Structural analysis (CH-314)

Week 4

Problems

Problem 1. Ions of mass m are analyzed by an Orbitrap mass spectrometer. How much the frequency of the axial oscillations of the doubly charged ions is higher than that of the singly charged?

Problem 2. Determine the nominal, monoisotopic, and average masses of peptide bradykinin (H-RPPGFSPFR-OH). Monoisotopic masses of the elements: m(^{1}H) = 1.007825 Da, m(^{12}C) = 12.00000 Da, m(^{14}N) = 14.00307 Da, m(^{16}O) = 15.99491 Da. Average masses of the elements: m(H) = 1.00794 Da, m(C) = 12.011 Da, m(N) = 14.00674 Da, m(O) = 15.9994 Da. What are the protonation/deprotonation sites in this peptide? Calculate the mass-to-charge ratio of protonated/deprotonated bradykinin ions.

Problem 3. Which resolution one needs to resolve monoisotopic peaks of triply protonated peptides H-RSHRGHR-OH and H-RVMRGMR-OH?

Problem 4. Doubly protonated peptide substance P (H-RPKPQQFFGLM-OH) is subjected to collision-induced dissociation (CID). Calculate at what m/z you would expect to see the following fragment ions: a) b_5^+, b_6^+; b) y_4^+, y_6^+; c) b_4^{2+}.

Problem 5. A doubly protonated peptide was subjected to CID MS/MS. The obtained mass spectrum contains peaks given below. Assuming the mass accuracy of 5 ppm, perform *de novo* sequencing:

182.081 Th
241.075 Th
338.182 Th
370.118 Th
439.230 Th
501.158 Th
526.262 Th
570.252 Th (precursor ion)
614.242 Th
639.346 Th
701.274 Th
770.386 Th
802.322 Th
899.429 Th
958.423 Th
1036.488 Th