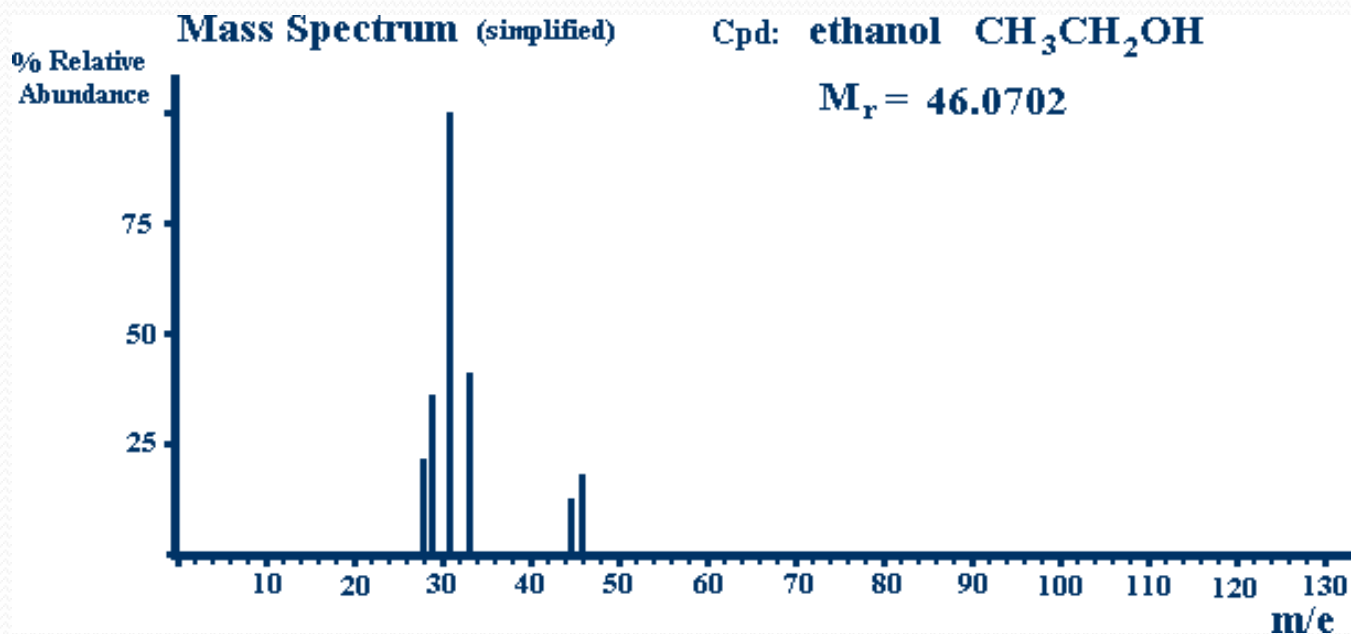


Spektrální metody

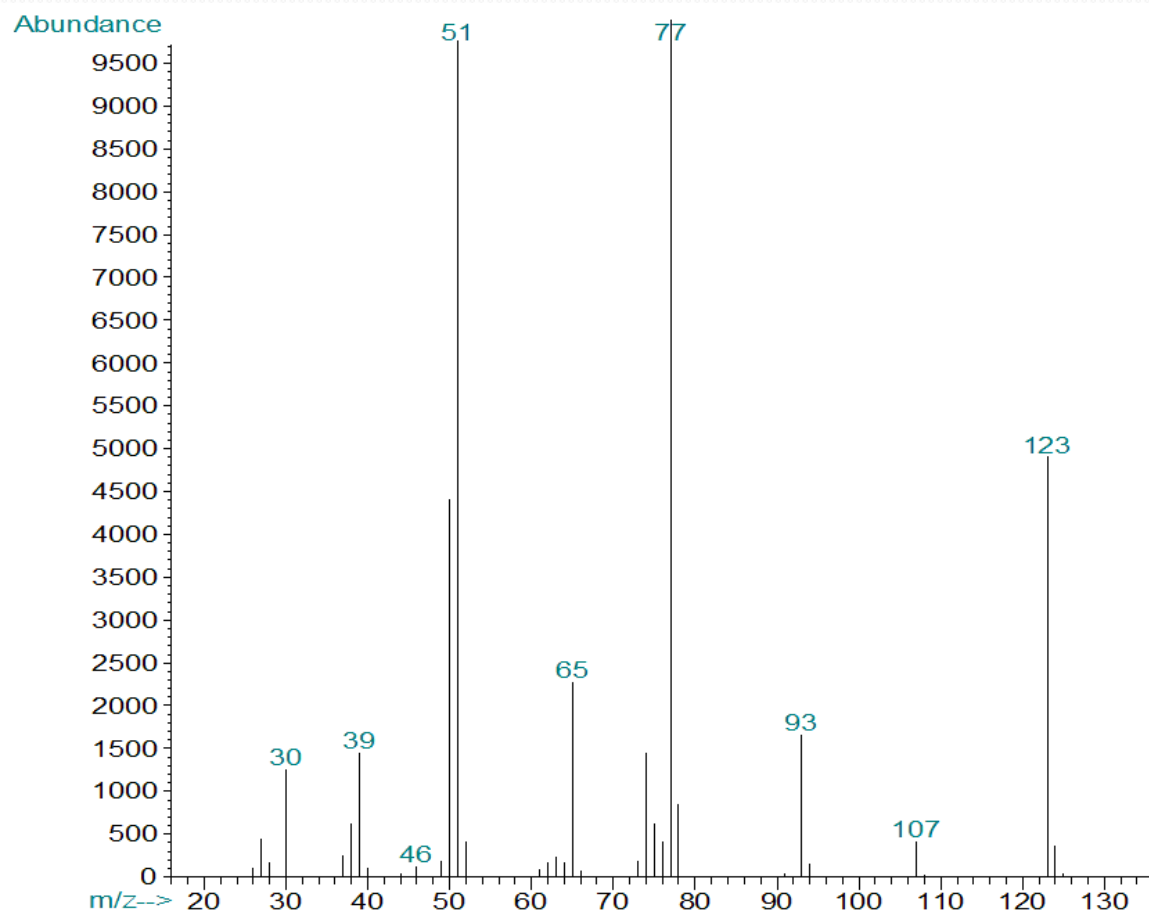
C2022 Organická chemie - seminář

Hmotnostní spektrometrie

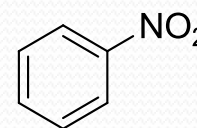
- Analýza iontů vznikajících ionizací vzorku
- Lze určit M_r a informace o struktuře na základě fragmentů



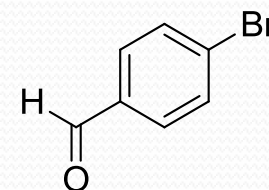
Které z následujících molekul přísluší daný hmotnostní chromatogram?



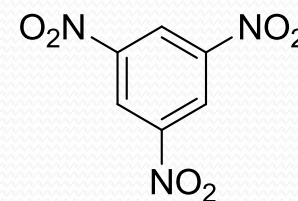
A.



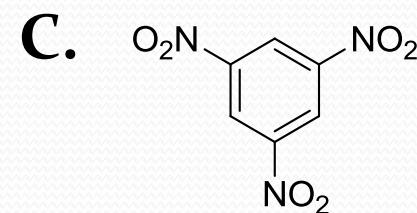
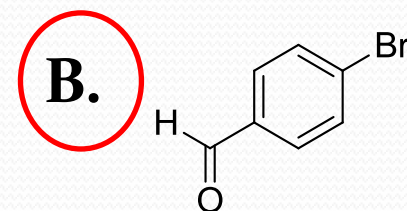
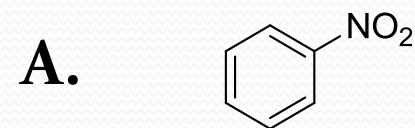
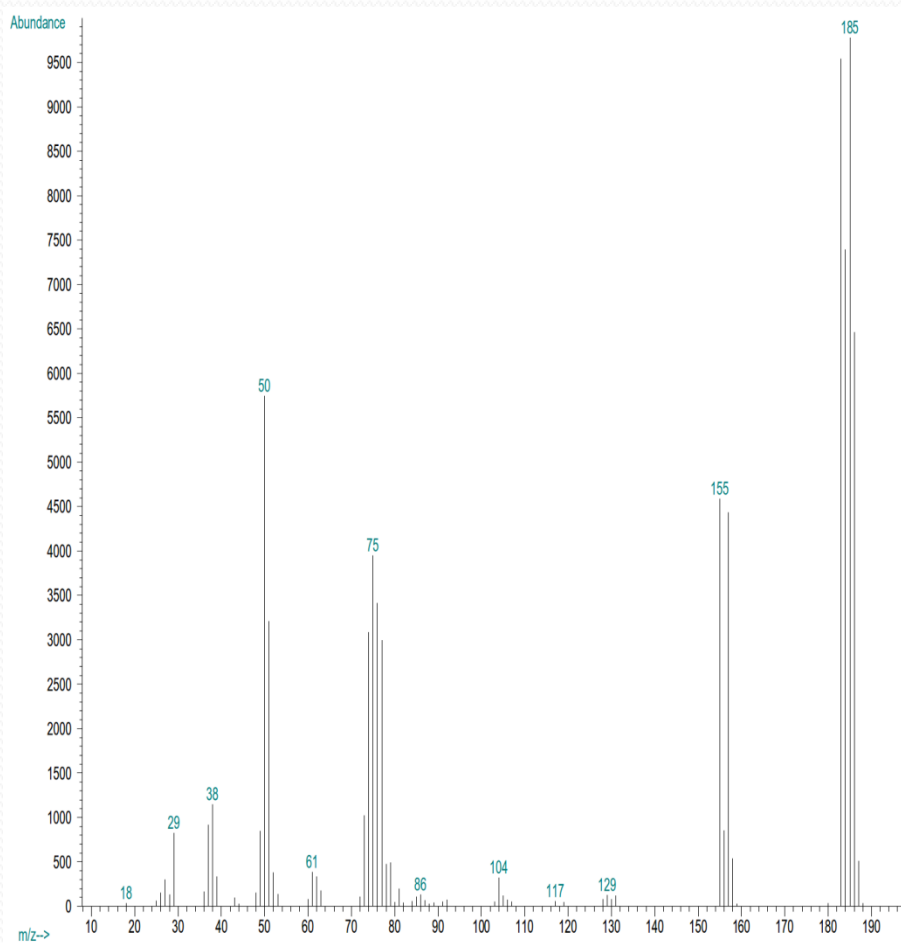
B.



C.

