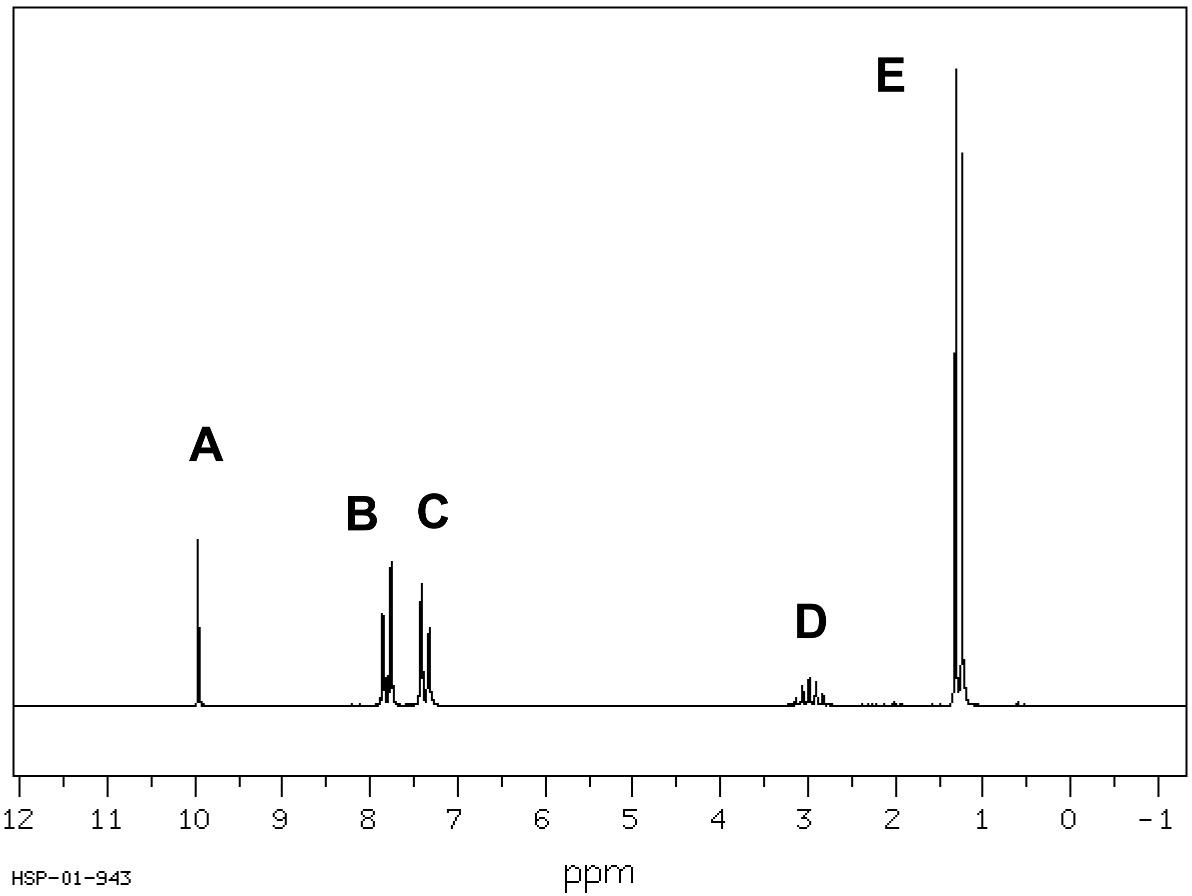
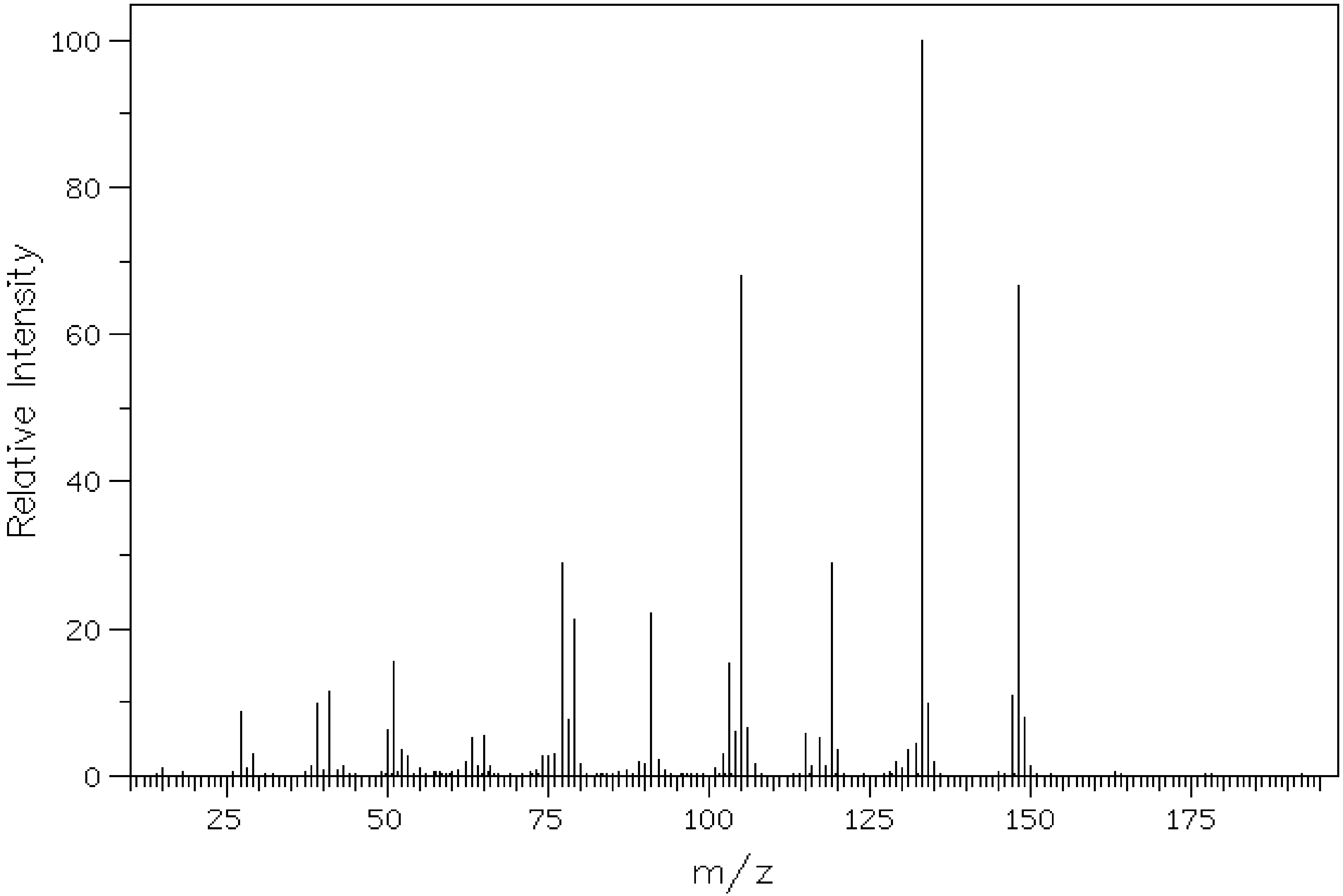
Příklad 8 – ^{1}H NMR

Zadání: Elementární analýzou kapalné organické látky bylo nalezeno 81.05 hm. % uhlíku a 8.02 hm. % vodíku. V UV spektru se projevuje silná absorpce v oblasti okolo 250 nm ($\varepsilon \approx 17000$), 290 nm ($\varepsilon \approx 1000$) a 370 nm ($\varepsilon \approx 15$). Na základě těchto údajů a přiložených 1H-NMR, MS a IČ spekter určete strukturu látky a interpretujte spektra.

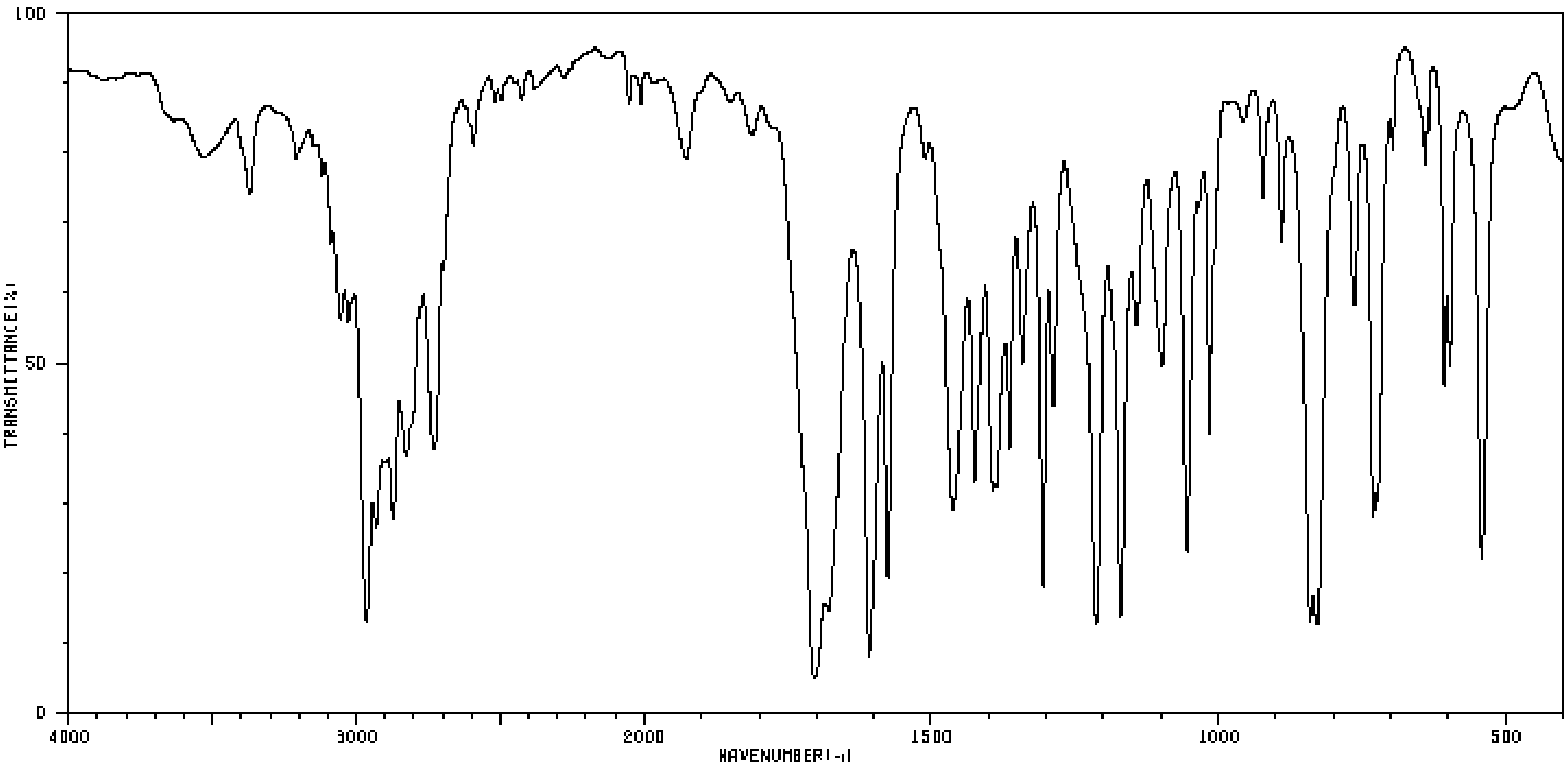


Poměr integrálních intenzit A : B : C : D : E = 1 : 2 : 2 : 1 : 6

Příklad 8 – EI-MS spektrum



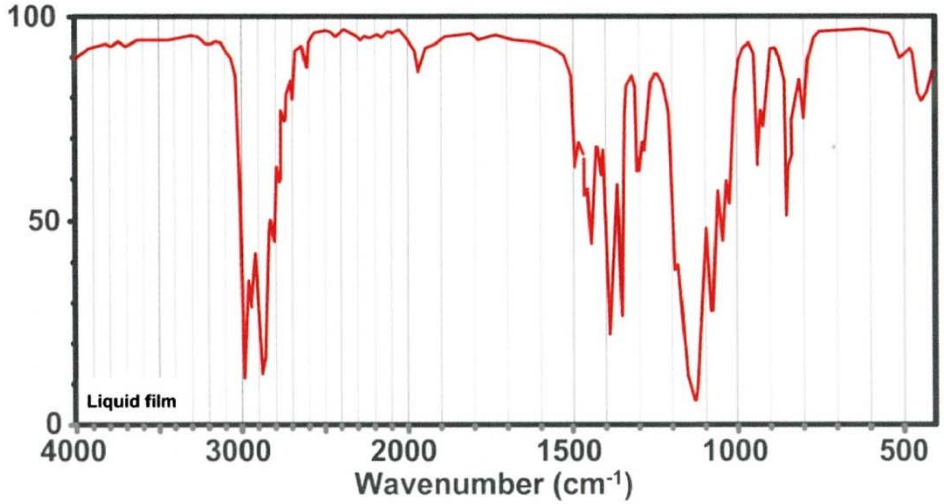
Příklad 8 – IČ spektrum

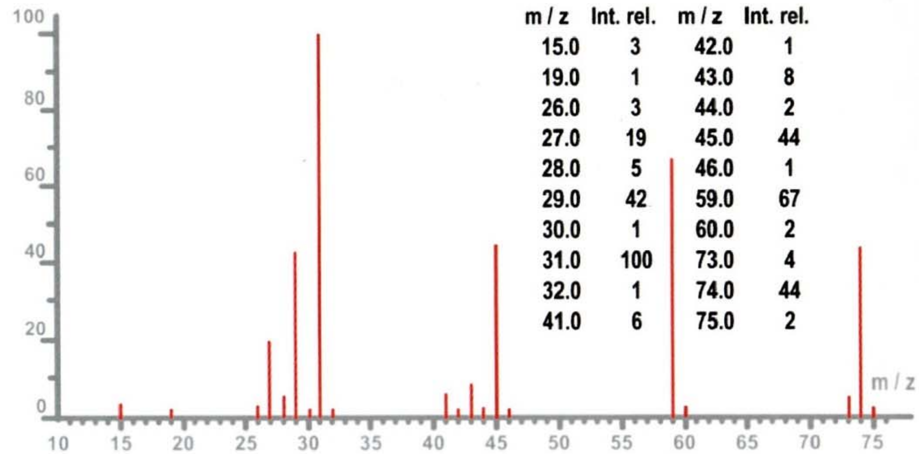


3090	64	2733	36	1386	31	1144	63	829	12
3056	53	1703	4	1364	36	1098	47	764	55
3029	53	1608	7	1342	47	1055	22	731	26
2964	12	1576	18	1306	17	1016	38	724	29
2931	25	1462	27	1288	42	1009	62	608	44
2872	26	1425	31	1213	12	890	64	596	47
2827	36	1393	30	1170	13	841	12	542	21

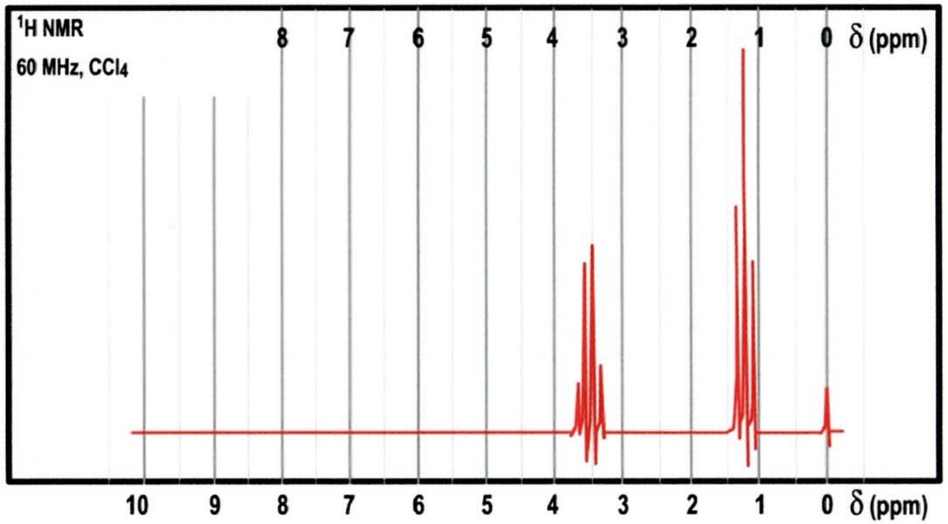
Příklad 9

Exercise 001 (001)

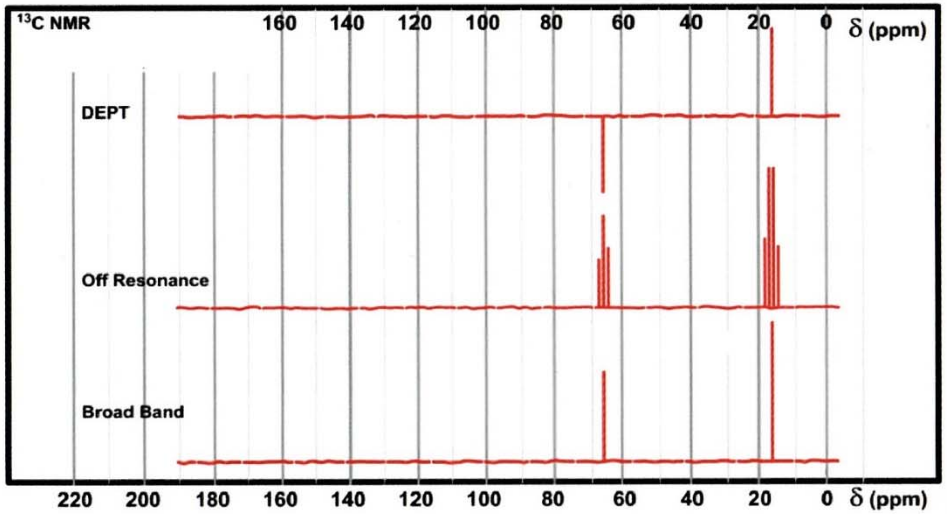




m / z	Int. rel.	m / z	Int. rel.
15.0	3	42.0	1
19.0	1	43.0	8
26.0	3	44.0	2
27.0	19	45.0	44
28.0	5	46.0	1
29.0	42	59.0	67
30.0	1	60.0	2
31.0	100	73.0	4
32.0	1	74.0	44
41.0	6	75.0	2



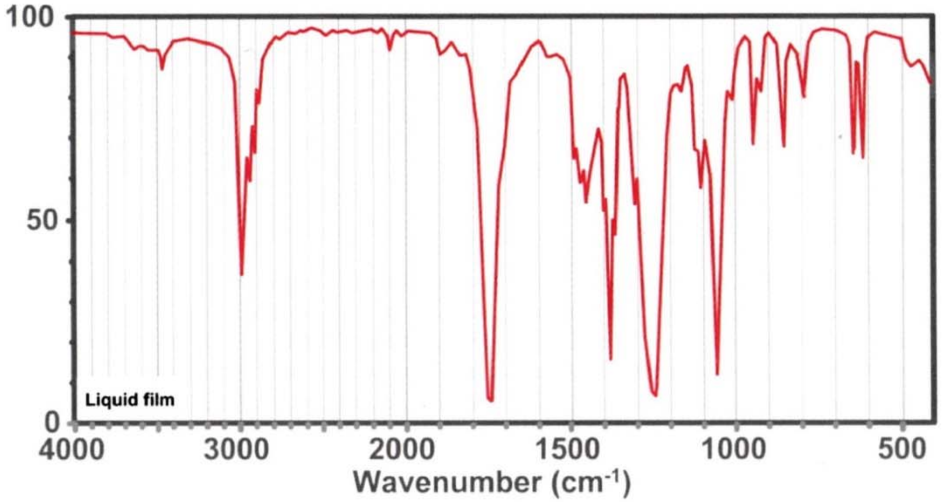
δ (integration): 1.3 (3), 3.5 (2)

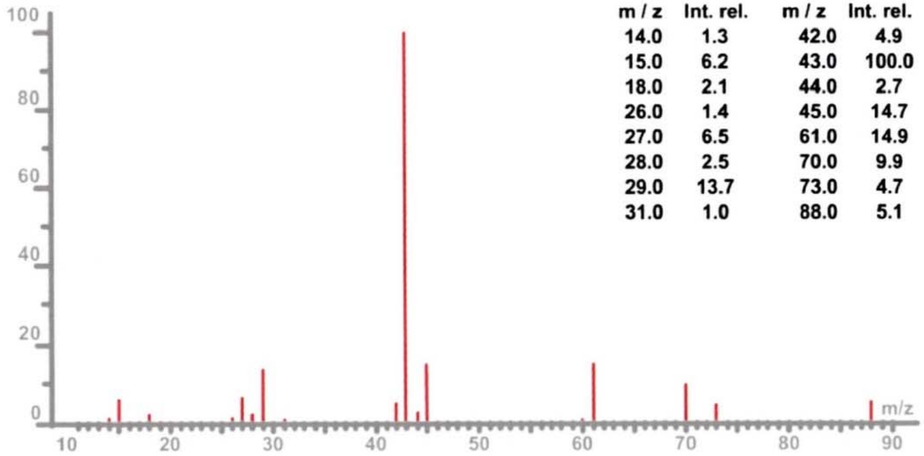


δ: 15.19, 65.88

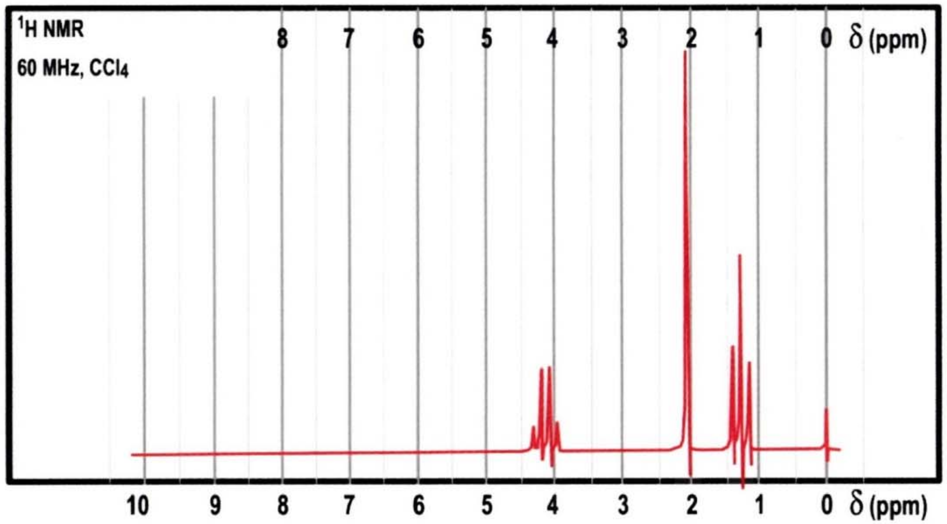
Příklad 10

Exercise 002 (003)

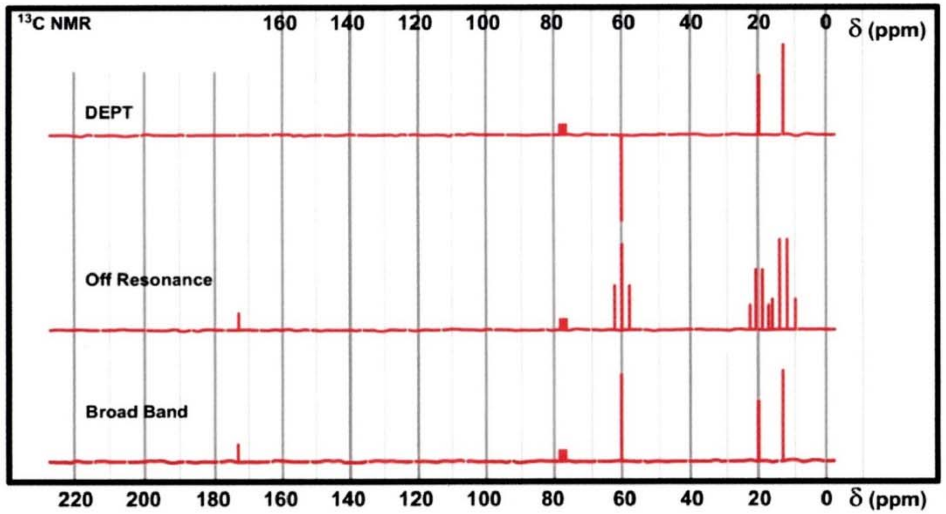




m / z	Int. rel.	m / z	Int. rel.
14.0	1.3	42.0	4.9
15.0	6.2	43.0	100.0
18.0	2.1	44.0	2.7
26.0	1.4	45.0	14.7
27.0	6.5	61.0	14.9
28.0	2.5	70.0	9.9
29.0	13.7	73.0	4.7
31.0	1.0	88.0	5.1



