



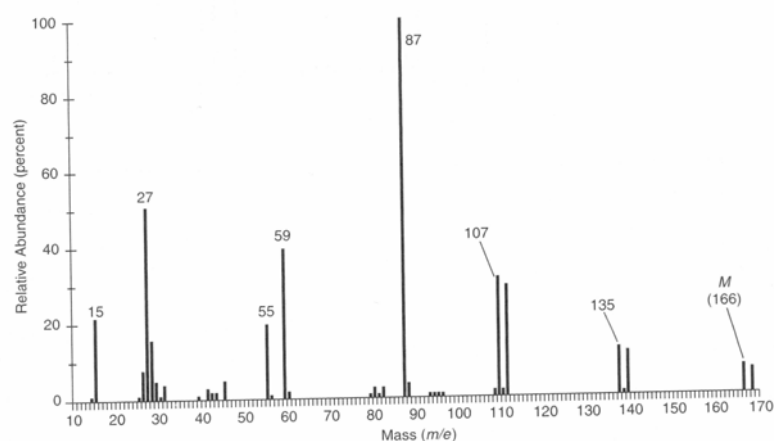
NMR, MS, IR, UV/Vis

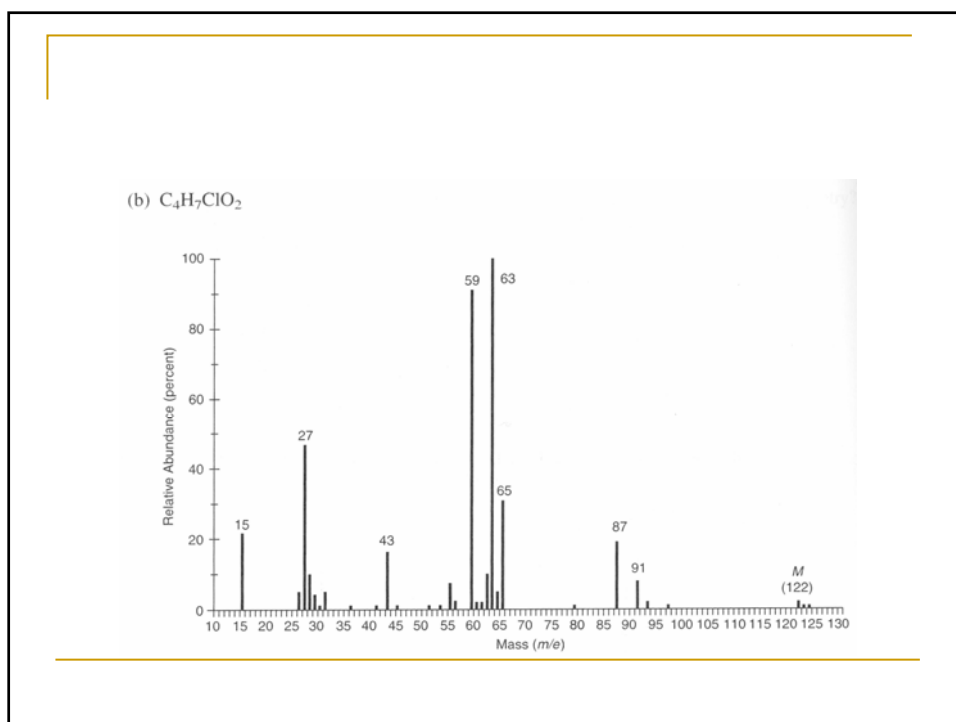
