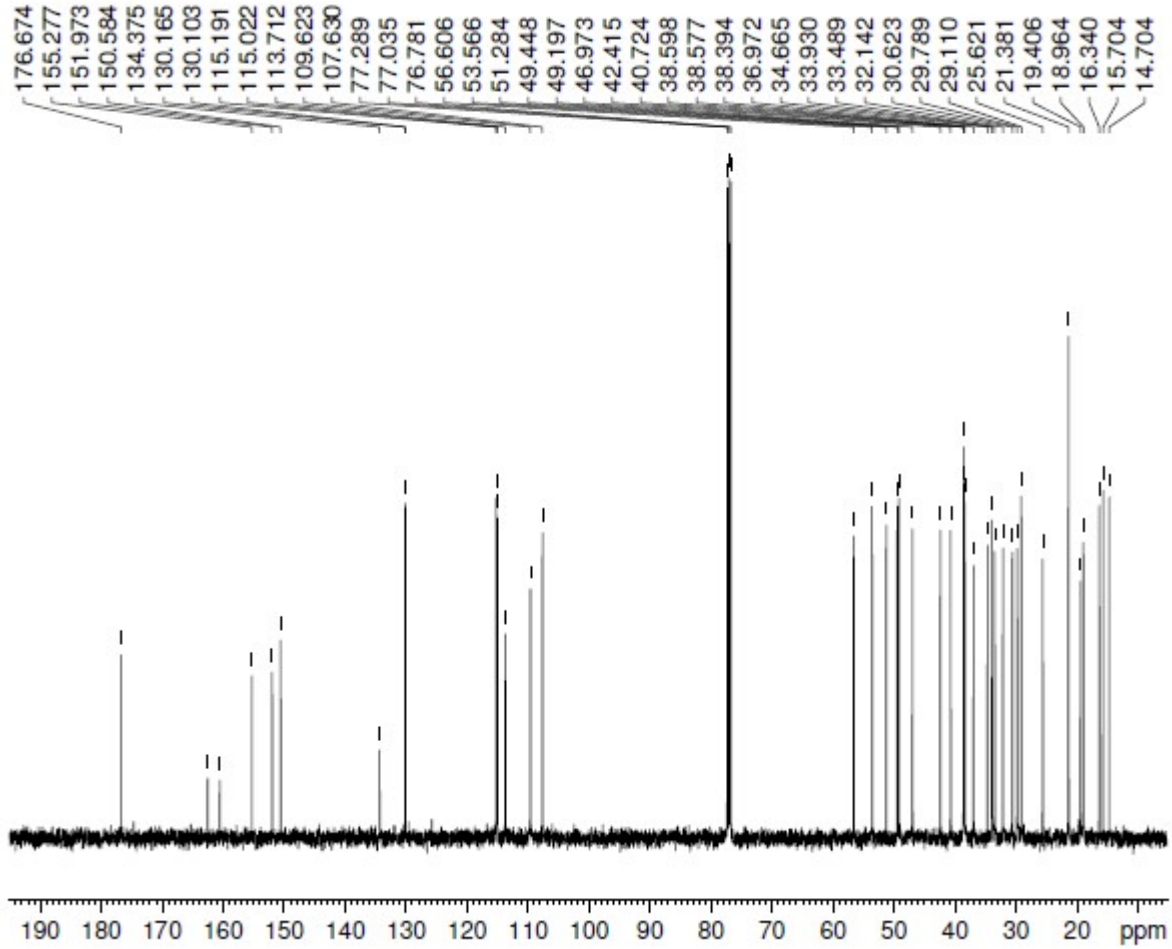


Methyl 5'-(4-fluorobenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15d** ^{1}H NMR spectra ($CDCl_3$)

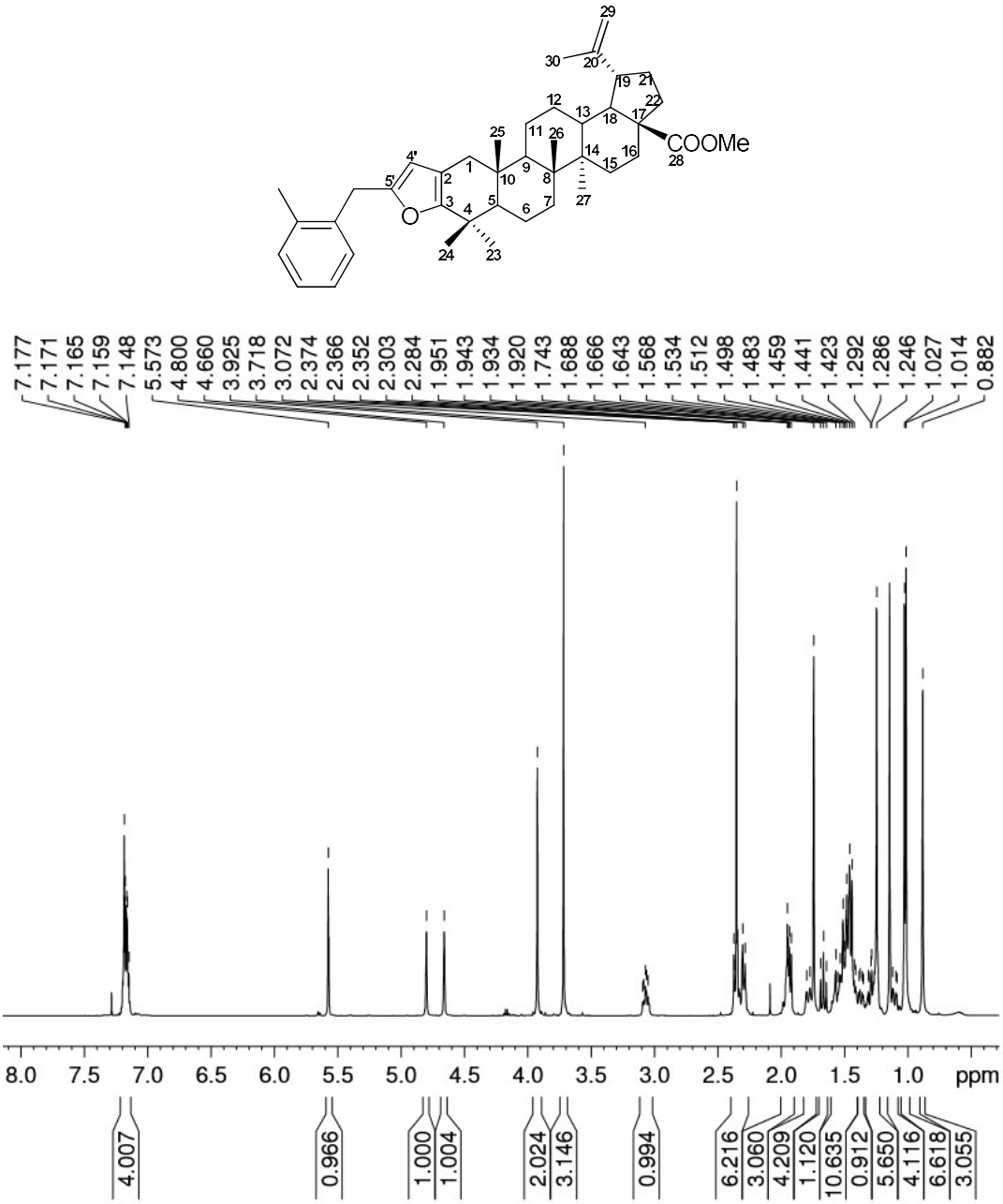




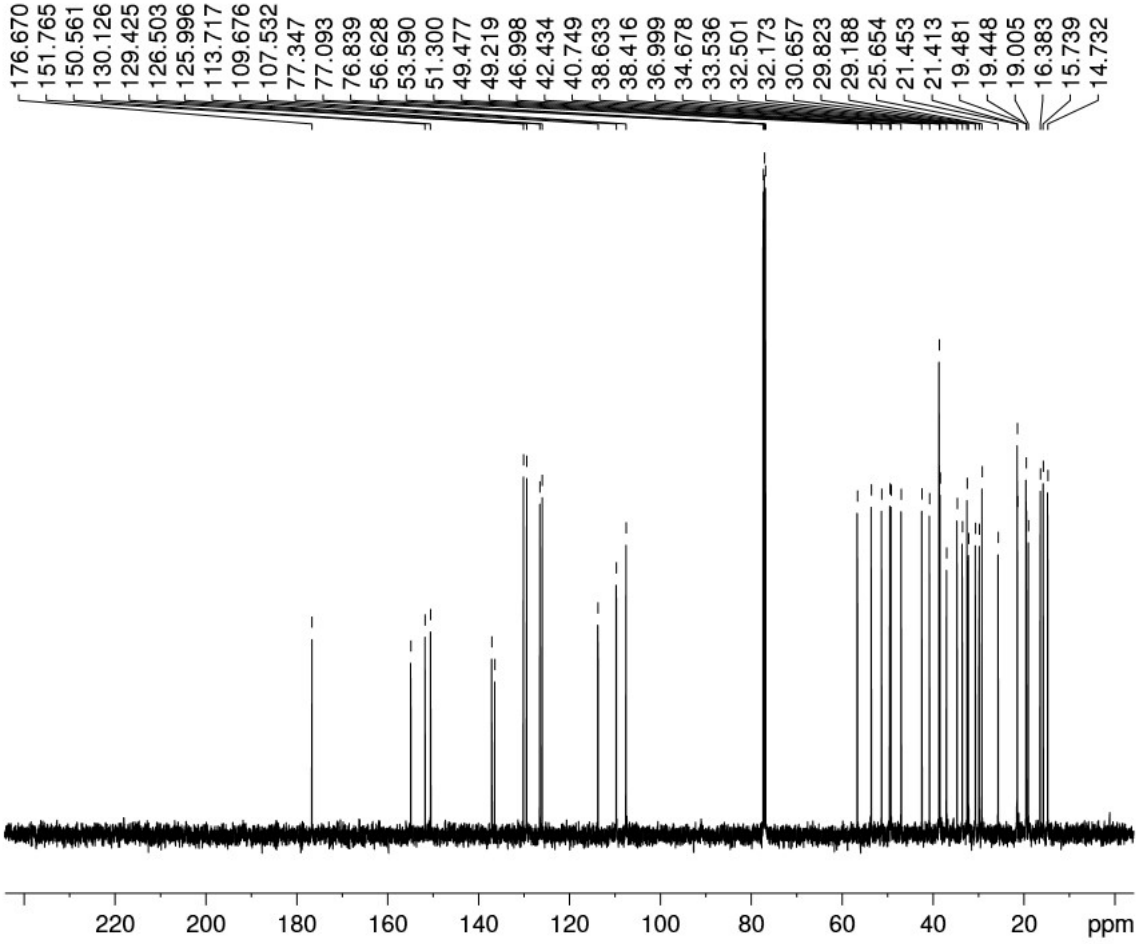
Methyl 5'-(4-fluorobenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15d** ^{13}C NMR spectra ($CDCl_3$)



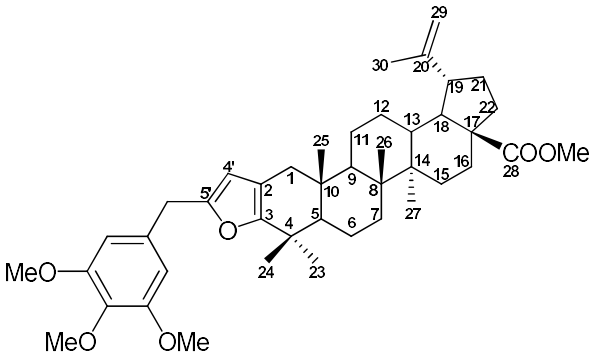
Methyl 5'-(2-methylbenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15e** ^{1}H NMR spectra ($CDCl_3$)

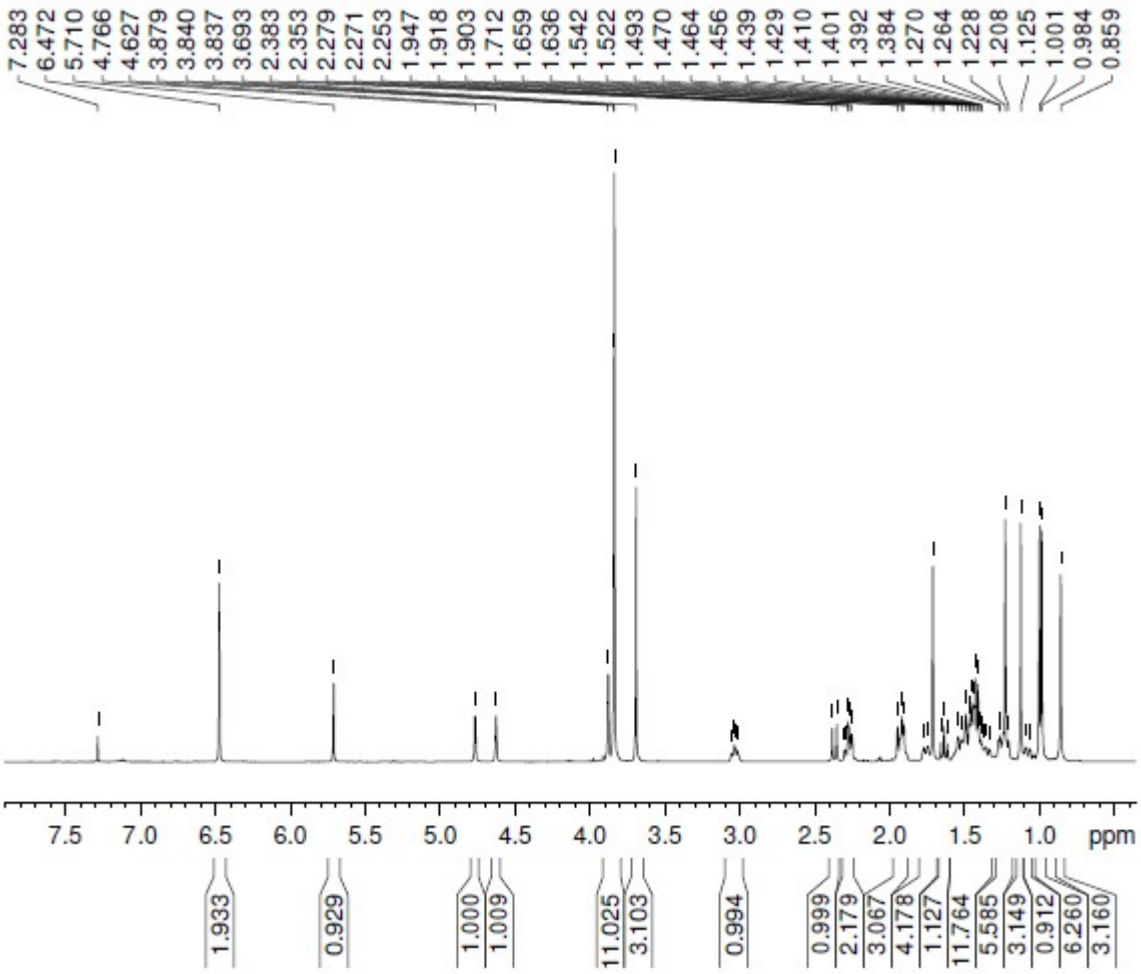


Methyl 5'-(2-methylbenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15e** ^{13}C NMR spectra ($CDCl_3$)