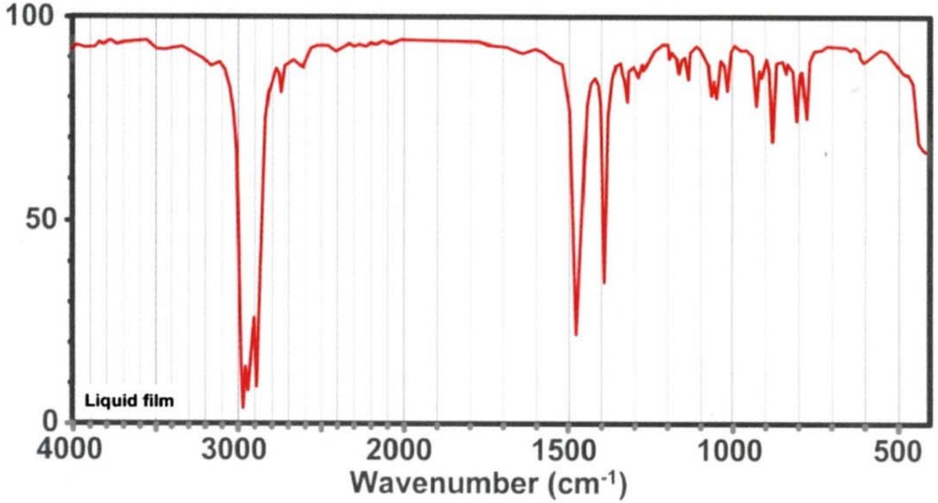
δ (integration): 4.12 (2), 2.04 (3), 1.26 (3)

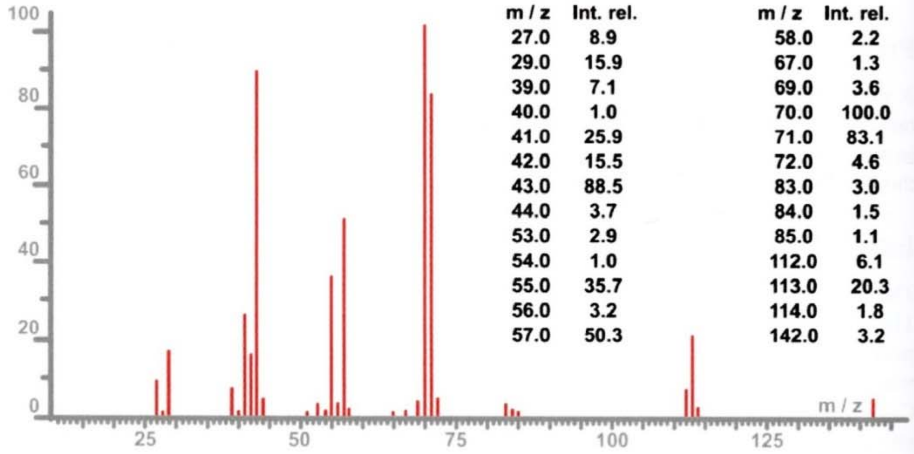


δ: 171.1, 60.4, 21.0, 14.3

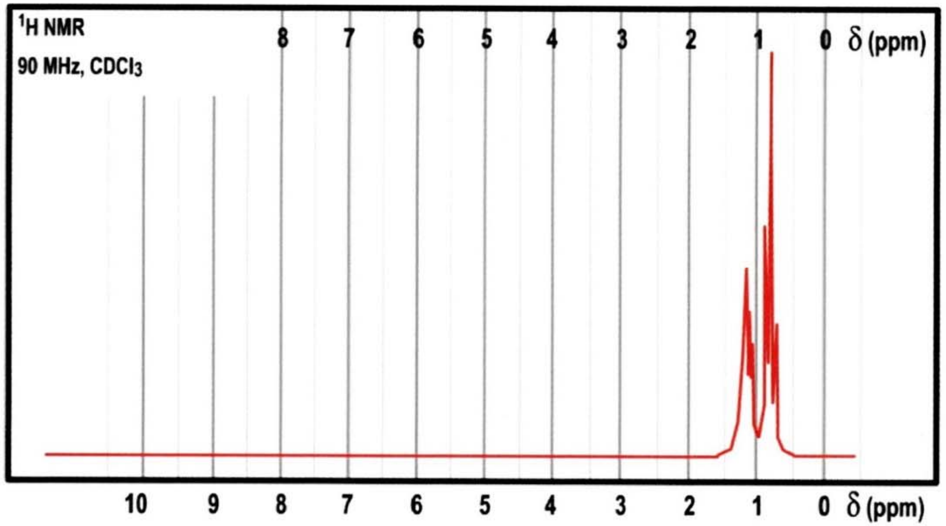
Příklad 11

Exercise 005 (094)

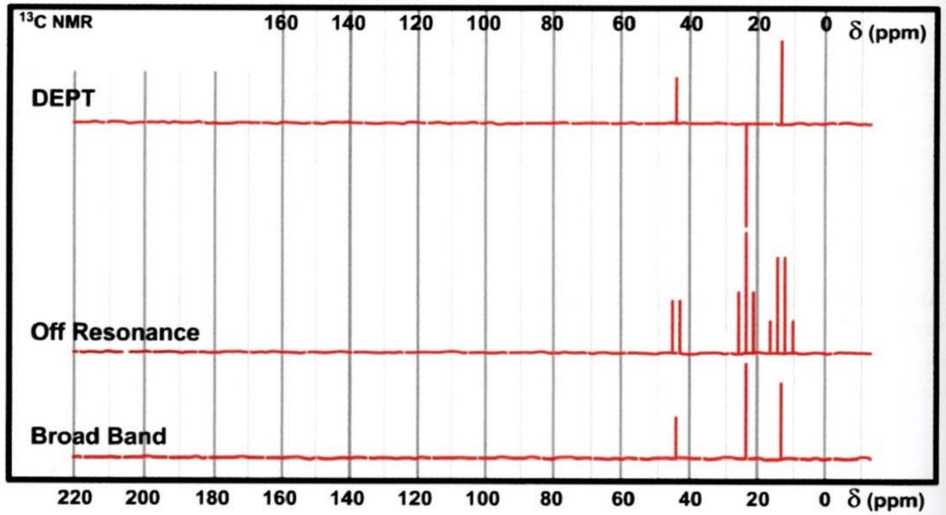




m / z	Int. rel.	m / z	Int. rel.
27.0	8.9	58.0	2.2
29.0	15.9	67.0	1.3
39.0	7.1	69.0	3.6
40.0	1.0	70.0	100.0
41.0	25.9	71.0	83.1
42.0	15.5	72.0	4.6
43.0	88.5	83.0	3.0
44.0	3.7	84.0	1.5
53.0	2.9	85.0	1.1
54.0	1.0	112.0	6.1
55.0	35.7	113.0	20.3
56.0	3.2	114.0	1.8
57.0	50.3	142.0	3.2



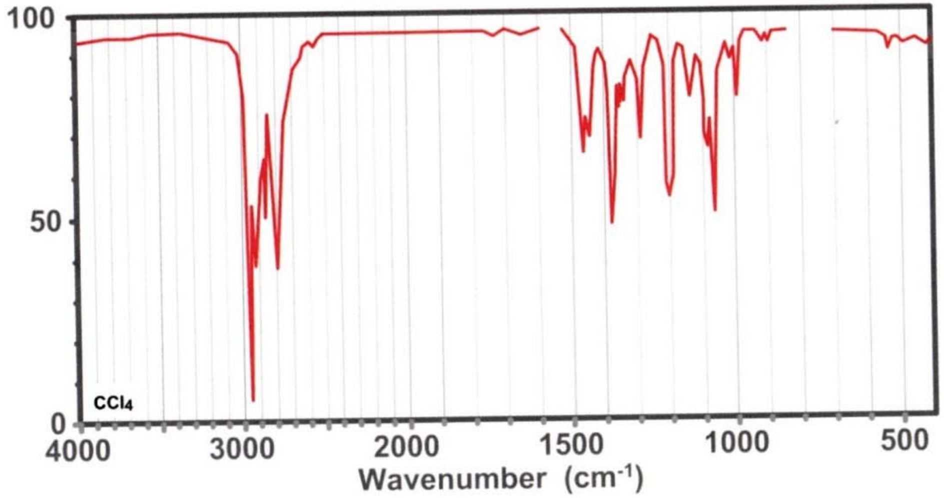
δ (integration): 1.05 (5), 0.86 (6)

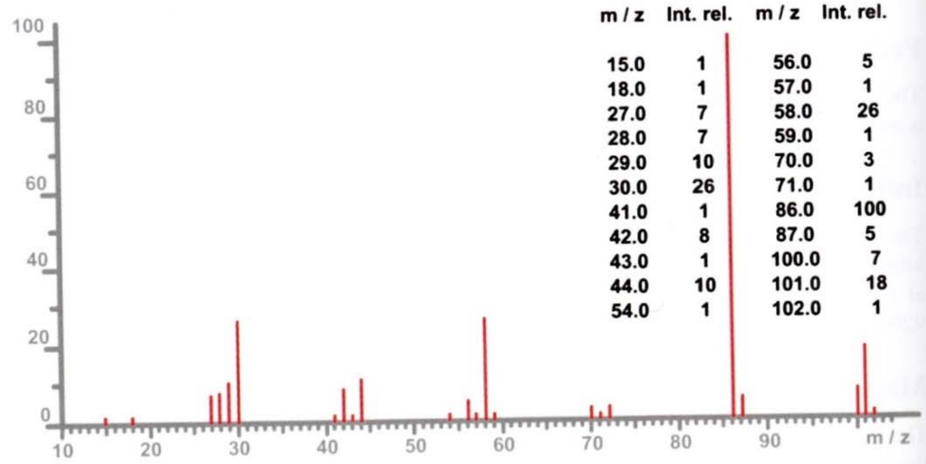


δ: 43.08, 22.88, 12.61

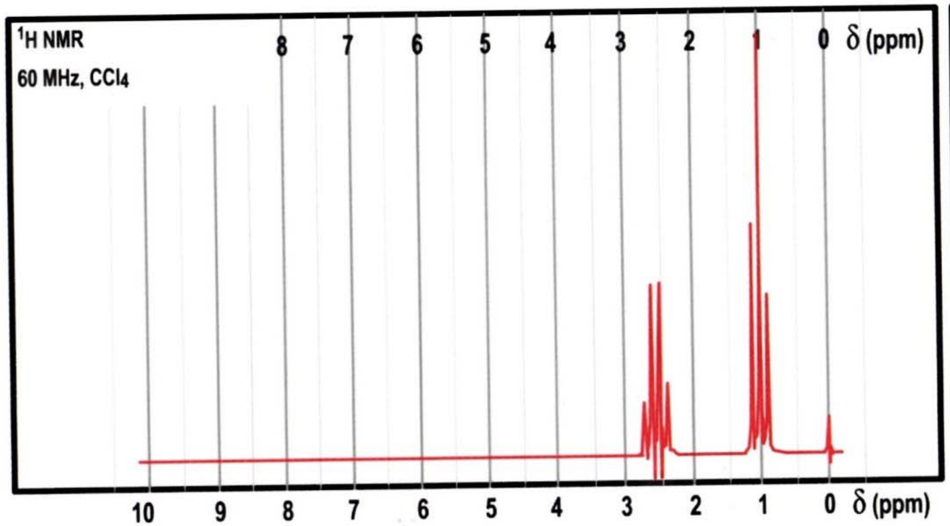
Příklad 12

Exercise 008 (011)

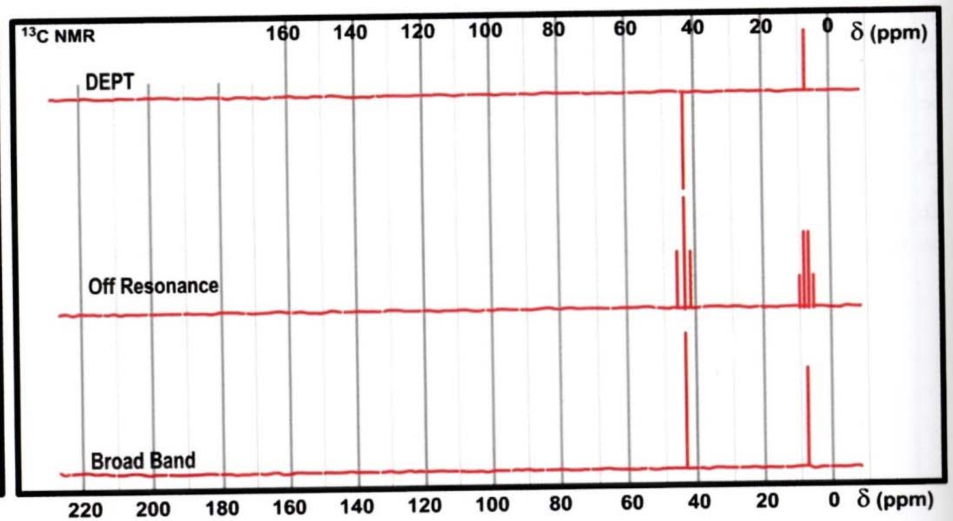




m / z	Int. rel.	m / z	Int. rel.
15.0	1	56.0	5
18.0	1	57.0	1
27.0	7	58.0	26
28.0	7	59.0	1
29.0	10	70.0	3
30.0	26	71.0	1
41.0	1	86.0	100
42.0	8	87.0	5
43.0	1	100.0	7
44.0	10	101.0	18
54.0	1	102.0	1



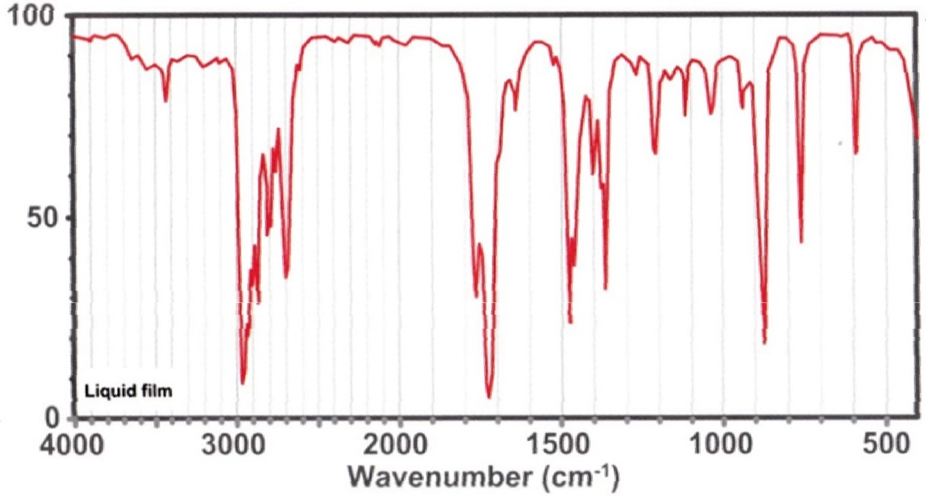
δ (integration): 2.42 (2), 0.97 (3)

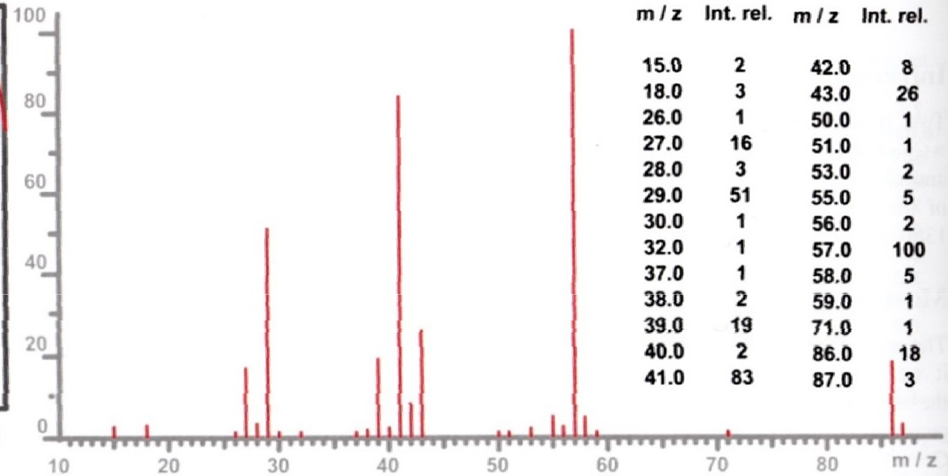


δ: 46.5, 11.8

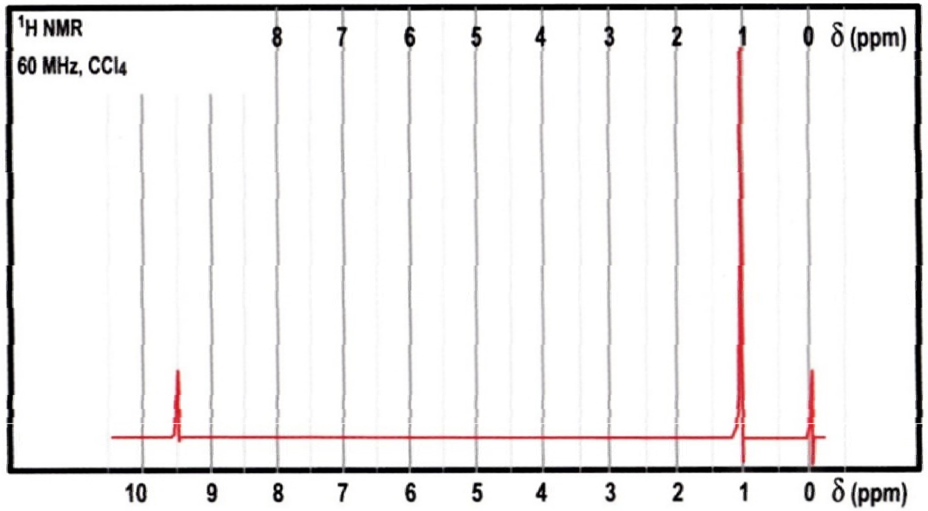
Příklad 13

Exercise 010 (005)

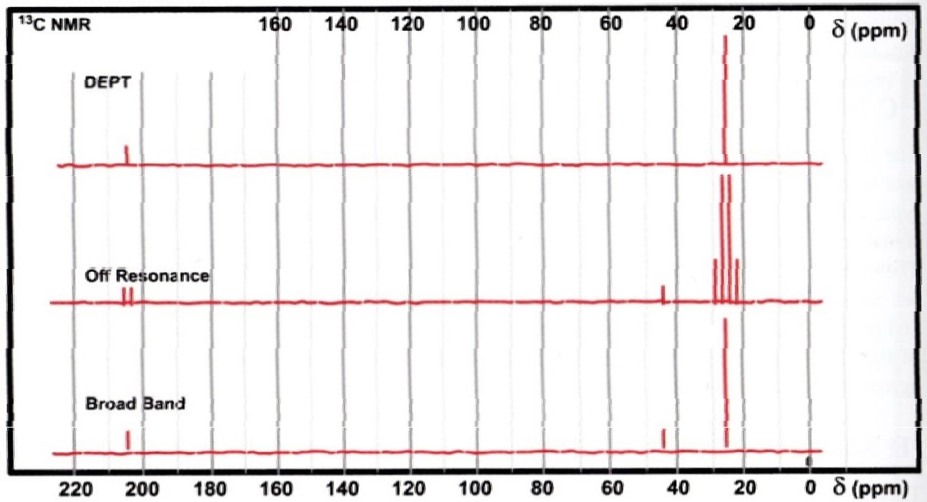




m / z	Int. rel.	m / z	Int. rel.
15.0	2	42.0	8
18.0	3	43.0	26
26.0	1	50.0	1
27.0	16	51.0	1
28.0	3	53.0	2
29.0	51	55.0	5
30.0	1	56.0	2
32.0	1	57.0	100
37.0	1	58.0	5
38.0	2	59.0	1
39.0	19	71.0	1
40.0	2	86.0	18
41.0	83	87.0	3



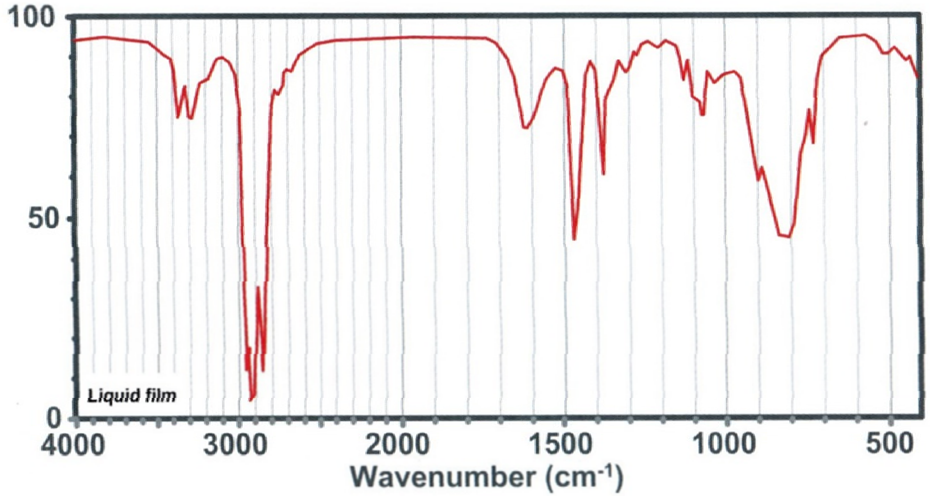
δ (integration): 9.48 (1), 1.08 (9)

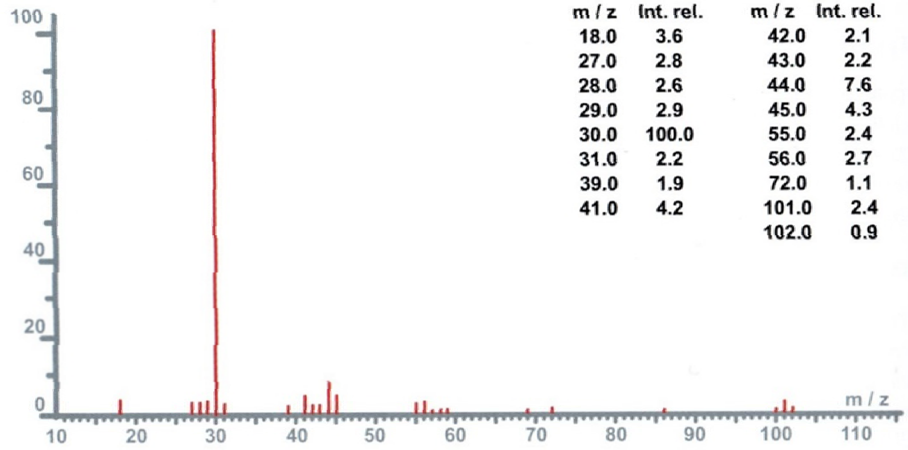


δ: 205.83, 42.50, 23.44

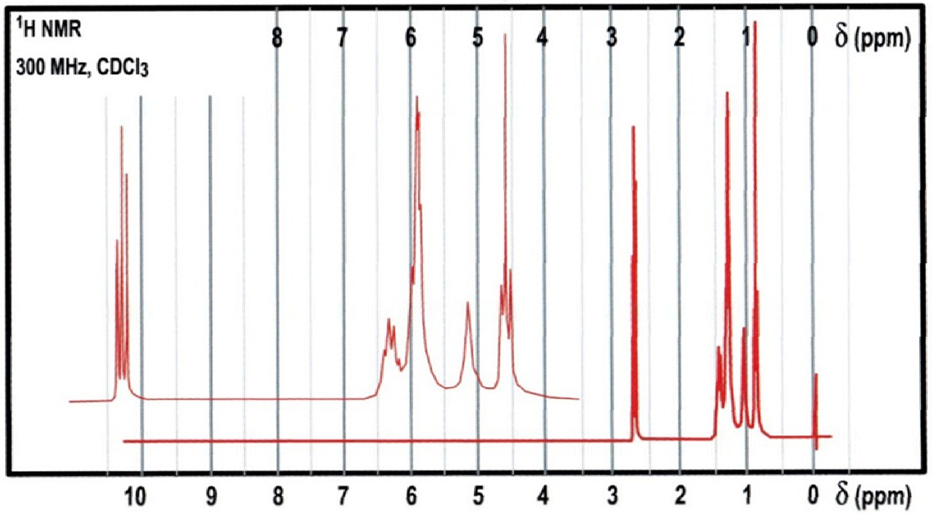
Příklad 14

Exercise 011 (066)