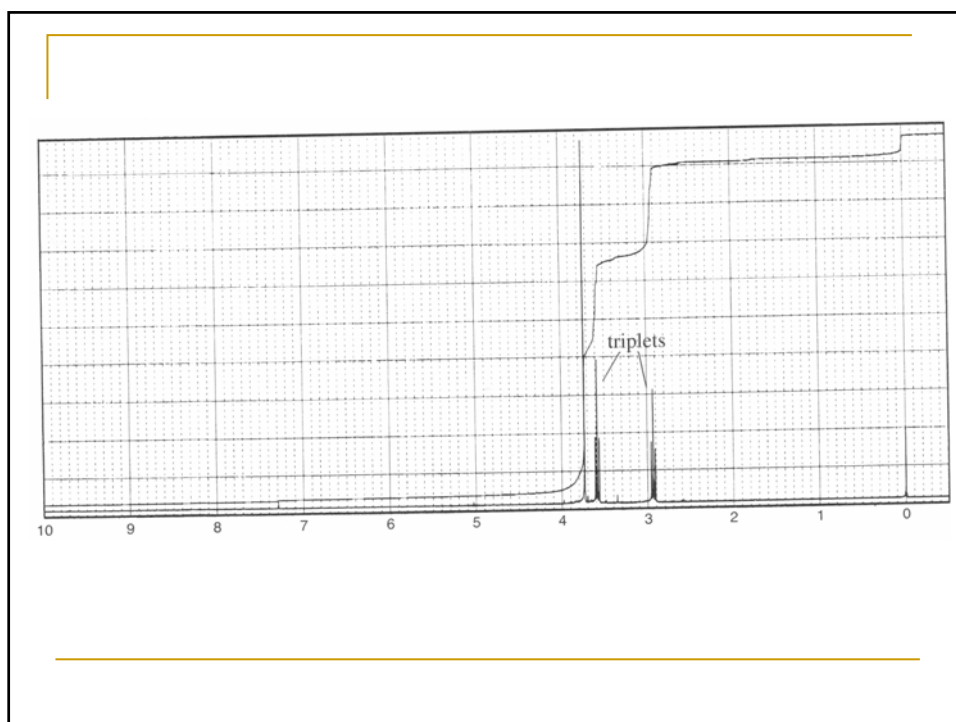
Kombinirani zadaci pri određivanju strukture organskih spojeva

