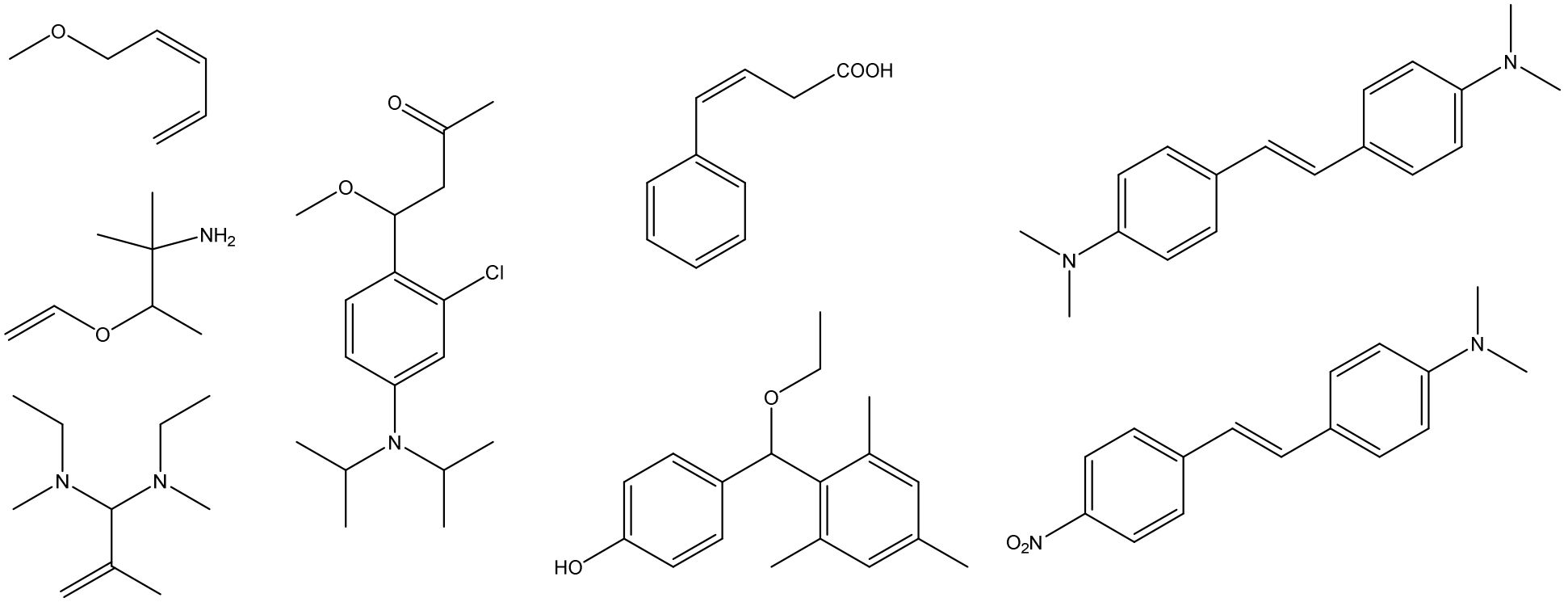
Zadanie 1. Narysuj przewidywane widma ^{1}H-NMR dla następujących struktur. Uważaj na protony diastereotopowe (3 przypadki) oraz symetrię związku. Podaj multipletowość sygnałów, stosunek intensywności w multipletach (jeśli nie jest to m), intensywność integralną sygnału.

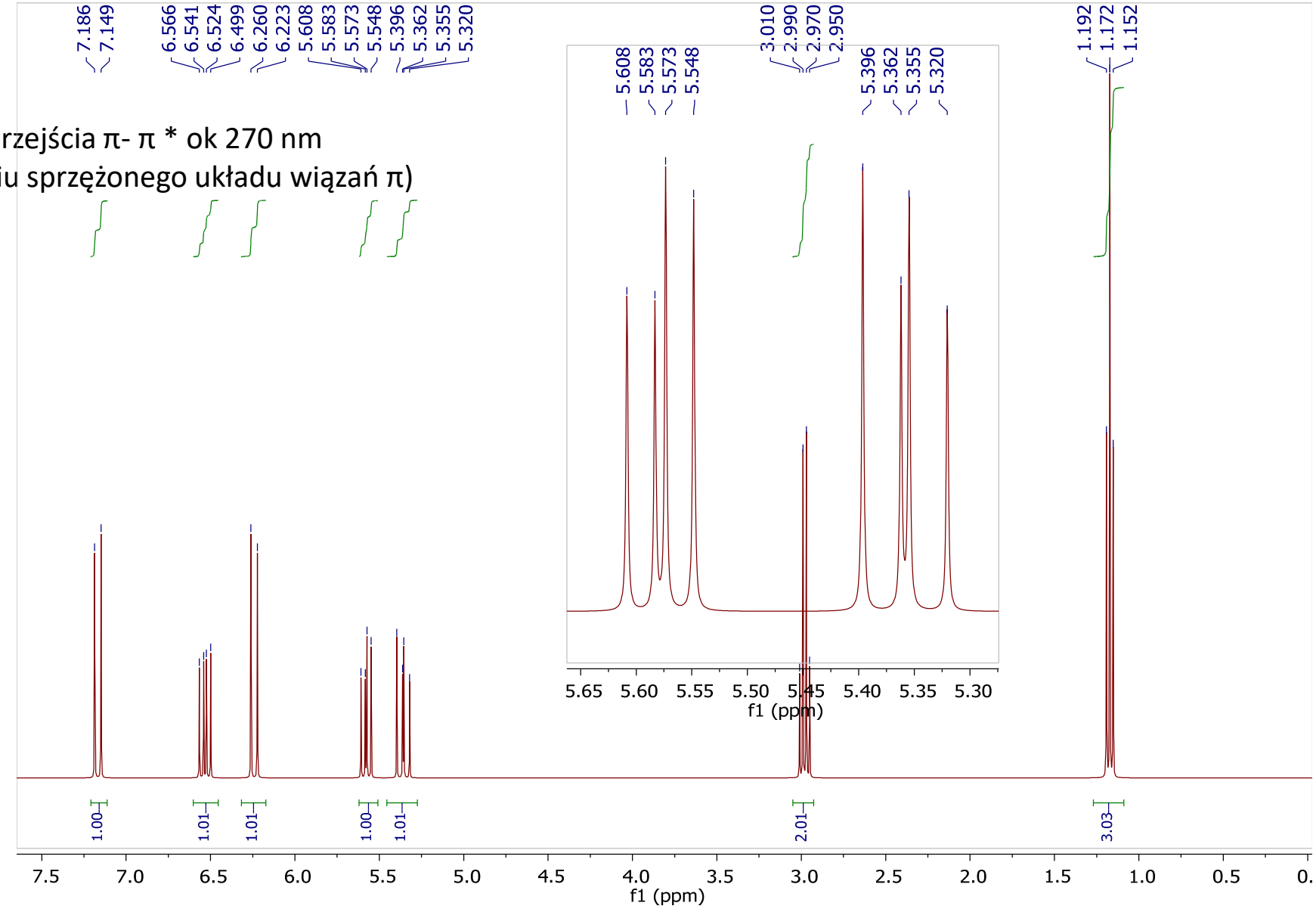


Zadanie 2. Na podstawie widma 1H NMR zmierzonych na aparacie Bruker 400 MHz ($CDCl_3$) określ strukturę związku chemicznego.

(a)

$C_7H_{10}O$

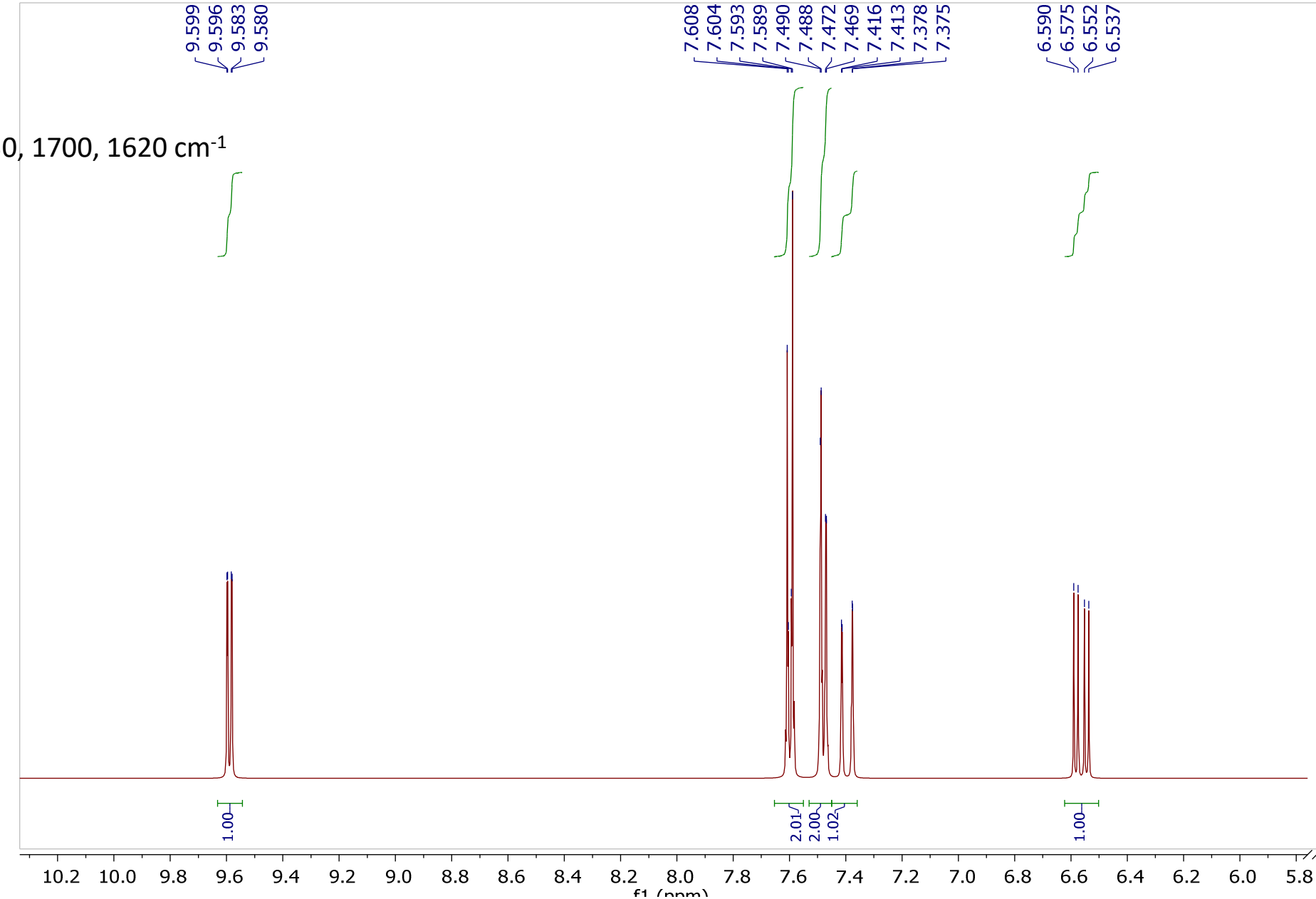
(W widmie UV-Vis sygnał przejścia π- π * ok 270 nm
Świadczący o występowaniu sprzężonego układu wiązań π)



(b)

C_9H_7ClO

IR: 3040, 2810, 2730, 1700, 1620 cm^{-1}

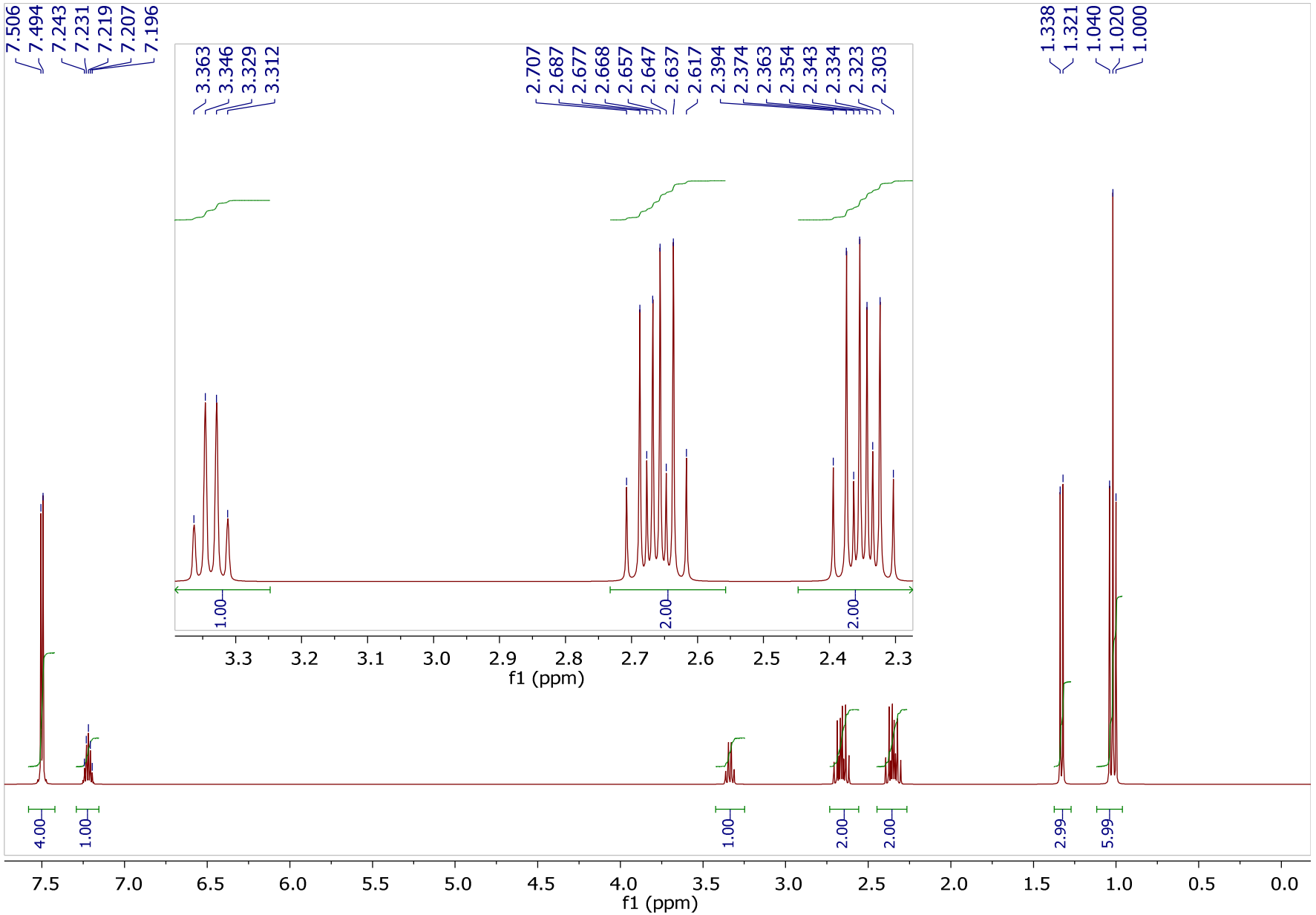


(c)