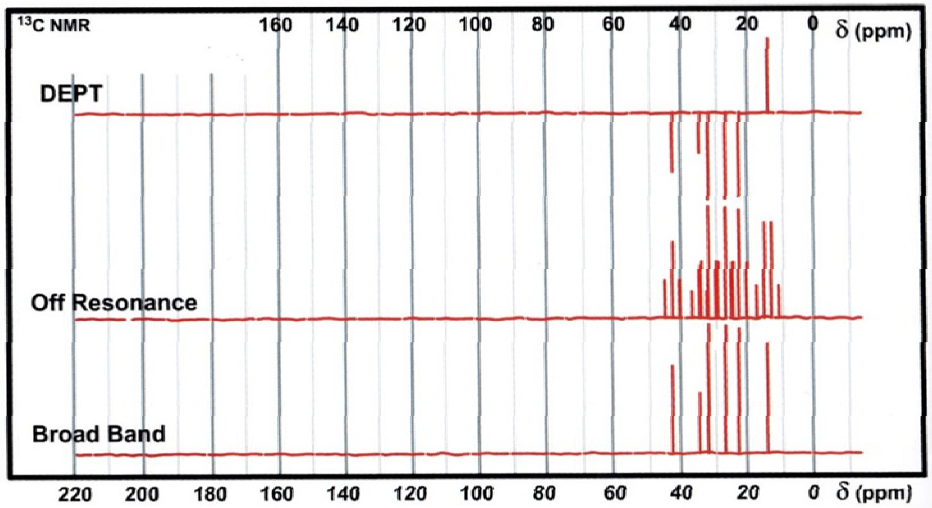




m / z	Int. rel.	m / z	Int. rel.
18.0	3.6	42.0	2.1
27.0	2.8	43.0	2.2
28.0	2.6	44.0	7.6
29.0	2.9	45.0	4.3
30.0	100.0	55.0	2.4
31.0	2.2	56.0	2.7
39.0	1.9	72.0	1.1
41.0	4.2	101.0	2.4
		102.0	0.9



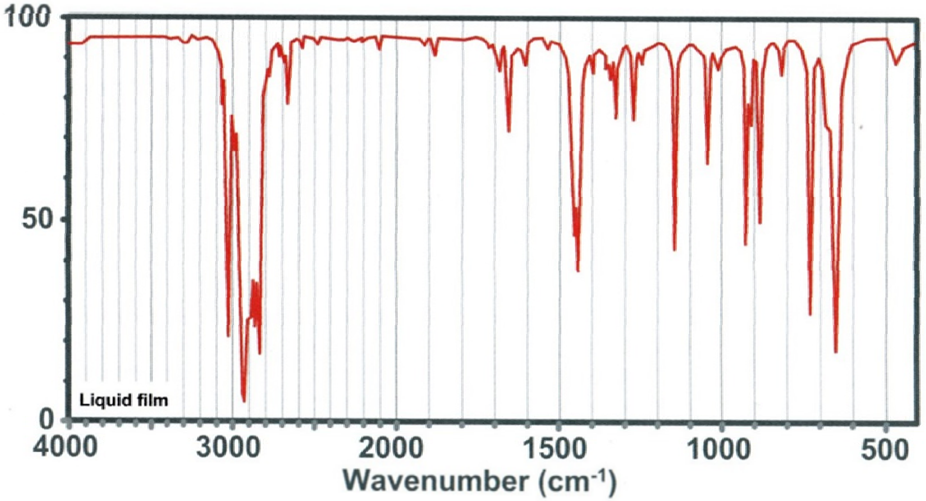
δ (integration): 2.7 (2), 1.1–1.4 (8), 1.2 (2), 0.9 (3)

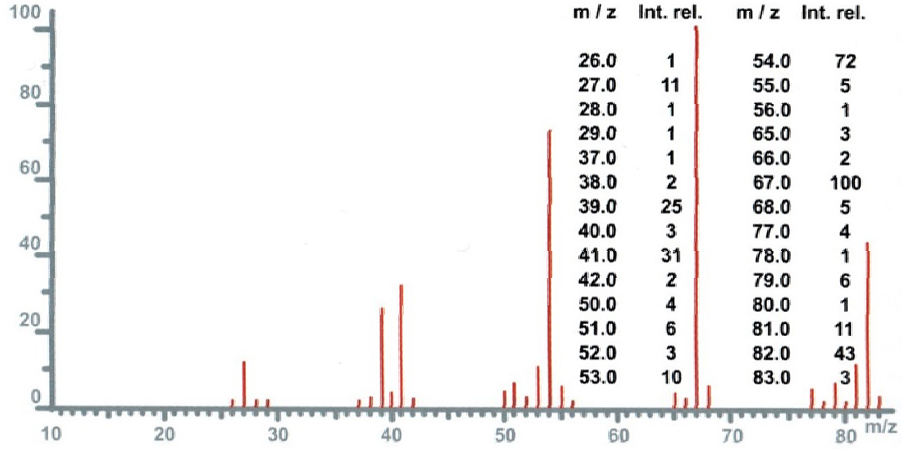


δ: 42.43, 34.09, 31.88, 26.72, 22.77, 14.09

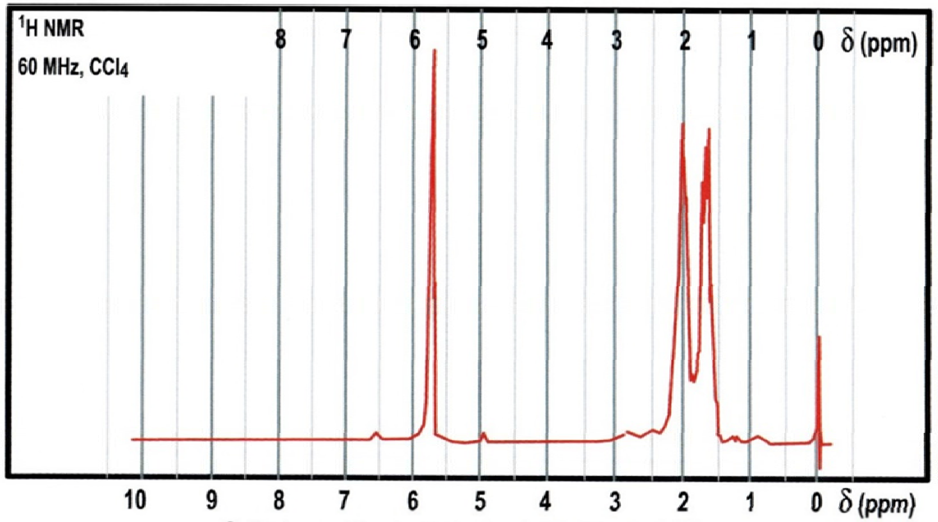
Příklad 15

Exercise 017 (018)

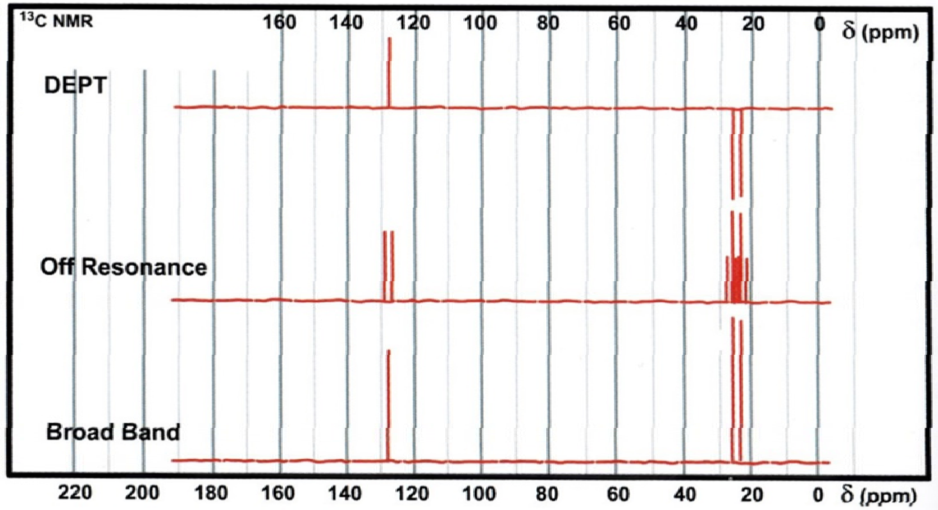




m / z	Int. rel.	m / z	Int. rel.
26.0	1	54.0	72
27.0	11	55.0	5
28.0	1	56.0	1
29.0	1	65.0	3
37.0	1	66.0	2
38.0	2	67.0	100
39.0	25	68.0	5
40.0	3	77.0	4
41.0	31	78.0	1
42.0	2	79.0	6
50.0	4	80.0	1
51.0	6	81.0	11
52.0	3	82.0	43
53.0	10	83.0	3



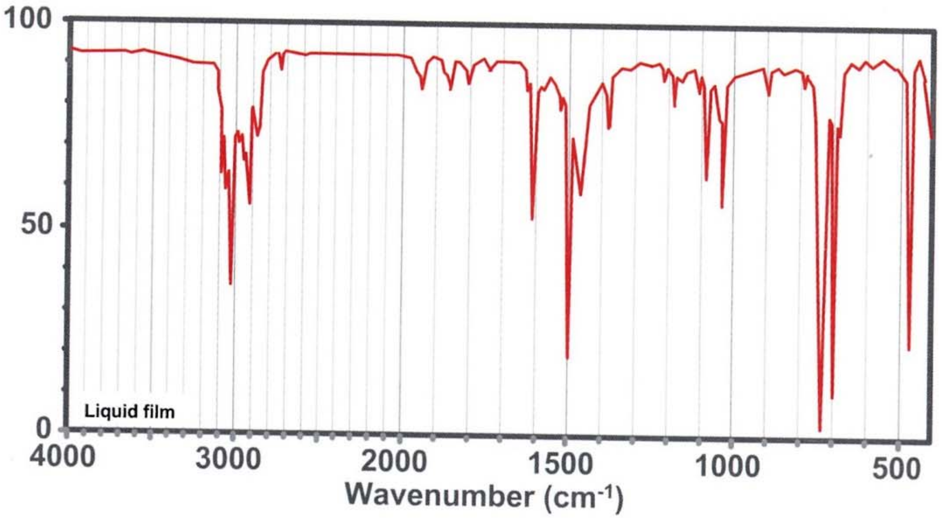
δ (integration): 5.6 (1), 1.98 (2), 1.6 (2)

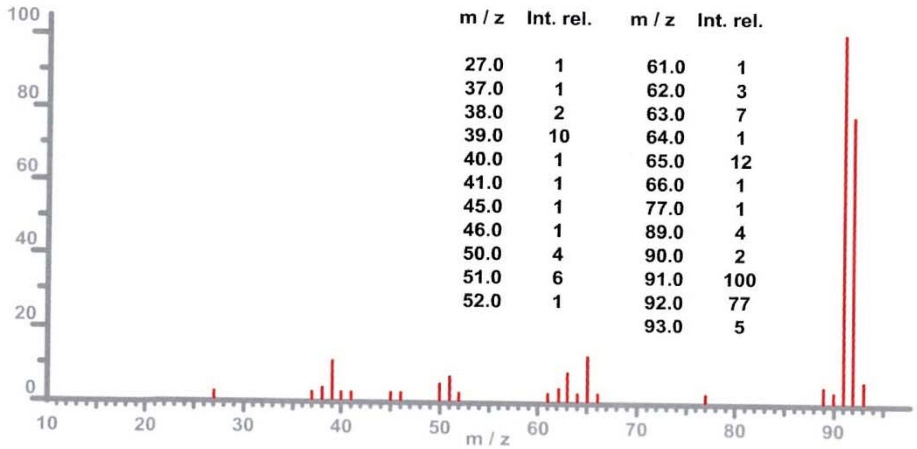


δ: 127.3, 25.3, 22.8

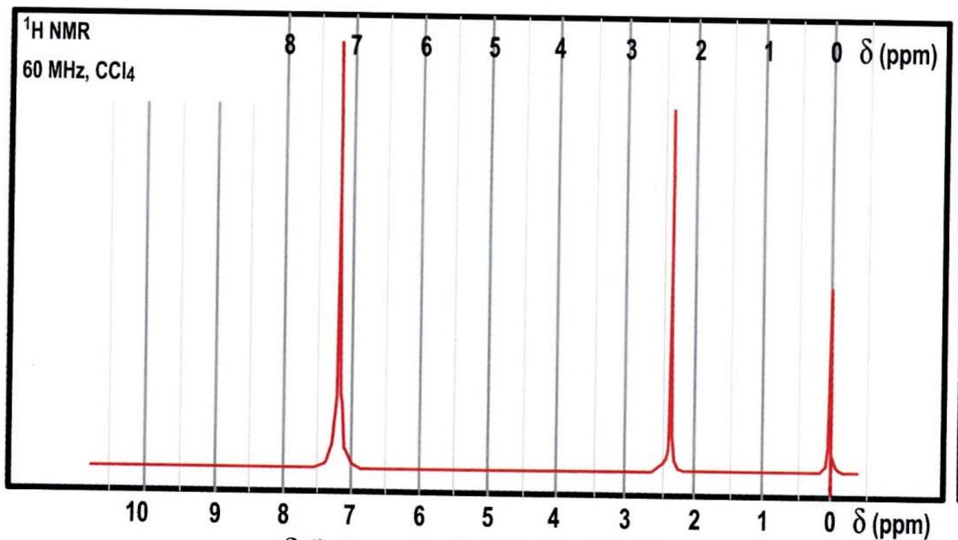
Příklad 16

Exercise 020 (012)

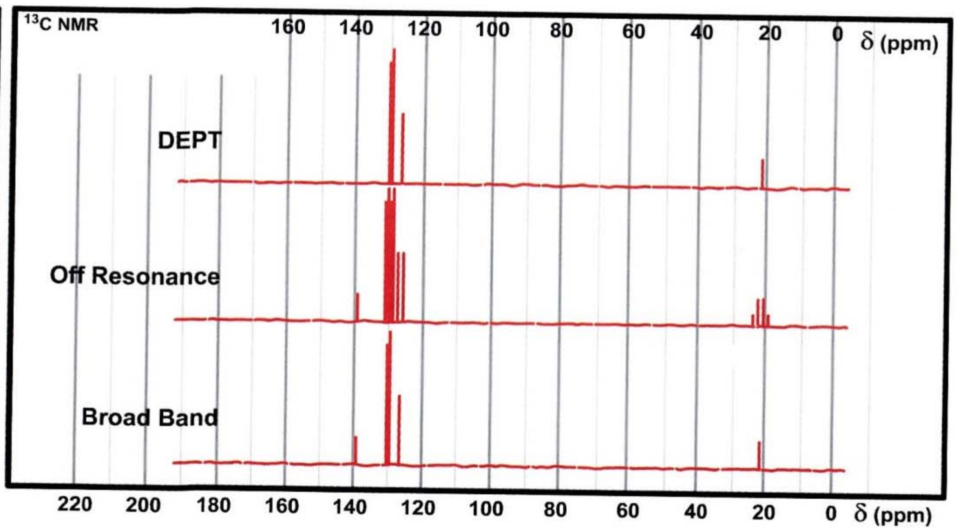




m / z	Int. rel.	m / z	Int. rel.
27.0	1	61.0	1
37.0	1	62.0	3
38.0	2	63.0	7
39.0	10	64.0	1
40.0	1	65.0	12
41.0	1	66.0	1
45.0	1	77.0	1
46.0	1	89.0	4
50.0	4	90.0	2
51.0	6	91.0	100
52.0	1	92.0	77
		93.0	5



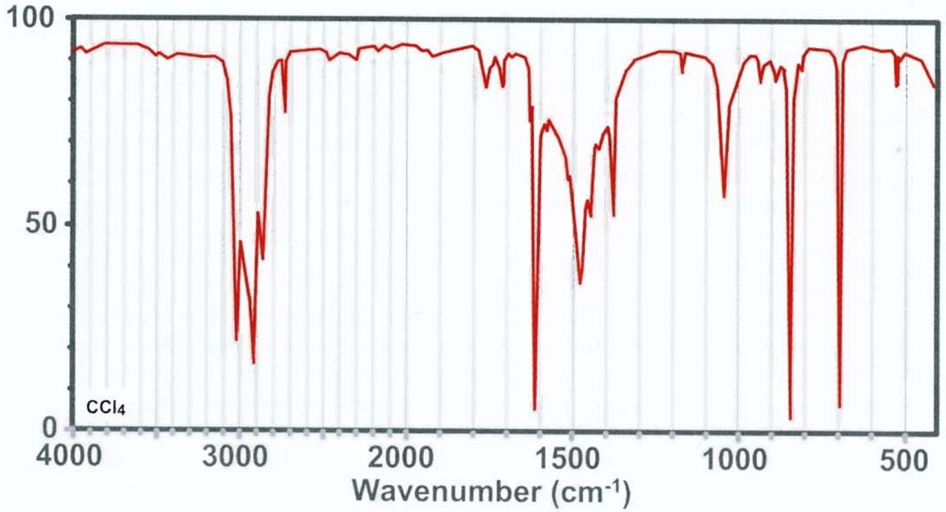
δ (integration): 7.2 (5), 2.4 (3).

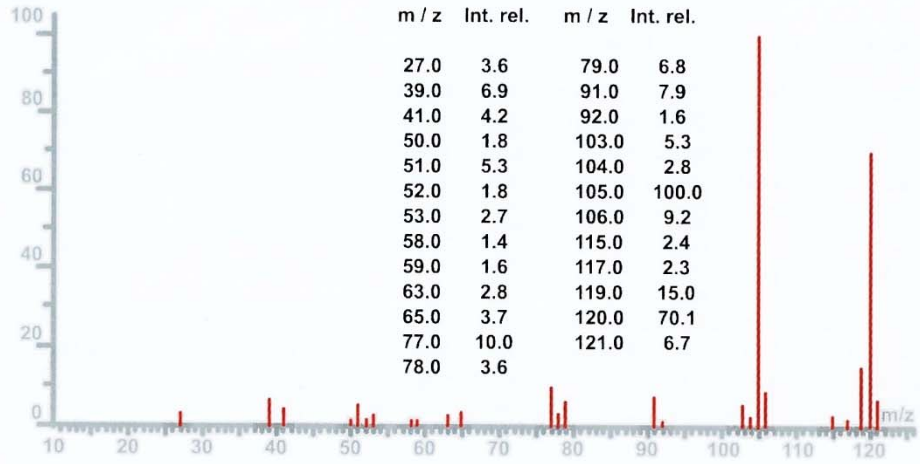


δ: 137.8, 129.1, 128.3, 125.4, 21.4

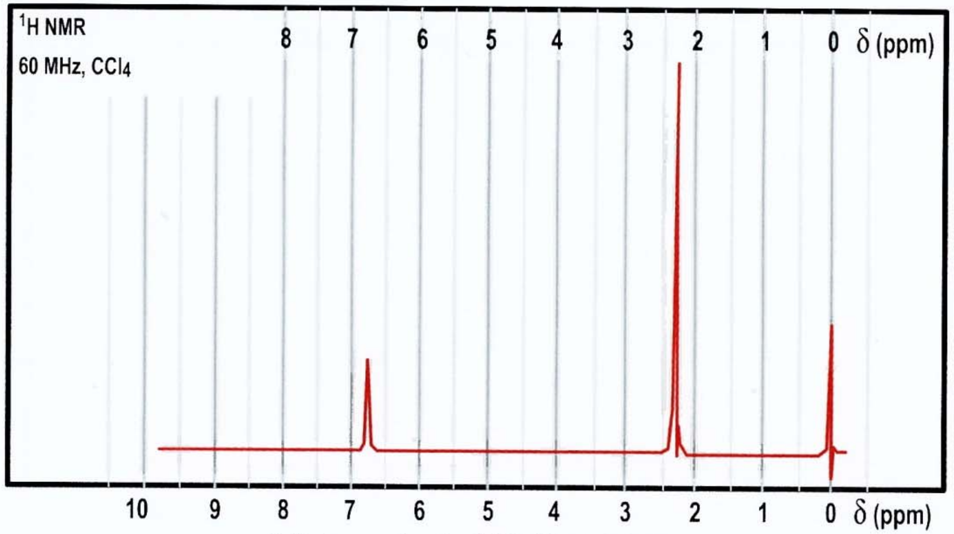
Příklad 17

Exercise 021 (013)

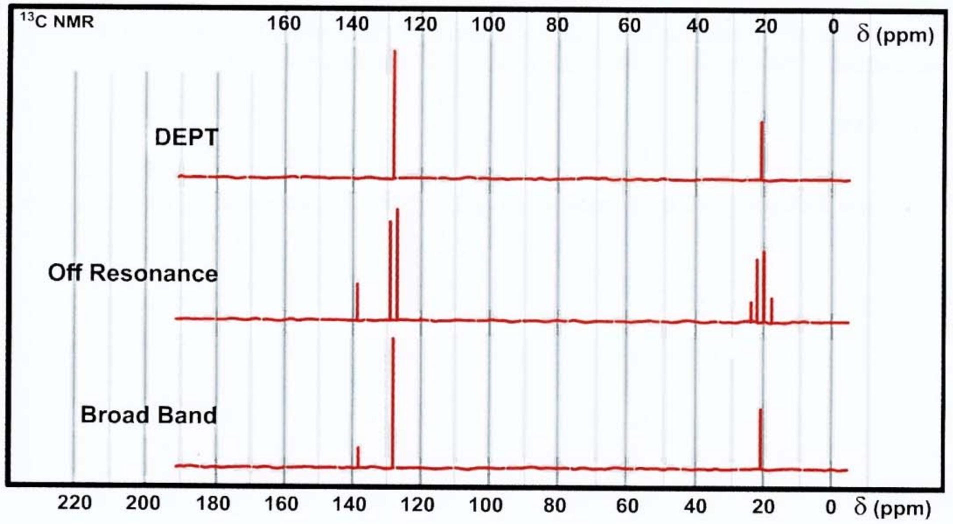




m / z	Int. rel.	m / z	Int. rel.
27.0	3.6	79.0	6.8
39.0	6.9	91.0	7.9
41.0	4.2	92.0	1.6
50.0	1.8	103.0	5.3
51.0	5.3	104.0	2.8
52.0	1.8	105.0	100.0
53.0	2.7	106.0	9.2
58.0	1.4	115.0	2.4
59.0	1.6	117.0	2.3
63.0	2.8	119.0	15.0
65.0	3.7	120.0	70.1
77.0	10.0	121.0	6.7
78.0	3.6		



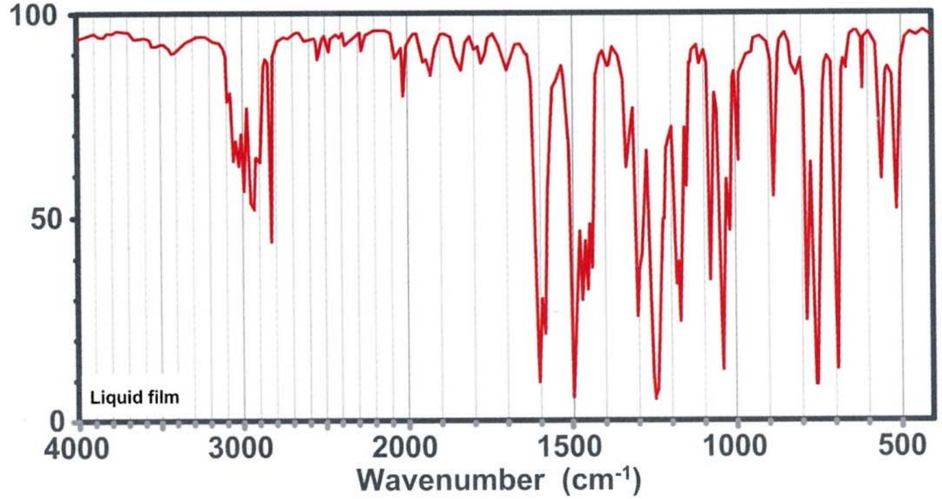
δ (integration): 6.78 (1), 2.26 (3)