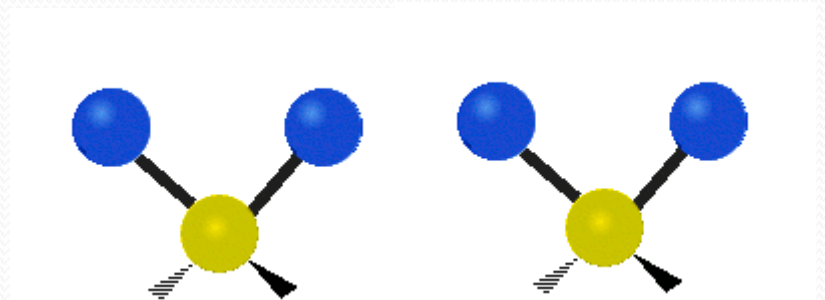
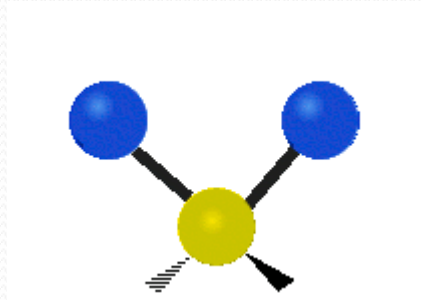
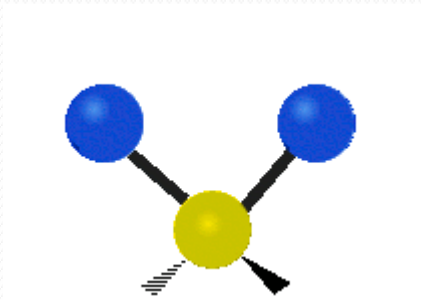
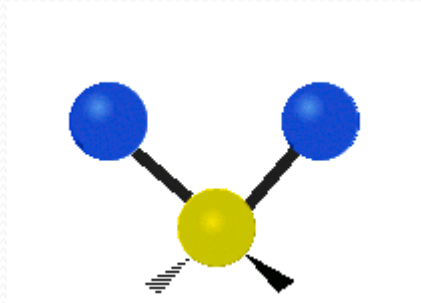
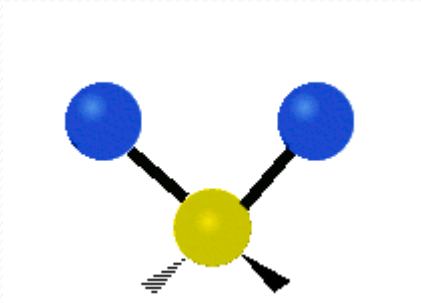
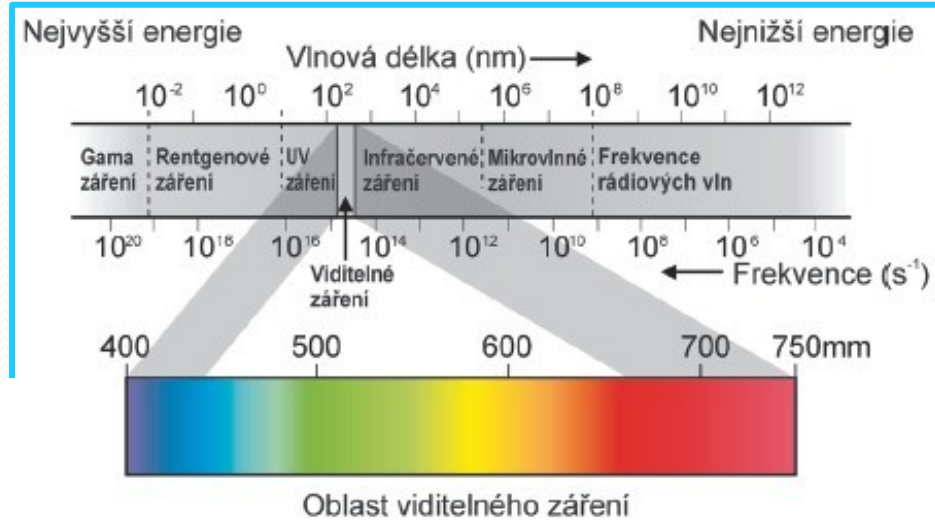


Které z následujících molekul přísluší daný hmotnostní chromatogram?



Infračervená spektroskopie

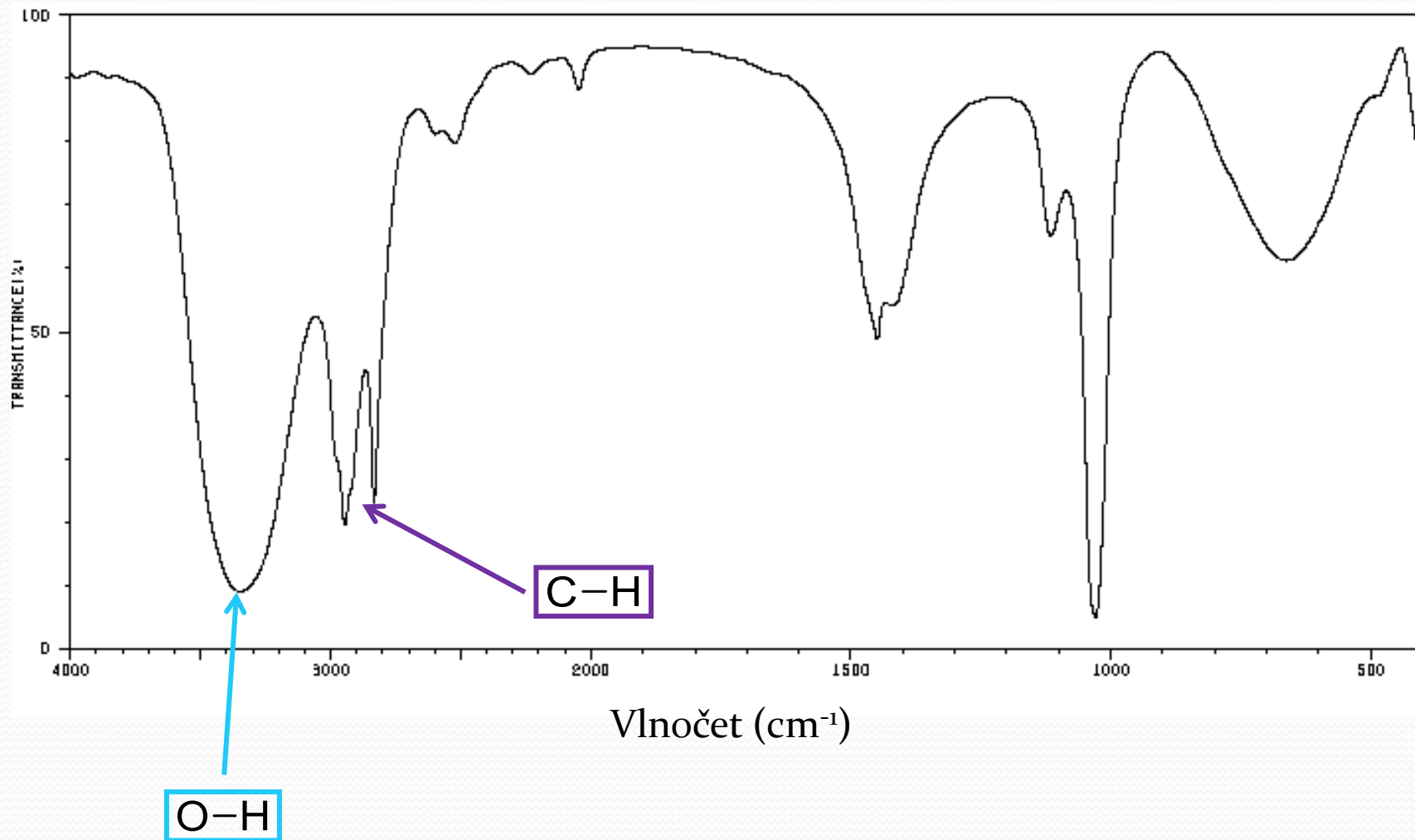
- Vibrace molekul



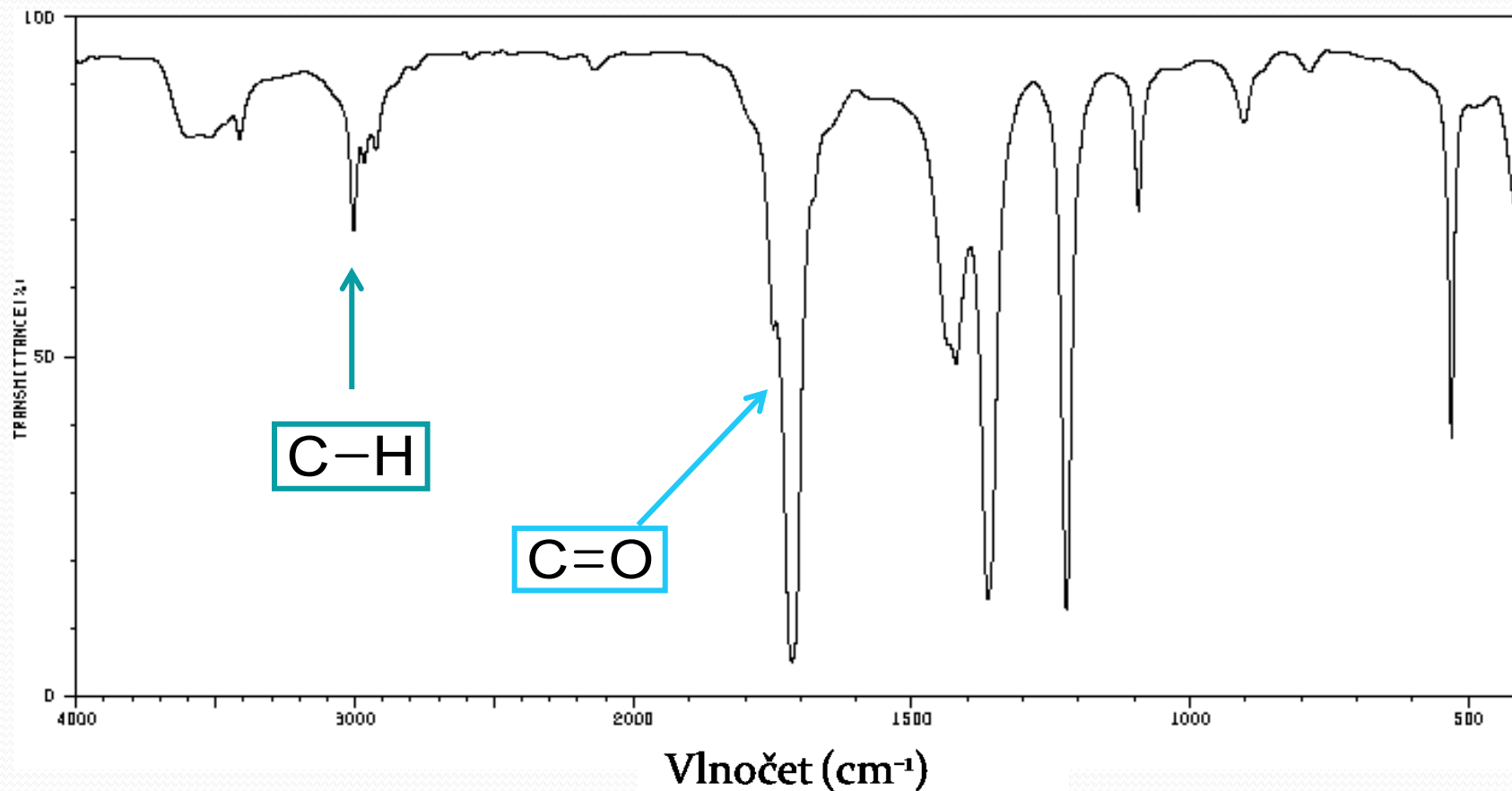
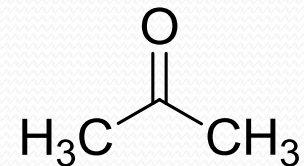
Charakteristické vibrační pásy