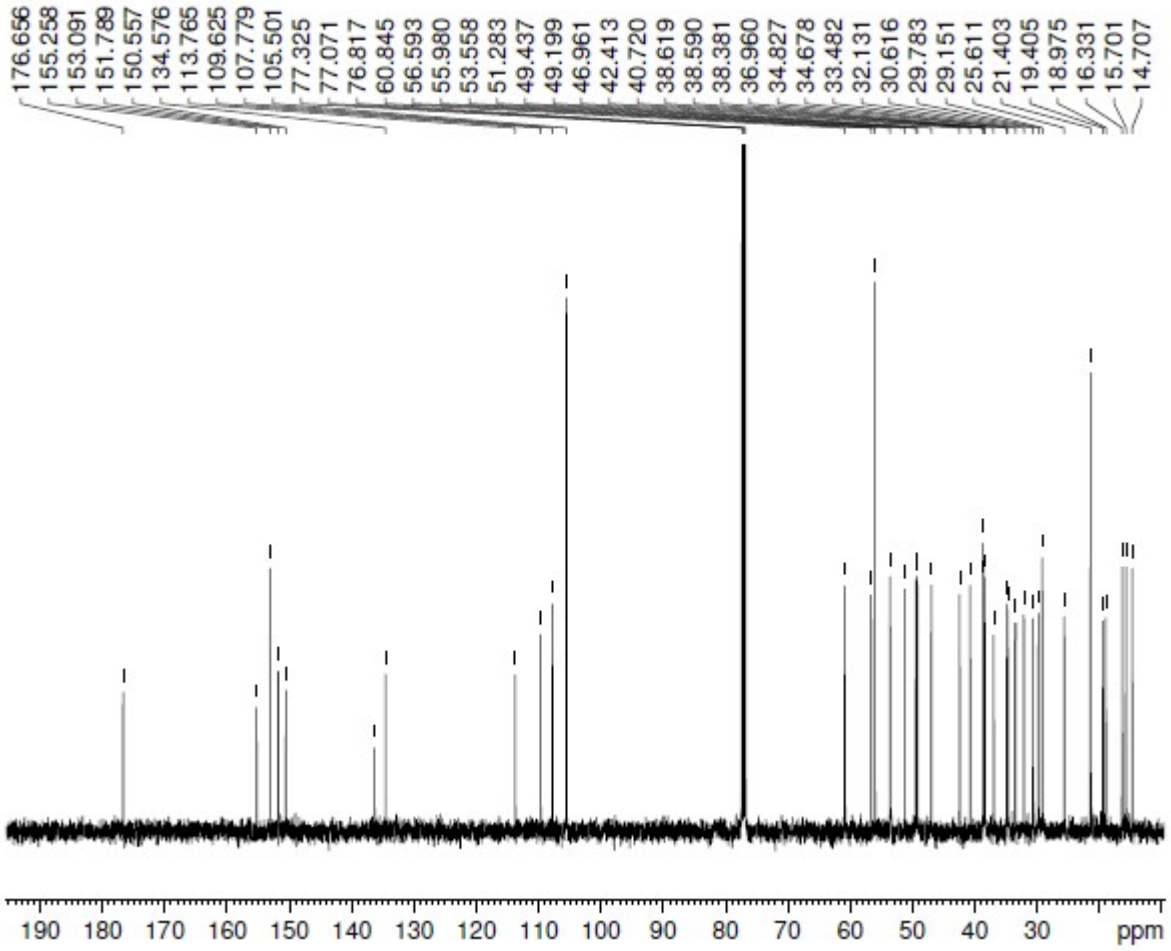


Methyl 5'-(3,4,5-trimethoxybenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15f** ^{1}H NMR spectra ($CDCl_3$)

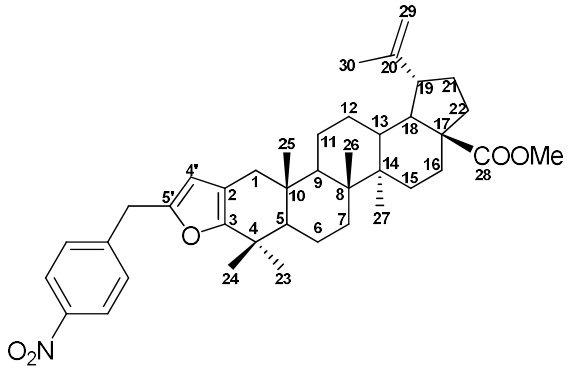


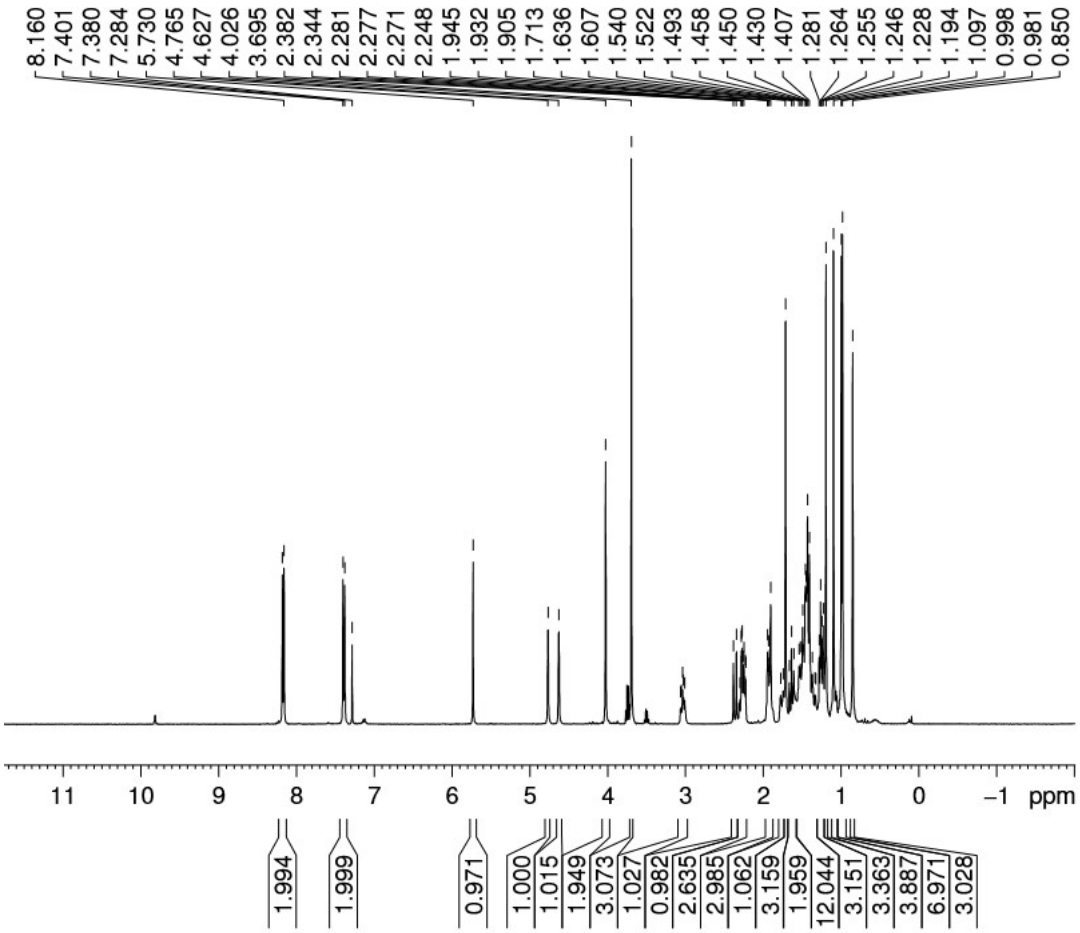


Methyl 5'-(3,4,5-trimethoxybenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15f** ^{13}C NMR spectra ($CDCl_3$)

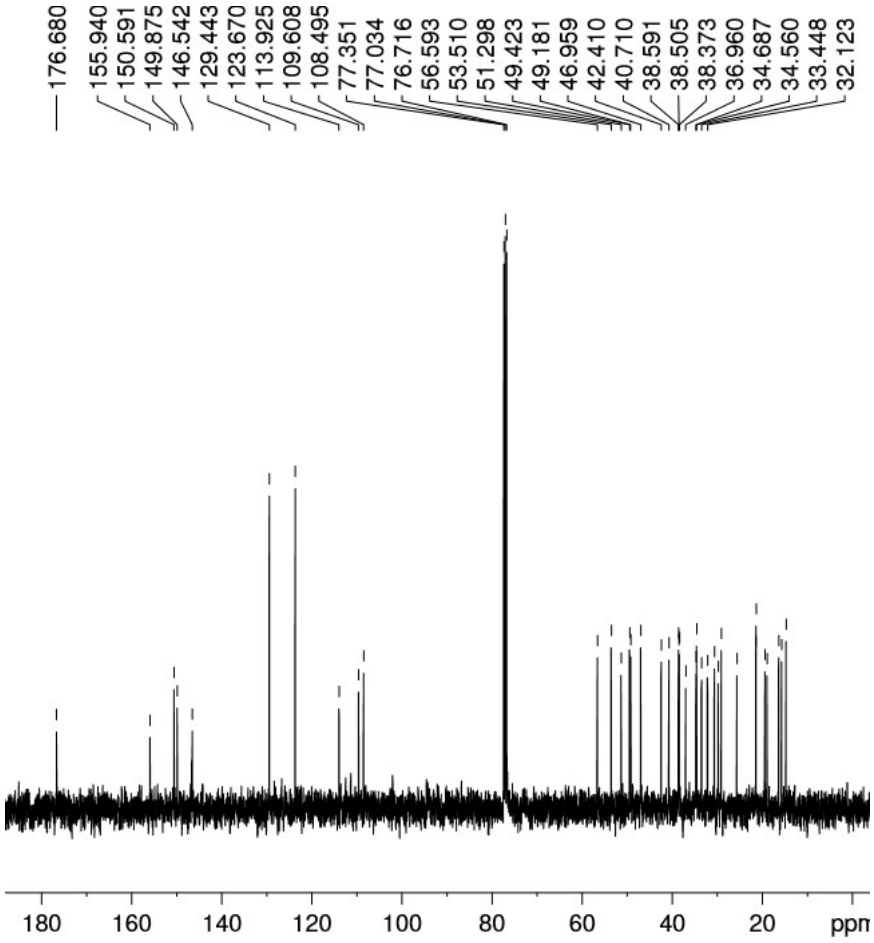


Methyl 5'-(4-nitrobenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15g** ^{1}H NMR spectra ($CDCl_3$)

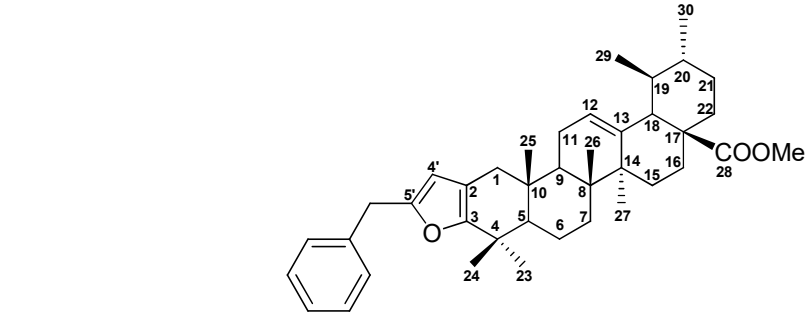


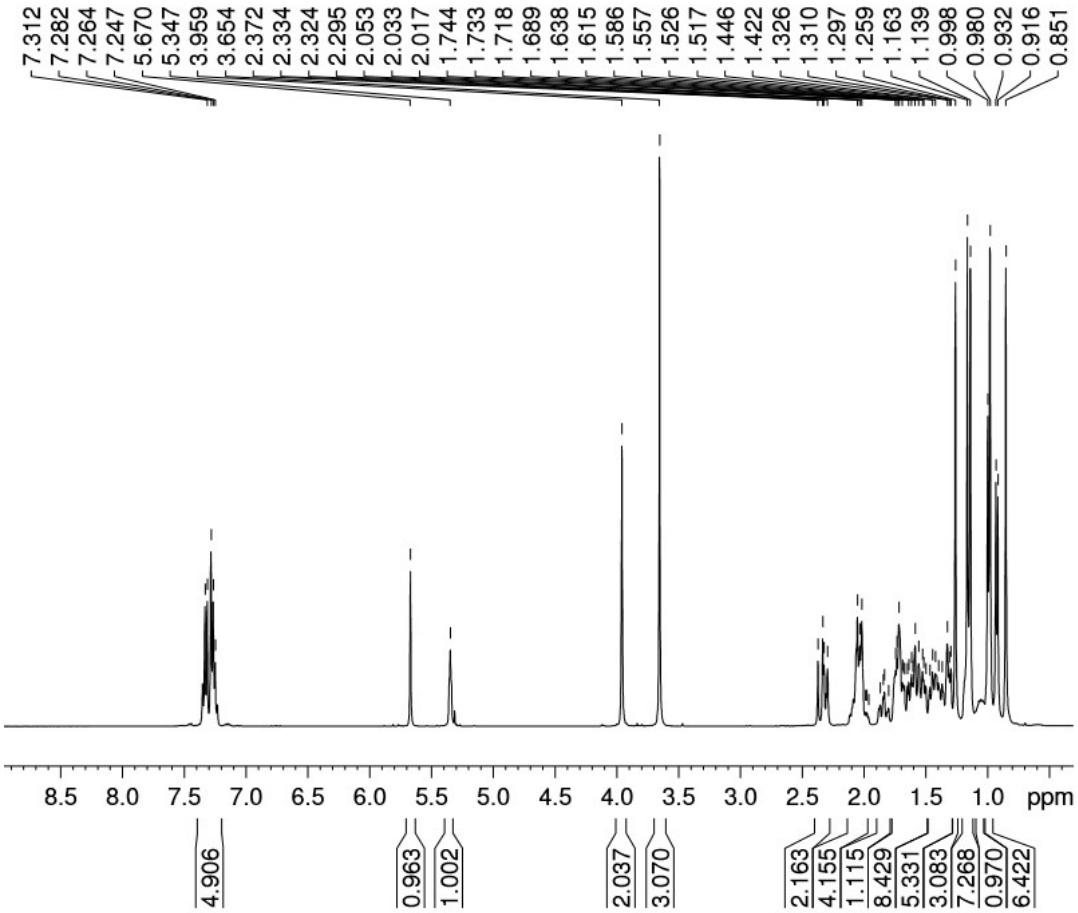


Methyl 5'-(4-nitrobenzyl)furano[3,2-b]lup-20(29)-en-28-oate **15g** ^{13}C NMR spectra ($CDCl_3$)

