

Informacje na podstawie których rozwiązujemy widmo ^1H NMR:

1. Wzór sumaryczny i stopień nienasycenia
2. Przesunięcie chemiczne dla danej grupy protonów
3. Integracja - ilość protonów w danej grupie
4. Układ spinowy – multipletowość

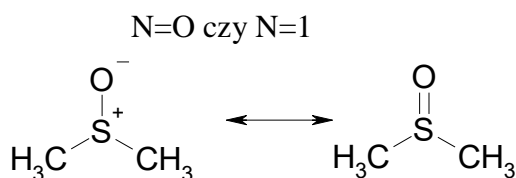
1. Stopień nienasycenia

$$N = \frac{1}{2} \{ 2(n_{IV} + 1) - n_I + n_{III} \}$$

gdzie n_I, n_{III}, n_{IV} ilość atomów jedno trój i cztero wiązalnych

Uwaga na siarkę, azot, fosfor

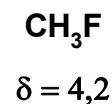
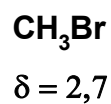
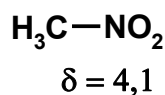
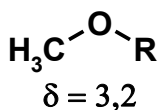
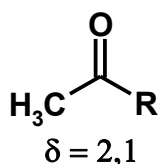
Np. dla DMSO $\text{C}_2\text{H}_6\text{SO}$



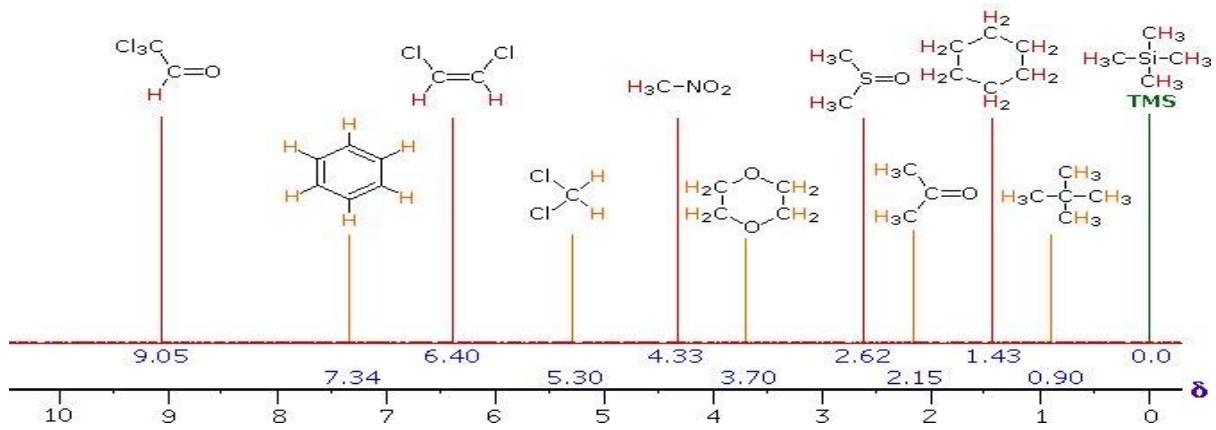
2. Przesunięcie chemiczne

Czynniki determinujące przesunięcie chemiczne:

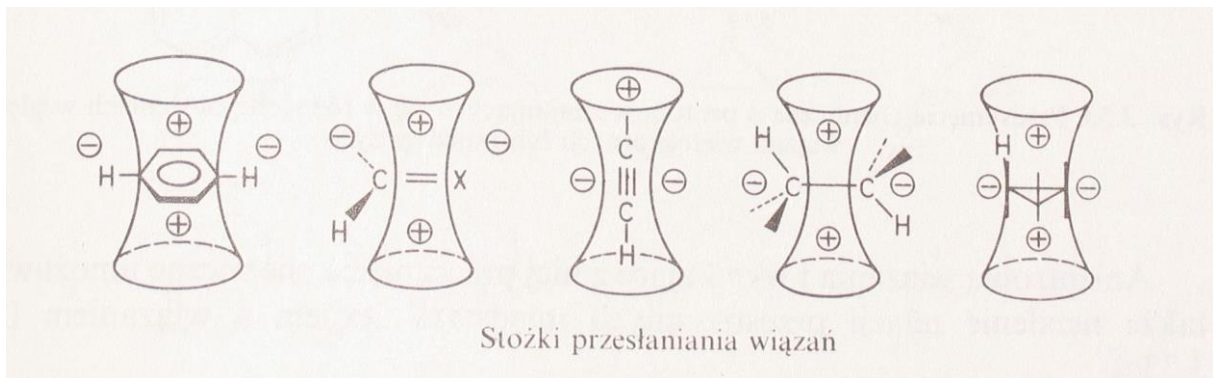
- elektroujemność,
- efekty mezomeryczne,
- anizotropia diamagnetyczna