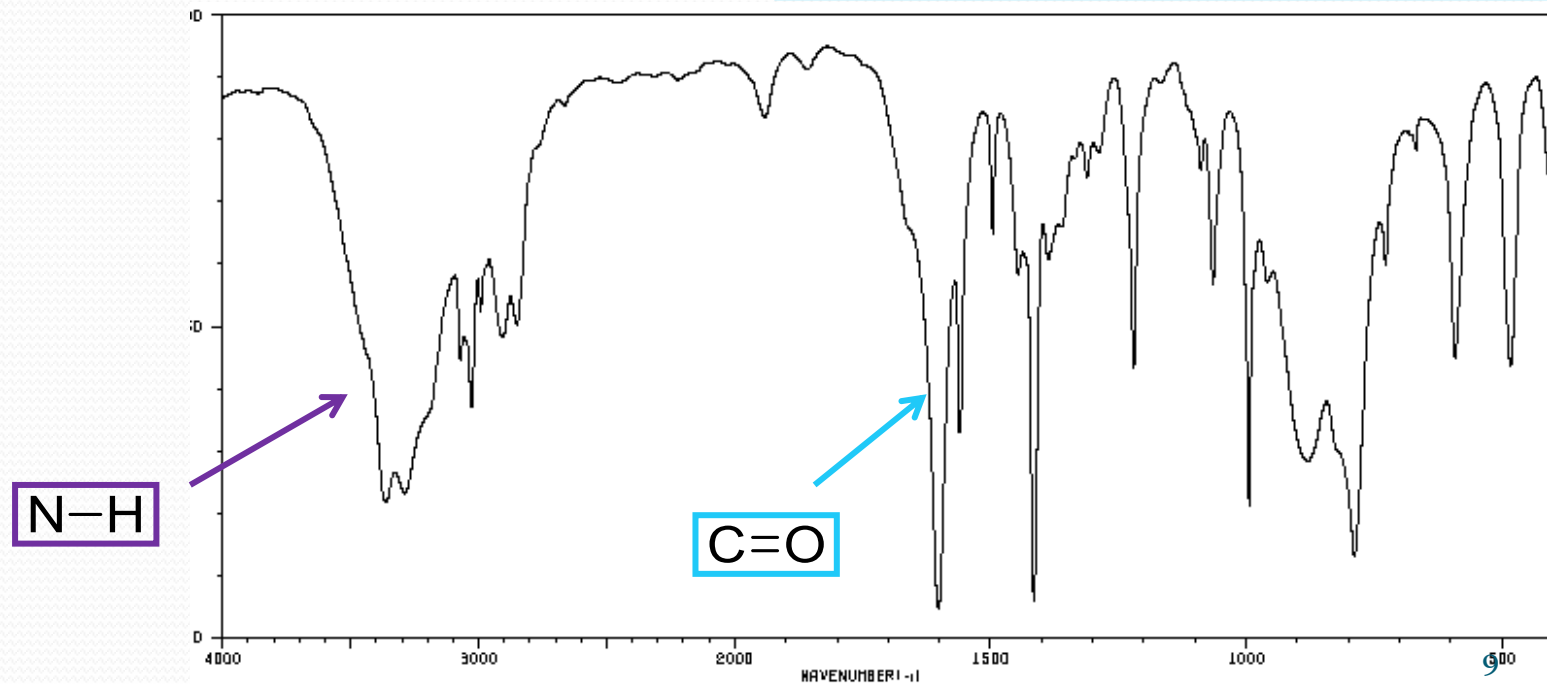
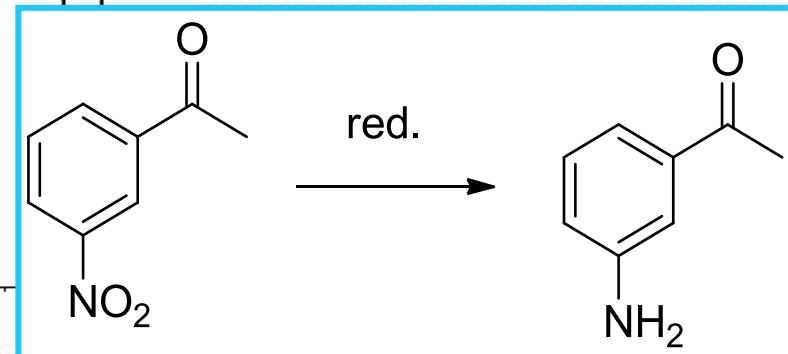
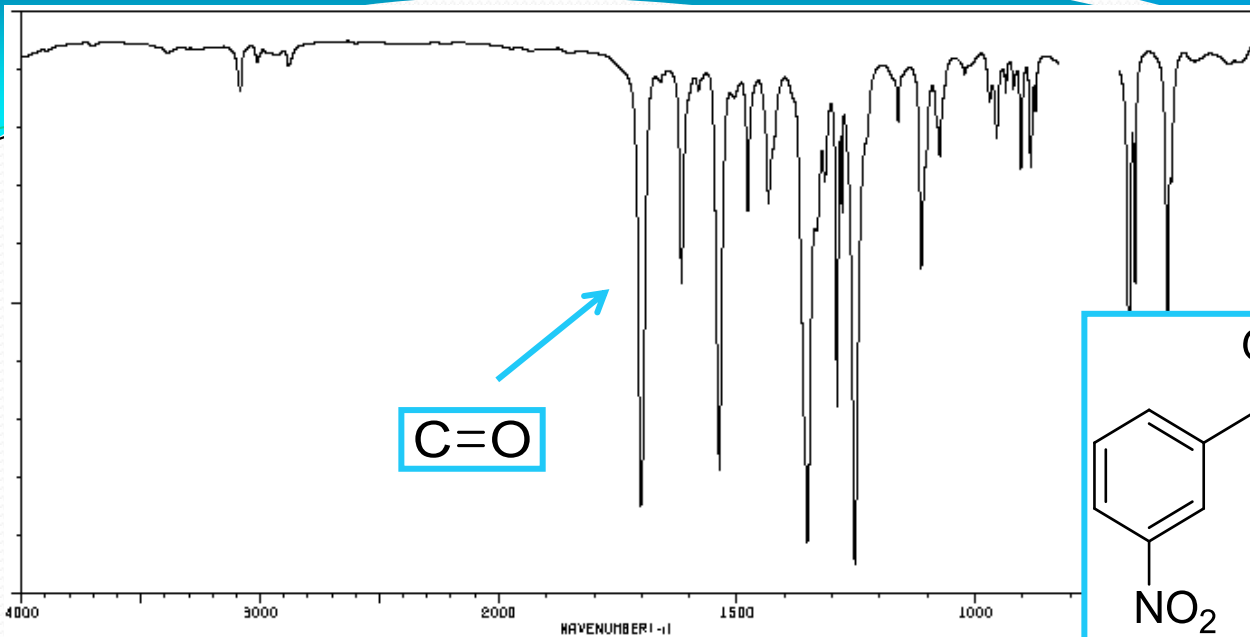
Major Functional Group	Absorption Frequency Region			
O-H	3650-3590			
N-H	3500-3300	1650-1590	900-650	
=CH-H	3100-3070	1420-1410	900-880	
=C-H	3100-3000	2000-1600		
C-H	2900-2700	1440-1320		
=-CH ₃	2880-2860	2970-2950	1380-1370	1470-1430
O-H	2700-2500	1320-1210	950-900	
C≡C	2140-2100			
C=O	1750-1700			
C=C	1600-1500			
C-N	1340-1250			
C-O-C	1200-1180			
-C-H	770-730			

IR spektrum methanolu



IR spektrum acetonu

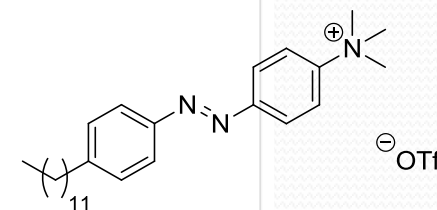
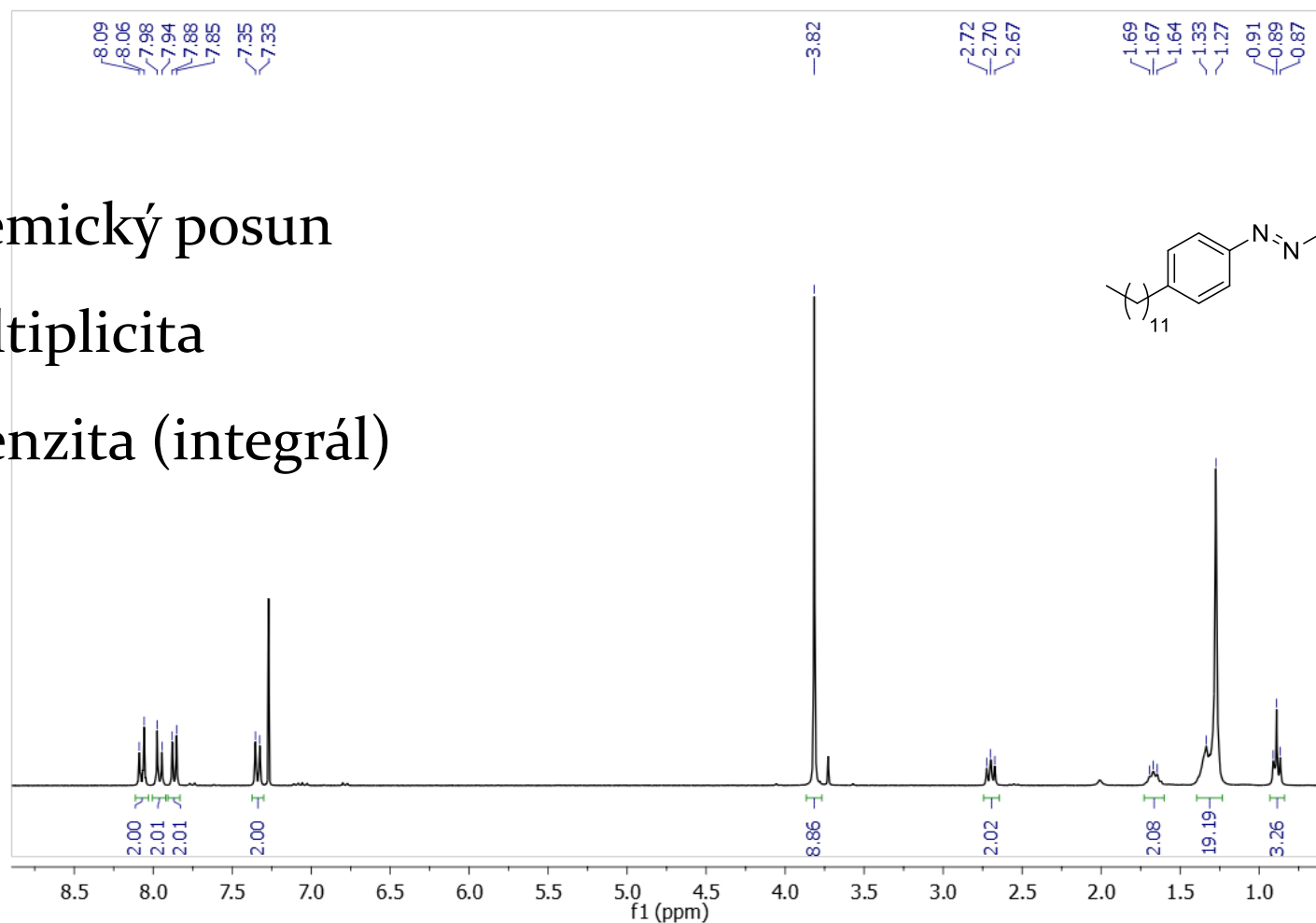




Nukleární magnetická rezonance

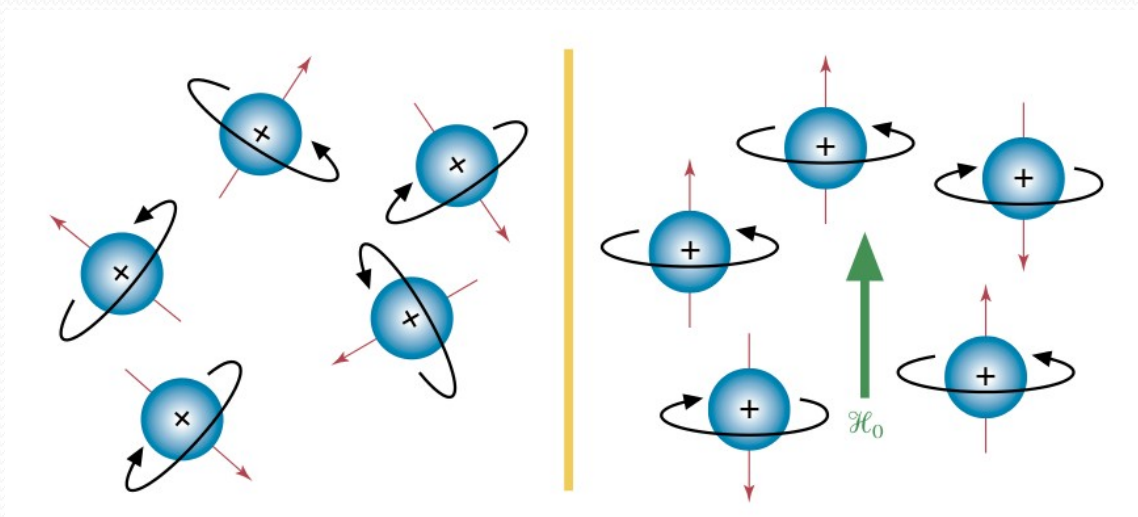
NMR

- ❖ Chemický posun
- ❖ Multiplicita
- ❖ Intenzita (integrál)



