

Structural analysis (CH-314)

Week 1

Problems

Problem 1. Calculate the nominal and monoisotopic masses as well as the atomic weights of the following elements:

- a) iodine (I);
- b) oxygen (O);
- c) lithium (Li).

Problem 2. Calculate the nominal and monoisotopic masses as well as the molecular weights of the following molecules:

- a) sodium iodide (NaI);
- b) amino acid glycine ($\text{C}_2\text{H}_5\text{NO}_2$).

Problem 3. Consider various types of molecular ions that can be produced from aminobenzoic acid ($\text{H}_2\text{N}-\text{C}_6\text{H}_4-\text{COOH}$). Calculate their monoisotopic masses.

Problem 4. Calculate the exact masses and the abundances of all hydrogen sulfide (H_2S) isotopologues (consider only the naturally occurring isotopes).

Problem 5. Calculate the abundances of the five lightest isotopologues (including the monoisotopic species) of the C_{90} fullerene.

Problem 6. For peptides, isotopic distribution is mainly due to ^{13}C . Estimate the minimum number of atoms that a peptide should contain for its A+1 peak to be the most abundant. And for its A+2 peak?

Problem 7. There are two sulfur-containing standard amino acids, methionine and cysteine. Considering isotopic distribution only due to the isotopes of sulfur, estimate the minimum number of such residues that a peptide should contain for its A+2 peak to be the most abundant.