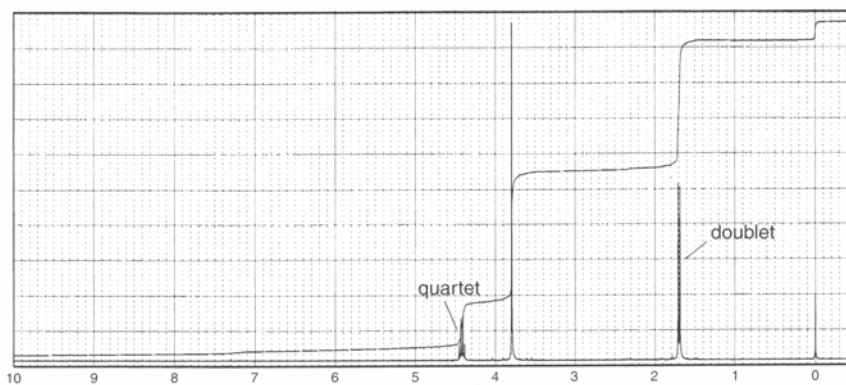
Prof. dr. sc. Irena Škorić

10. Use the mass spectrum and the additional spectral data provided to deduce the structure of each of the following compounds.

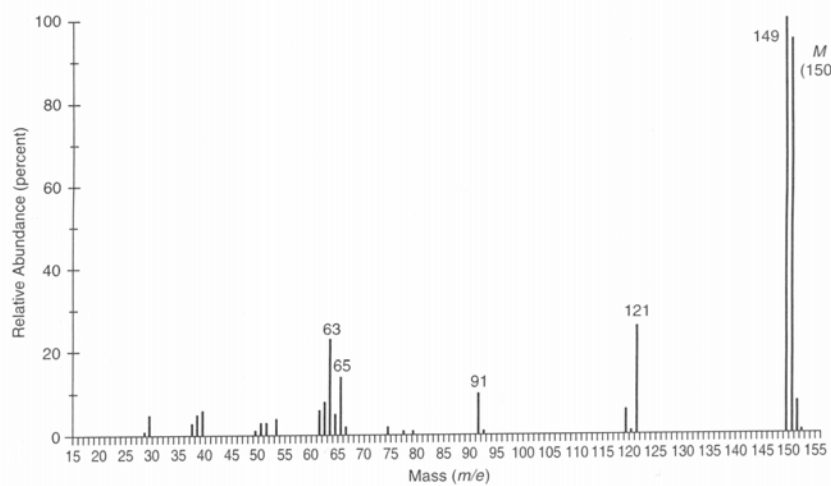
(a) $C_4H_7BrO_2$

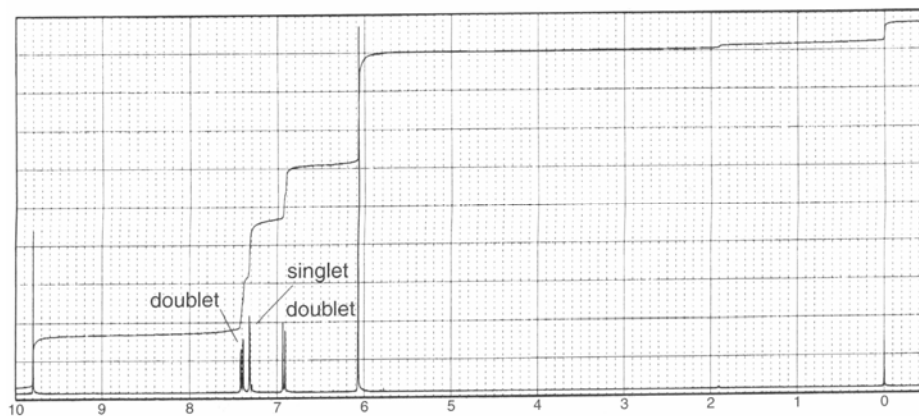