^1H spektrum

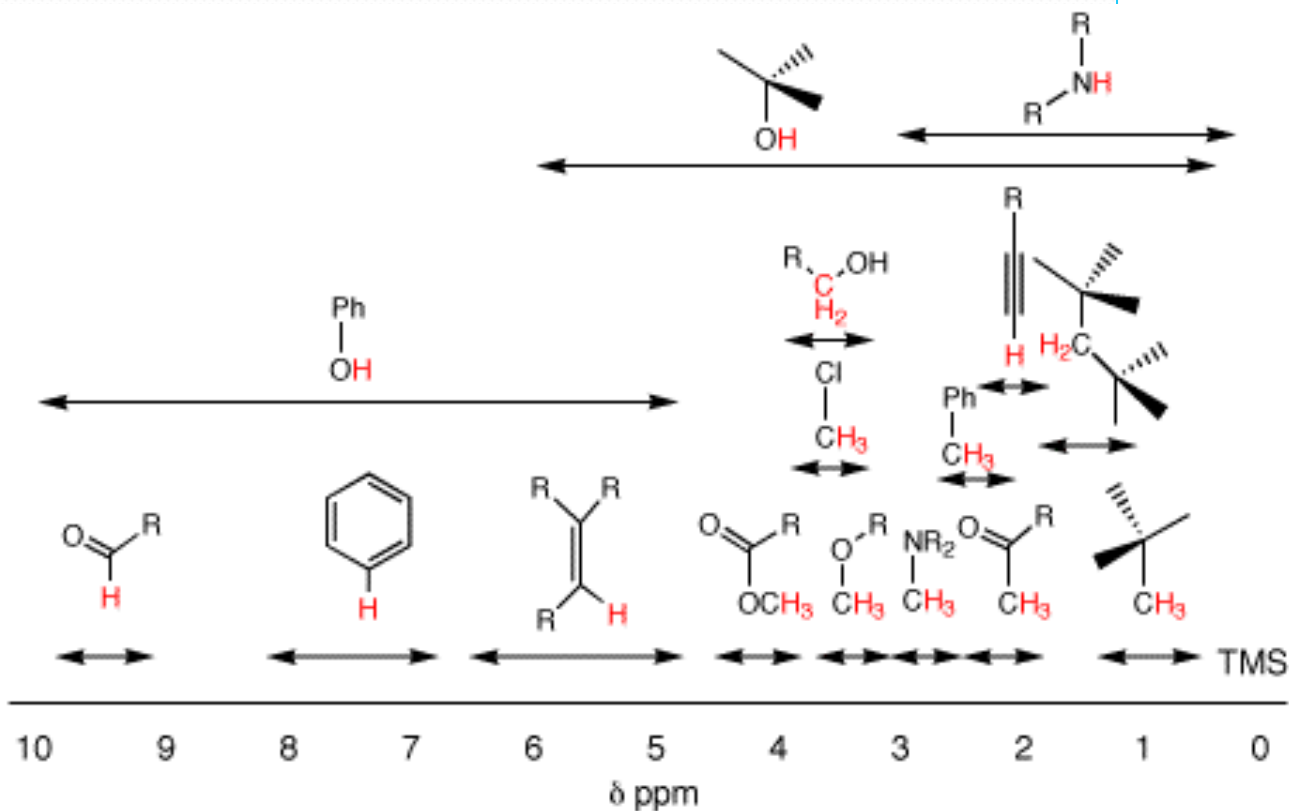
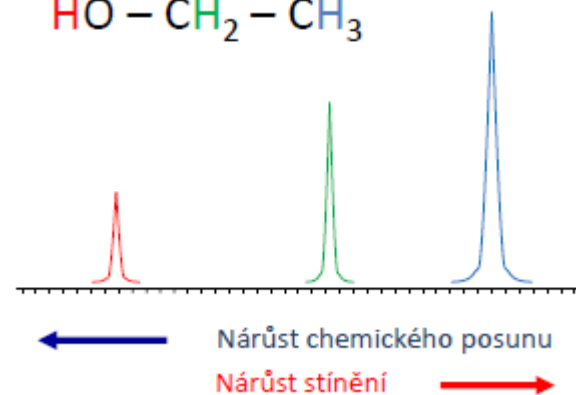
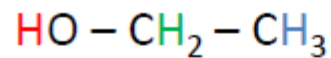
Princip NMR



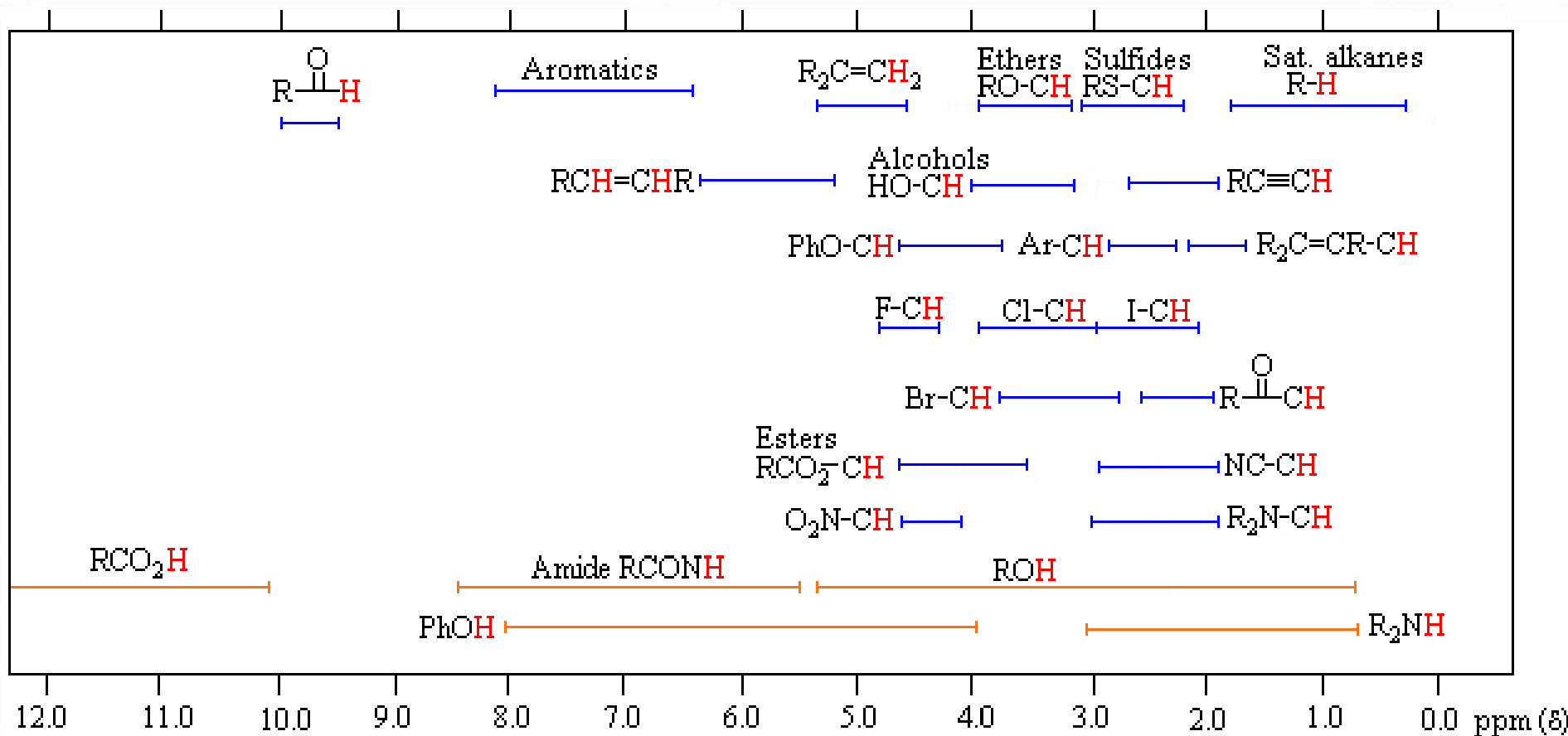
- Jádra s nenulovým jaderným spinem (^1H , ^{13}C , ^{15}N , ^{19}F , ^{31}P)
- Působení radiofrekvenčního záření v magnetickém poli

^1H NMR

- Chemický posun – δ (ppm)
 - - ovlivněný stíněním elektronů

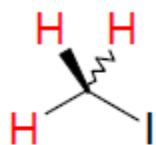


^1H NMR chemické posuny

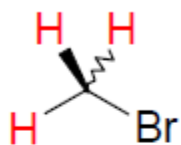


^1H NMR - trendy

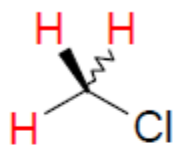
2,1 ppm



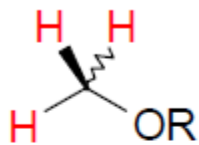
2,3 ppm



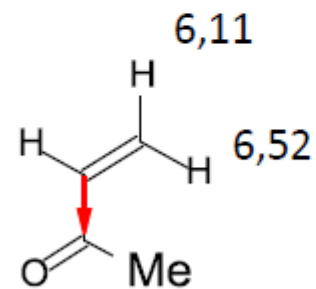
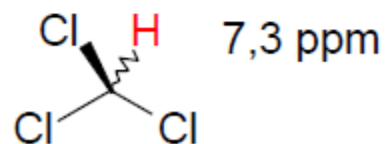
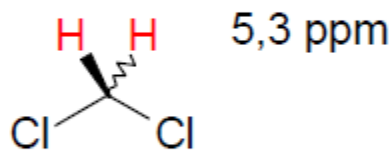
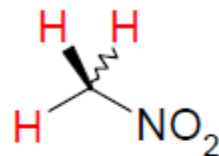
3 ppm



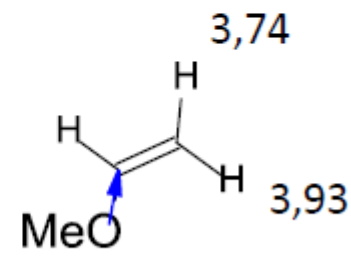
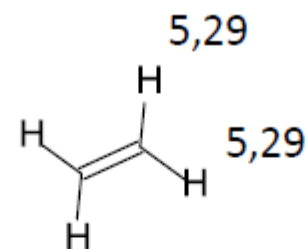
3,1 ppm