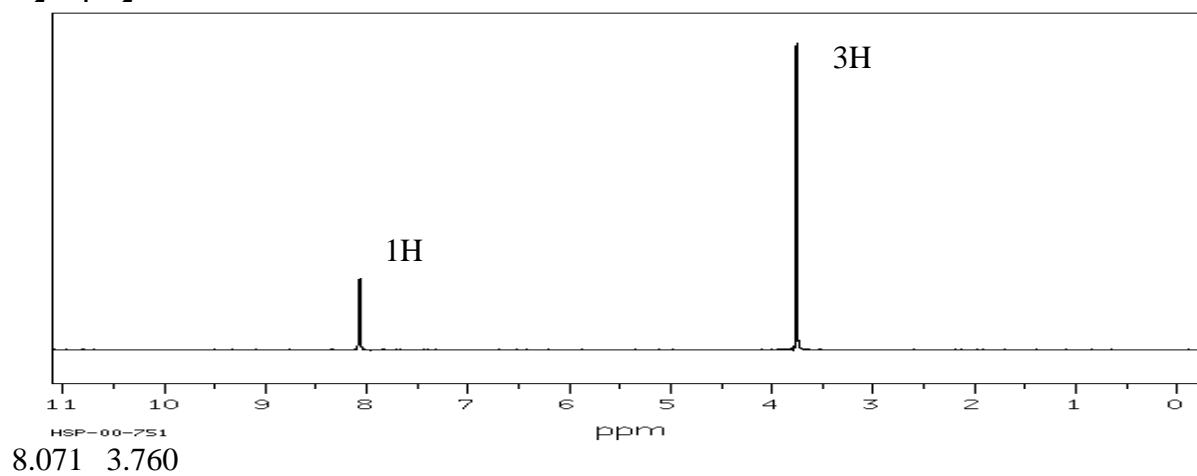
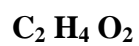
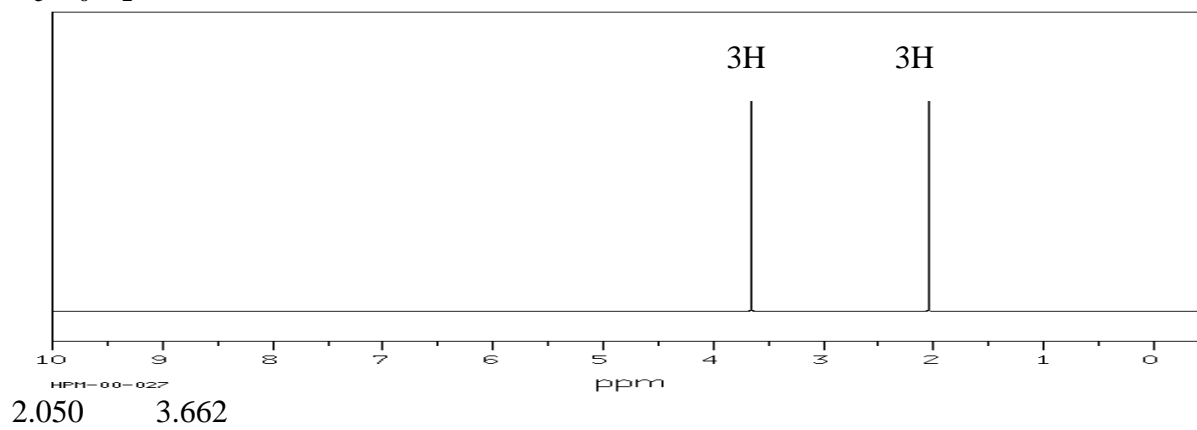
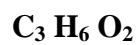
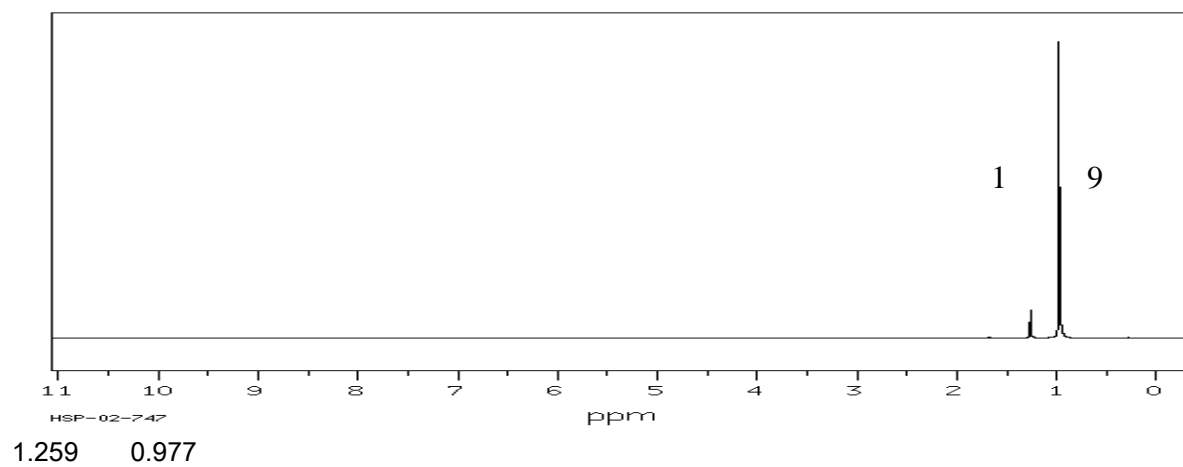


Związek	$(\text{CH}_3)_4\text{C}$	$(\text{CH}_3)_3\text{N}$	$(\text{CH}_3)_2\text{O}$	CH_3F
δ	0.9	2.1	3.2	4.2
Związek	$(\text{CH}_3)_4\text{Si}$	$(\text{CH}_3)_3\text{P}$	$(\text{CH}_3)_2\text{S}$	CH_3Cl
δ	0.0	0.9	2.1	3.0

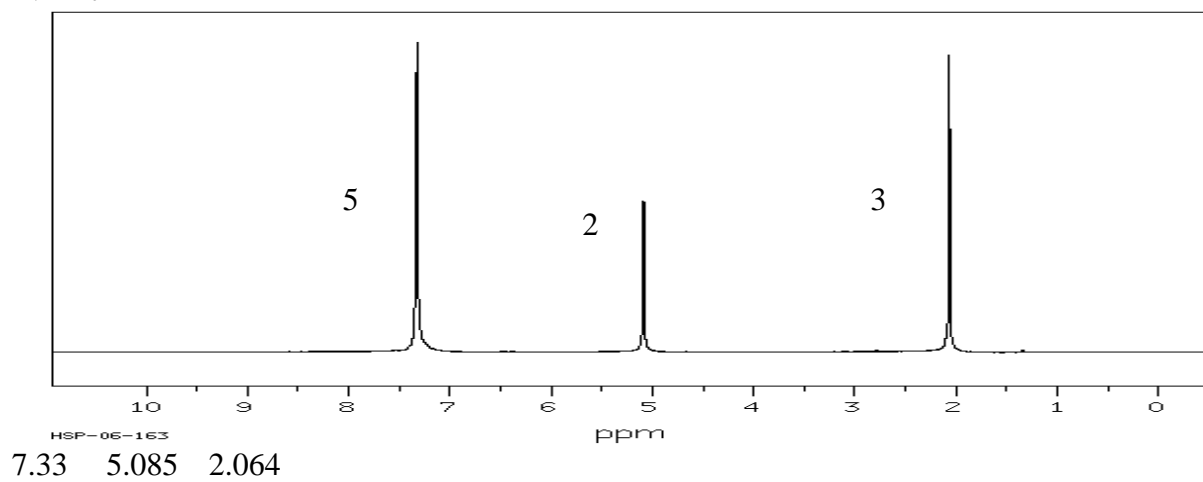


Przykłady przesunięć chemicznych protonów..