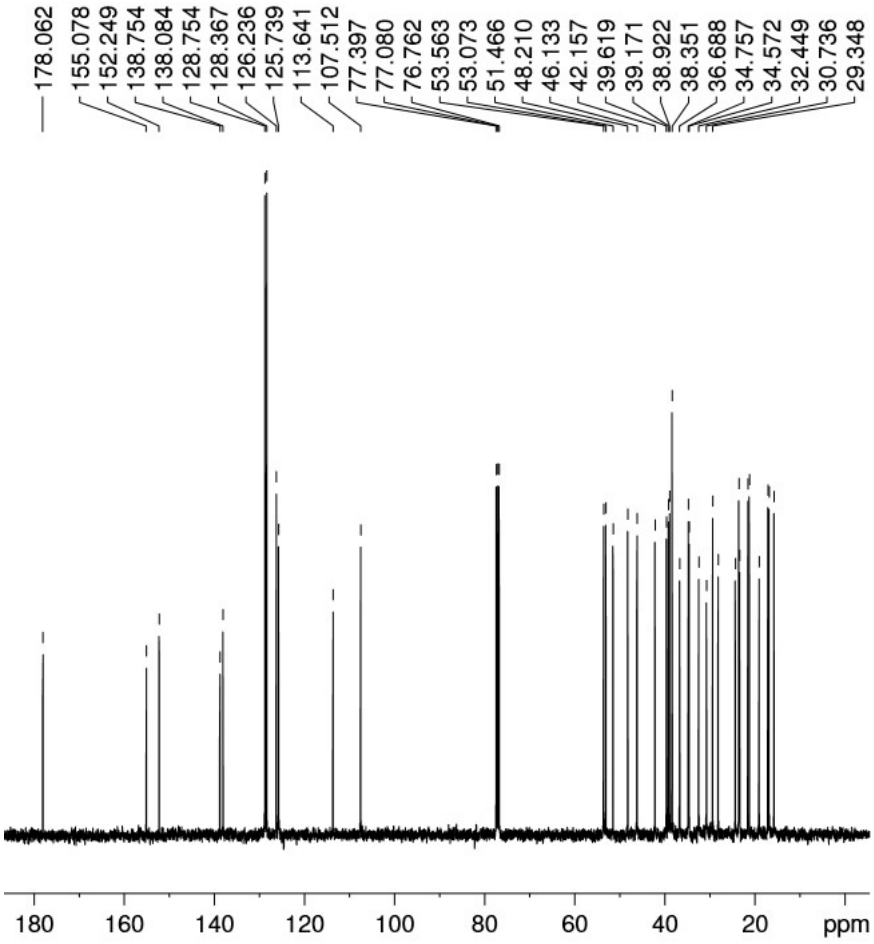


Methyl 5'-benzylfurano[3,2-b]urs-12-en-28-oate **18a** ^{1}H NMR spectra ($CDCl_3$)

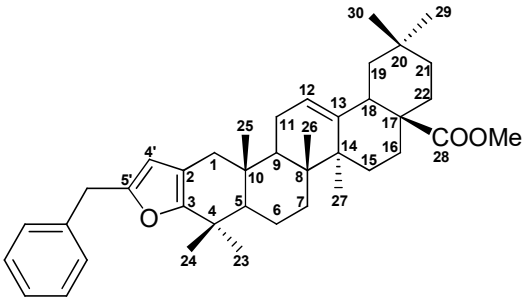


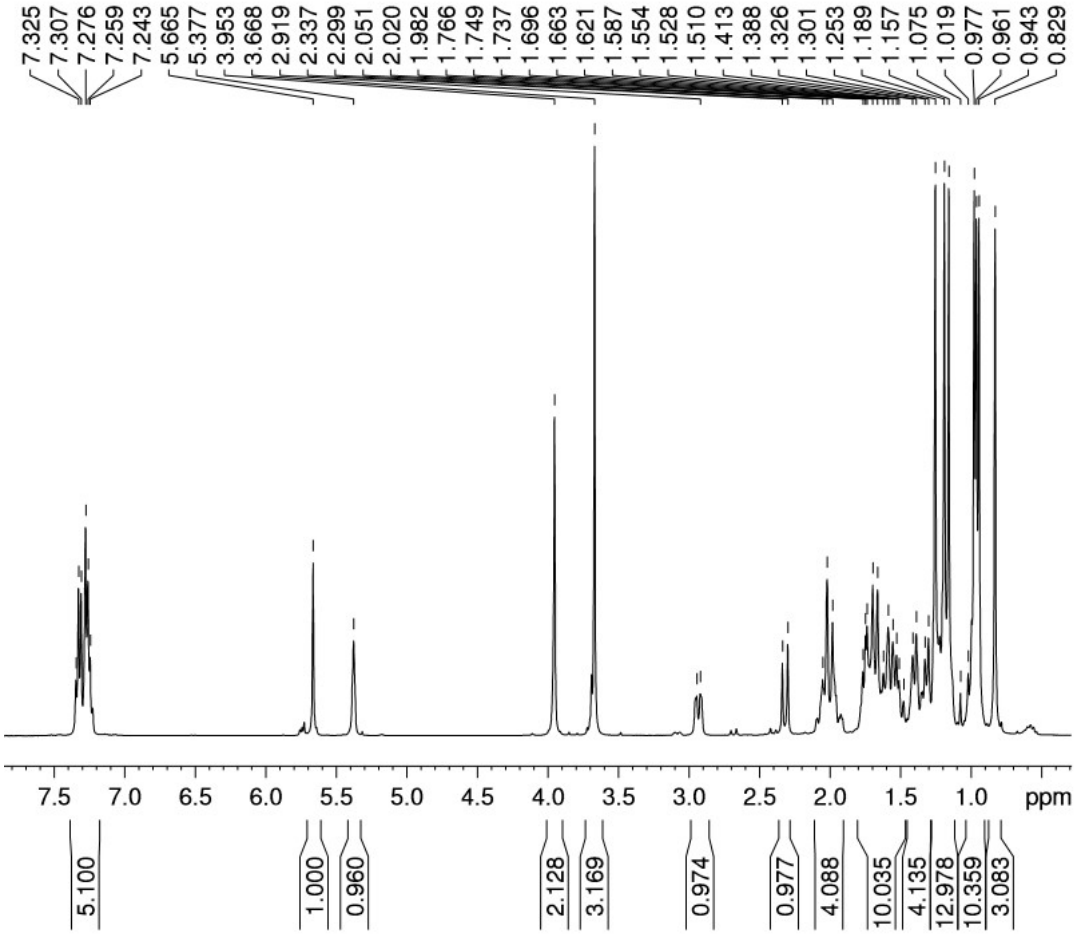


Methyl 5'-benzylfurano[3,2-b]urs-12-en-28-oate **18a** ^{13}C NMR spectra ($CDCl_3$)

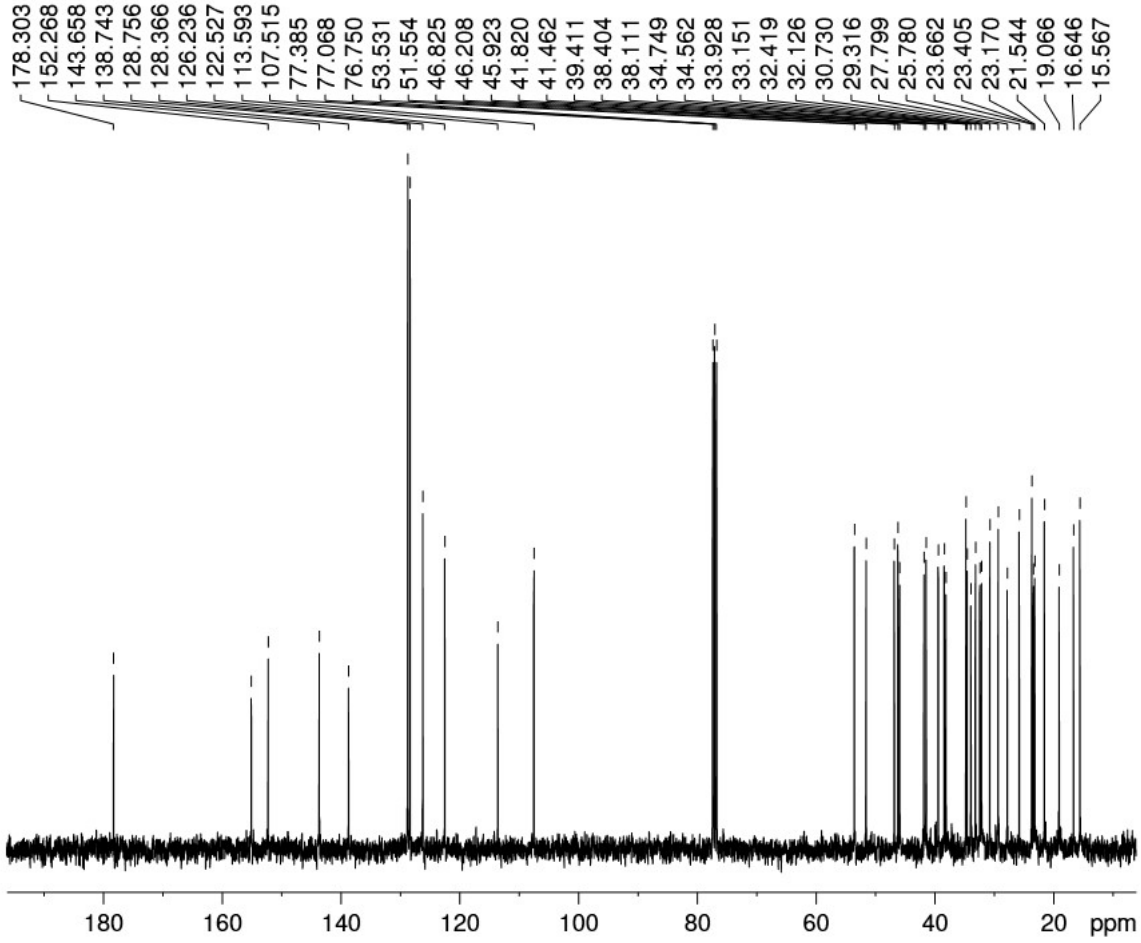


Methyl 5'-benzylfurano[3,2-b]olean-12-en-28-oate **20a** ^{1}H NMR spectra ($CDCl_3$)