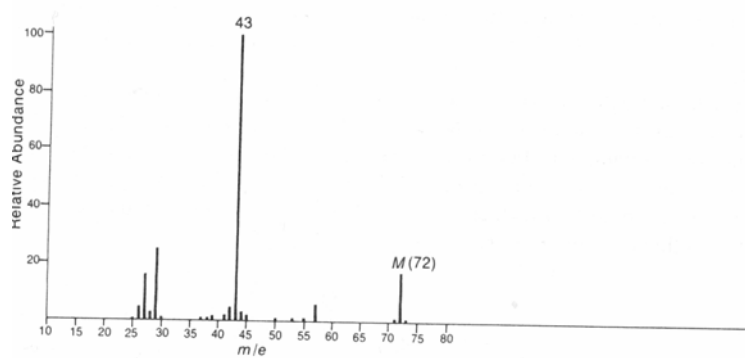
(c) $C_8H_6O_3$

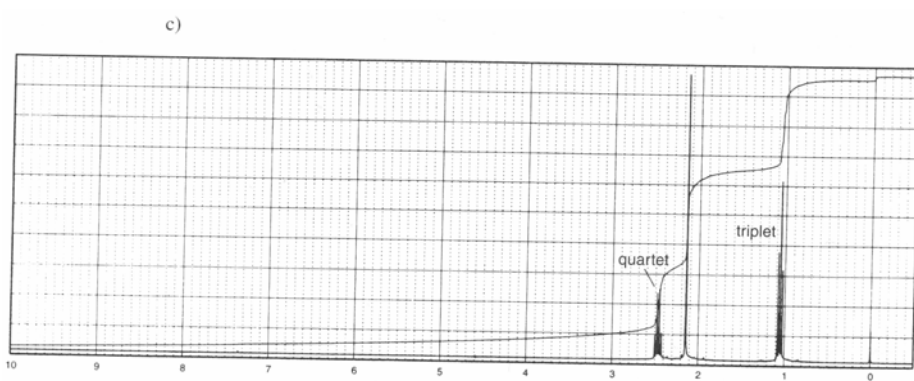
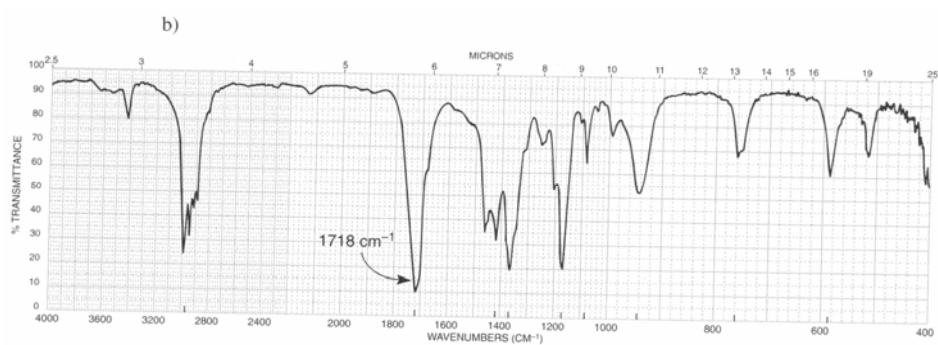




The UV spectrum of this compound is determined in 95% ethanol: λ_{max} 290 nm ($\log \epsilon$ 1.3).

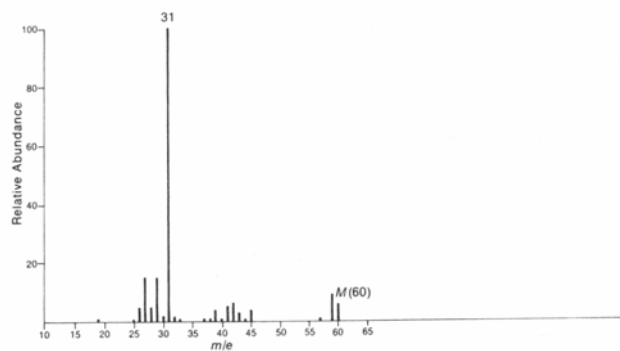
a)