4,5 ppm

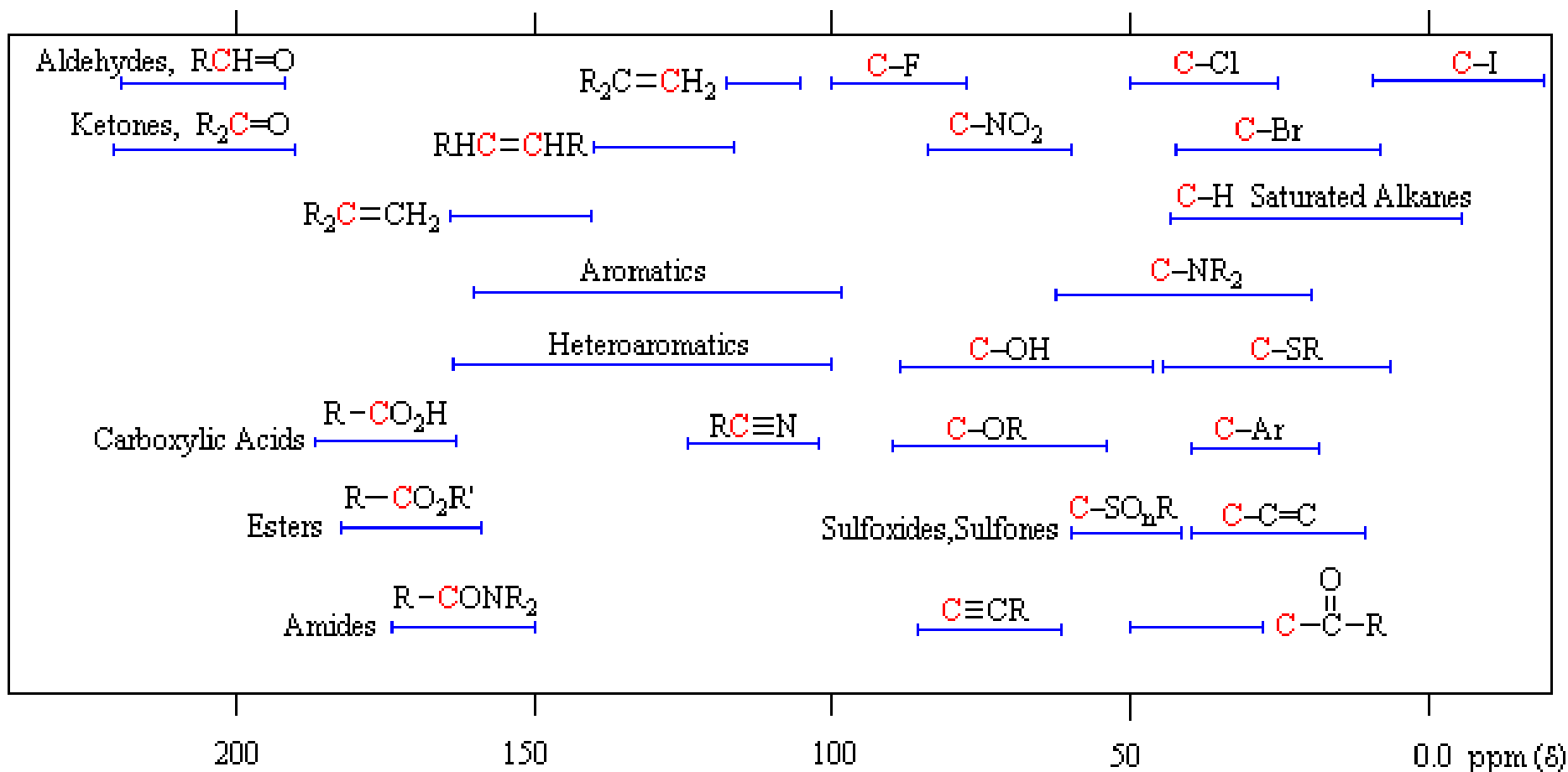


-M



+M

^{13}C NMR chemické posuny



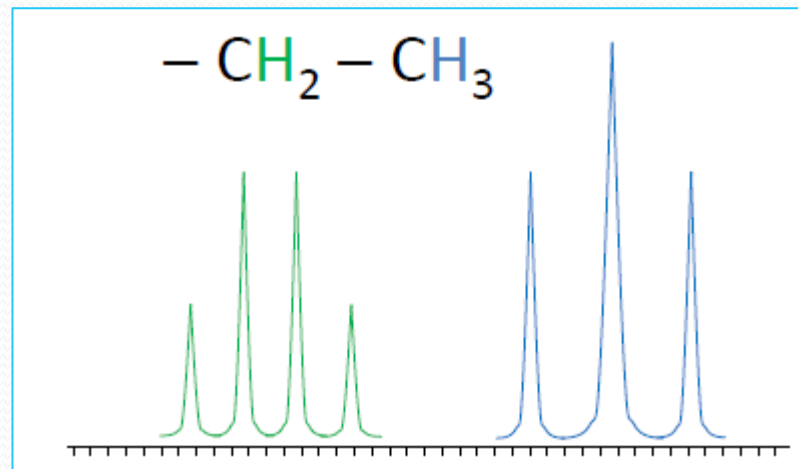
^1H NMR - multiplicita

- Jak stěpené jednotlivé signály jsou?

- $m = n + 1$ $n \dots$ počet interagujících jader

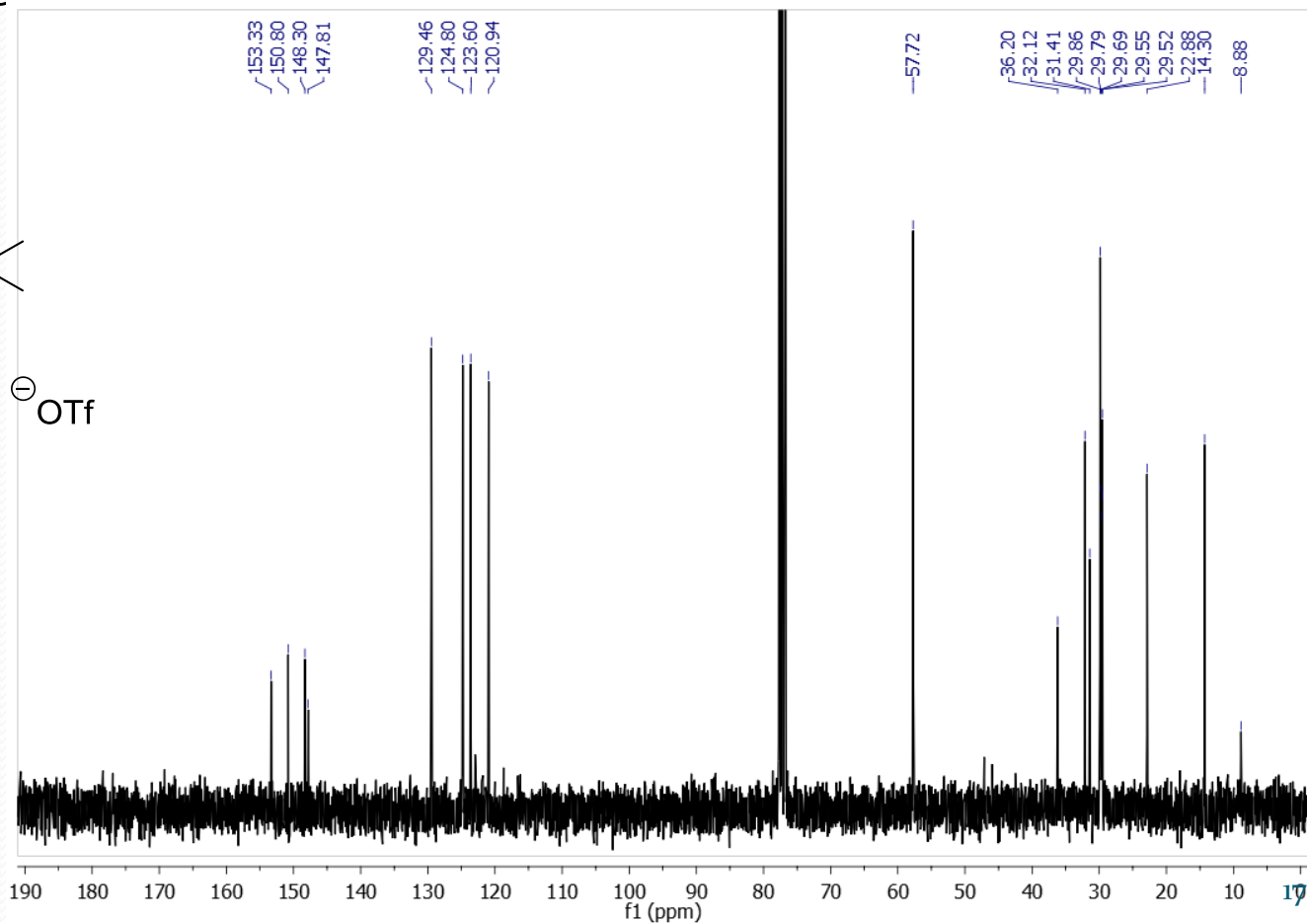
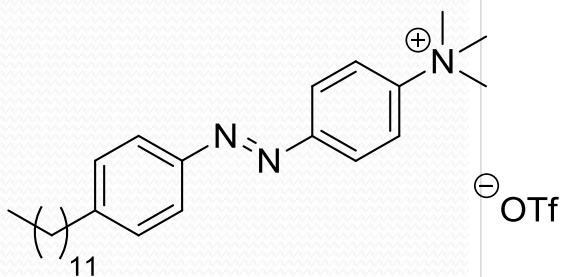
- Intenzita čar se řídí
Pascalovým trojúhelníkem