$C_{12}H_{19}N$

Racemat

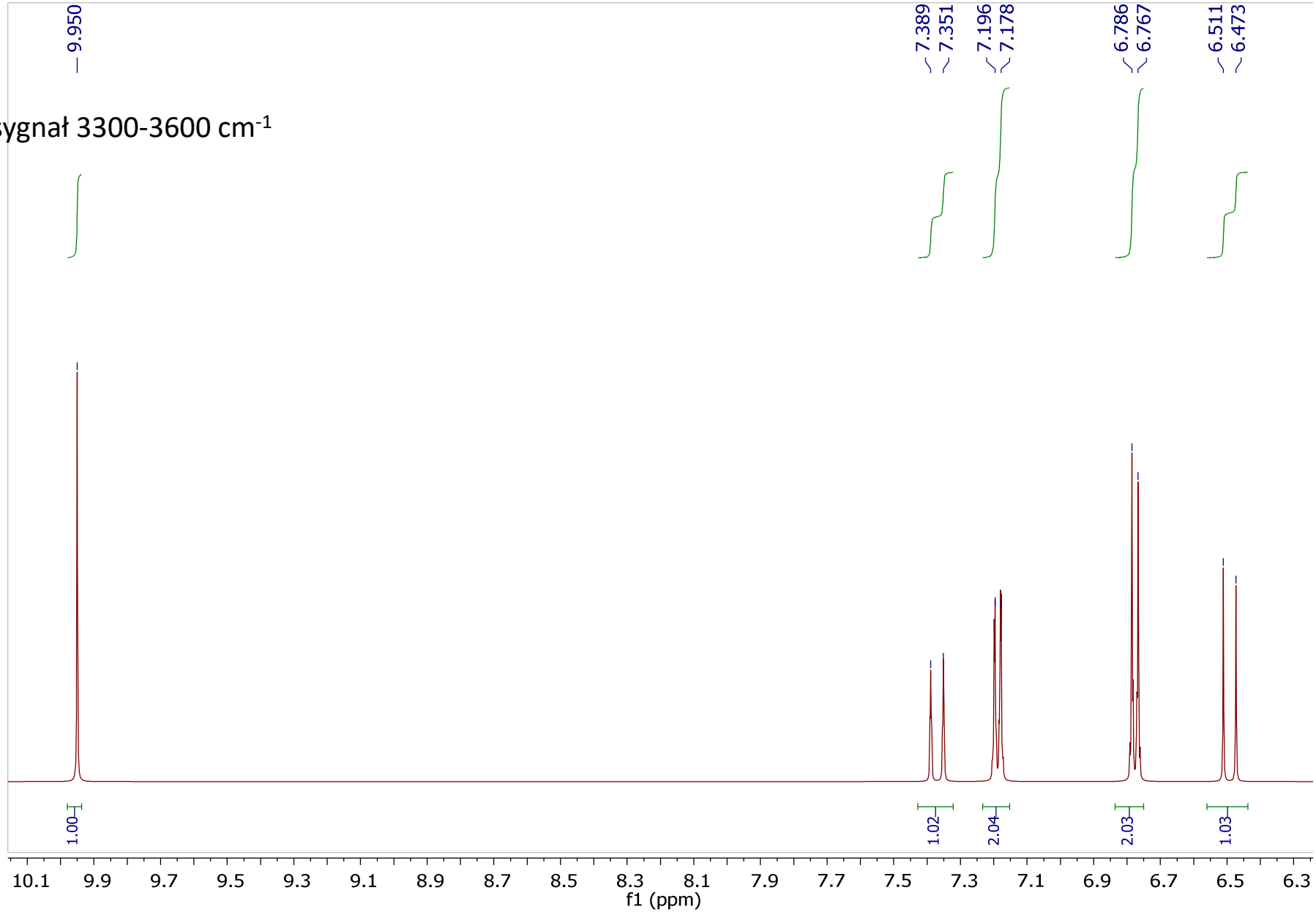
Pierścień aromatyczny monopodstawiony



(d)

C_8H_7IO

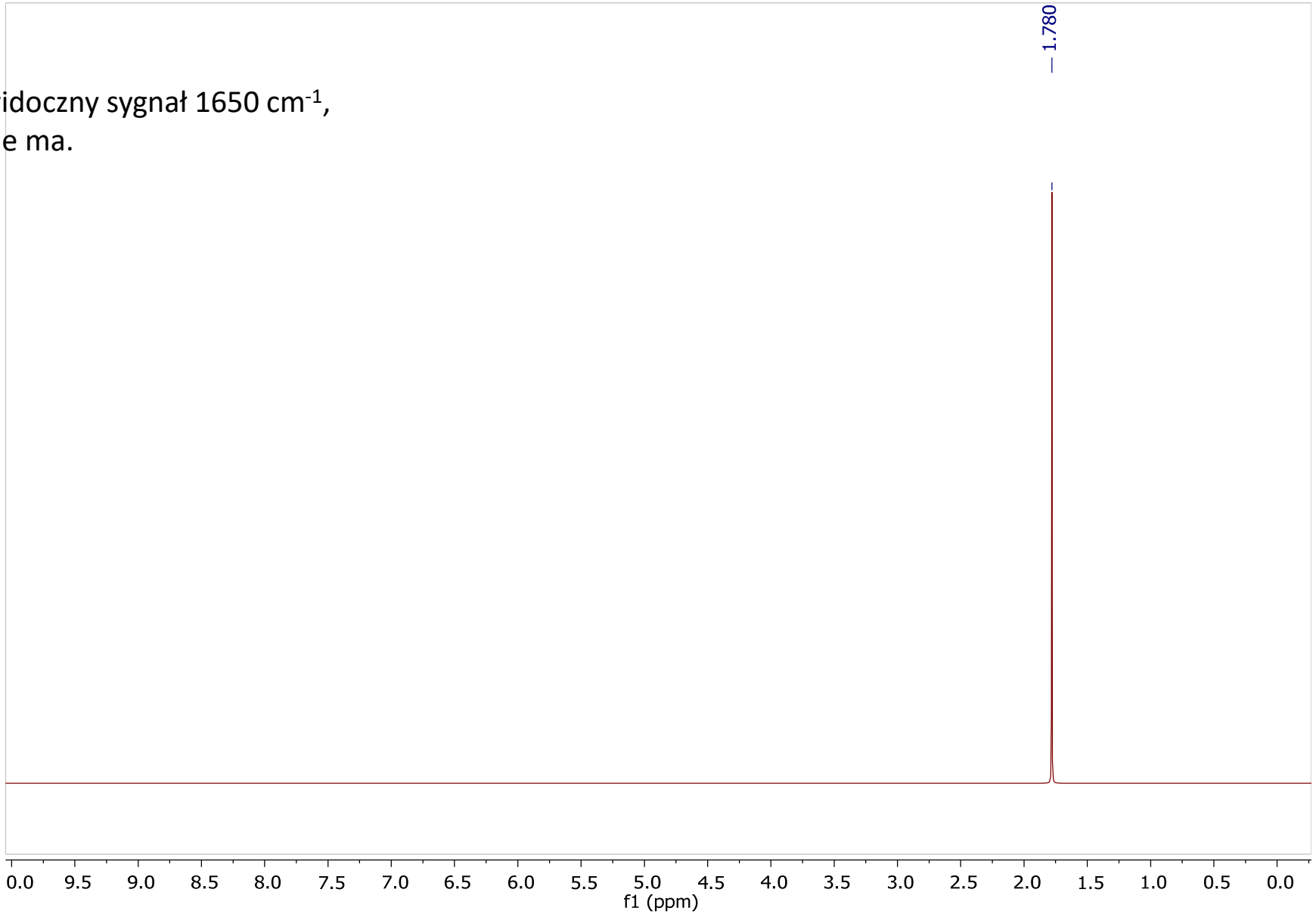
W Widmie IR szeroki sygnał 3300-3600 cm^{-1}



(e)

C_6H_{12}

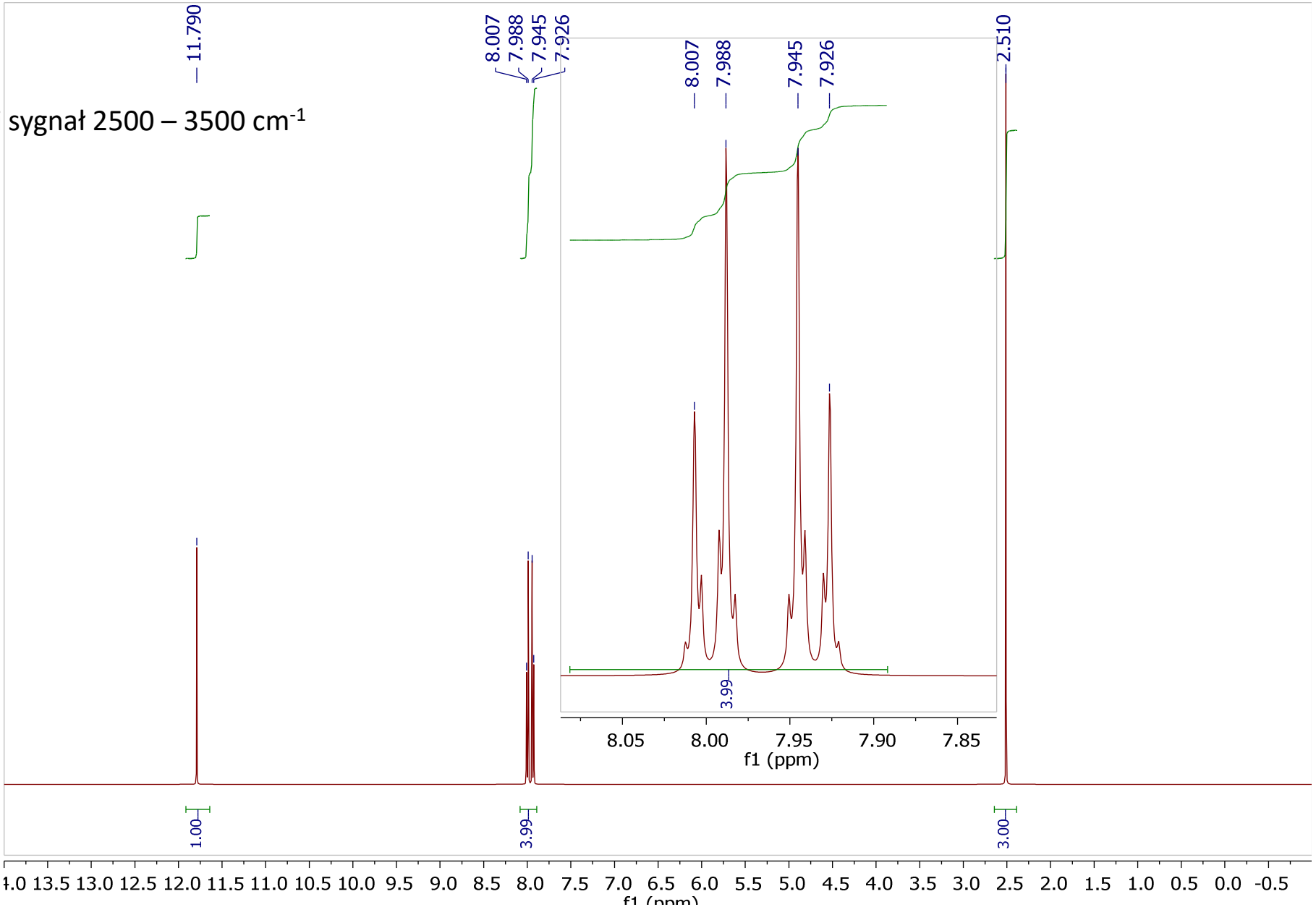
W widmie Ramana widoczny sygnał 1650 cm^{-1},
ale w widmie IR go nie ma.



