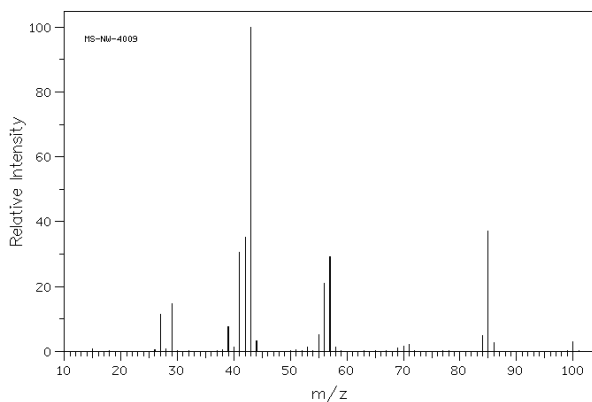
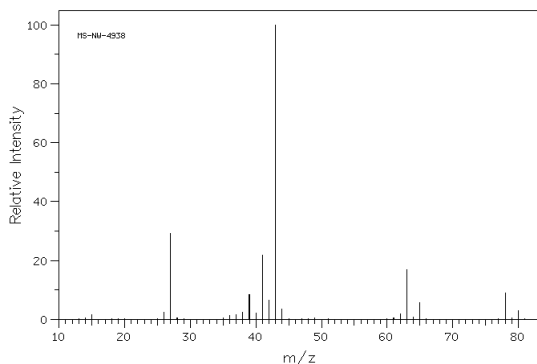


TUTORIAL SHEET MS + IR SPECTROSCOPY

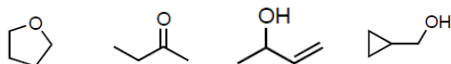
- Determine the degree of unsaturation (HDI) for the hydrocarbons with the following molecular formulas:
 - $C_{12}H_{16}$
 - $C_{14}H_{10}O_4$
 - $C_7H_7NH_2$
 - C_7H_7NO
 - C_8H_9ClO
- An unknown hydrocarbon has a molecular ion peak at $m/z = 84$, with a relative intensity of 31.3. The $M + 1$ peak has a relative intensity of 2.06, and the $M + 2$ peak has a relative intensity of 0.08. What is the molecular formula for this substance?
- Given below is the mass spectrum of 2-methylhexane. What is the m/z value of the M^+ peak and of the base peak? Give possible structures of the fragments giving rise to the large peaks at $m/z = 85$, 57, and 43.



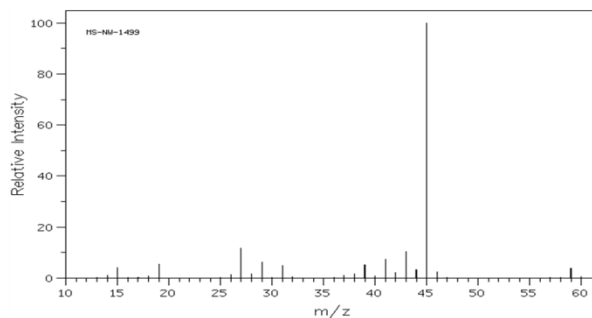
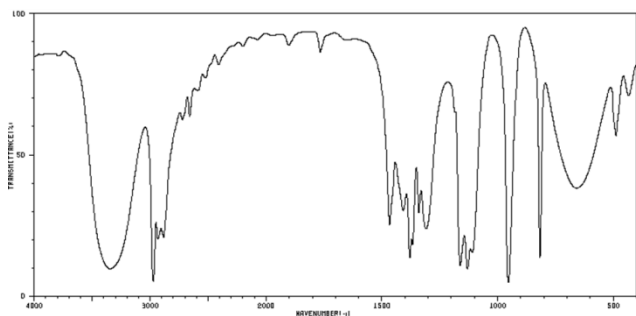
- Given below is the mass spectrum of compound with 46% of Carbon. Deduce the molecular formula/structure.



5. Which of the following compounds gives an IR spectrum with a peak at 3300 cm^{-1} (s, br) and at 1640 cm^{-1} (m)?



6. The O-H stretching vibration of phenol is observed at 3300 cm^{-1} . Assuming the bond strength of the following compounds to be identical to that of phenol, estimate the positions of the corresponding stretching vibrations. (a) thiophenol (d) deuterated phenol.
7. Given below is the IR and mass spectrum of compound. Take the value of molecular ion peak to be at $m/z = 60$. Get the structure.



8. A compound with pleasant smell has a following mass spectra and IR data. Deduce the structure of the compound.

Major IR Peaks (cm^{-1})
2880-2890
1737 (str)
1194, 1116 (str)

Major peaks in Mass spectrum (m/z)
29
41
56
57 base peak
73
85
101
116 molecular ion