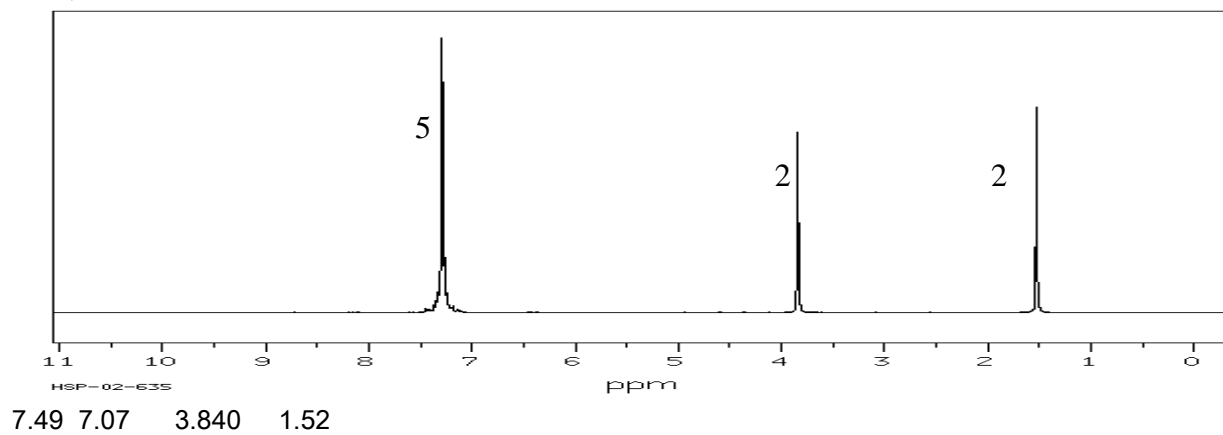




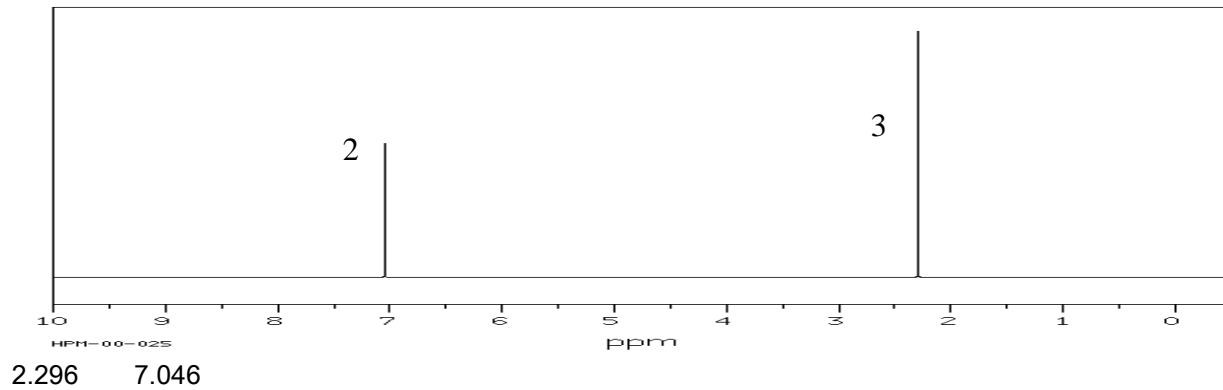
C₉H₁₀O₂

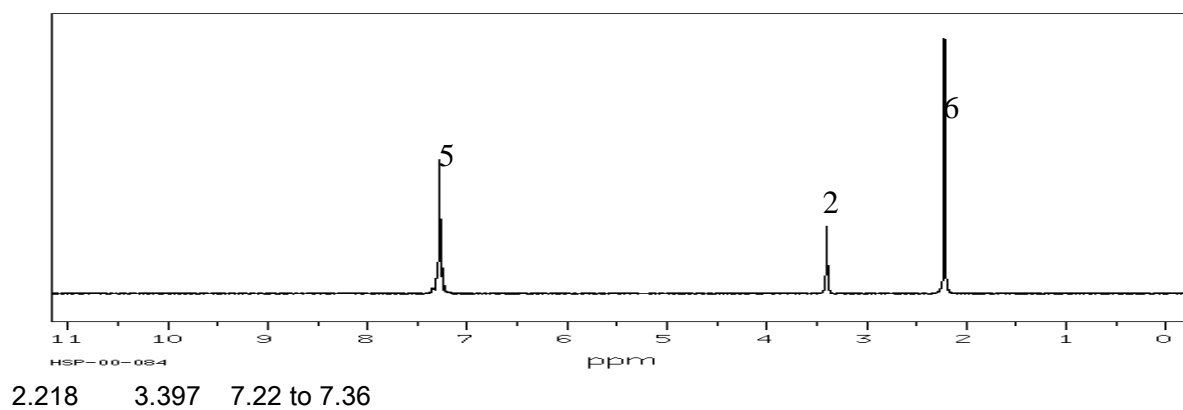
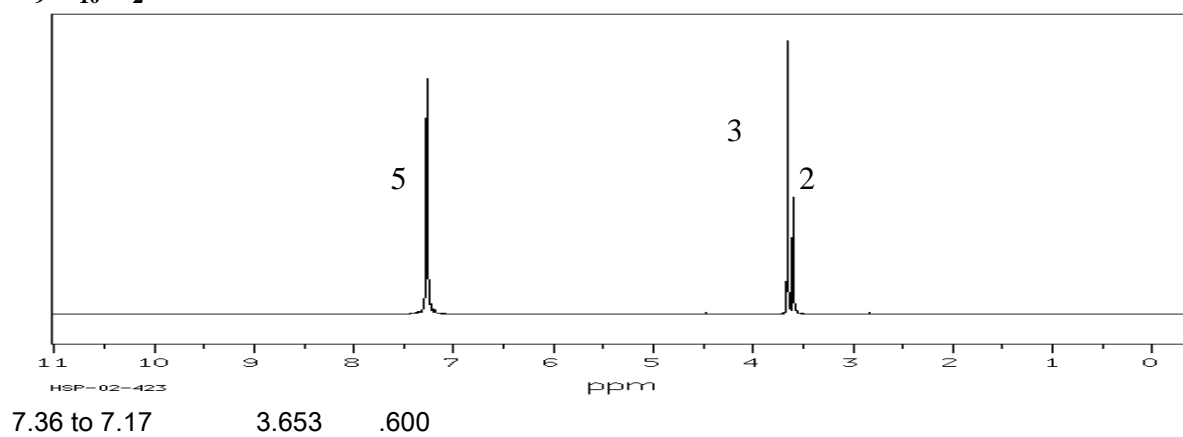
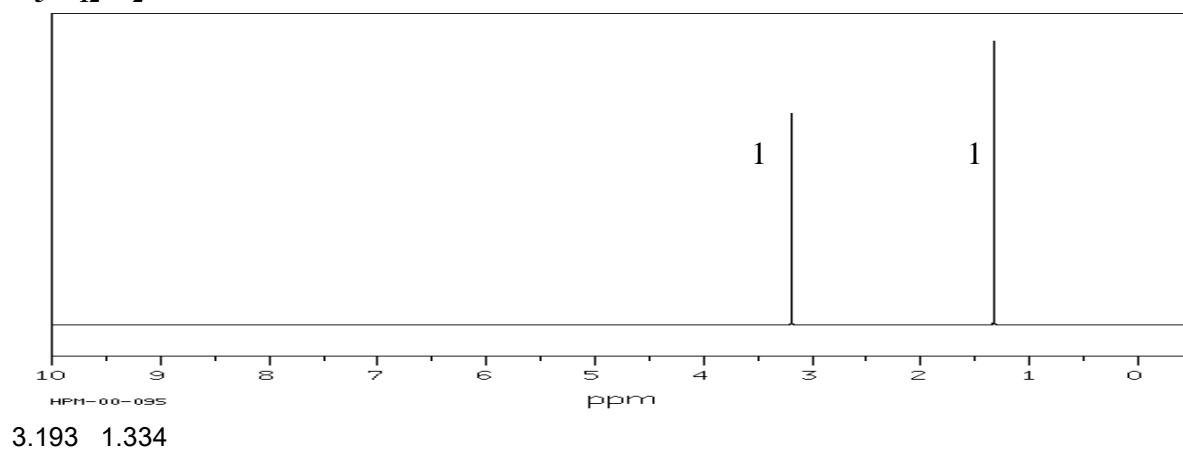
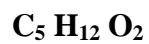


