L06. Chemometrical methods in expert systems for the molecular structure elucidation

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Conventionally, two following branches may be distinguished in chemomertics: quantitative and qualitative ones. Quantitative chemometrics is based on continue mathematics, where mathematical statistics plays the leading role. The major areas in this field include multivariate calibration, pattern recognition, mathematical mixture resolution, etc. The main attention is focused on quantitative aspects of chemical analysis. Qualitative chemometrics is based on discrete mathematics, mainly on mathematical logic, graph theory and combinatorial analysis. These methods allow realizing the basic stages of an analytical procedure which is commonly called Computer-Aided Structure Elucidation (CASE).

This procedure is successfully applied to the structure elucidation of unknown (newly separated or synthesized) organic compounds from their MS, NMR and optical spectra, that is for qualitative analysis. To automate the qualitative analysis, CASE expert systems were developed. Methodology of CASE expert systems includes the following main stages: 1) spectral parameters determination in molecular spectra of different nature; 2) selection of possible molecular fragments on the basis of spectral data; 3) generation of all molecular structures which met spectral data and additional constraints, the found fragments and molecular formula being used for this goal; 4) selection of the most probable structure by means of spectrum prediction for all candidate structures included into the output file; 5) determination of 3D model and relative stereochemistry of the preferable structure.

In our presentation, we consider how the methods intrinsic for both branches of chemometrics are combined within CASE expert systems. Important role of quantitative chemometrics and its impact on the entire CASE strategy is discussed and illustrated by series of examples taken from analytical practice. Expert system ACD/Structure Elucidator is used as an example of the most advanced CASE expert system.