Design, Synthesis and Preliminary Evaluation of the Cytotoxicity and Antibacterial Activity of Novel Triphenylphosphonium Derivatives of Betulin

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^{1}H NMR spectrum of betulin (**1**); 600 MHz/CDCl₃/TMS; δ (ppm).

150.45
109.66
78.97
77.20
76.99
76.77
60.57
55.30
50.41
48.78
47.79
42.72
40.93
38.86
38.71
37.32
37.17
34.25
33.97
29.77
29.19
27.98
27.41
27.06
25.23
20.84
19.08
18.30
16.10
15.98
15.34
14.76
-0.02

170   160   150   140   130   120   110   100   90   80   70   60   50   40   30   20   10   0
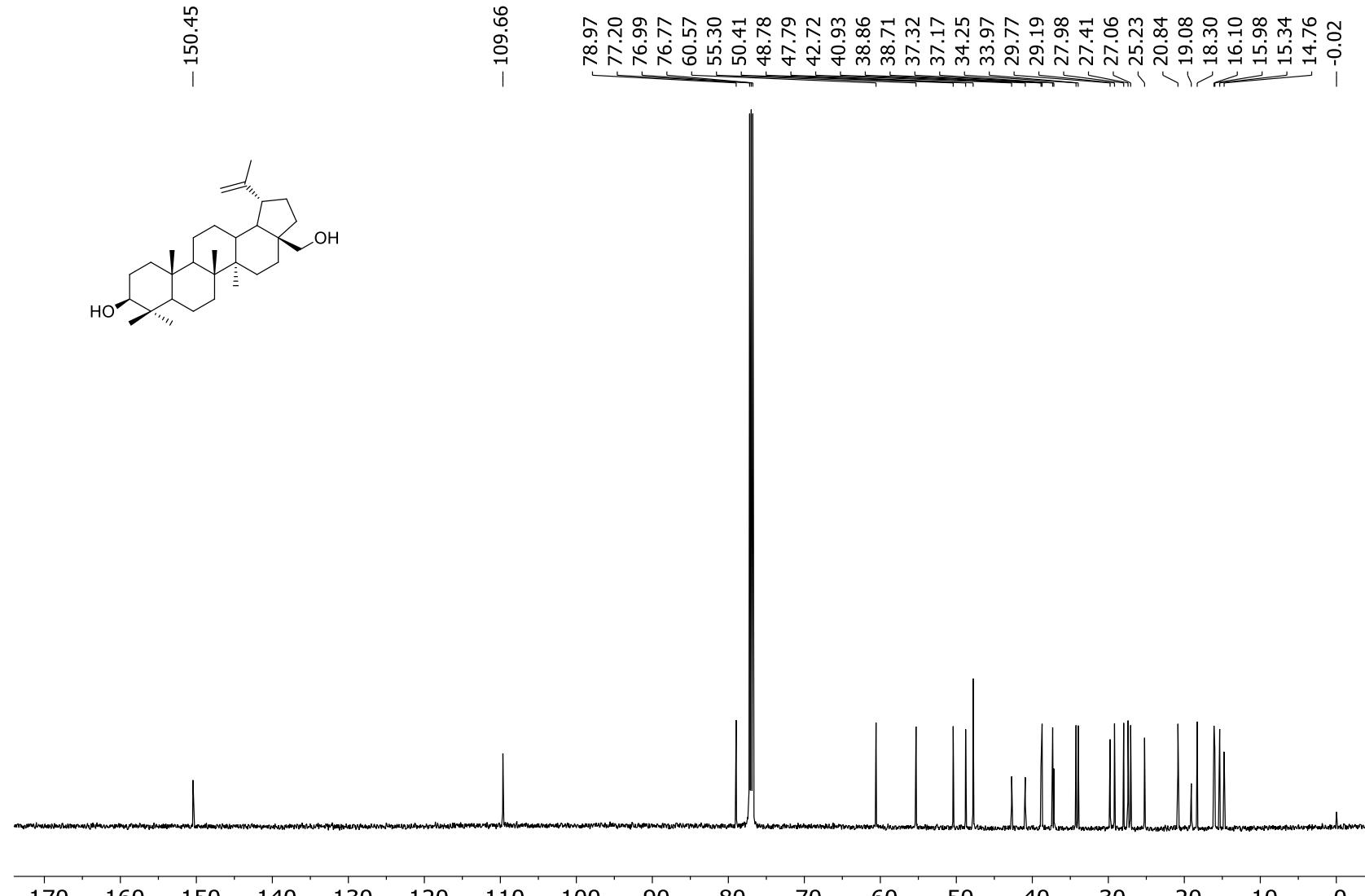
^{13}C NMR spectrum of betulin (**1**); 150 MHz/CDCl$_3$/TMS; δ (ppm).
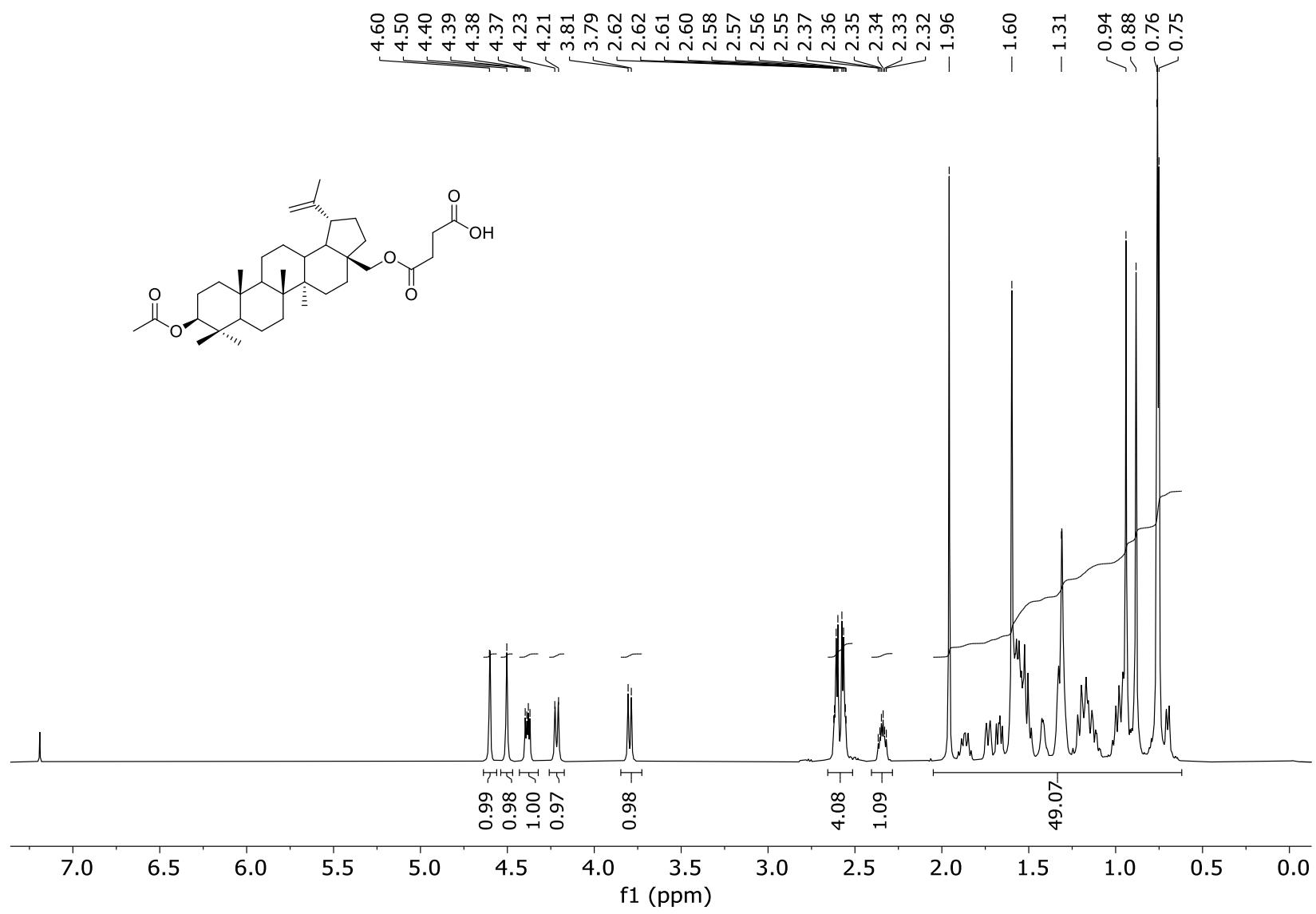
^{1}H NMR spectrum of 3-*O*-acetyl-28-*O*-(3'-carboxypropanoyl)betulin (**4a**); 600 MHz/CDCl$_3$/TMS; δ (ppm).
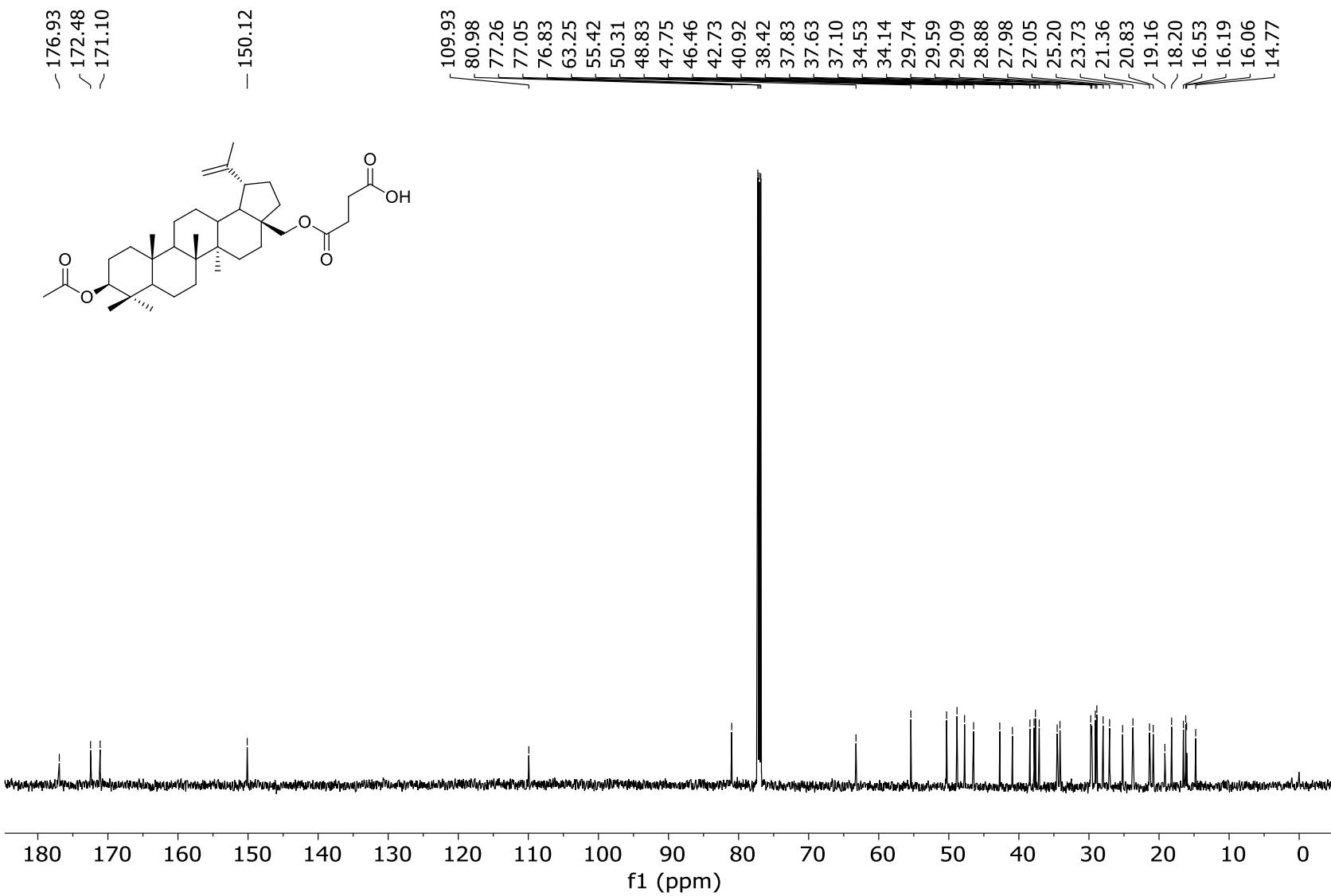
^{13}C NMR spectrum of 3-*O*-acetyl-28- *O*-(3'-carboxypropanoyl)betulin (**4a**); 150 MHz/CDCl$_3$/TMS; δ (ppm).
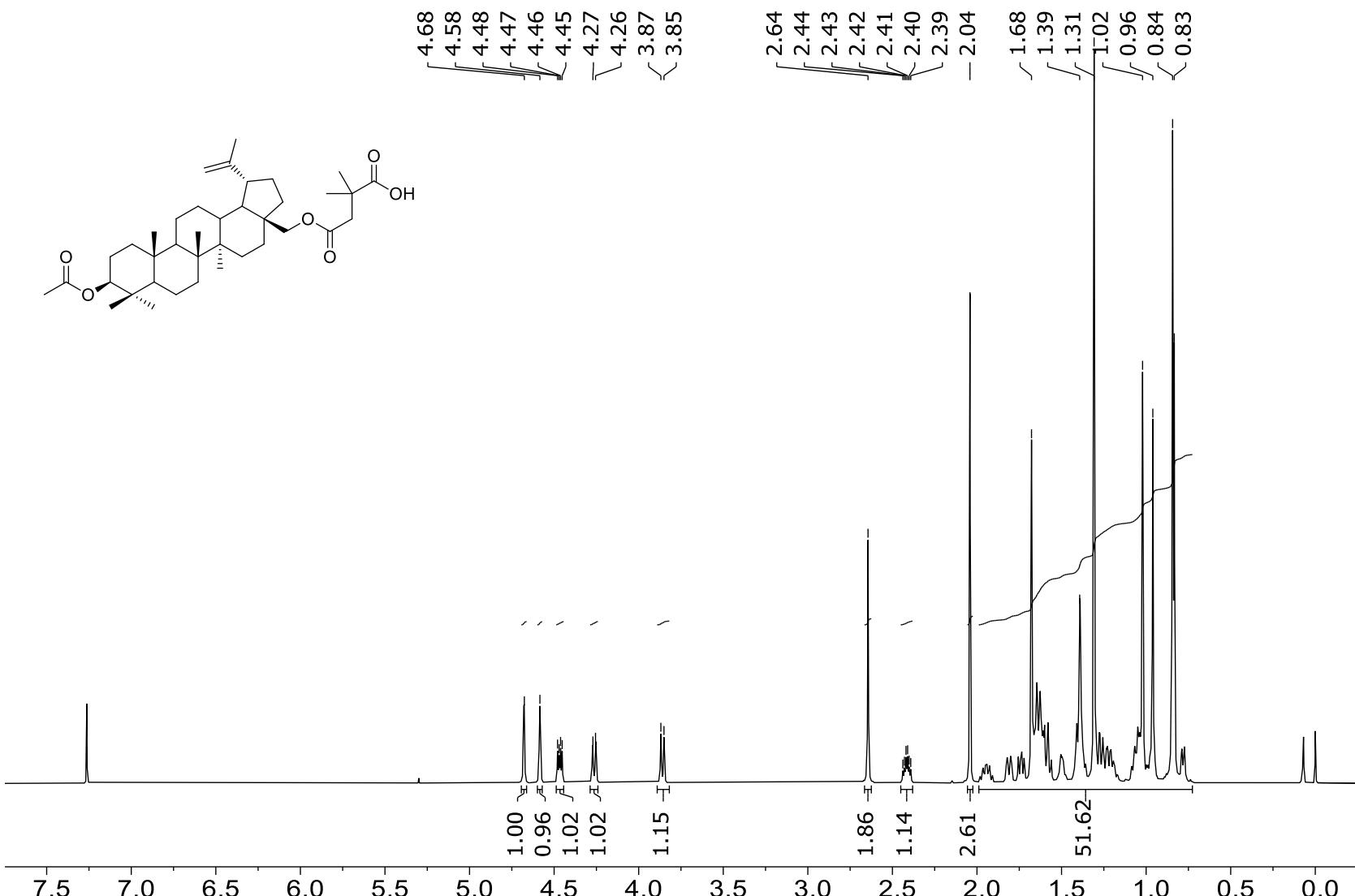
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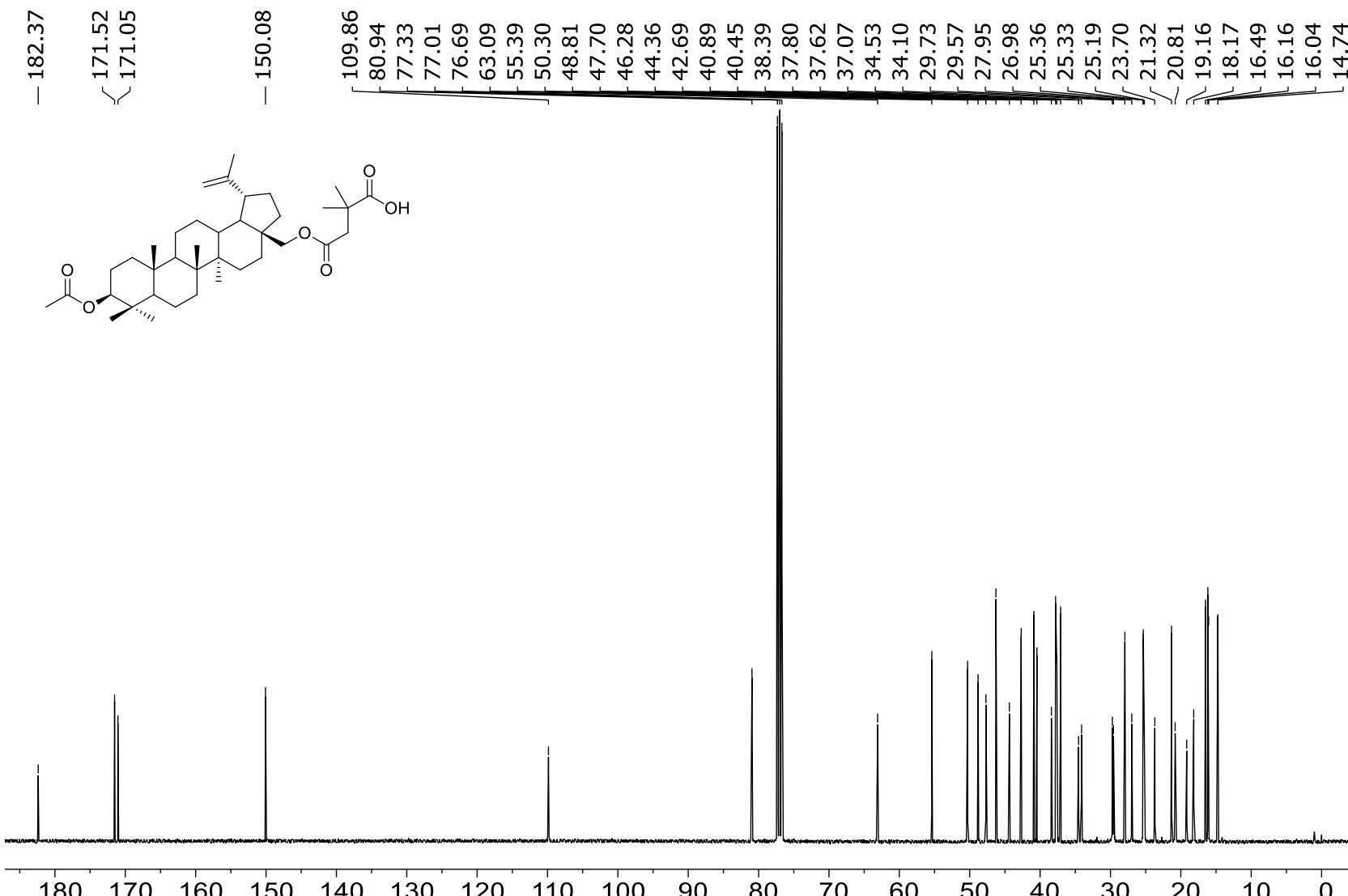
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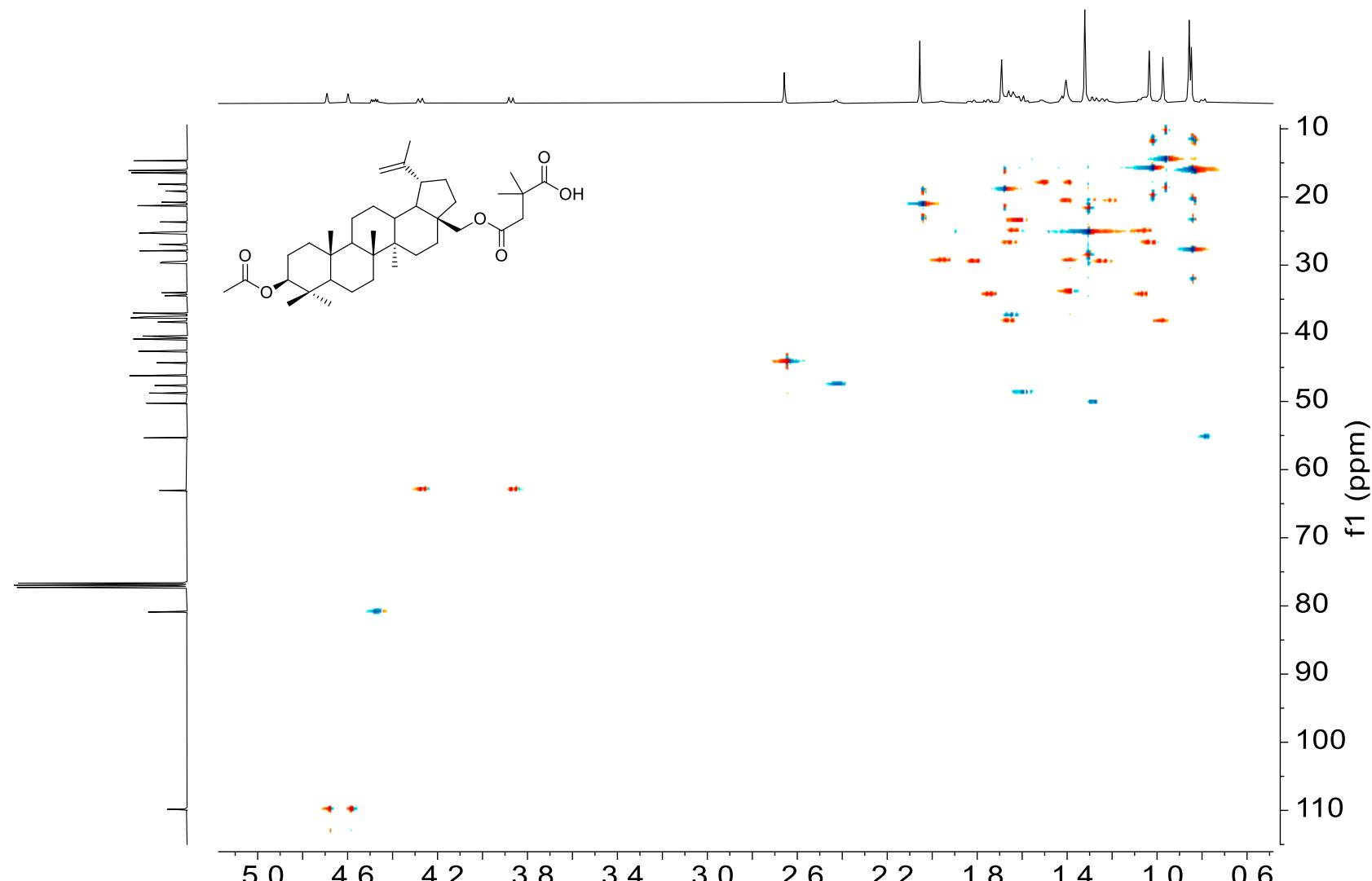
gHSQC spectrum of 3-*O*-acetyl-28-*O*-(3',3'-dimethyl-3'-carboxypropanoyl)betulin (**4b**)

4.69
4.68
4.59
4.59
4.59
4.59
4.51
4.50
4.49
4.48
4.32
4.30
3.89
3.87
2.69
2.68
2.68
2.67
2.67
2.66
2.63
2.63
2.62
2.61
2.45
2.44
2.43
2.42
2.41
2.40
1.69
1.03
0.98
0.85
0.84
0.83

1.00
1.01
1.00
0.99

1.00

8.48
1.04

46.15

7.5   7.0   6.5   6.0   5.5   5.0   4.5   4.0   3.5   3.0   2.5   2.0   1.5   1.0   0.5   0.0
f1 (ppm)

^{1}H NMR spectrum of 3,28-*O,O*′-bis(3′-carboxypropanoyl)betulin (**5**); 600 MHz/CDCl₃/TMS; δ (ppm).
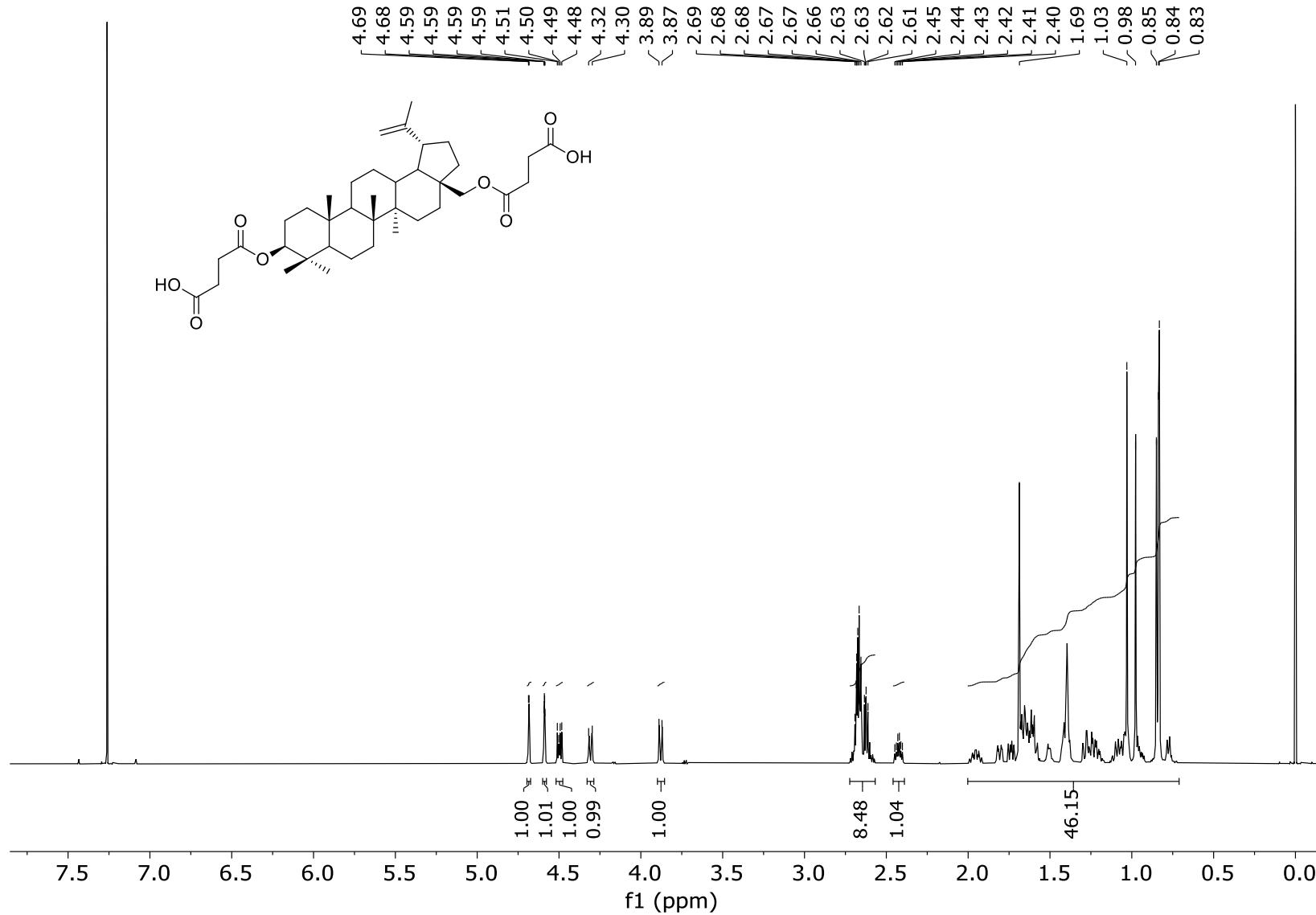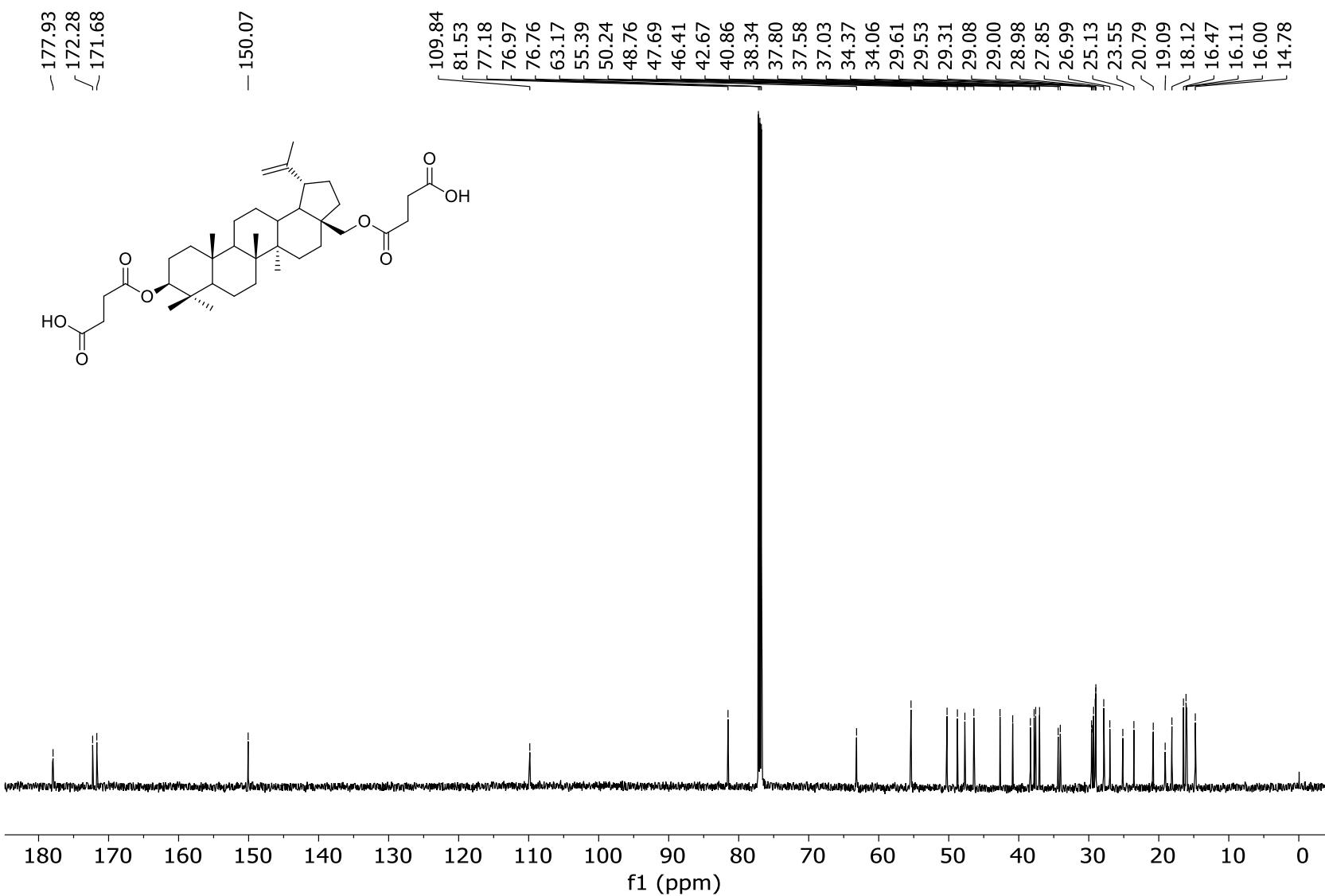
^{13}C NMR spectrum of 3,28-*O,O′*-bis(3′-carboxypropanoyl)betulin (**5**); 150 MHz/CDCl$_3$/TMS; δ (ppm).