			1			
		1		1		
	1		2		1	
	1	3		3		1
	1	4	6	4	1	
1	5	10	10	5	1	



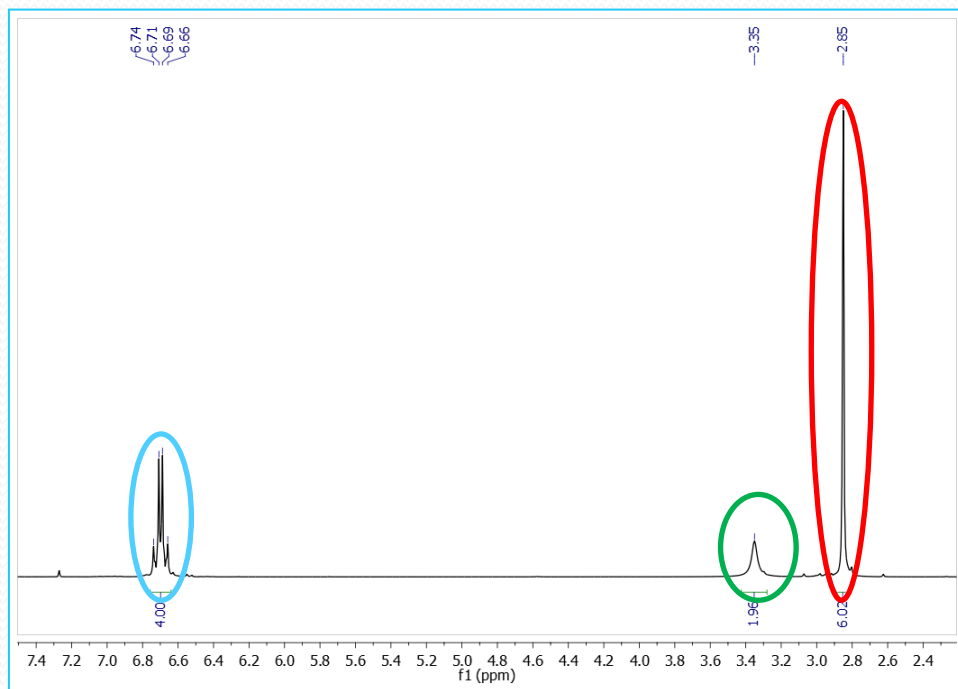
^{13}C NMR

- Decoupling

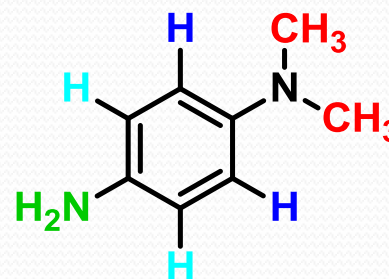


^1H NMR - integrály

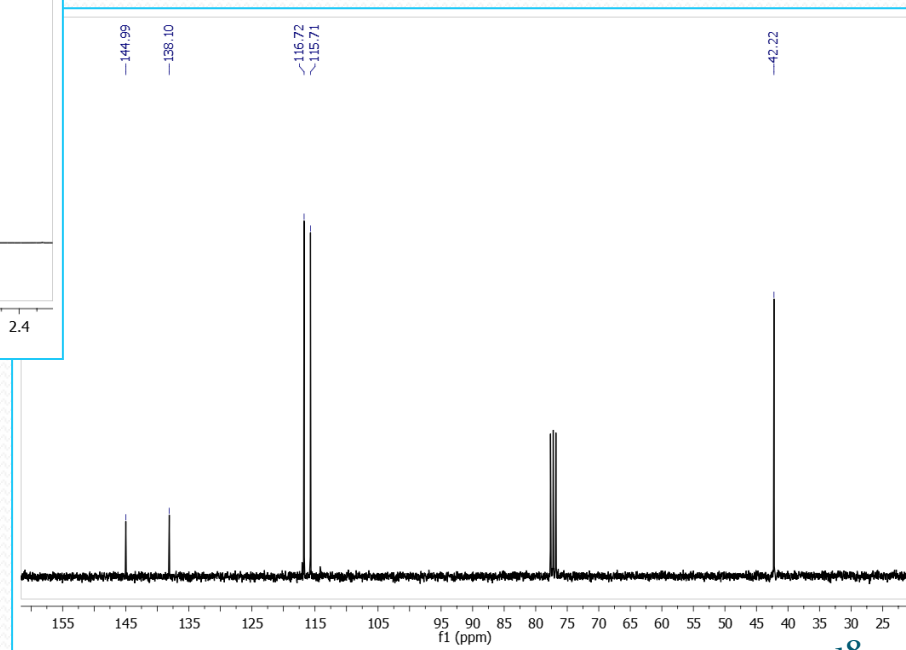
Příklad č. 1



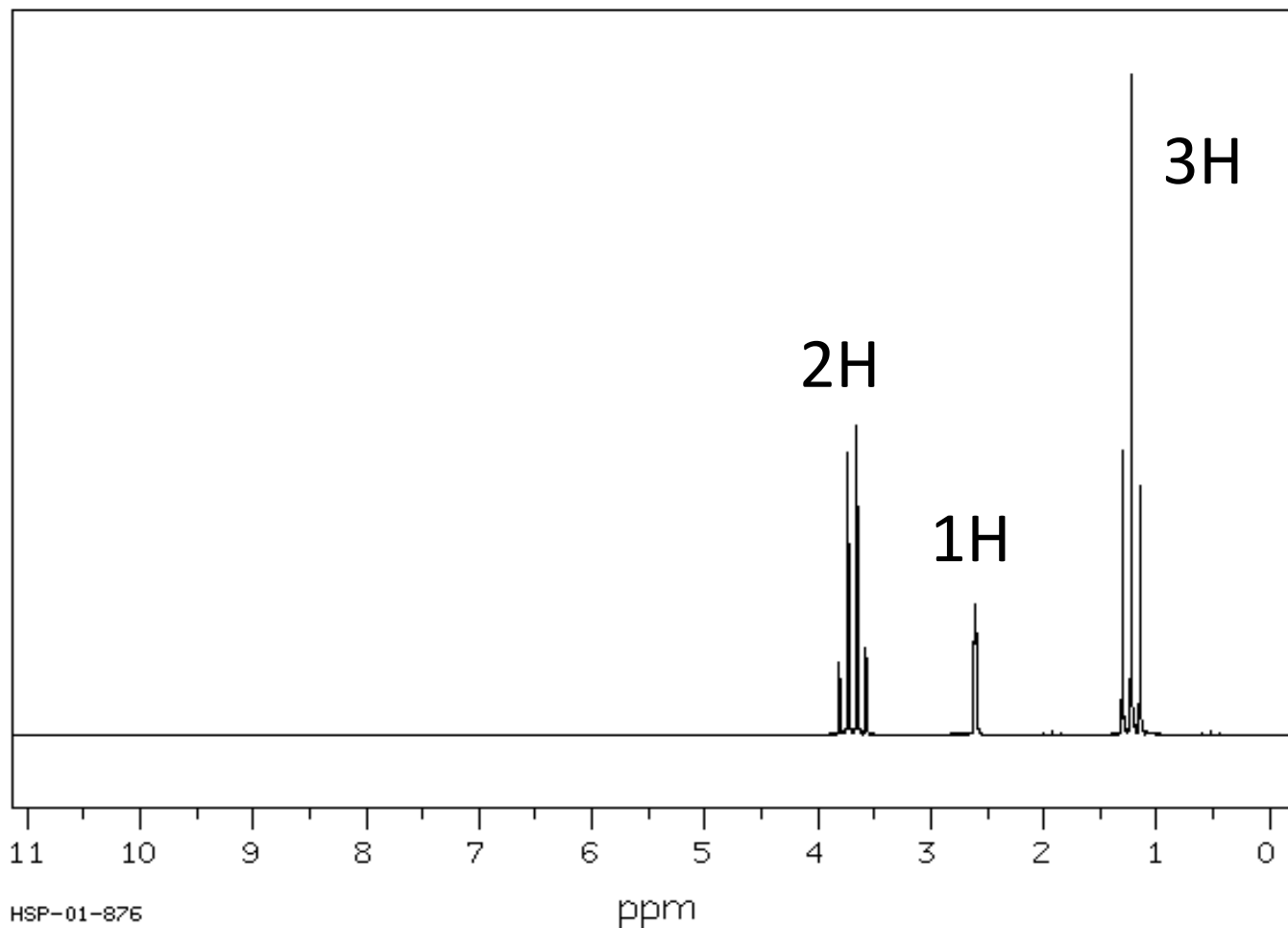
^1H NMR



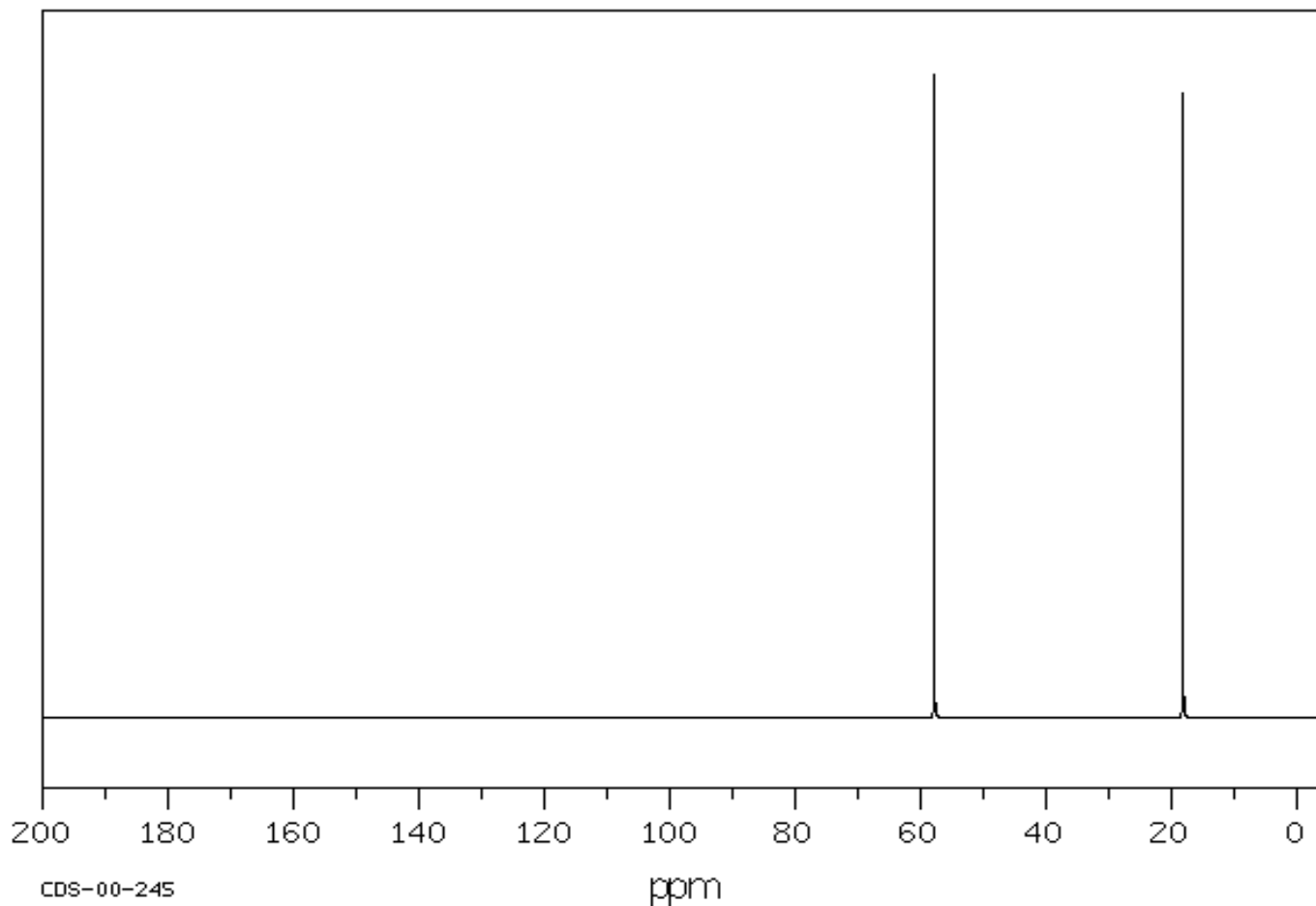
^{13}C NMR



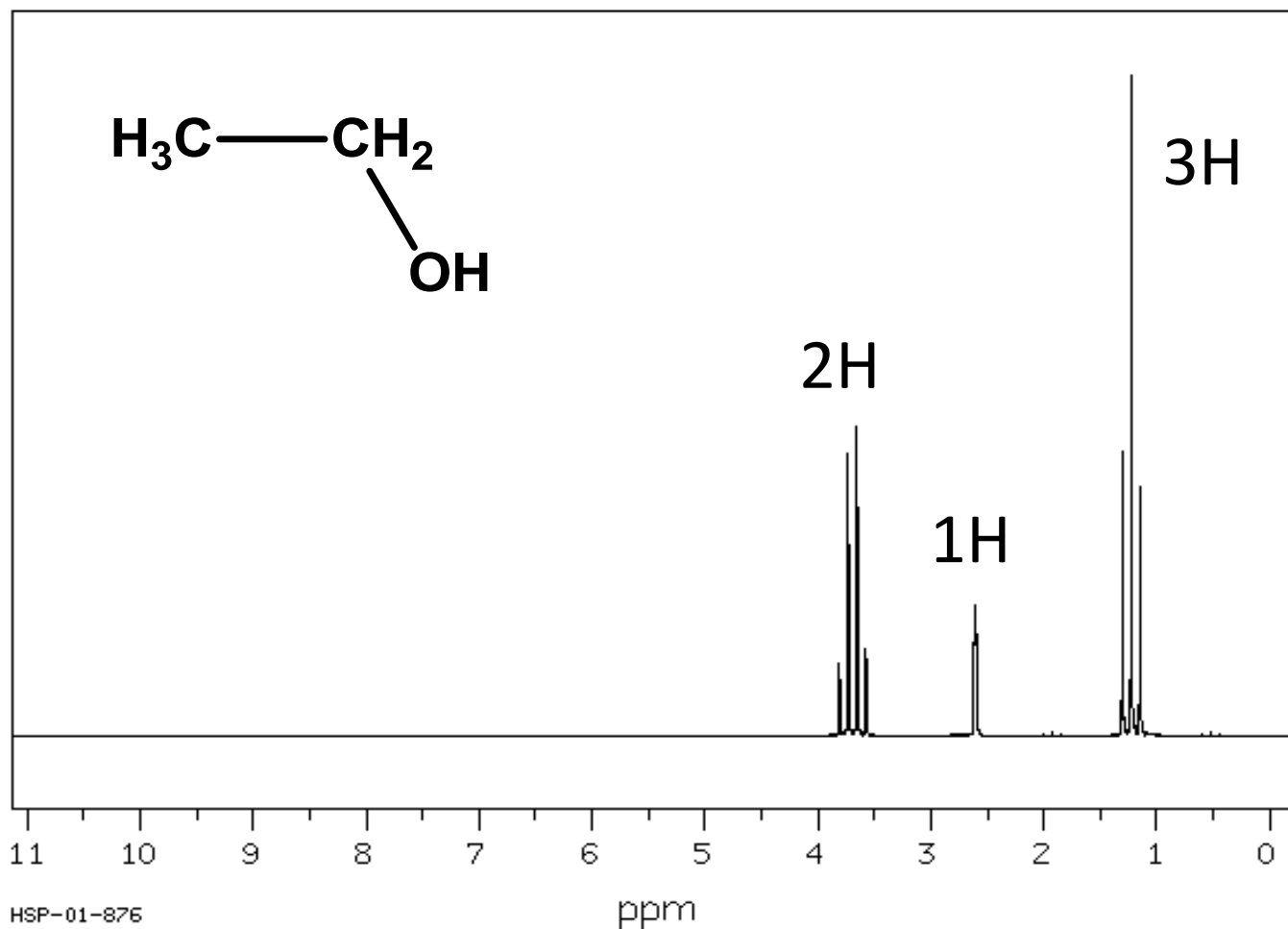
Nakreslete sktrukturu alkoholu, jemuž přísluší následující NMR spektra. (^1H)