C₇H₉N

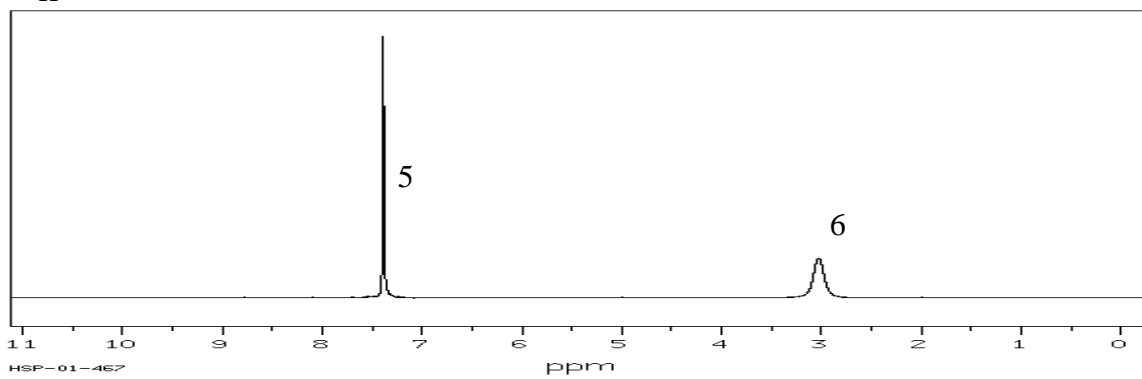


C₈H₁₀



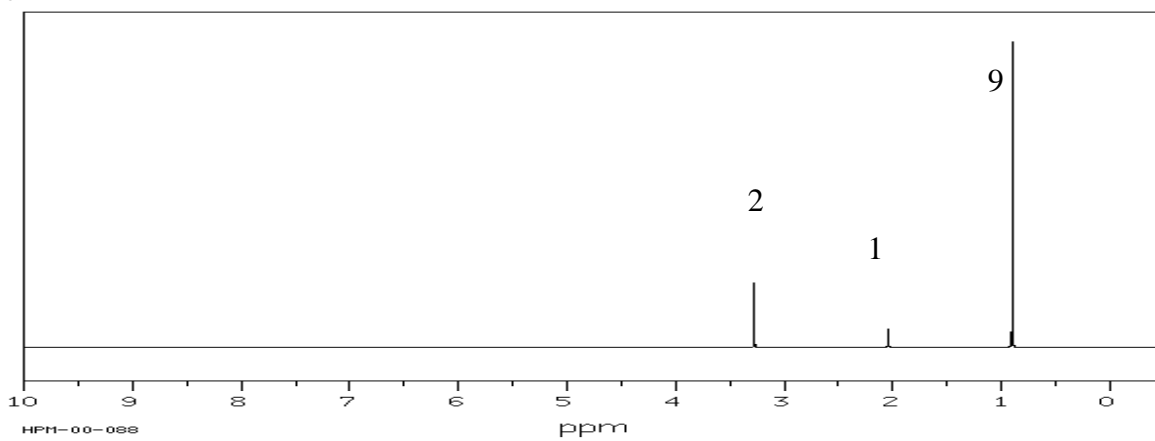


C₉H₁₁NO



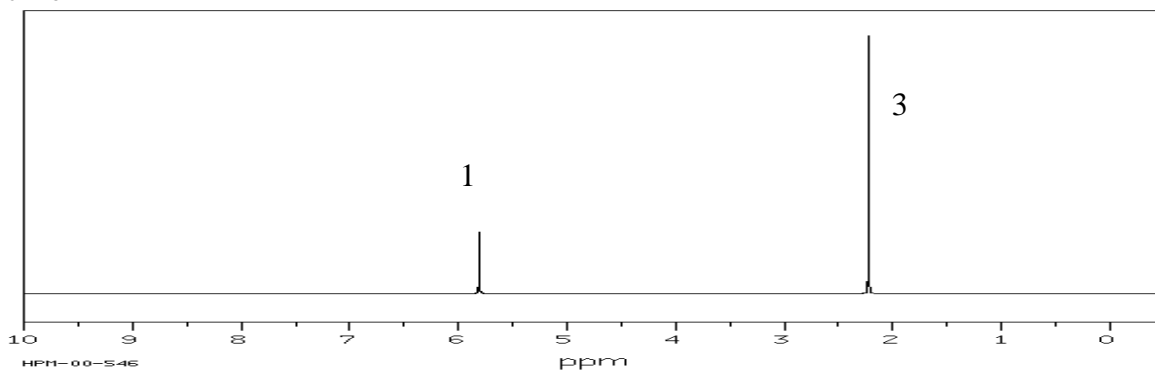
7.39 3.03

C₅H₁₂O



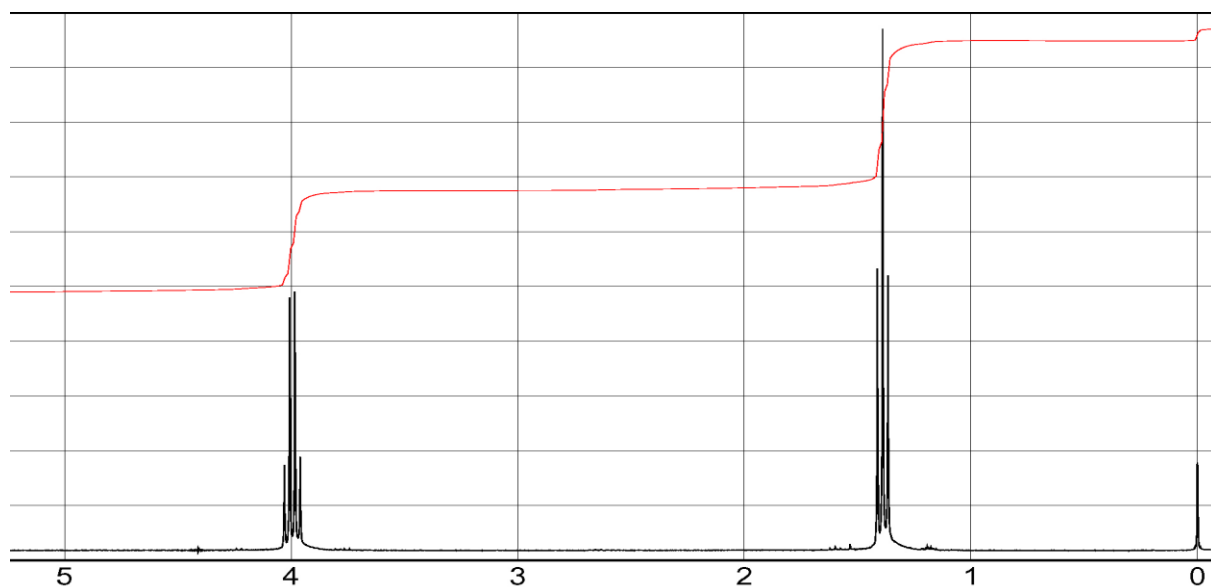
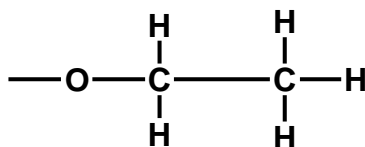
3.280 0.906 2.05

C₆H₈O

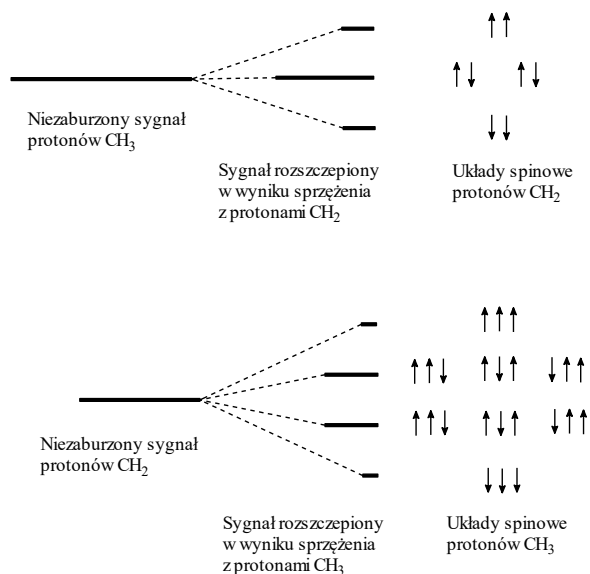


5.812 2.228

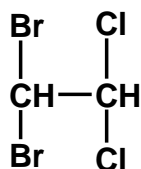
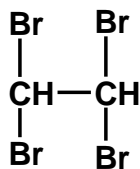