^{1}H NMR spectrum of analogue **6a**; 600 MHz/CDCl$_3$/TMS; δ (ppm).
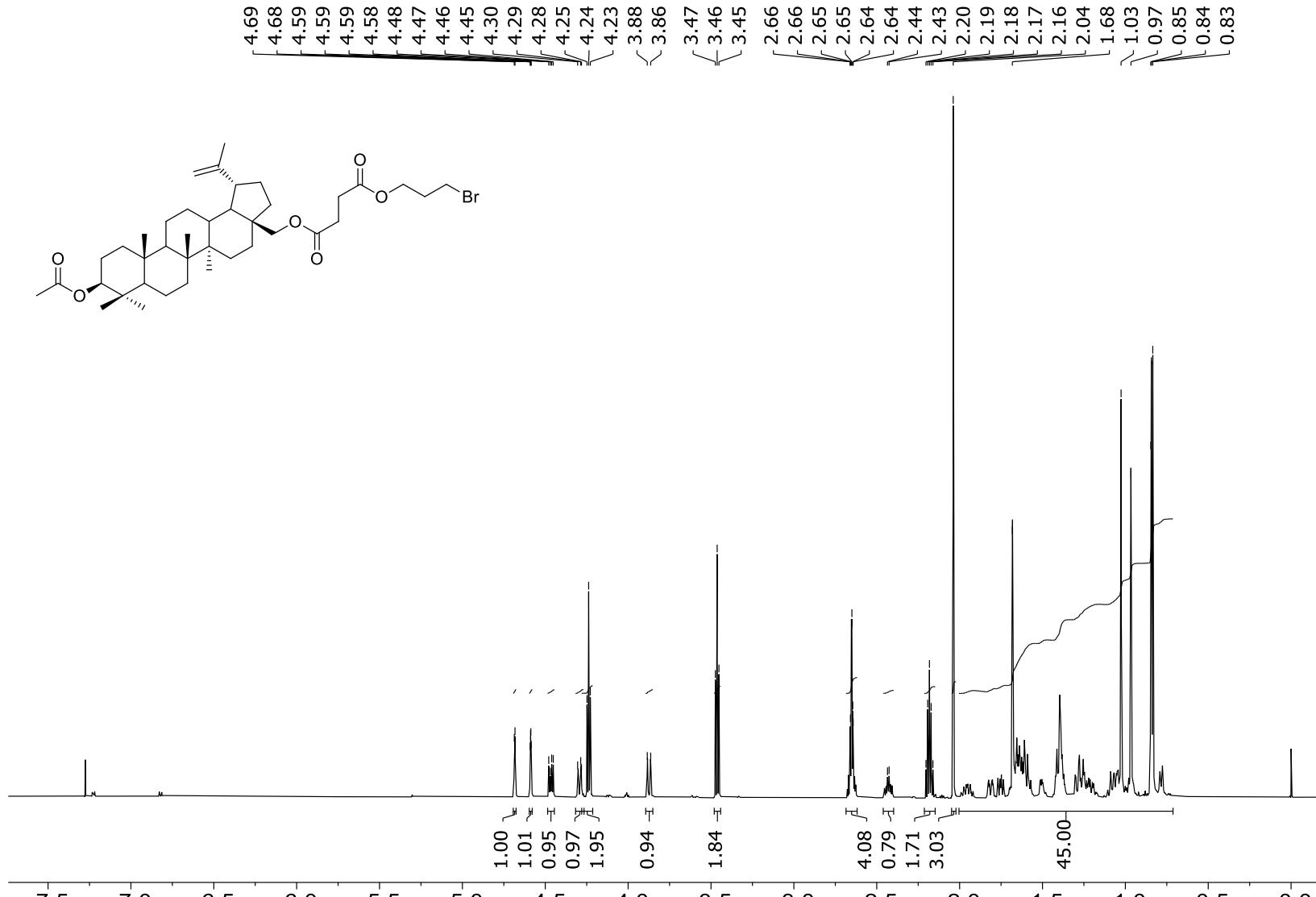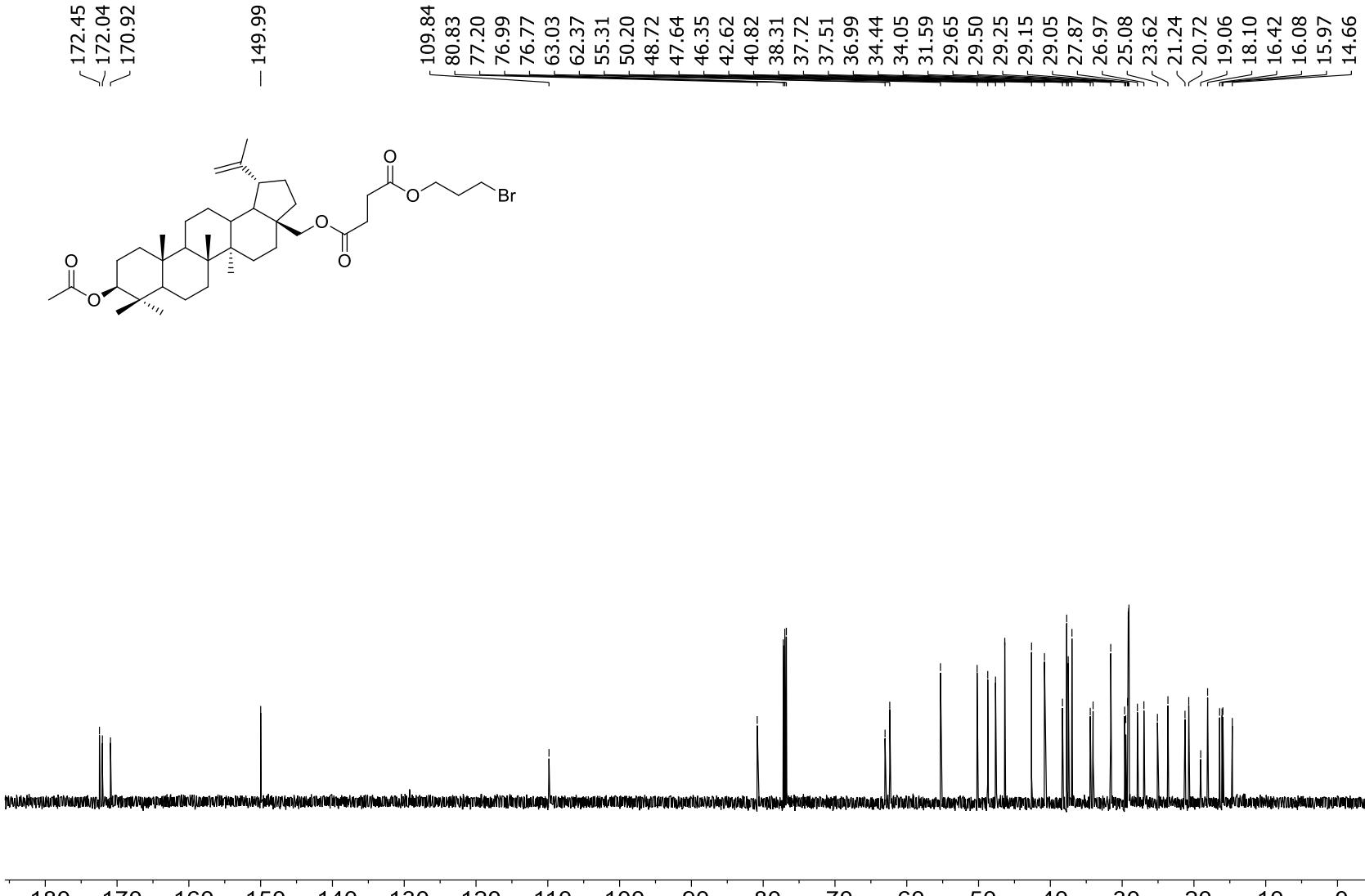
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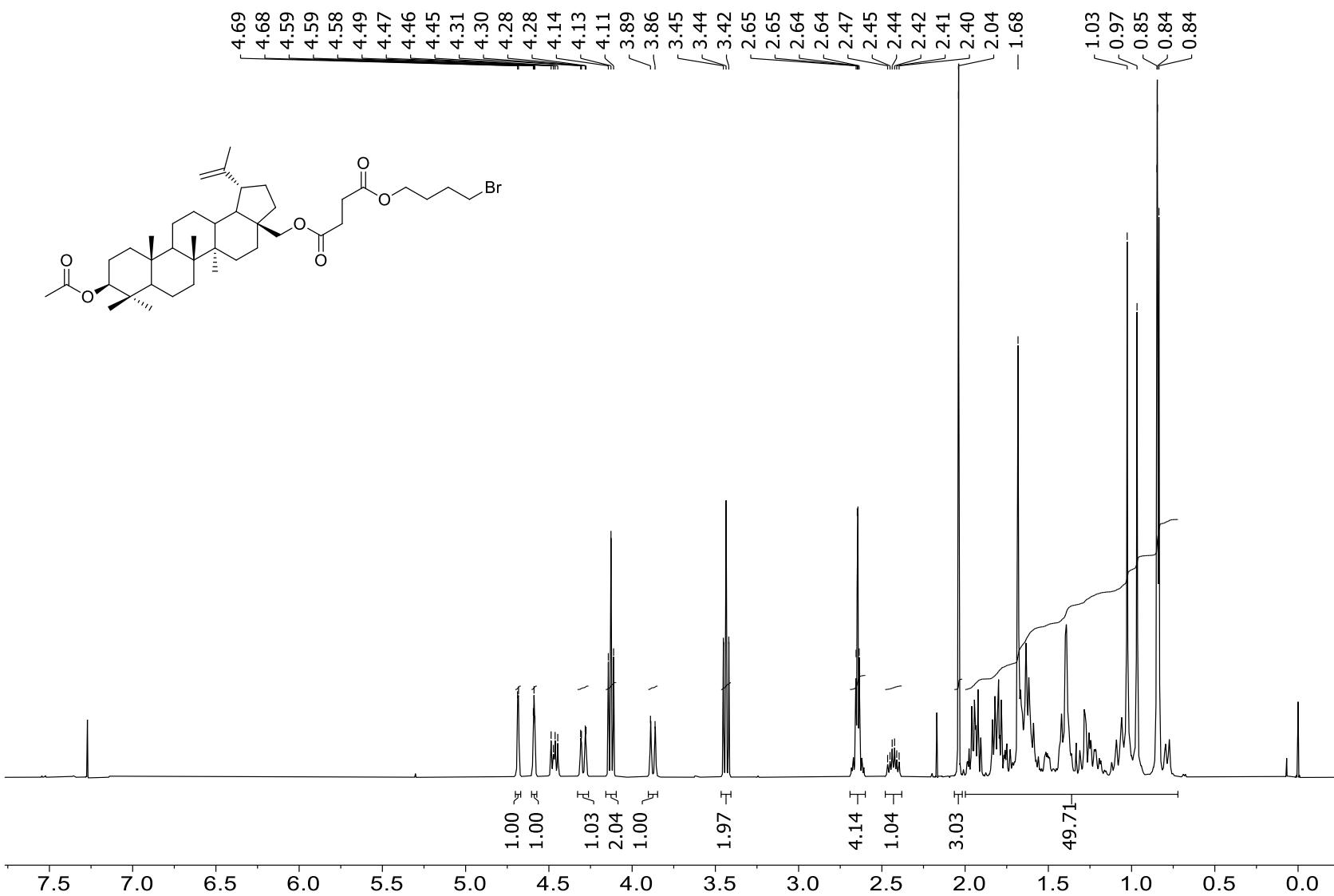
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^{13}C NMR spectrum of analogue **6b**; 100 MHz/CDCl$_3$/TMS; δ (ppm).

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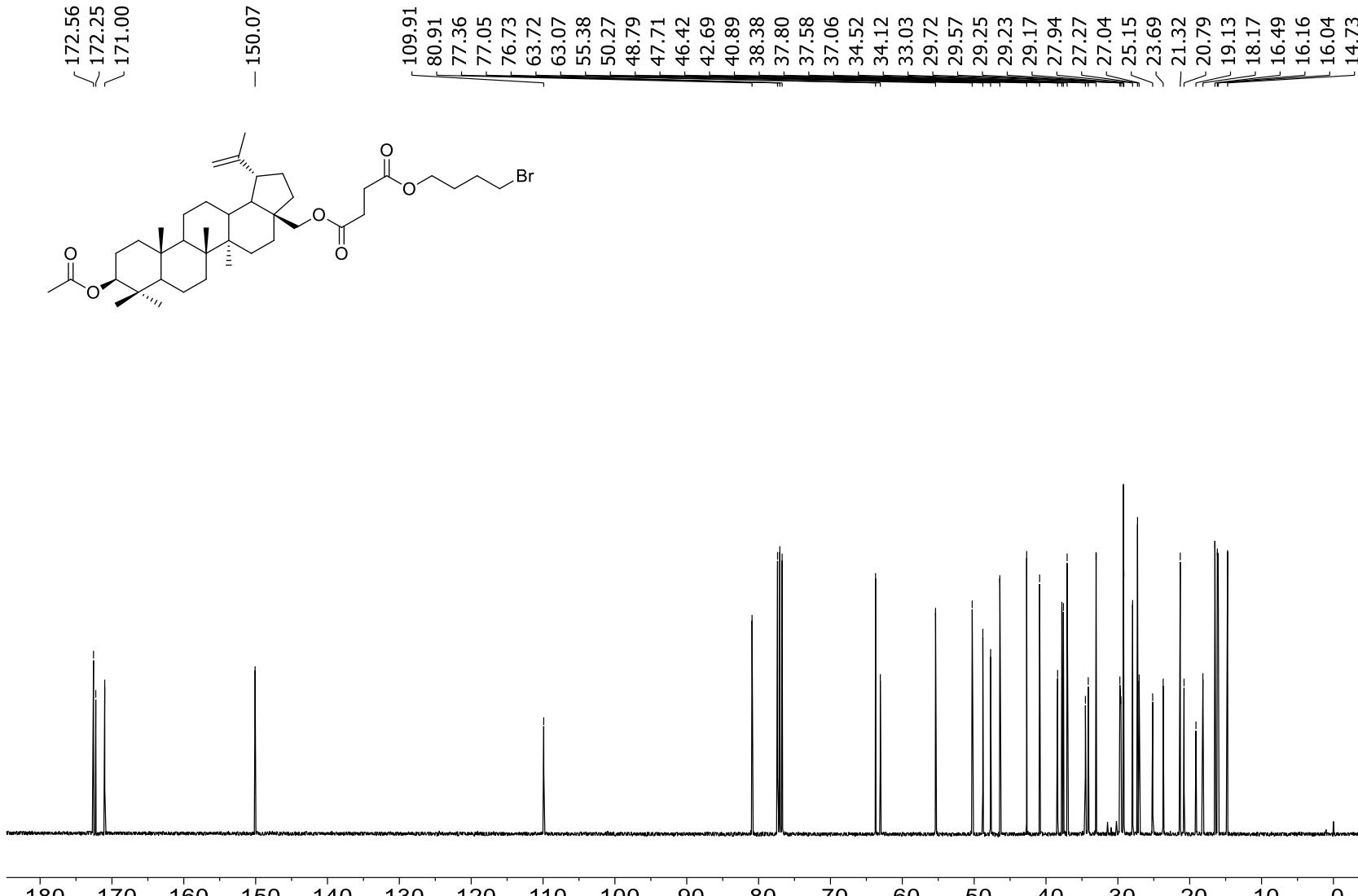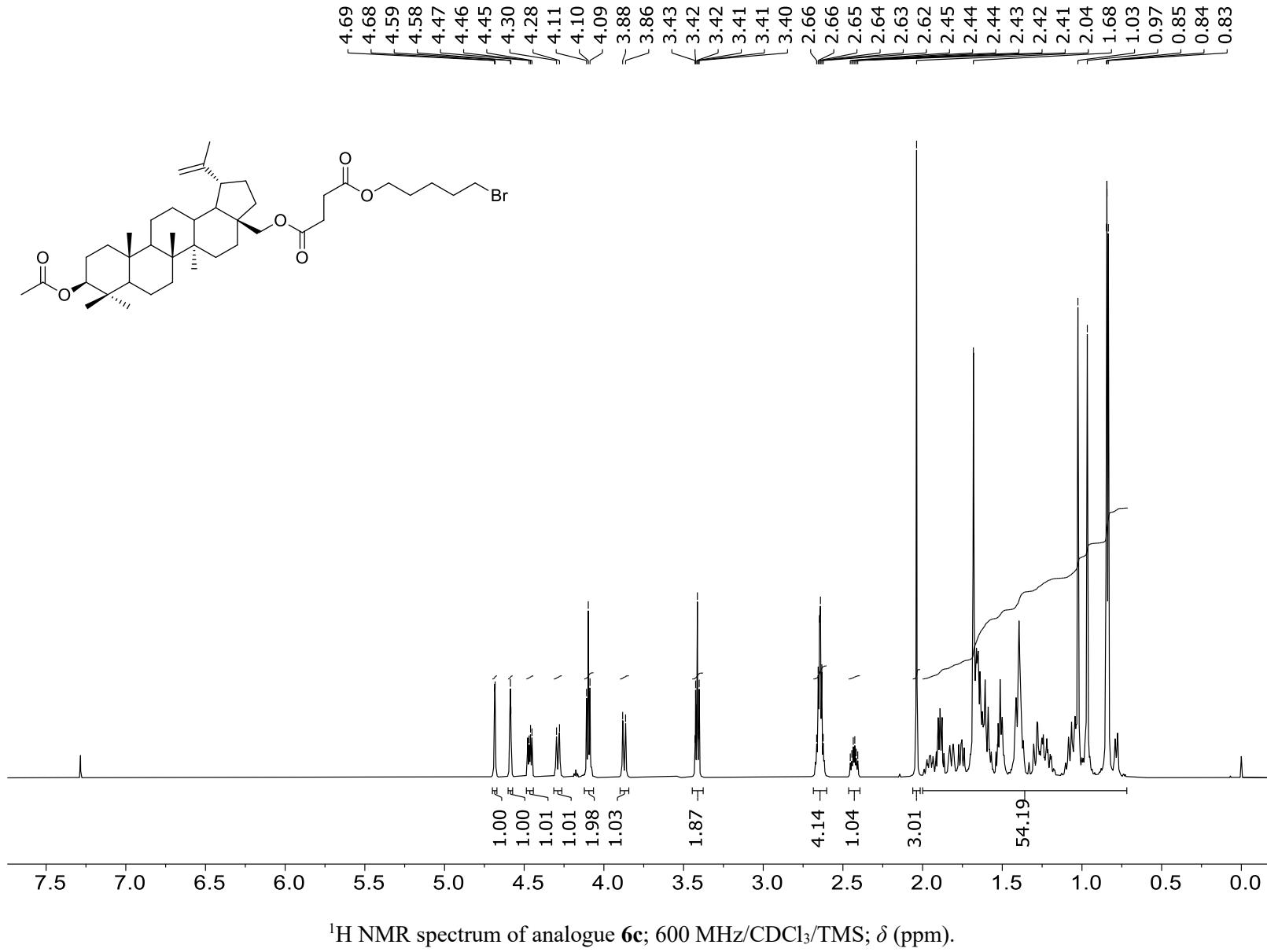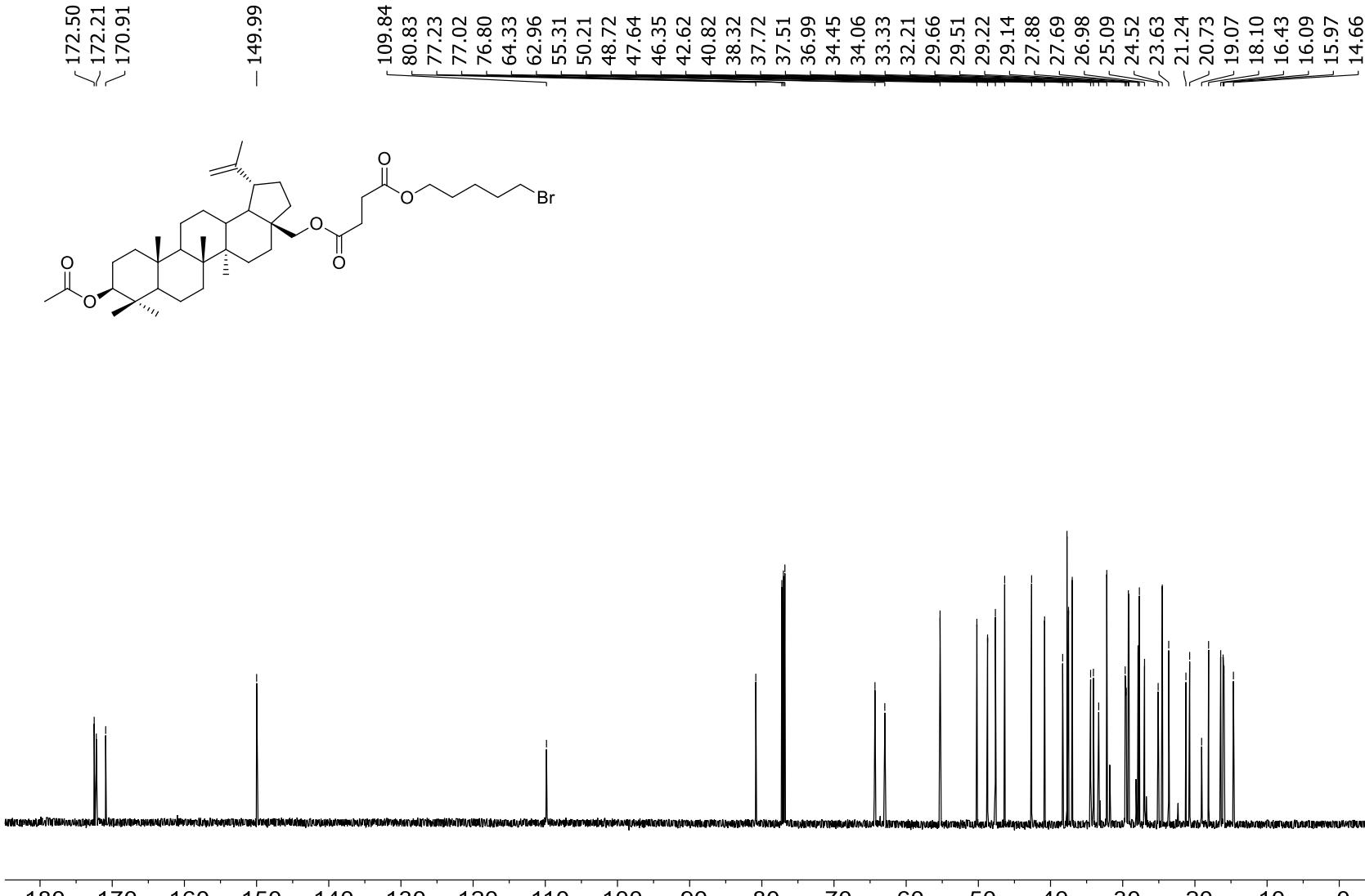
^{13}C NMR spectrum of analogue **6c**; 150 MHz/CDCl$_3$/TMS; δ (ppm).

^{1}H NMR spectrum of analogue **6d**; 400 MHz/CDCl$_3$/TMS; δ (ppm).

^{13}C NMR spectrum of analogue **6d**; 100 MHz/CDCl$_3$/TMS; δ (ppm).

Peak labels: 176.47, 171.59, 170.98, 150.05, 109.88, 80.90, 77.31, 77.00, 76.68, 62.87, 62.46, 55.36, 50.26, 48.78, 47.66, 46.29, 44.47, 42.67, 40.87, 40.59, 38.37, 37.78, 37.57, 37.04, 34.52, 34.10, 31.70, 29.72, 29.55, 29.46, 27.93, 26.98, 25.50, 25.45, 25.15, 23.68, 21.30, 20.77, 19.12, 18.14, 16.47, 16.14, 16.04, 14.70
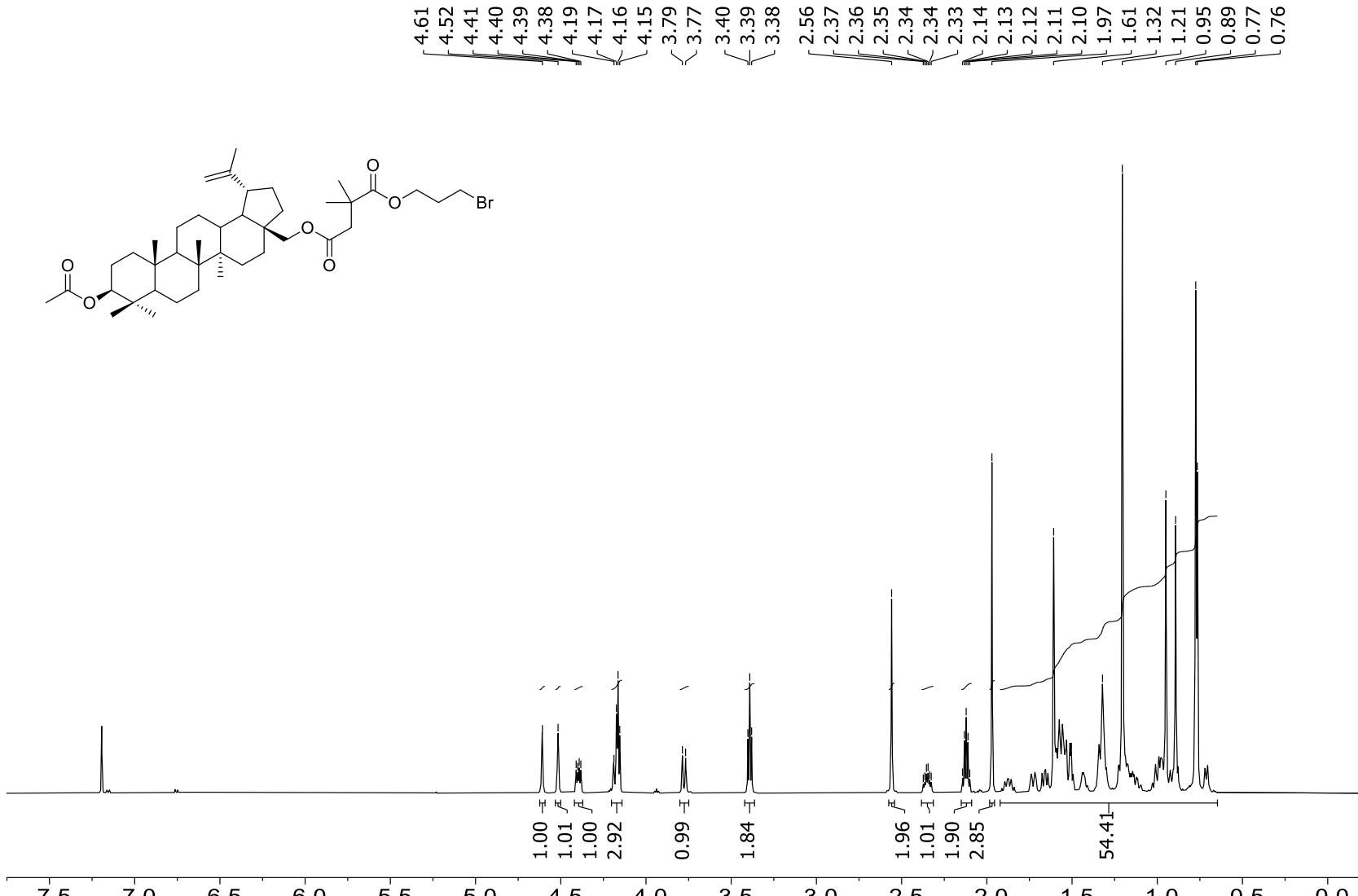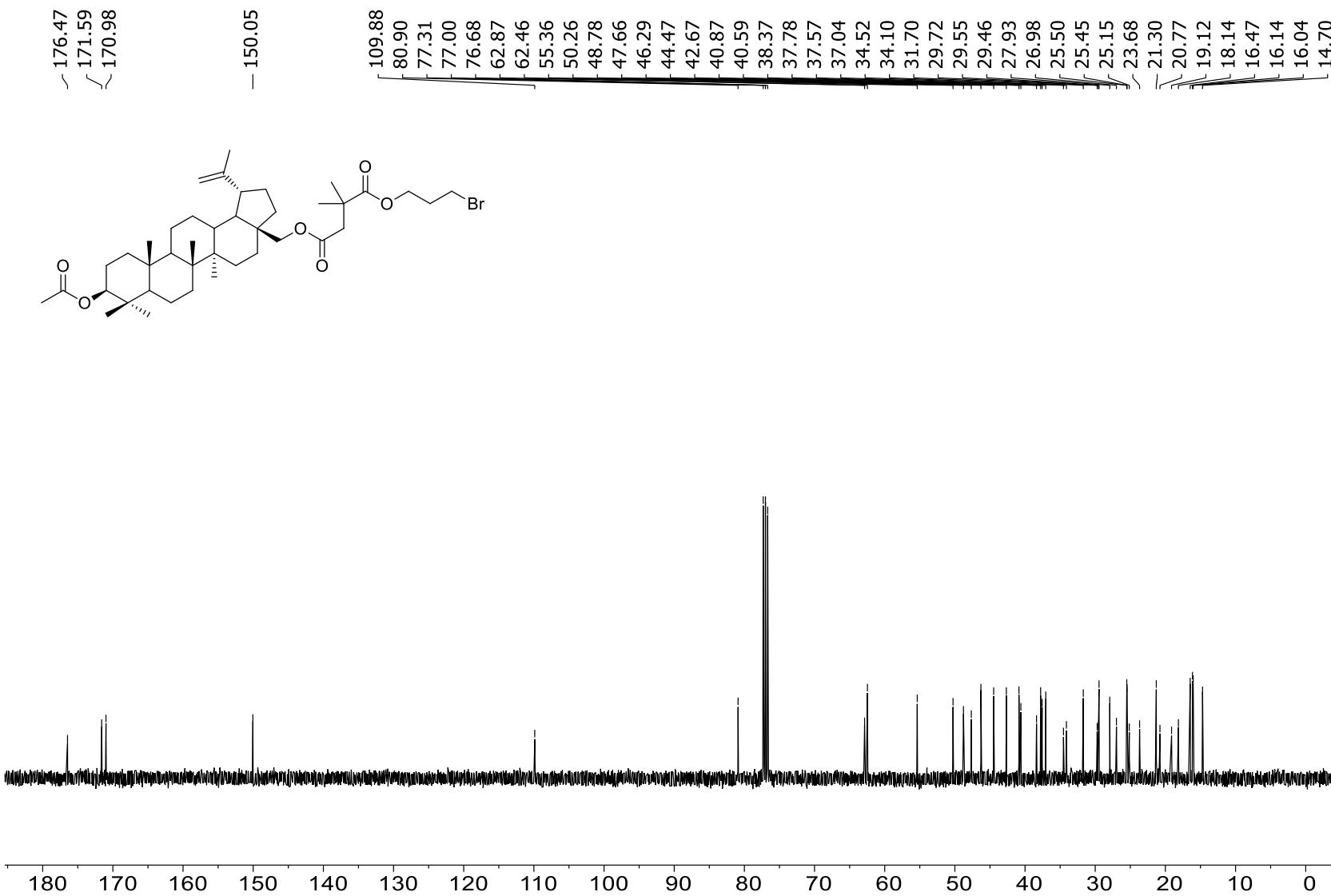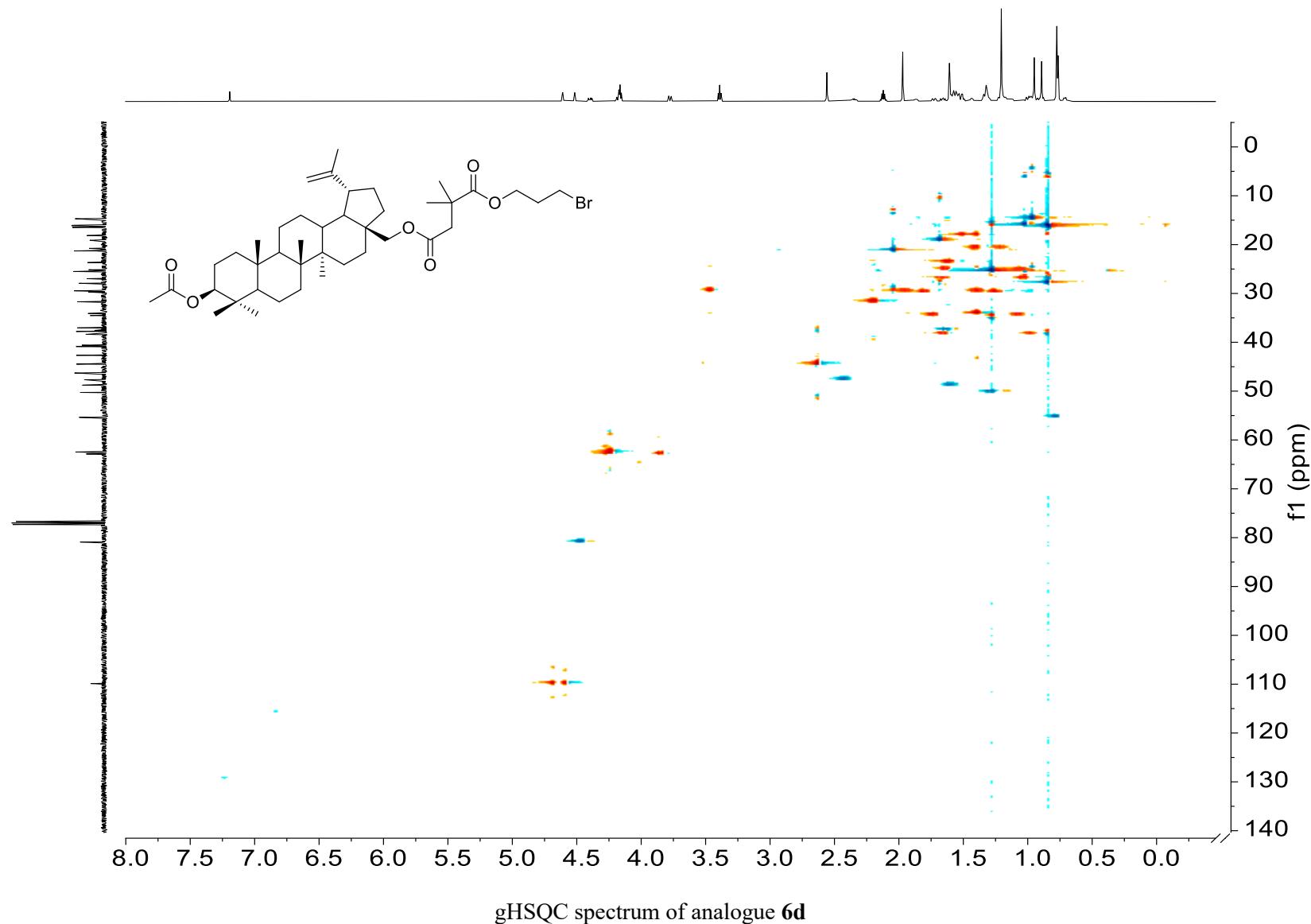
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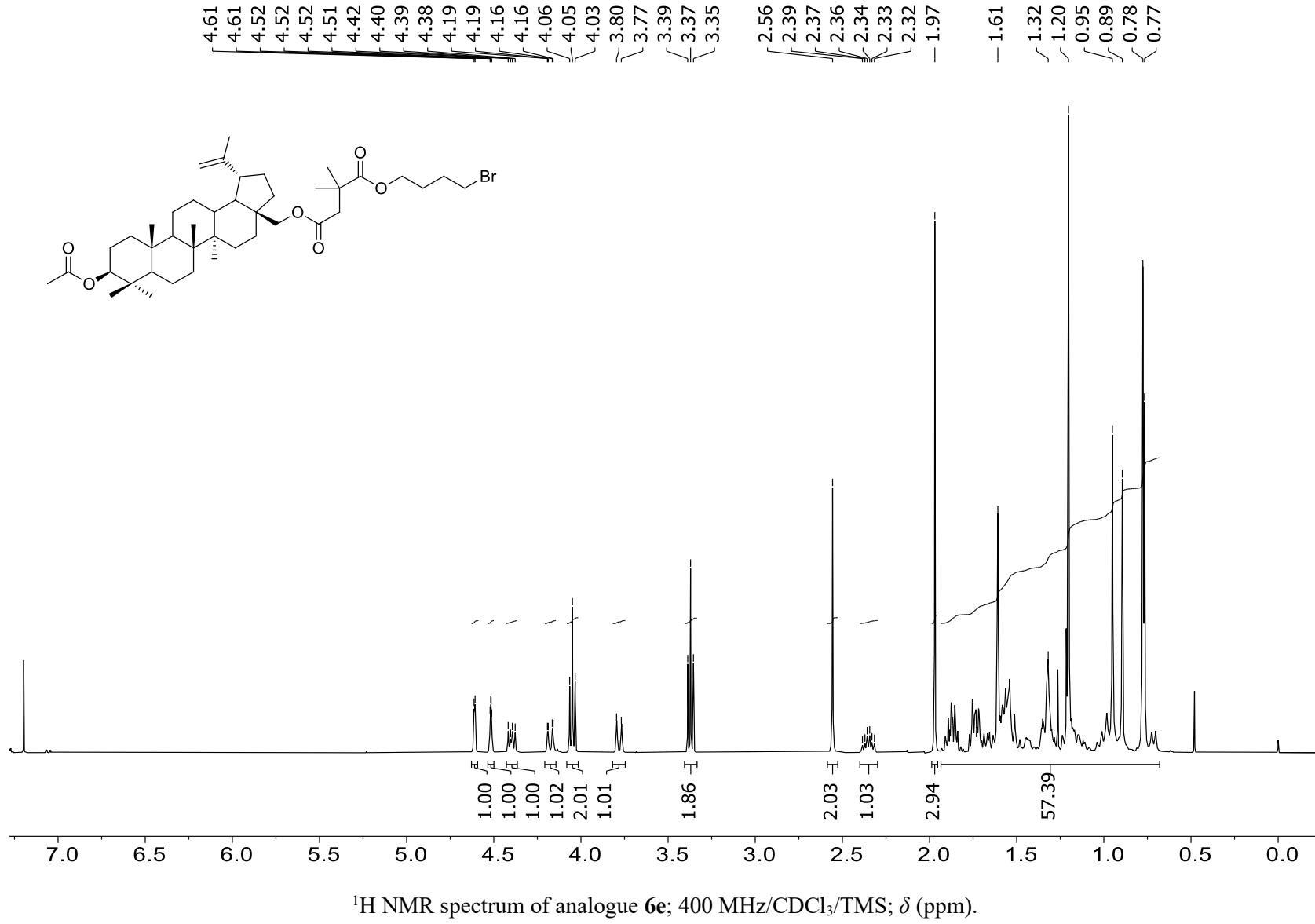
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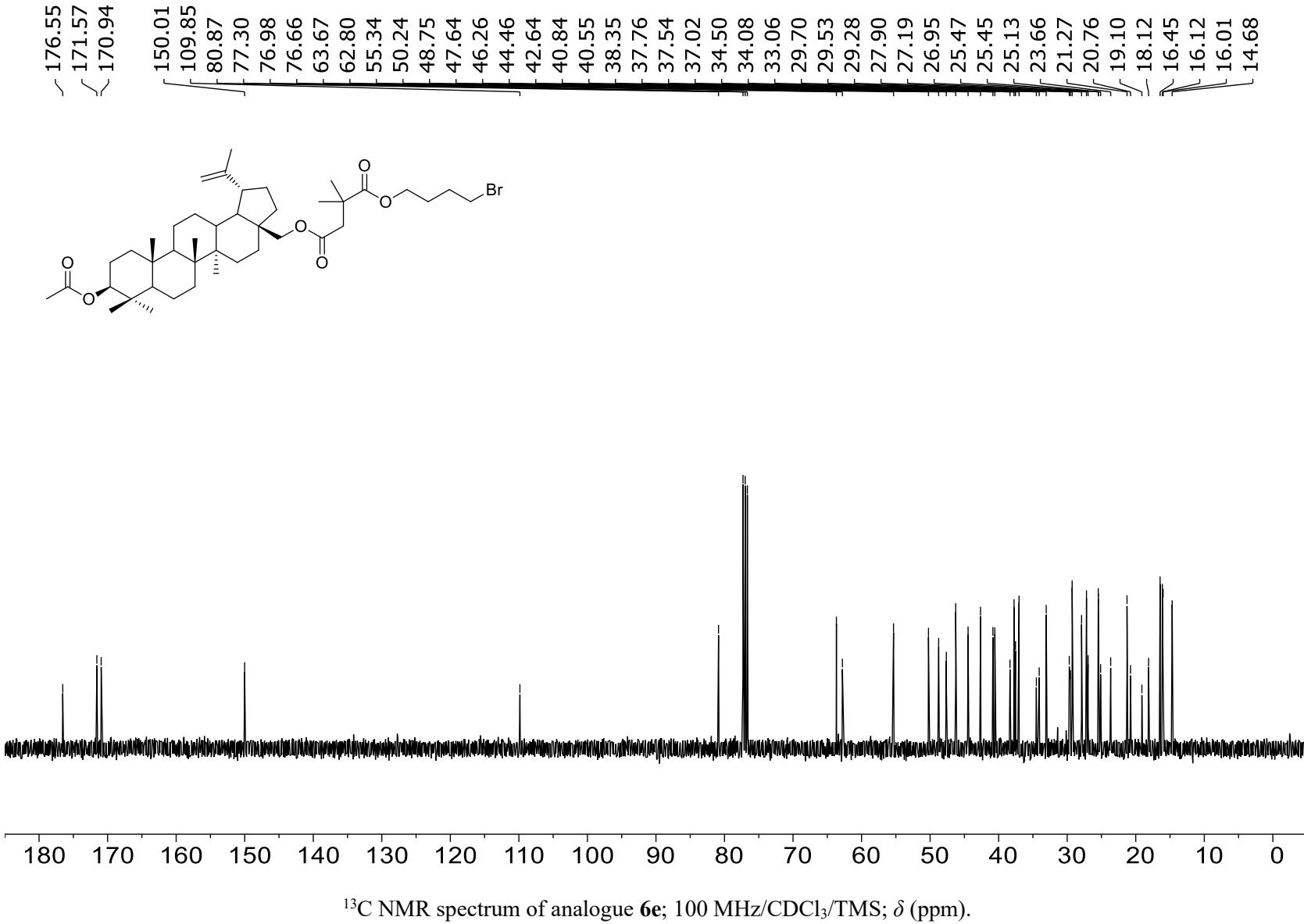
^{13}C NMR spectrum of analogue **6e**; 100 MHz/CDCl$_3$/TMS; δ (ppm).