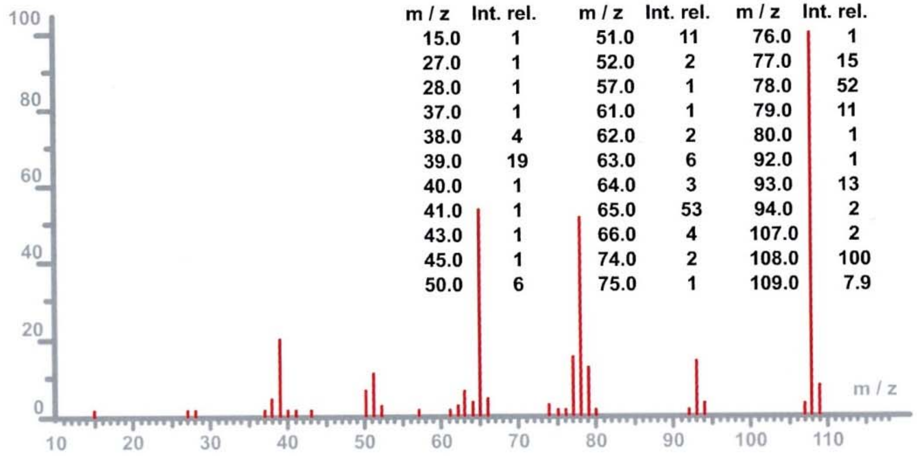


δ: 137.7, 127.0, 21.8

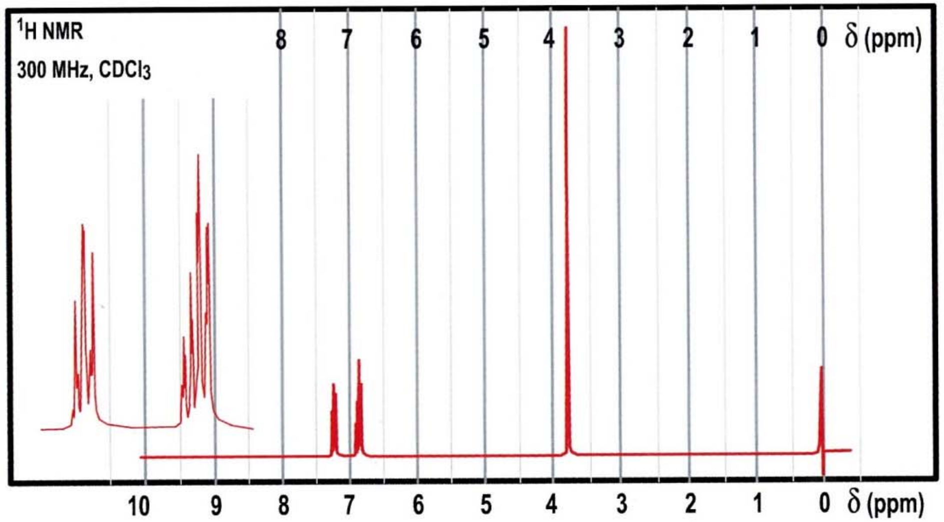
Příklad 18

Exercise 022 (025)

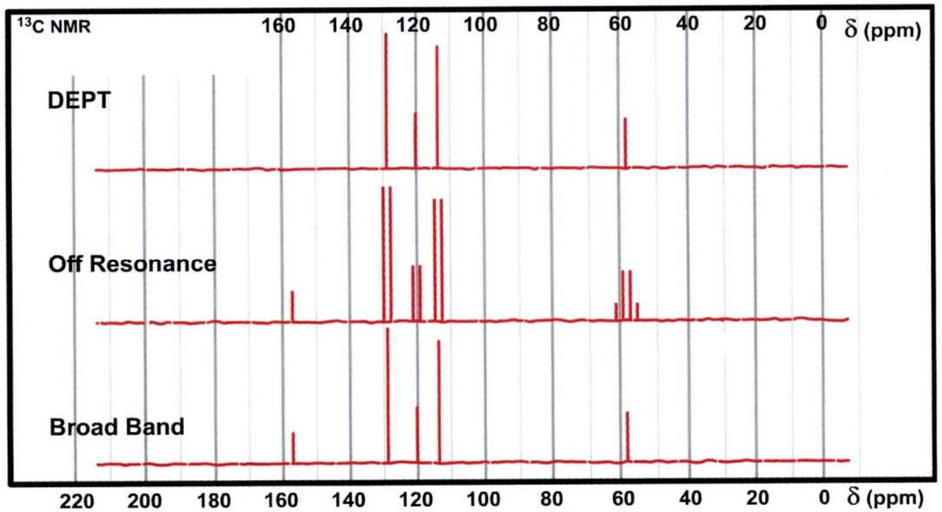




m / z	Int. rel.	m / z	Int. rel.	m / z	Int. rel.
15.0	1	51.0	11	76.0	1
27.0	1	52.0	2	77.0	15
28.0	1	57.0	1	78.0	52
37.0	1	61.0	1	79.0	11
38.0	4	62.0	2	80.0	1
39.0	19	63.0	6	92.0	1
40.0	1	64.0	3	93.0	13
41.0	1	65.0	53	94.0	2
43.0	1	66.0	4	107.0	2
45.0	1	74.0	2	108.0	100
50.0	6	75.0	1	109.0	7.9



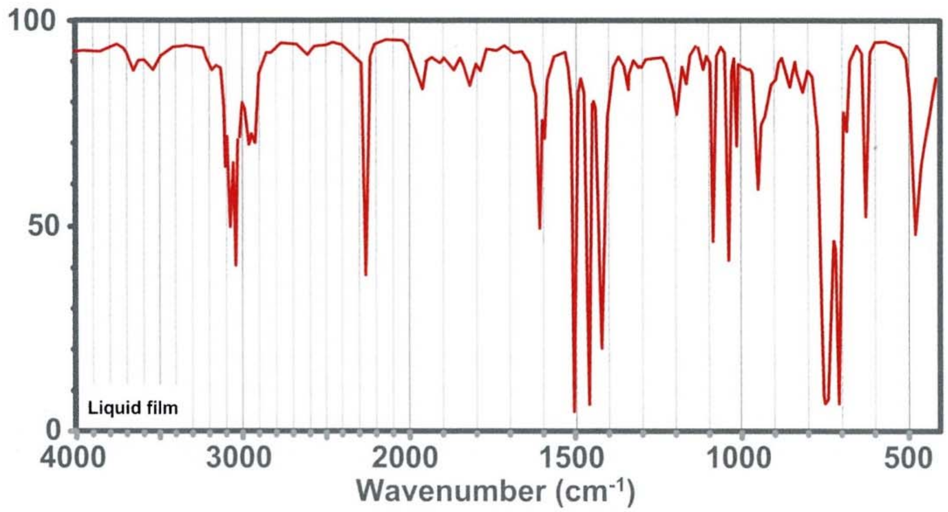
δ (integration): 7.3 (2), 6.9 (3), 3.7 (3)

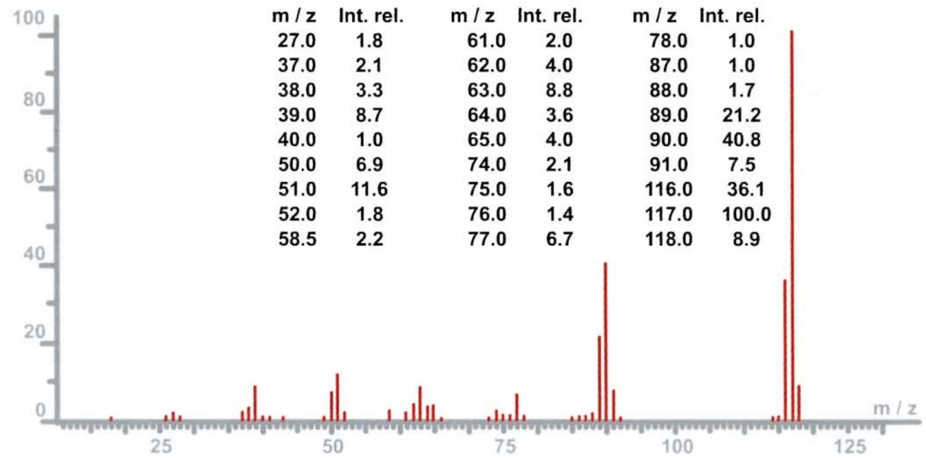


δ: 159.7, 129.5, 120.7, 114.0, 55.1

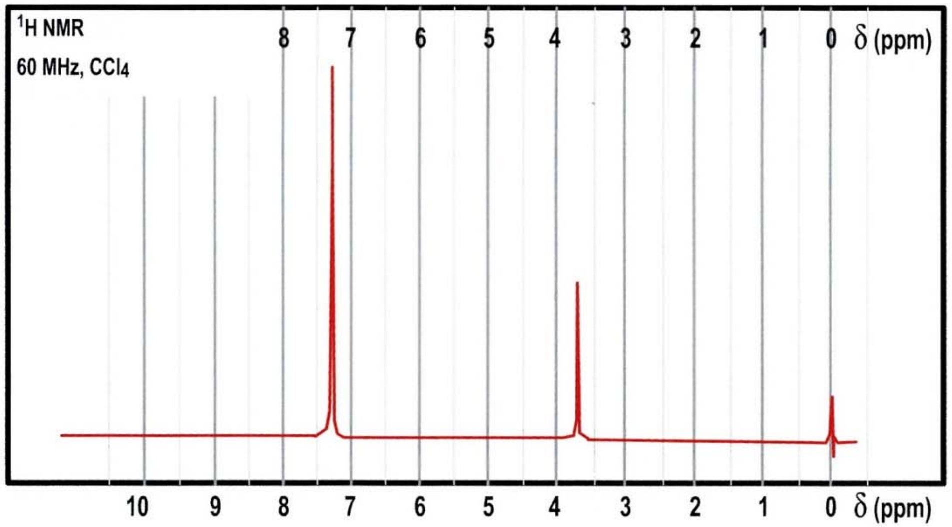
Příklad 19

Exercise 029 (027)

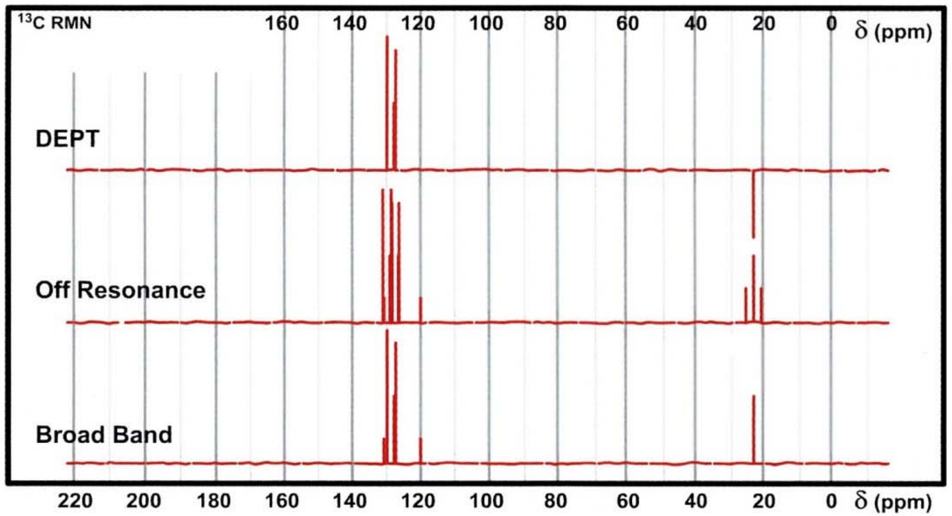




m / z	Int. rel.	m / z	Int. rel.	m / z	Int. rel.
27.0	1.8	61.0	2.0	78.0	1.0
37.0	2.1	62.0	4.0	87.0	1.0
38.0	3.3	63.0	8.8	88.0	1.7
39.0	8.7	64.0	3.6	89.0	21.2
40.0	1.0	65.0	4.0	90.0	40.8
50.0	6.9	74.0	2.1	91.0	7.5
51.0	11.6	75.0	1.6	116.0	36.1
52.0	1.8	76.0	1.4	117.0	100.0
58.5	2.2	77.0	6.7	118.0	8.9



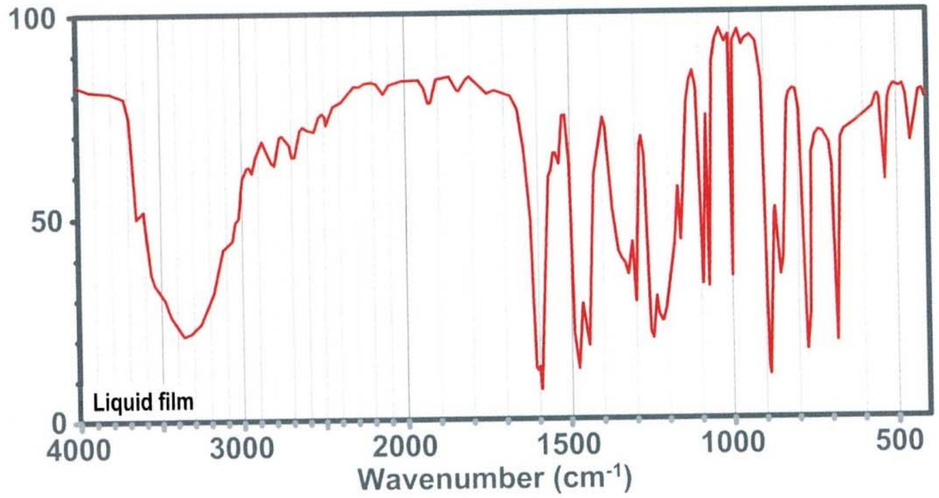
δ (integration): 7.3 (5), 3.7 (2)

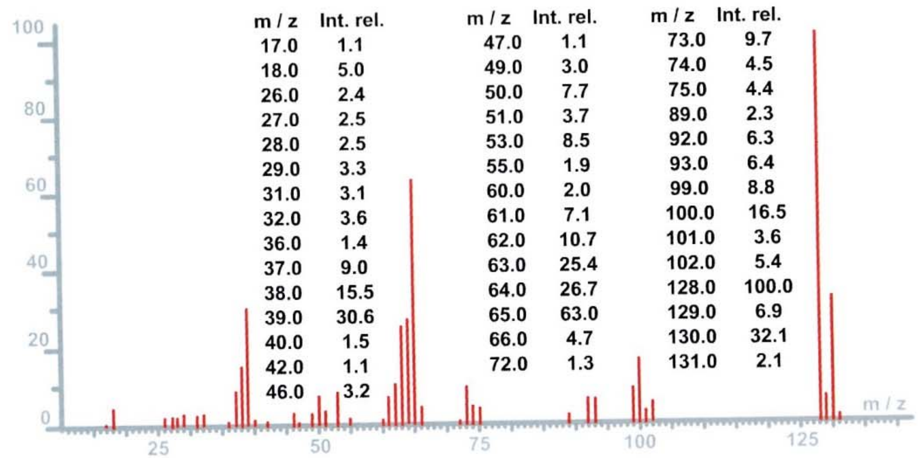


δ: 131, 130, 128, 127, 120, 25

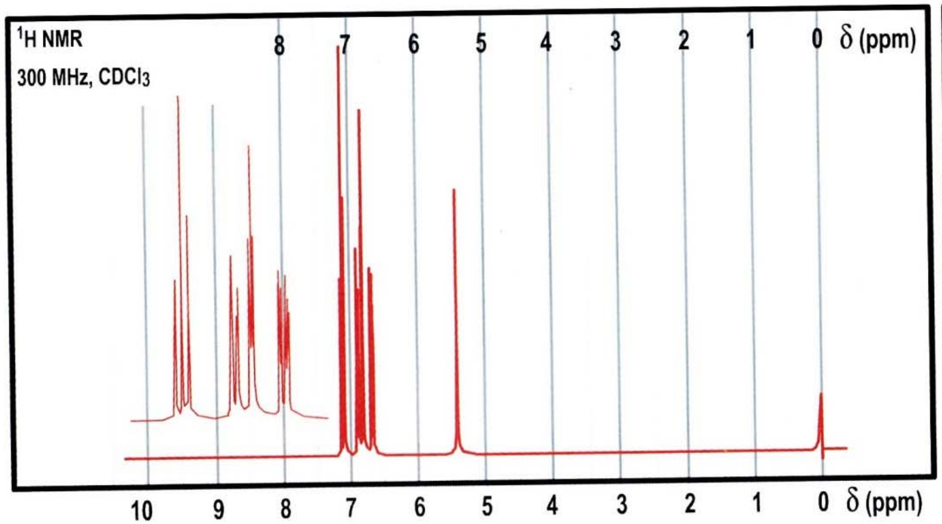
Příklad 21

Exercise 035 (082)

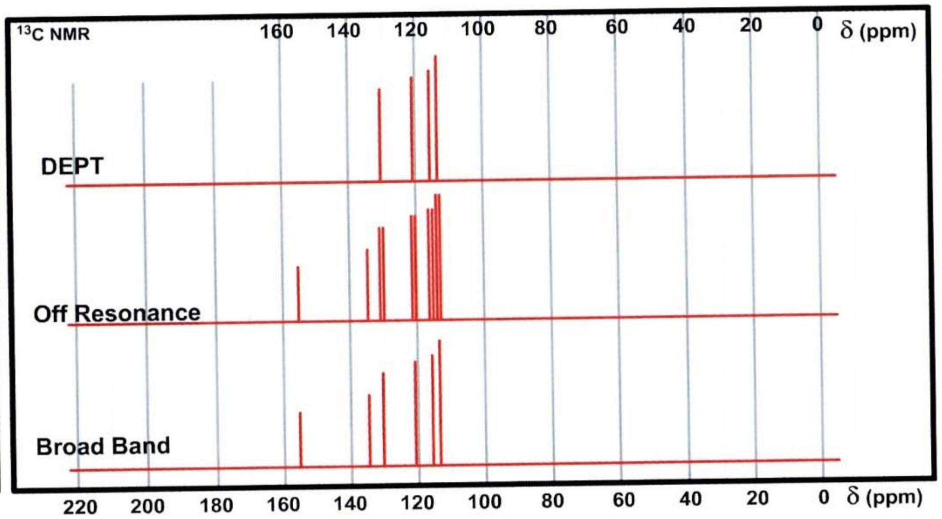




m / z	Int. rel.	m / z	Int. rel.	m / z	Int. rel.
17.0	1.1	47.0	1.1	73.0	9.7
18.0	5.0	49.0	3.0	74.0	4.5
26.0	2.4	50.0	7.7	75.0	4.4
27.0	2.5	51.0	3.7	89.0	2.3
28.0	2.5	53.0	8.5	92.0	6.3
29.0	3.3	55.0	1.9	93.0	6.4
31.0	3.1	60.0	2.0	99.0	8.8
32.0	3.6	61.0	7.1	100.0	16.5
36.0	1.4	62.0	10.7	101.0	3.6
37.0	9.0	63.0	25.4	102.0	5.4
38.0	15.5	64.0	26.7	128.0	100.0
39.0	30.6	65.0	63.0	129.0	6.9
40.0	1.5	66.0	4.7	130.0	32.1
42.0	1.1	72.0	1.3	131.0	2.1
46.0	3.2				



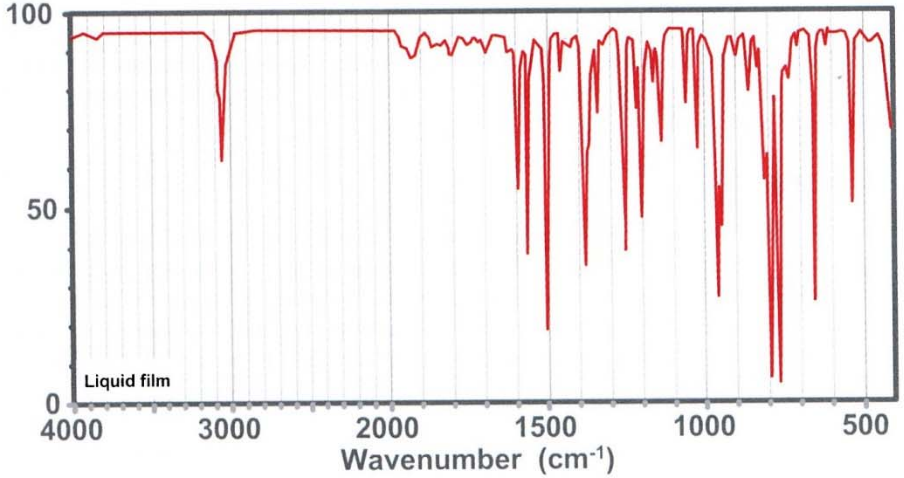
δ (integration): 7.1 (1) 6.9 (1), 6.8 (1),6.7 (1), 5.4 (1)

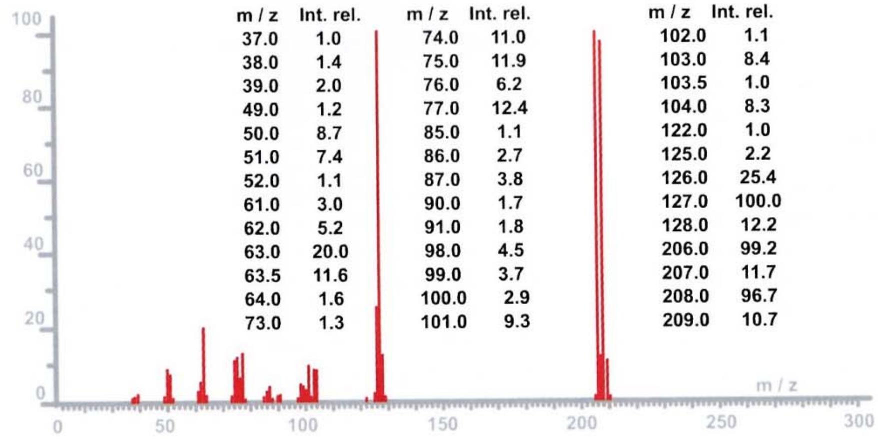


δ: 155.8, 135.0, 130.6, 121.5, 116.0, 113.9

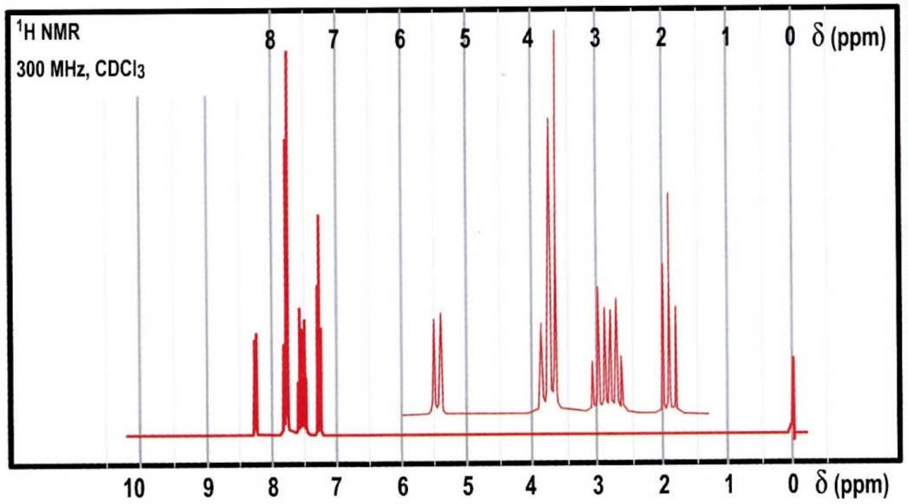
Příklad 22

Exercise 036 (091)