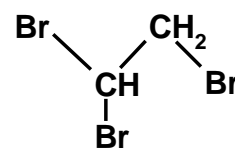
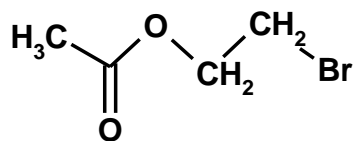
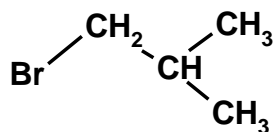
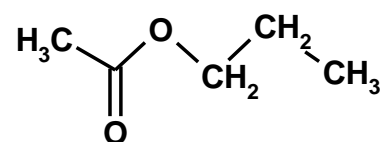
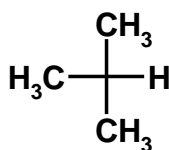
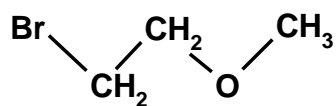
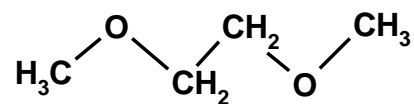
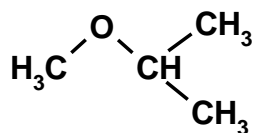
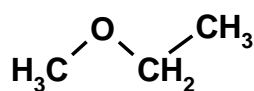
Układy spinowe - multipletowość