^{1}H NMR spectrum of analogue **6f**; 600 MHz/CDCl$_3$/TMS; δ (ppm).
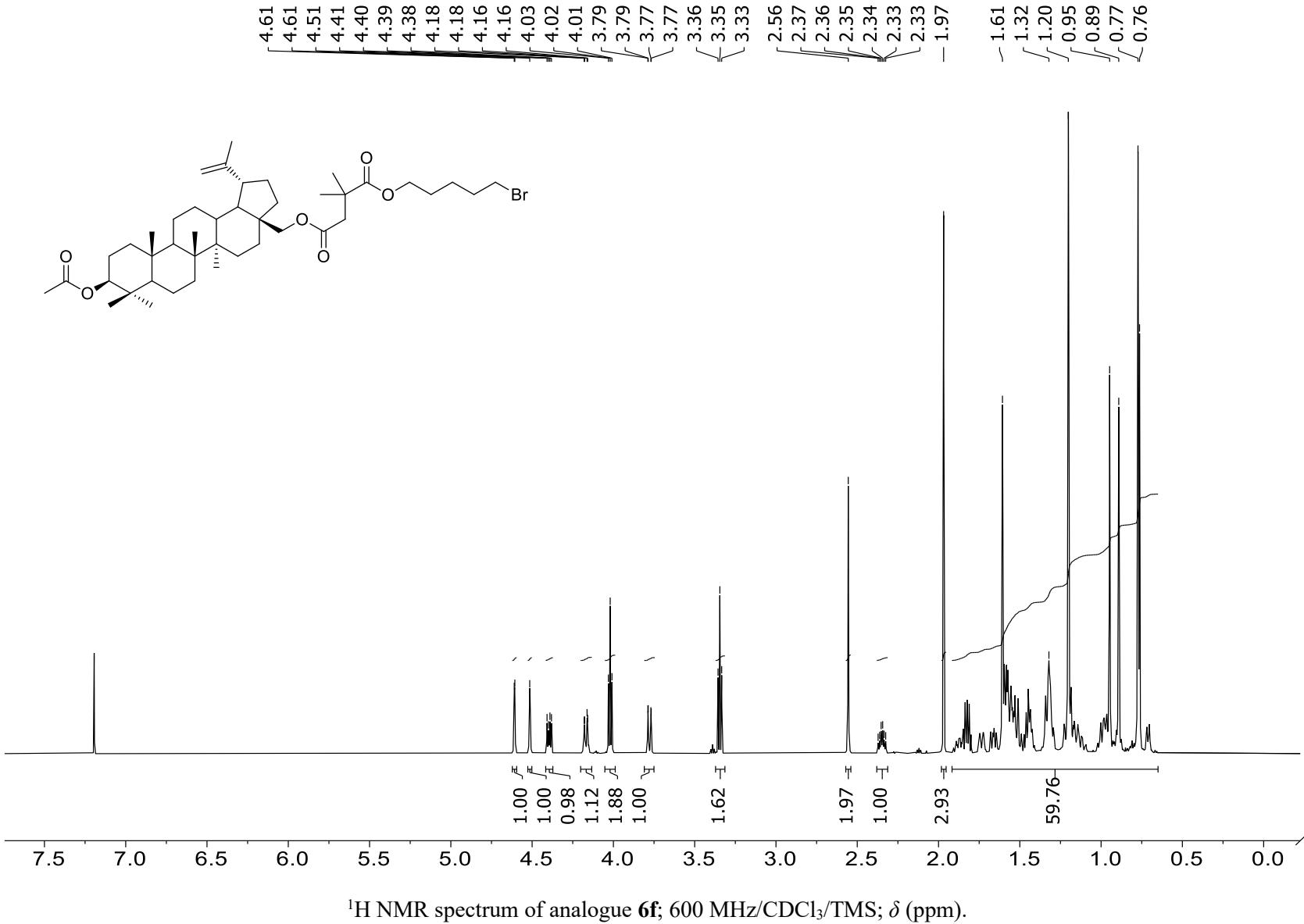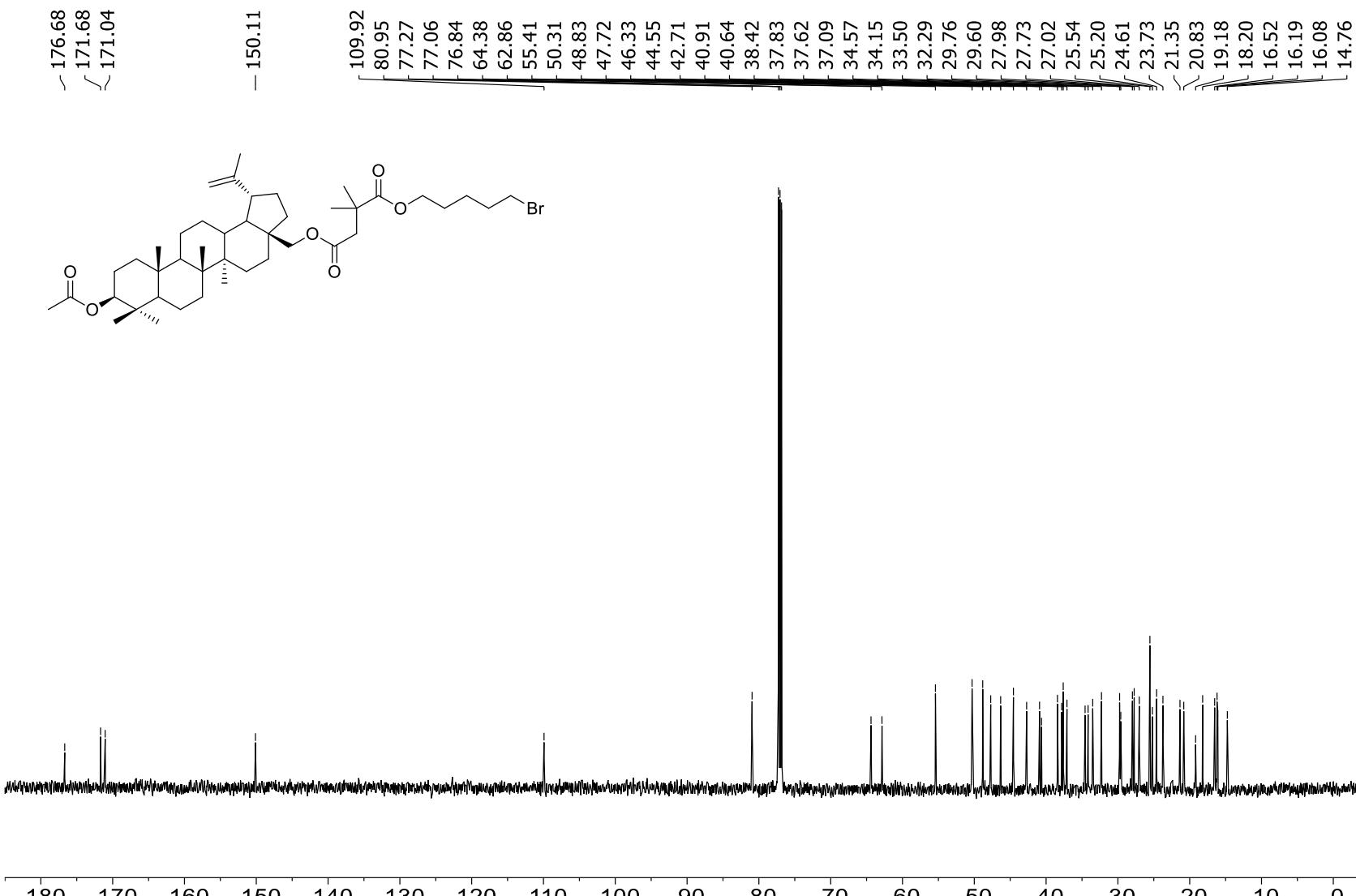
^{13}C NMR spectrum of analogue **6f**; 150 MHz/CDCl$_3$/TMS; δ (ppm).

^{1}H NMR spectrum of analogue **7a**; 600 MHz/CDCl$_3$/TMS; δ (ppm).
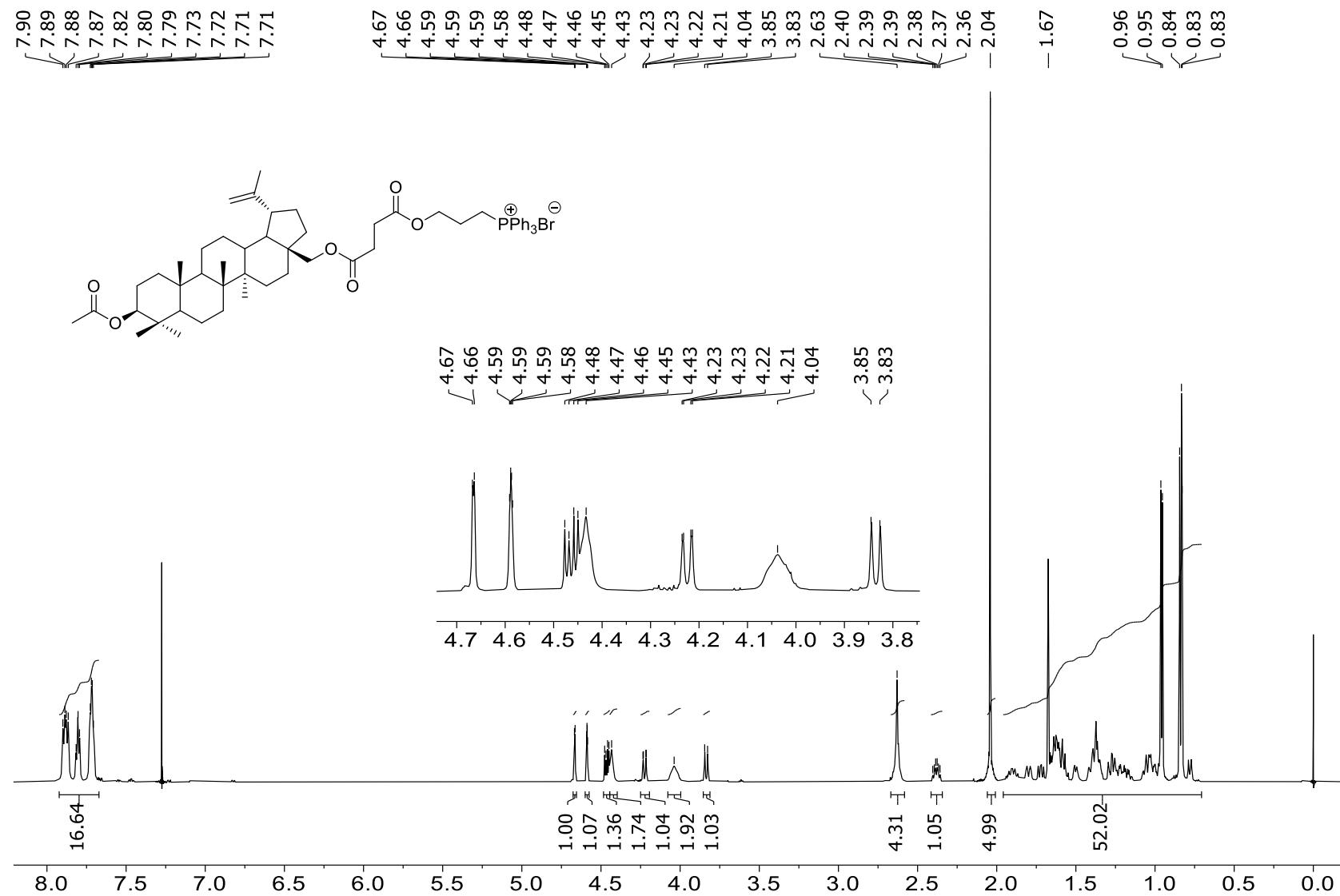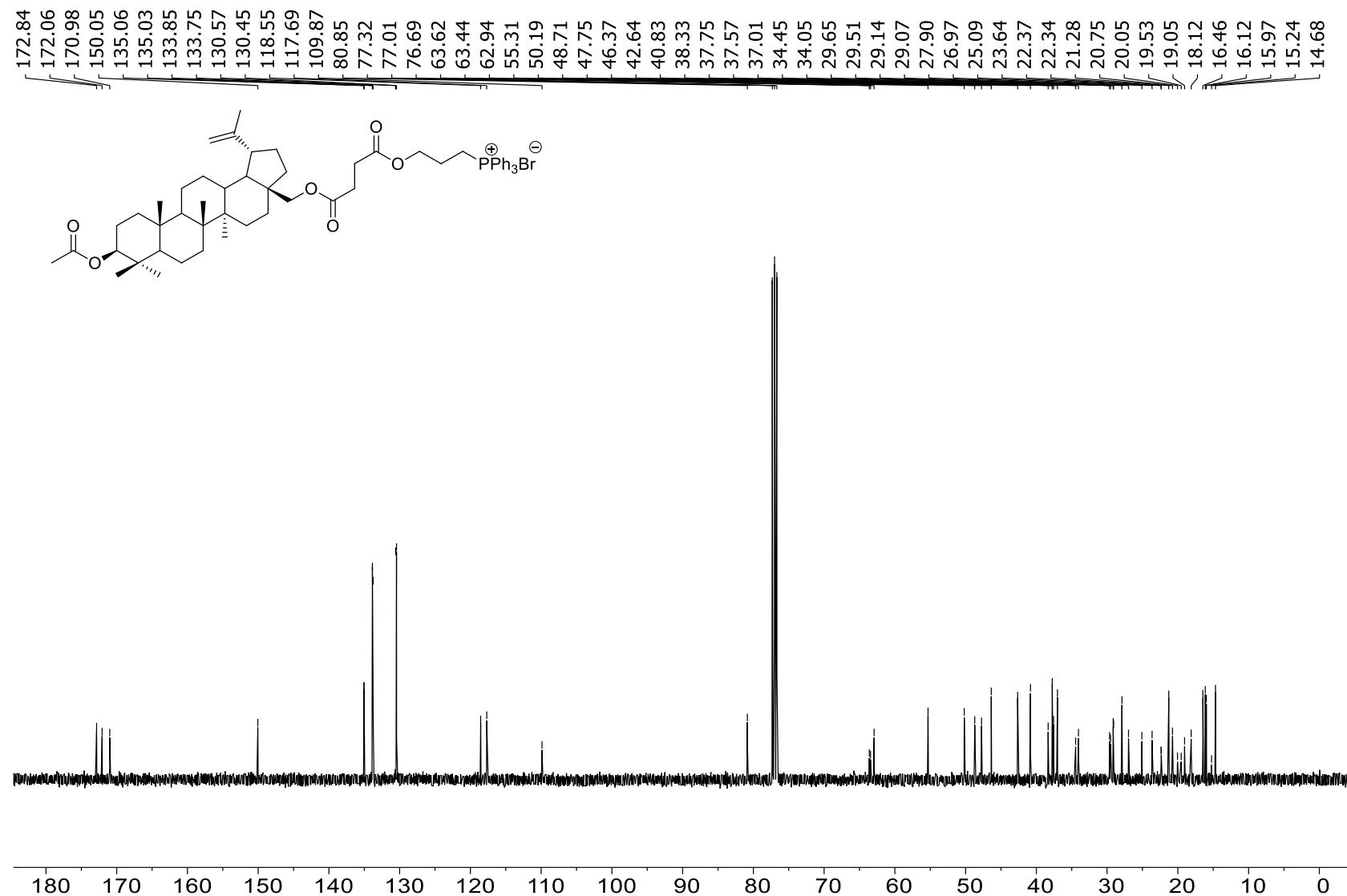
^{13}C NMR spectrum of analogue **7a**; 100 MHz/CDCl$_3$/TMS; δ (ppm).
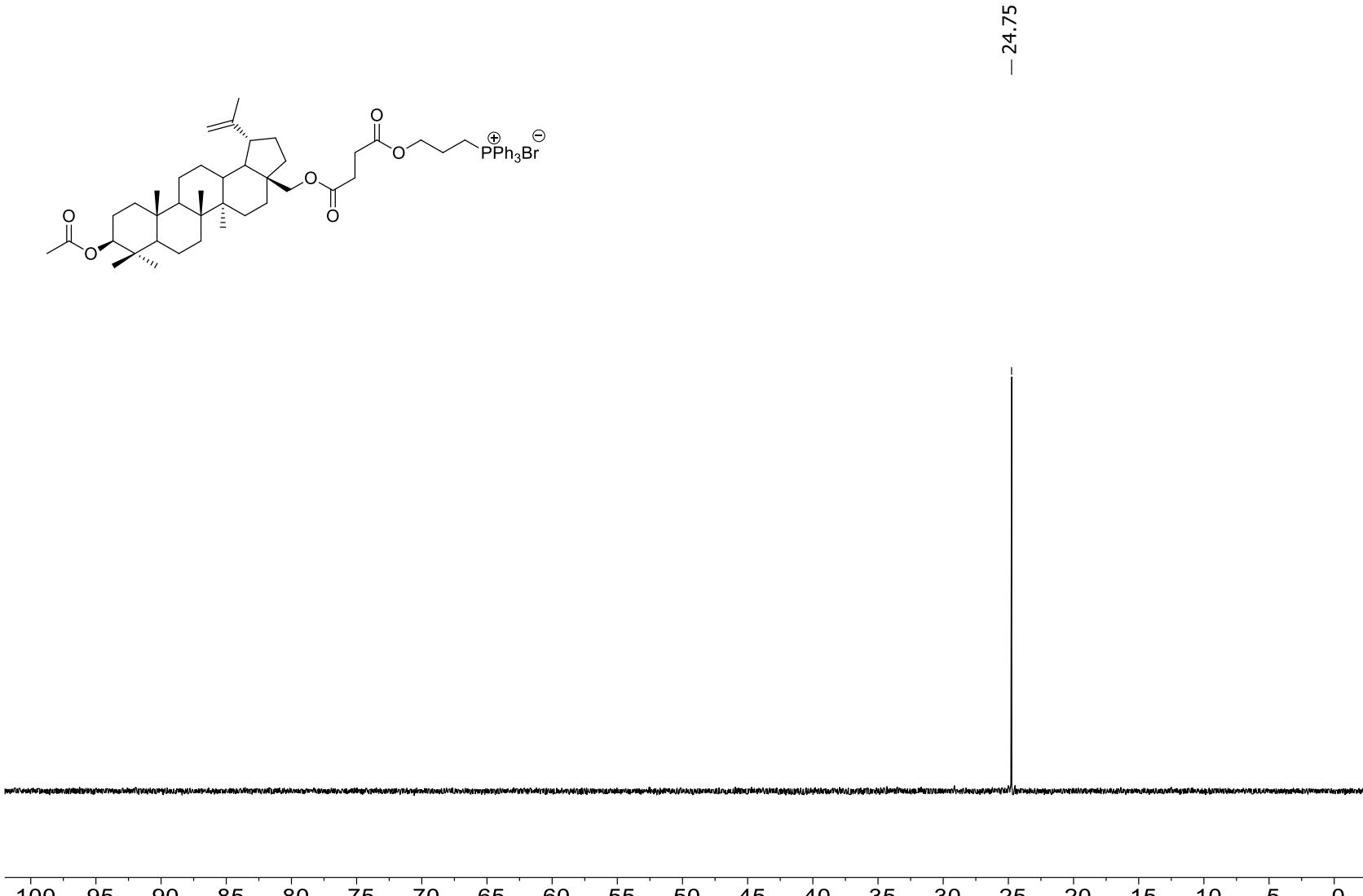
^{31}P NMR spectrum of analogue **7a**; 161.9 MHz/CDCl$_3$/TMS; δ (ppm).

— 24.75
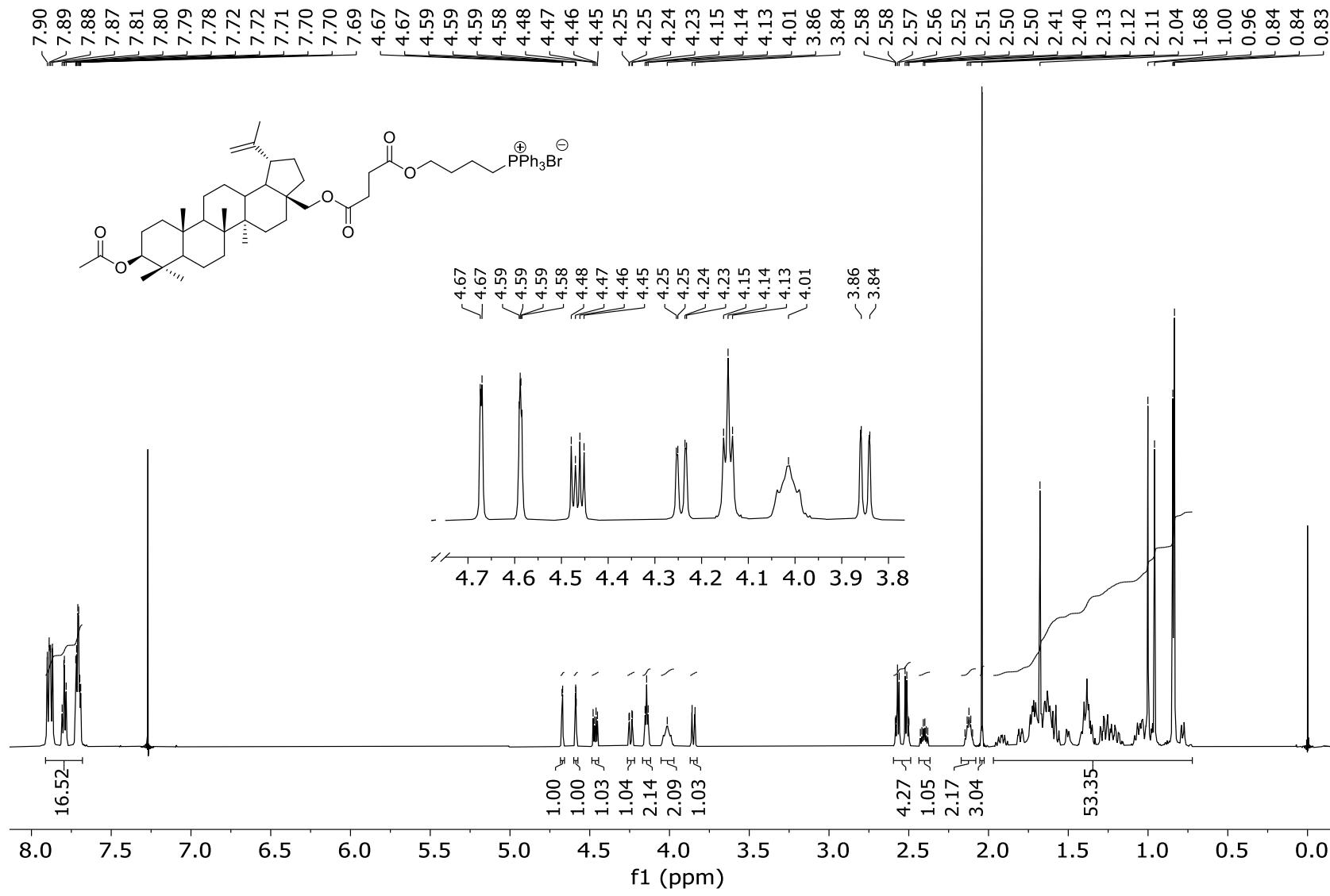
^{1}H NMR spectrum of analogue **7b**; 600 MHz/CDCl$_3$/TMS; δ (ppm).
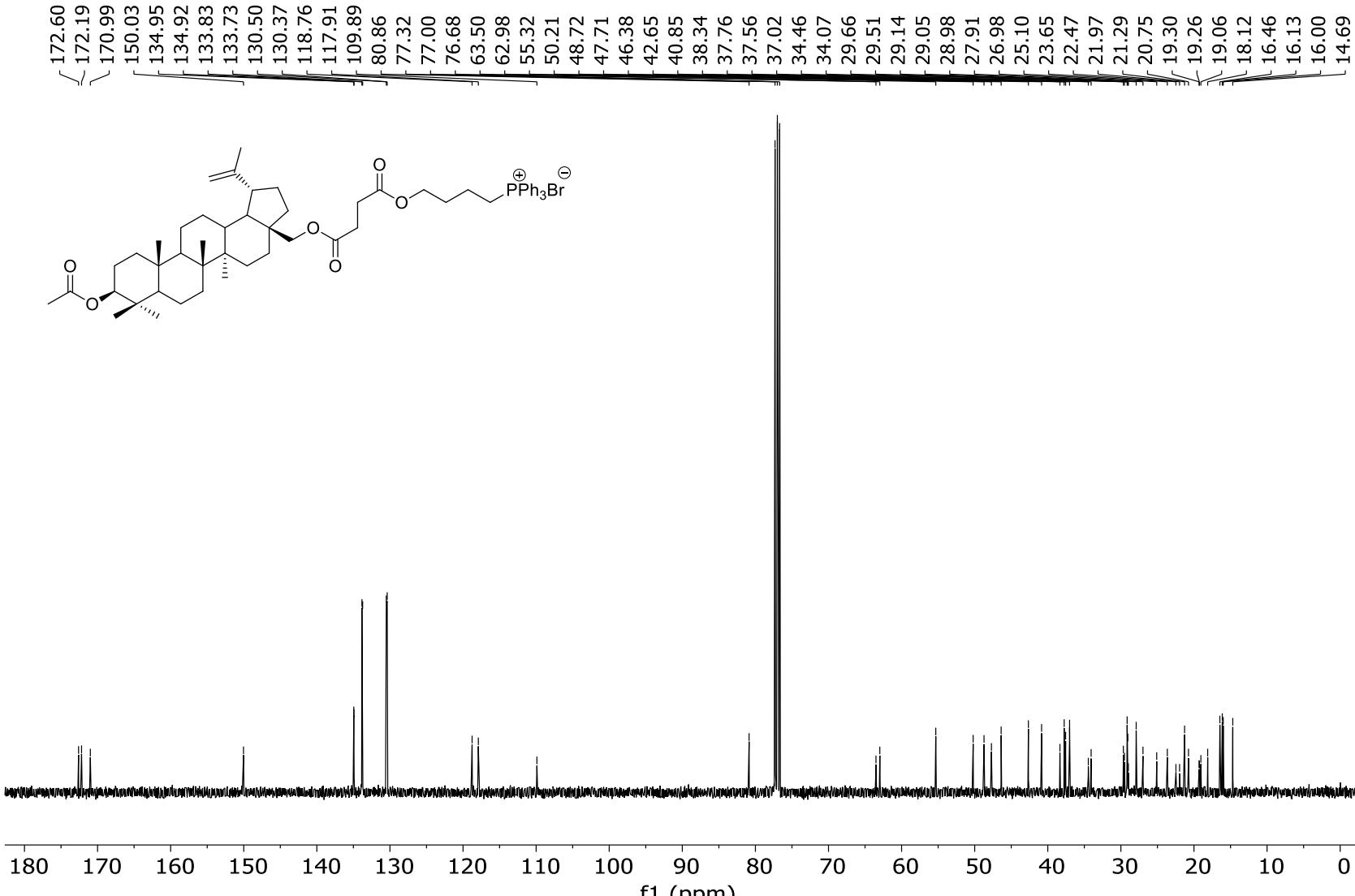
^{13}C NMR spectrum of analogue **7b**; 100 MHz/CDCl$_3$/TMS; δ (ppm).