(f)

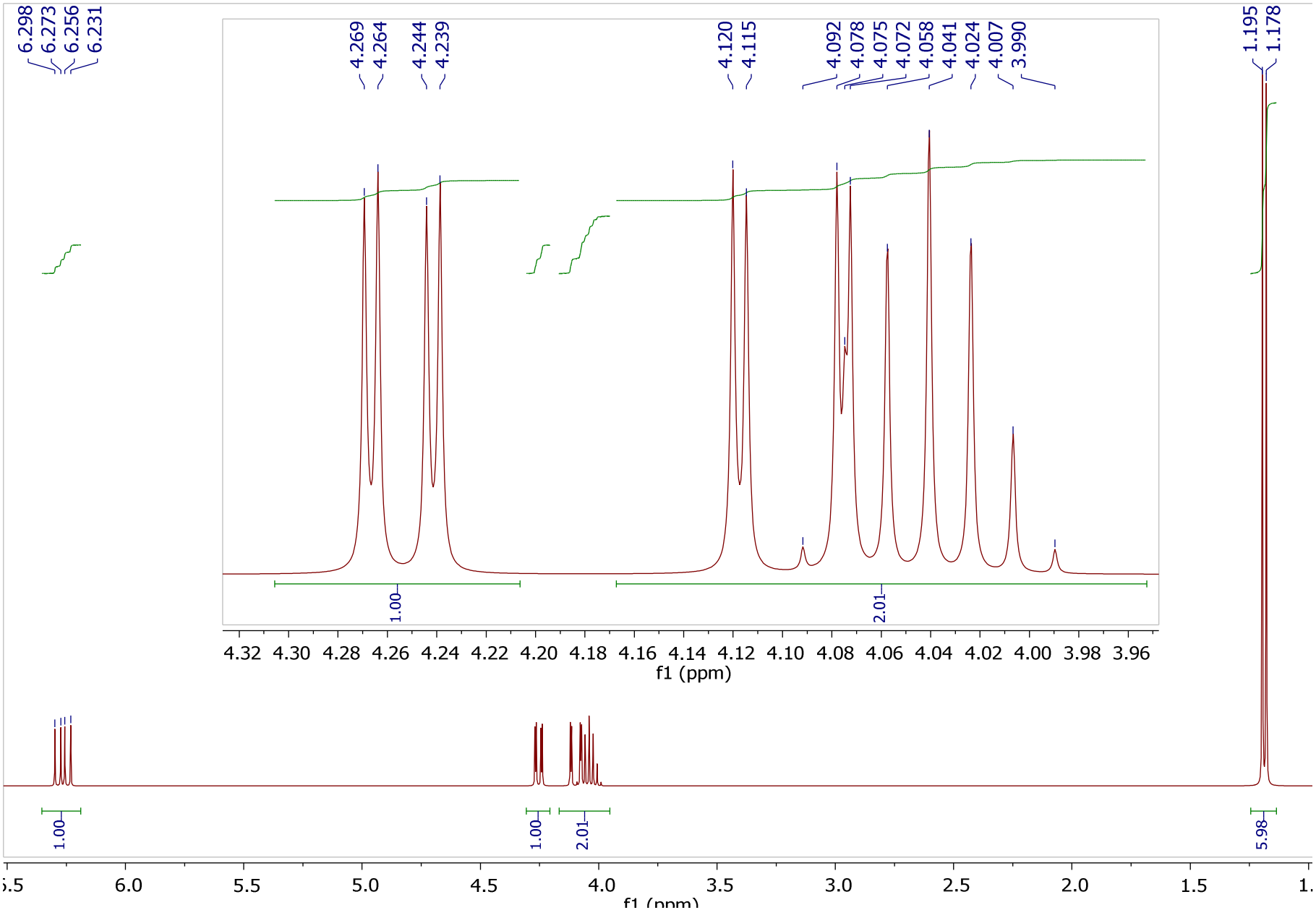
$C_9H_8O_3$

W widmie IR szeroki sygnał 2500 – 3500 cm^{-1}



(g)

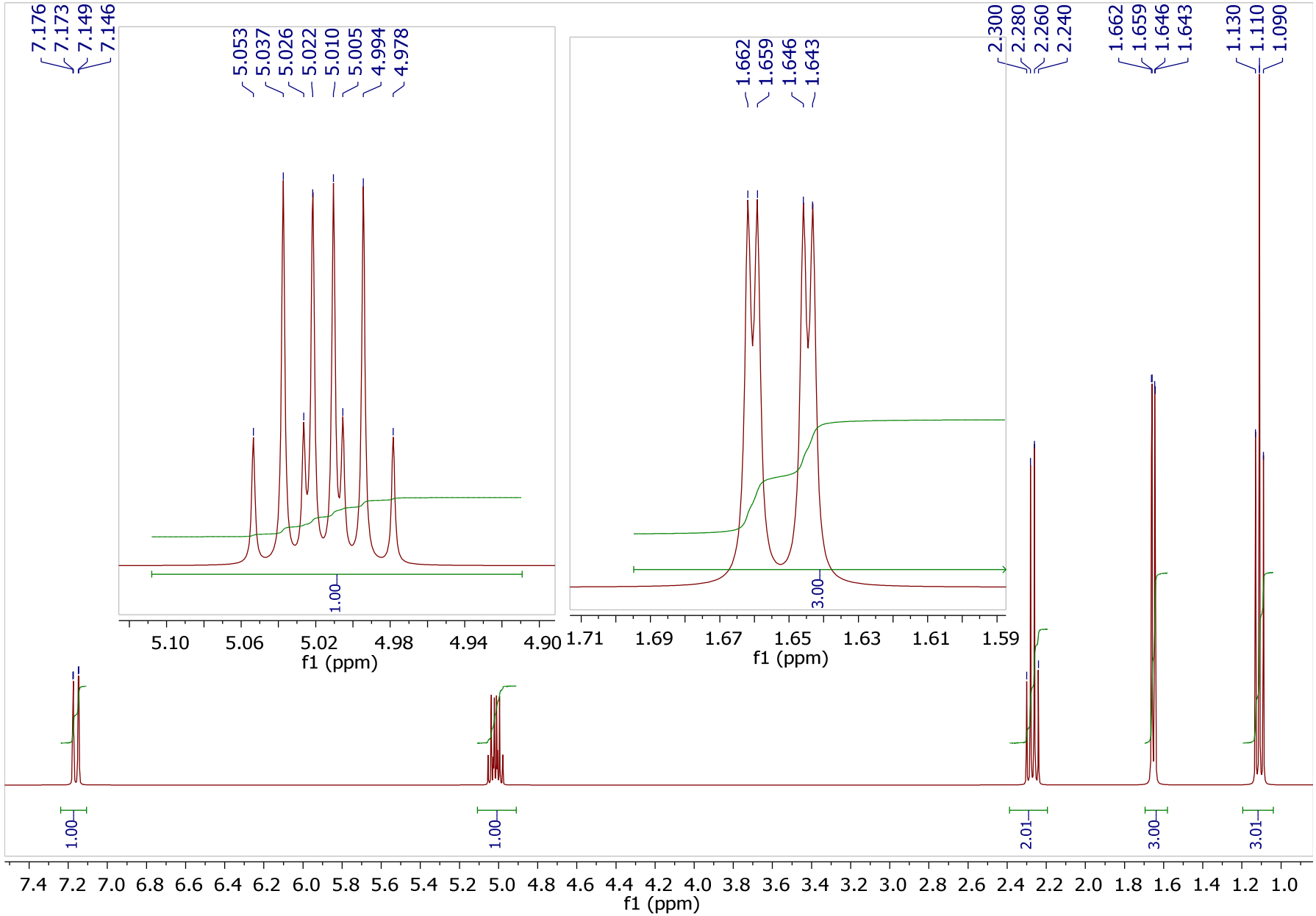
$C_5H_{10}O$


6.298
6.273
6.256
6.231
4.269
4.264
4.244
4.239
4.120
4.115
4.092
4.078
4.075
4.072
4.058
4.041
4.024
4.007
3.990
1.195
1.178
1.00
2.01
4.32 4.30 4.28 4.26 4.24 4.22 4.20 4.18 4.16 4.14 4.12 4.10 4.08 4.06 4.04 4.02 4.00 3.98 3.96
f1 (ppm)
1.00
1.00
2.01
5.98
6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)

(h)

$C_6H_{10}O_2$

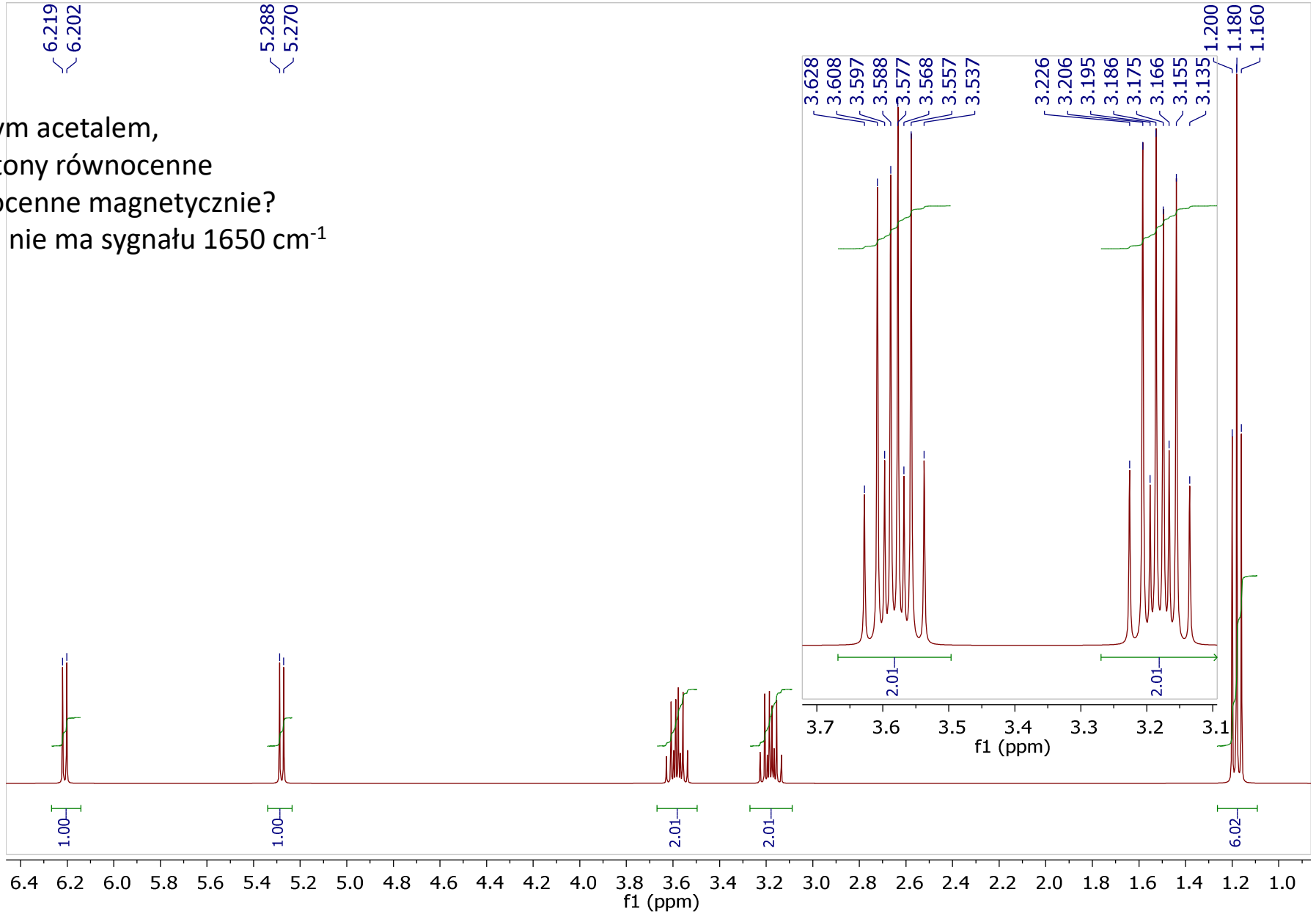
Ester



(i)