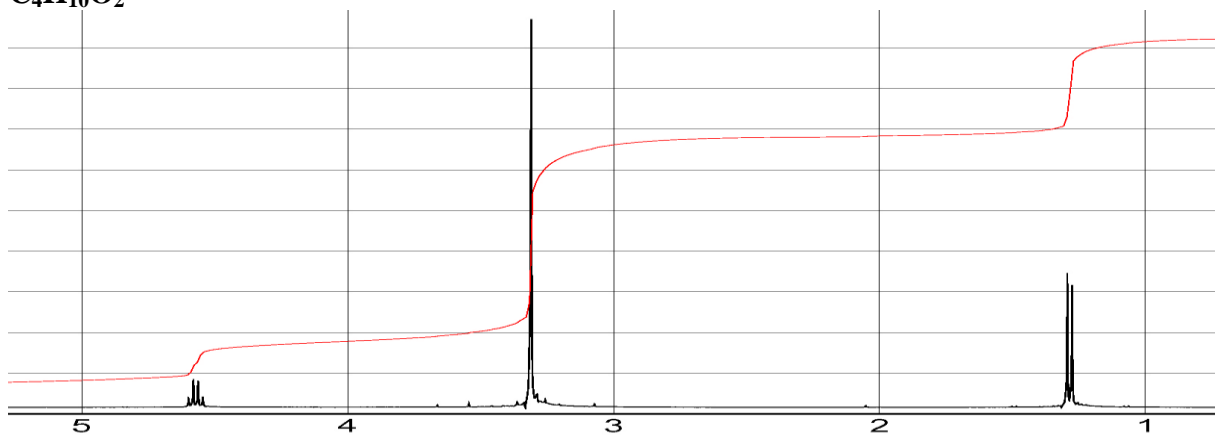
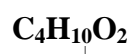
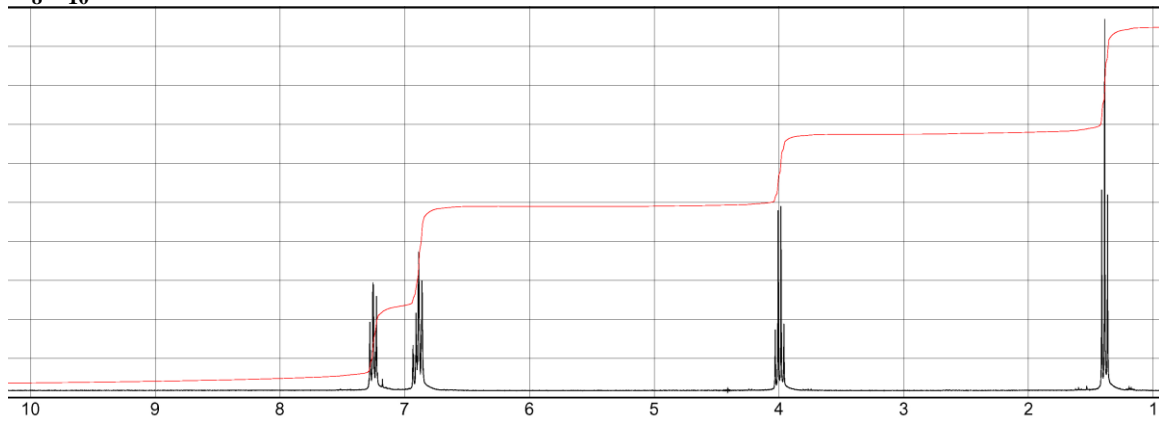
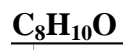
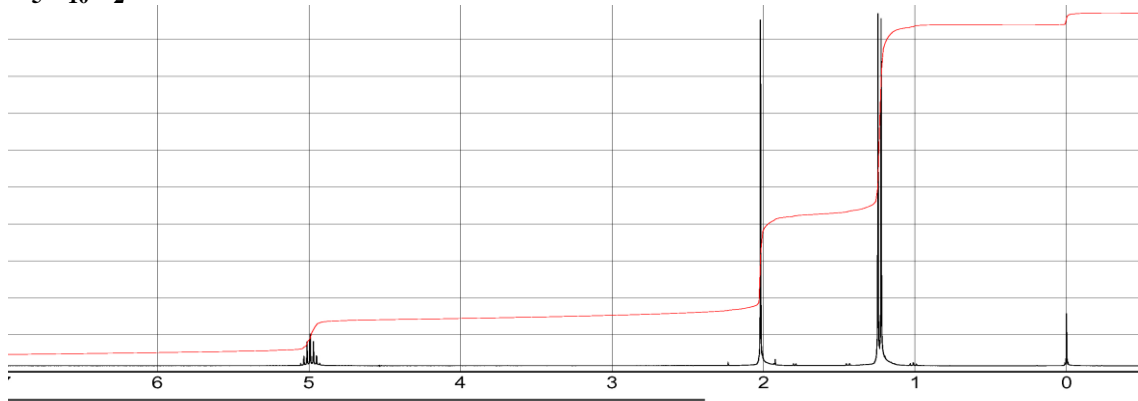
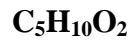