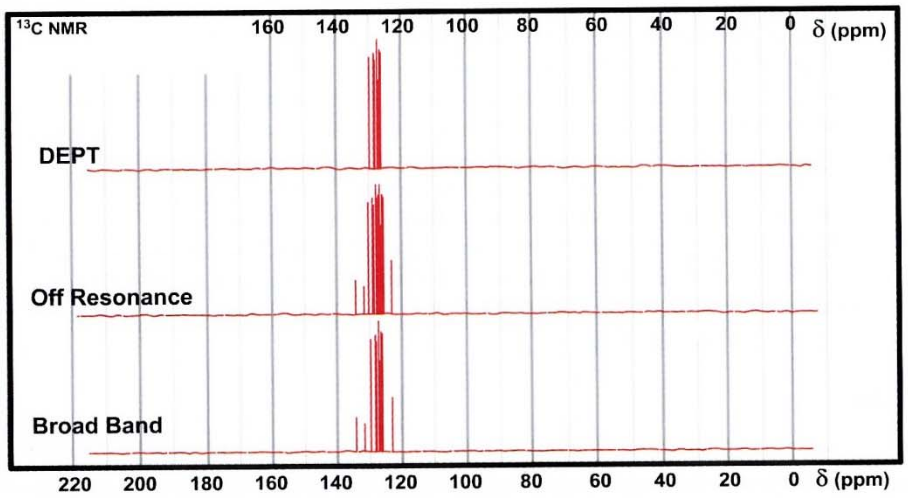




m / z	Int. rel.	m / z	Int. rel.	m / z	Int. rel.
37.0	1.0	74.0	11.0	102.0	1.1
38.0	1.4	75.0	11.9	103.0	8.4
39.0	2.0	76.0	6.2	103.5	1.0
49.0	1.2	77.0	12.4	104.0	8.3
50.0	8.7	85.0	1.1	122.0	1.0
51.0	7.4	86.0	2.7	125.0	2.2
52.0	1.1	87.0	3.8	126.0	25.4
61.0	3.0	90.0	1.7	127.0	100.0
62.0	5.2	91.0	1.8	128.0	12.2
63.0	20.0	98.0	4.5	206.0	99.2
63.5	11.6	99.0	3.7	207.0	11.7
64.0	1.6	100.0	2.9	208.0	96.7
73.0	1.3	101.0	9.3	209.0	10.7



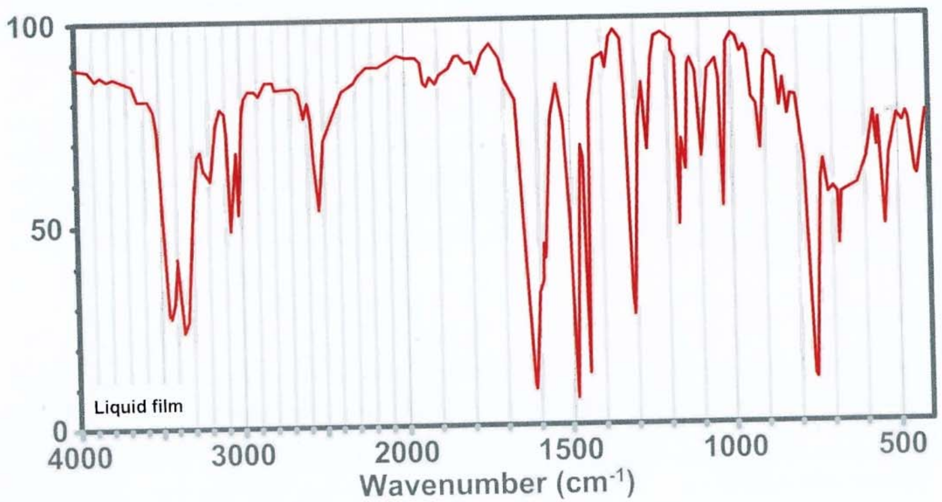
δ (integration): 8.19 (1), 7.73–7.70 (3), 7.51–7.44 (2), 7.21 (1)

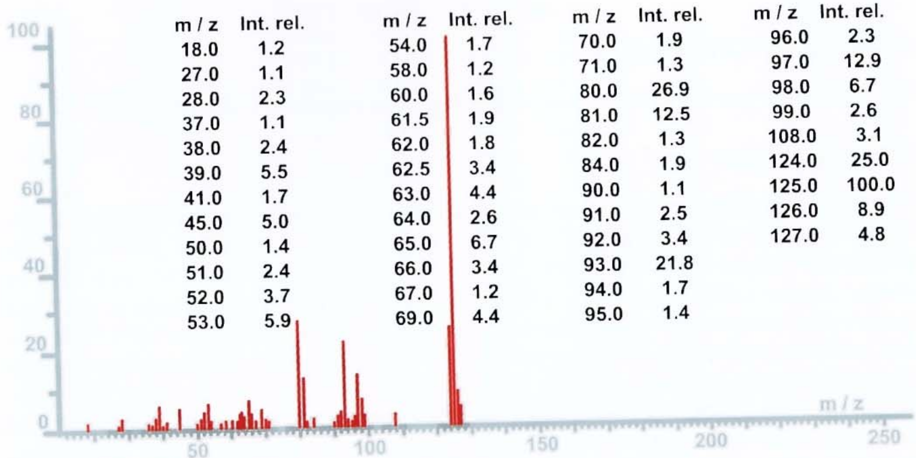


δ: 134.5, 131.9, 129.8, 128.2, 127.8, 127.2, 127.0, 126.6, 126.0, 122.8

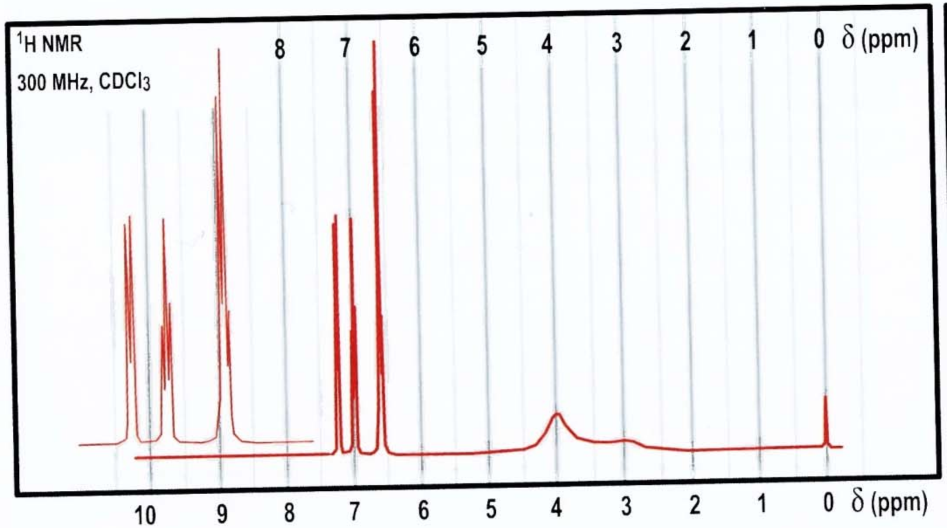
Příklad 23

Exercise 039 (087)

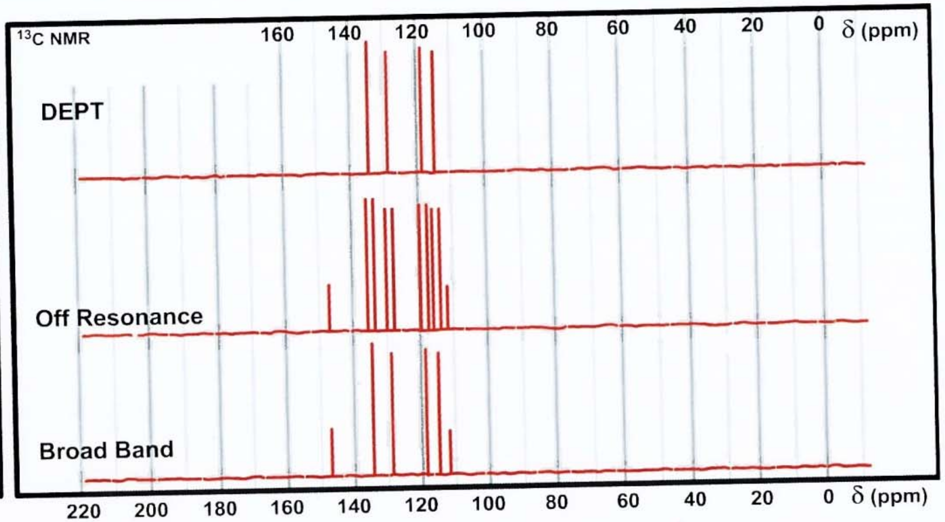




m / z	Int. rel.	m / z	Int. rel.	m / z	Int. rel.	m / z	Int. rel.
18.0	1.2	54.0	1.7	70.0	1.9	96.0	2.3
27.0	1.1	58.0	1.2	71.0	1.3	97.0	12.9
28.0	2.3	60.0	1.6	80.0	26.9	98.0	6.7
37.0	1.1	61.5	1.9	81.0	12.5	99.0	2.6
38.0	2.4	62.0	1.8	82.0	1.3	108.0	3.1
39.0	5.5	62.5	3.4	84.0	1.9	124.0	25.0
41.0	1.7	63.0	4.4	90.0	1.1	125.0	100.0
45.0	5.0	64.0	2.6	91.0	2.5	126.0	8.9
50.0	1.4	65.0	6.7	92.0	3.4	127.0	4.8
51.0	2.4	66.0	3.4	93.0	21.8		
52.0	3.7	67.0	1.2	94.0	1.7		
53.0	5.9	69.0	4.4	95.0	1.4		



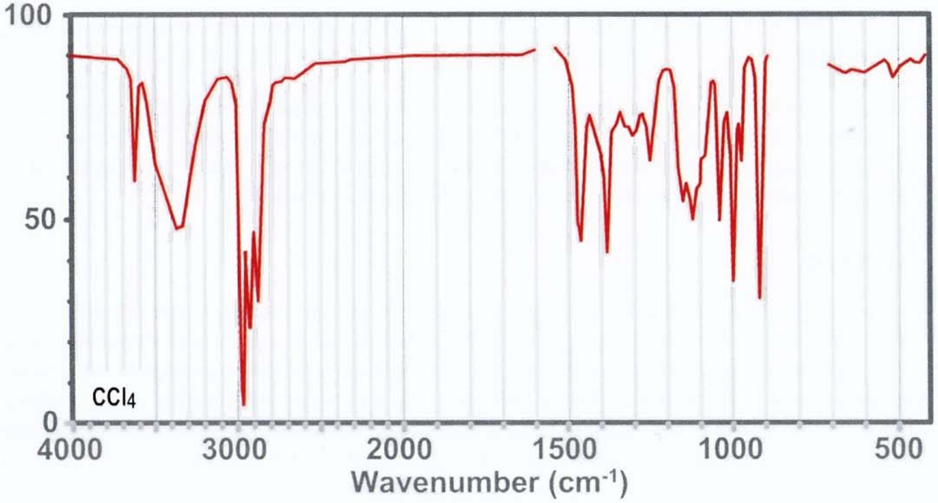
δ (integration): 7.3 (1), 7.0 (1), 6.6 (2), 3–4 (3)

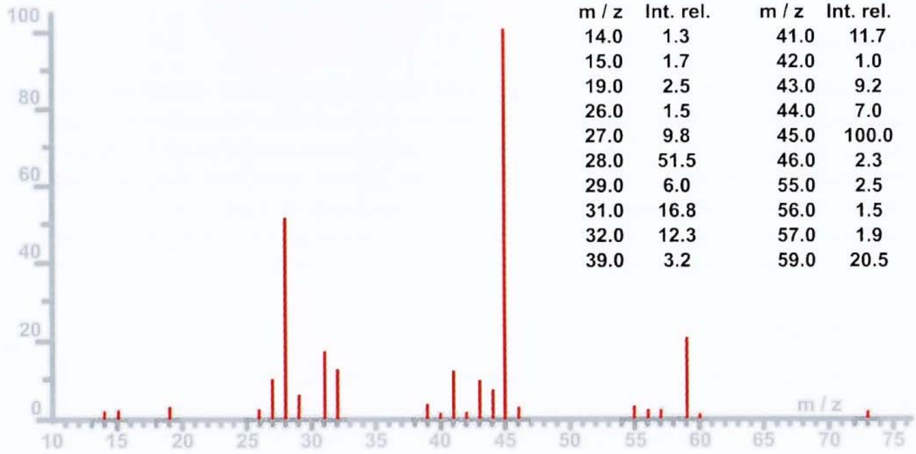


δ: 147.1, 134.7, 128.9, 118.6, 115.1, 111.8

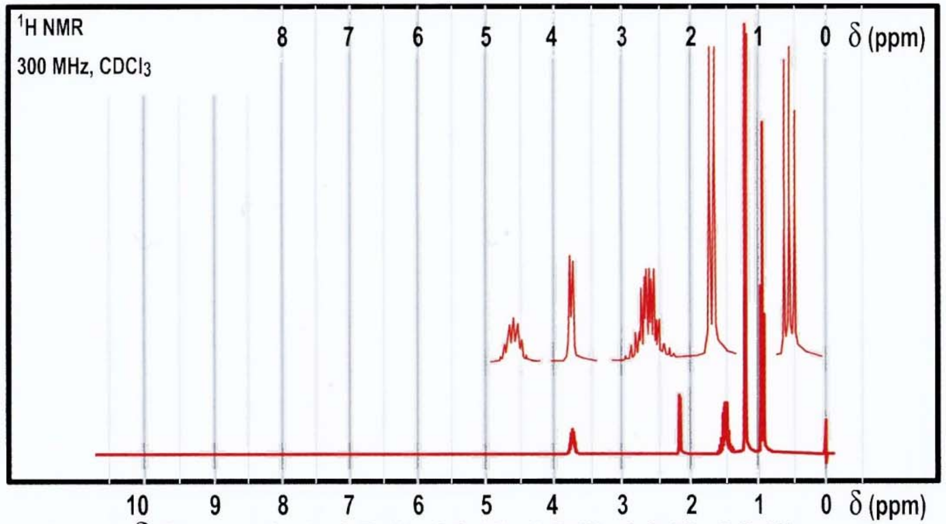
Příklad 24

Exercise 040 (070)

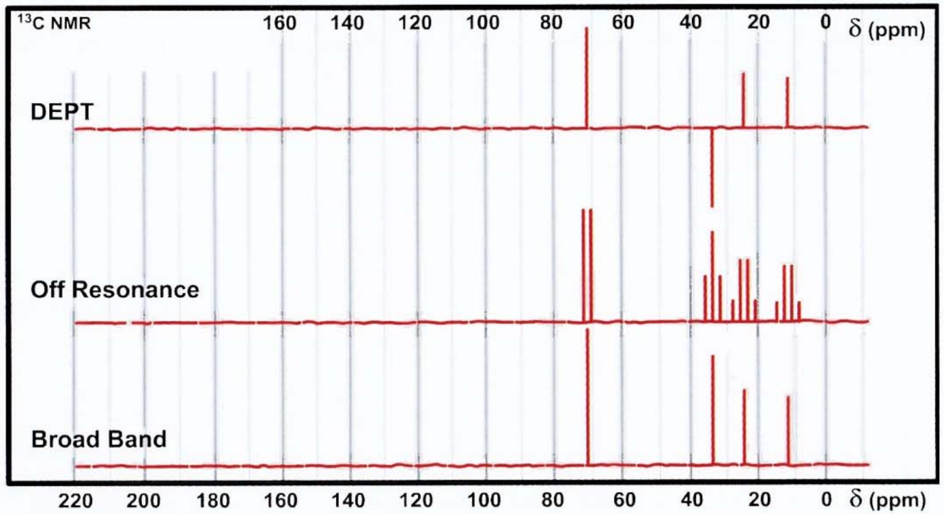




m / z	Int. rel.	m / z	Int. rel.
14.0	1.3	41.0	11.7
15.0	1.7	42.0	1.0
19.0	2.5	43.0	9.2
26.0	1.5	44.0	7.0
27.0	9.8	45.0	100.0
28.0	51.5	46.0	2.3
29.0	6.0	55.0	2.5
31.0	16.8	56.0	1.5
32.0	12.3	57.0	1.9
39.0	3.2	59.0	20.5



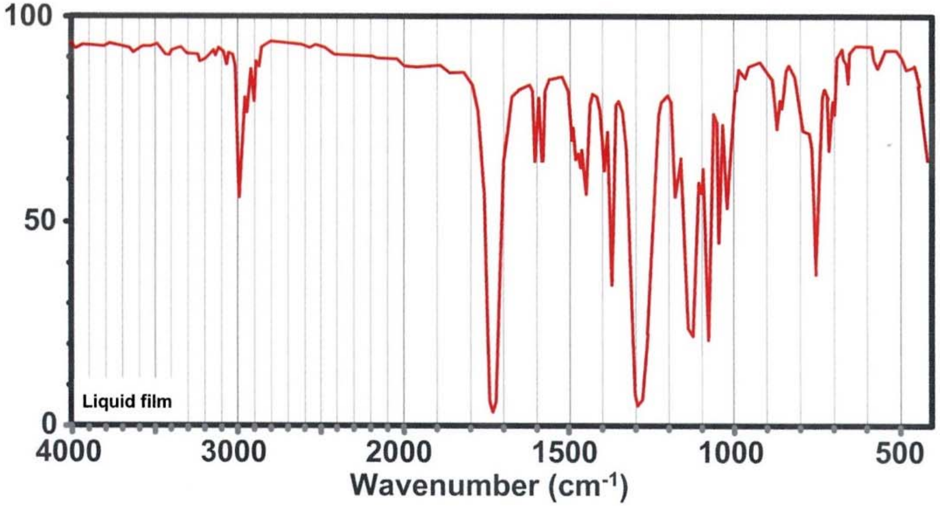
δ (integration): 3.7 (1), 2.2 (1), 1.5 (2), 1.2 (3), 0.9 (3)

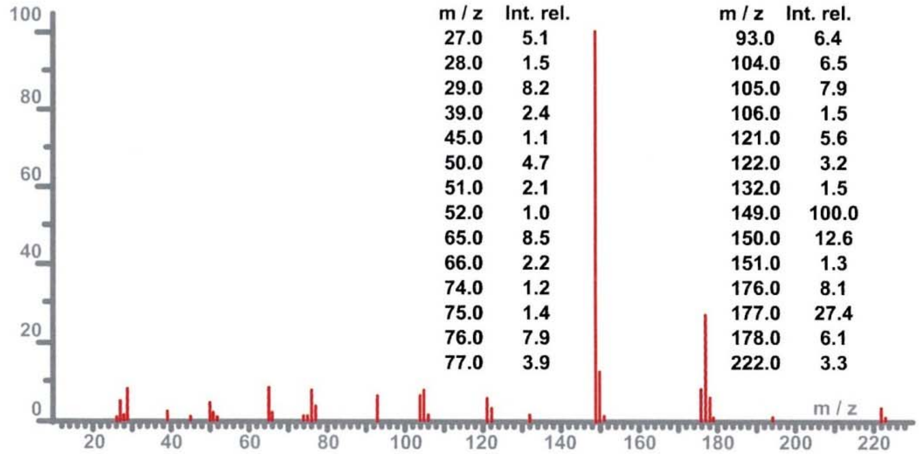


δ: 69.2, 32.1, 22.8, 10.0

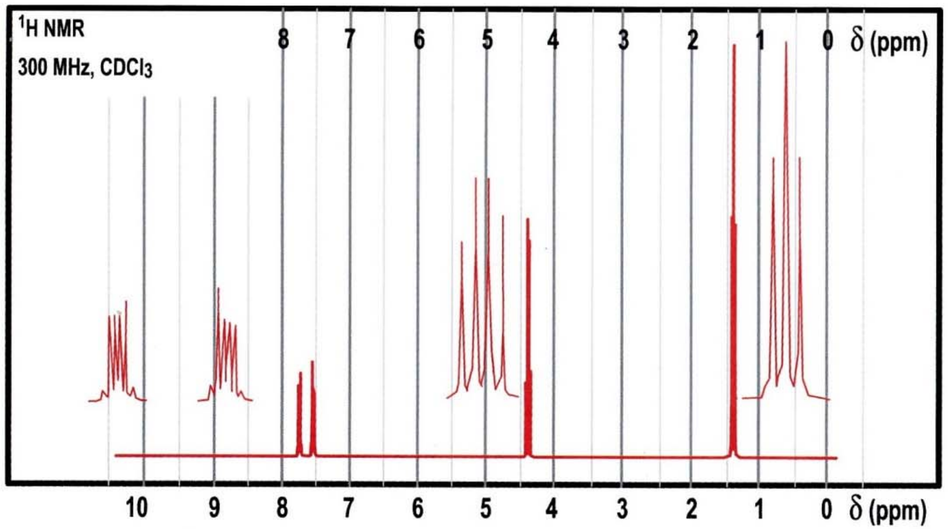
Příklad 25

Exercise 076 (064)

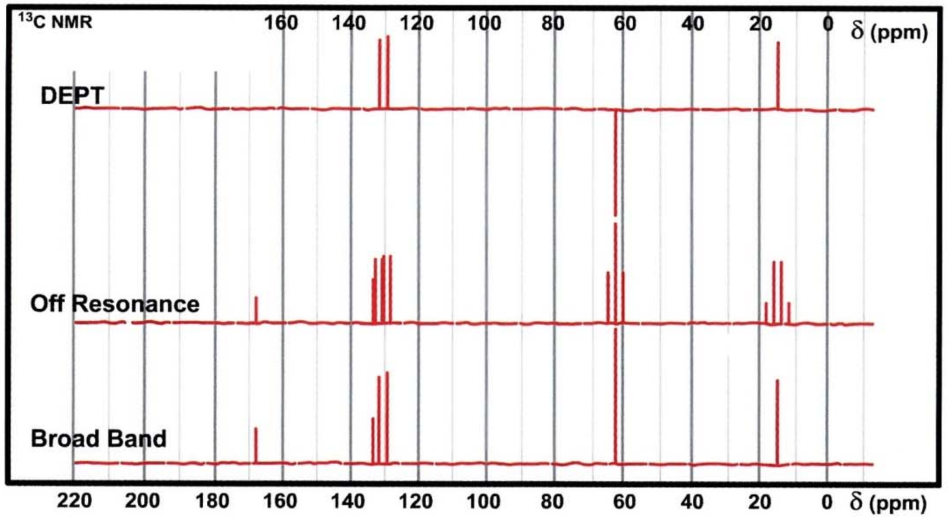




m / z	Int. rel.	m / z	Int. rel.
27.0	5.1	93.0	6.4
28.0	1.5	104.0	6.5
29.0	8.2	105.0	7.9
39.0	2.4	106.0	1.5
45.0	1.1	121.0	5.6
50.0	4.7	122.0	3.2
51.0	2.1	132.0	1.5
52.0	1.0	149.0	100.0
65.0	8.5	150.0	12.6
66.0	2.2	151.0	1.3
74.0	1.2	176.0	8.1
75.0	1.4	177.0	27.4
76.0	7.9	178.0	6.1
77.0	3.9	222.0	3.3



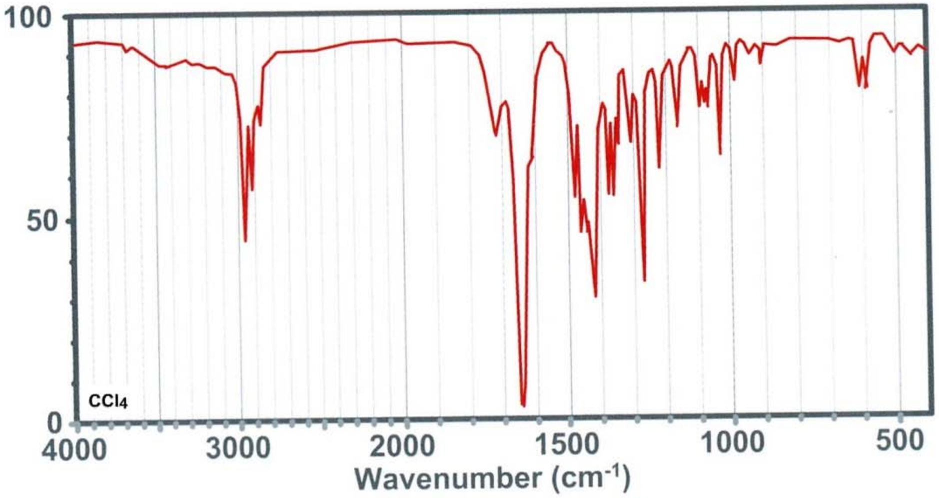
δ (integration): 7.7 (1), 7.5 (1), 4.3 (2), 1.4 (3)