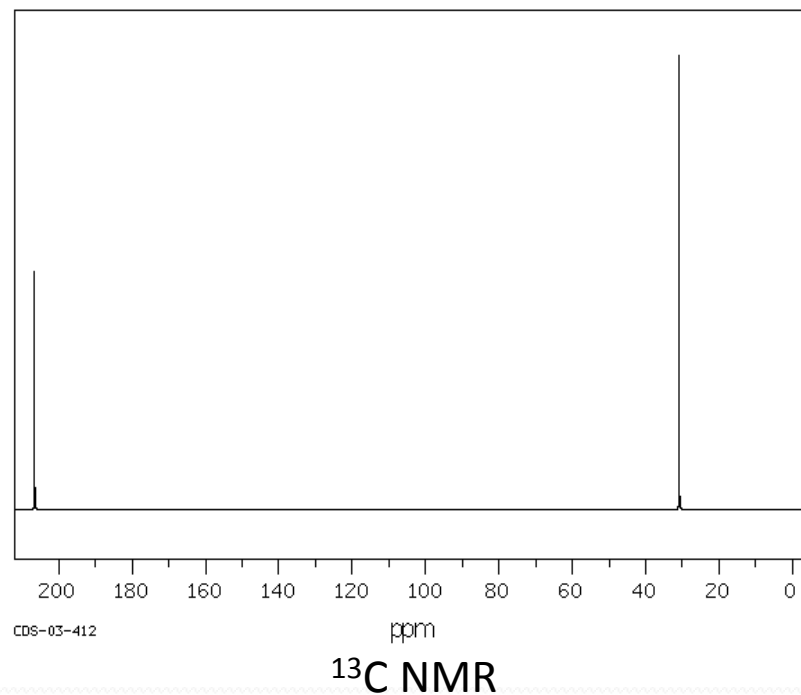
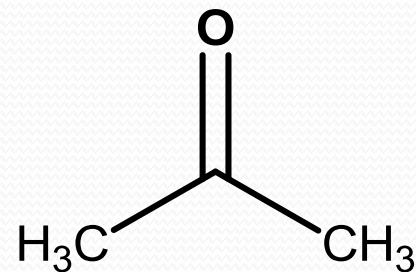
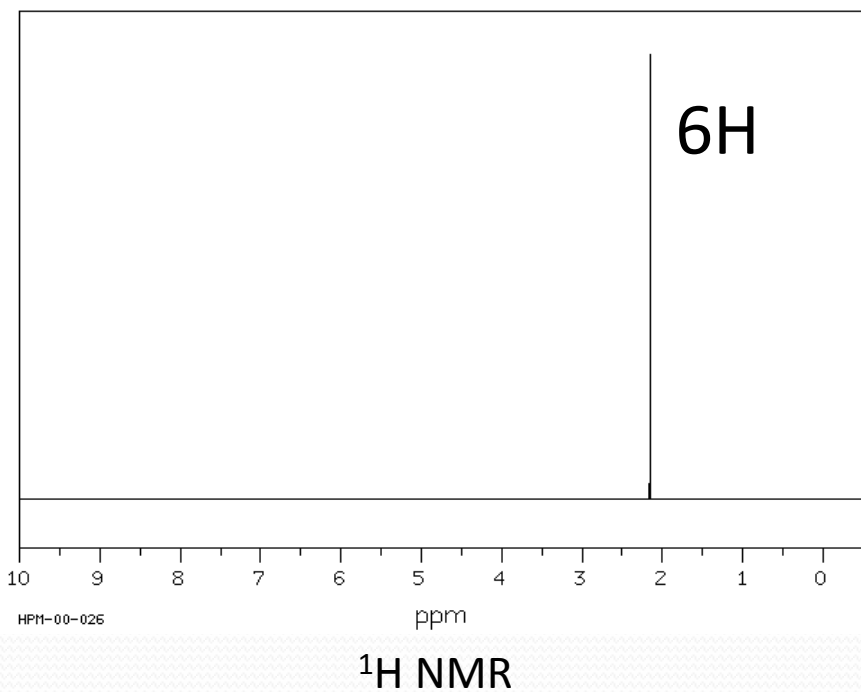
Nakreslete sktrukturu alkoholu, jemuž
přísluší následující NMR spektra. (^{13}C)



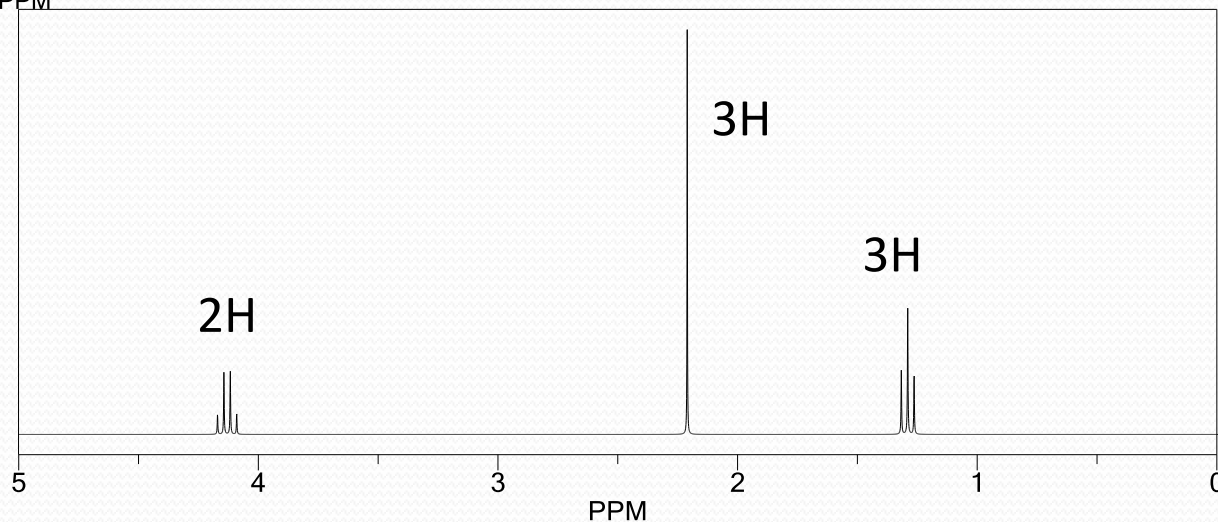
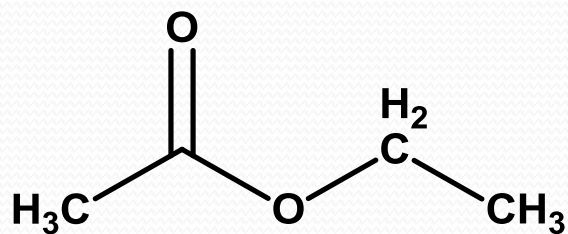
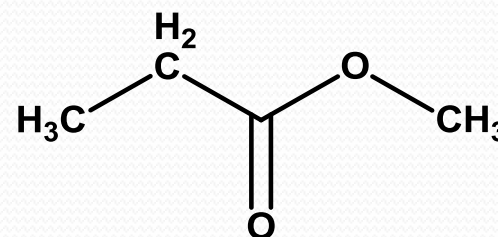
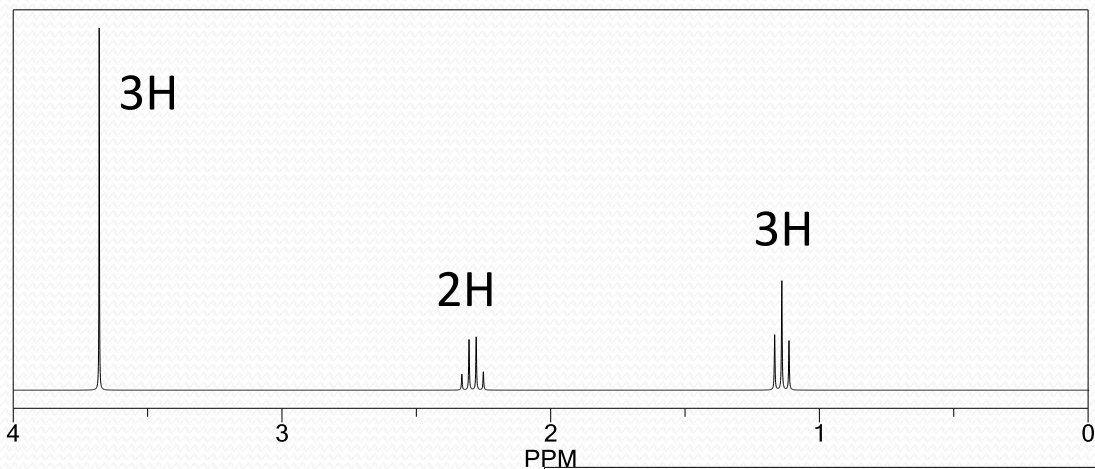
Nakreslete sktrukturu alkoholu, jemuž přísluší následující NMR spektra. (^1H)



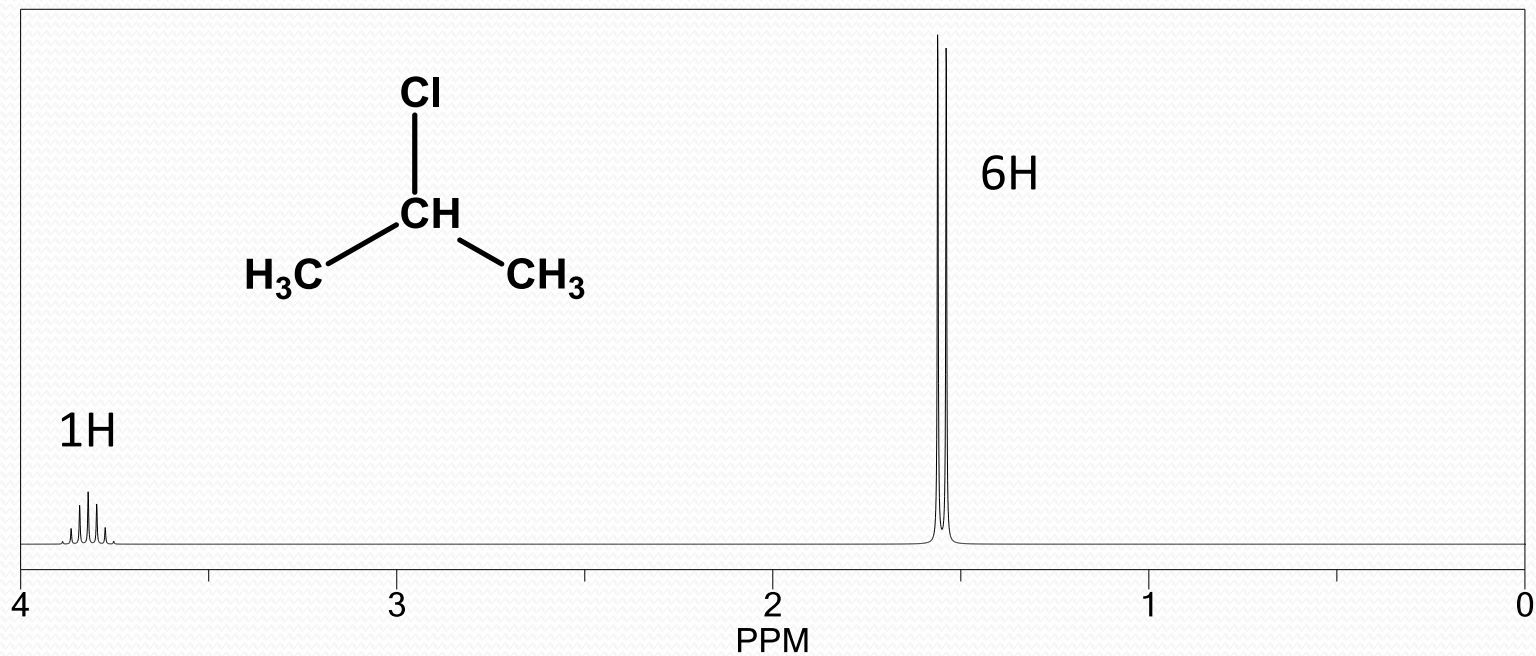
Nakreslete strukturu sloučeniny se
sumárním vzorcem C_3H_6O



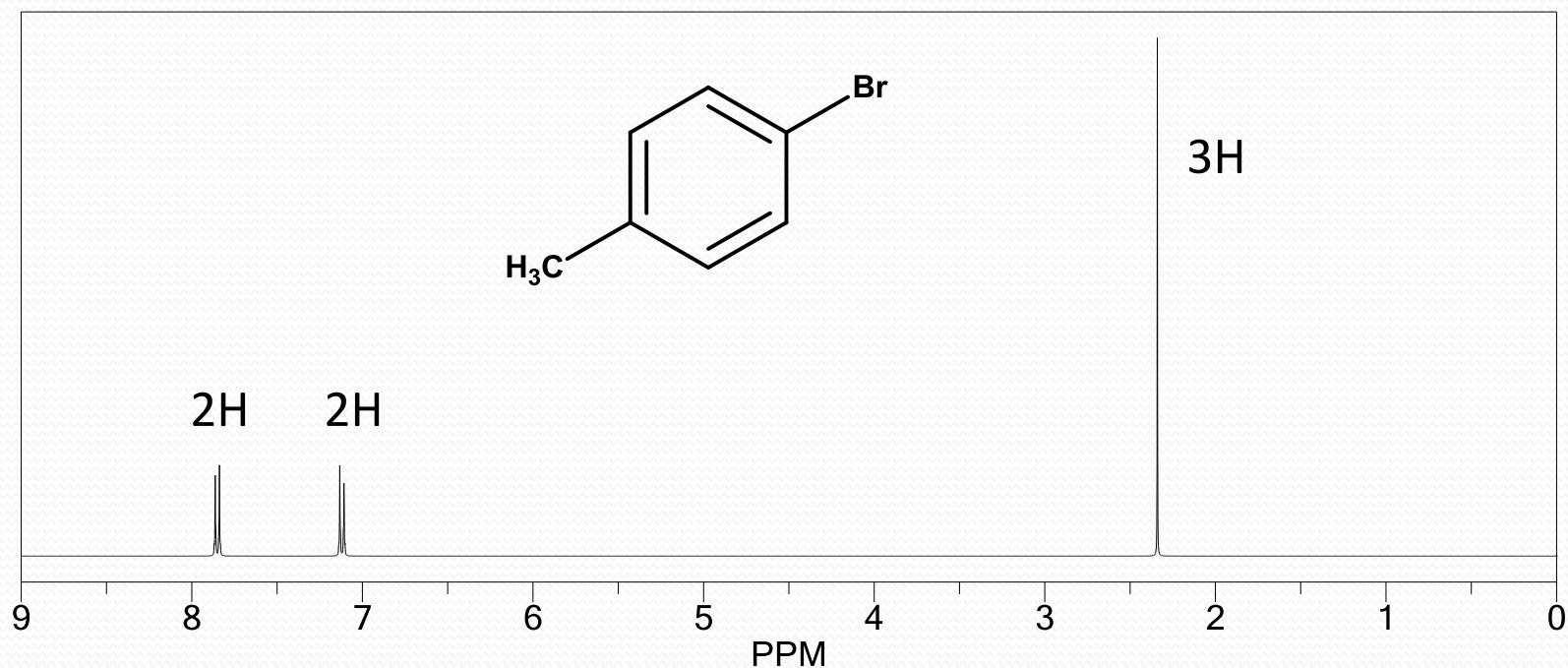
Určete, kterým 2 esterům se sumárním vzorcem $C_4H_8O_2$ přísluší následující dvě 1H NMR spectra