$C_6H_{12}Cl_2O_2$

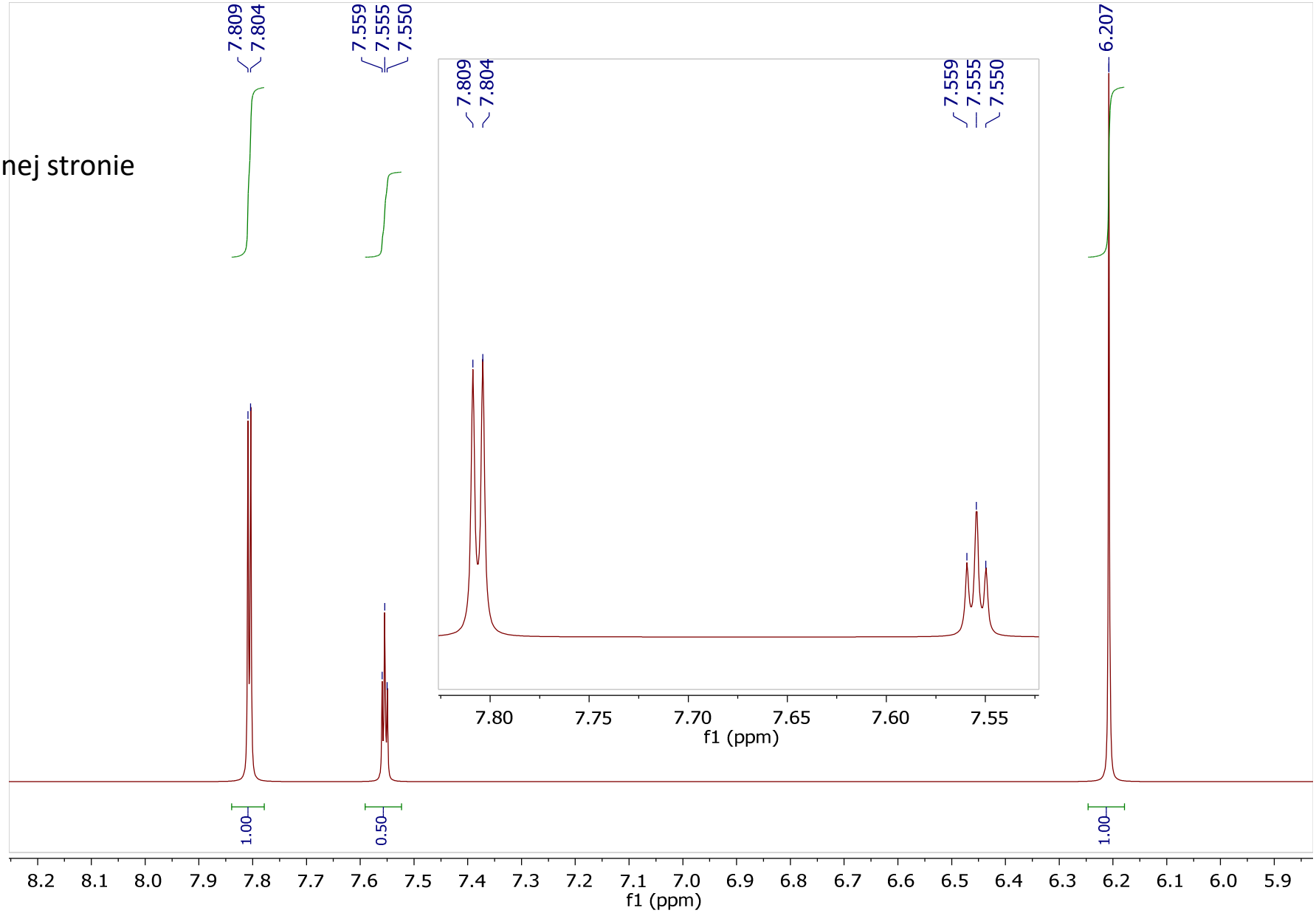
Związek jest achiralnym acetalem,
ale czy wszystkie protony równocenne
chemicznie, są równocenne magnetycznie?
W widmie IR i Raman nie ma sygnału 1650 cm^{-1}



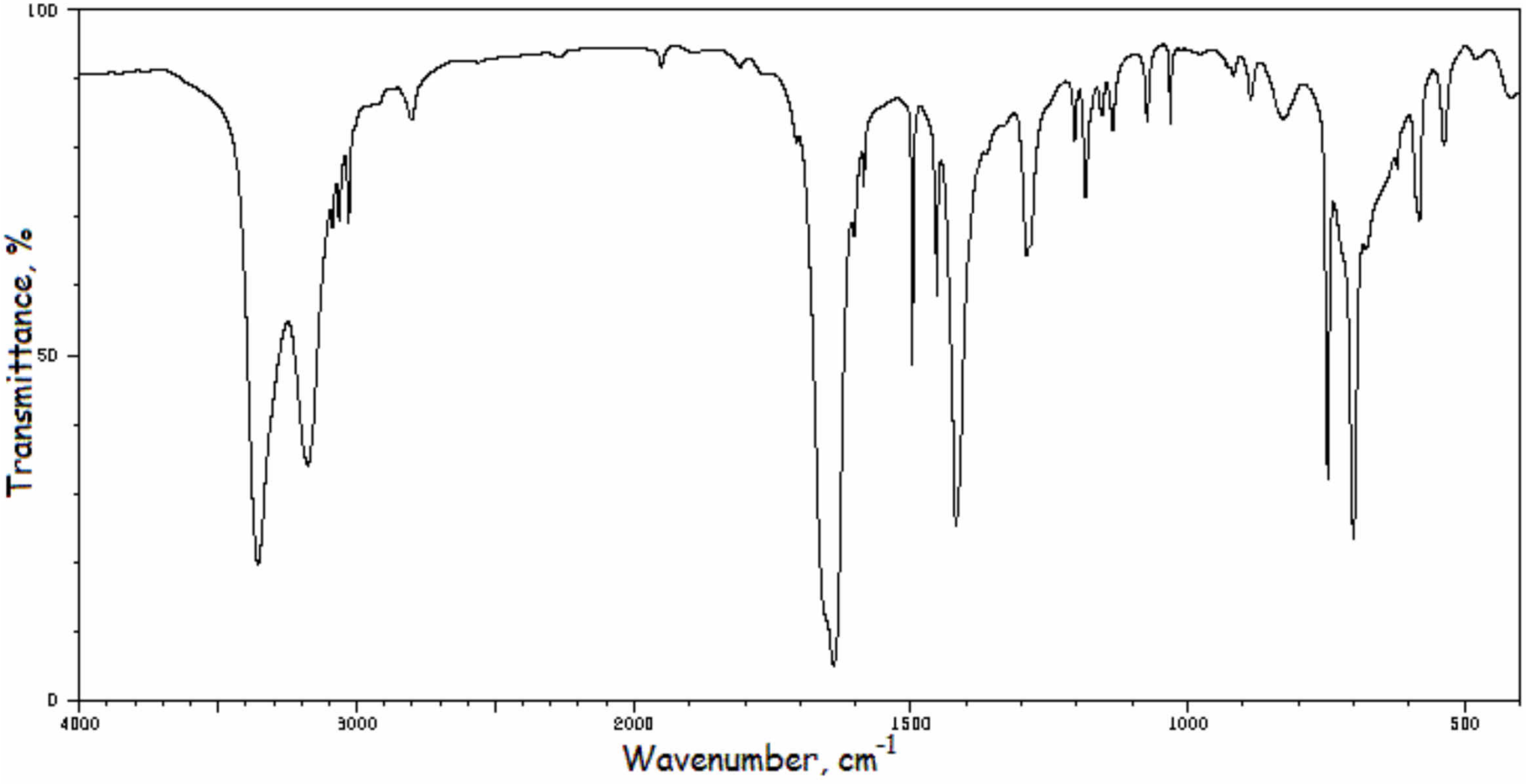
(j)

$C_7H_5Cl_2NO$

IR załączone na następnej stronie



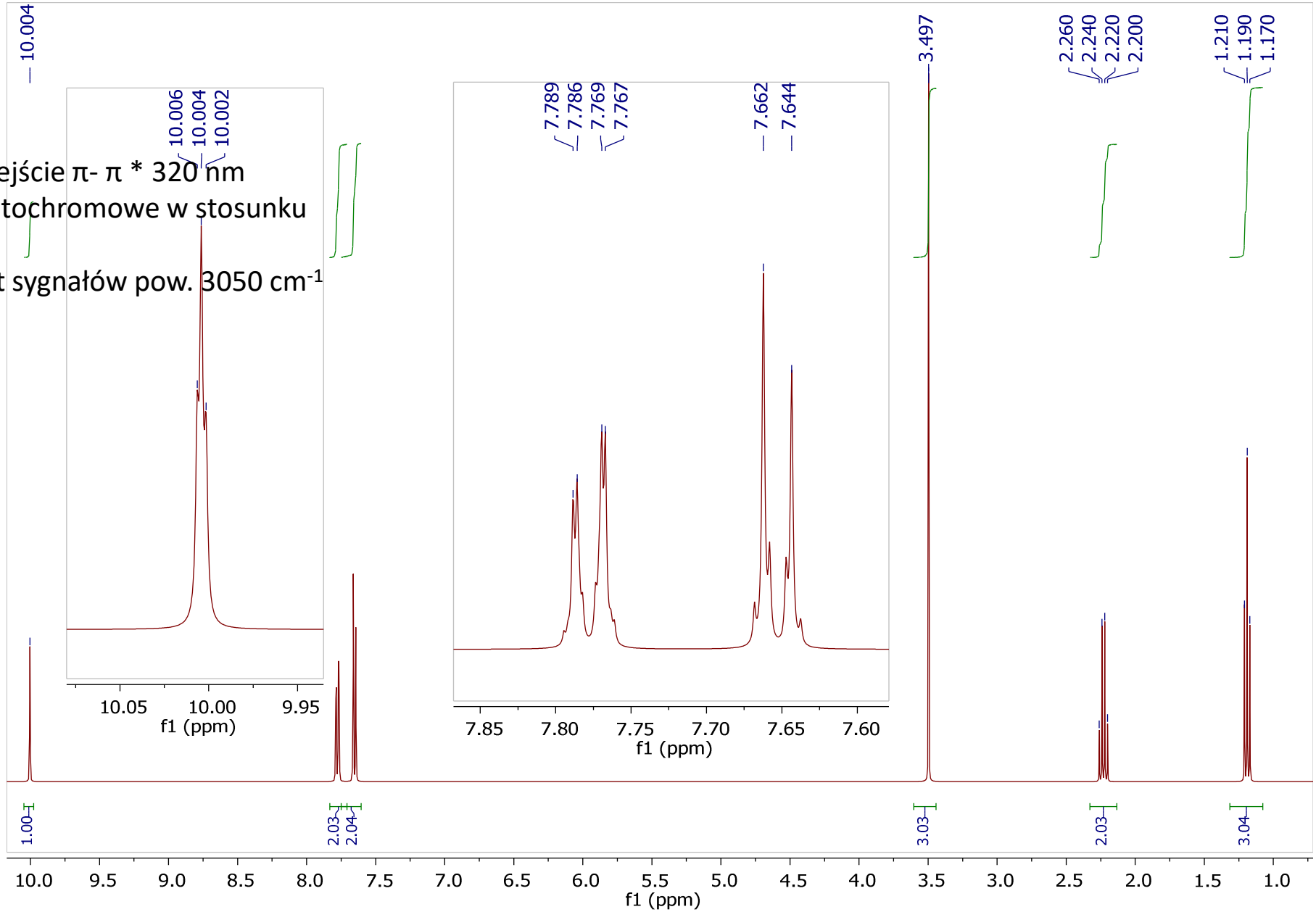
(j)


100
50
0
Transmittance, %
4000
3000
2000
1500
1000
500
Wavenumber, cm-1

(k)

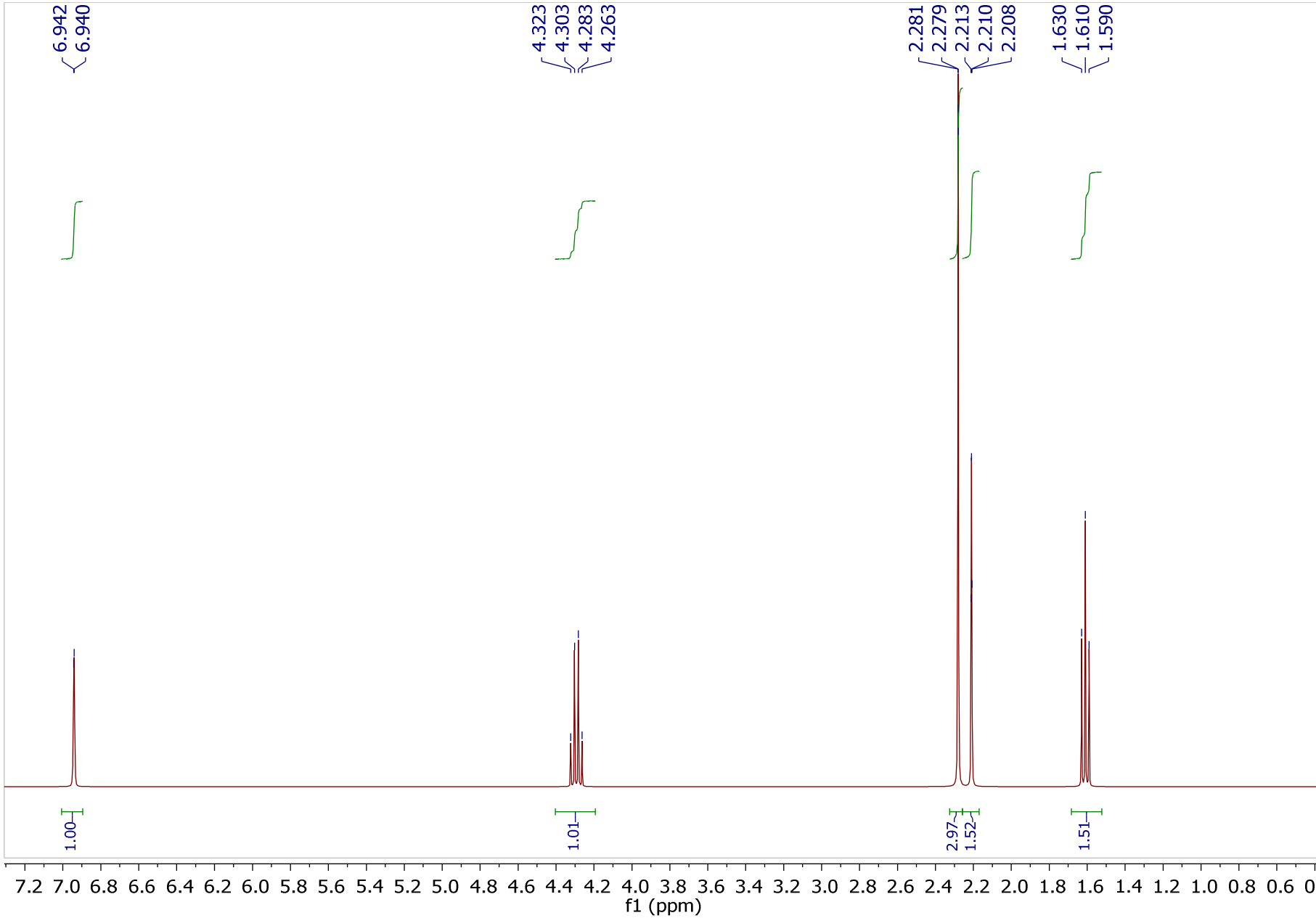
$C_{11}H_{13}NO_2$

W widmie UV-Vis przejście π- π * 320 nm
(silne przesunięcie batochromowe w stosunku do benzenu)
W widmie IR brak jest sygnałów pow. 3050 cm^{-1}