— 24.61
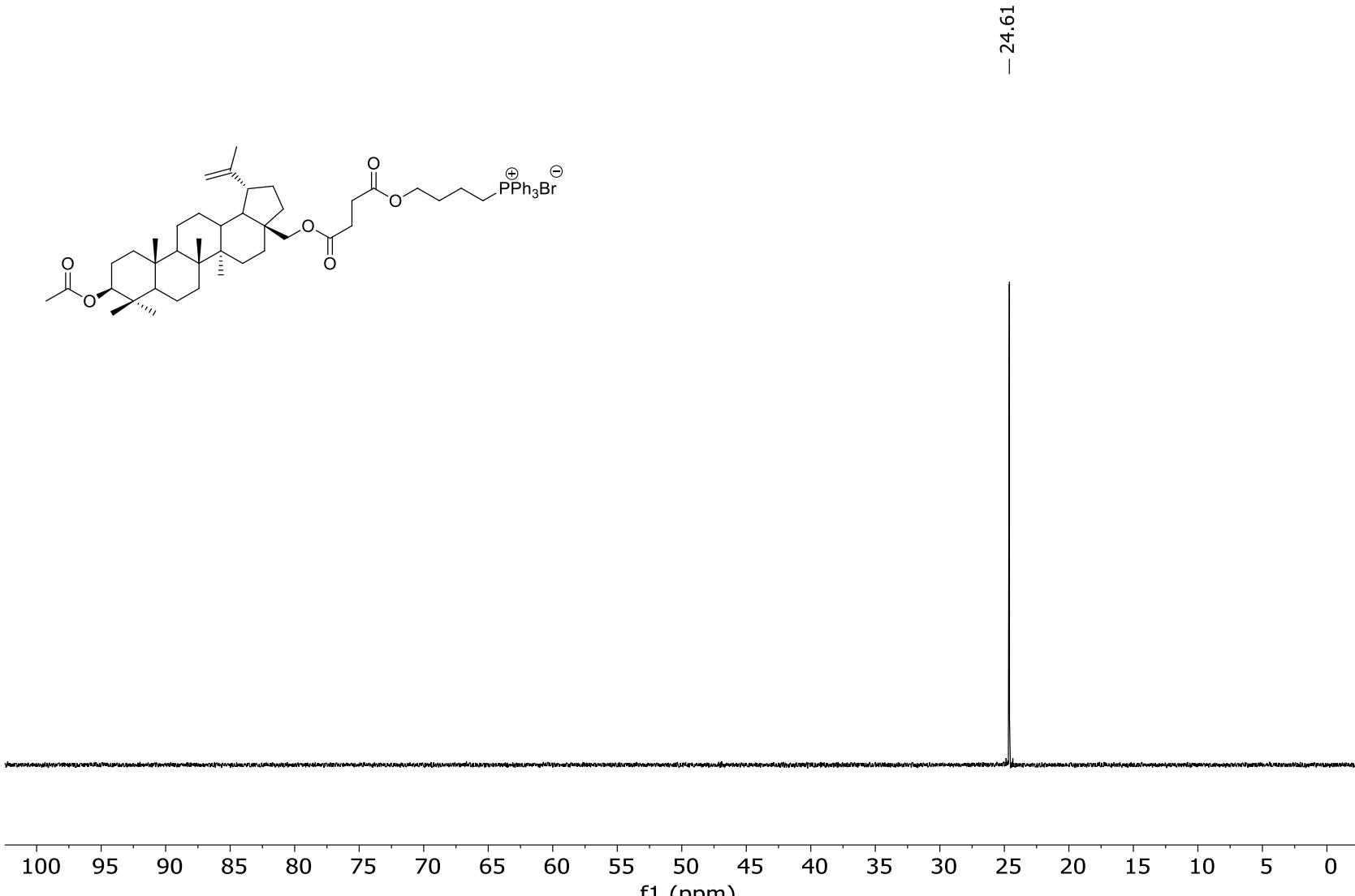
^{31}P NMR spectrum of analogue **7b**; 161.9 MHz/CDCl$_3$/TMS; δ (ppm).
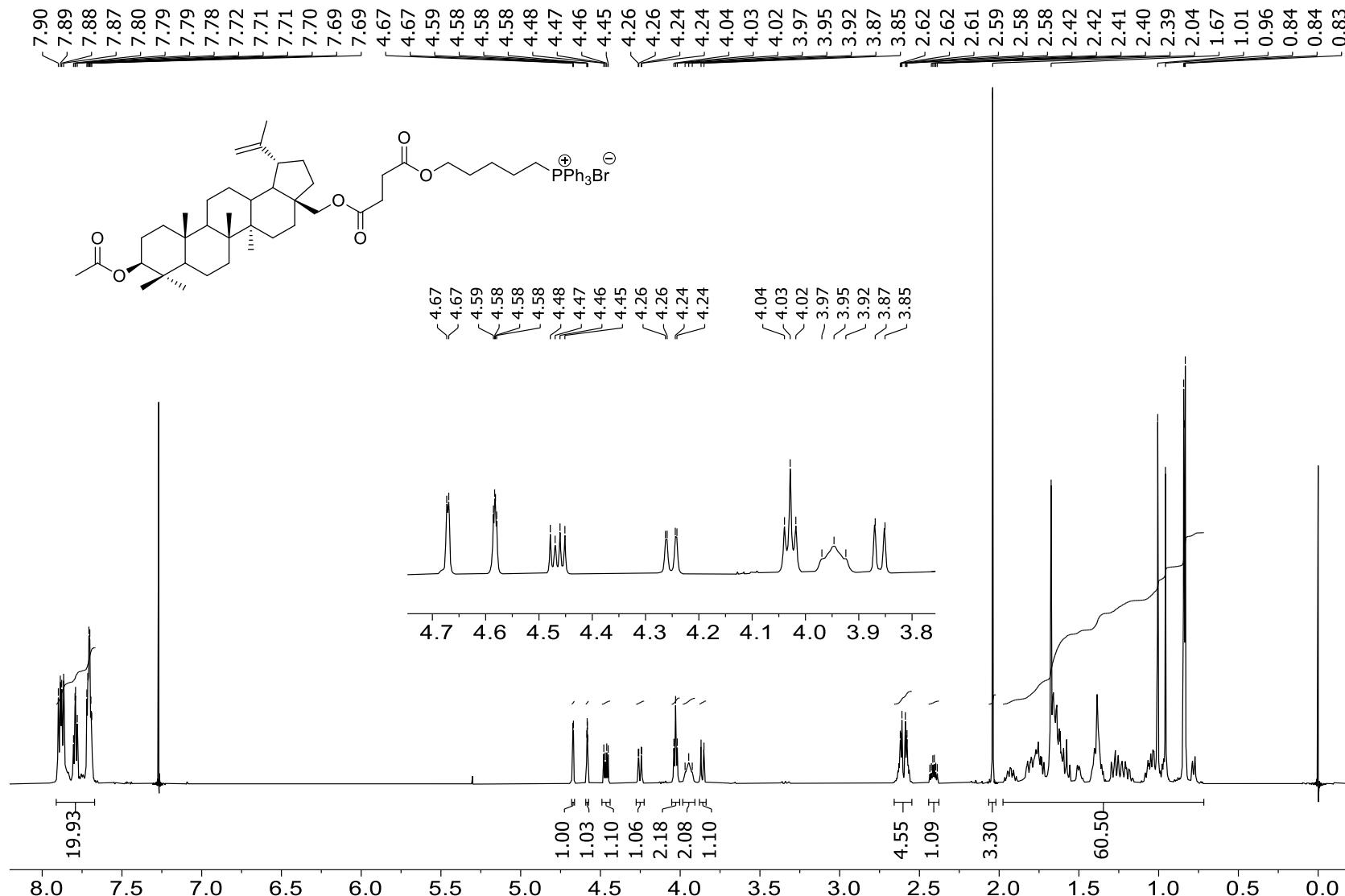
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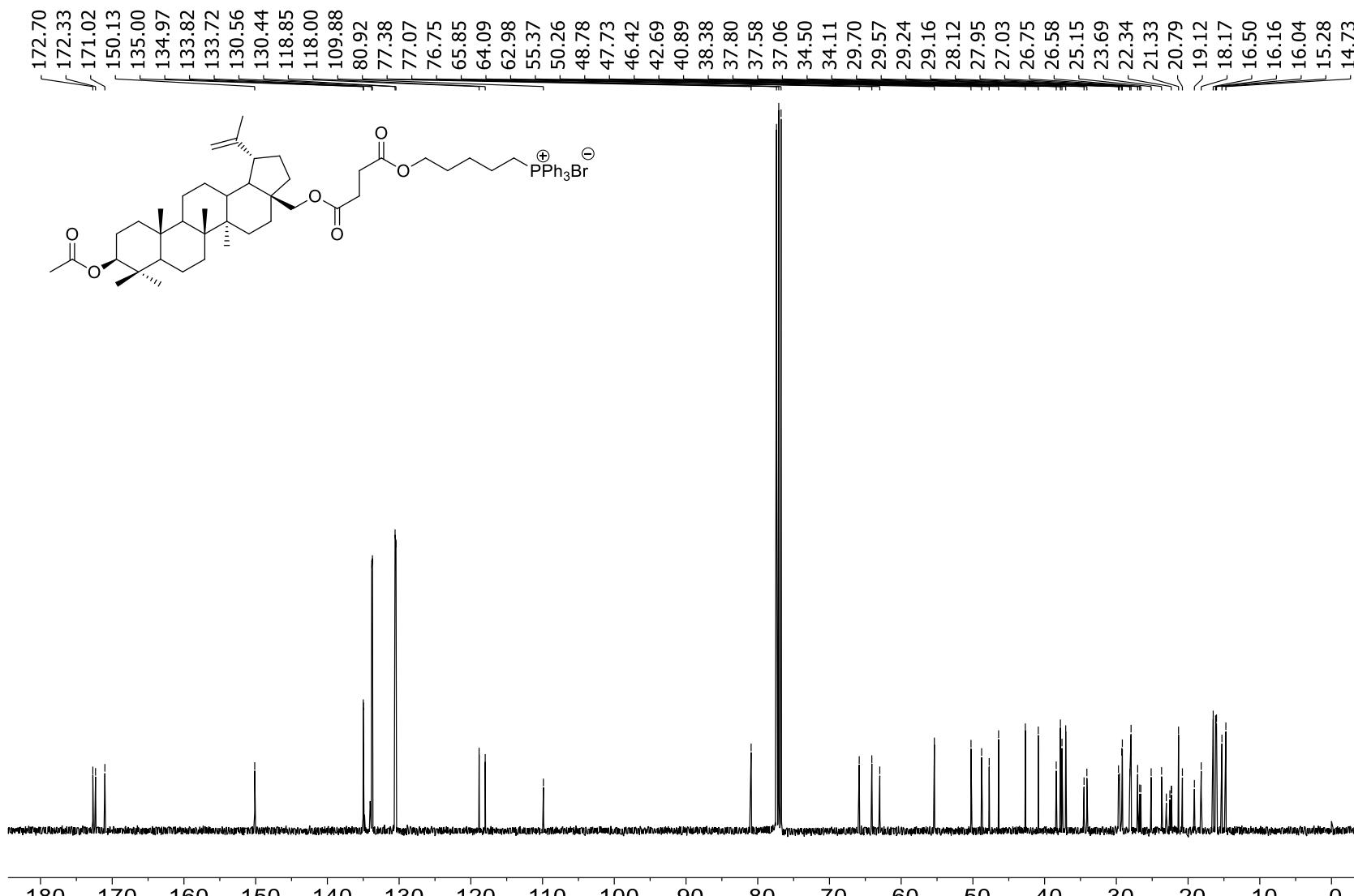
^{13}C NMR spectrum of analogue **7c**; 100 MHz/CDCl$_3$/TMS; δ (ppm).
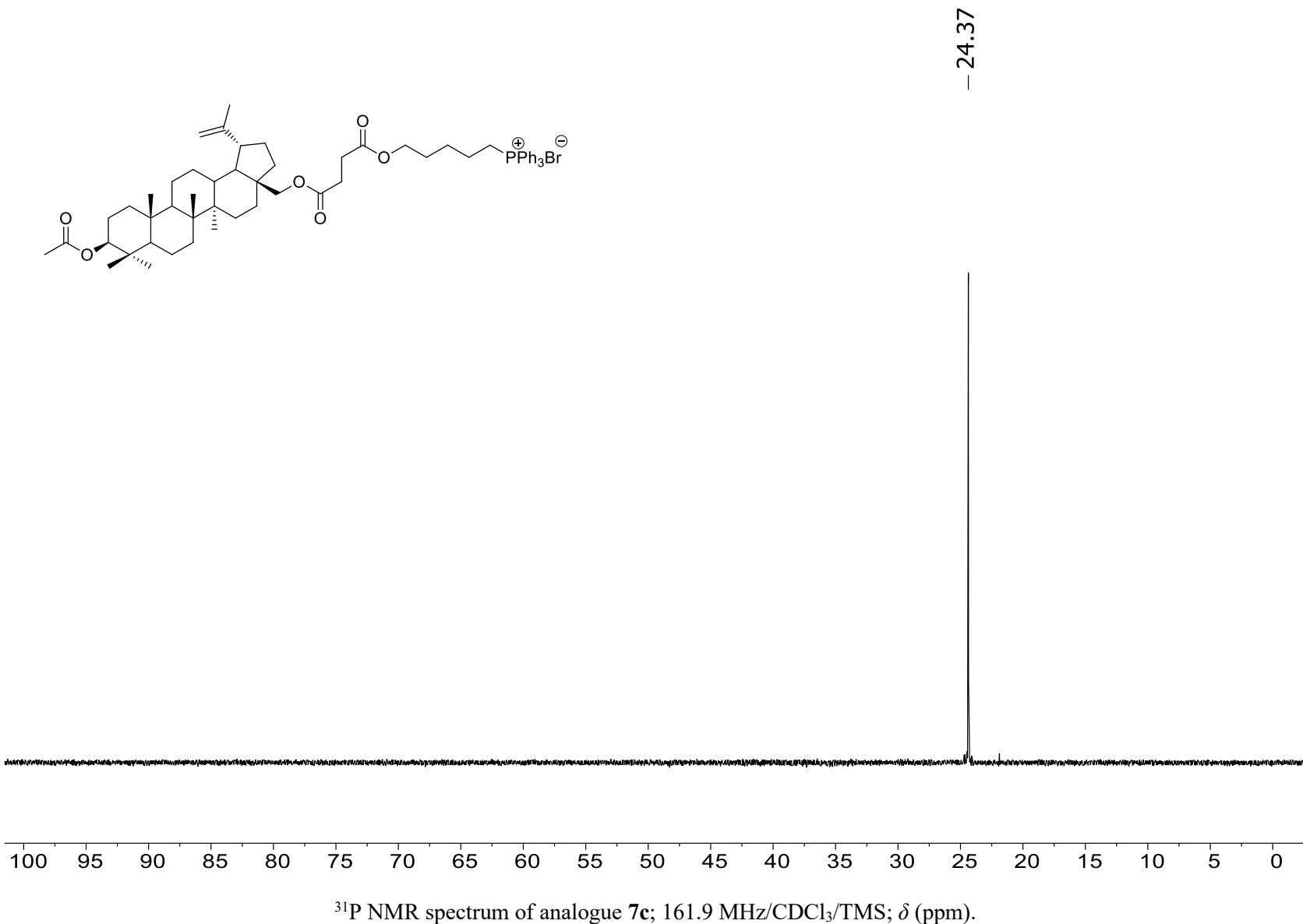
^{31}P NMR spectrum of analogue **7c**; 161.9 MHz/CDCl$_3$/TMS; δ (ppm).

— 24.37
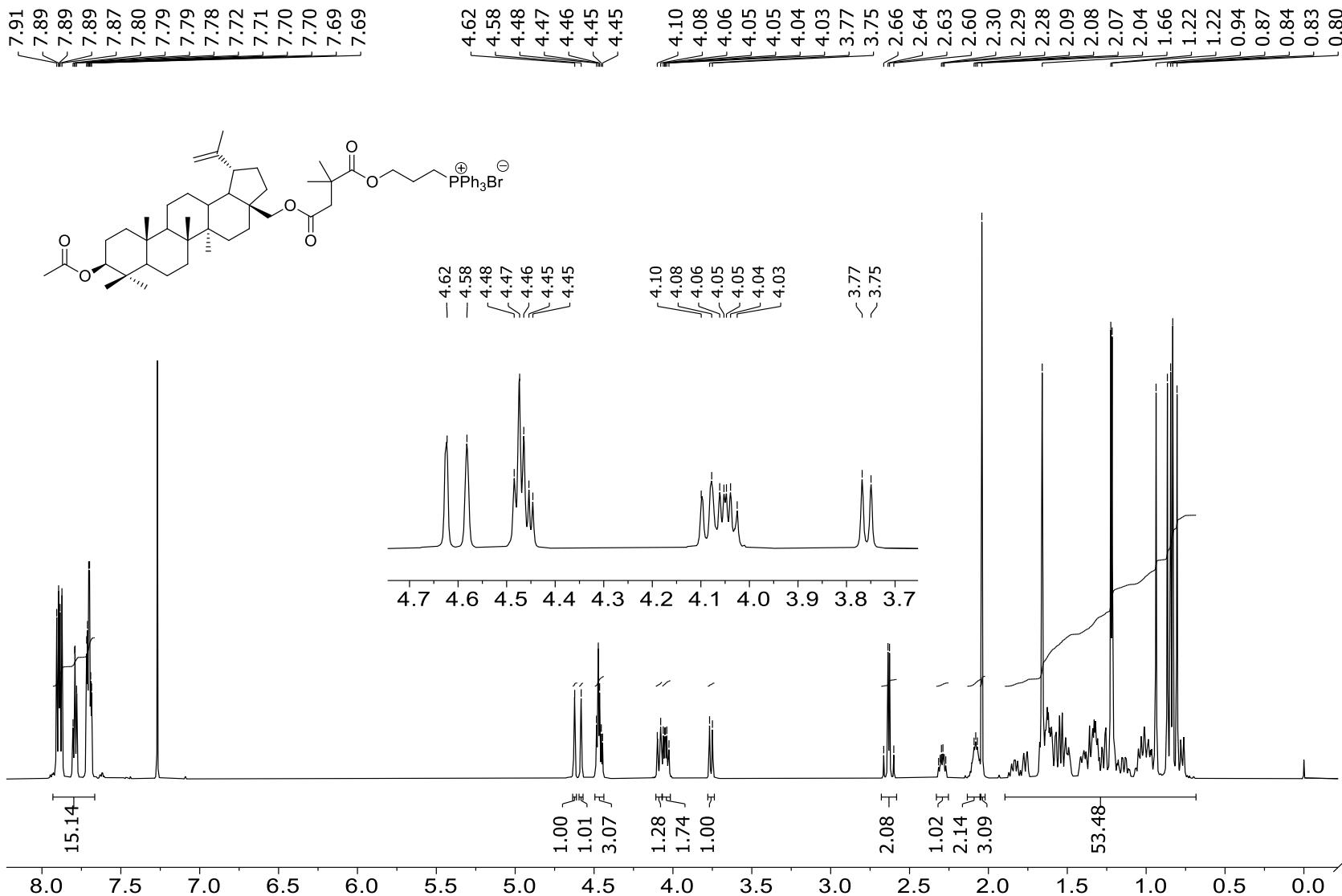
^{1}H NMR spectrum of analogue **7d**; 600 MHz/CDCl$_3$/TMS; δ (ppm).
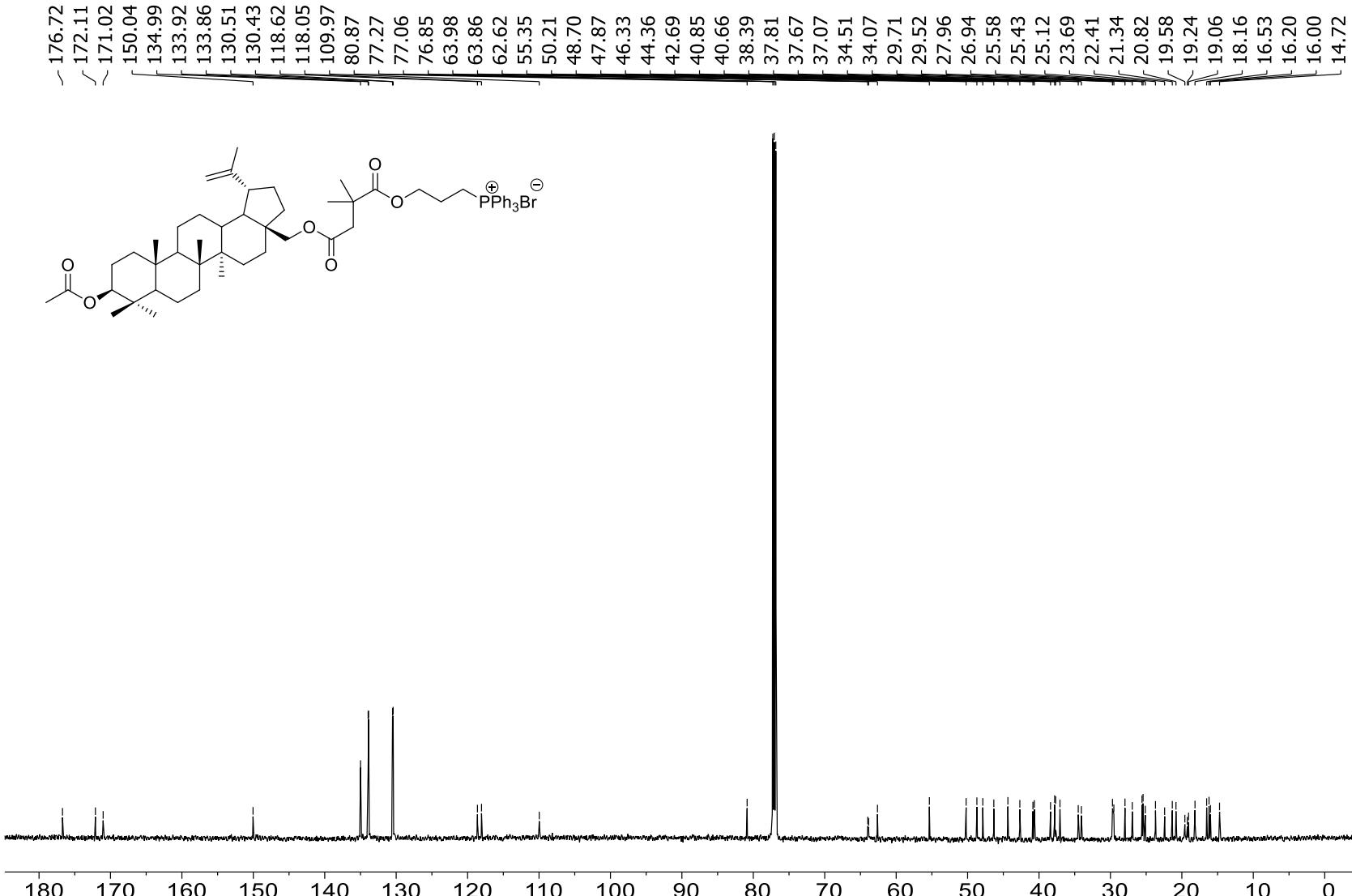
^{13}C NMR spectrum of analogue **7d**; 150 MHz/CDCl$_3$/TMS; δ (ppm).

176.72
172.11
171.02
150.04
134.99
133.92
133.86
130.51
130.43
118.62
118.05
109.97
80.87
77.27
77.06
76.85
63.98
63.86
62.62
55.35
50.21
48.70
47.87
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14.72
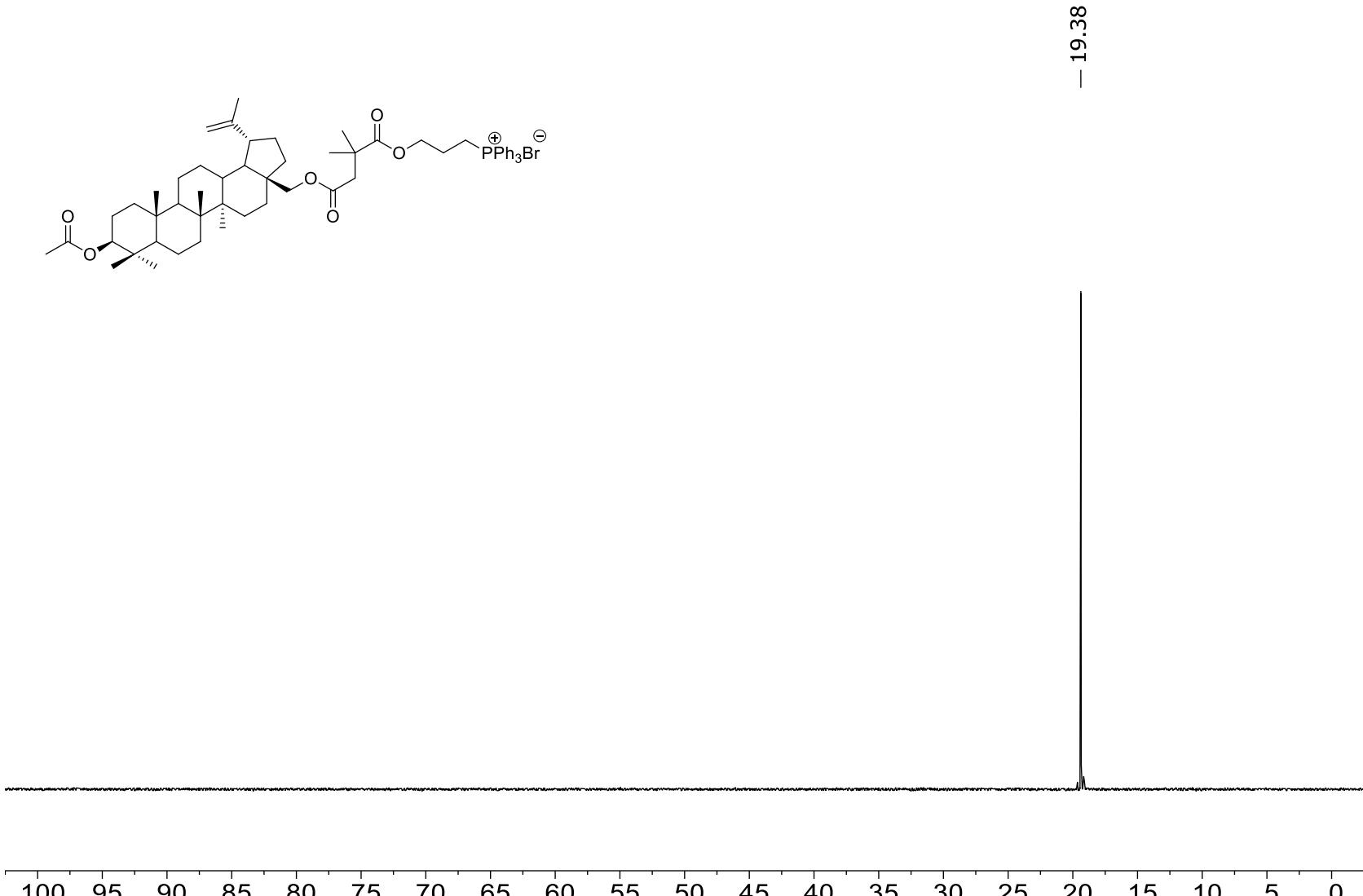
^{31}P NMR spectrum of analogue **7d**; 161.9 MHz/CDCl$_3$/TMS; δ (ppm).