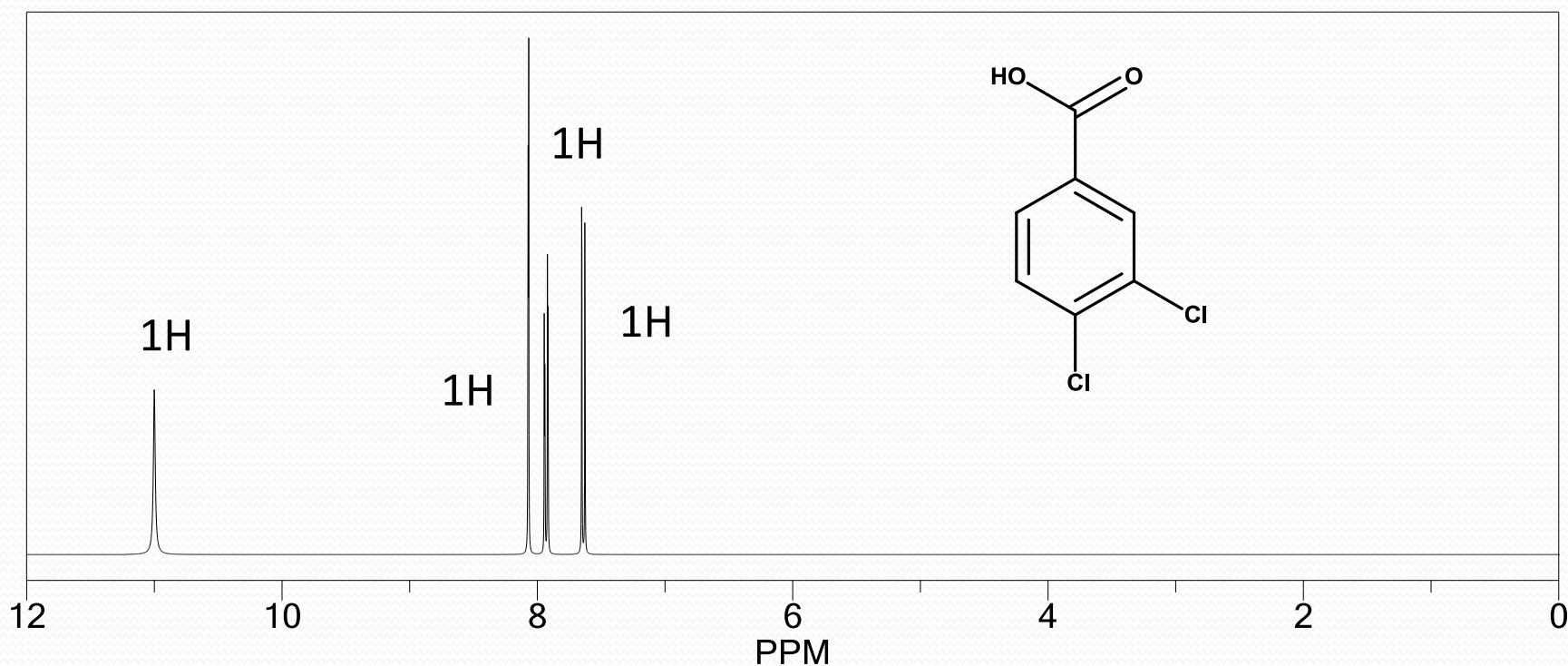
Navrhněte strukturu molekuly se sumárním vzorcem C_3H_7Cl podle následujícího 1H NMR spektra



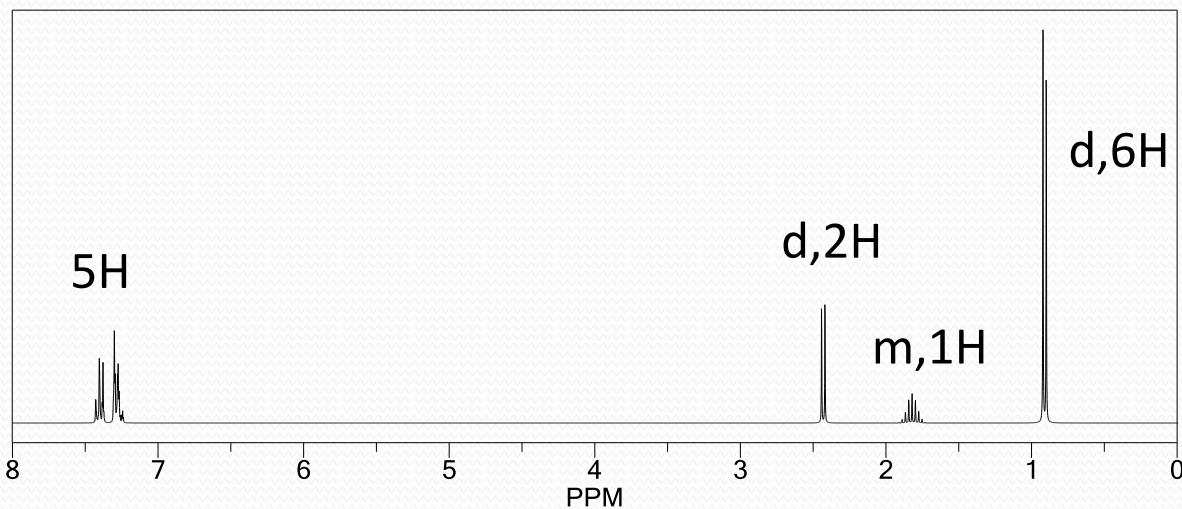
Navrhněte strukturu molekuly se sumárním vzorcem C_7H_7Br podle následujícího 1H NMR spektra



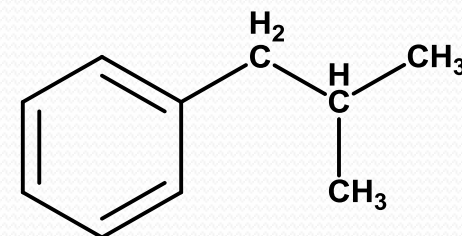
Navrhněte strukturu kyseliny se sumárním vzorcem $C_7H_4Cl_2O_2$ podle následujícího 1H NMR spektra



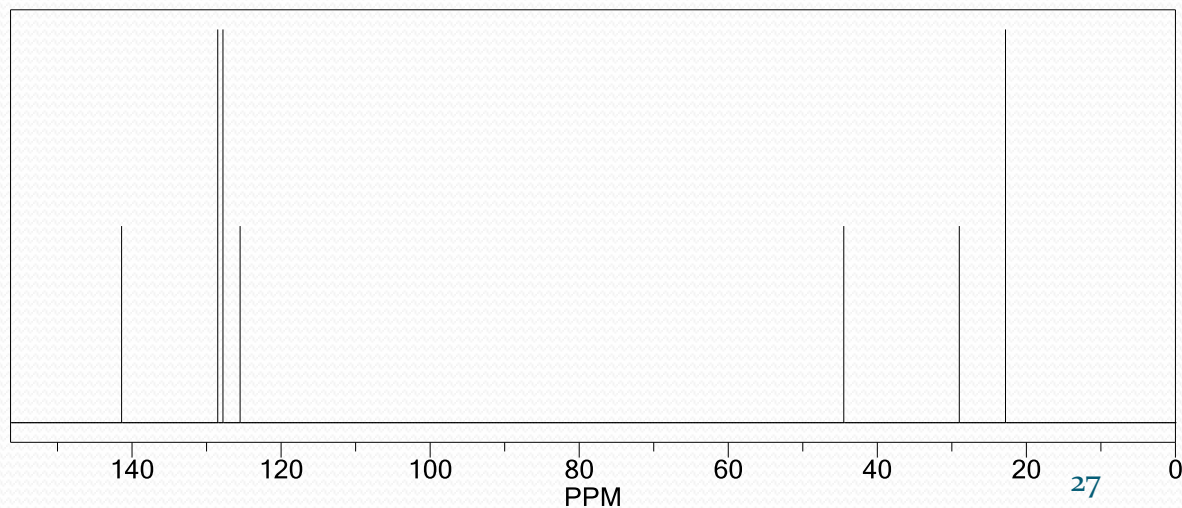
Navrhněte strukturu molekuly se sumárním vzorcem $C_{10}H_{14}$ podle následujících NMR spekter



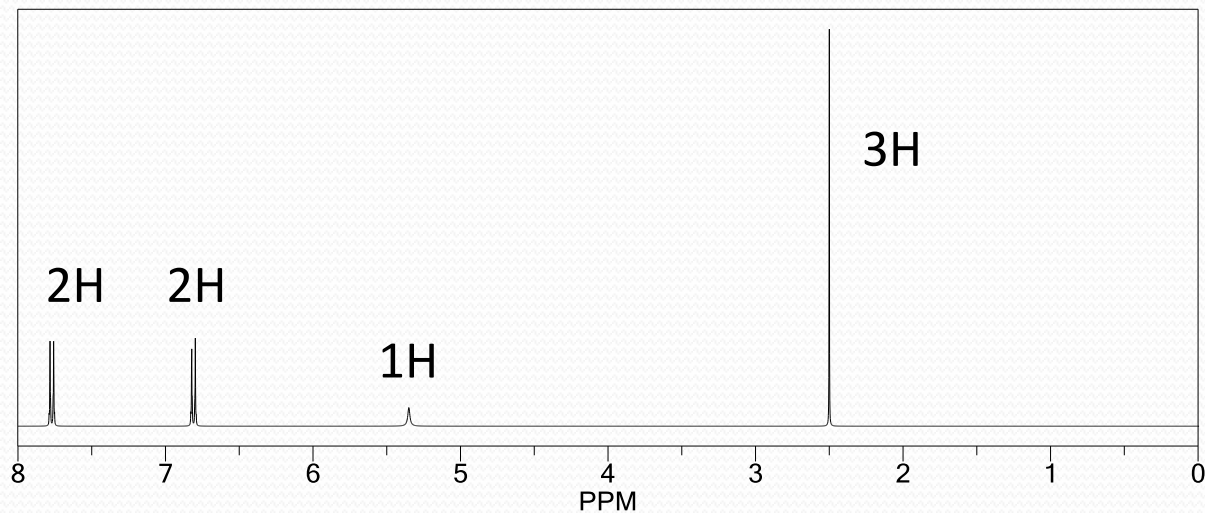
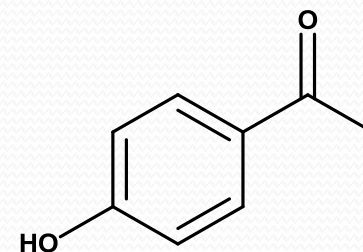
1H NMR



^{13}C NMR



Navrhněte strukturu molekuly se sumárním vzorcem $C_8H_8O_2$ podle následujících NMR spekter

 1H NMR ^{13}C NMR