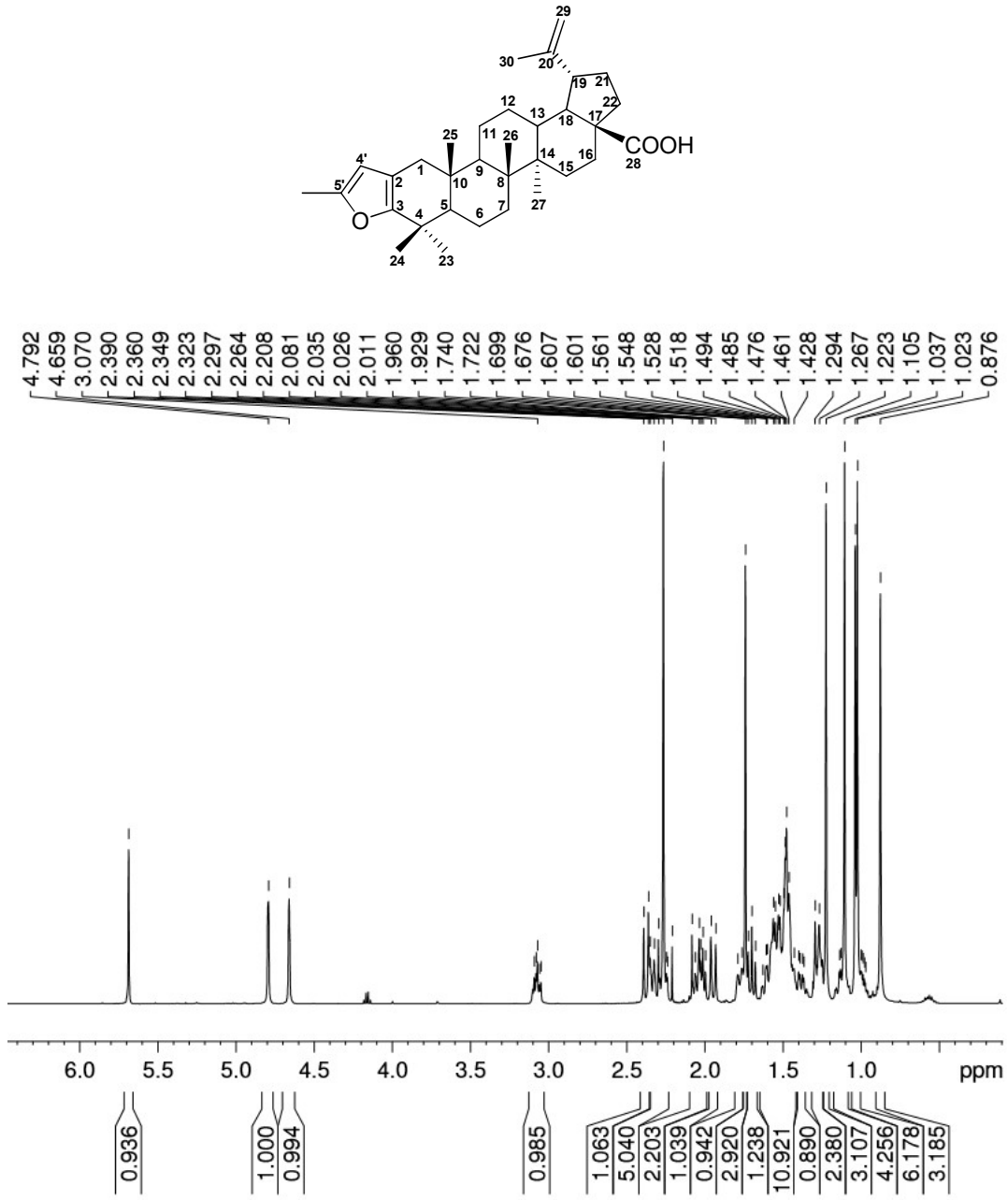




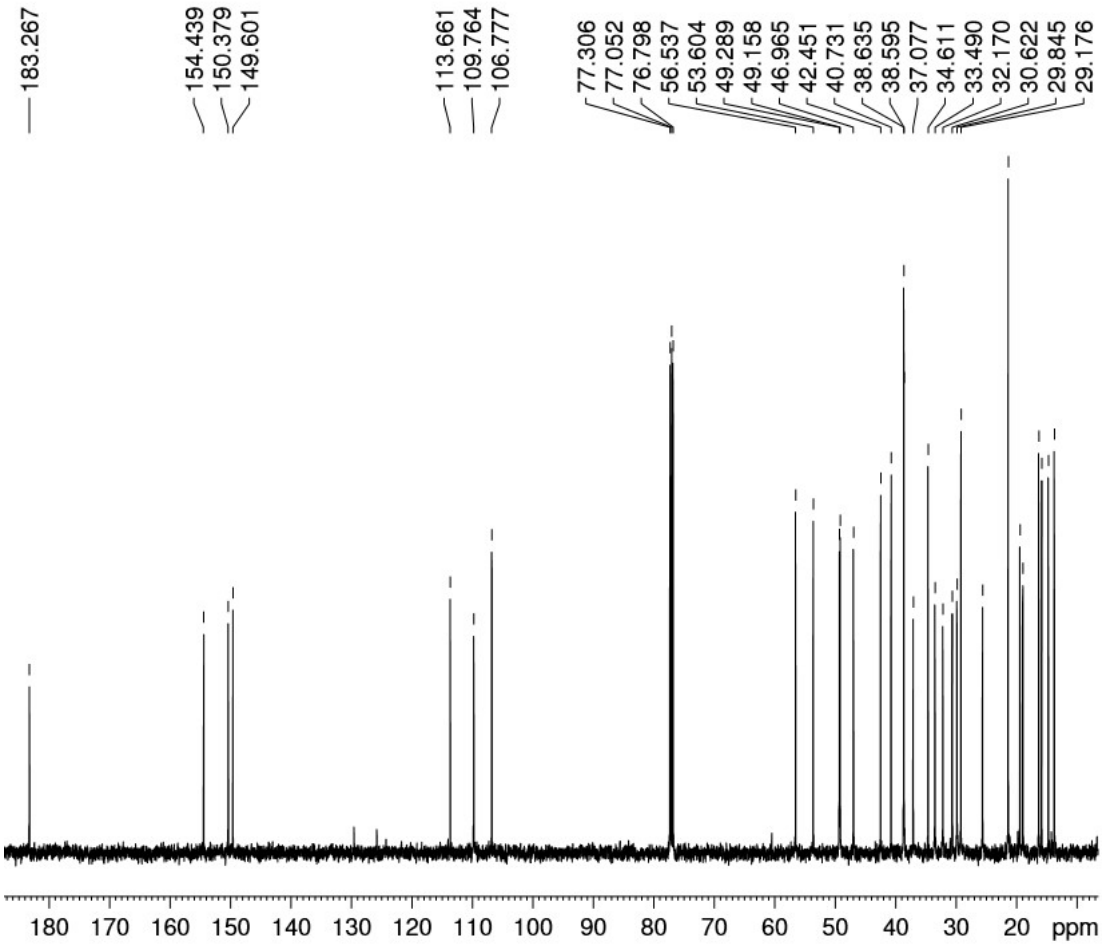
Methyl 5'-benzylfurano[3,2-b]olean-12-en-28-oate **20a** ^{13}C NMR spectra ($CDCl_3$)



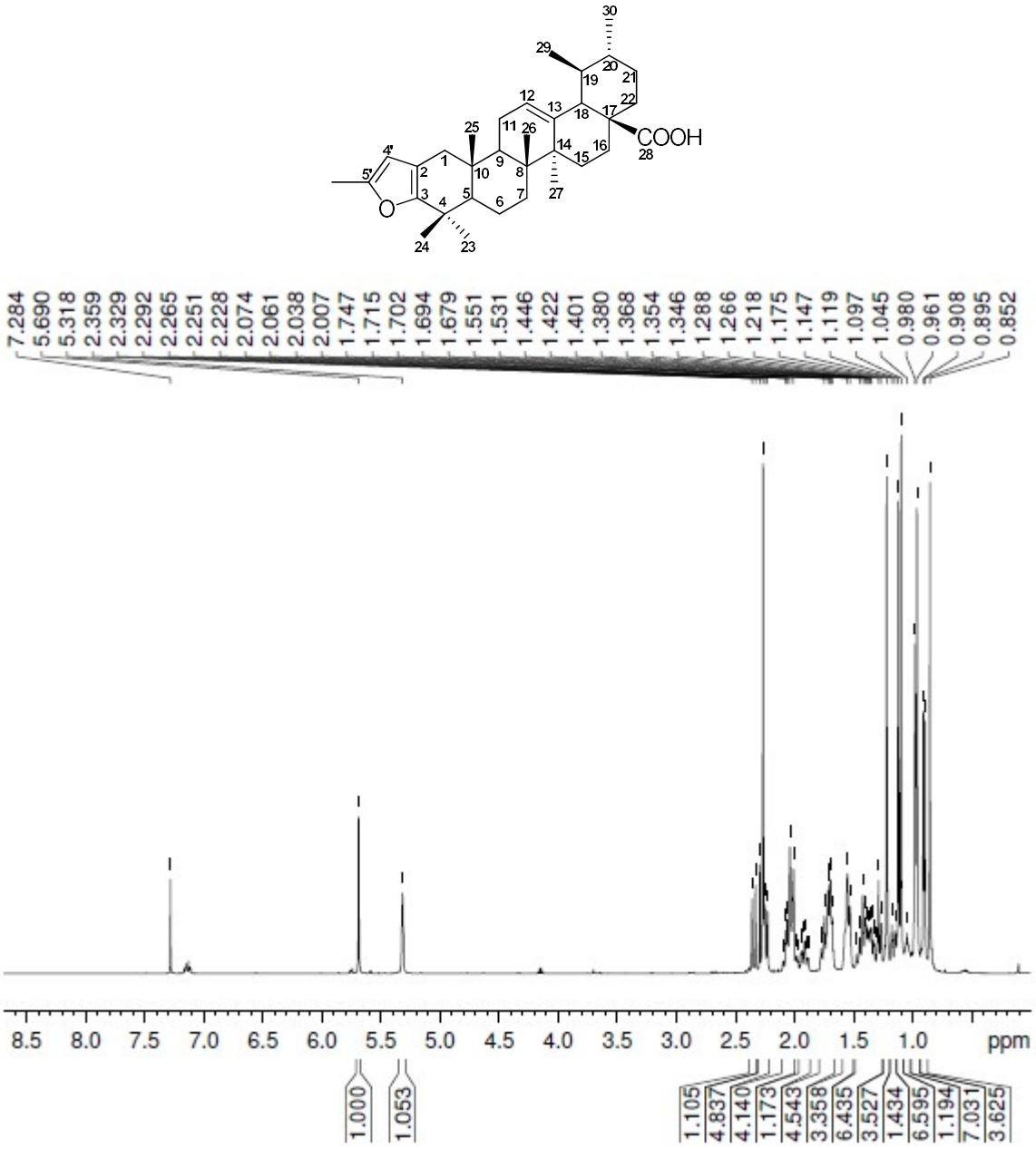
5'-Methylfurano[3,2-b]lup-20(29)-en-28-oic acid **11b** ^{1}H NMR spectra ($CDCl_3$)



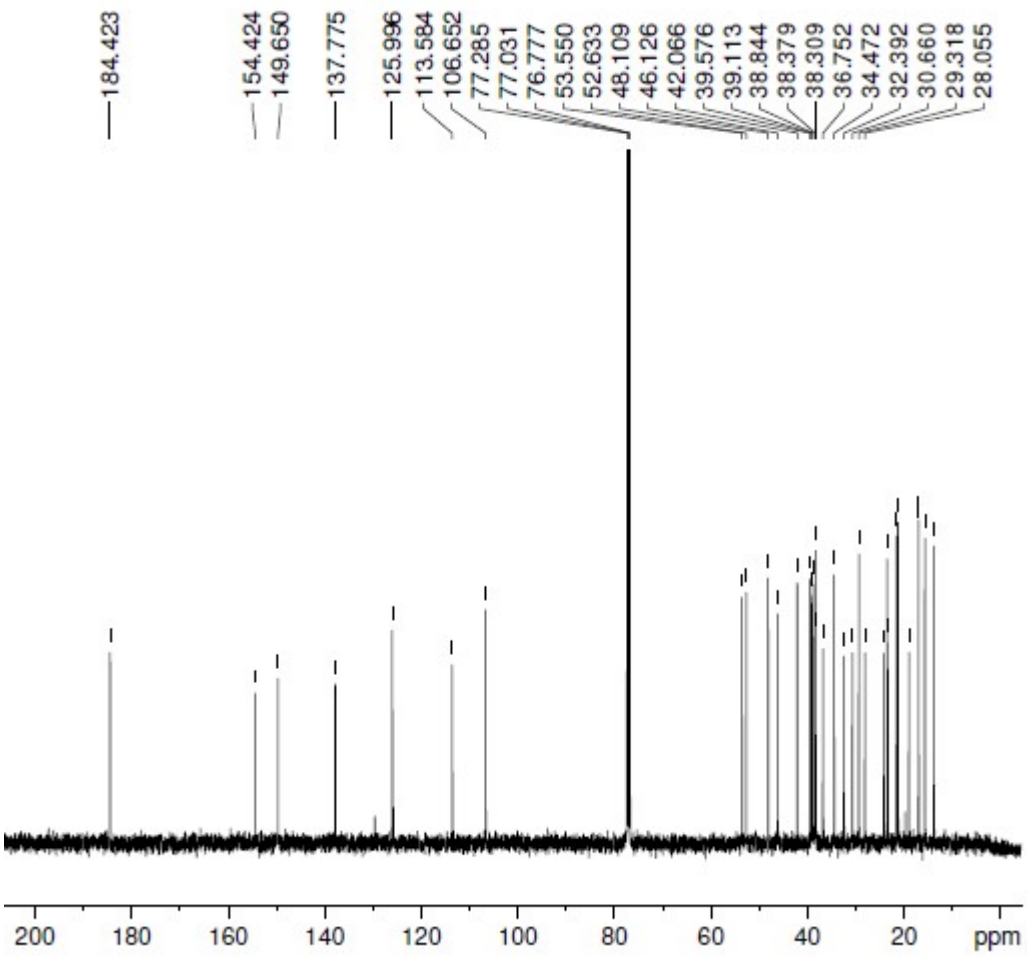
5'-Methylfurano[3,2-b]lup-20(29)-en-28-oic acid **11b** ^{13}C NMR spectra ($CDCl_3$)



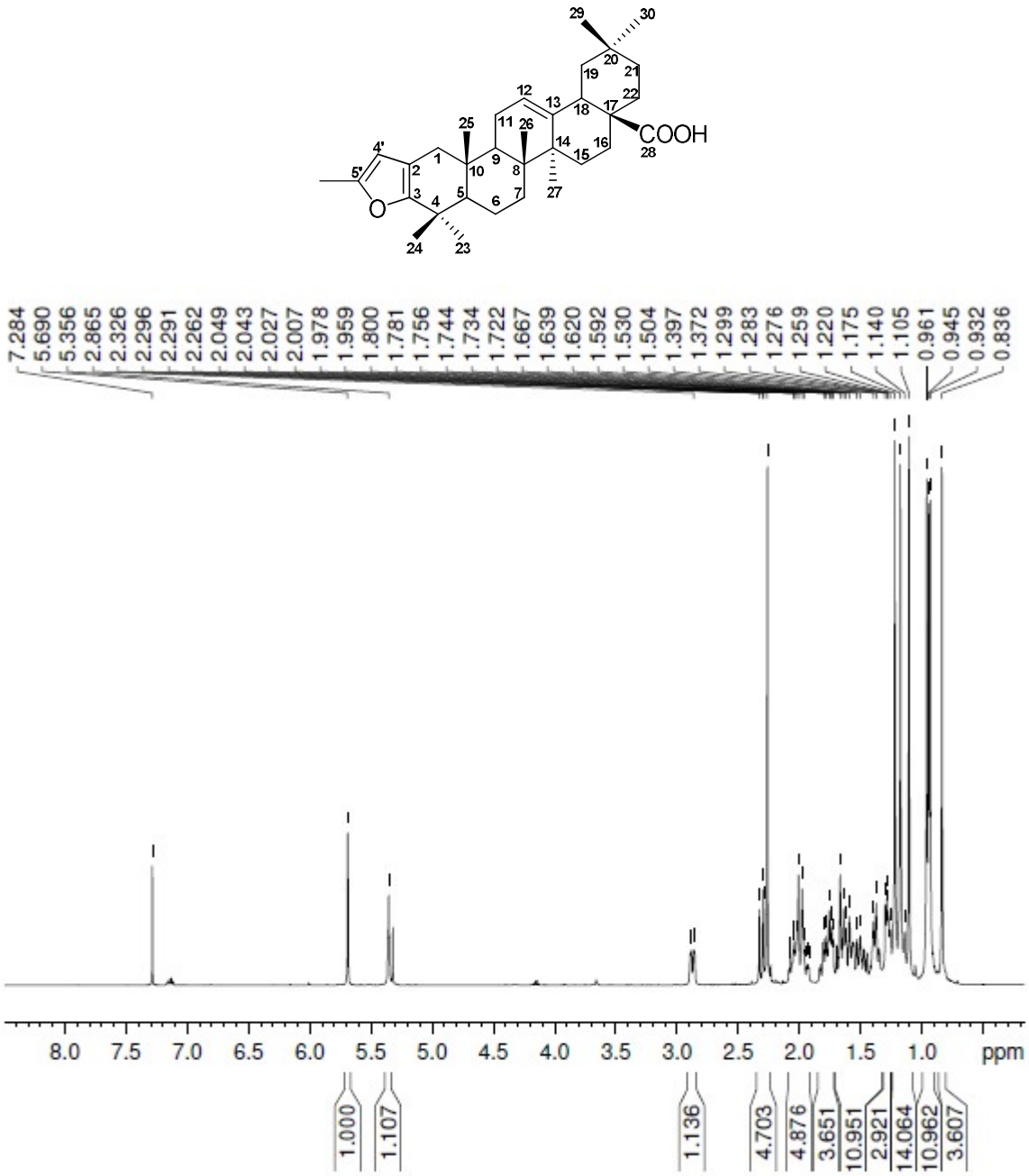
5'-Methylfurano[3,2-b]urs-12-en-28-oic acid **12b** ^{1}H NMR spectra ($CDCl_3$)