— 19.38

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
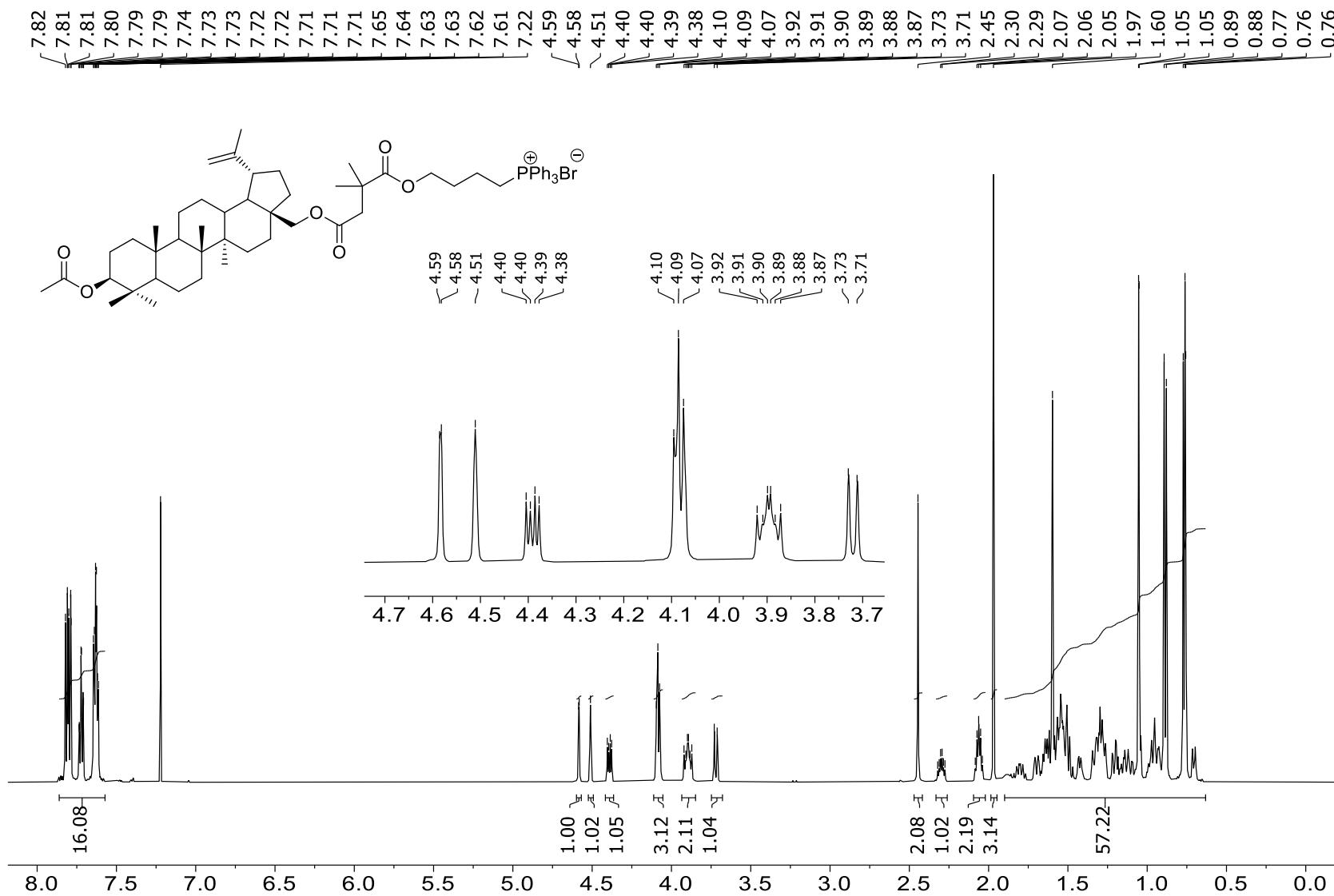
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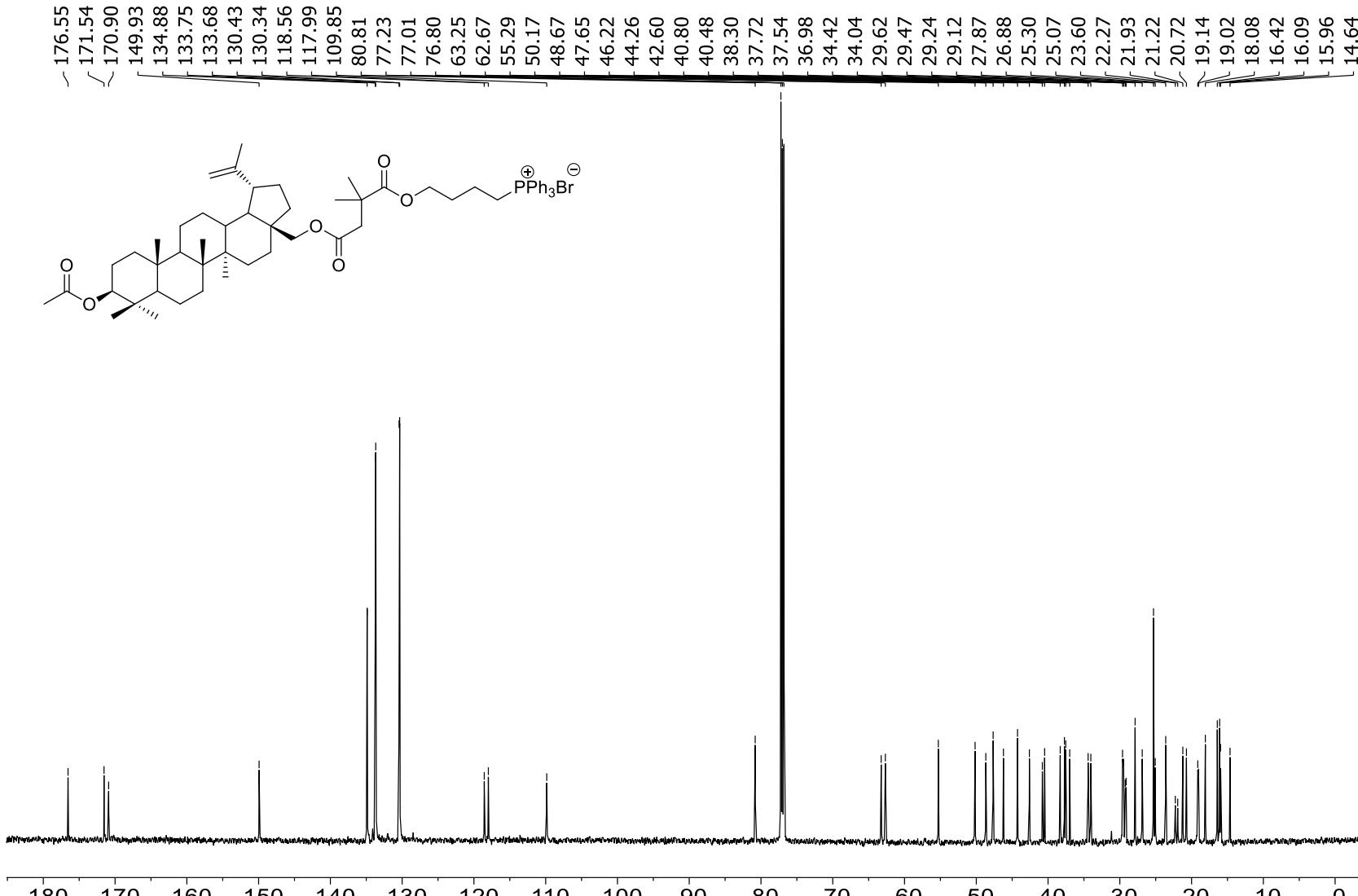
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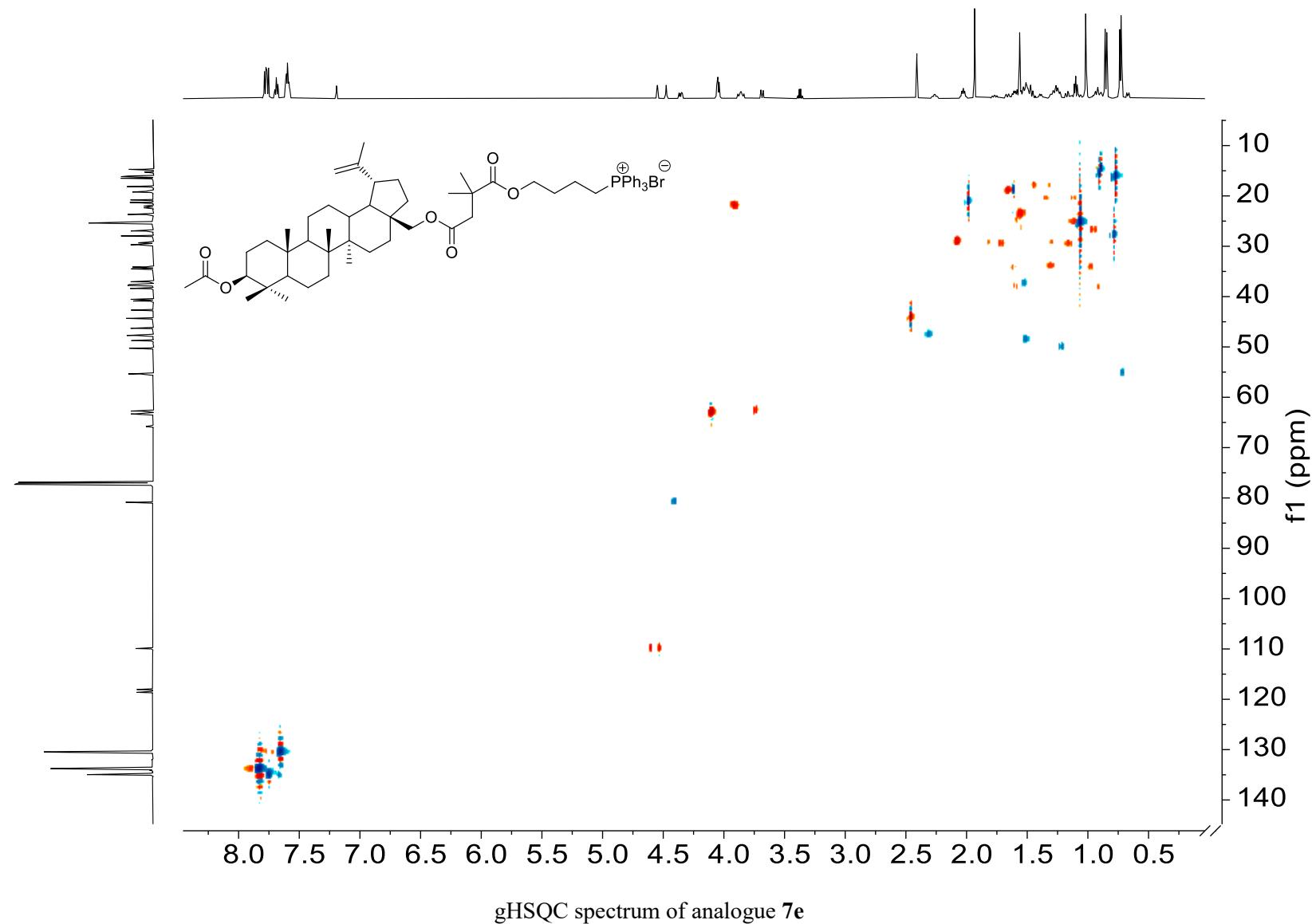
gHSQC spectrum of analogue **7e**
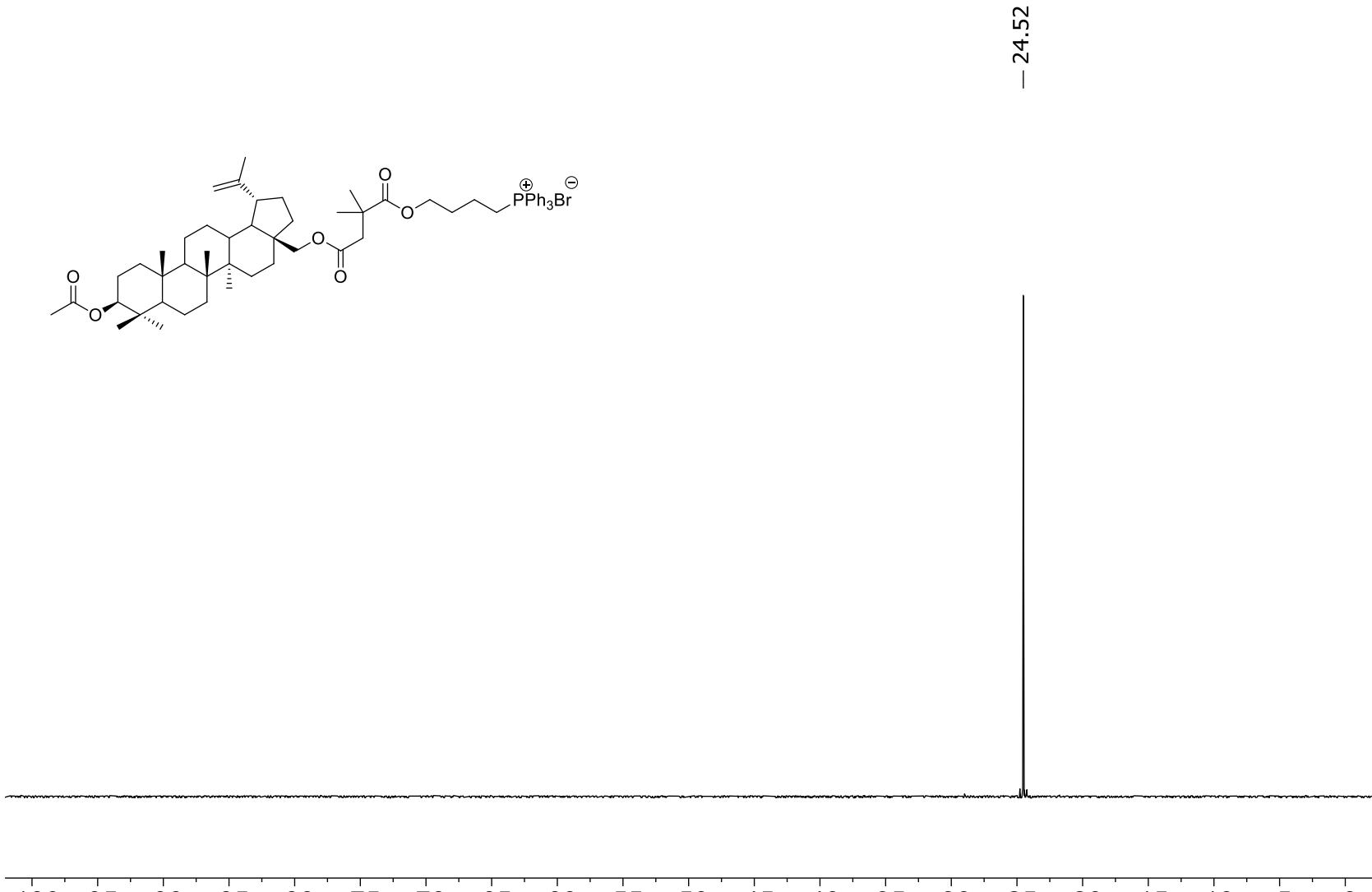
^{31}P NMR spectrum of analogue **7e**; 161.9 MHz/CDCl$_3$/TMS; δ (ppm).

— 24.52

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

^{1}H NMR spectrum of analogue **7f**; 400 MHz/CDCl$_3$/TMS; δ (ppm).

176.61
171.69
170.95
150.06
134.94
134.91
133.76
133.67
130.50
130.37
118.82
117.97
109.83
80.85
63.94
62.71
55.32
50.21
48.72
47.66
46.24
44.37
42.63
40.82
40.53
38.34
37.75
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27.90
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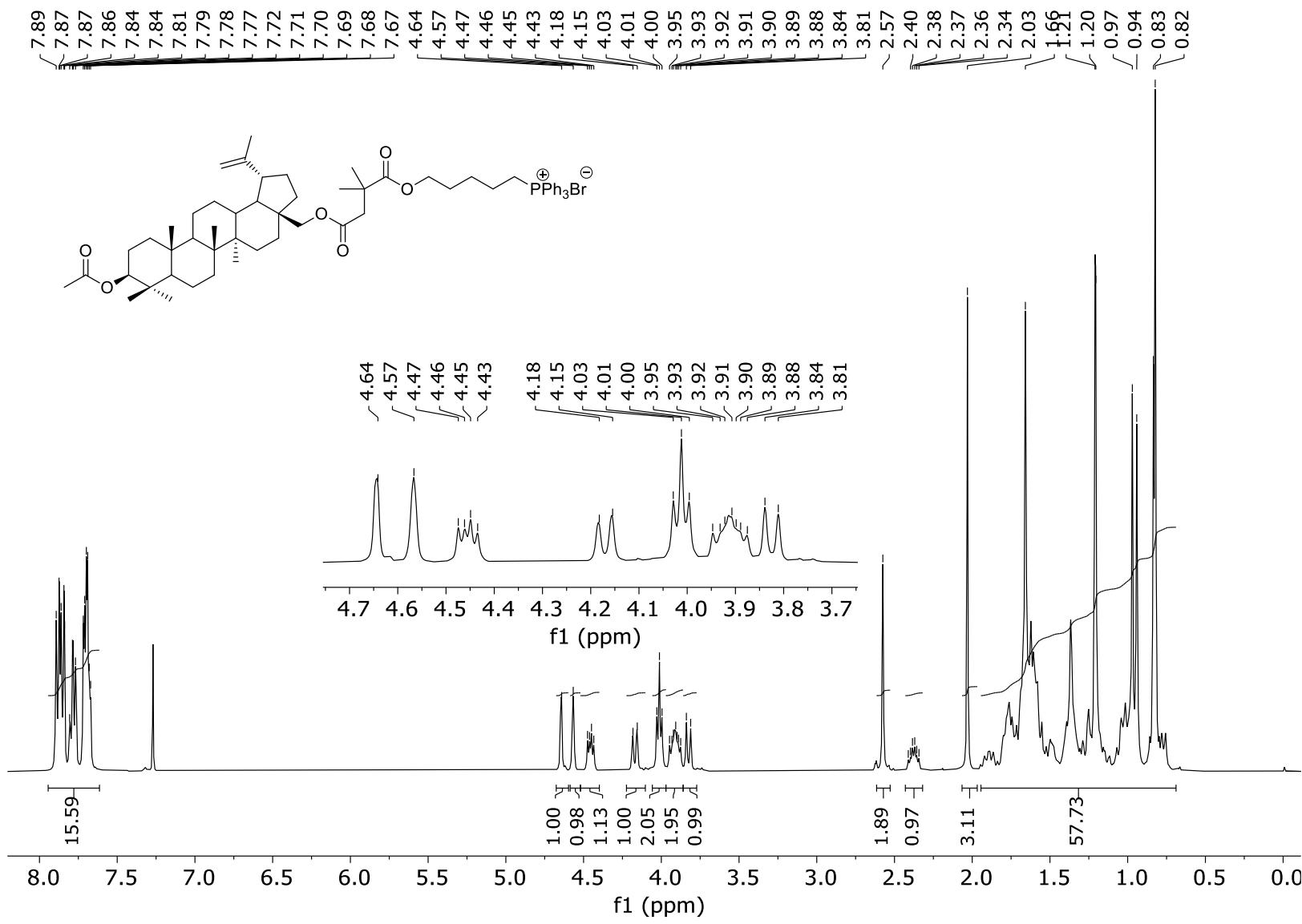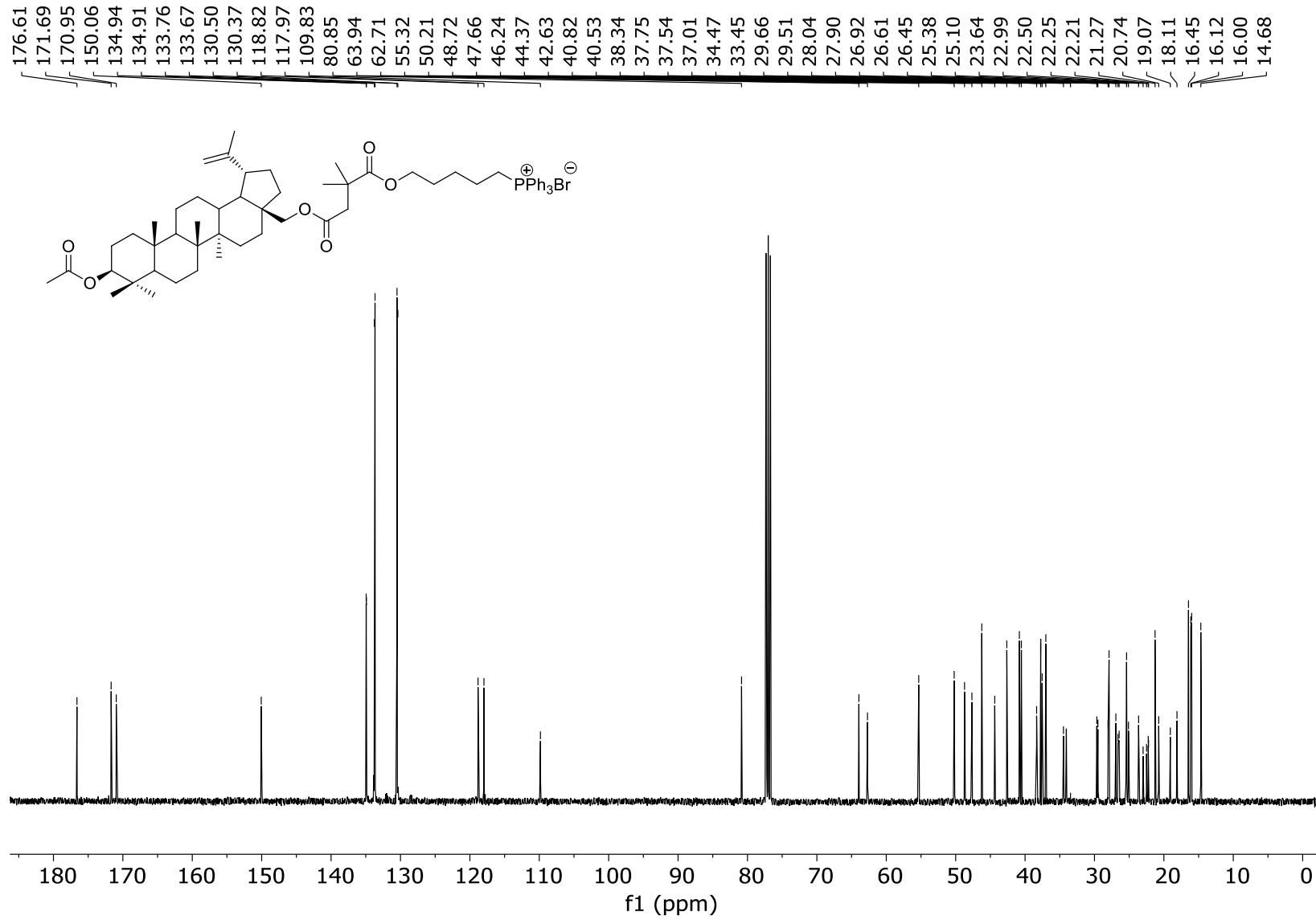
^{13}C NMR spectrum of analogue **7f**; 100 MHz/CDCl$_3$/TMS; δ (ppm).

— 24.35

^{31}P NMR spectrum of analogue **7f**; 161.9 MHz/CDCl$_3$/TMS; δ (ppm).
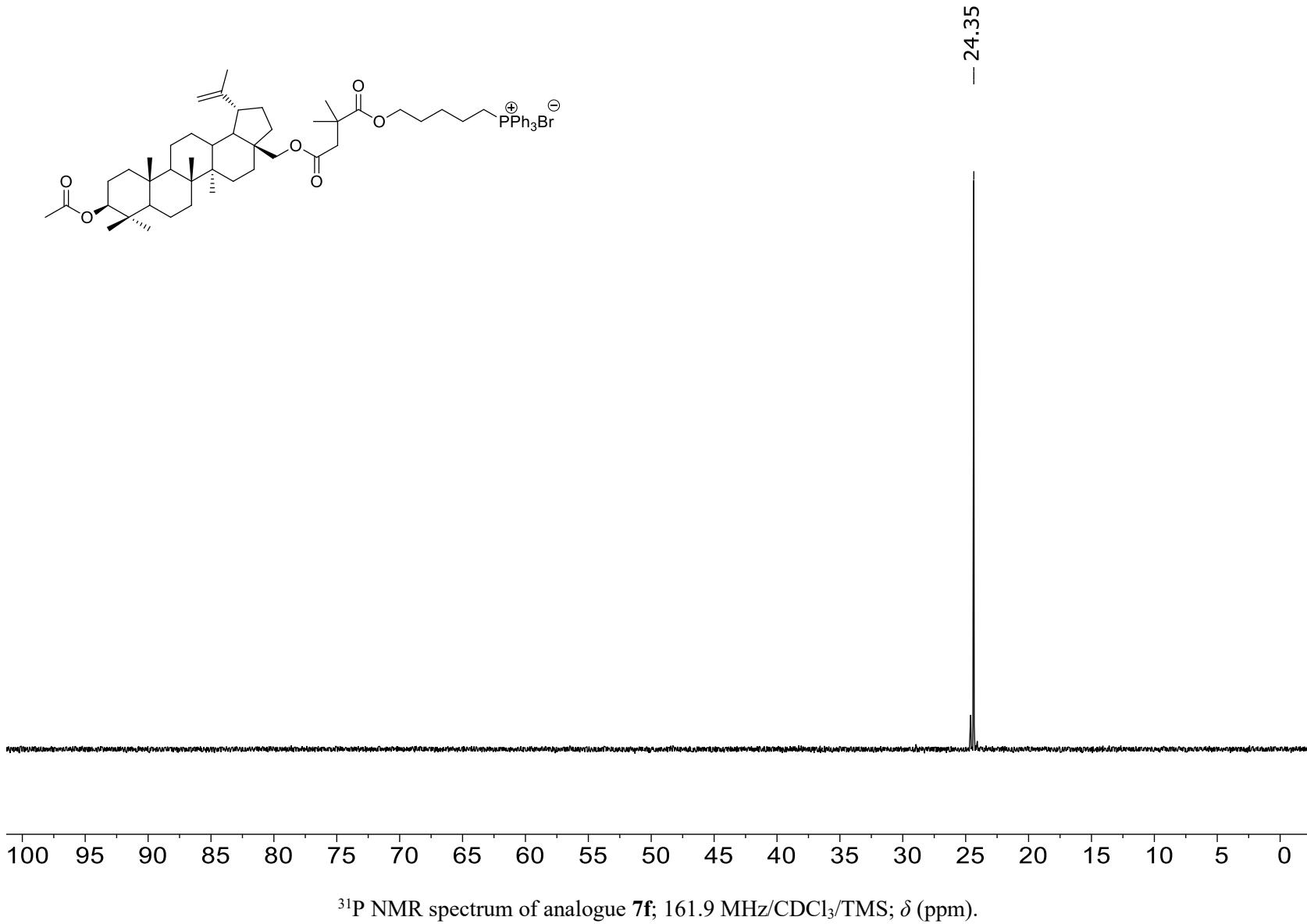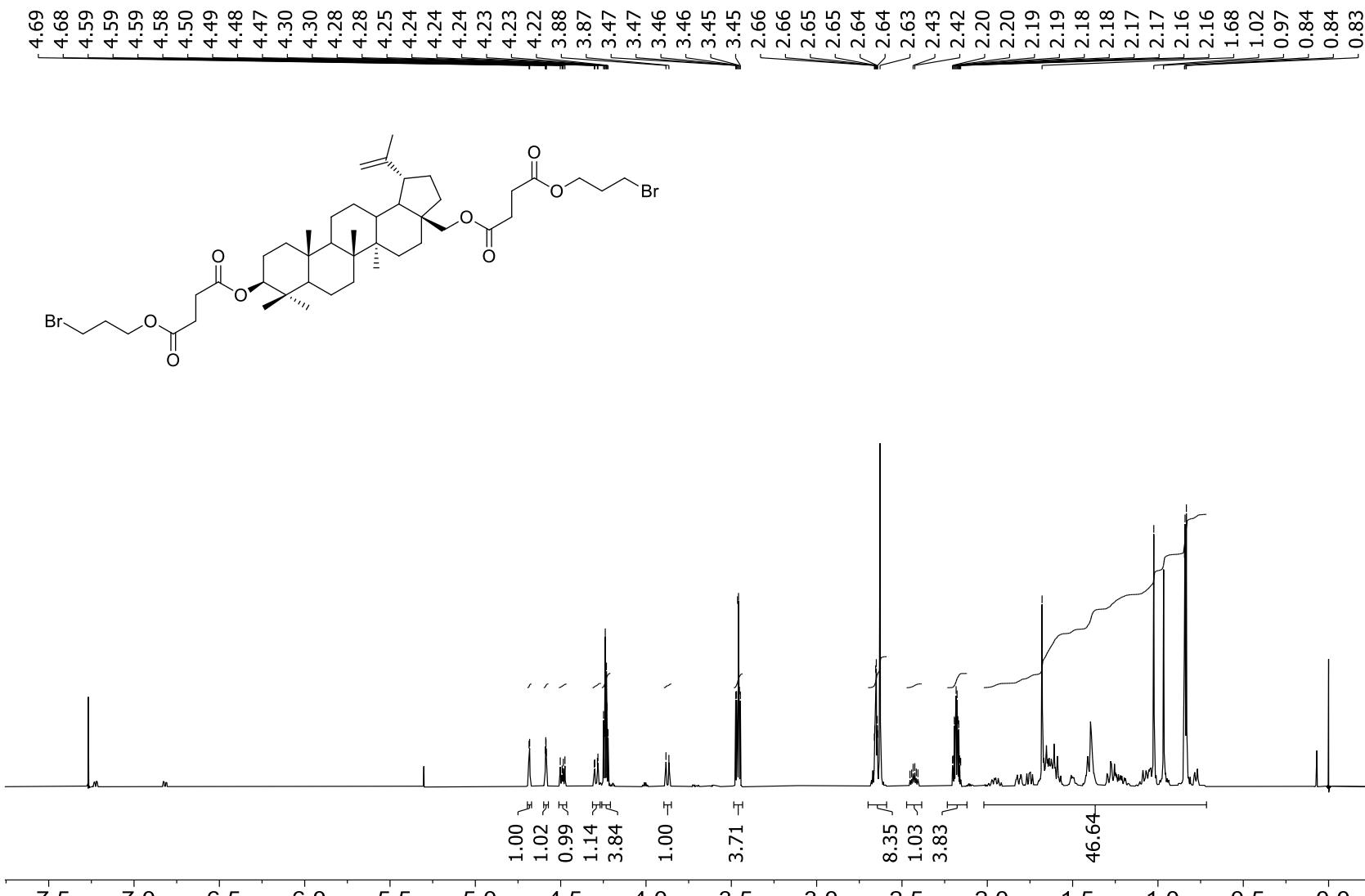
^{1}H NMR spectrum of analogue **8a**; 600 MHz/CDCl$_3$/TMS; δ (ppm).

^{13}C NMR spectrum of analogue **8a**; 150 MHz/CDCl$_3$/TMS; δ (ppm).

^{1}H NMR spectrum of analogue **8b**; 600 MHz/CDCl$_3$/TMS; δ (ppm).

^{13}C NMR spectrum of analogue **8b**; 150 MHz/CDCl$_3$/TMS; δ (ppm).