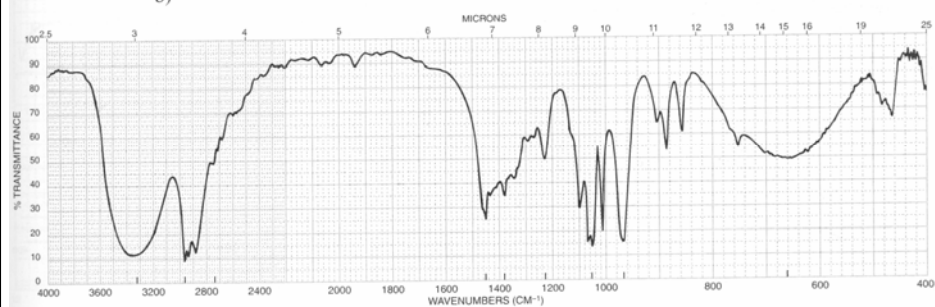


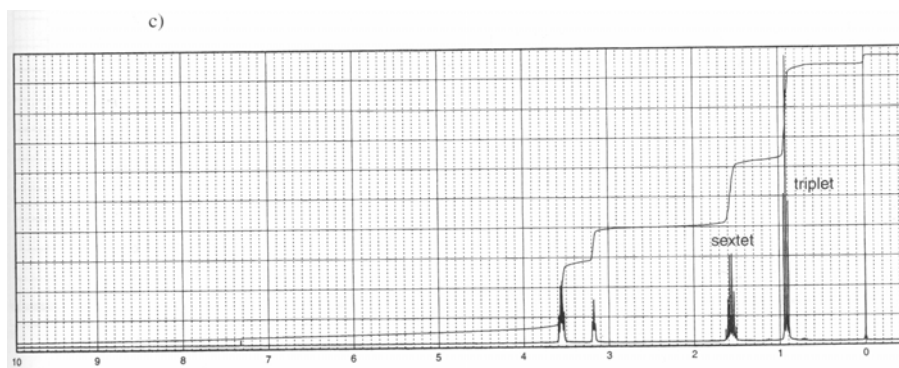
The UV spectrum of this compound shows no maximum above 205 nm. When a drop of aqueous acid is added to the sample, the pattern at 3.6 ppm in the proton NMR spectrum simplifies to a triplet, and the pattern at 3.2 ppm simplifies to a singlet.

a)



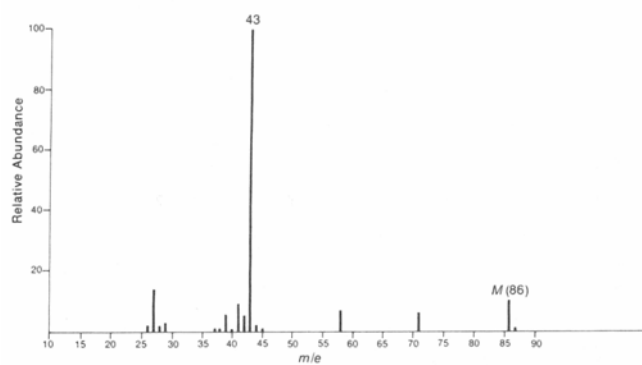
b)

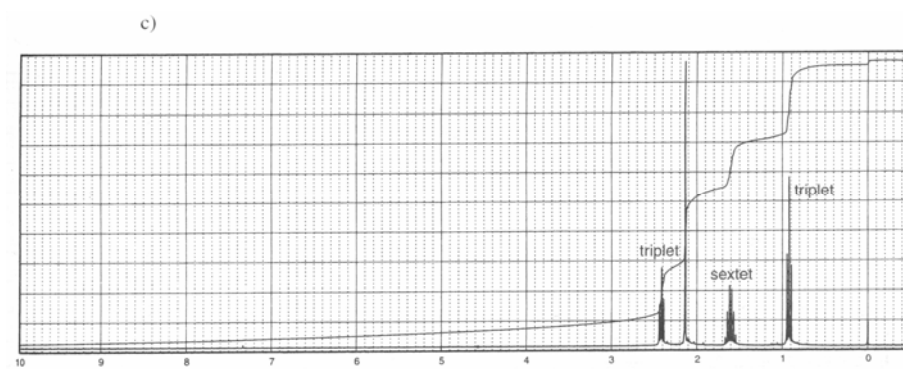
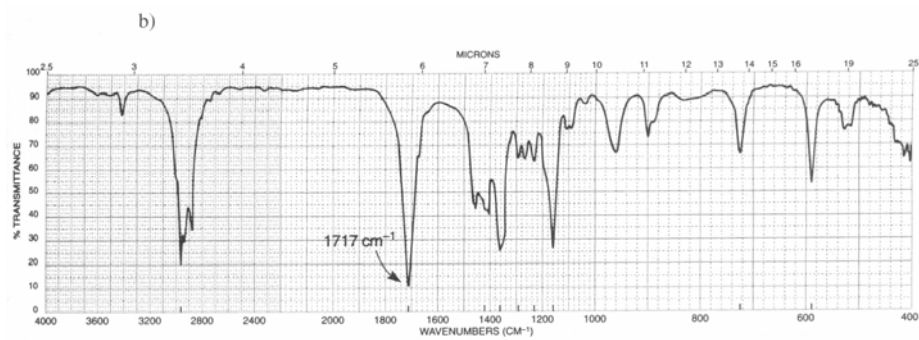




The UV spectrum of this compound is determined in 95% ethanol: λ_{max} 280 nm ($\log \epsilon$ 1.3)
 This compound has the formula $\text{C}_5\text{H}_{10}\text{O}$.