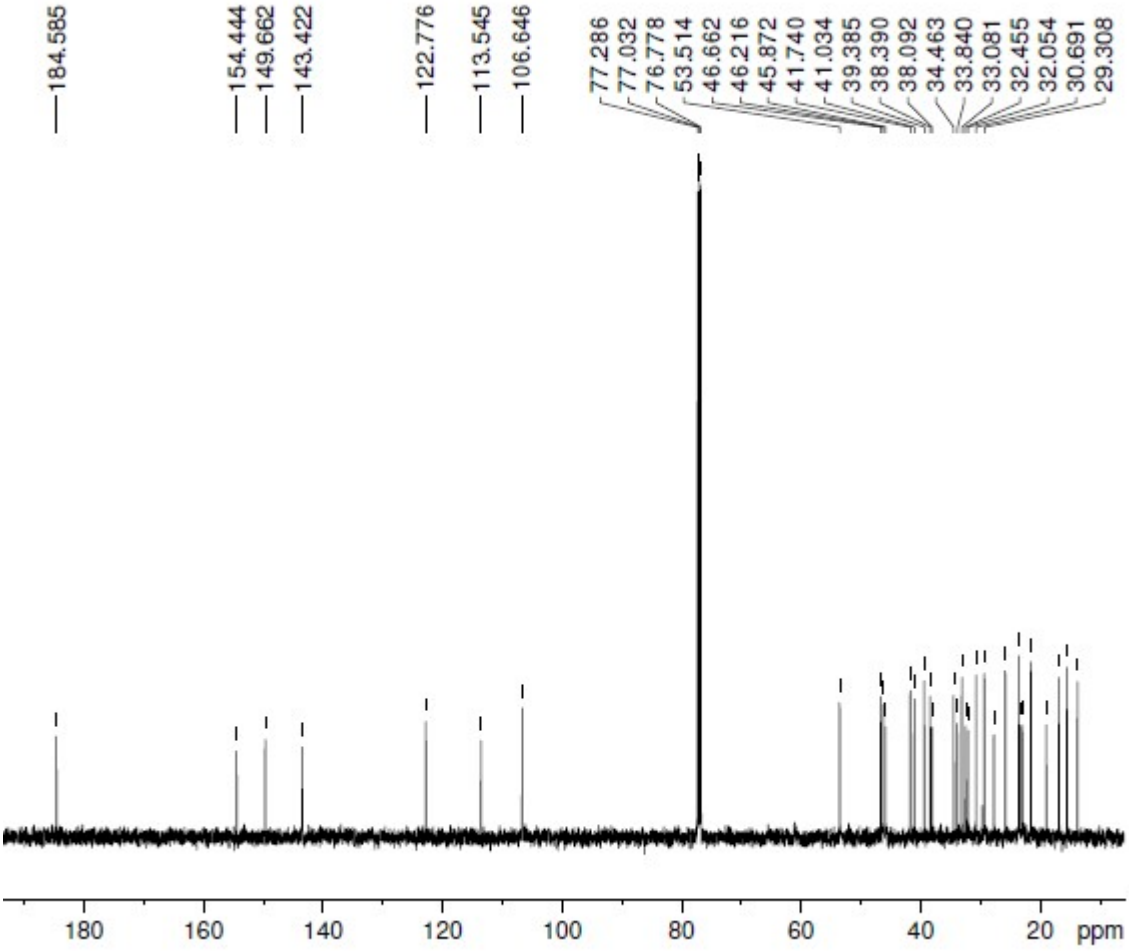
5'-Methylfurano[3,2-b]urs-12-en-28-oic acid **12b** ^{13}C NMR spectra ($CDCl_3$)



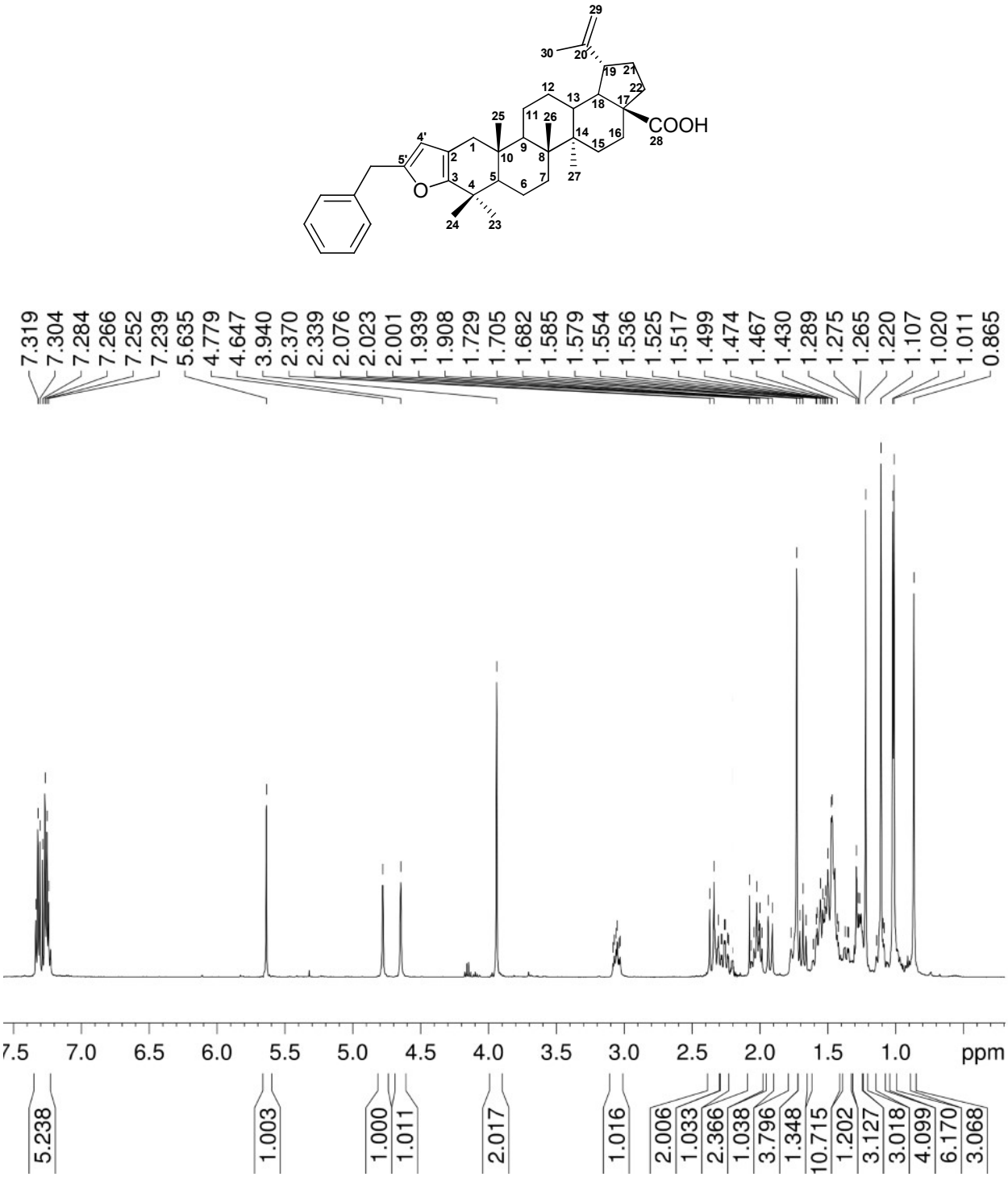
5'-Methylfurano[3,2-b]olean-12-en-28-oic acid **13b** ^{1}H NMR spectra ($CDCl_3$)



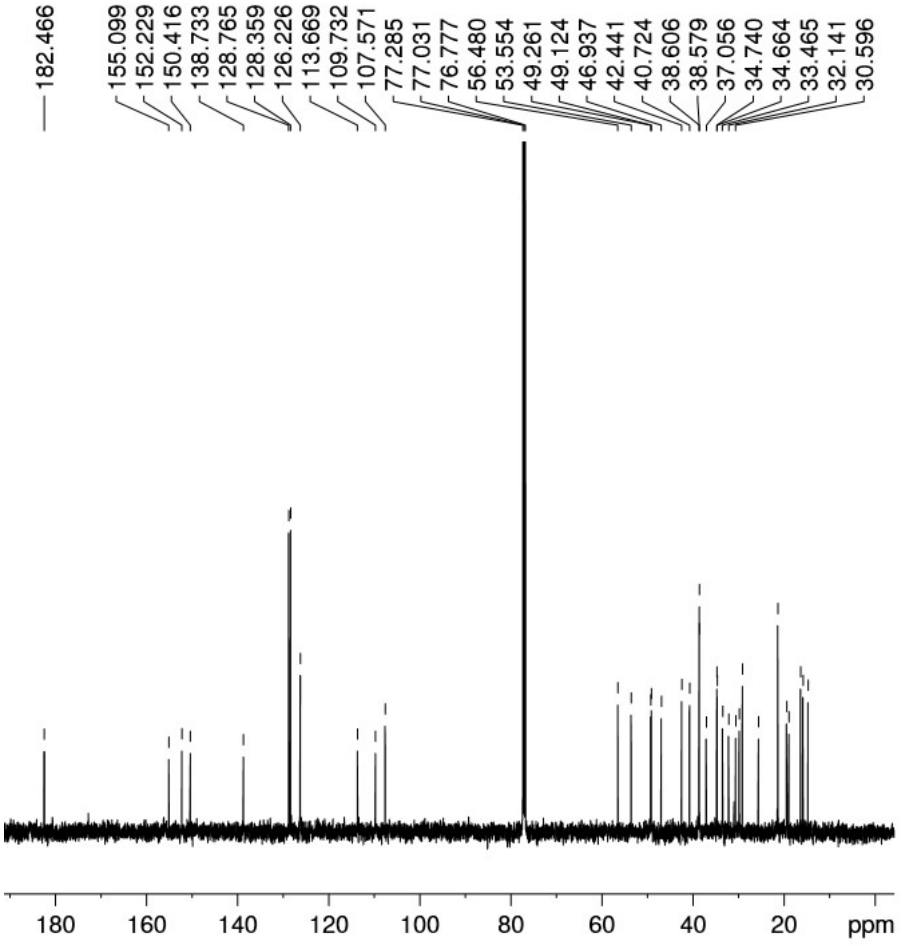
5'-Methylfurano[3,2-b]olean-12-en-28-oic acid **13b** ^{13}C NMR spectra ($CDCl_3$)



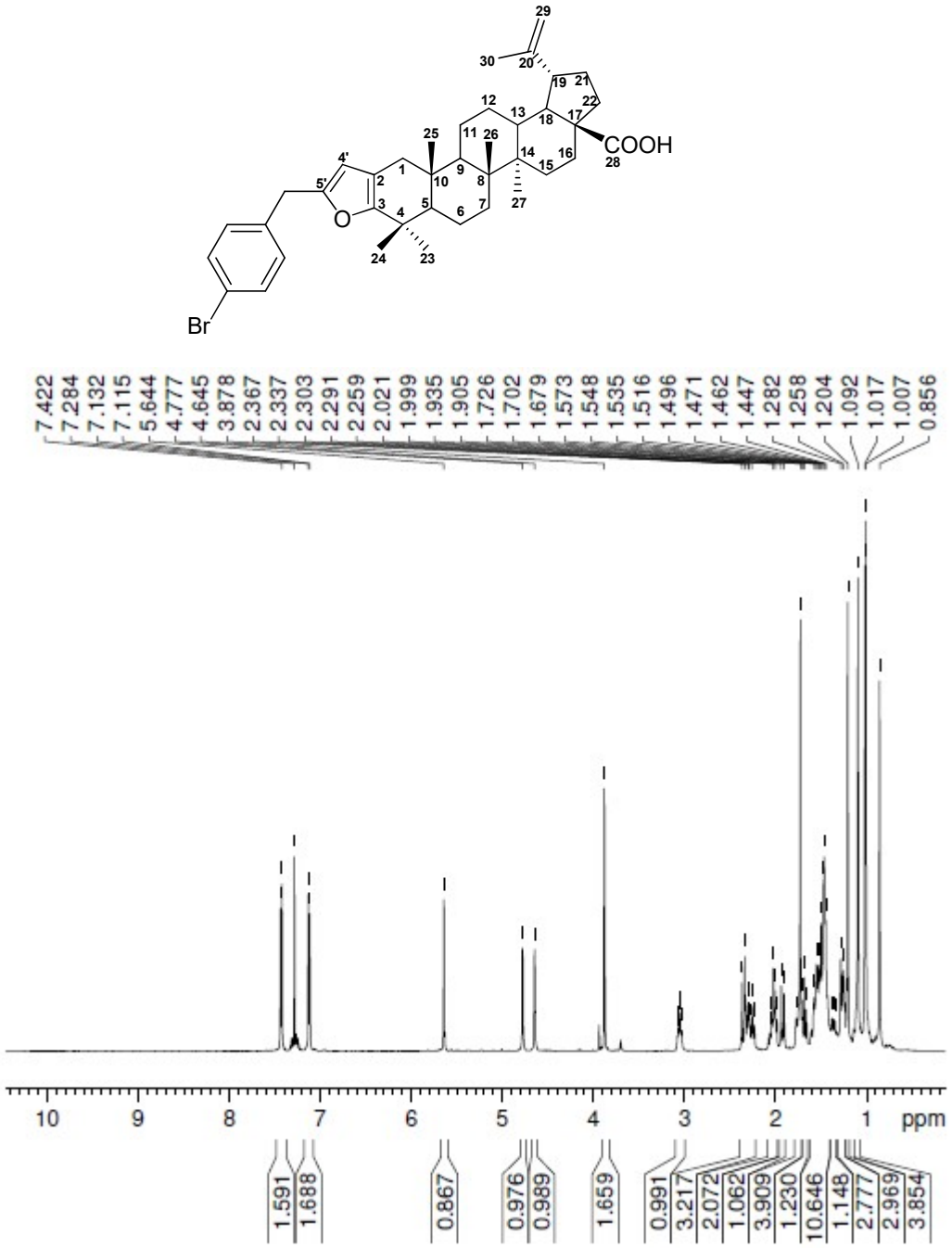
5'-Benzylfurano[3,2-b]lup-20(29)-en-28-oic acid **16a** ^{1}H NMR spectra ($CDCl_3$)



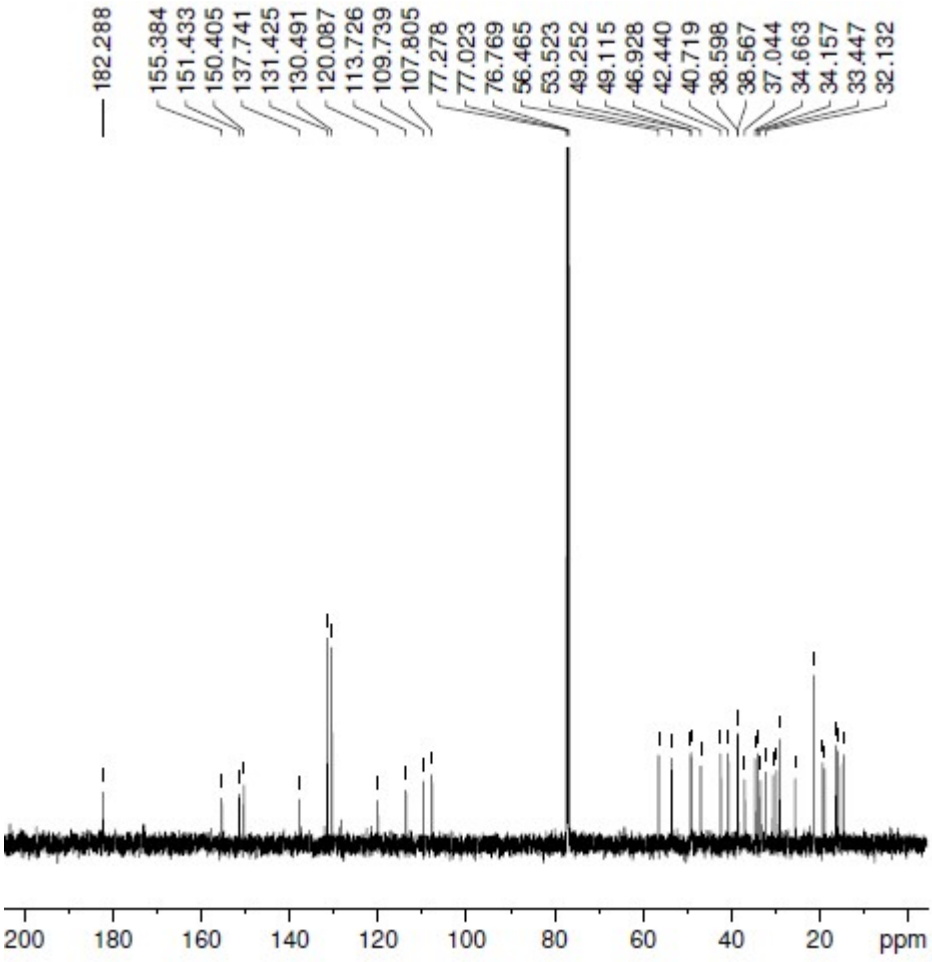
5'-Benzylfurano[3,2-b]lup-20(29)-en-28-oic acid **16a** ^{13}C NMR spectra ($CDCl_3$)