^{1}H NMR spectrum of analogue **8c**; 600 MHz/CDCl$_3$/TMS; δ (ppm).
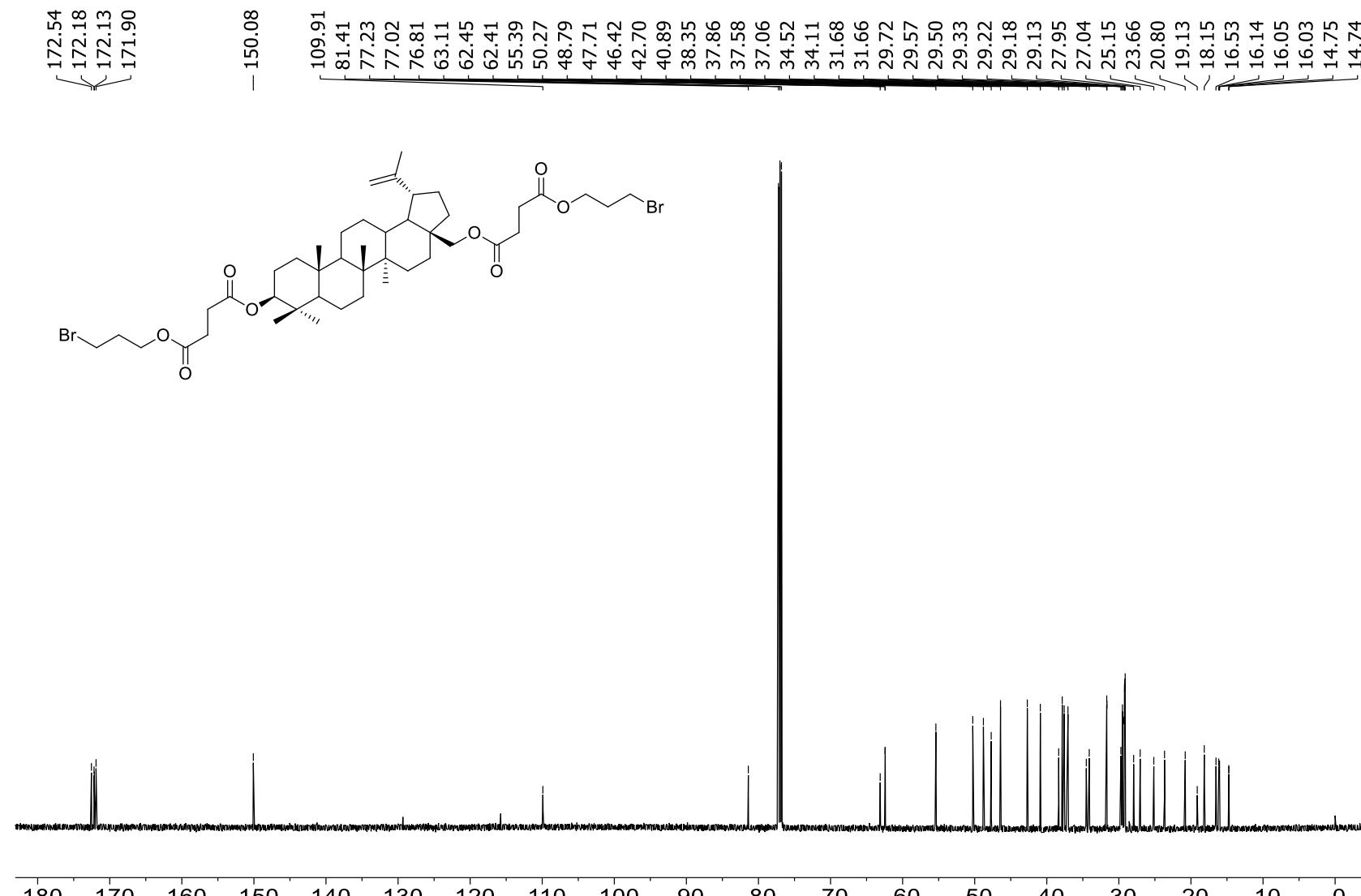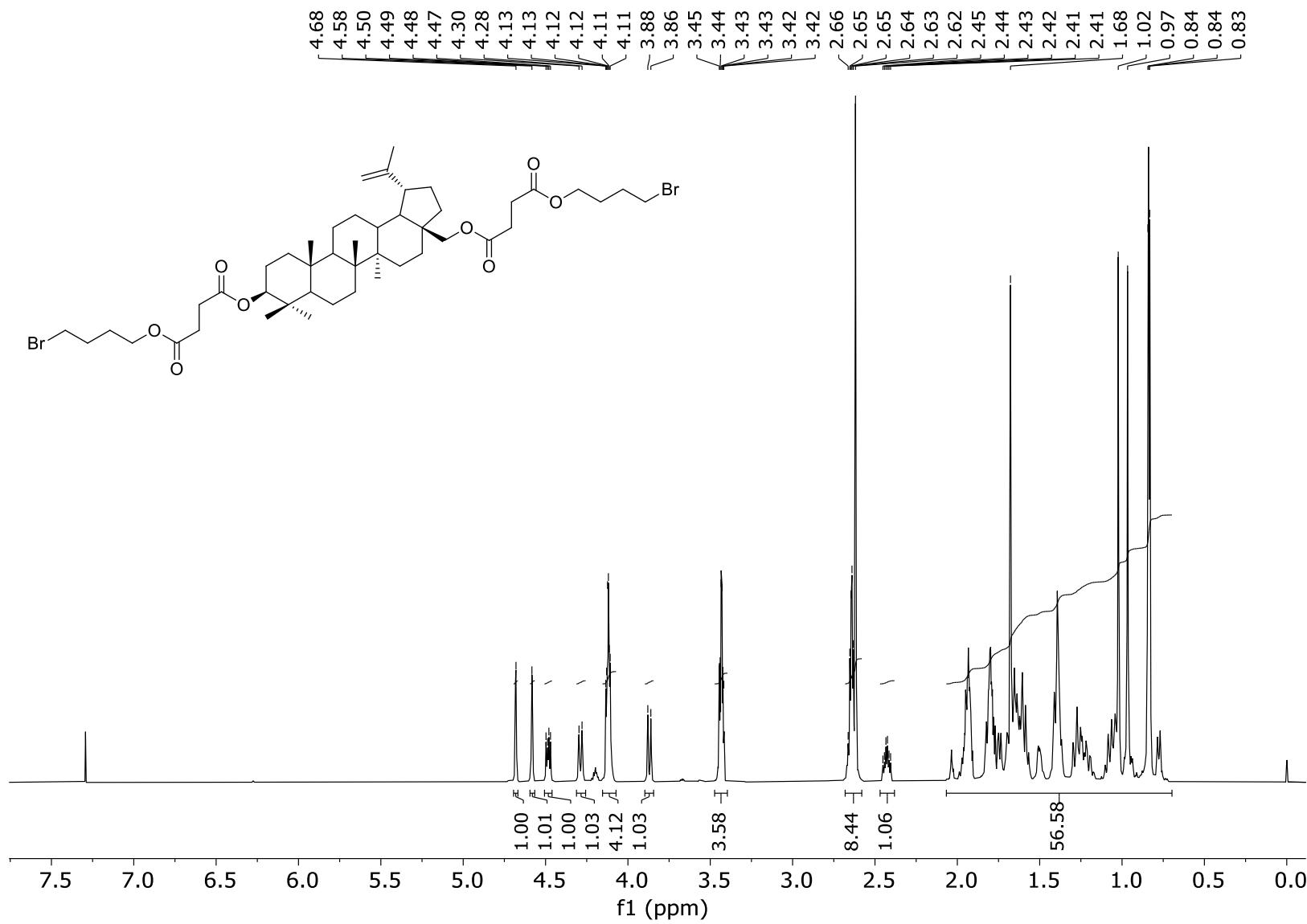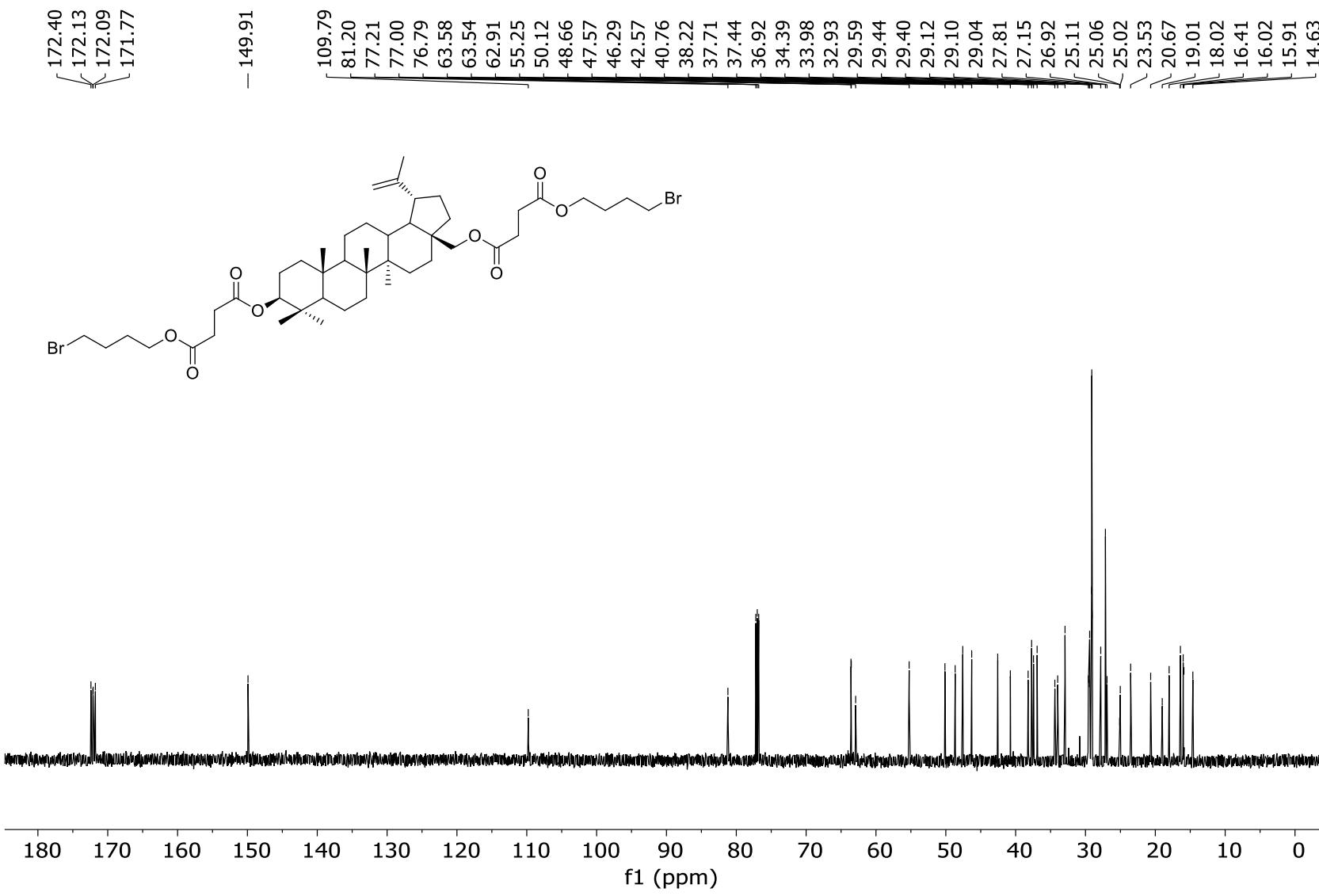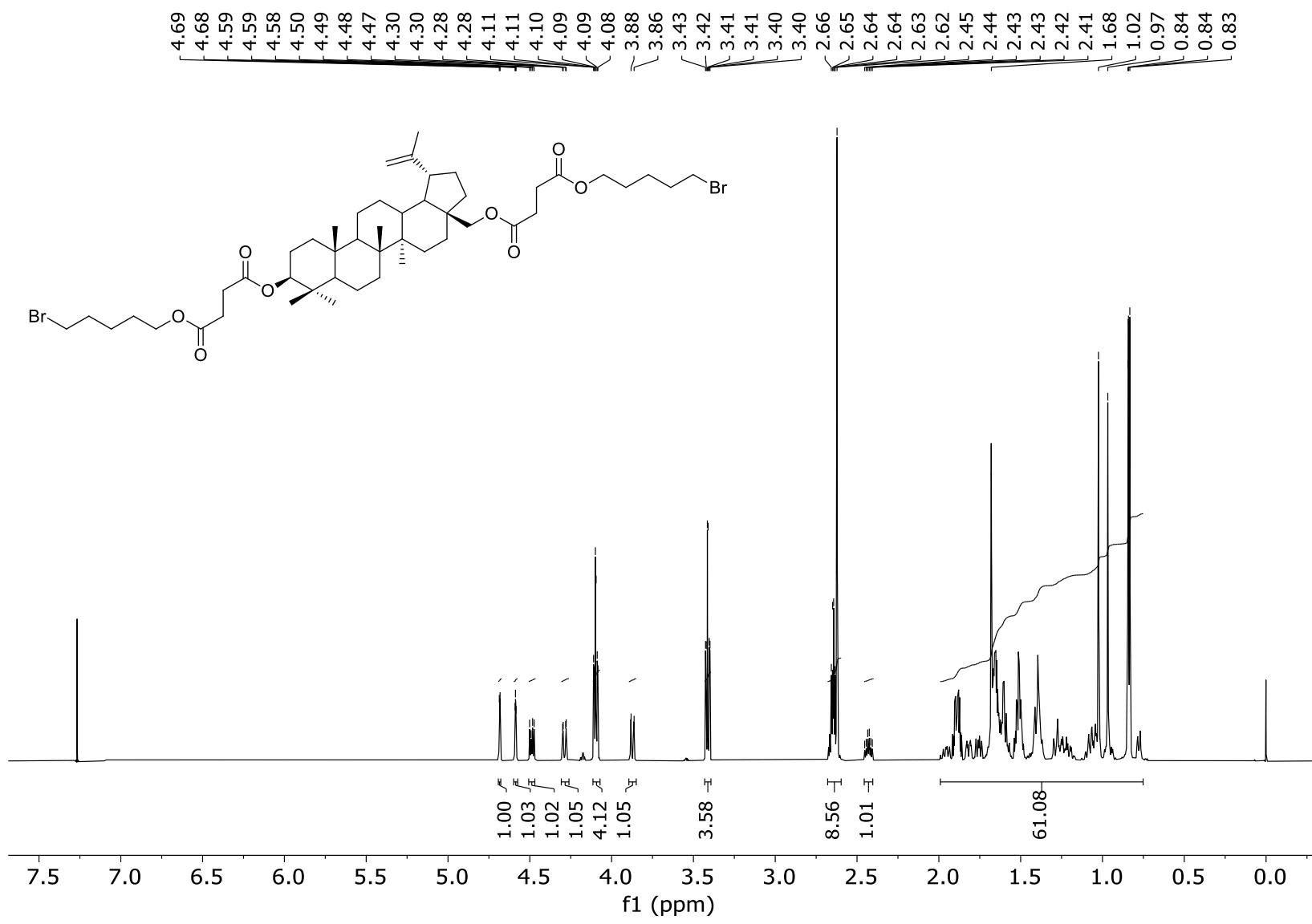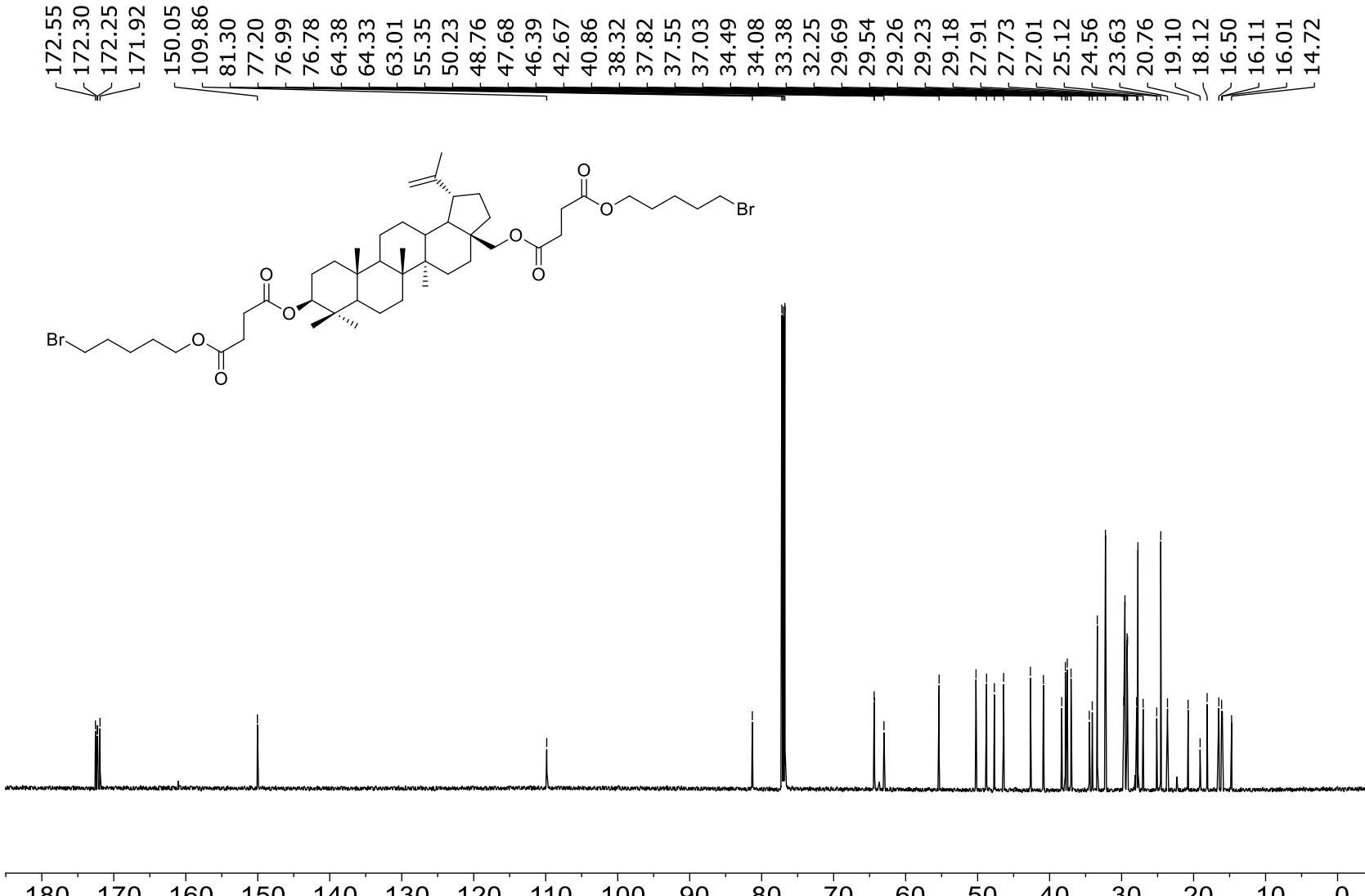
^{13}C NMR spectrum of analogue **8c**; 150 MHz/CDCl$_3$/TMS; δ (ppm).

Peak values (ppm): 172.55, 172.30, 172.25, 171.92, 150.05, 109.86, 81.30, 77.20, 76.99, 76.78, 64.38, 64.33, 63.01, 55.35, 50.23, 48.76, 47.68, 46.39, 42.67, 40.86, 38.32, 37.82, 37.55, 37.03, 34.49, 34.08, 33.38, 32.25, 29.69, 29.54, 29.26, 29.23, 29.18, 27.91, 27.73, 27.01, 25.12, 24.56, 23.63, 20.76, 19.10, 18.12, 16.50, 16.11, 16.01, 14.72

^{1}H NMR spectrum of analogue **9a**; 600 MHz/CDCl$_3$/TMS; δ (ppm).
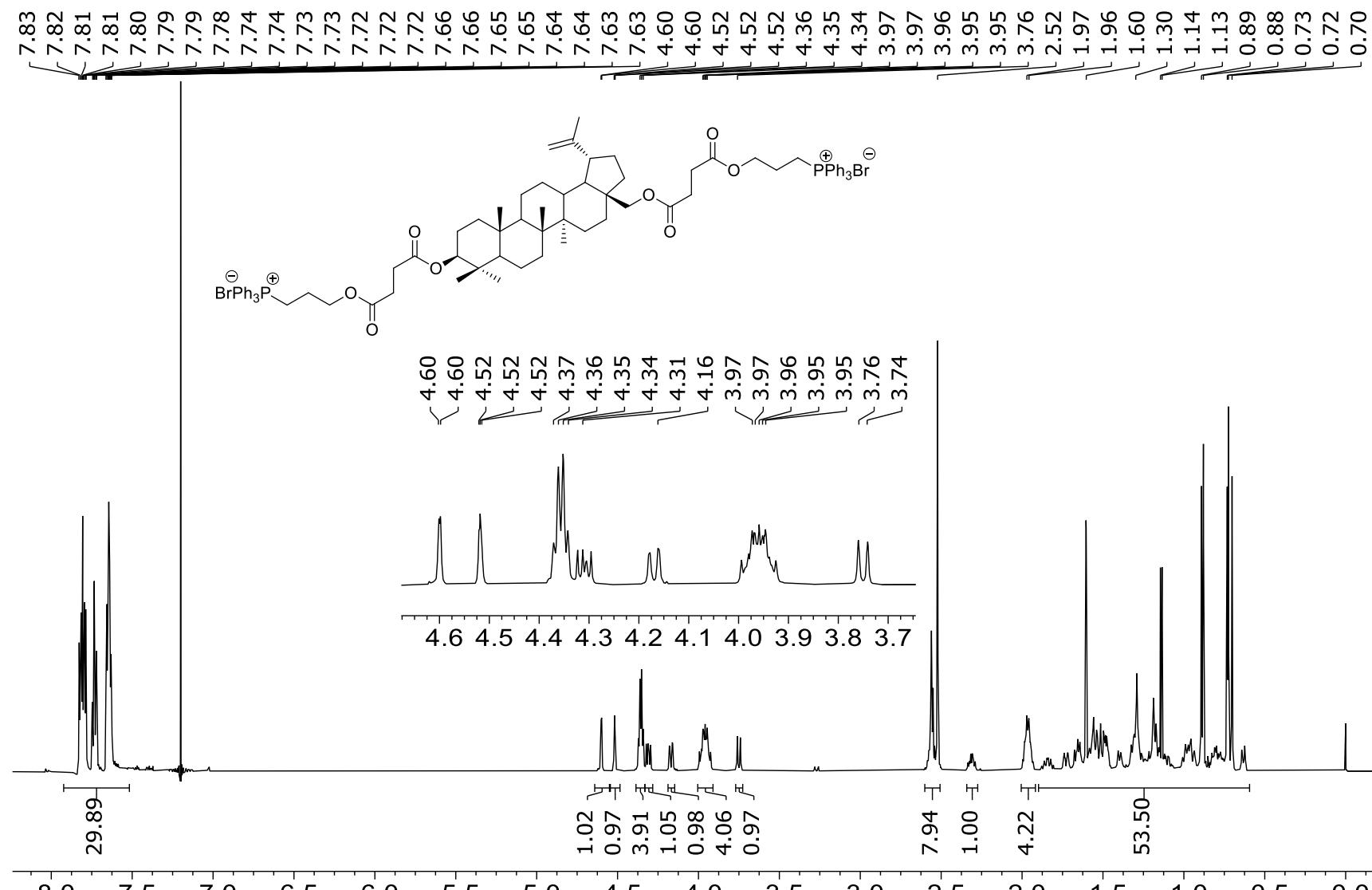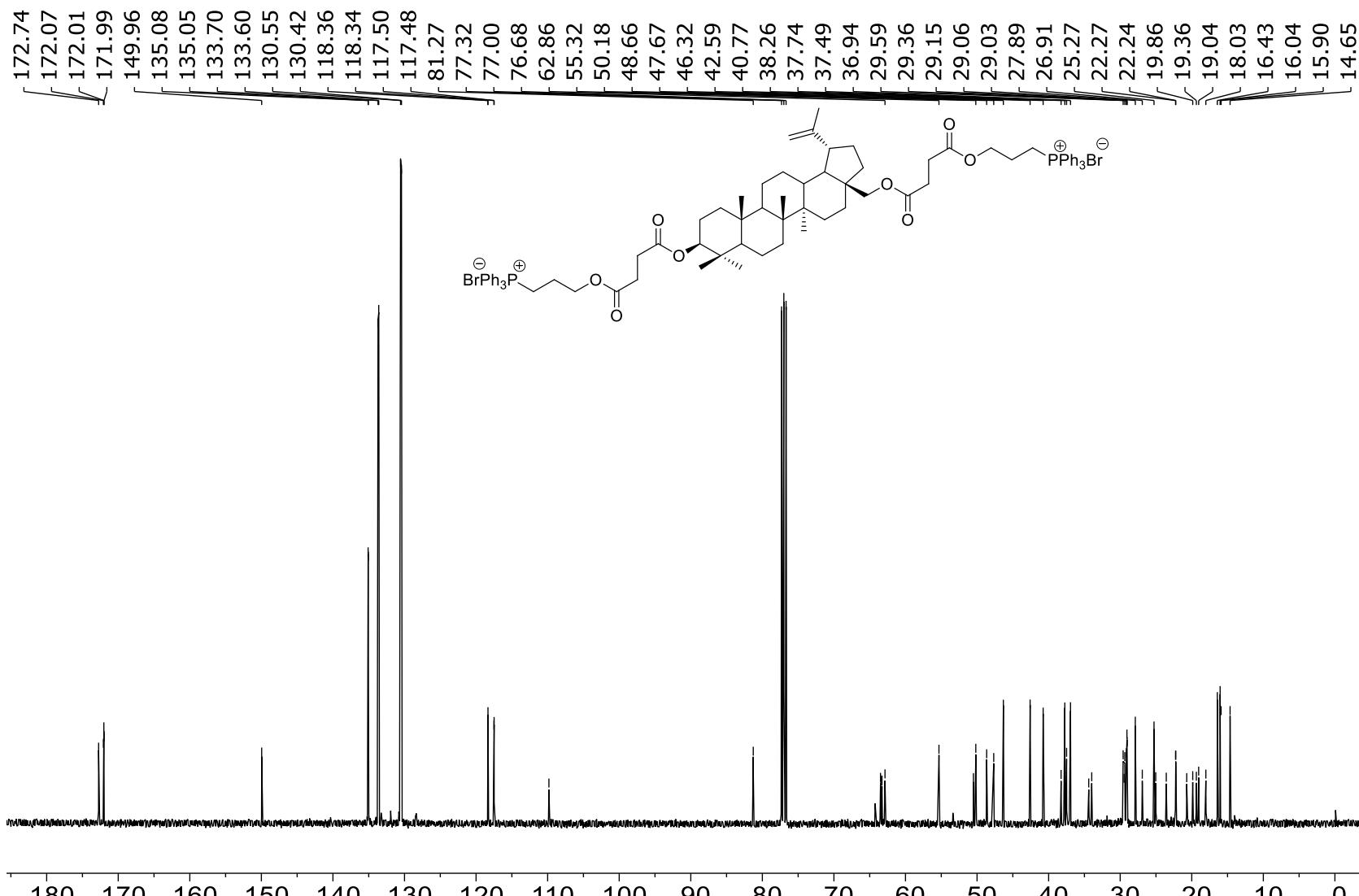
^{13}C NMR spectrum of analogue **9a**; 150 MHz/CDCl$_3$/TMS; δ (ppm).

24.61
24.54
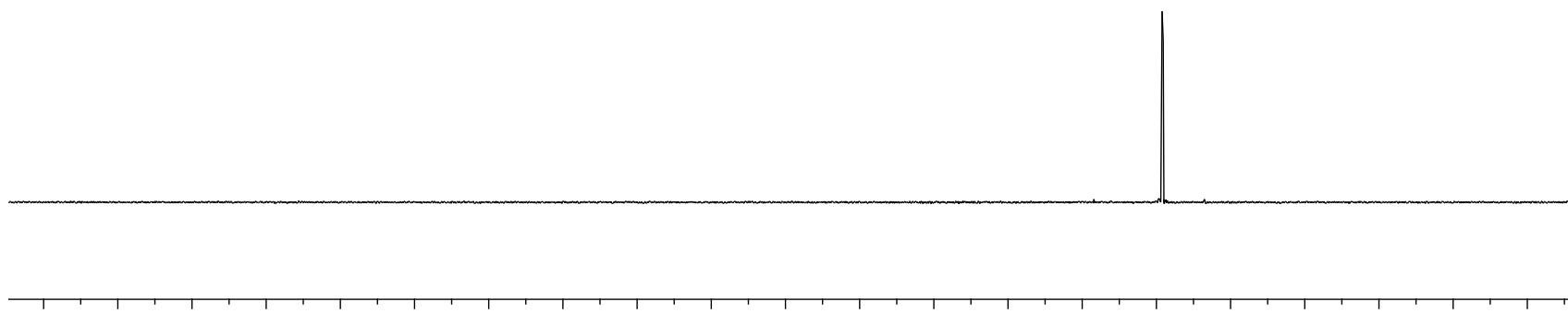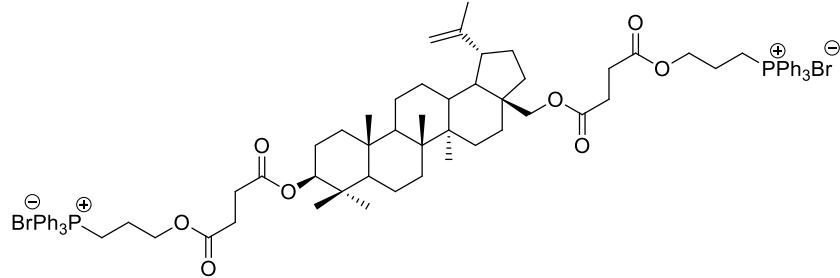
^{31}P NMR spectrum of analogue **9a**; 161.9 MHz/CDCl$_3$/TMS; δ (ppm).
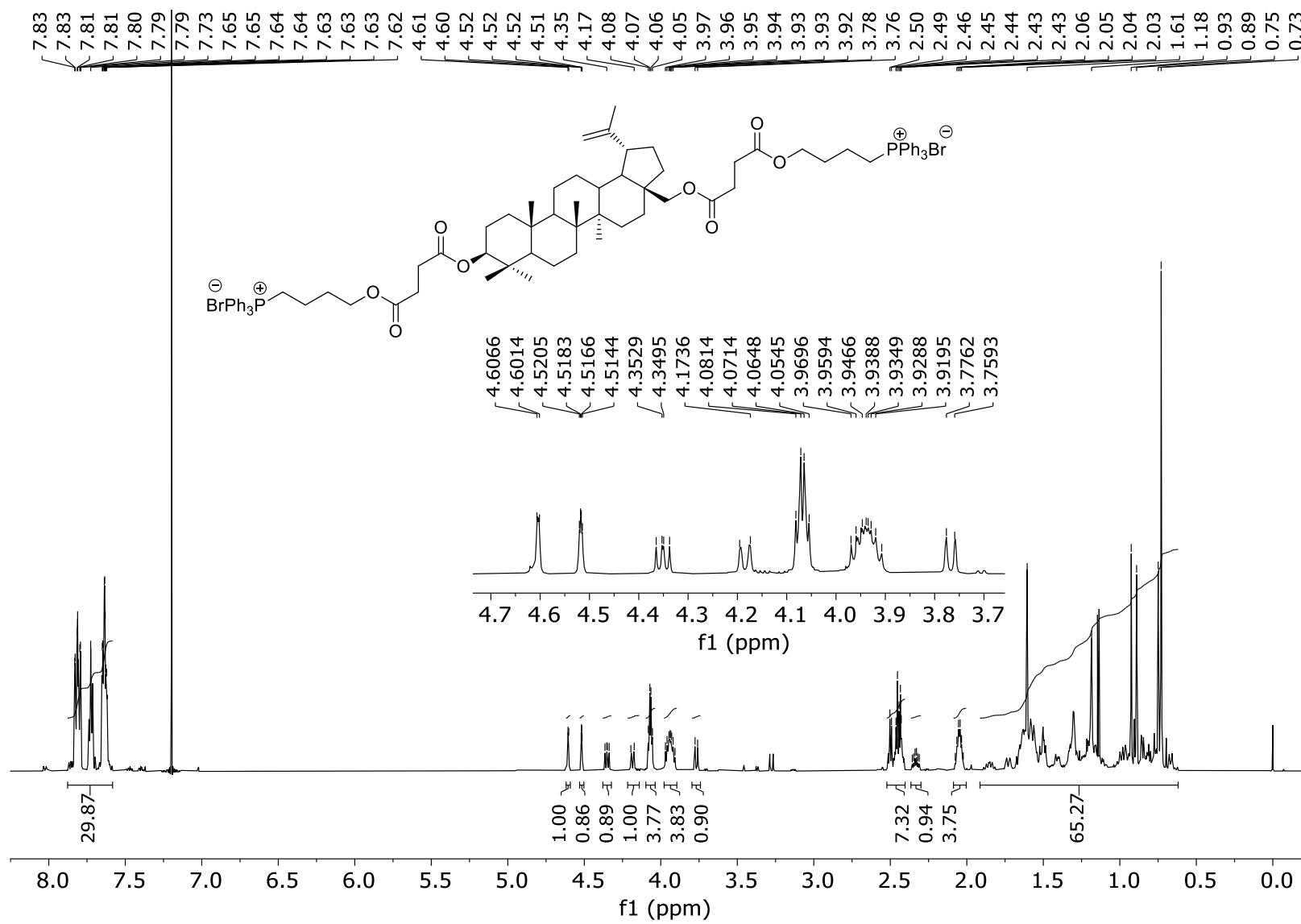
^{1}H NMR spectrum of analogue **9b**; 600 MHz/CDCl$_3$/TMS; δ (ppm).

172.56, 172.18, 172.16, 171.87, 150.00, 134.96, 134.94, 133.77, 133.68, 130.49, 130.37, 118.69, 117.83, 81.28, 63.42, 62.95, 55.35, 50.21, 48.71, 47.69, 46.37, 42.65, 40.83, 38.29, 37.79, 37.54, 37.00, 34.04, 29.64, 29.47, 29.12, 29.04, 28.94, 27.91, 26.97, 25.32, 25.09, 23.61, 22.41, 21.91, 20.75, 19.29, 19.24, 19.07, 18.09, 16.49, 16.10, 15.98, 14.71
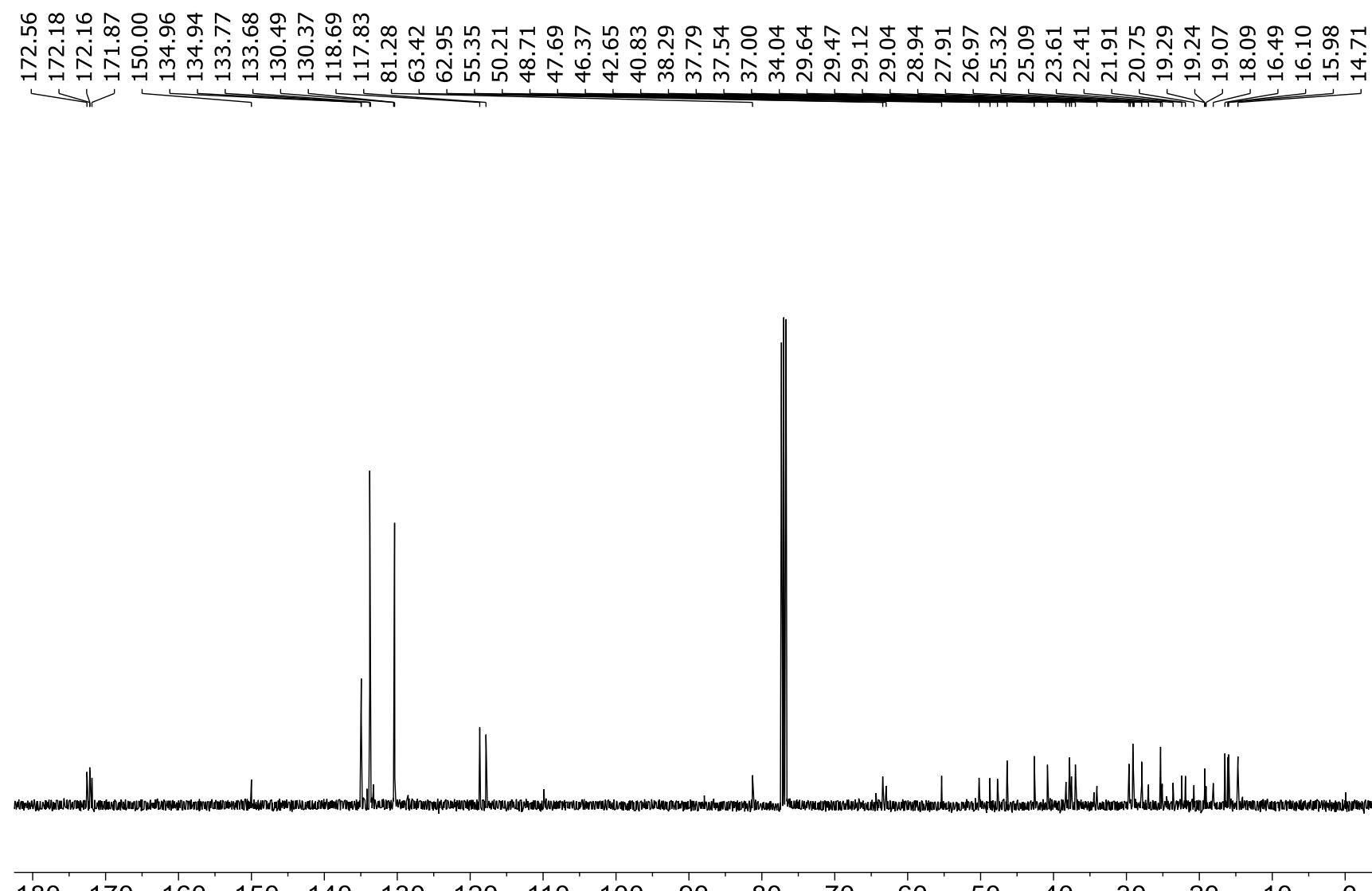
^{13}C NMR spectrum of analogue **9b**; 100 MHz/CDCl$_3$/TMS; δ (ppm).