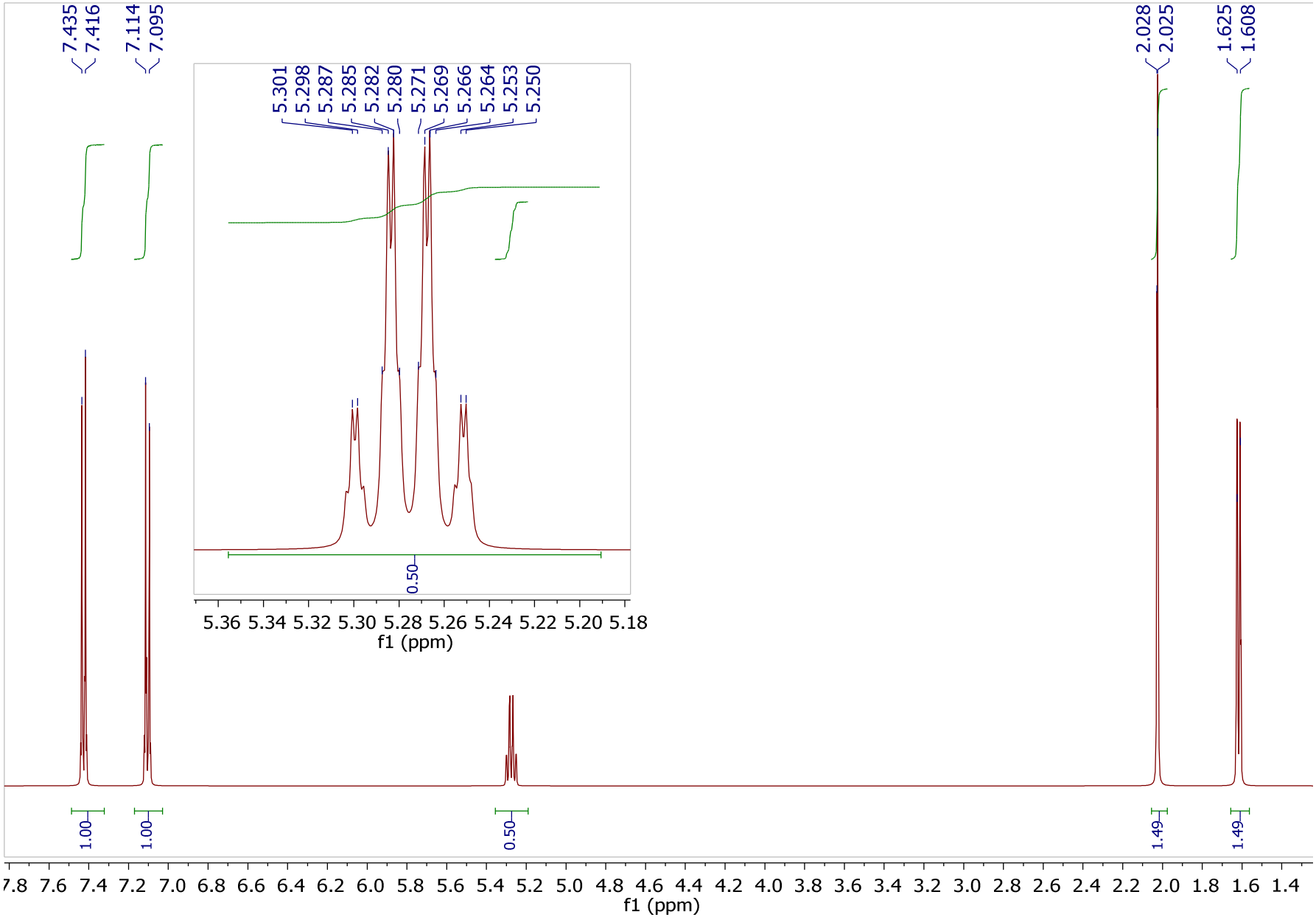
(l)

$C_{11}H_{16}O$


6.942
6.940
4.323
4.303
4.283
4.263
2.281
2.279
2.213
2.210
2.208
1.630
1.610
1.590
1.00
1.01
2.97
1.52
1.51
7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0
f1 (ppm)

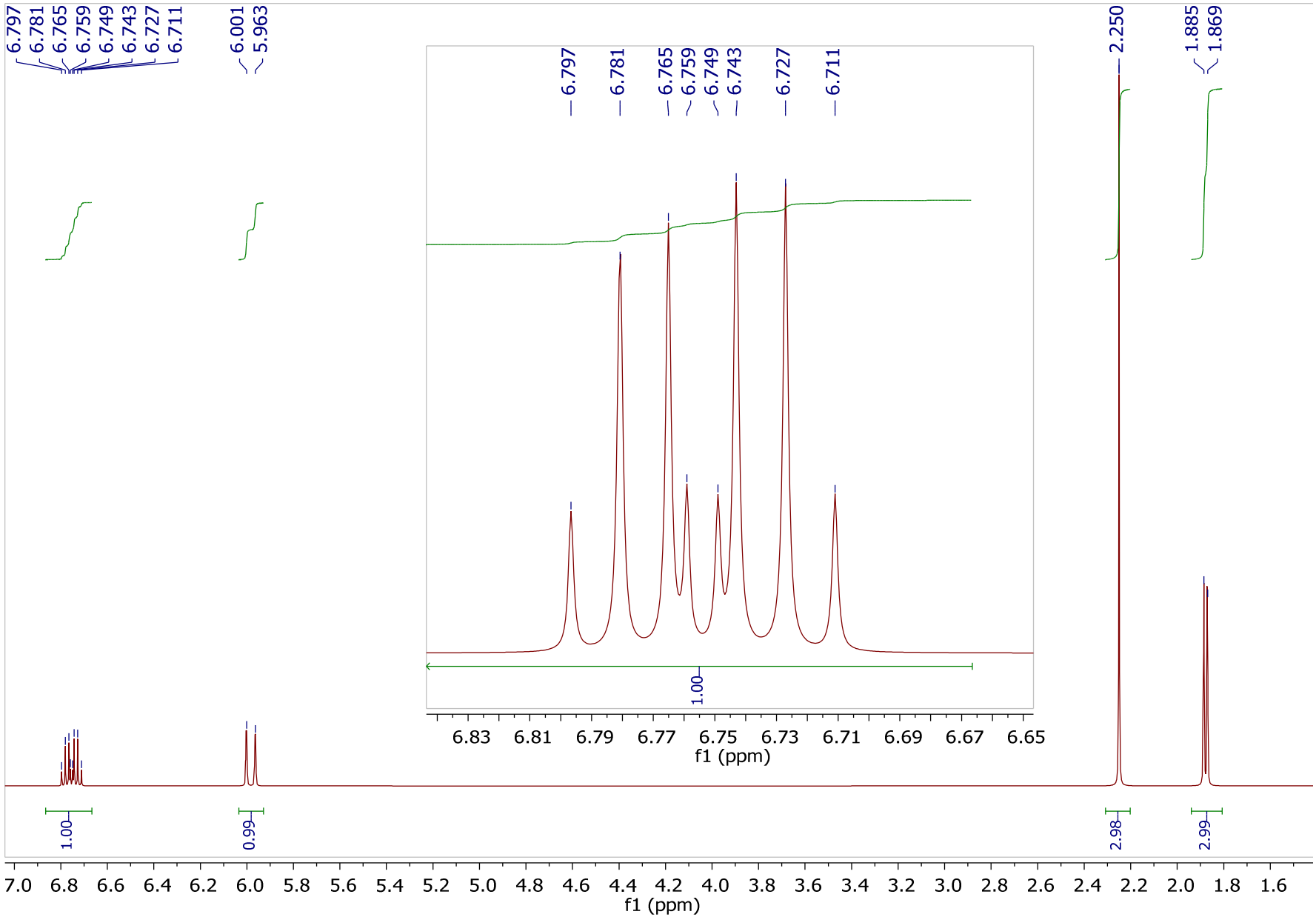
(m)

$C_{10}H_{11}Cl$


7.435
7.416
7.114
7.095
2.028
2.025
1.625
1.608
5.301
5.298
5.287
5.285
5.282
5.280
5.271
5.269
5.266
5.264
5.253
5.250
0.50
5.36 5.34 5.32 5.30 5.28 5.26 5.24 5.22 5.20 5.18
f1 (ppm)
1.00
1.00
0.50
1.49
1.49
7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4
f1 (ppm)

(n)

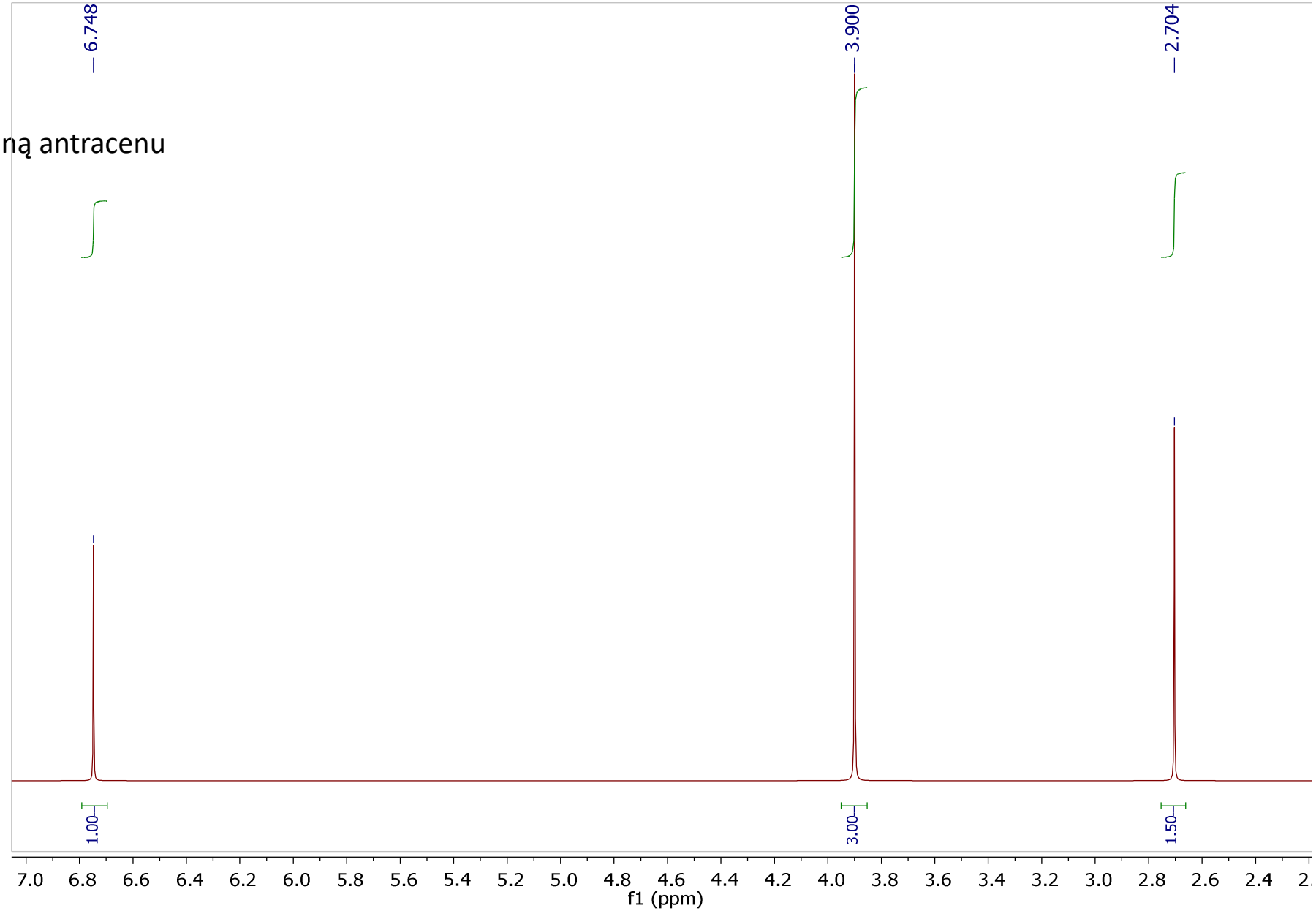
C_5H_8O


6.797
6.781
6.765
6.759
6.749
6.743
6.727
6.711
6.001
5.963
2.250
1.885
1.869
1.00
0.99
2.98
2.99
f1 (ppm)