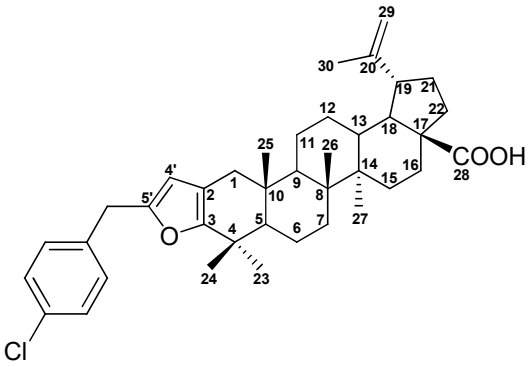
5'-(4-Brombenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16b** ^{1}H NMR spectra ($CDCl_3$)

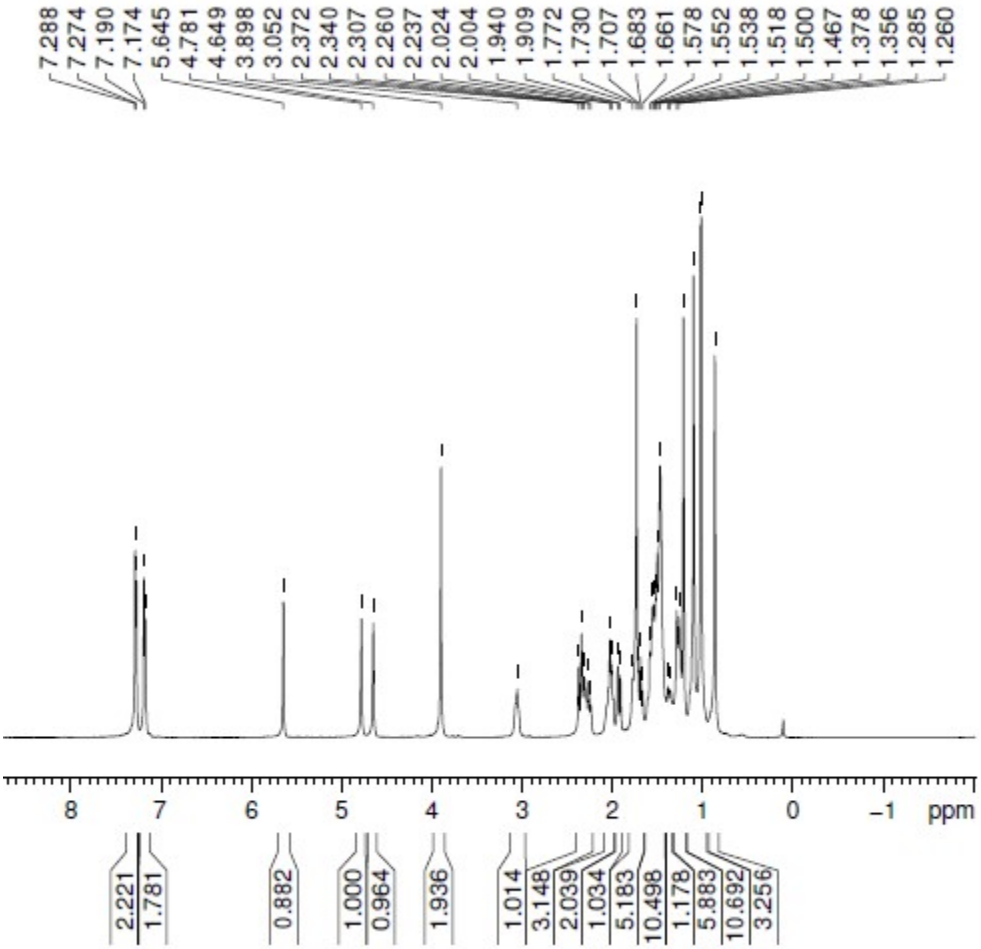


5'-(4-Brombenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16b** ^{13}C NMR spectra ($CDCl_3$)

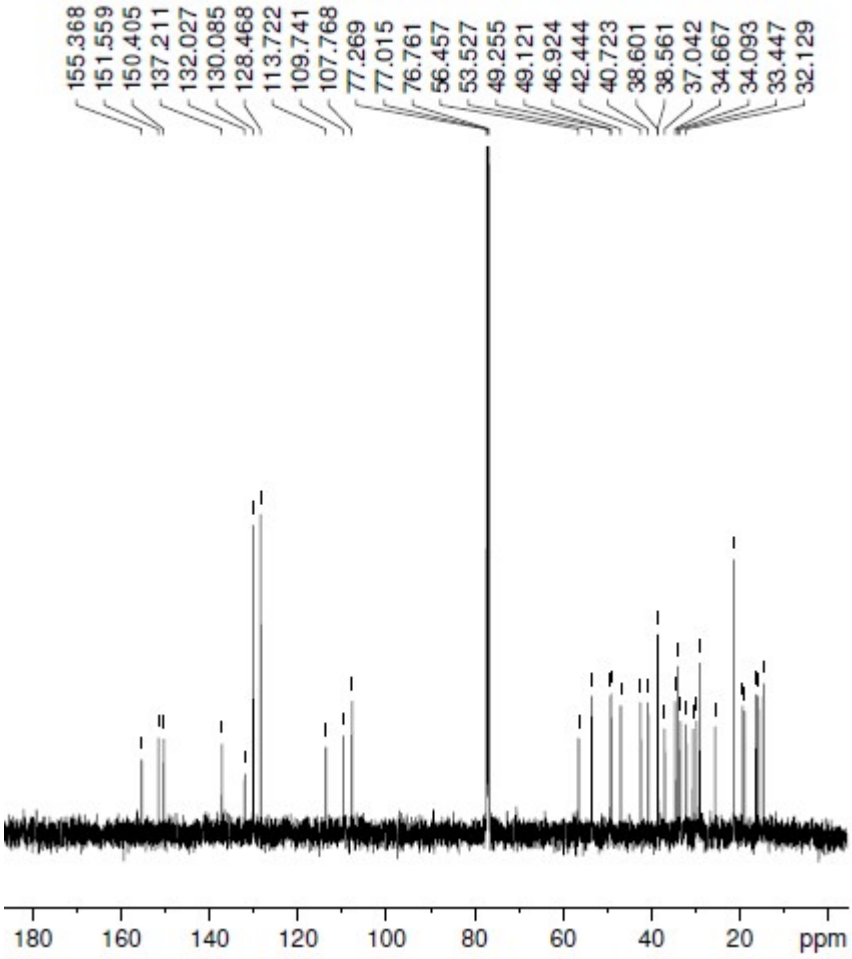


5'-(4-Chlorobenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16c** ^{1}H NMR spectra ($CDCl_3$)

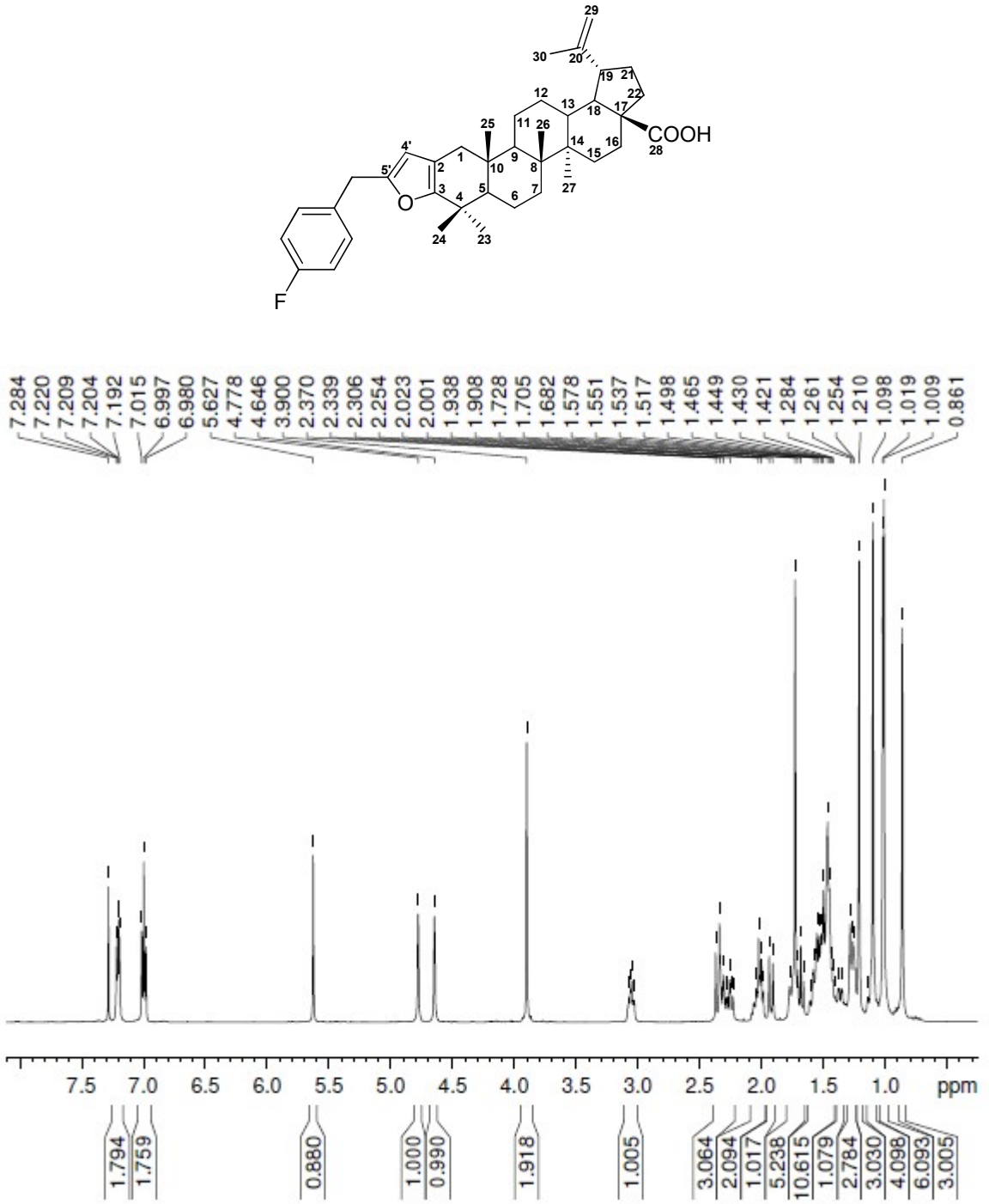




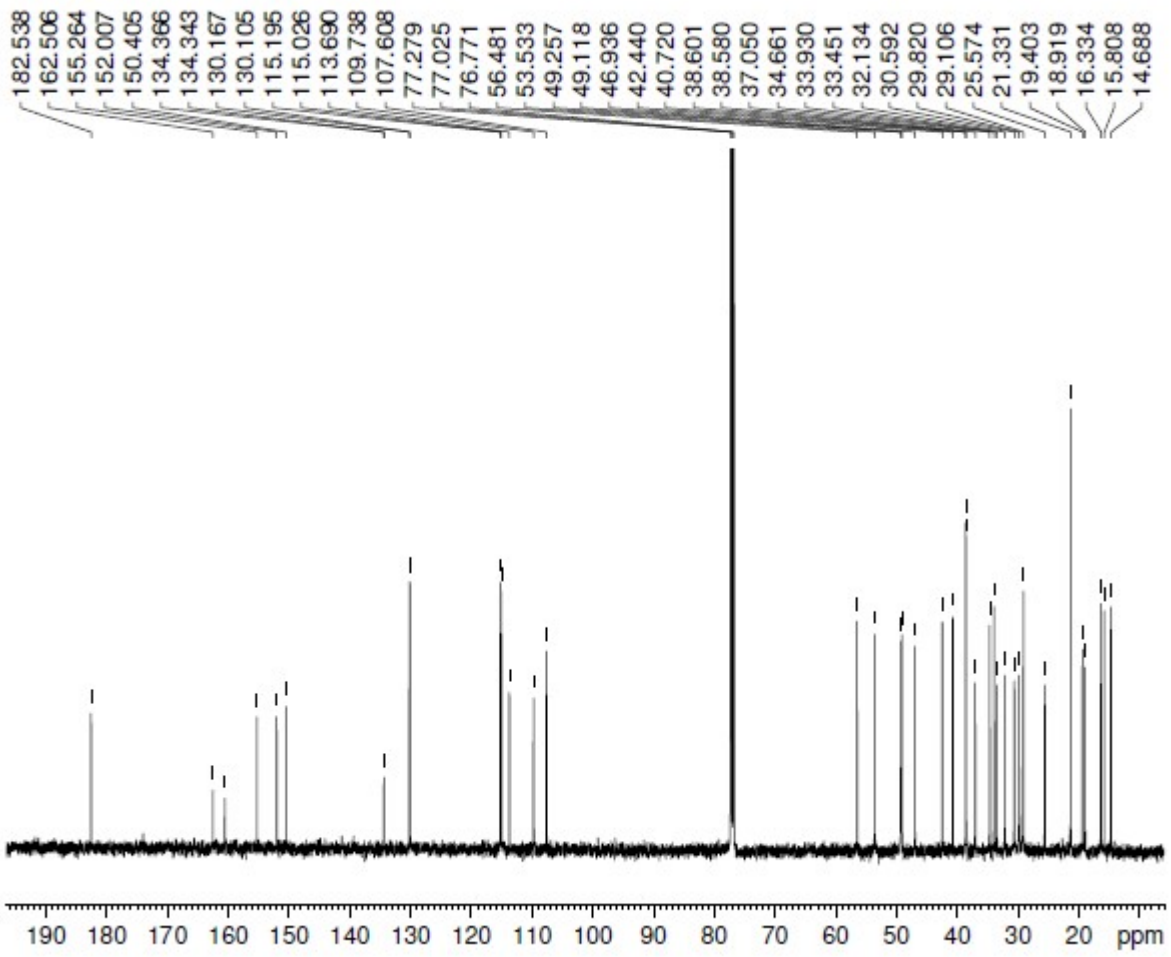
5'-(4-Chlorobenzyl)furano[3,2-b]lup-20,29-en-28-oic acid **16c** ^{13}C NMR spectra ($CDCl_3$)