— 24.51
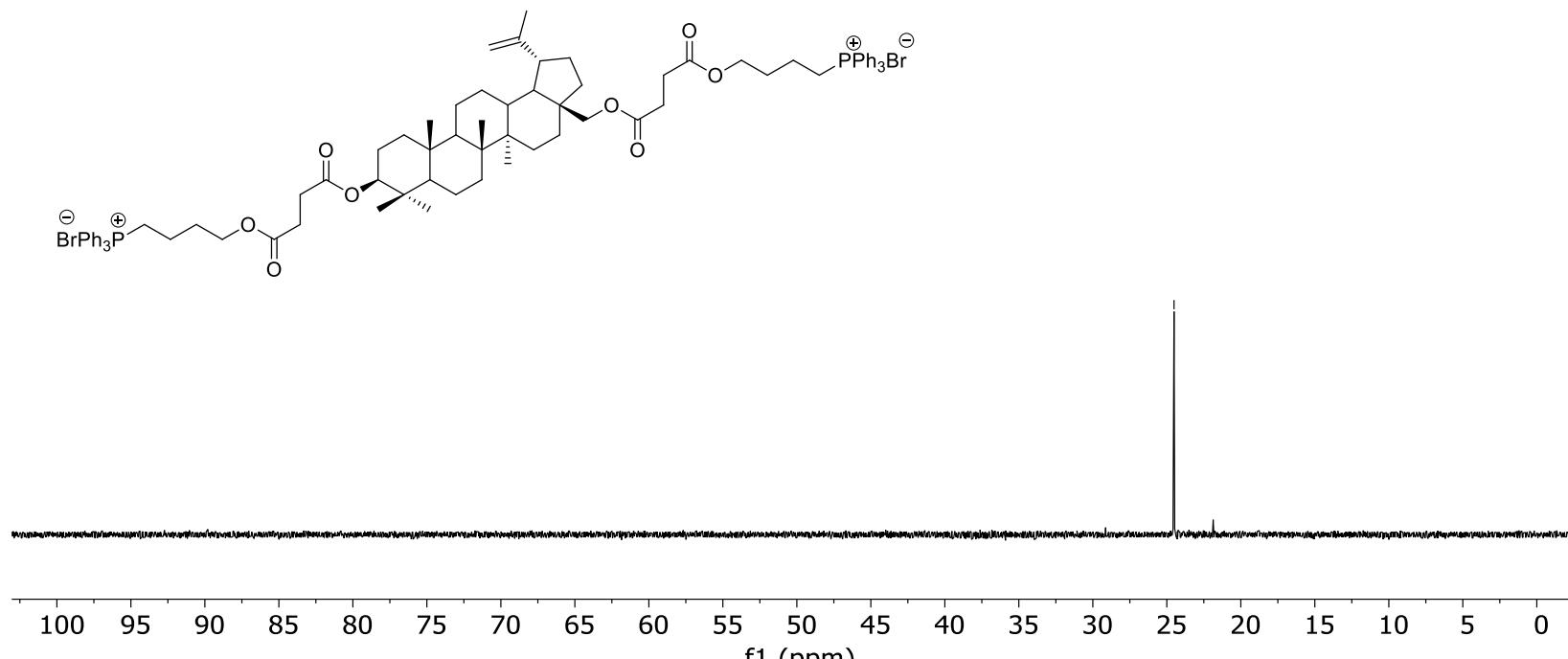
^{31}P NMR spectrum of analogue **9b**; 161.9 MHz/CDCl$_3$/TMS; δ (ppm).
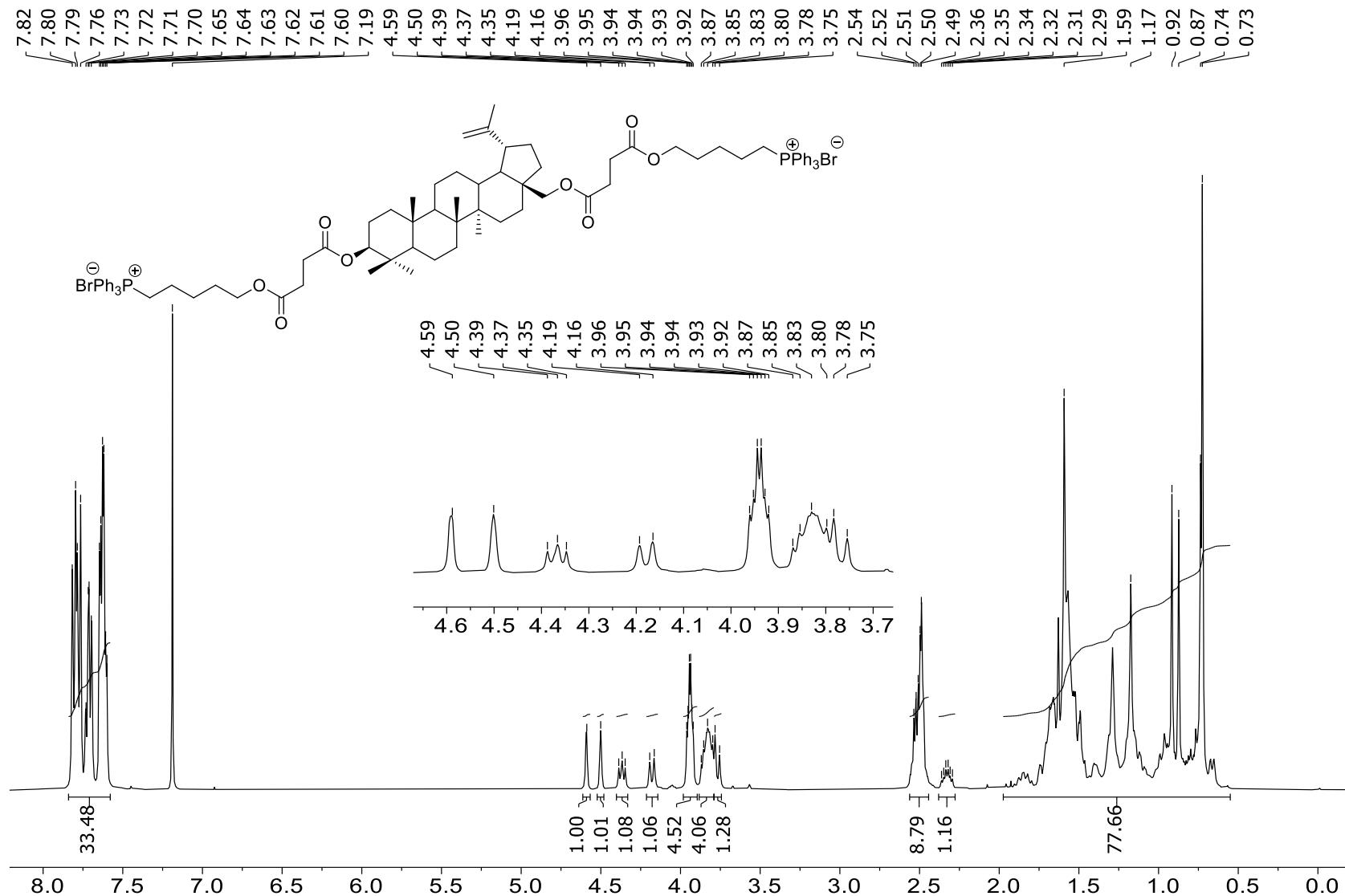
^{1}H NMR spectrum of analogue **9c**; 400 MHz/CDCl$_3$/TMS; δ (ppm).
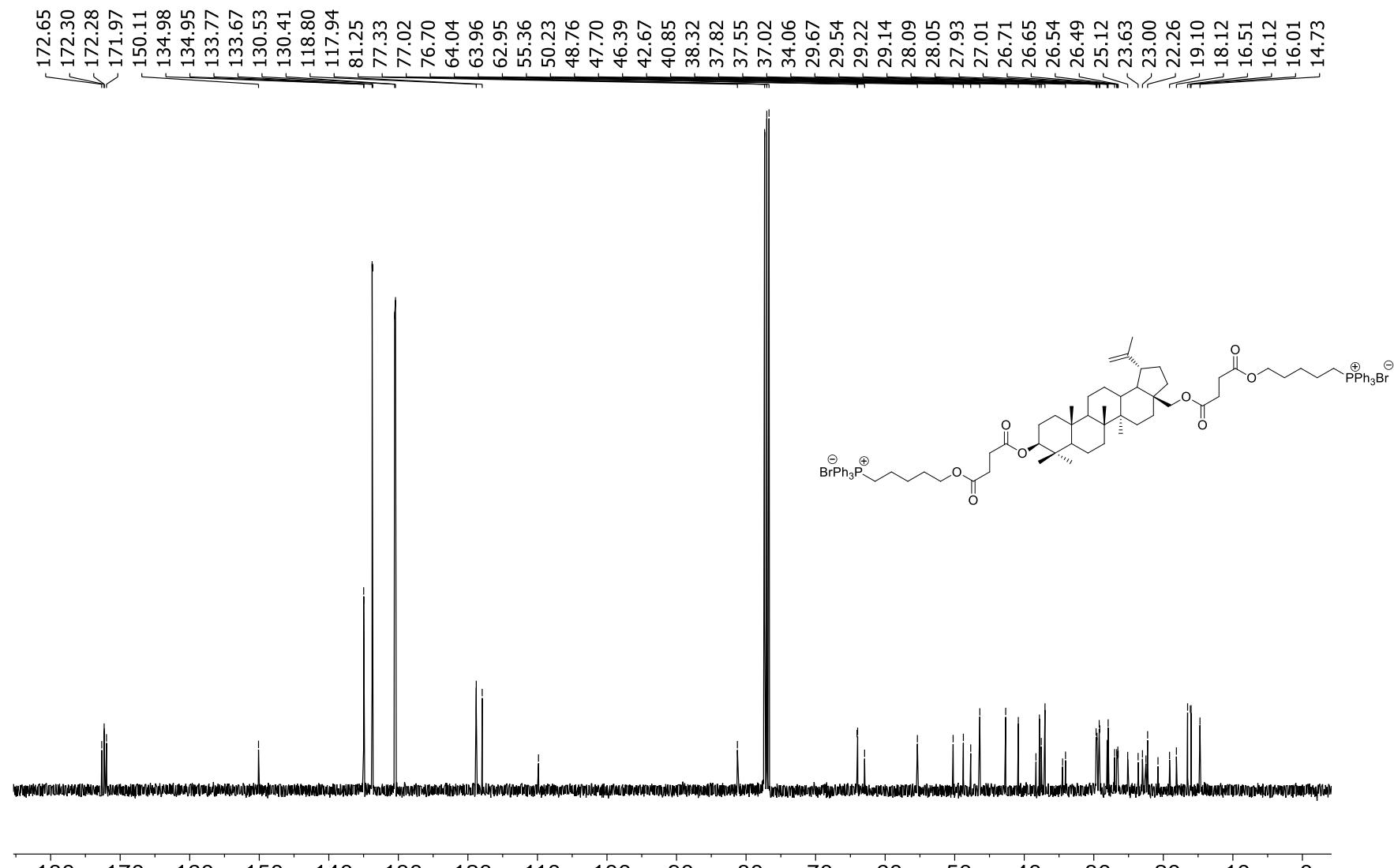
^{13}C NMR spectrum of analogue **9c**; 100 MHz/CDCl$_3$/TMS; δ (ppm).