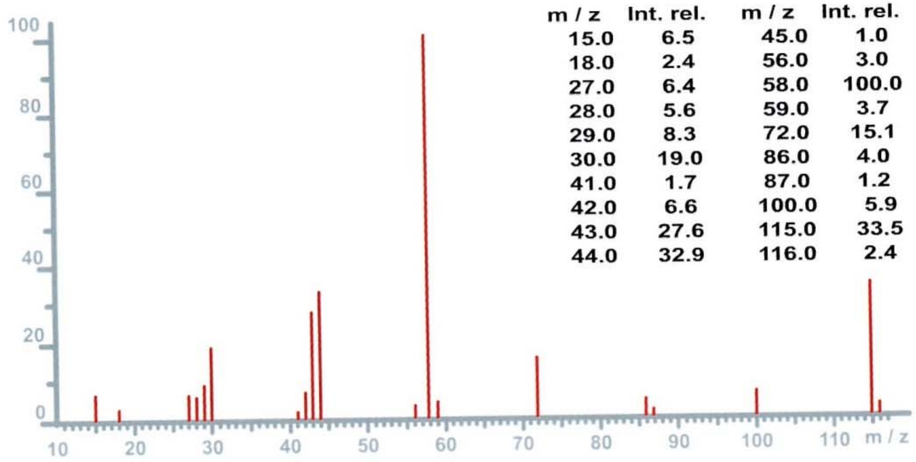


δ: 168, 132, 131, 129, 62, 14

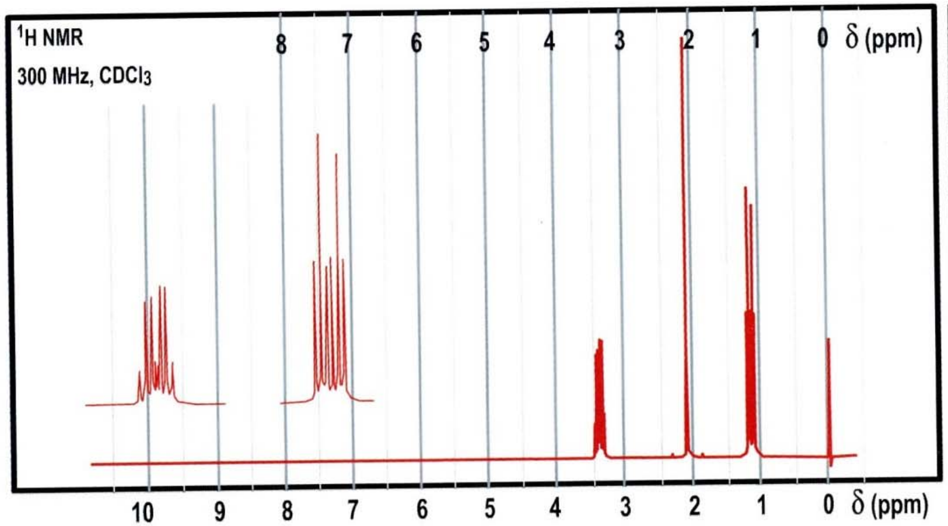
Příklad 26

Exercise 045 (008)

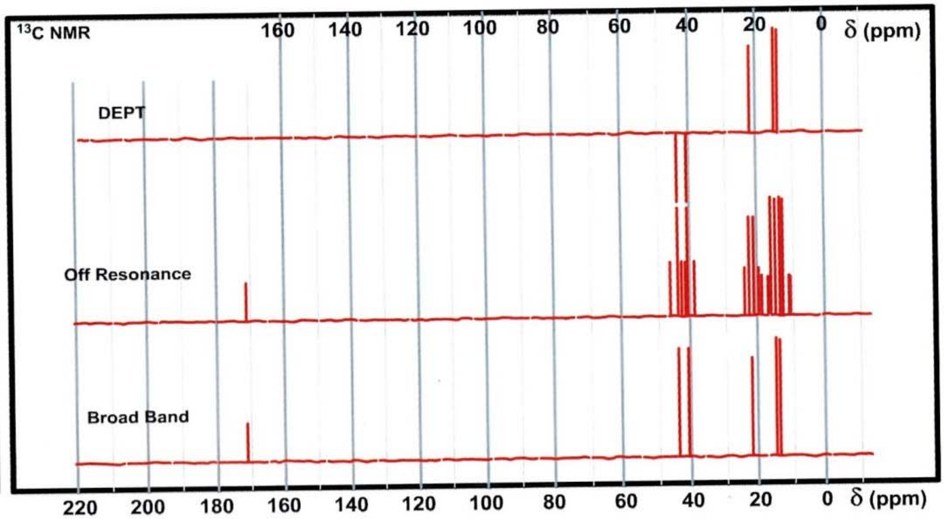




m / z	Int. rel.	m / z	Int. rel.
15.0	6.5	45.0	1.0
18.0	2.4	56.0	3.0
27.0	6.4	58.0	100.0
28.0	5.6	59.0	3.7
29.0	8.3	72.0	15.1
30.0	19.0	86.0	4.0
41.0	1.7	87.0	1.2
42.0	6.6	100.0	5.9
43.0	27.6	115.0	33.5
44.0	32.9	116.0	2.4



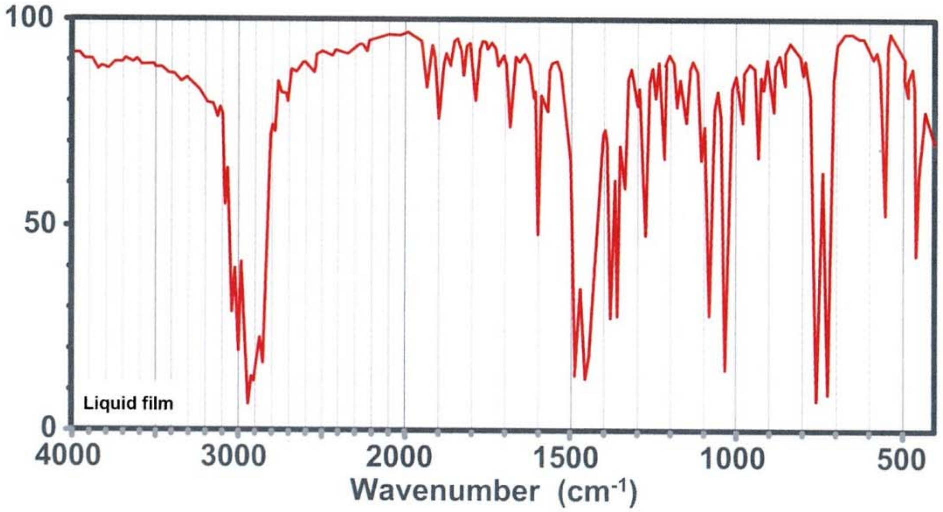
δ (integration): 3.3 (4), 2.1 (3), 1.2 (6)

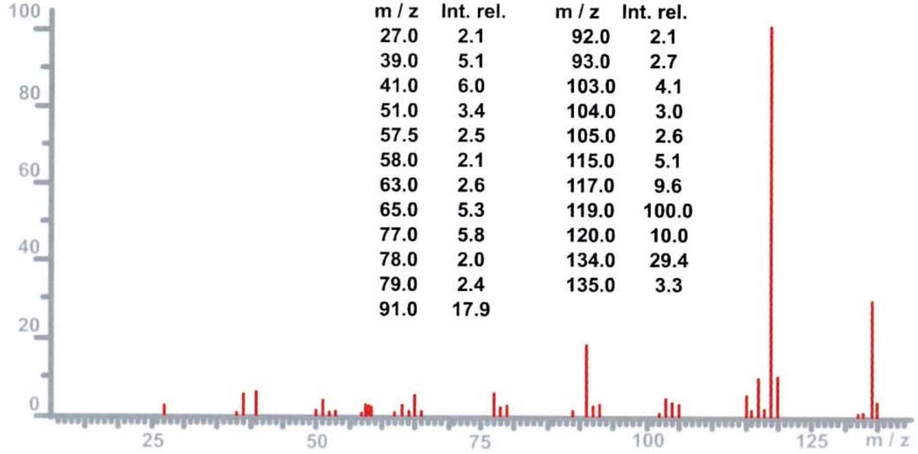


δ: 169.6, 42.9, 40.0, 21.4, 14.2, 13.1

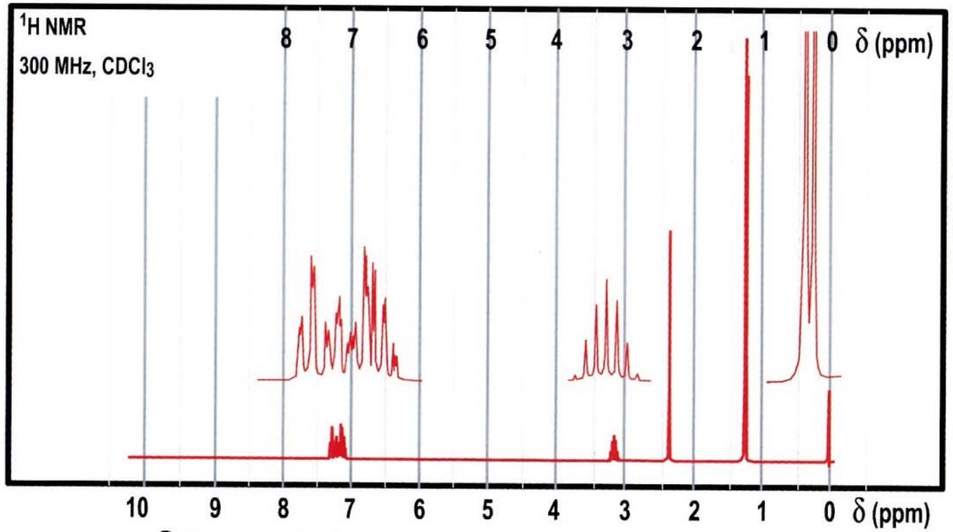
Příklad 27

Exercise 048 (032)

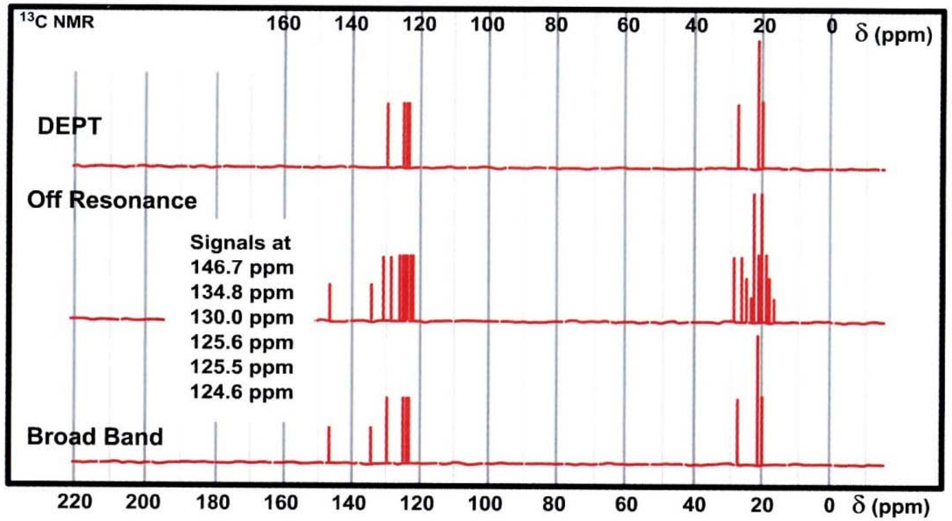




m / z	Int. rel.	m / z	Int. rel.
27.0	2.1	92.0	2.1
39.0	5.1	93.0	2.7
41.0	6.0	103.0	4.1
51.0	3.4	104.0	3.0
57.5	2.5	105.0	2.6
58.0	2.1	115.0	5.1
63.0	2.6	117.0	9.6
65.0	5.3	119.0	100.0
77.0	5.8	120.0	10.0
78.0	2.0	134.0	29.4
79.0	2.4	135.0	3.3
91.0	17.9		



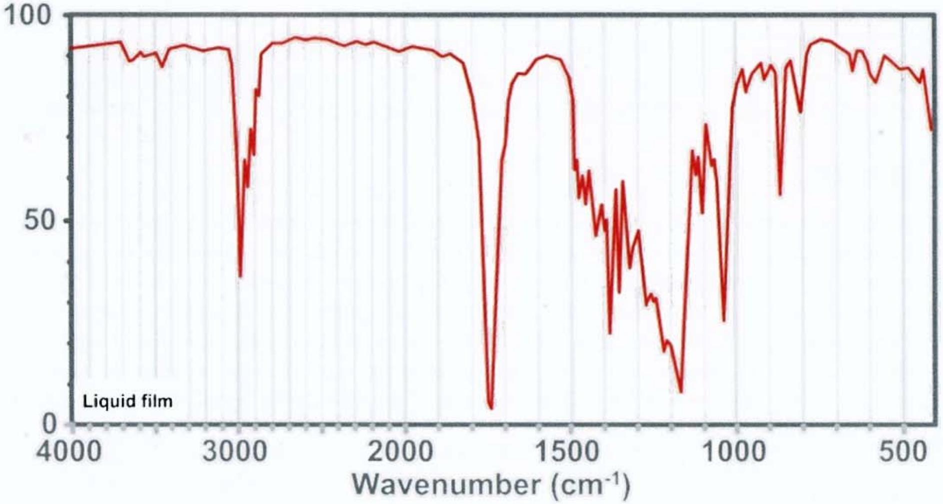
δ (integration): 7.0–7.3 (4), 3.1 (1), 2.3 (3), 1.2 (6)

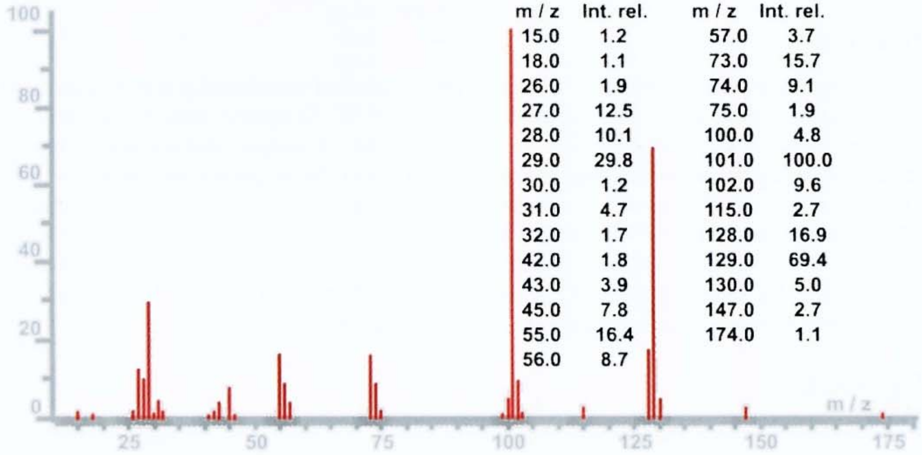


δ: 146.7, 134.8, 130.0, 125.6, 125.5, 124.6, 29, 22, 19

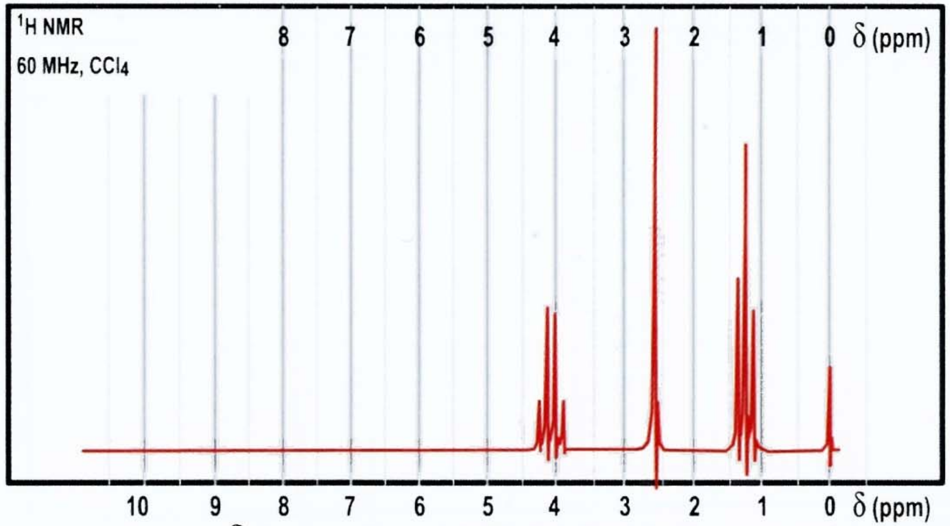
Příklad 28

Exercise 053 (042)

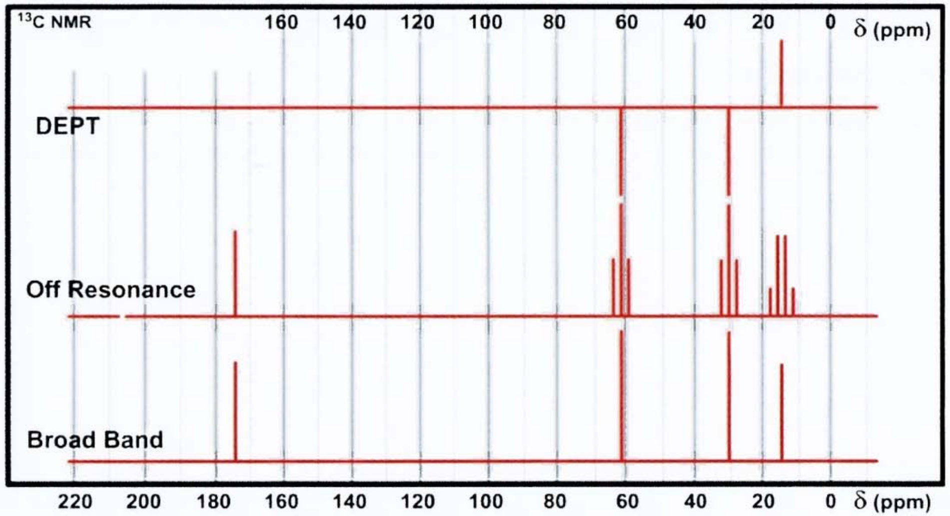




m / z	Int. rel.	m / z	Int. rel.
15.0	1.2	57.0	3.7
18.0	1.1	73.0	15.7
26.0	1.9	74.0	9.1
27.0	12.5	75.0	1.9
28.0	10.1	100.0	4.8
29.0	29.8	101.0	100.0
30.0	1.2	102.0	9.6
31.0	4.7	115.0	2.7
32.0	1.7	128.0	16.9
42.0	1.8	129.0	69.4
43.0	3.9	130.0	5.0
45.0	7.8	147.0	2.7
55.0	16.4	174.0	1.1
56.0	8.7		



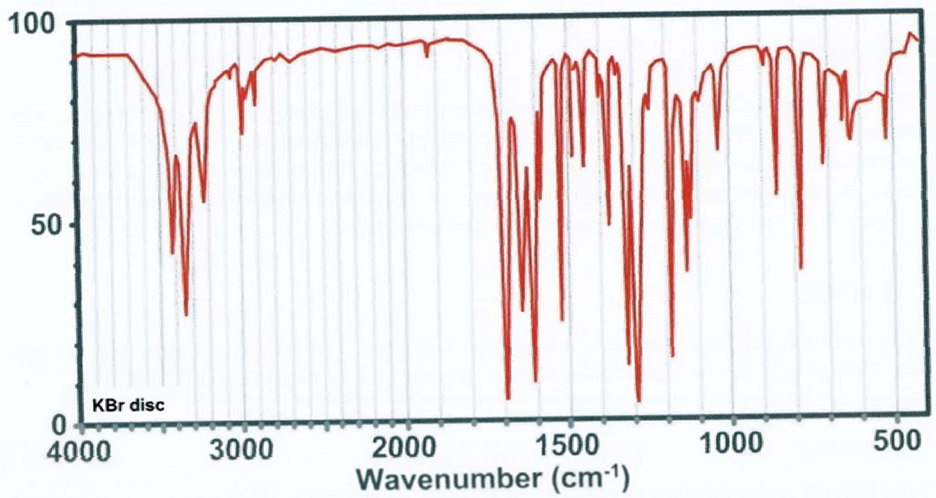
δ (integration): 4.1 (2), 2.6 (2), 1.2 (3)

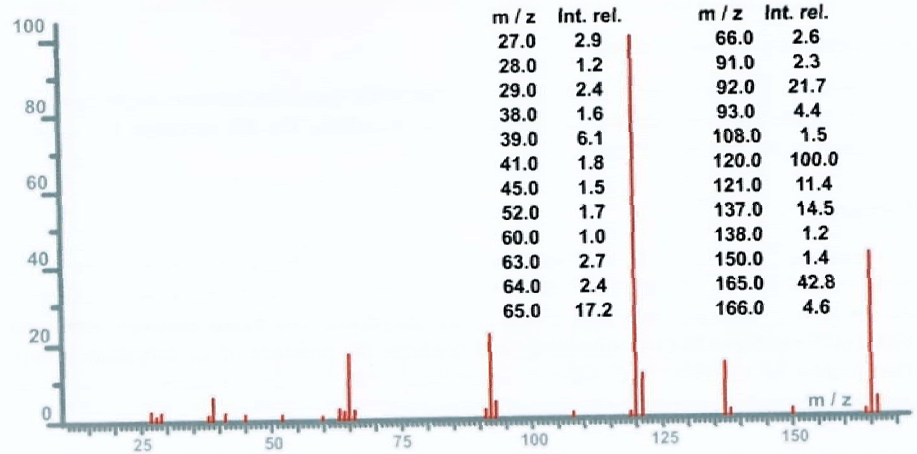


δ: 172.36, 60.67, 29.26, 14.24

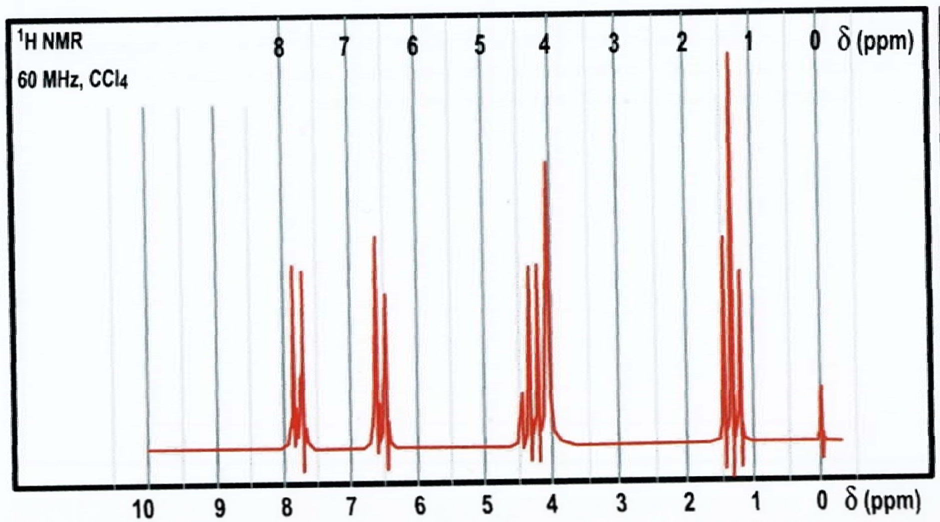
Příklad 29

Exercise 055 (048)

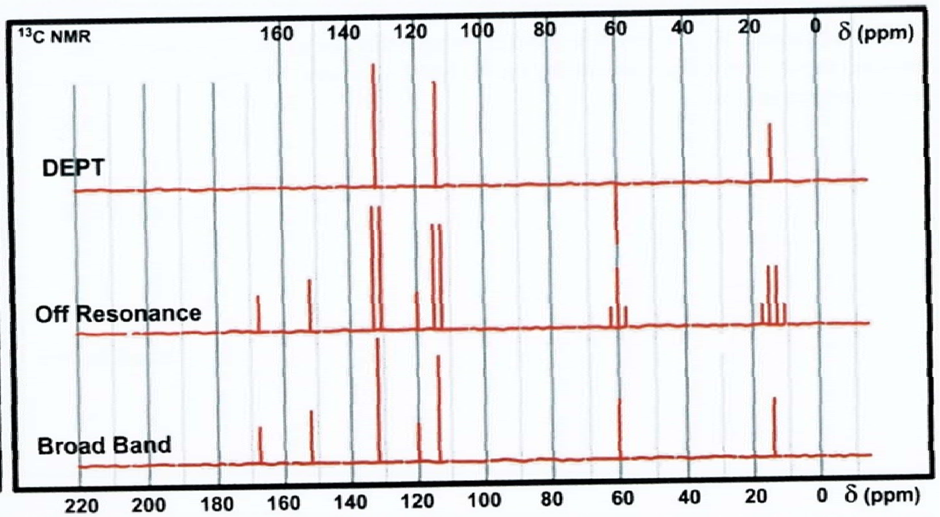




m / z	Int. rel.	m / z	Int. rel.
27.0	2.9	66.0	2.6
28.0	1.2	91.0	2.3
29.0	2.4	92.0	21.7
38.0	1.6	93.0	4.4
39.0	6.1	108.0	1.5
41.0	1.8	120.0	100.0
45.0	1.5	121.0	11.4
52.0	1.7	137.0	14.5
60.0	1.0	138.0	1.2
63.0	2.7	150.0	1.4
64.0	2.4	165.0	42.8
65.0	17.2	166.0	4.6