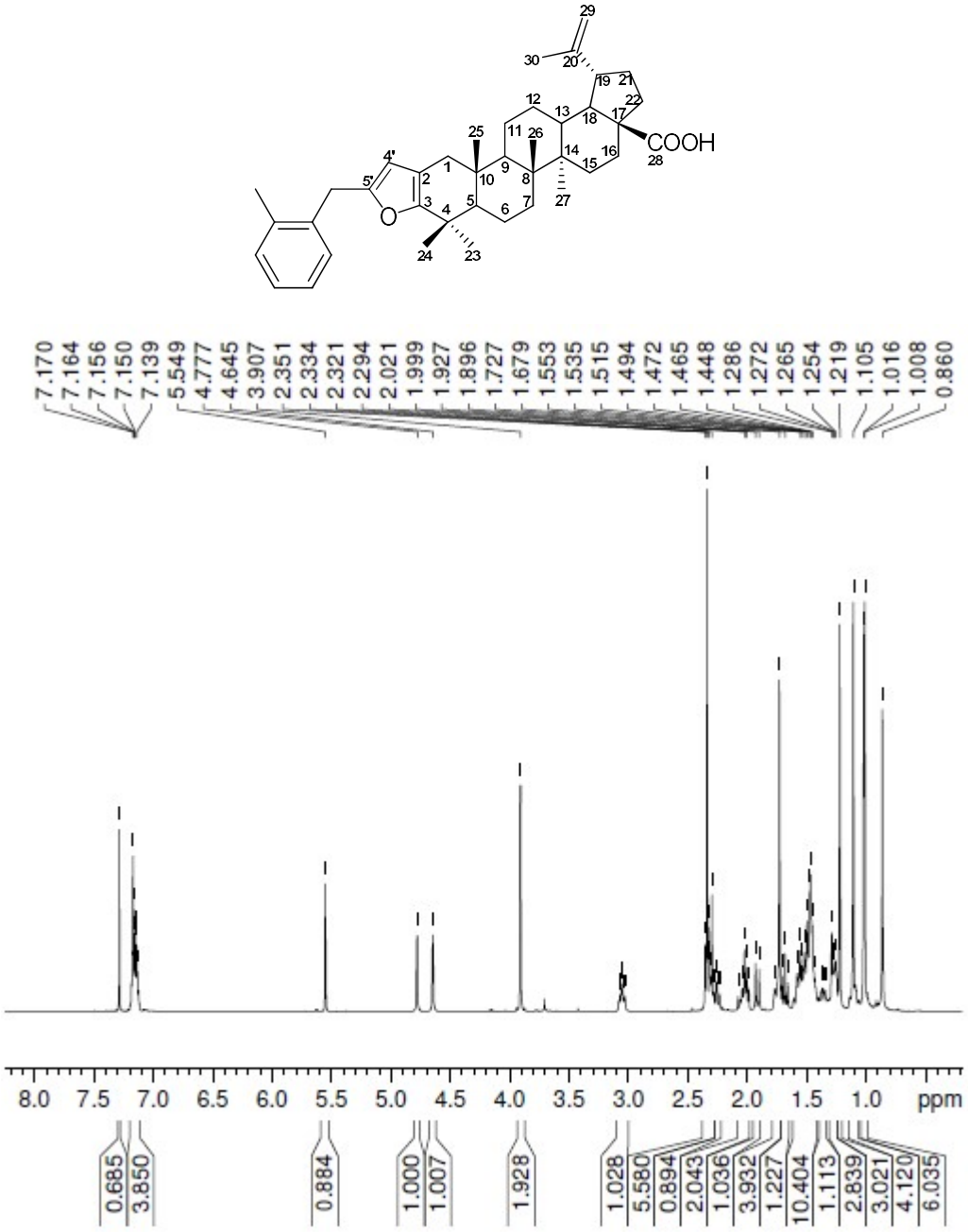
5'-(4-Fluorobenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16d** ^{1}H NMR spectra ($CDCl_3$)



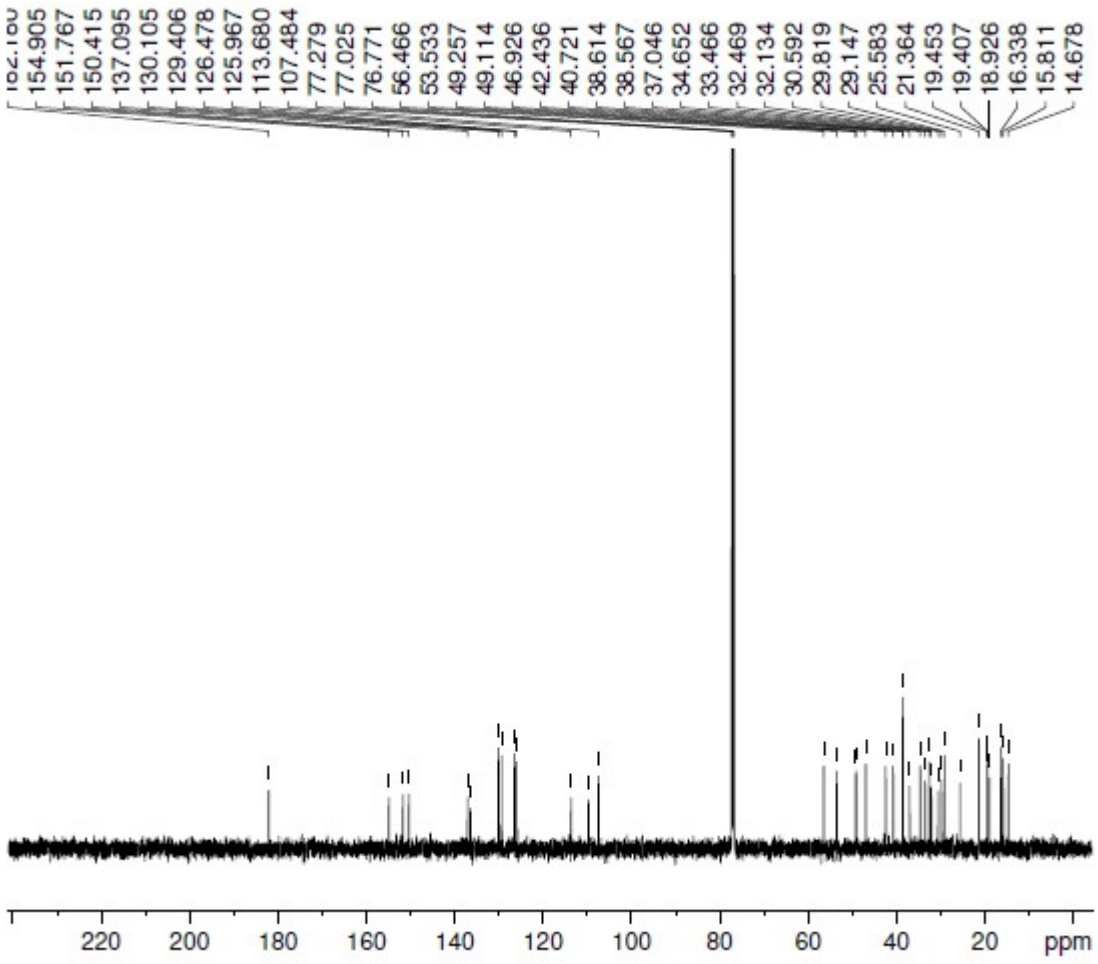
5'-(4-Fluorobenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16d** ^{13}C NMR spectra ($CDCl_3$)



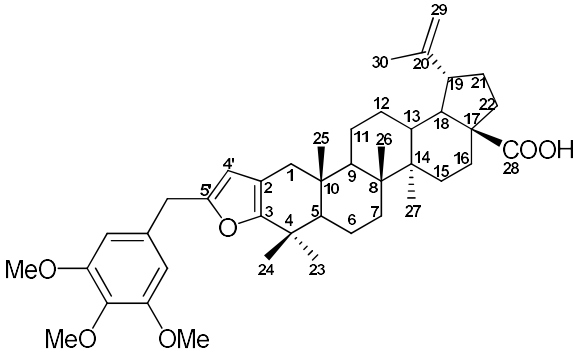
5'-(4-Methylbenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16e** ^{1}H NMR spectra ($CDCl_3$)

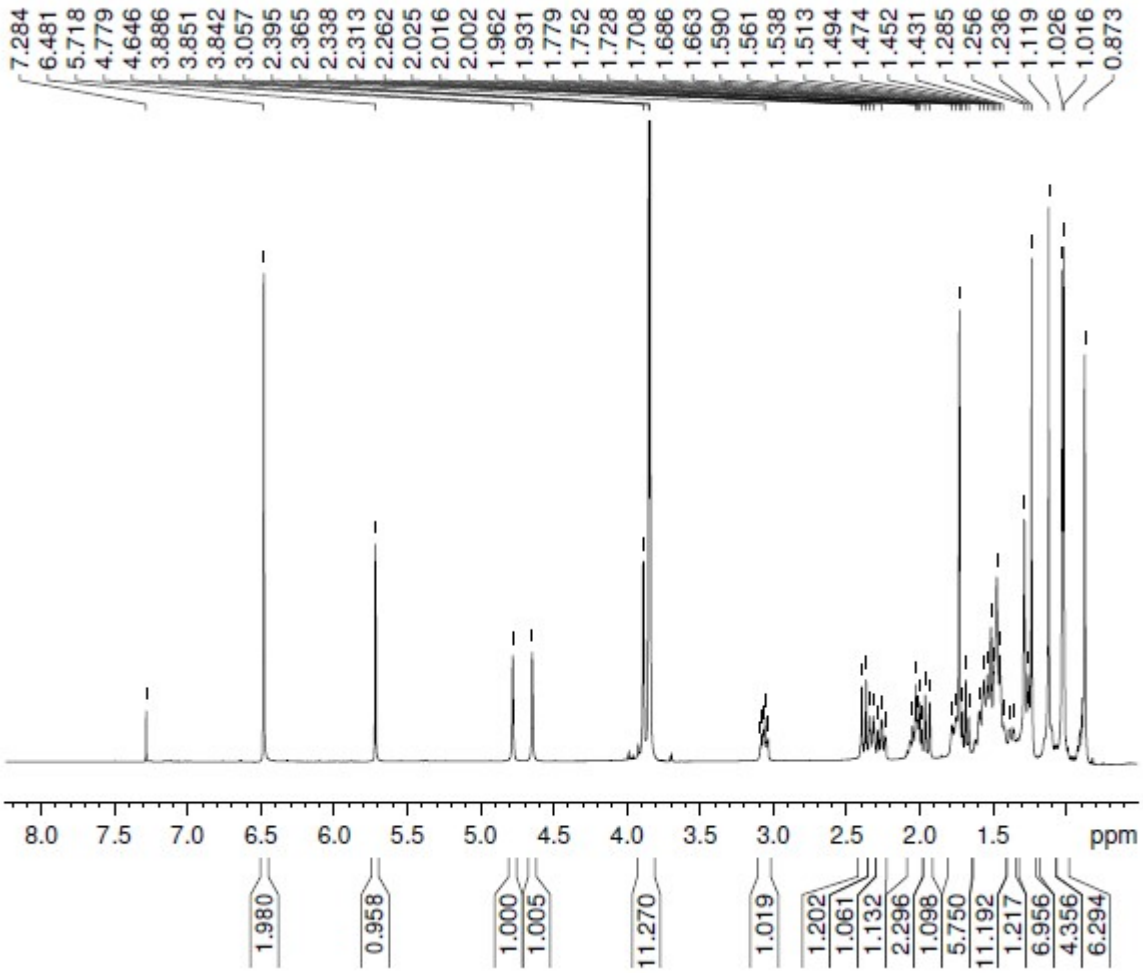


5'-(4-Methylbenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16e** ^{13}C NMR spectra ($CDCl_3$)

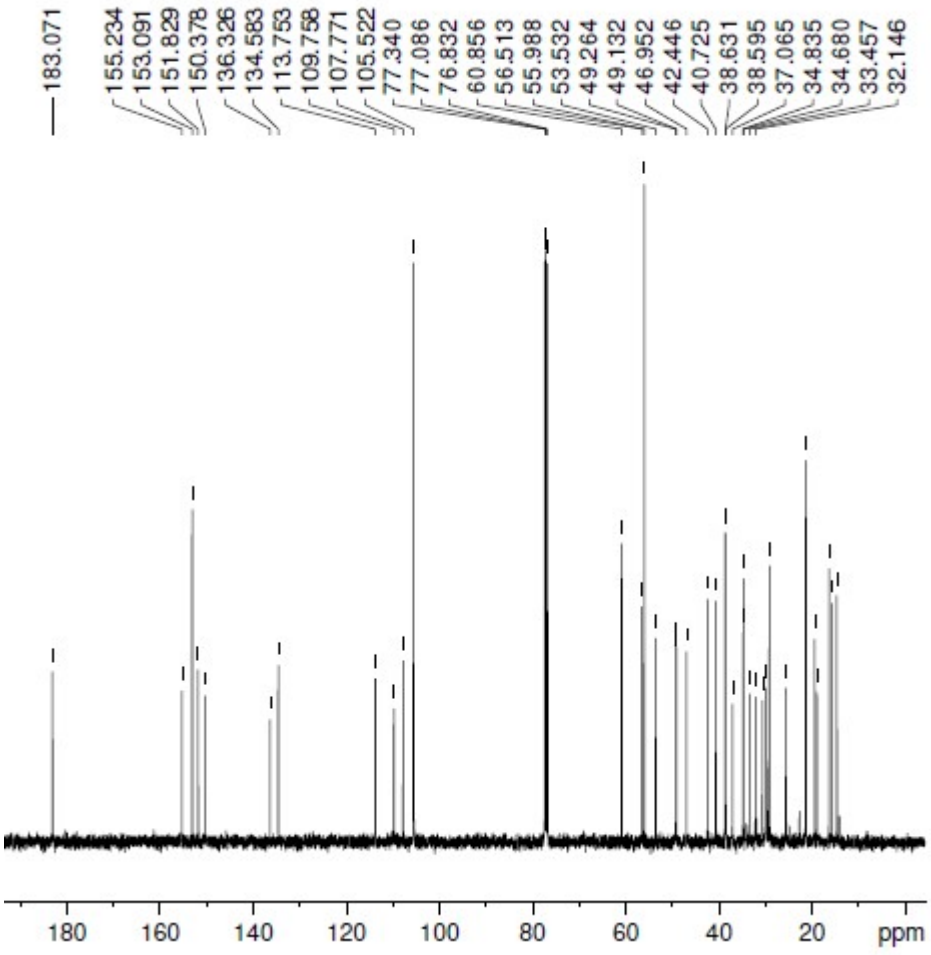


5'-(3,4,5-Trimethoxybenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16f** ^{1}H NMR spectra ($CDCl_3$)