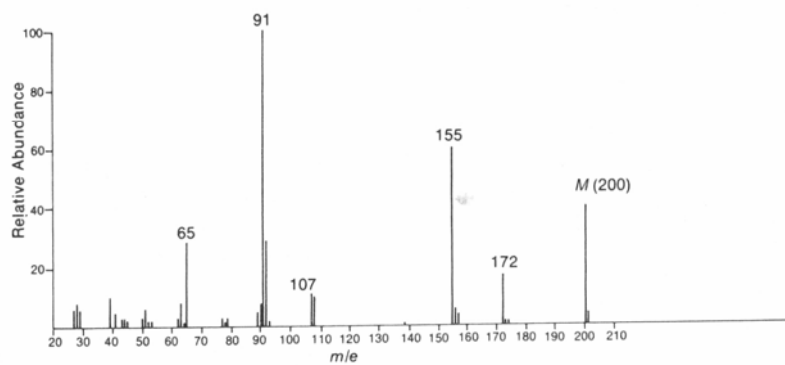
a)



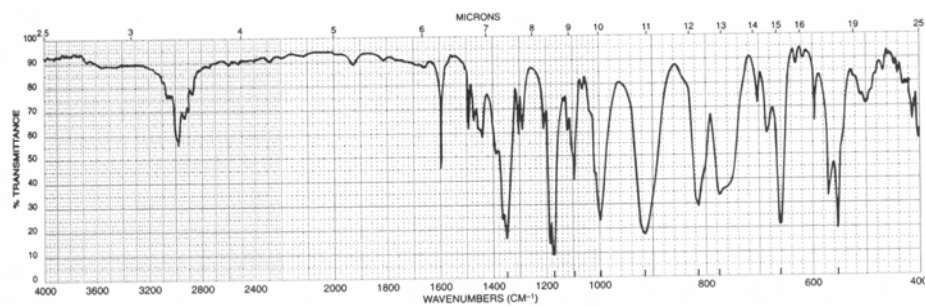


The UV spectrum of this compound is determined in 95% ethanol: λ_{max} 225 nm ($\log \epsilon$ 4.0) and 270 nm ($\log \epsilon$ 2.8). This compound has the formula $\text{C}_9\text{H}_{12}\text{O}_3\text{S}$.

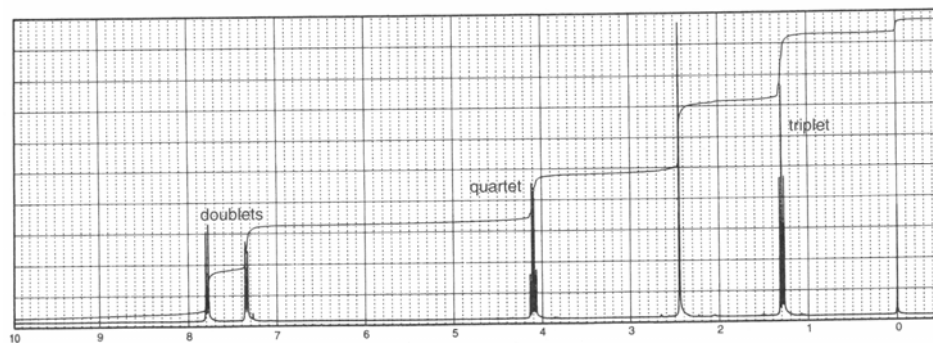
a)



b)



c)



This compound has the formula $C_6H_{11}BrO_2$. Determine the structure of this compound. Draw the structures of the fragments observed in the mass spectrum at 121/123 and 149/151. The carbon-13 spectrum shows peaks at 14, 31, 56, 62, and 172 ppm.