(o)

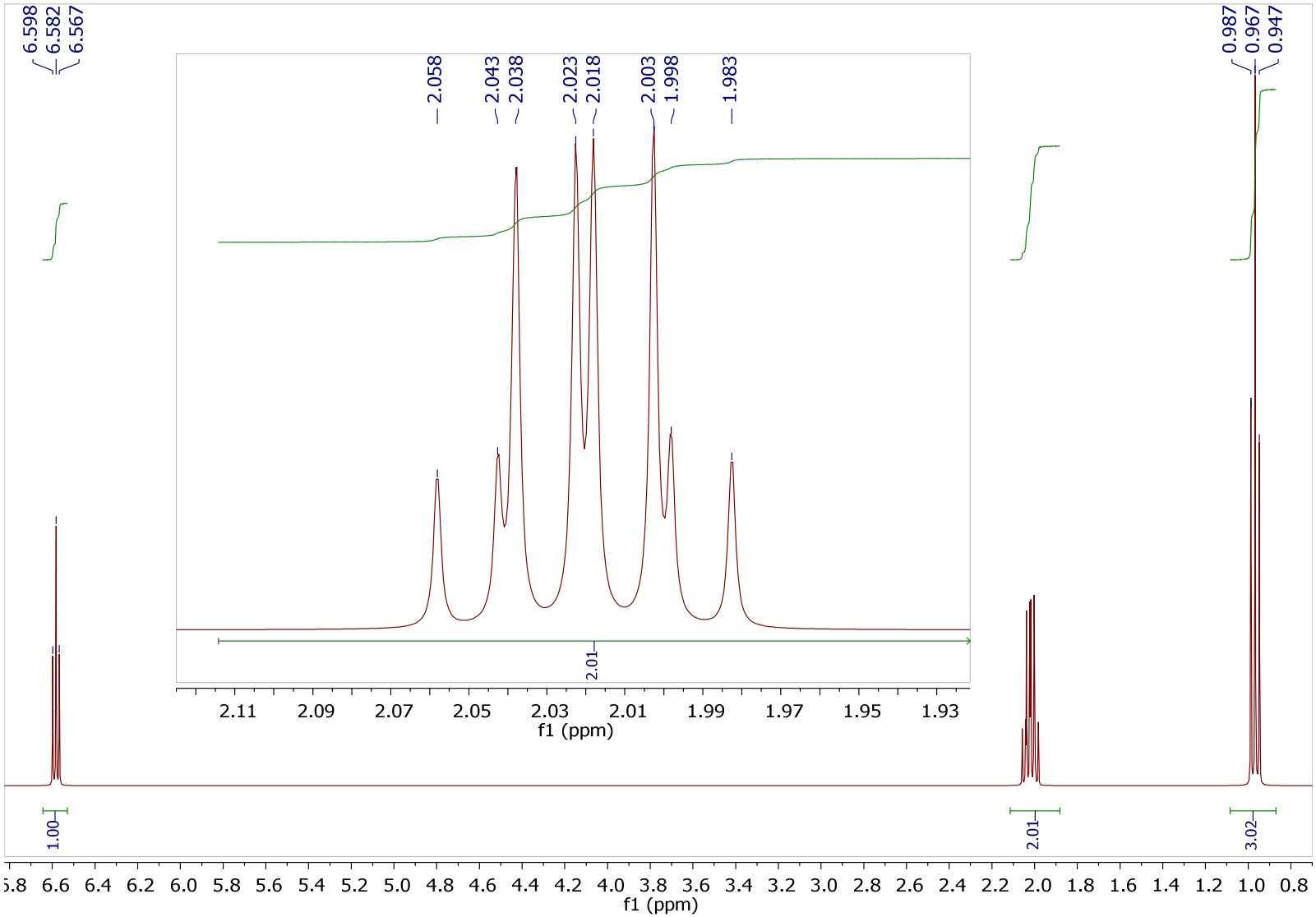
$C_{20}H_{22}O_4$

Związek jest pochodną antracenu



(p)

$C_4H_6Br_2$

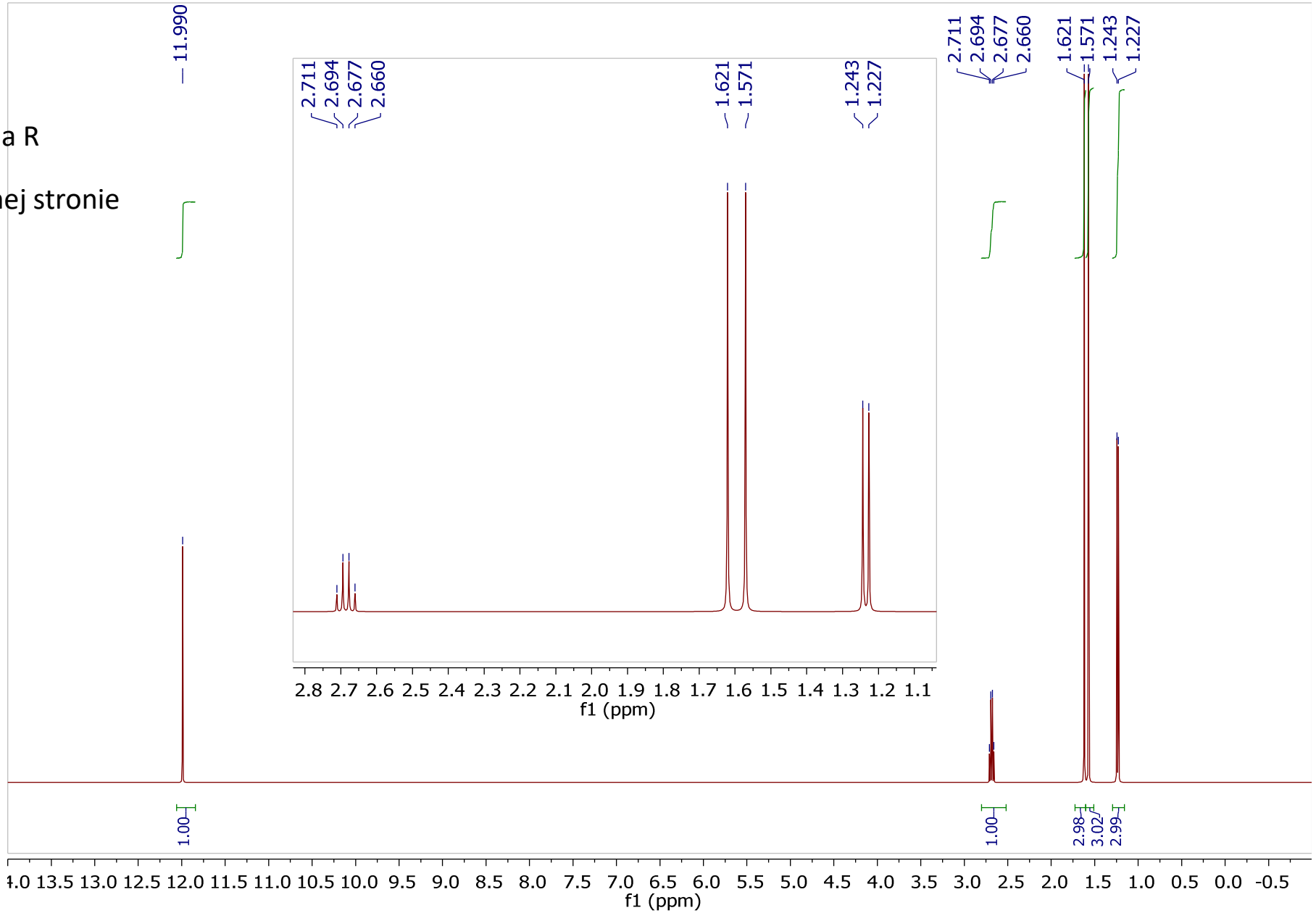

6.598
6.582
6.567
2.058
2.043
2.038
2.023
2.018
2.003
1.998
1.983
0.987
0.967
0.947
2.01
2.11 2.09 2.07 2.05 2.03 2.01 1.99 1.97 1.95 1.93
f1 (ppm)
1.00
2.01
3.02
6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8
f1 (ppm)

(r)