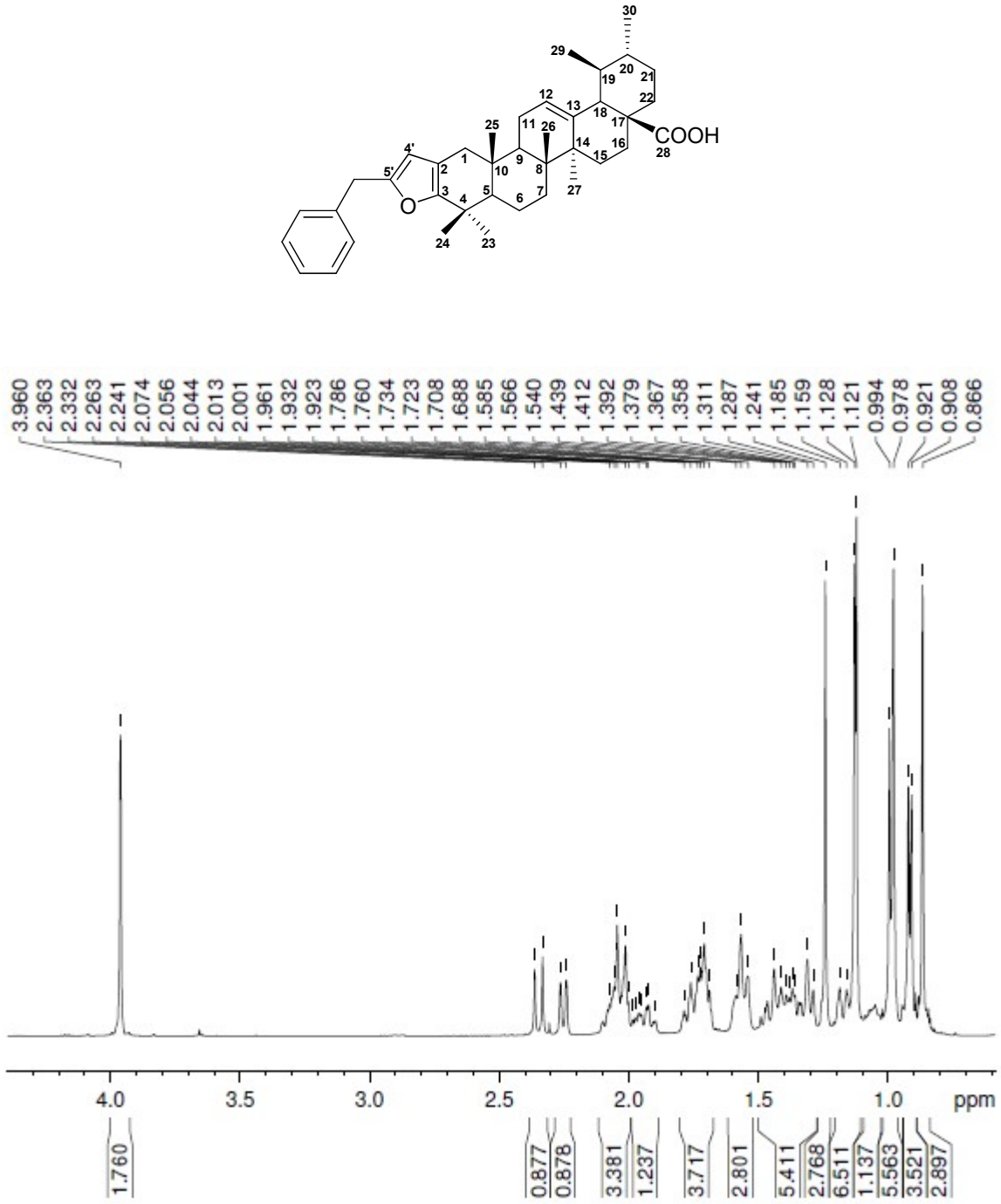




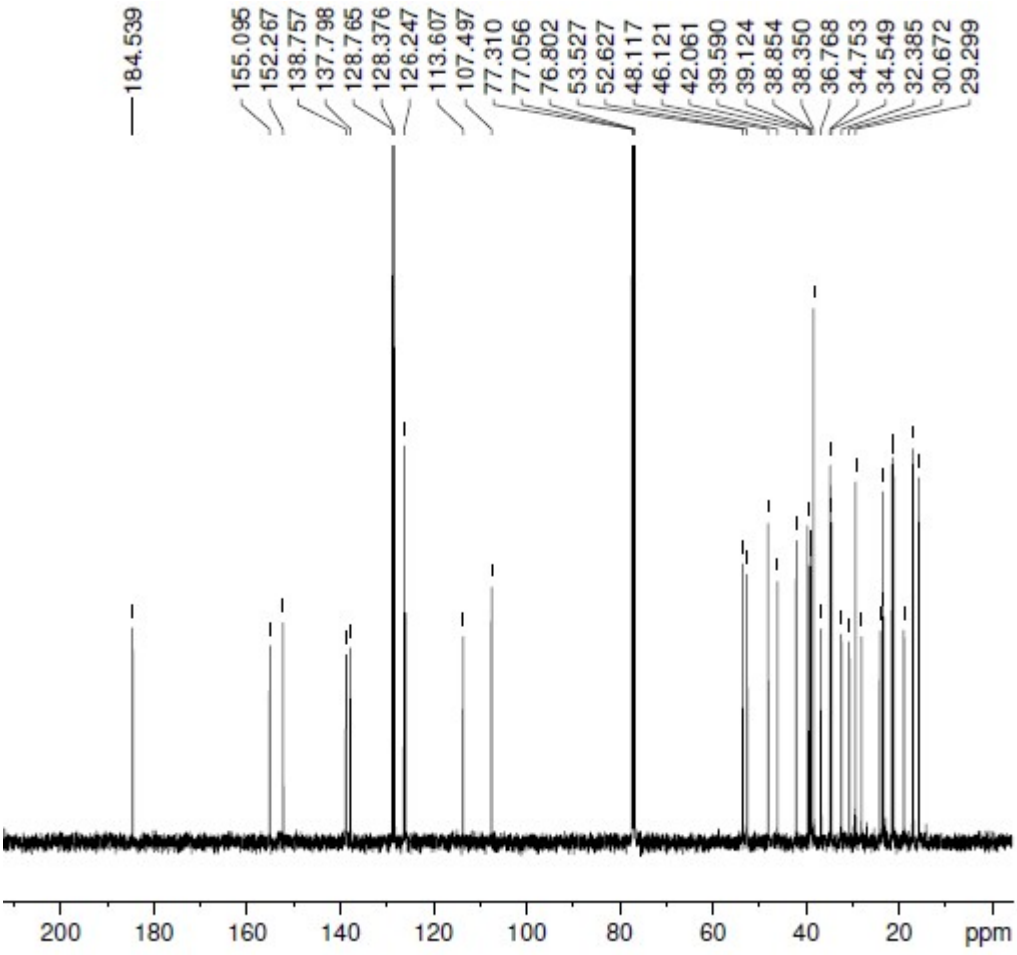
5'-(3,4,5-Trimethoxybenzyl)furano[3,2-b]lup-20(29)-en-28-oic acid **16f** ^{13}C NMR spectra ($CDCl_3$)



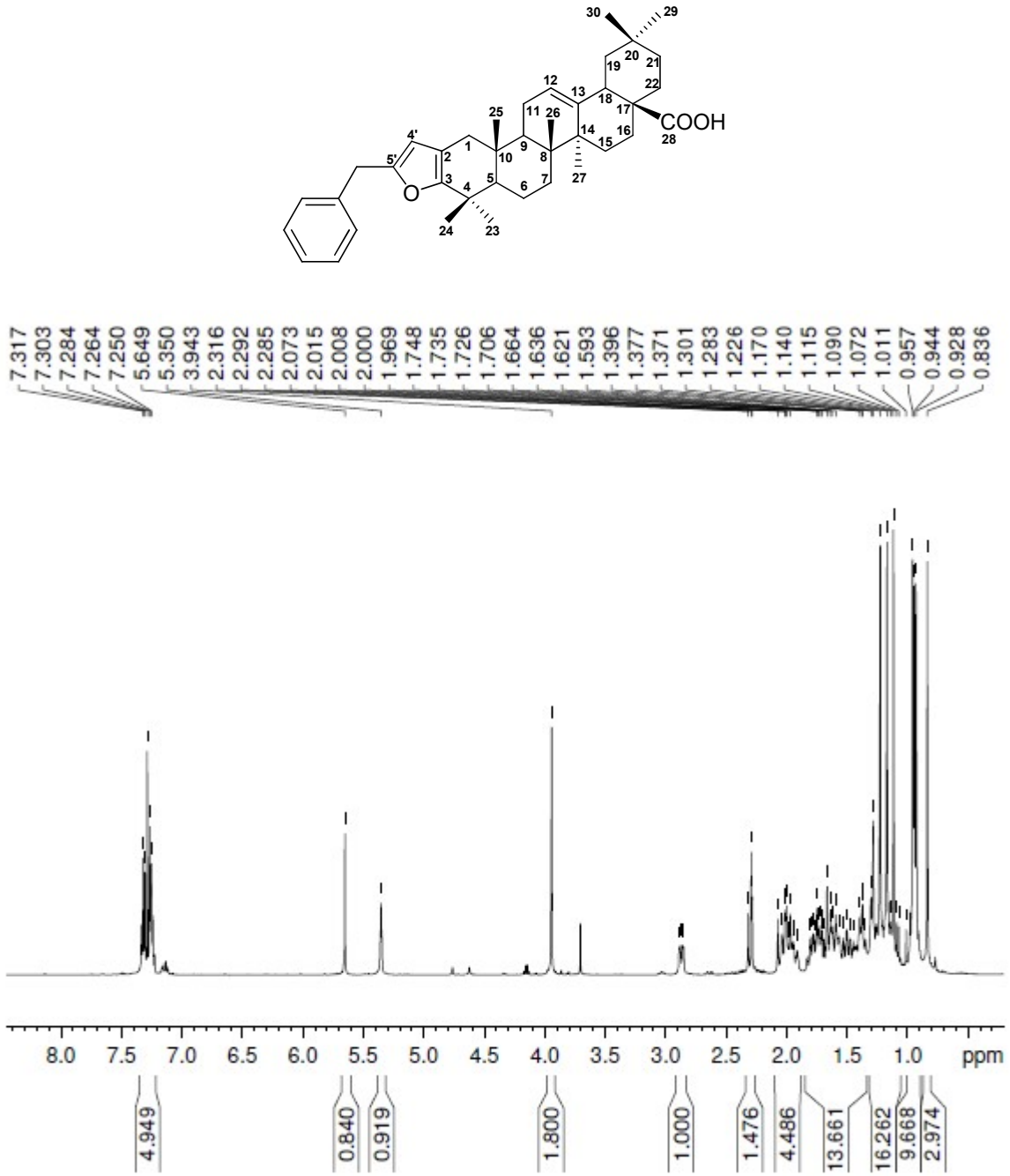
5'-Benzylfurano[3,2-b]urs-12-en-28-oic acid **18b** ^{1}H NMR spectra ($CDCl_3$)



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** ^{1}H NMR spectra ($CDCl_3$)



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

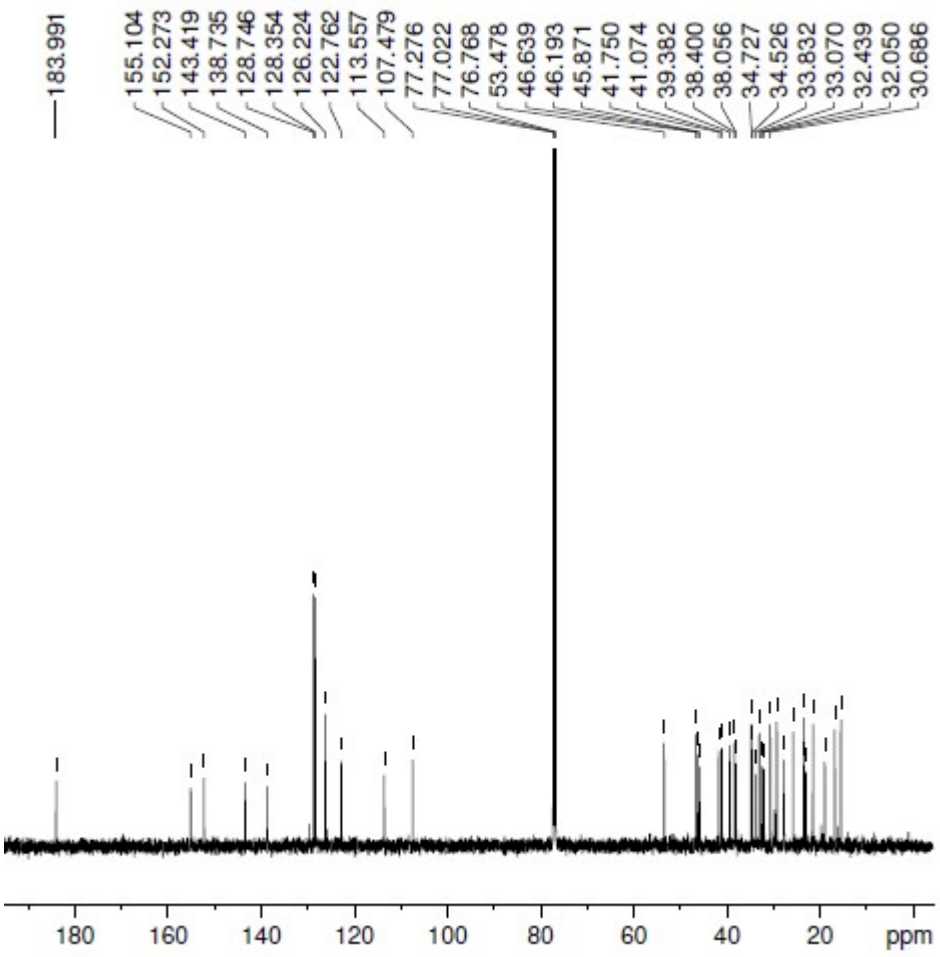


Table 1. ^{13}C NMR spectra of compounds **14a-g, 17** and **19**

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, $^1J_{C,F}$ = 8) 115.37 (d, $^1J_{C,F}$ = 22) 162.34 (d, $^1J_{C,F}$ = 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_6H_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, $^1J_{C,F}$ = 8) 115.10 (d, $^1J_{C,F}$ = 21) 162.53 (d, $^1J_{C,F}$ = 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_6H_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, $^1J_{C,F}$ = 3,25) 130.13 (d, $^1J_{C,F}$ = 8) 115.10 (d, $^1J_{C,F}$ = 21) 161.53 (d, $^1J_{C,F}$ = 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_6H_4	-	-	-	-	-	-	-	19.45	-	-	-
(O-Me)$_2$ O-Me	-	-	-	-	-	-	-	-	55.98 60.85	-	-