— 24.36
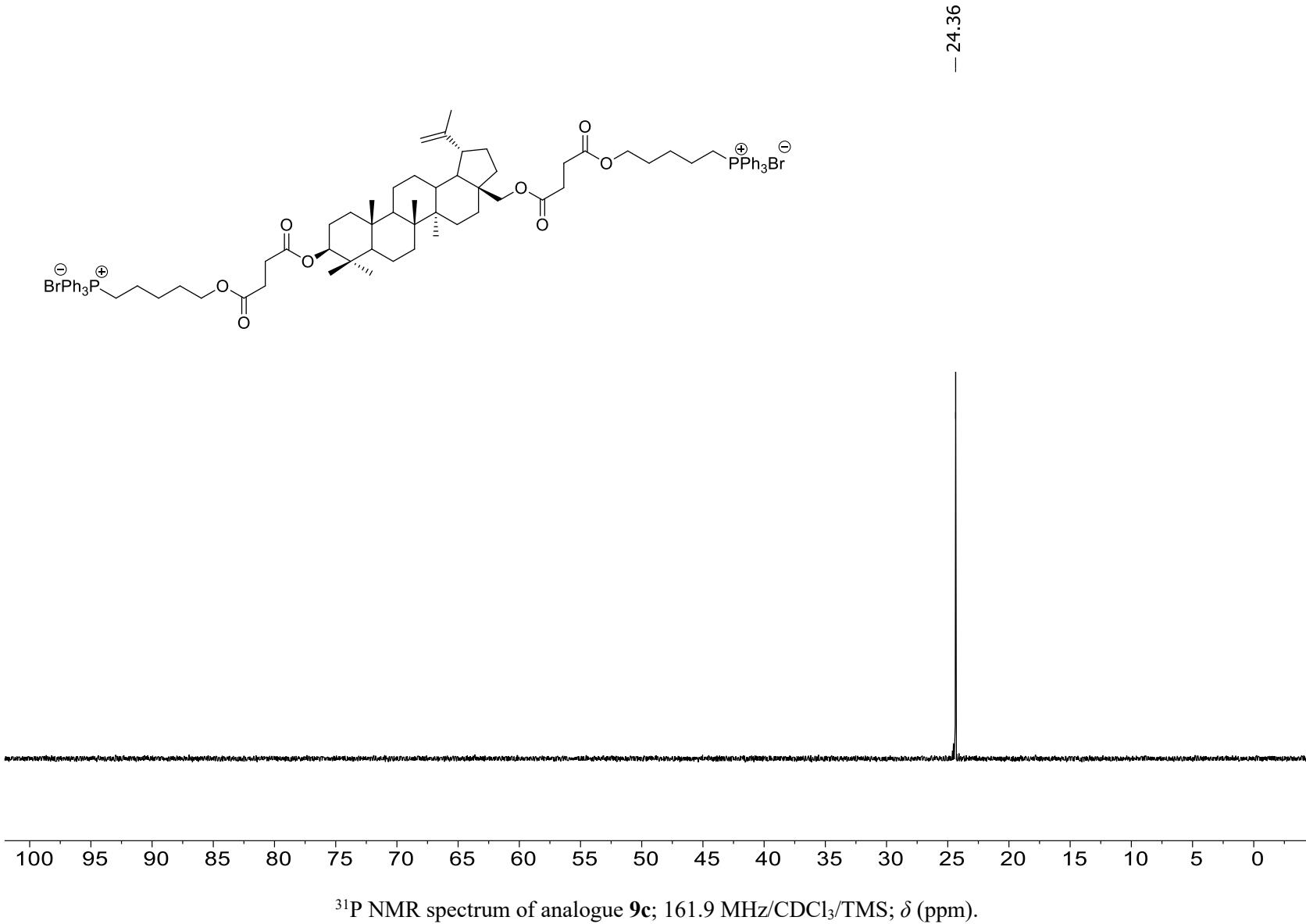
^{31}P NMR spectrum of analogue **9c**; 161.9 MHz/CDCl$_3$/TMS; δ (ppm).
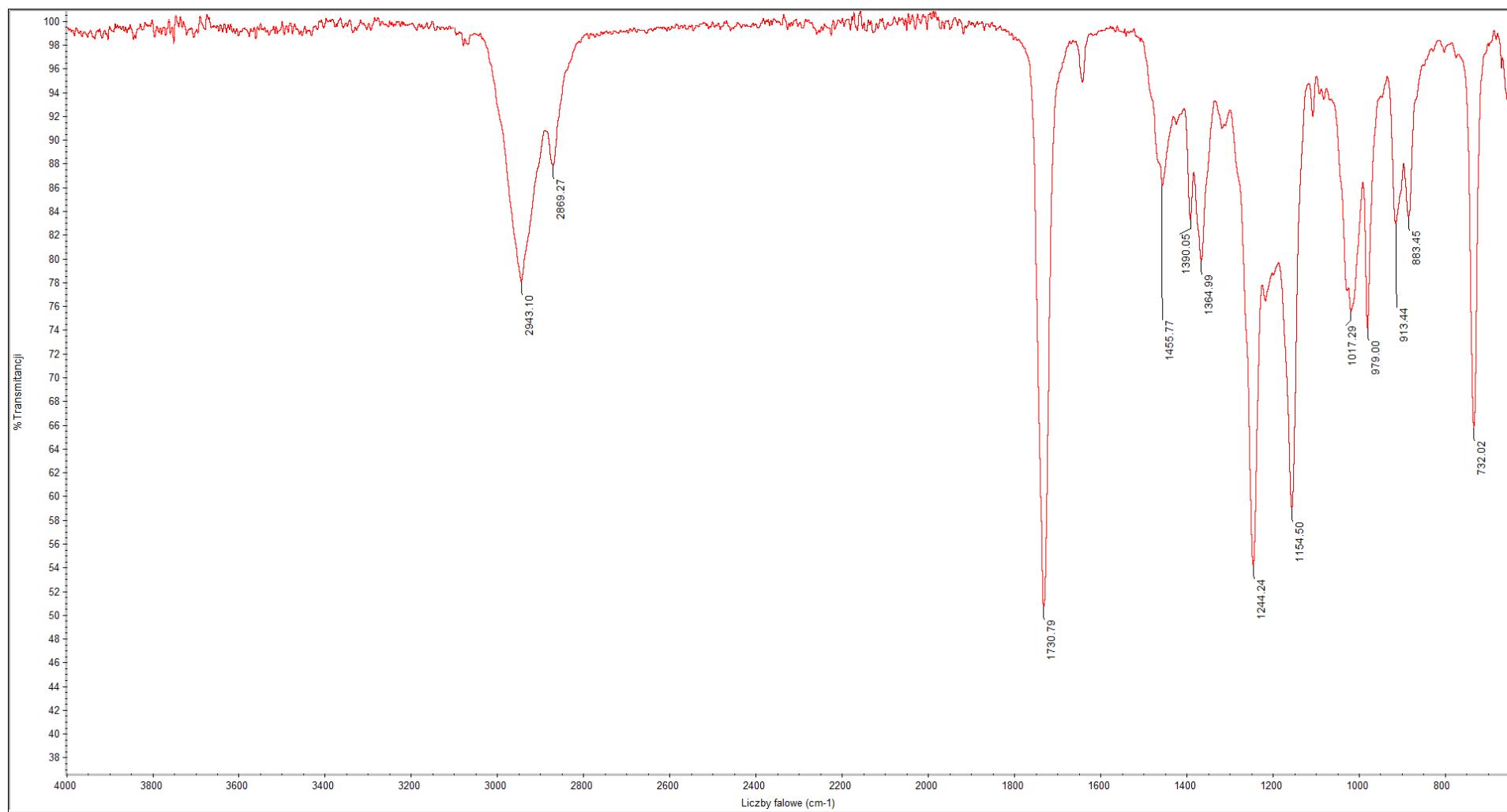
IR spectrum of product **6a**; ATR (cm^{-1}).
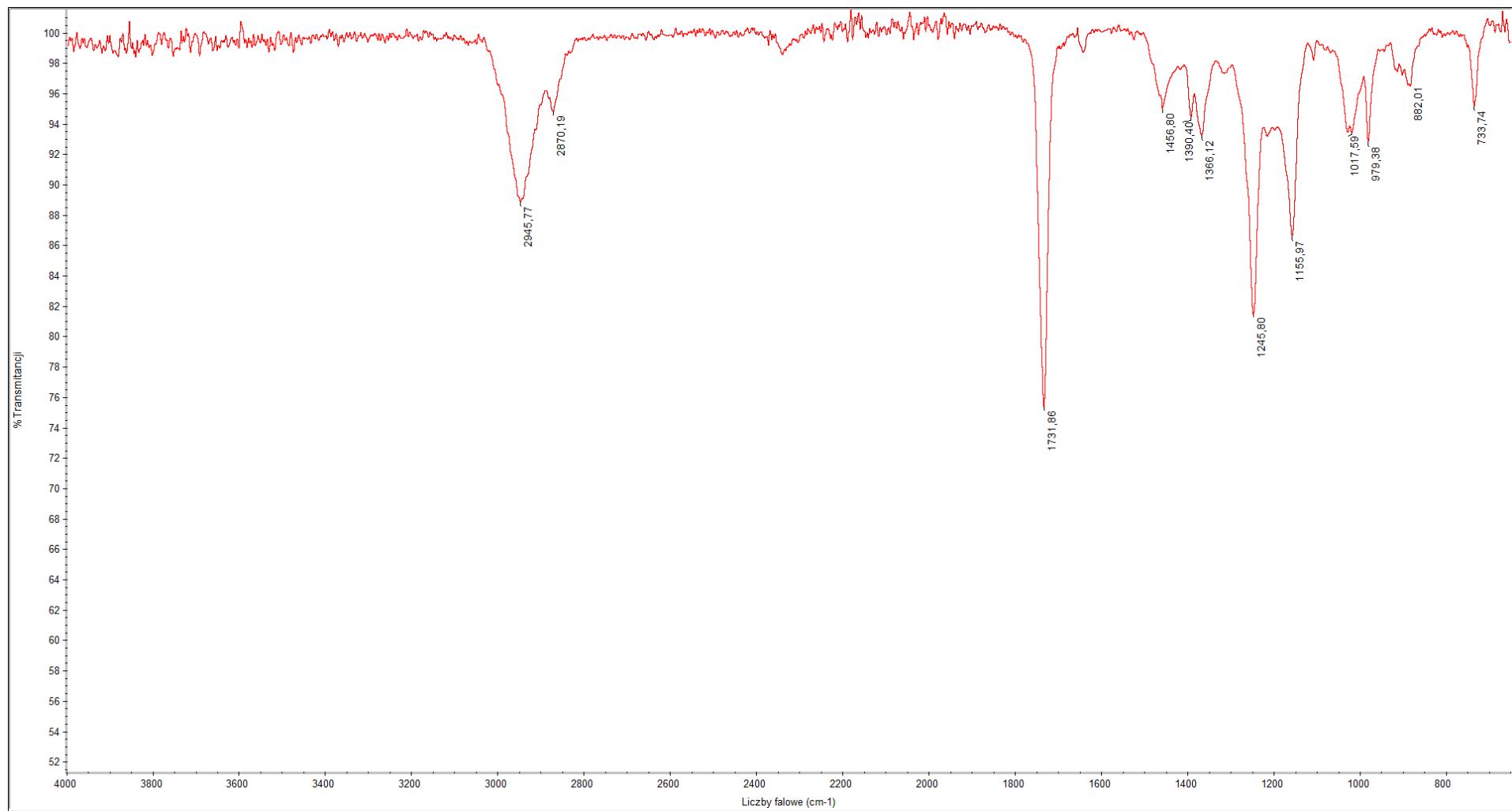
IR spectrum of product **6b**; ATR (cm^{-1}).
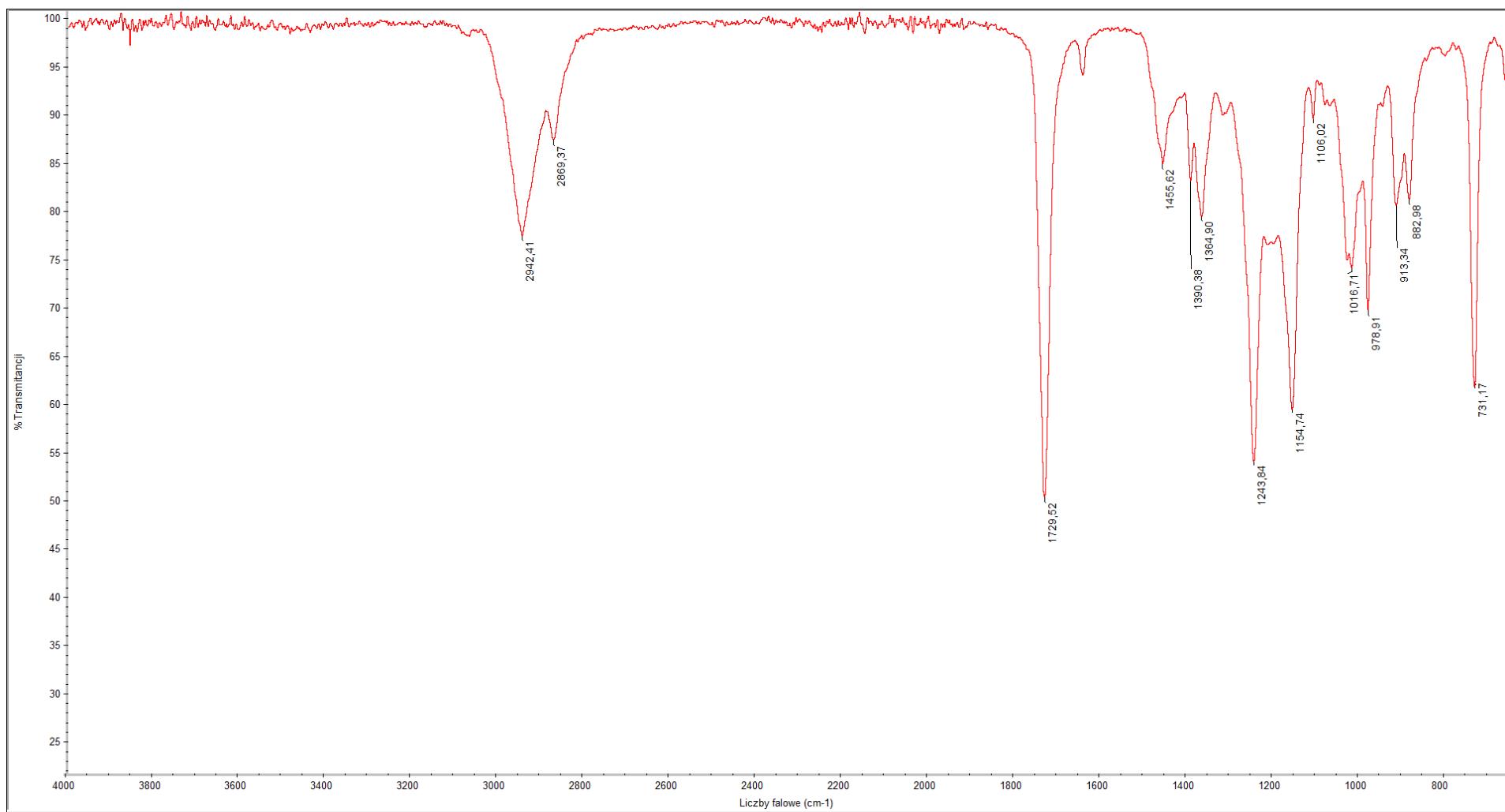
IR spectrum of product **6c**; ATR (cm^{-1}).
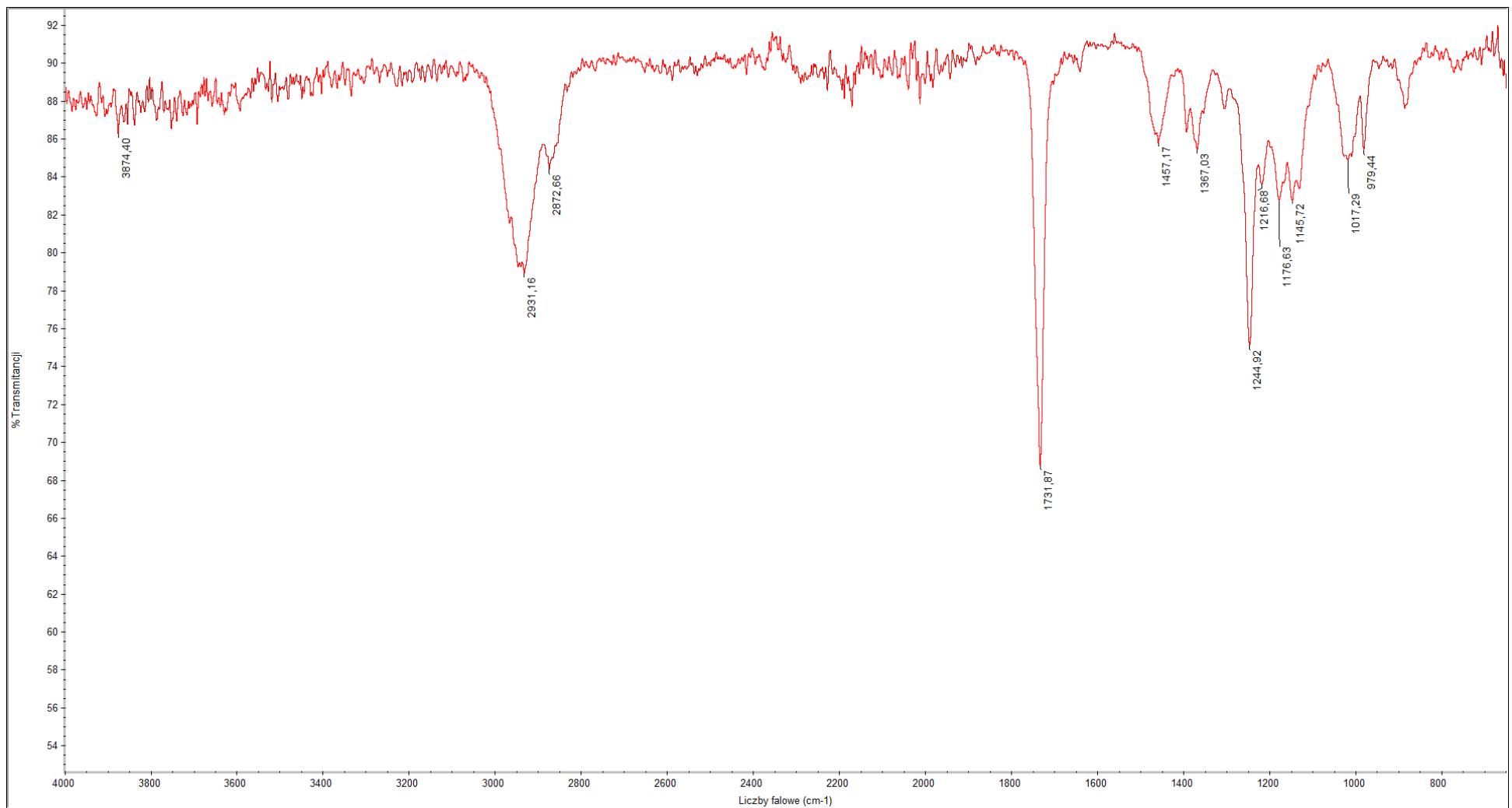
IR spectrum of product **6d**; ATR (cm⁻¹).
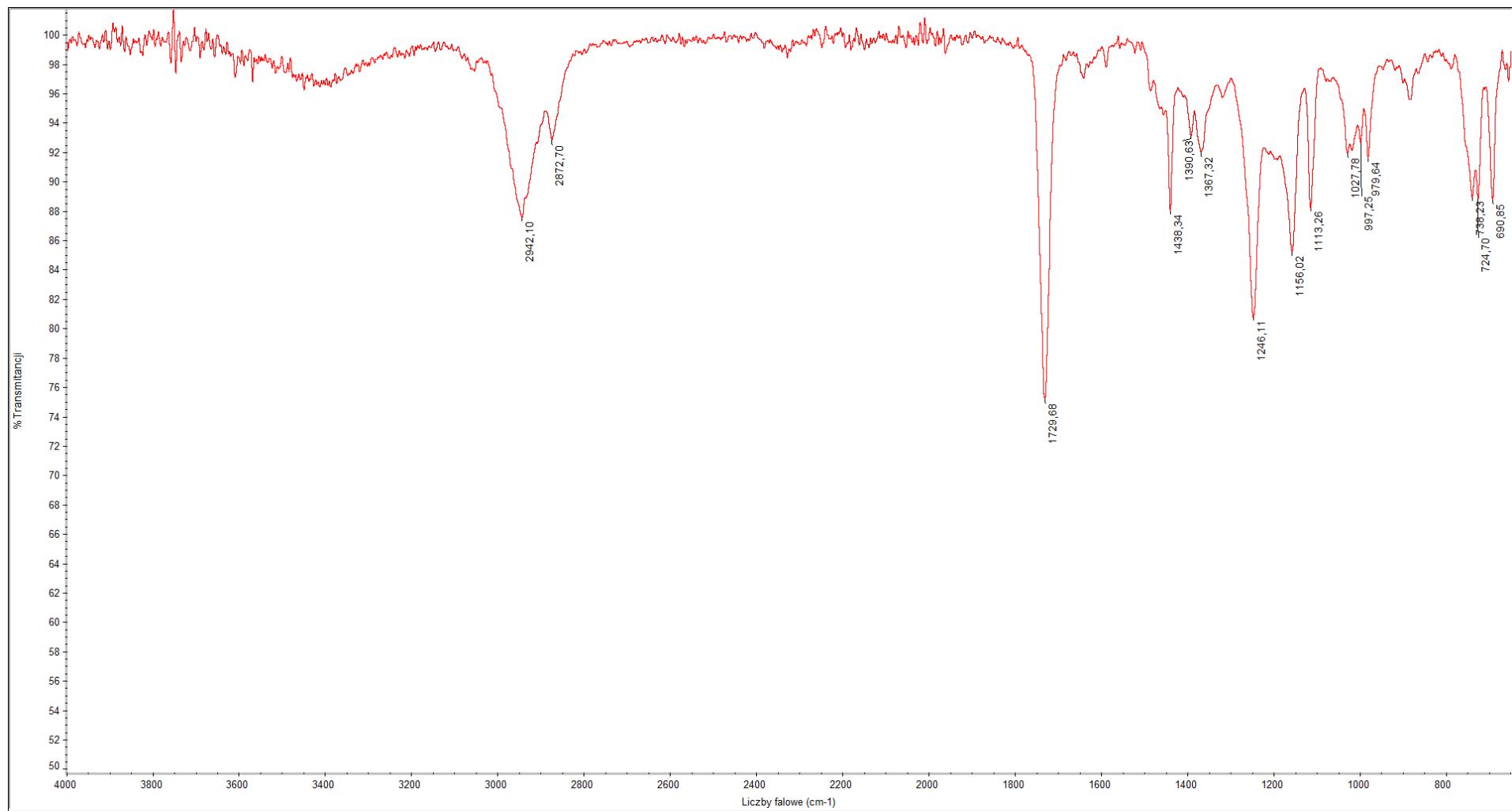
IR spectrum of product **7a**; ATR (cm⁻¹).
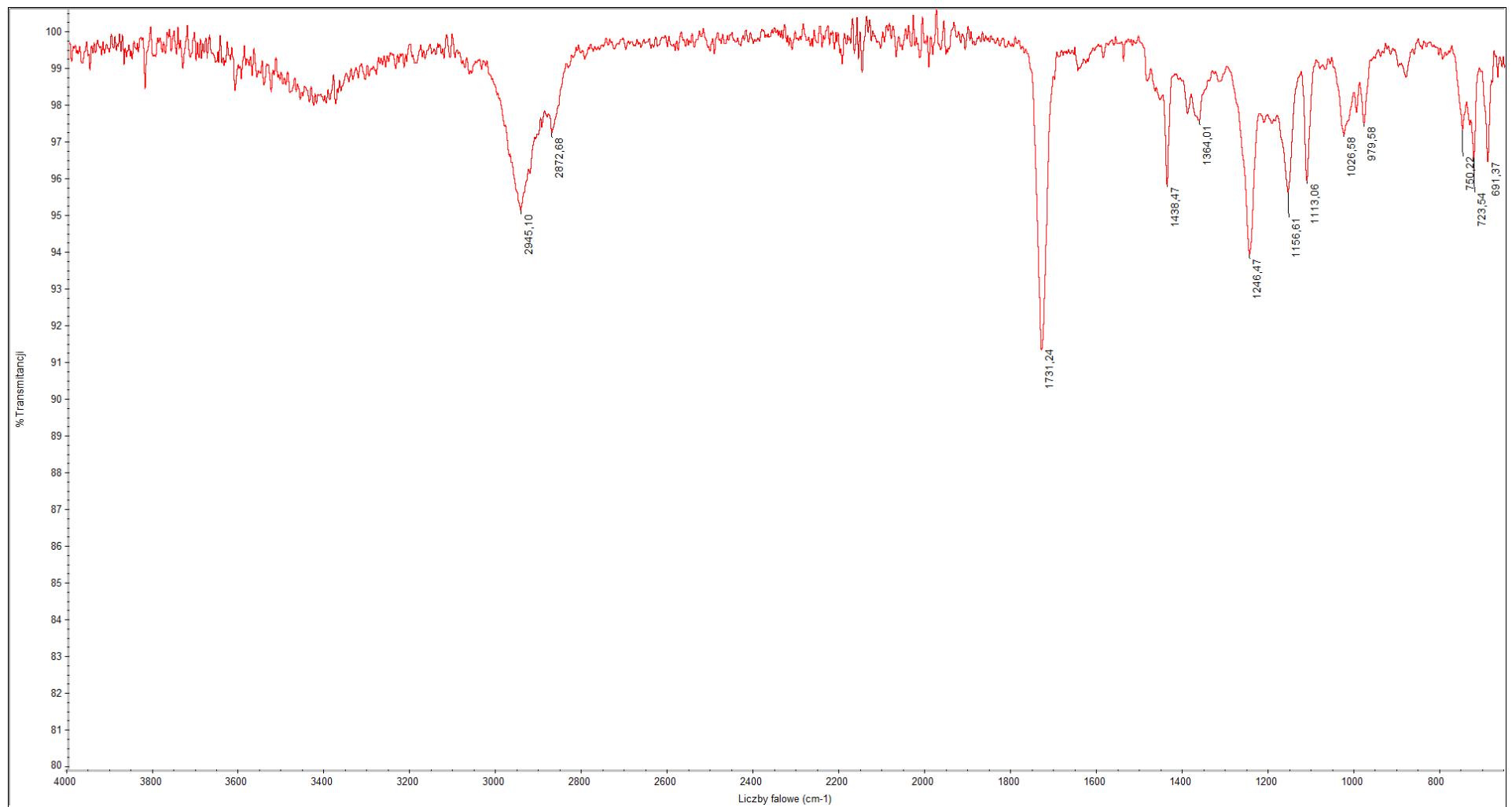
IR spectrum of product **7b**; ATR (cm^{-1}).
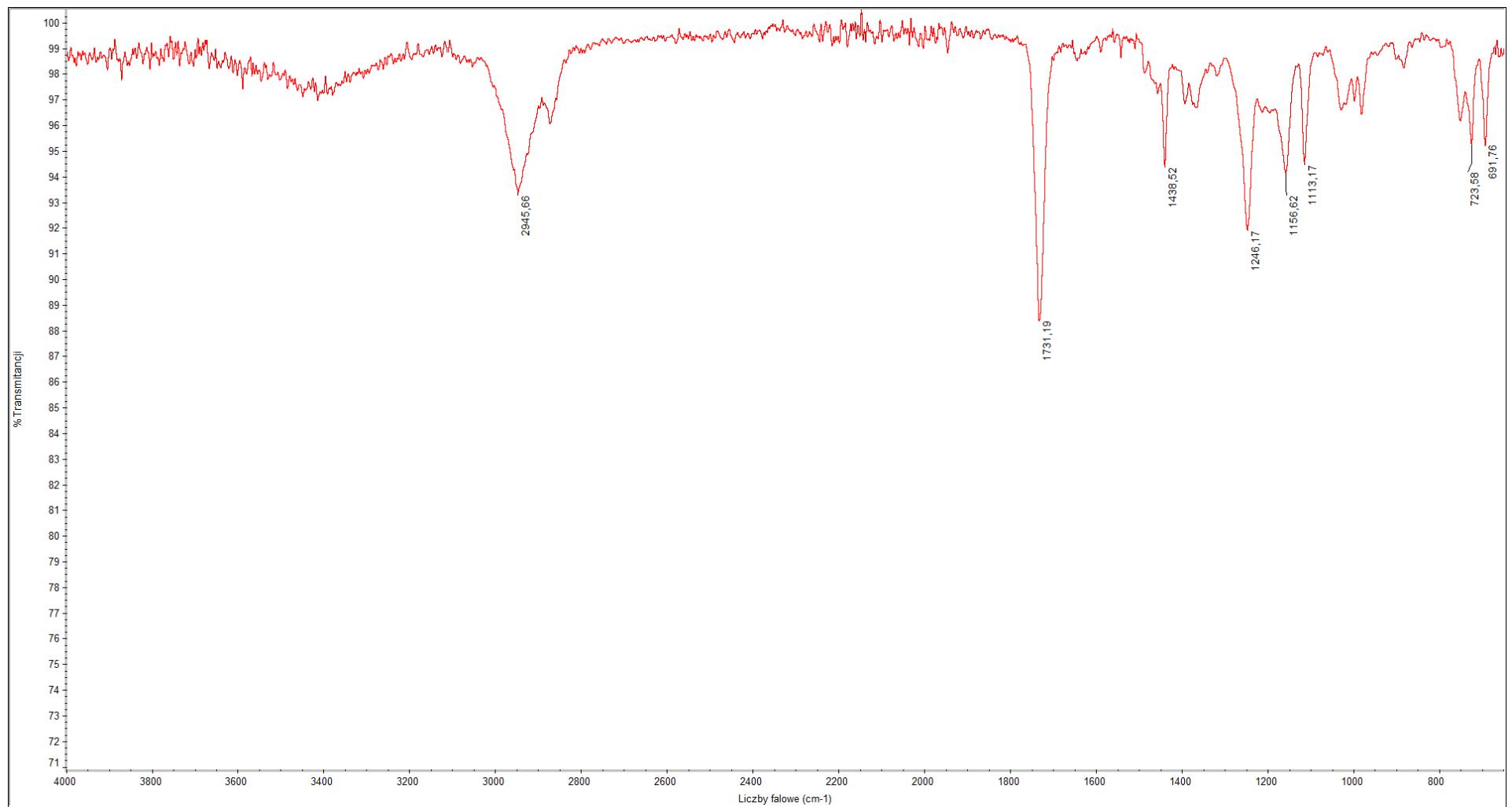
IR spectrum of product **7c**; ATR (cm⁻¹).
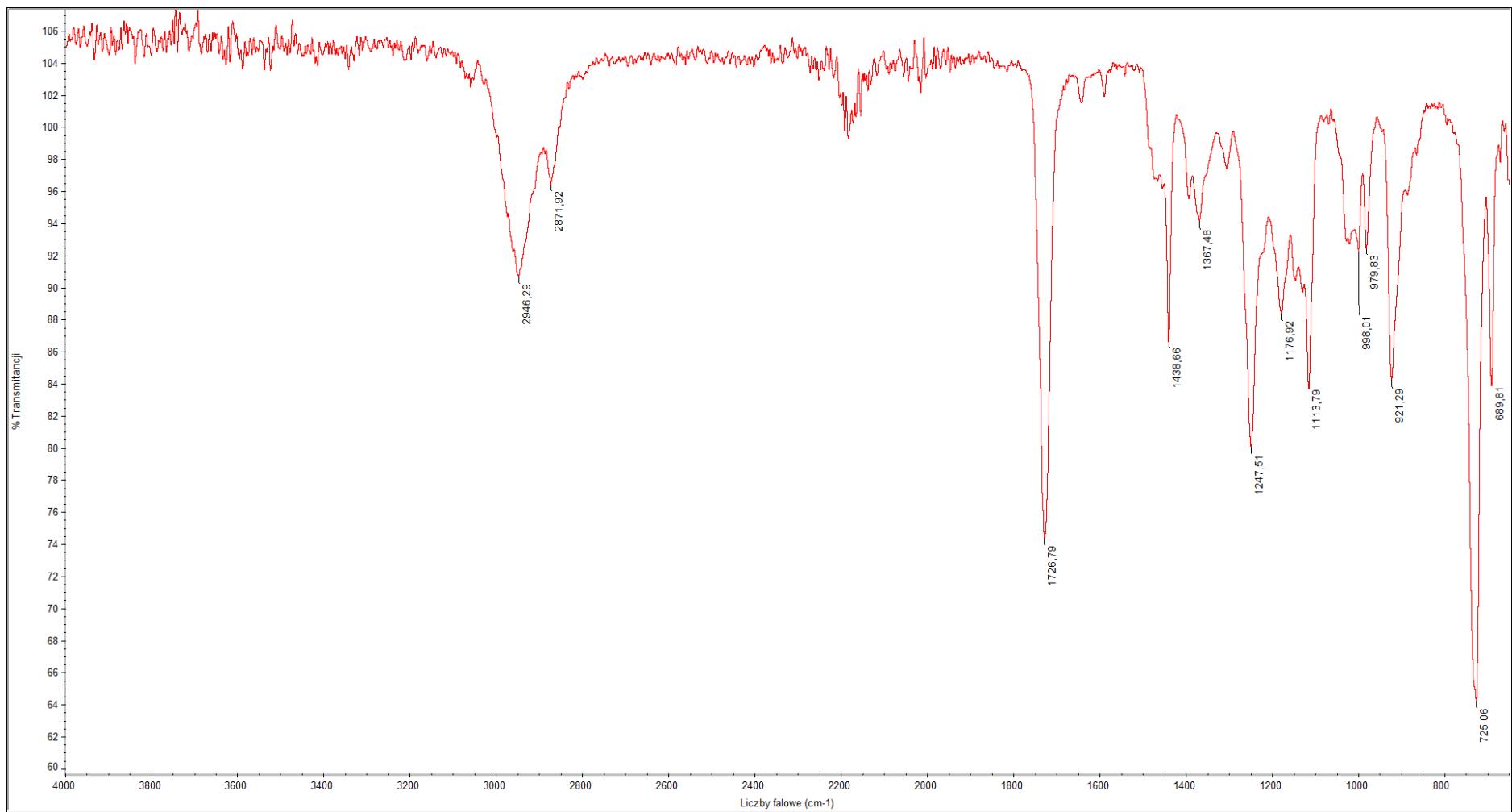
IR spectrum of product **7d**; ATR (cm^{-1}).
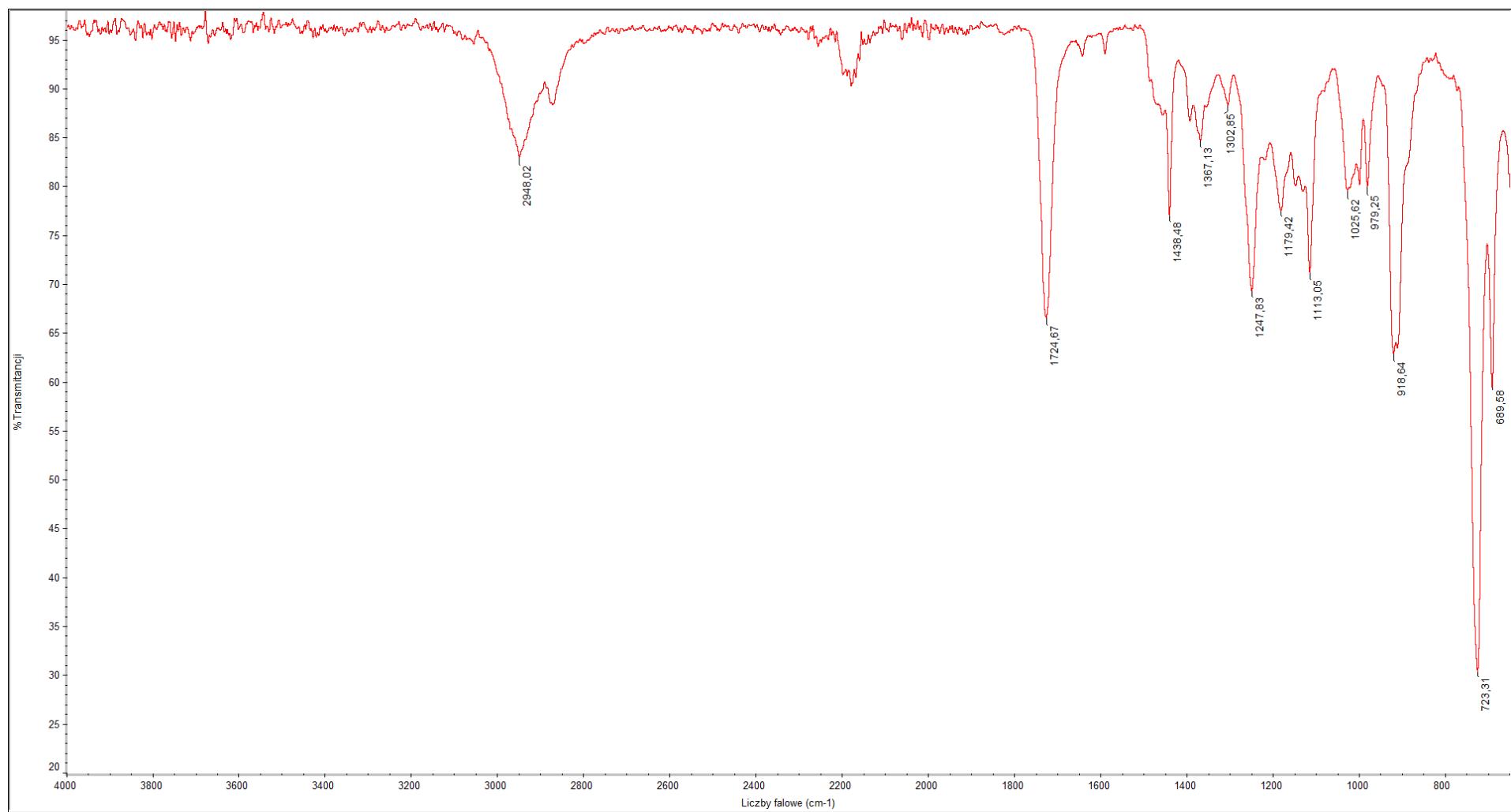
IR spectrum of product **7e**; ATR (cm^{-1}).
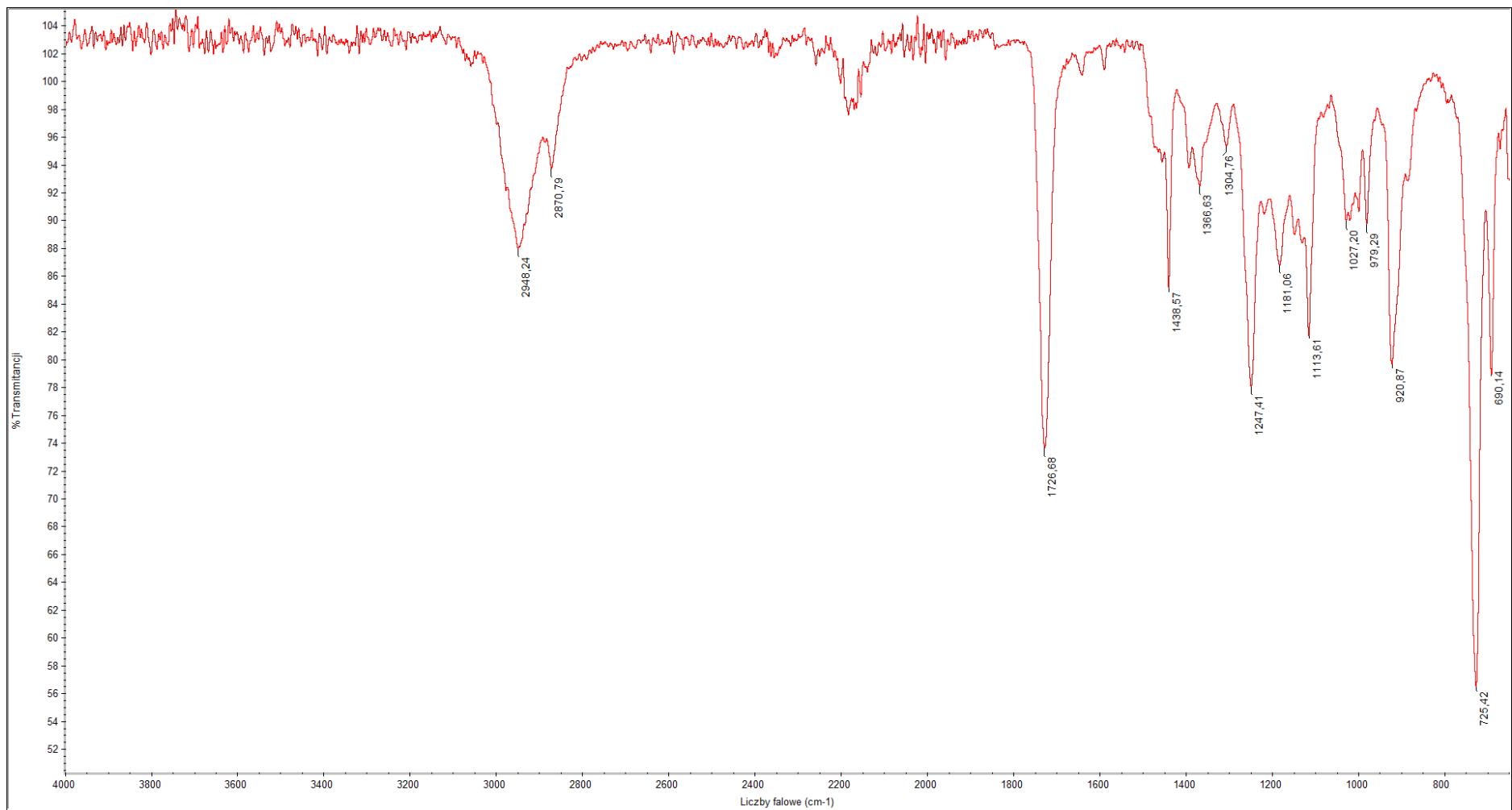
IR spectrum of product **7f**; ATR (cm⁻¹).
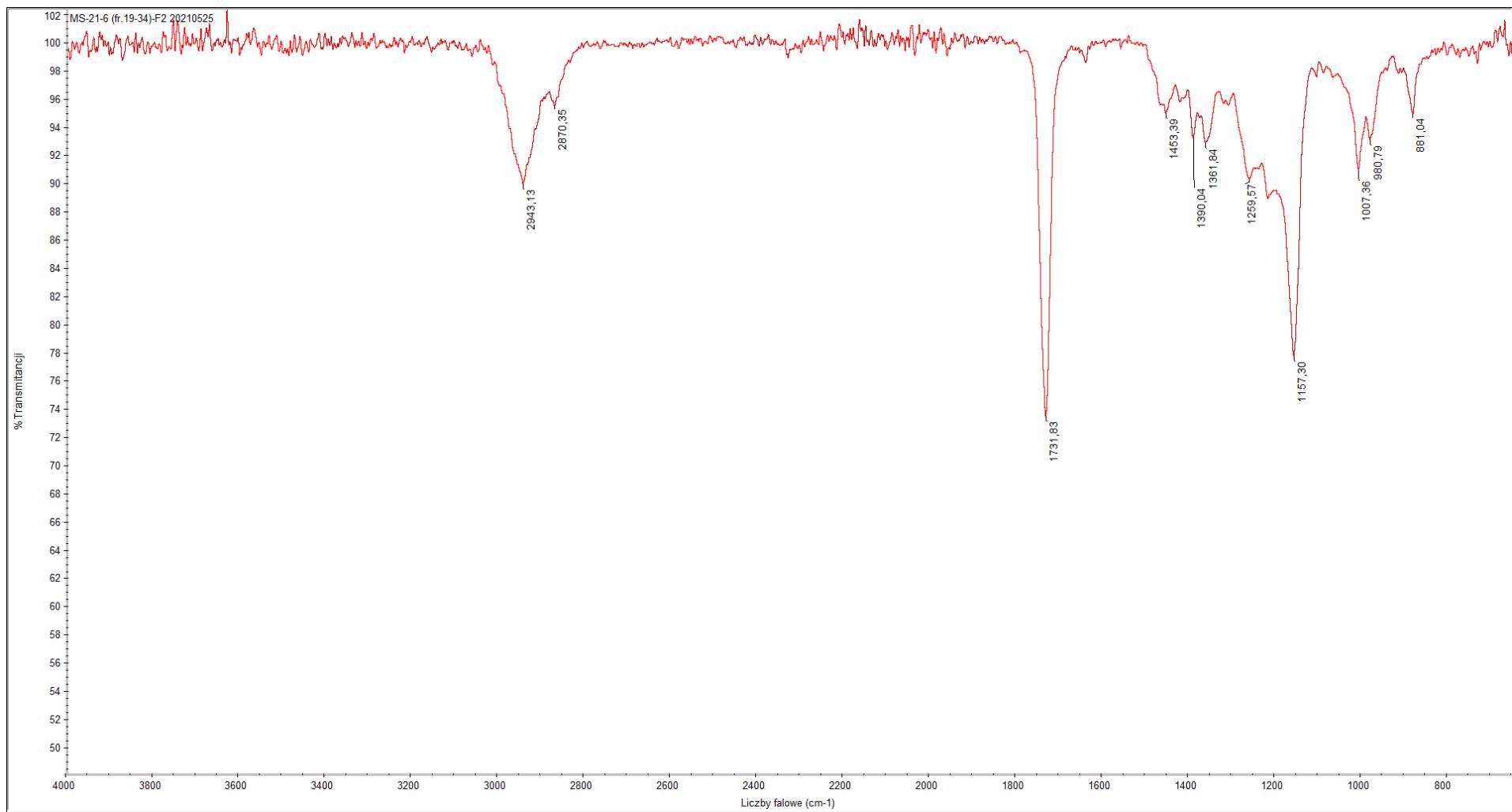
IR spectrum of product **8a**; ATR (cm-1).
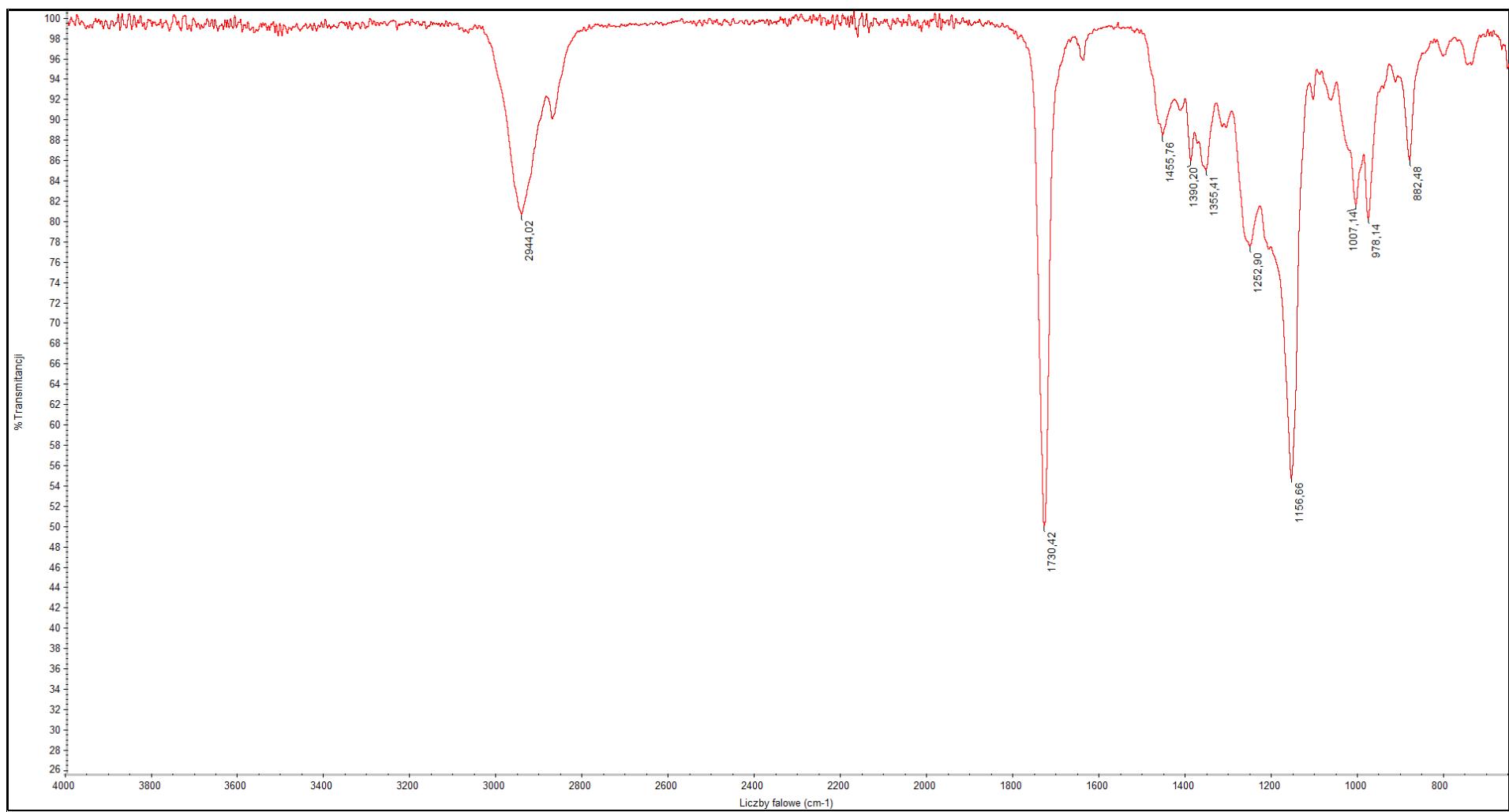
IR spectrum of product **8b**; ATR (cm^{-1}).
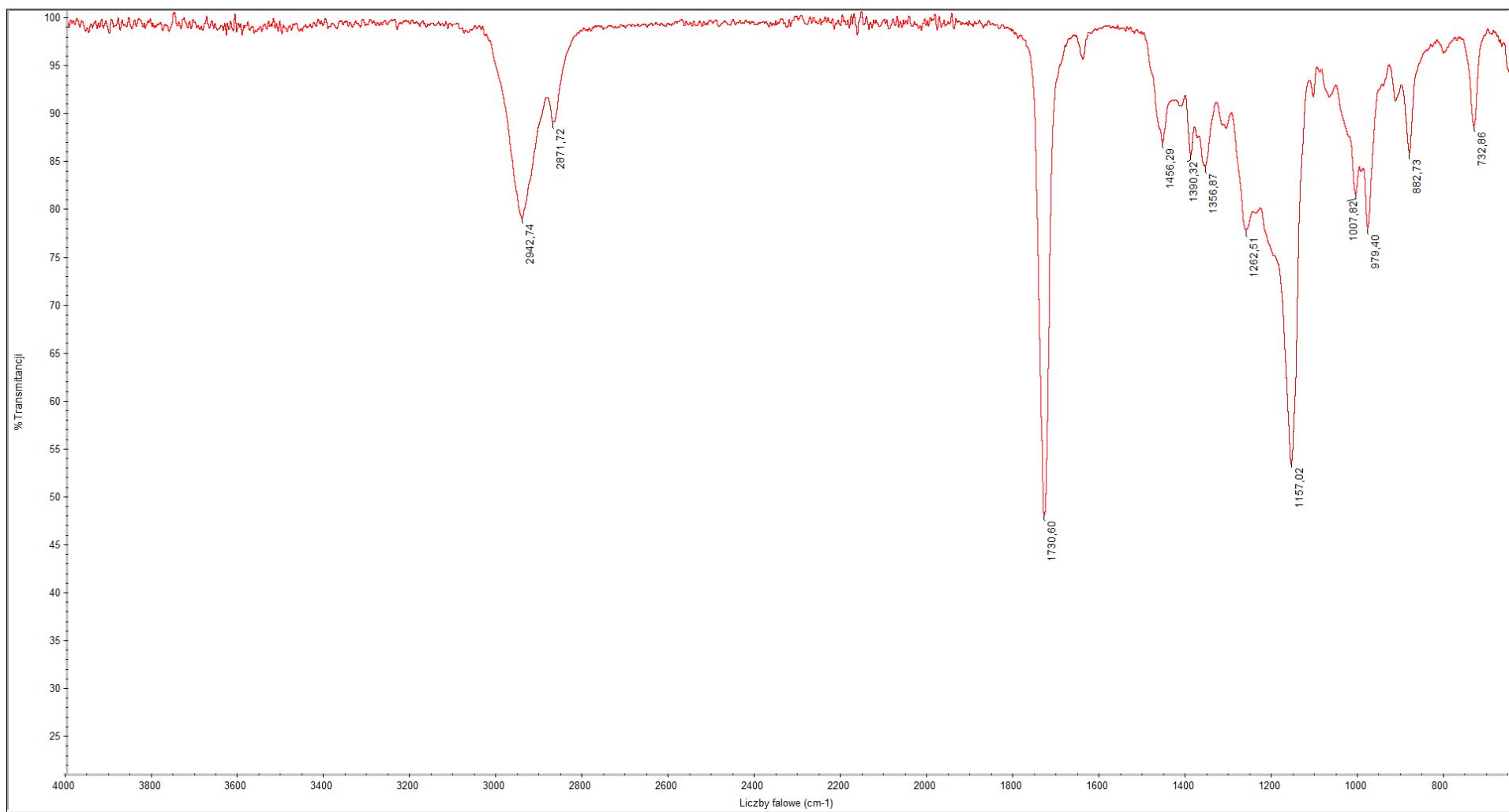
IR spectrum of product **8c**; ATR (cm⁻¹).
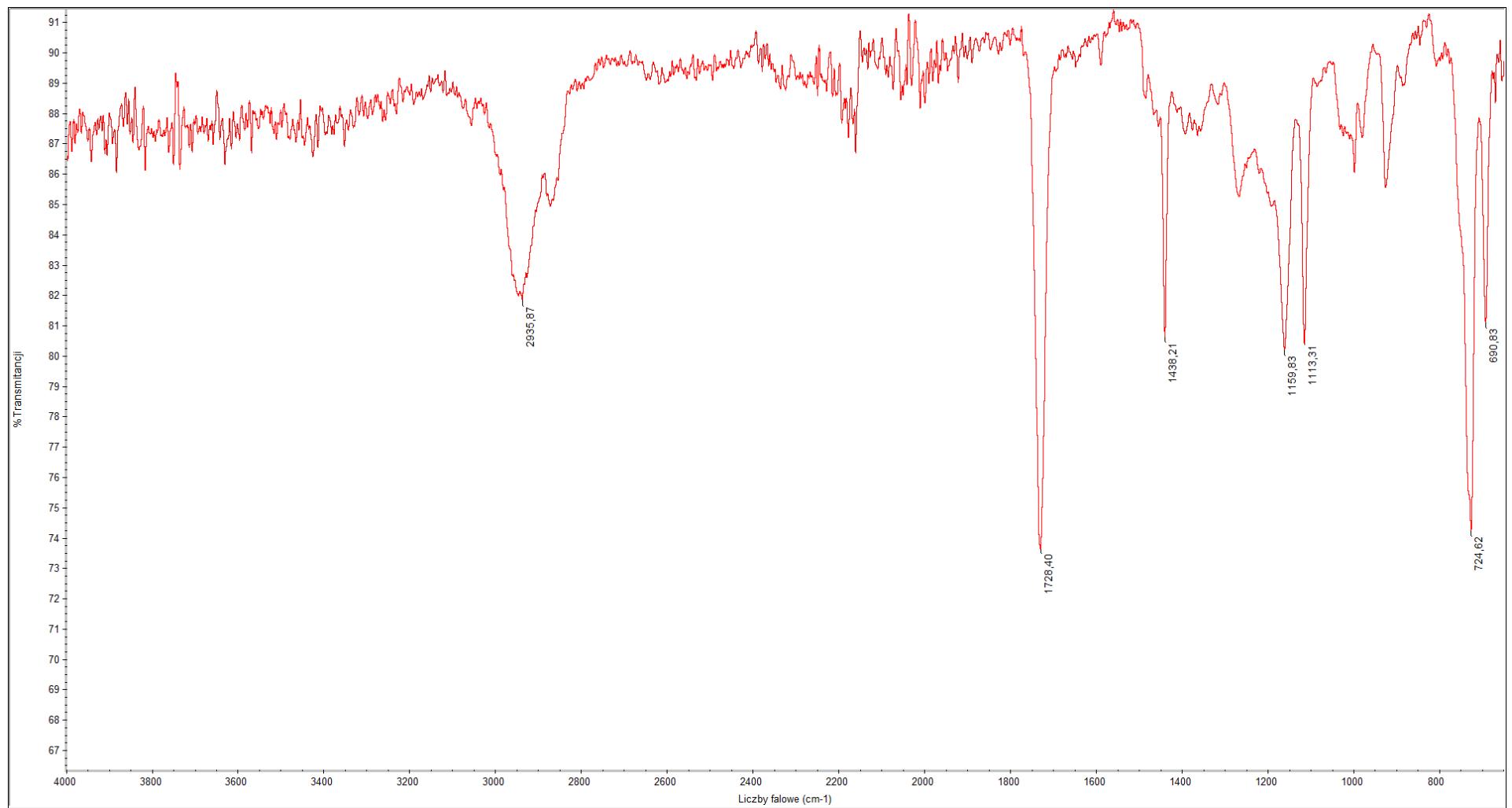
IR spectrum of product **9b**; ATR (cm^{-1}).
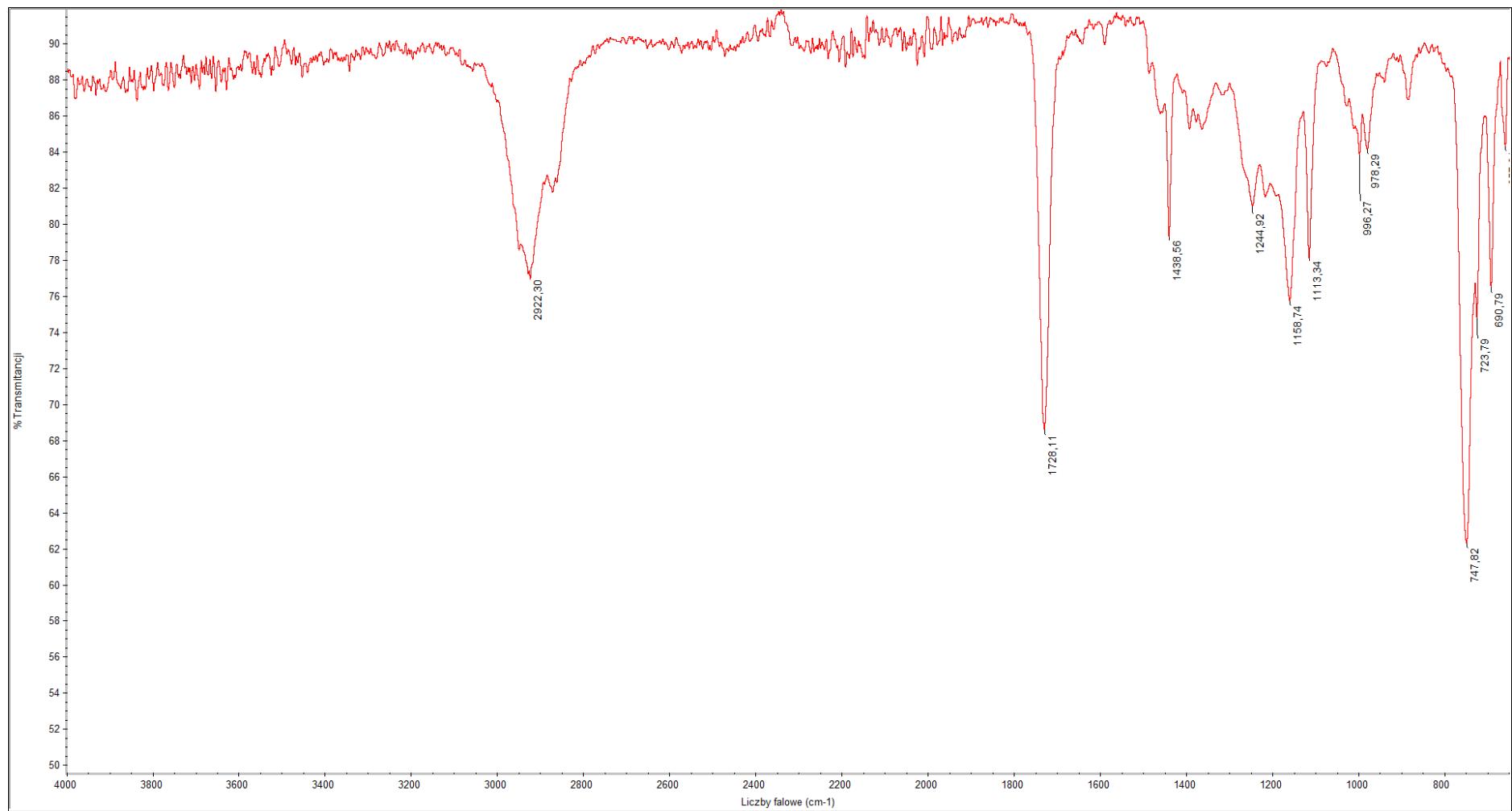
IR spectrum of product **9c**; ATR (cm⁻¹).