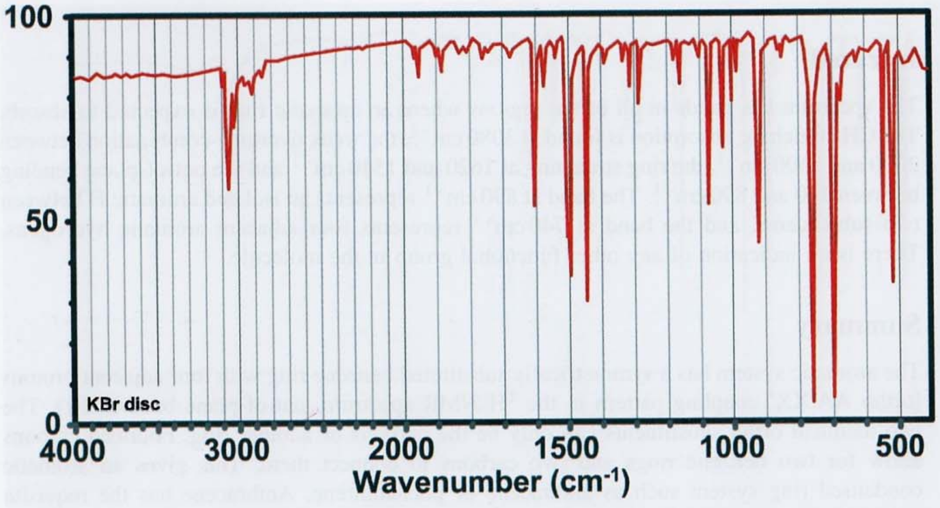
δ: (integration): 7.8 (2), 6.6 (2), 4.3 (2), 4.1 (2), 1.4 (3)

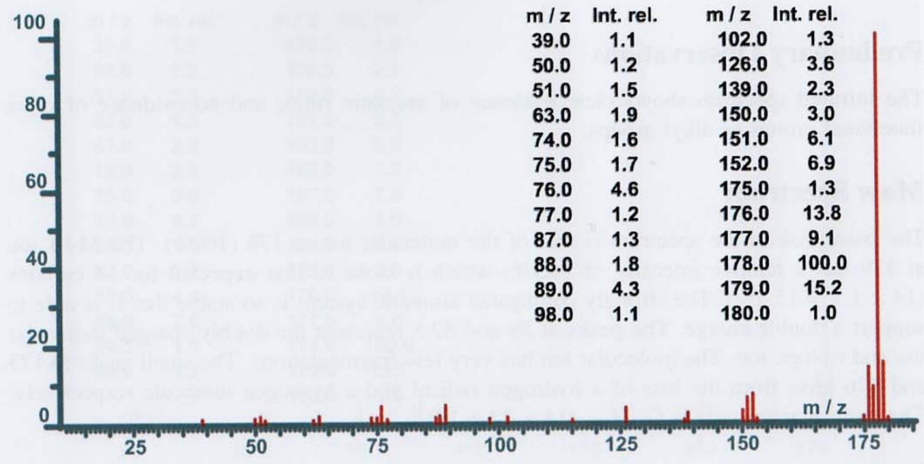


δ: 166.9, 151.4, 131.6, 119.6, 113.7, 60.3, 14.4

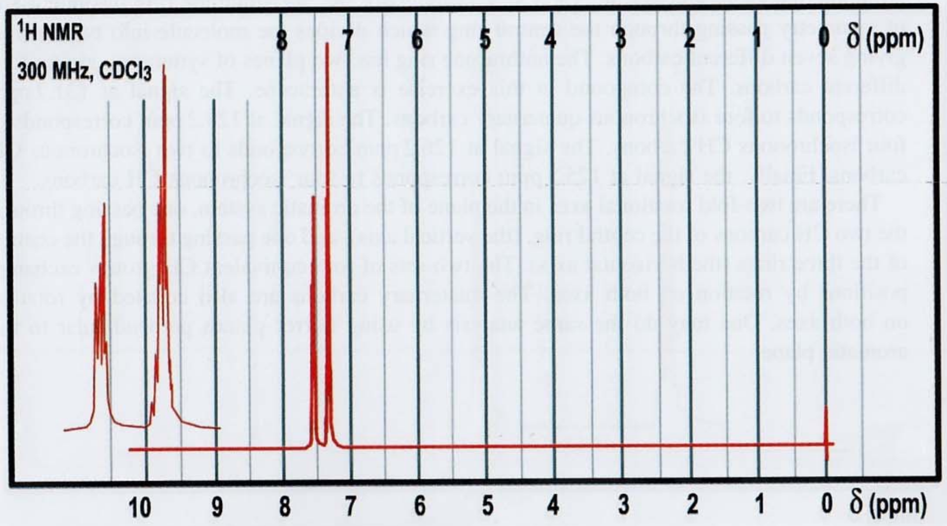
Příklad 30

Exercise 059 (097)

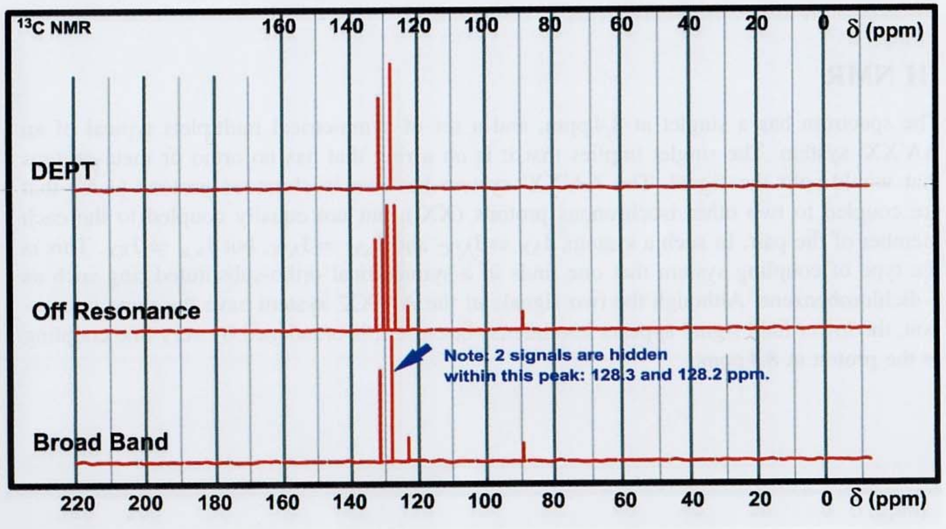




m / z	Int. rel.	m / z	Int. rel.
39.0	1.1	102.0	1.3
50.0	1.2	126.0	3.6
51.0	1.5	139.0	2.3
63.0	1.9	150.0	3.0
74.0	1.6	151.0	6.1
75.0	1.7	152.0	6.9
76.0	4.6	175.0	1.3
77.0	1.2	176.0	13.8
87.0	1.3	177.0	9.1
88.0	1.8	178.0	100.0
89.0	4.3	179.0	15.2
98.0	1.1	180.0	1.0



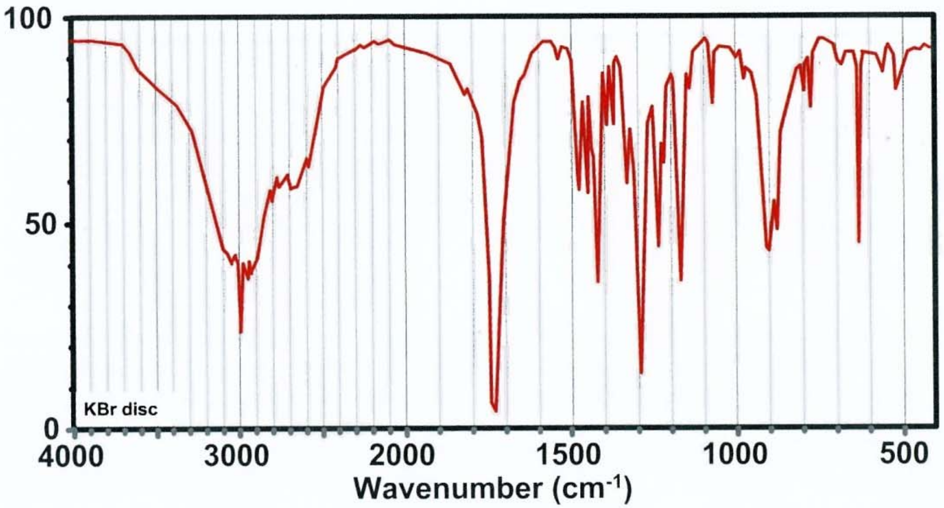
δ (integration): 7.5 (2), 7.3 (3)

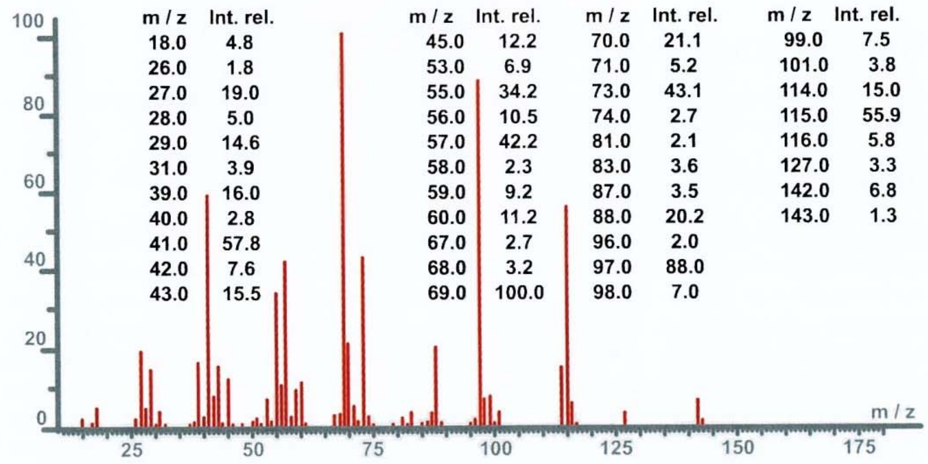


δ: 131.59, 128.33, 128.26, 123.31, 89.43

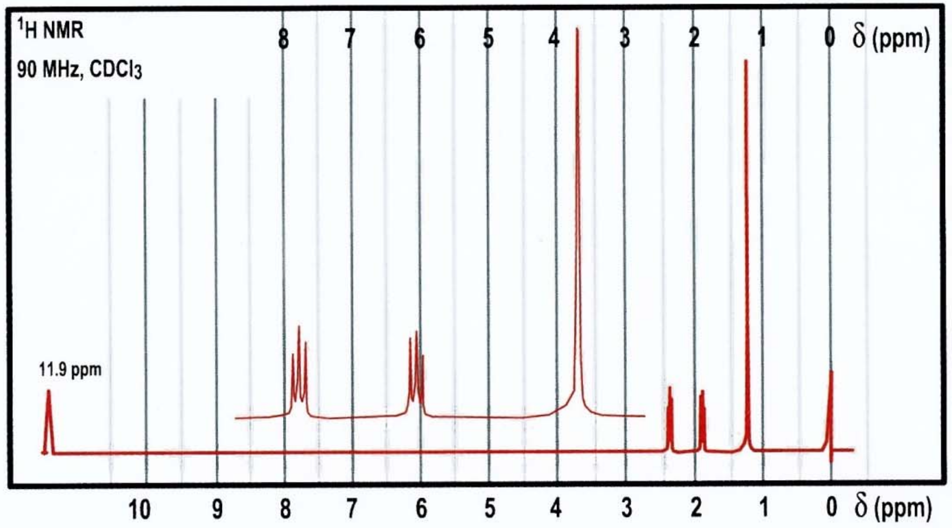
Příklad 31

Exercise 061 (077)

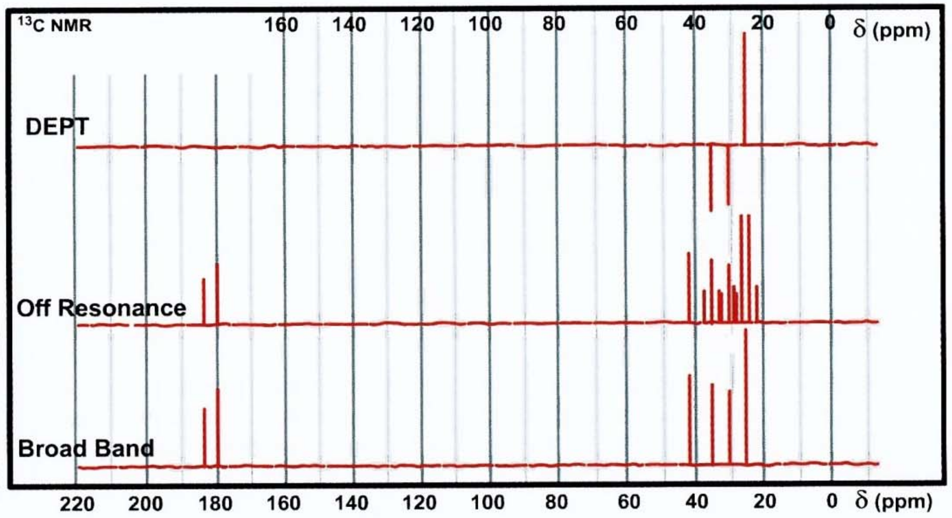




m / z	Int. rel.	m / z	Int. rel.	m / z	Int. rel.	m / z	Int. rel.
18.0	4.8	45.0	12.2	70.0	21.1	99.0	7.5
26.0	1.8	53.0	6.9	71.0	5.2	101.0	3.8
27.0	19.0	55.0	34.2	73.0	43.1	114.0	15.0
28.0	5.0	56.0	10.5	74.0	2.7	115.0	55.9
29.0	14.6	57.0	42.2	81.0	2.1	116.0	5.8
31.0	3.9	58.0	2.3	83.0	3.6	127.0	3.3
39.0	16.0	59.0	9.2	87.0	3.5	142.0	6.8
40.0	2.8	60.0	11.2	88.0	20.2	143.0	1.3
41.0	57.8	67.0	2.7	96.0	2.0		
42.0	7.6	68.0	3.2	97.0	88.0		
43.0	15.5	69.0	100.0	98.0	7.0		



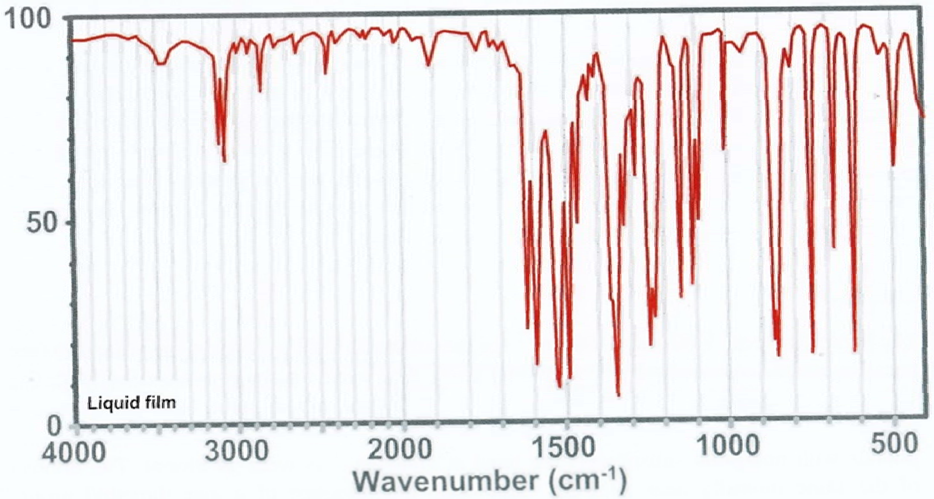
δ (integration): 11.9 (1), 2.4 (1), 1.9 (1), 1.2 (3)

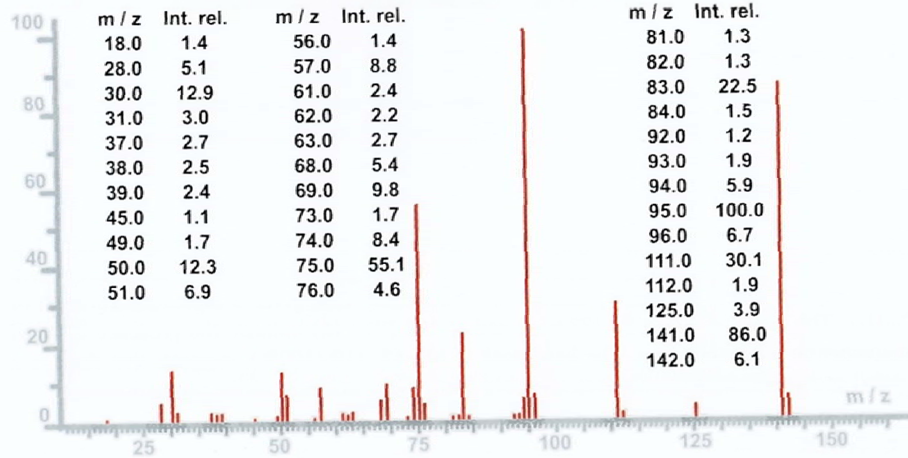


δ: 184.2, 180.0, 41.4, 34.8, 30.1, 24.8

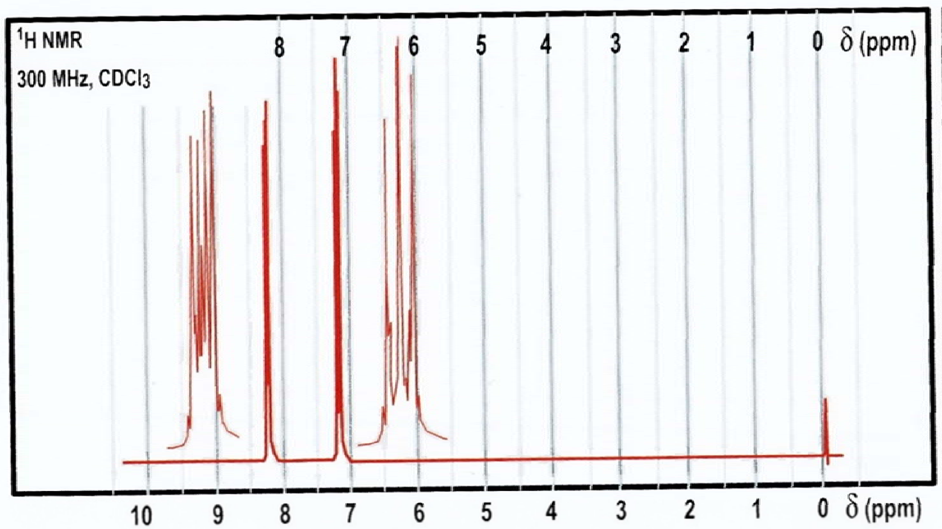
Příklad 32

Exercise 065 (074)

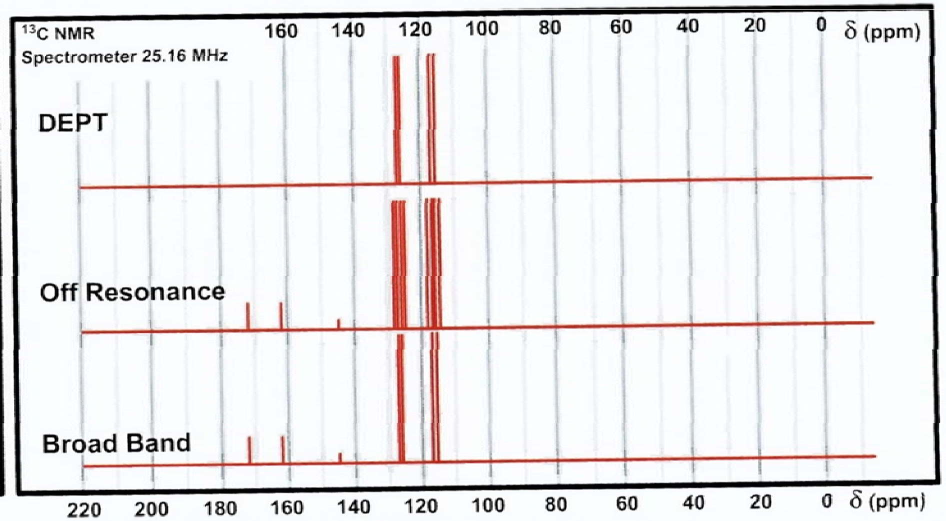




m / z	Int. rel.	m / z	Int. rel.	m / z	Int. rel.
18.0	1.4	56.0	1.4	81.0	1.3
28.0	5.1	57.0	8.8	82.0	1.3
30.0	12.9	61.0	2.4	83.0	22.5
31.0	3.0	62.0	2.2	84.0	1.5
37.0	2.7	63.0	2.7	92.0	1.2
38.0	2.5	68.0	5.4	93.0	1.9
39.0	2.4	69.0	9.8	94.0	5.9
45.0	1.1	73.0	1.7	95.0	100.0
49.0	1.7	74.0	8.4	96.0	6.7
50.0	12.3	75.0	55.1	111.0	30.1
51.0	6.9	76.0	4.6	112.0	1.9
				125.0	3.9
				141.0	86.0
				142.0	6.1



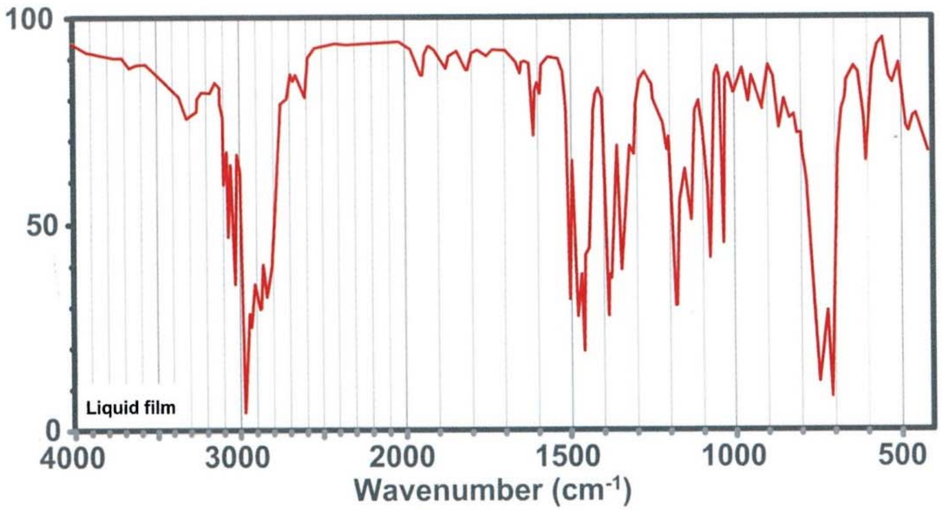
δ (integration): 8.3 (1), (7.2 (1)