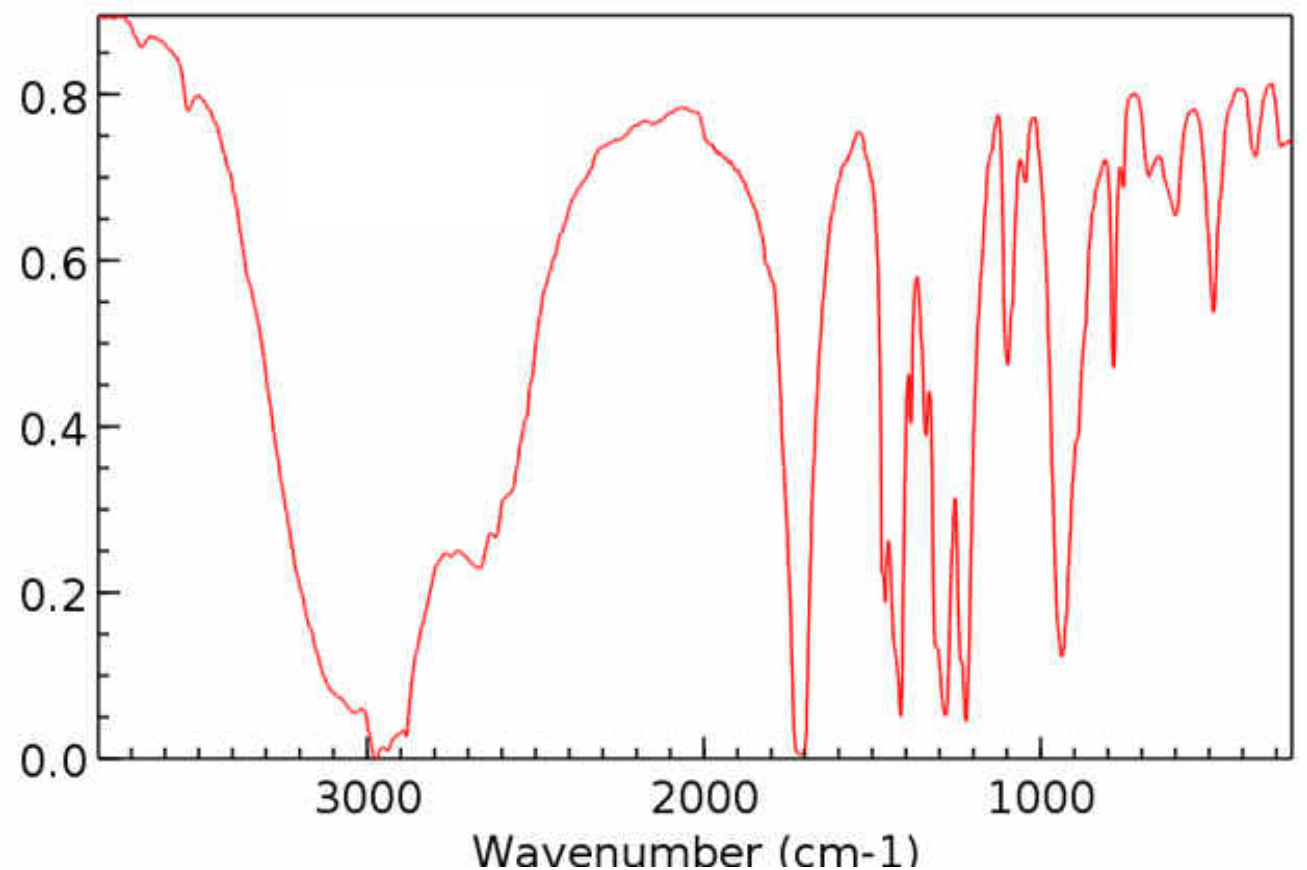
$C_6H_{11}ClO_2$

Konfiguracja absolutna R

Widmo IR na następnej stronie



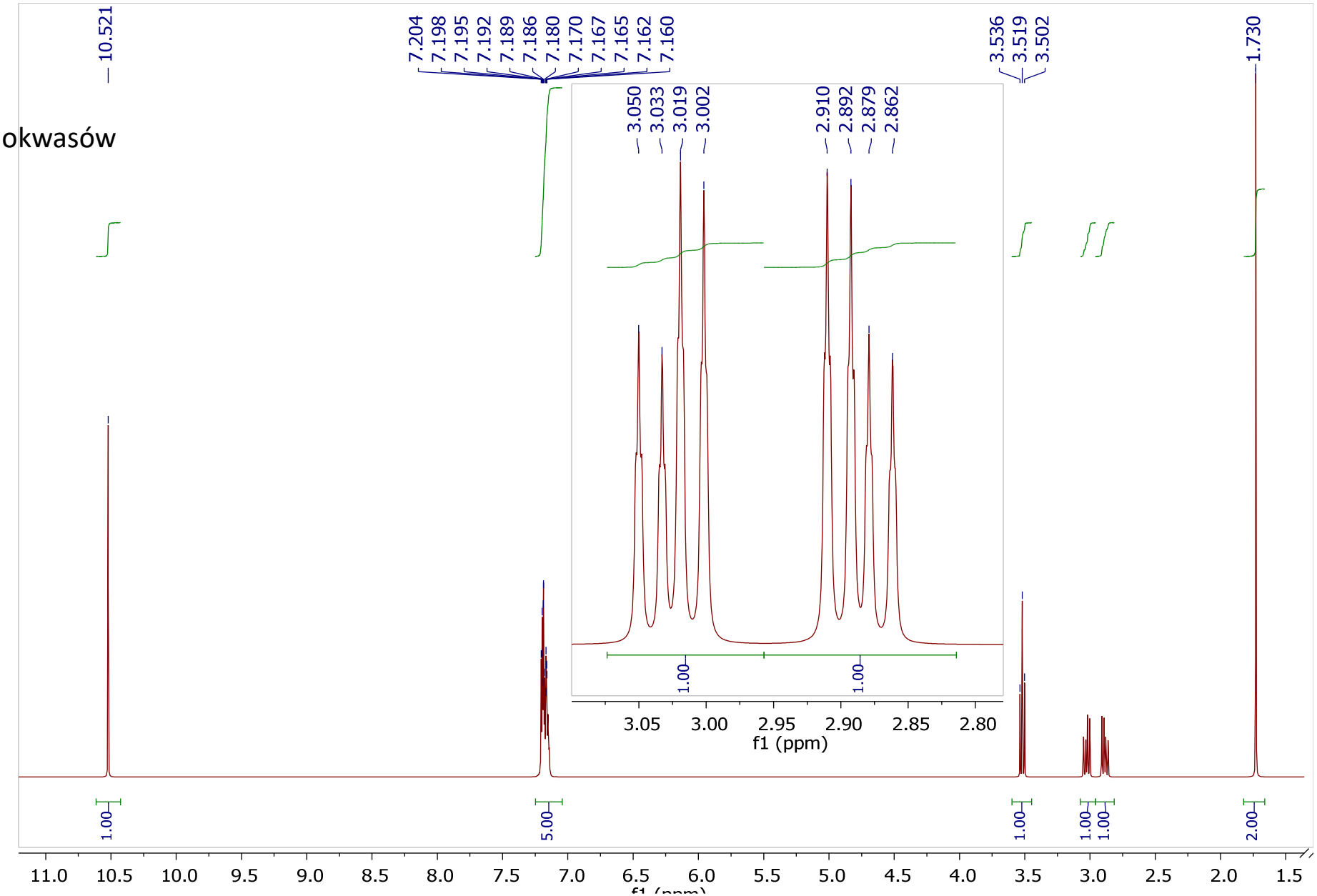
(r)



(s)

$C_9H_{11}NO_2$

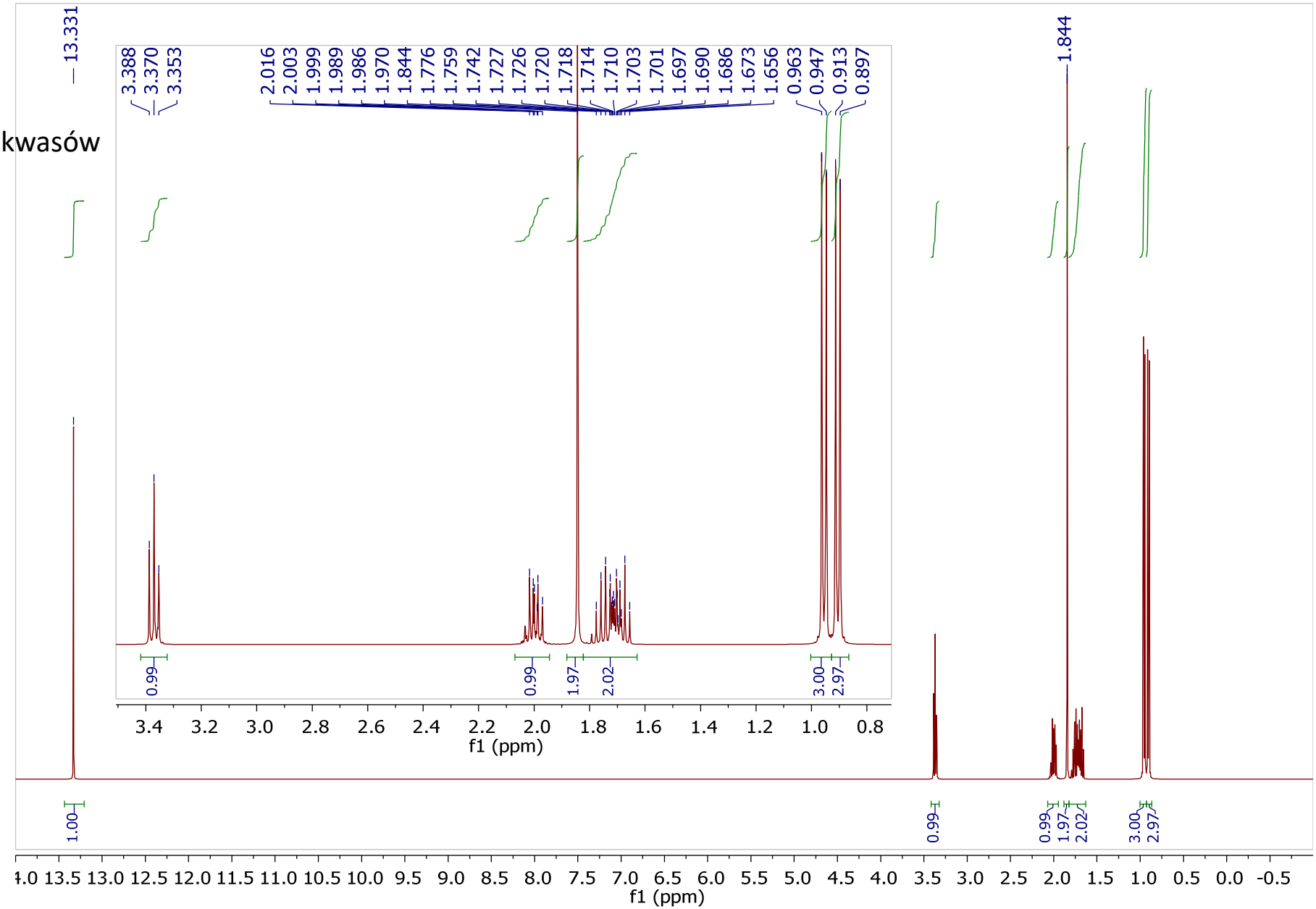
Jeden z alfa-aminokwasów



(t)

$C_6H_{13}NO_2$

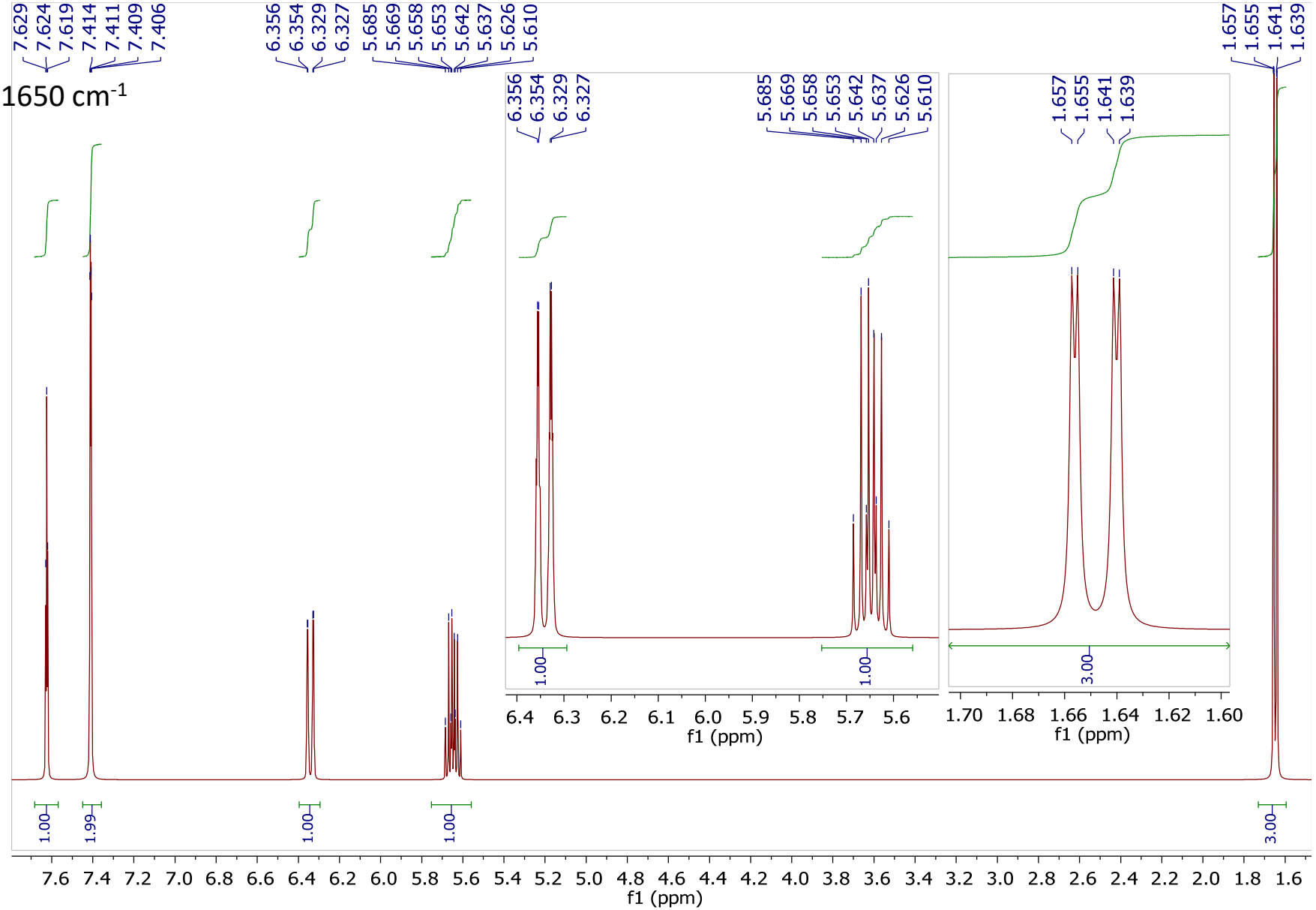
Jeden z alfa-aminokwasów



(u)