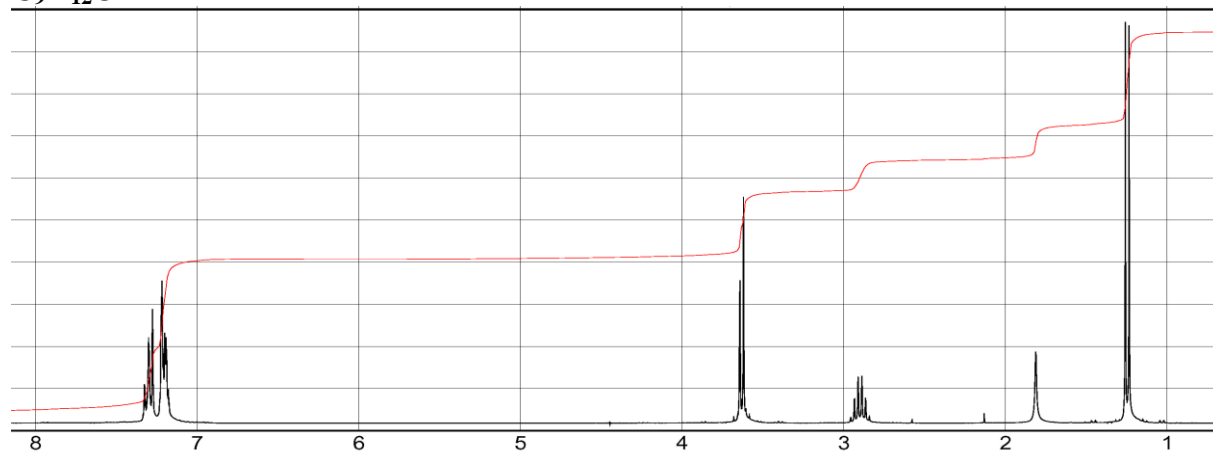
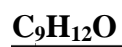
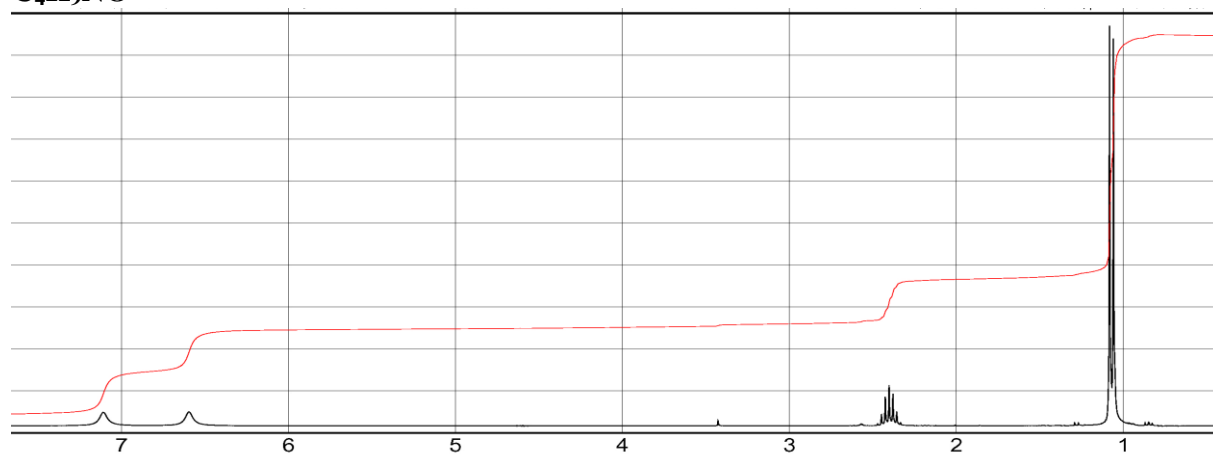
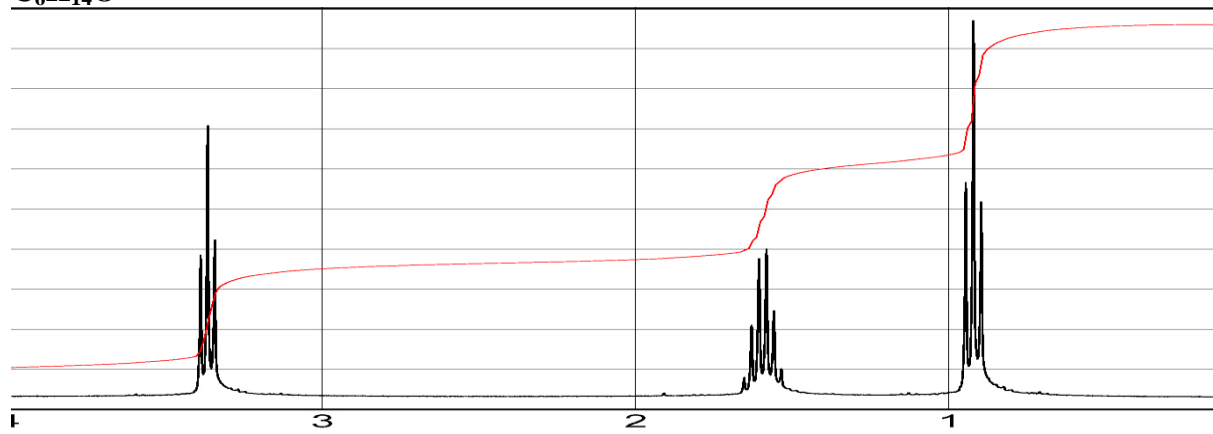
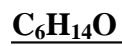
Krotność multipletu dla układów protonowych można obliczyć ze wzoru $(n+1)$, gdzie n jest liczbą równocennych protonów przy sąsiednim węglu. Protony grupy CH_3 mają 2 sąsiadów w grupie CH_2 , czyli krotność multipletu metylowego wyniesie 3, natomiast grupa CH_2 ma 3 sąsiadów (CH_3), czyli jej sygnał zostanie rozszczepiony 4 części.