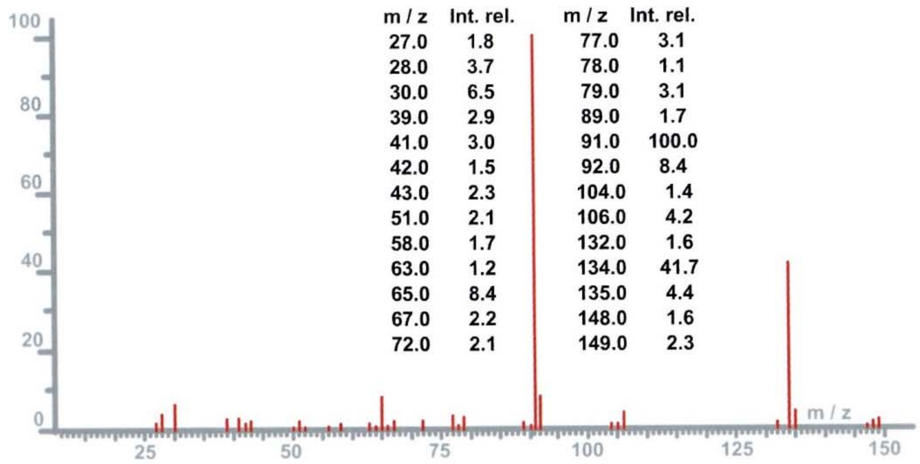


δ: 171.57, 161.34, 144.60, 126.66, 126.26, 117.02, 116.07

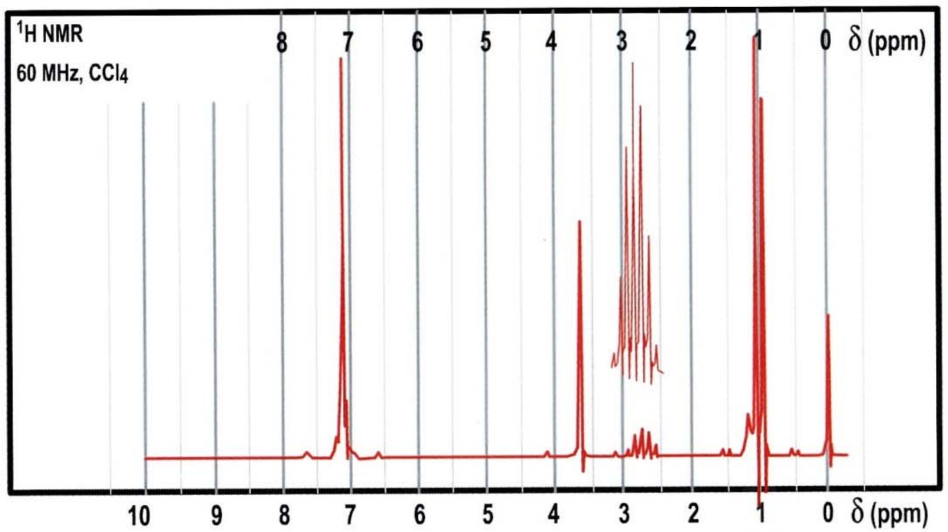
Příklad 33

Exercise 075 (059)

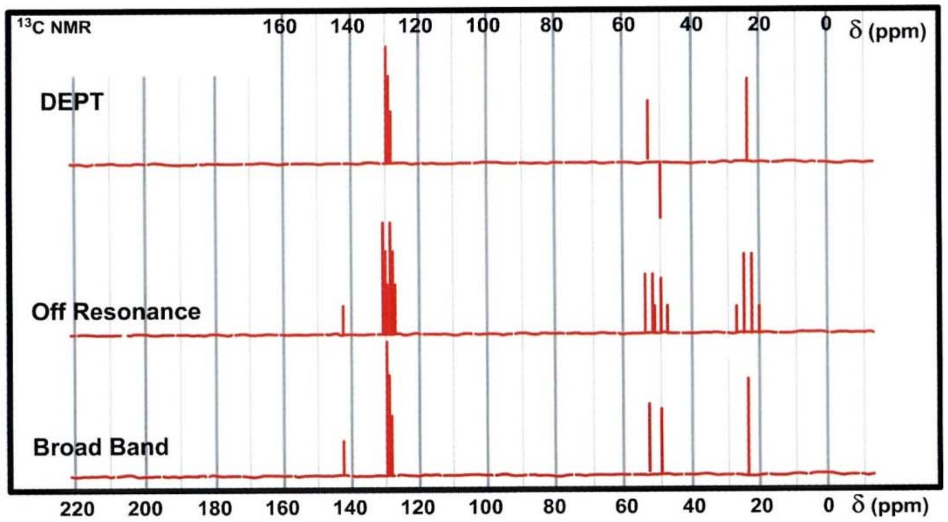




m / z	Int. rel.	m / z	Int. rel.
27.0	1.8	77.0	3.1
28.0	3.7	78.0	1.1
30.0	6.5	79.0	3.1
39.0	2.9	89.0	1.7
41.0	3.0	91.0	100.0
42.0	1.5	92.0	8.4
43.0	2.3	104.0	1.4
51.0	2.1	106.0	4.2
58.0	1.7	132.0	1.6
63.0	1.2	134.0	41.7
65.0	8.4	135.0	4.4
67.0	2.2	148.0	1.6
72.0	2.1	149.0	2.3

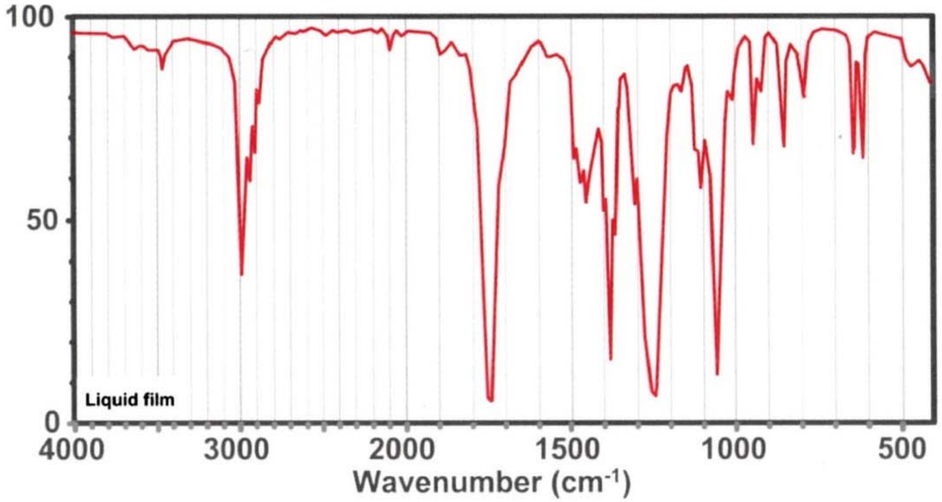


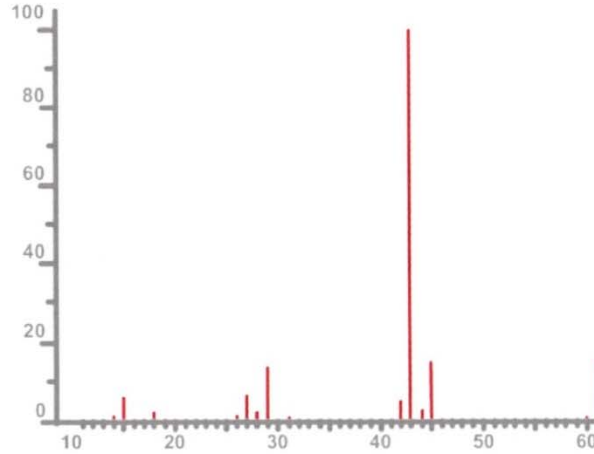
δ (integration): 7.3 (5), 3.8 (2), 2.8 (1), 1.25 – 1.1 (7)



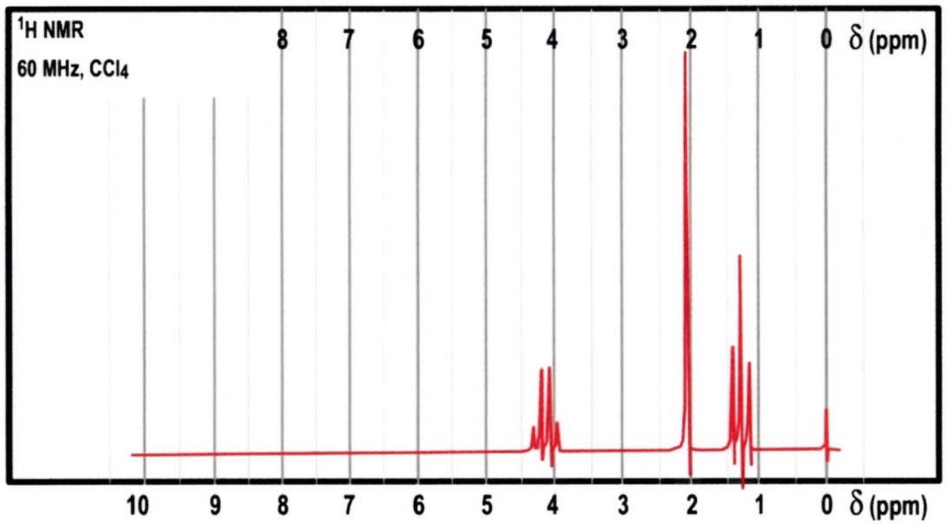
δ: 142, 128.3, 128.0, 126, 51, 48, 23

Příklad 34

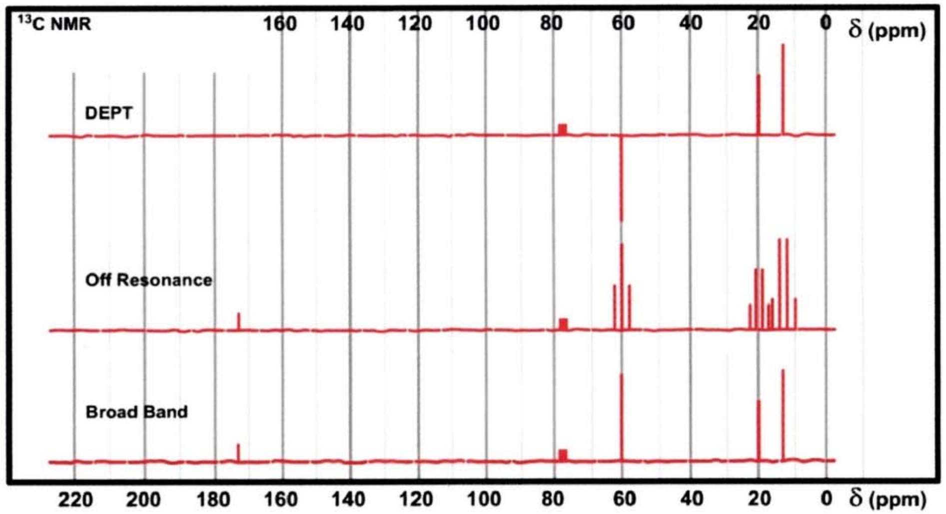




m / z	Int. rel.	m / z	Int. rel.
14.0	1.3	42.0	4.9
15.0	6.2	43.0	100.0
18.0	2.1	44.0	2.7
26.0	1.4	45.0	14.7
27.0	6.5	61.0	14.9
28.0	2.5	70.0	9.9
29.0	13.7	73.0	4.7
31.0	1.0	88.0	5.1

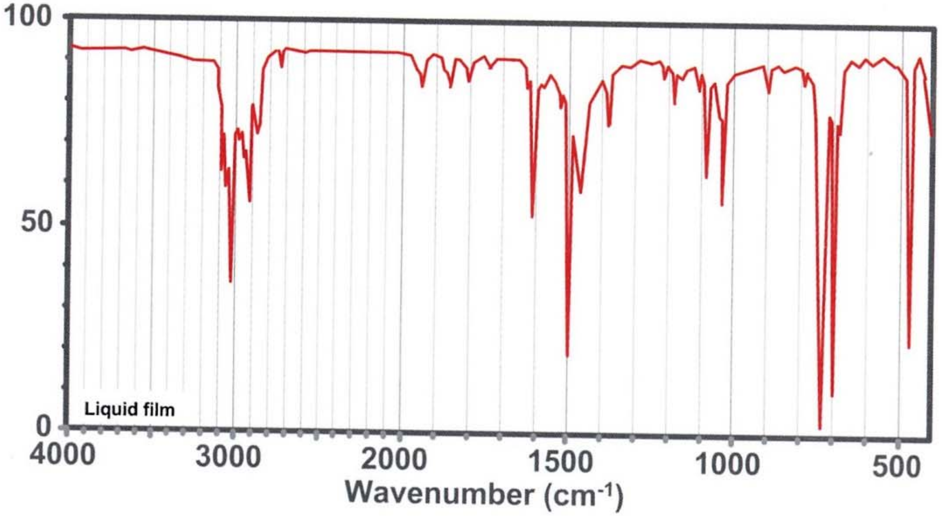


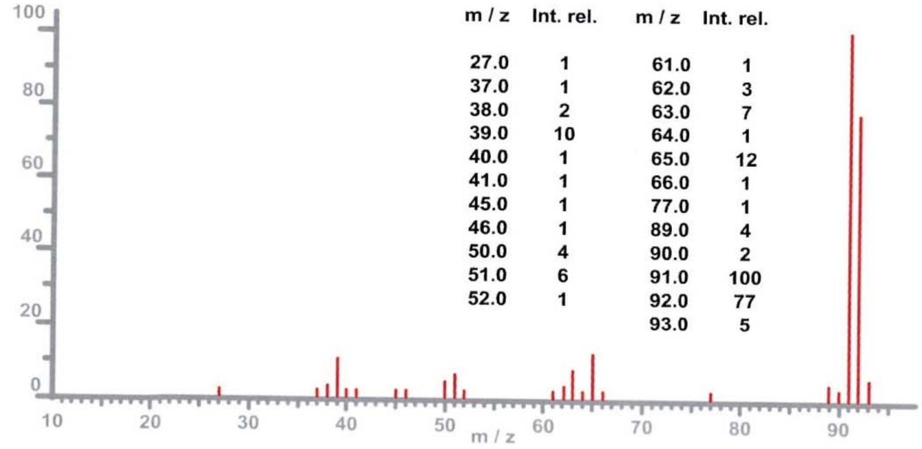
δ (integration): 4.12 (2), 2.04 (3), 1.26 (3)



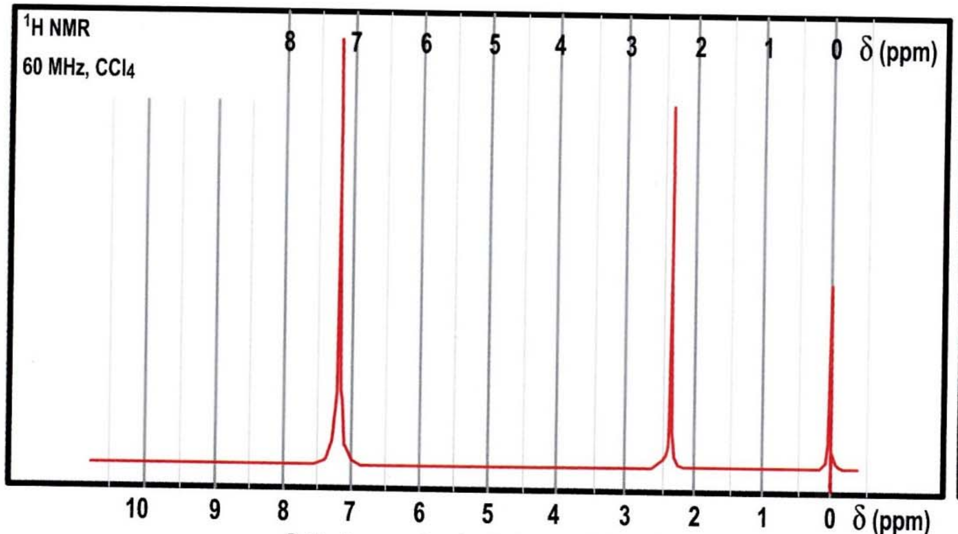
δ: 171.1, 60.4, 21.0, 14.3

Příklad 35

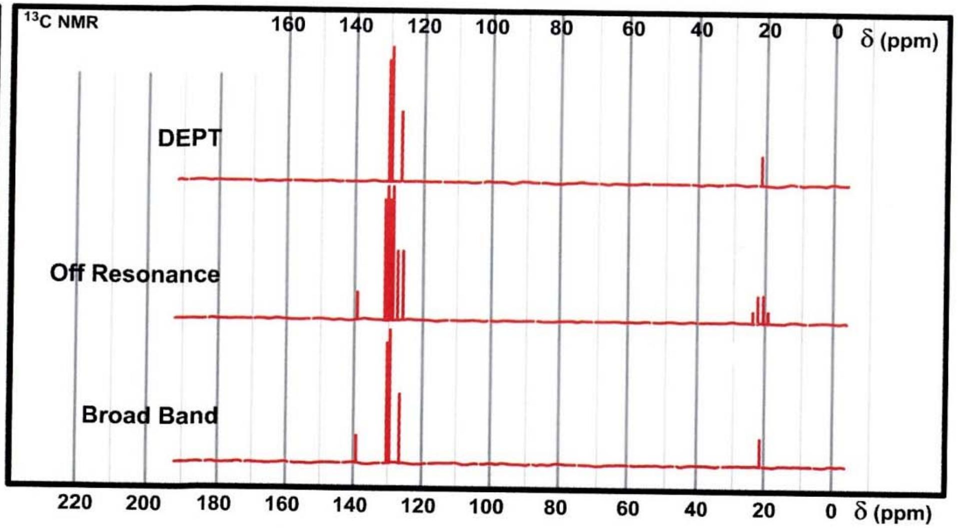




m / z	Int. rel.	m / z	Int. rel.
27.0	1	61.0	1
37.0	1	62.0	3
38.0	2	63.0	7
39.0	10	64.0	1
40.0	1	65.0	12
41.0	1	66.0	1
45.0	1	77.0	1
46.0	1	89.0	4
50.0	4	90.0	2
51.0	6	91.0	100
52.0	1	92.0	77
		93.0	5

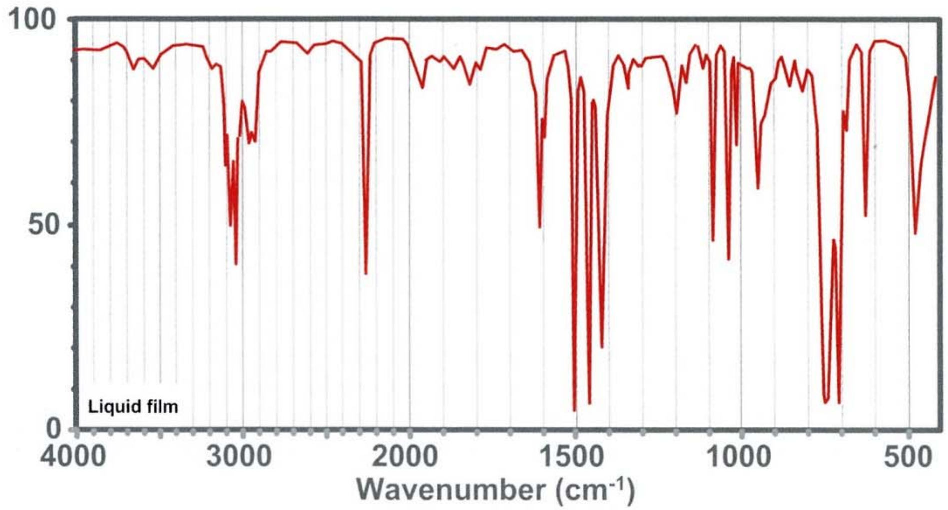


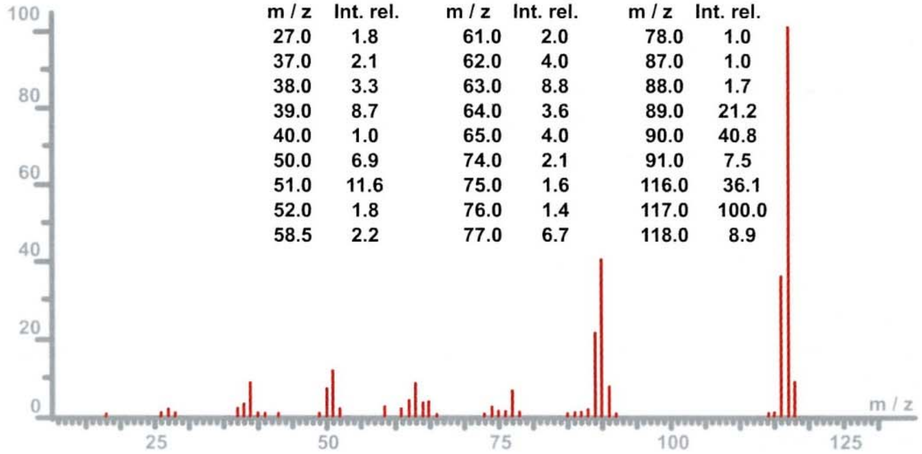
δ (integration): 7.2 (5), 2.4 (3).



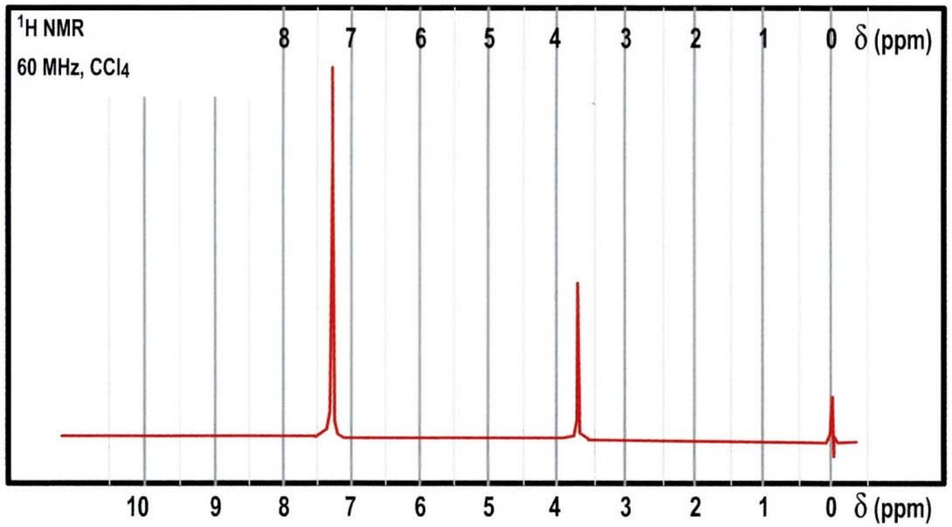
δ: 137.8, 129.1, 128.3, 125.4, 21.4

Příklad 36

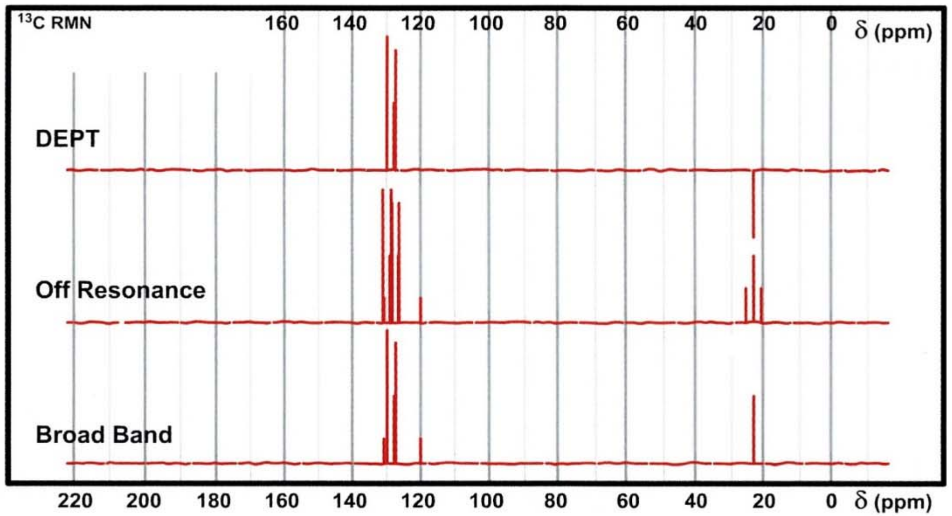




m / z	Int. rel.	m / z	Int. rel.	m / z	Int. rel.
27.0	1.8	61.0	2.0	78.0	1.0
37.0	2.1	62.0	4.0	87.0	1.0
38.0	3.3	63.0	8.8	88.0	1.7
39.0	8.7	64.0	3.6	89.0	21.2
40.0	1.0	65.0	4.0	90.0	40.8
50.0	6.9	74.0	2.1	91.0	7.5
51.0	11.6	75.0	1.6	116.0	36.1
52.0	1.8	76.0	1.4	117.0	100.0
58.5	2.2	77.0	6.7	118.0	8.9



δ (integration): 7.3 (5), 3.7 (2)



δ: 131, 130, 128, 127, 120, 25