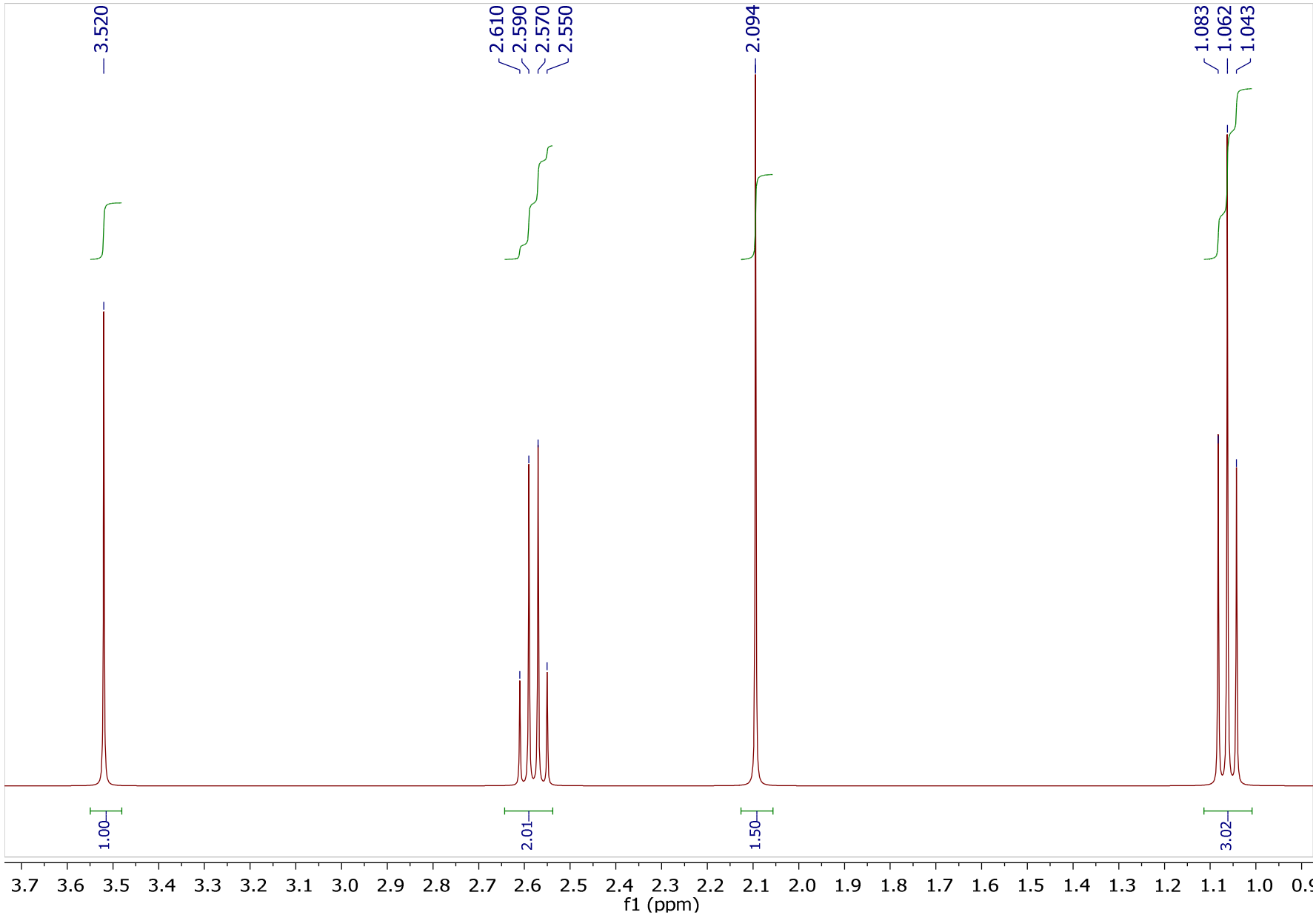
$C_9H_8Br_2$

W widmie IR min. sygnał 1650 cm^{-1}



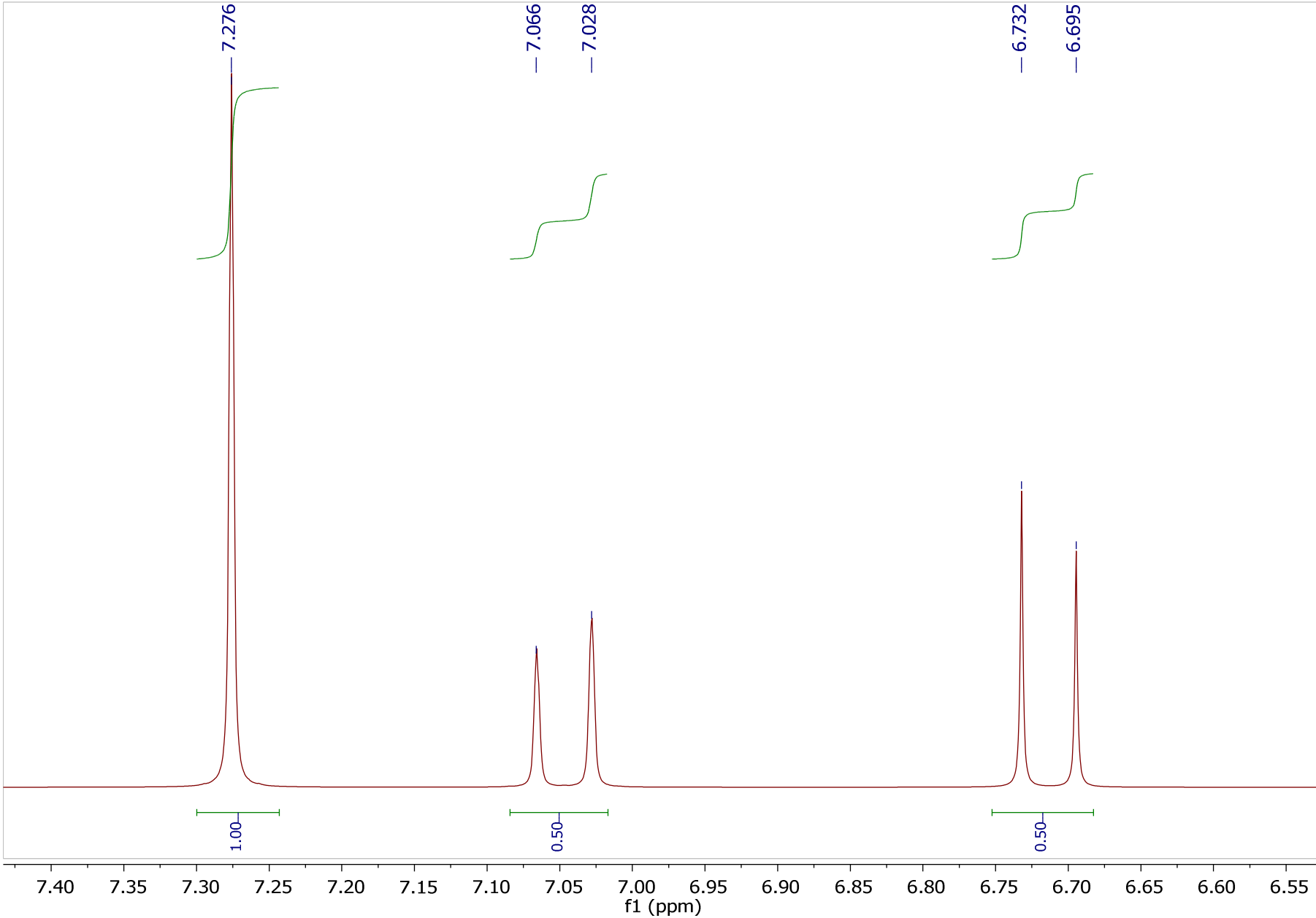
(w)

$C_7H_{15}NO$


3.520
2.610
2.590
2.570
2.550
2.094
1.083
1.062
1.043
1.00
2.01
1.50
3.02
3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9
f1 (ppm)

(x)

$C_{10}H_8Br_2$

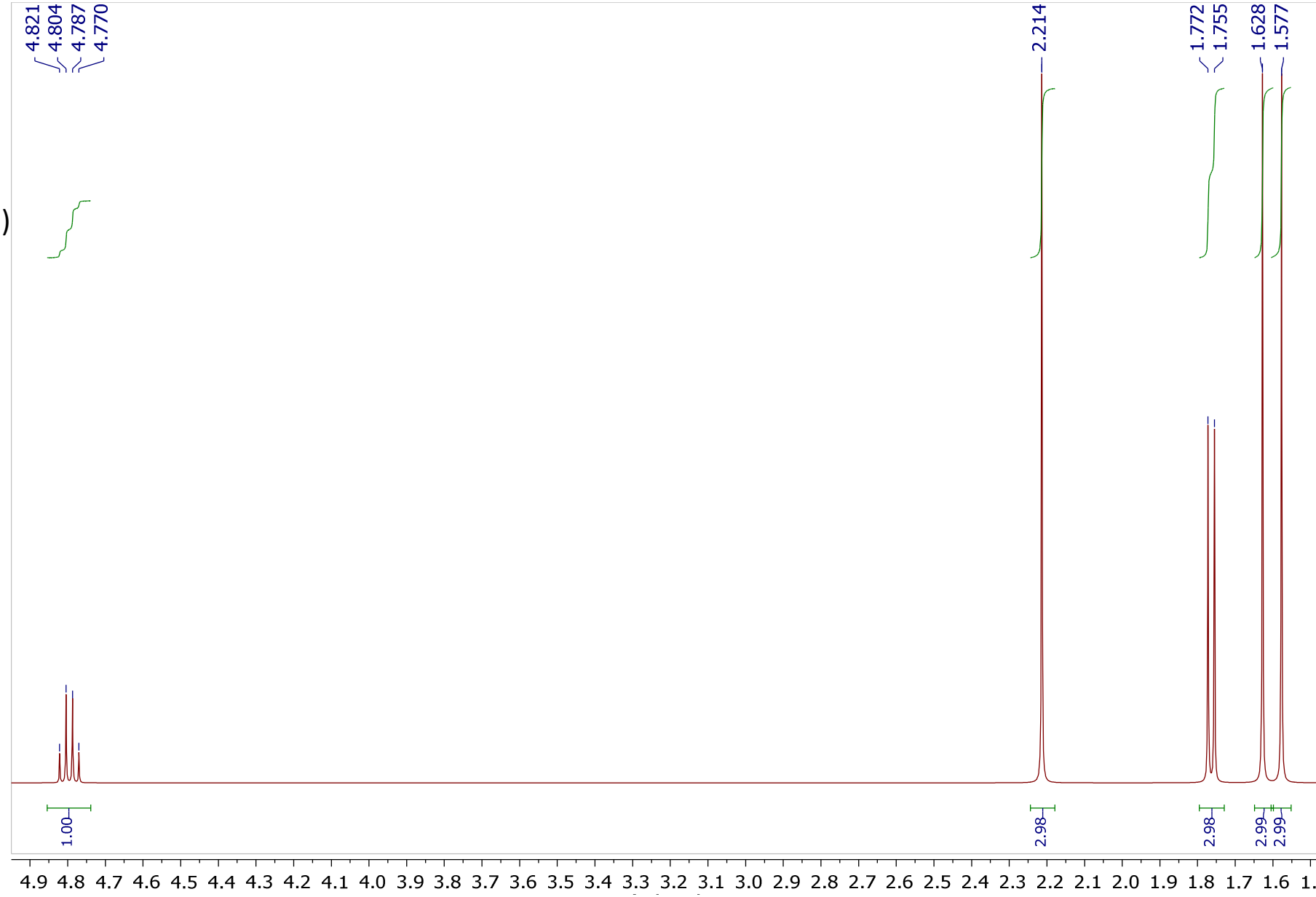

7.276
7.066
7.028
6.732
6.695
1.00
0.50
0.50
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
6.80
6.75
6.70
6.65
6.60
6.55
f1 (ppm)

(y)

$C_8H_{13}ClO_2$

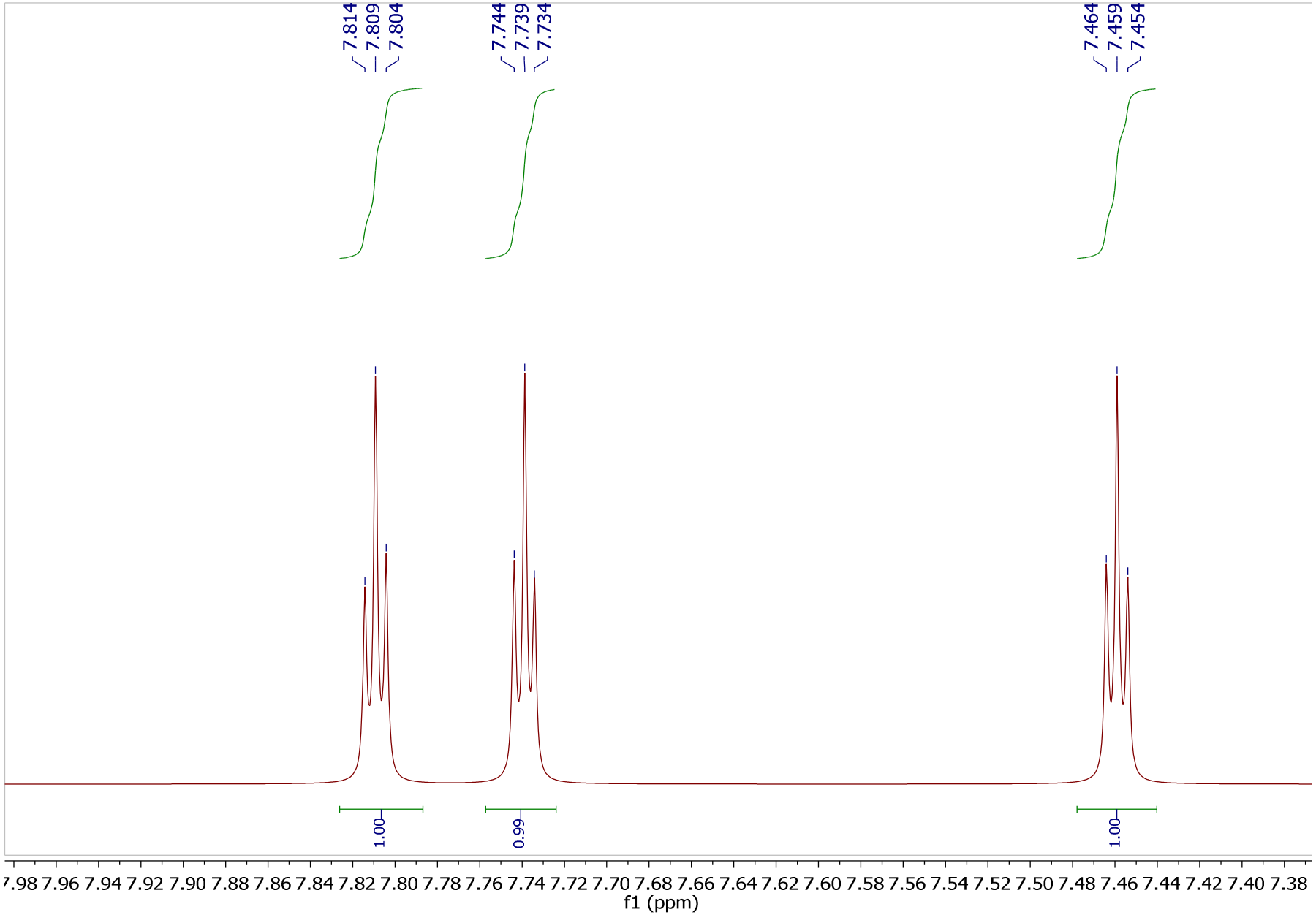
Konfiguracja S

2 grupy karbonylowe
(pozycja względna 1,3)



(z)

C_6H_3BrICl


7.814
7.809
7.804
7.744
7.739
7.734
7.464
7.459
7.454
1.00
0.99
1.00
7.98 7.96 7.94 7.92 7.90 7.88 7.86 7.84 7.82 7.80 7.78 7.76 7.74 7.72 7.70 7.68 7.66 7.64 7.62 7.60 7.58 7.56 7.54 7.52 7.50 7.48 7.46 7.44 7.42 7.40 7.38
f1 (ppm)