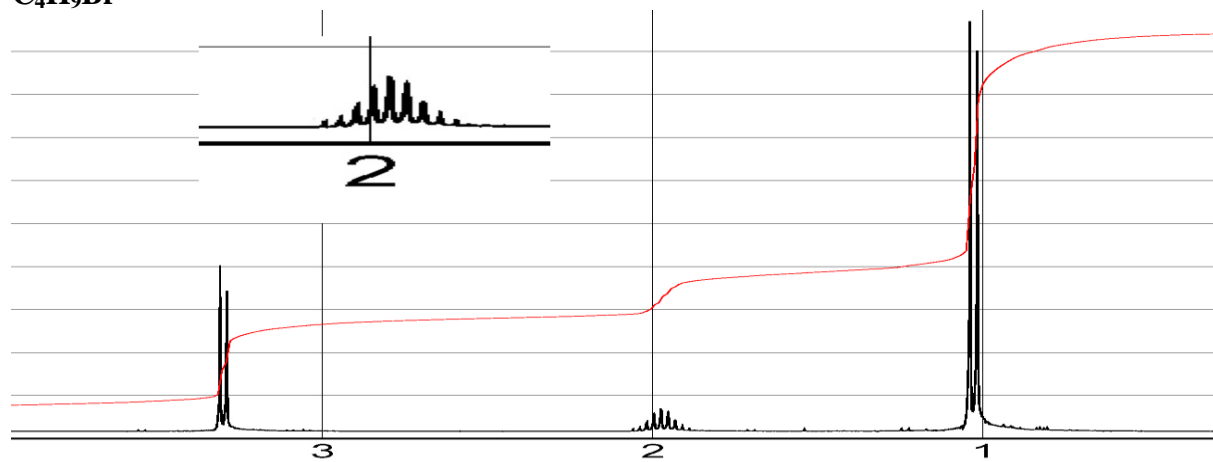
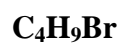
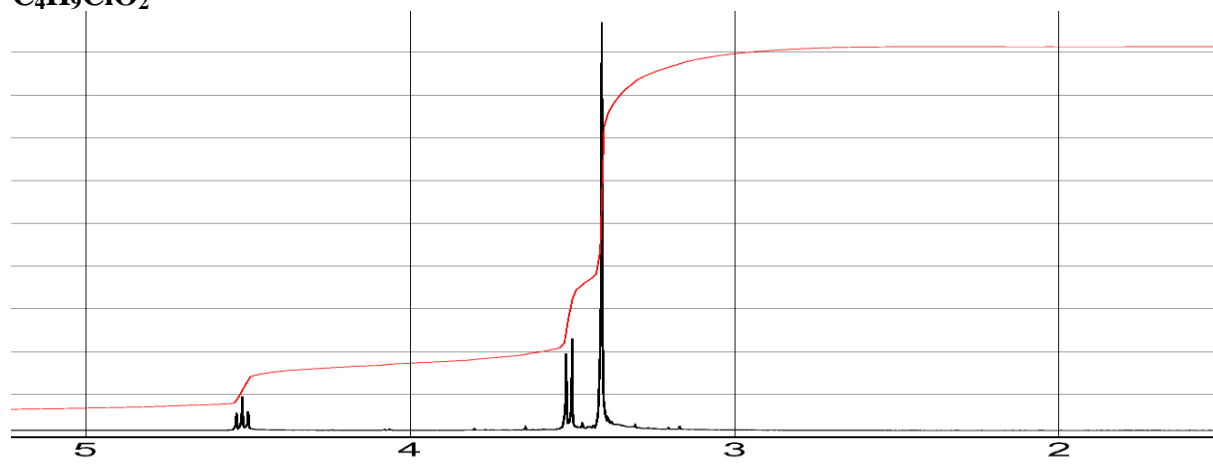
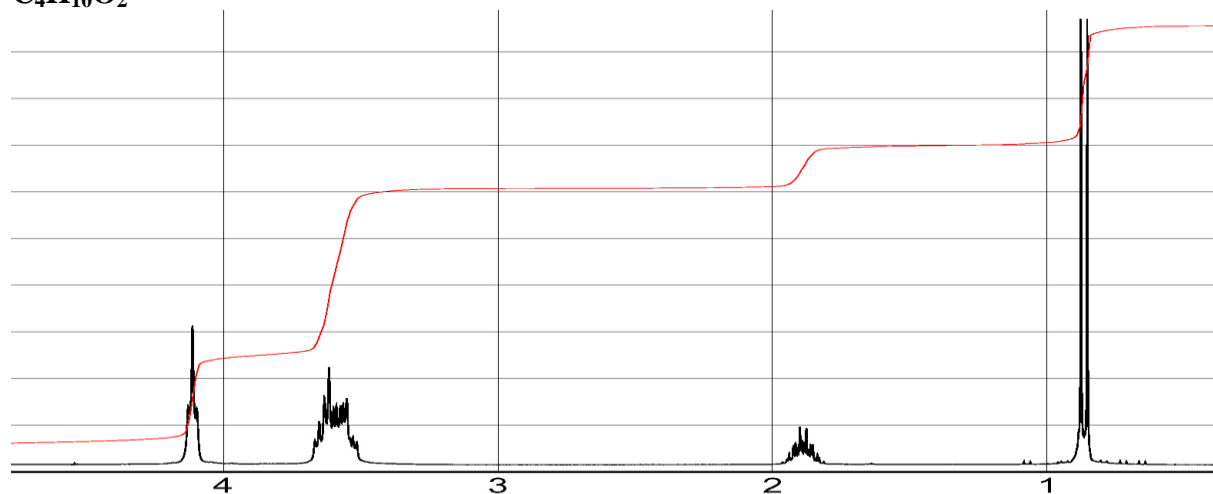


Narysuj widma (układy spinowe) dla podanych poniżej związków.

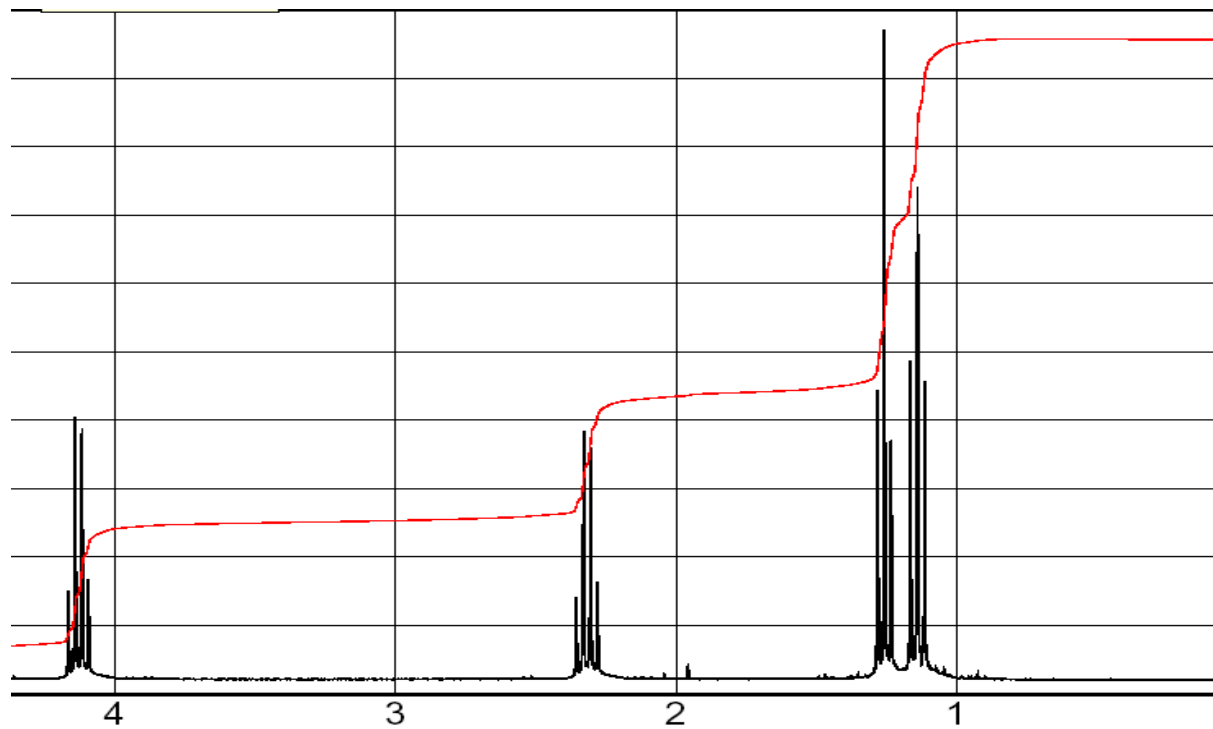








$C_5H_{10}O_2$



$C_{11}H_{14}O_2$

