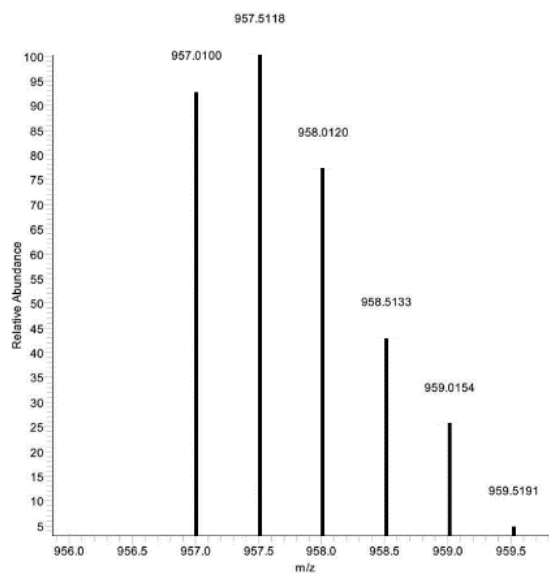


Structural analysis (CH-314)

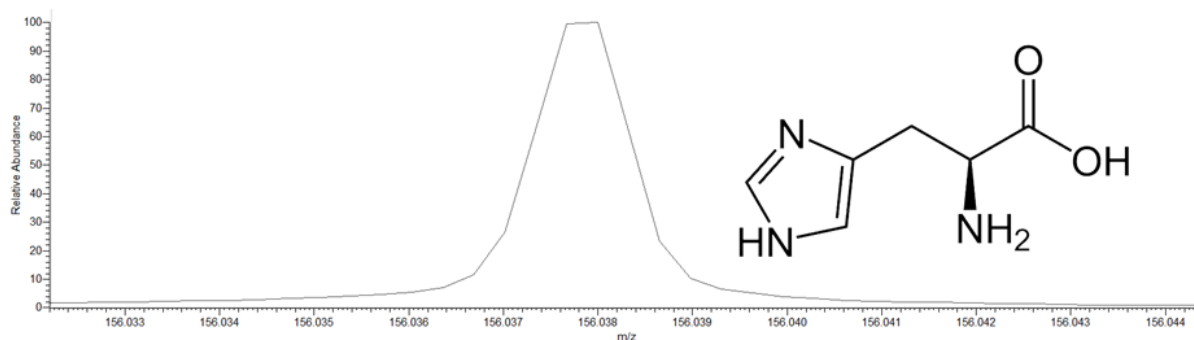
Week 2

Problems

Problem 1. Consider the isotopic distribution of a protonated peptide shown below. Estimate the charge state (z) of this peptide, its monoisotopic and average masses (of the neutral species), and the number of carbon atoms in it.

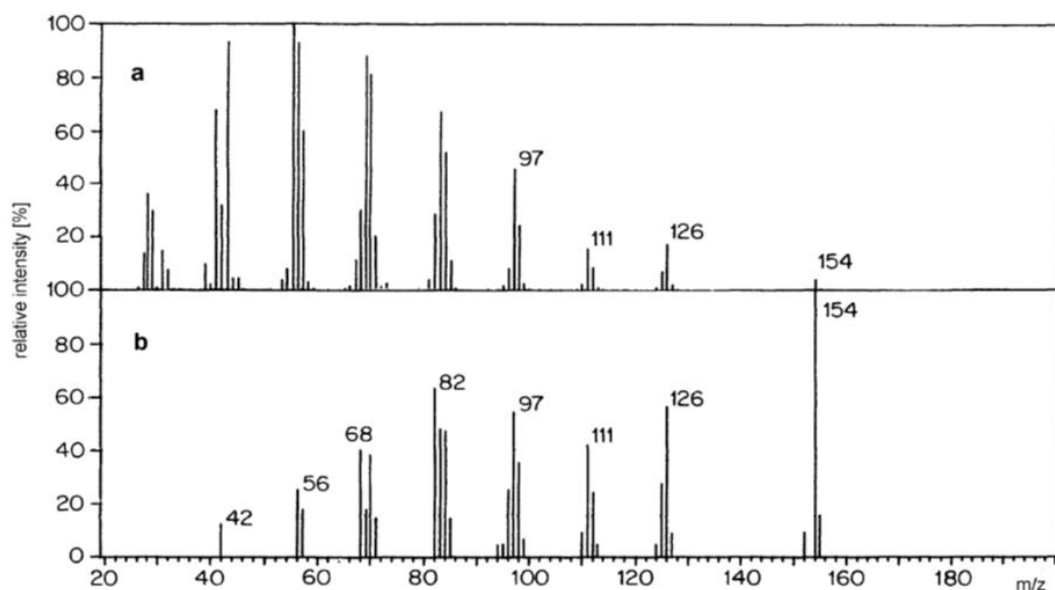


Problem 2. Shown below is the monoisotopic peak of a singly protonated amino acid, histidine. Estimate mass measurement accuracy and mass resolution.

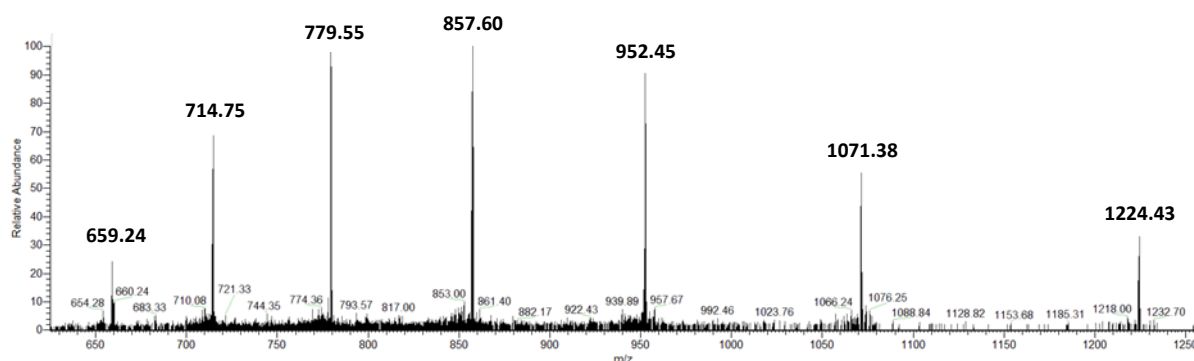


Problem 3. Which resolution is required to distinguish monoisotopic peaks of deprotonated aspirin ($C_9H_8O_4$) and deprotonated glucose ($C_6H_{12}O_6$)? And to resolve isotopic distribution (due to ^{13}C) of a 24 kDa protein?

Problem 4. Electron ionization mass spectra of undecan-1-ol ($C_{11}H_{23}OH$) recorded at two different electron energies are shown below. Which of them, do you think, corresponds to higher electron energy? Explain why.



Problem 5. Shown below is the mass spectrum of a small protein recorded using positive mode electrospray ionization (ESI). Estimate the molecular weight of the protein?



Problem 6. Shown below is the mass spectrum of a mixture of proteins. Which ionization technique, do you think, was used? Why?

