# T07. Analysis of complex mixtures using self-modeling decomposition of different spectral data

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A system where no a priori information about chemical components is available is classified as a black system. The aim of performing curve resolution on black systems is to estimate the spectra (qualitative analysis) and concentration profiles (quantitative analysis) of the entire chemical component present in the mixture.

In this work we have compared performances of different self-modeling curve resolution techniques in identification and quantitative analysis of substances of different nature. Traditional self-modeling (SIMPLISMA, ALS) and independent component analysis (MILCA, SNICA, RADICAL, FASTICA and JADE) algorithms were applied to experimental standardless analysis of complex mixtures and real objects. Results are presented for several types of spectroscopic signals: UV-VIS, IR, and fluorescence.

Consideration of the composition of waste waters in the petroleum industry and widespread environmental contaminants has defined our choice to study certain organic compounds. We have investigated up to five component mixtures with various concentrations of benzene, toluene and o-xylenes in the UV-region. We have also examined various multicomponent mixtures of different compositions (up to six substances) of PAHs in their solid and liquid states by means of IR, UV spectroscopy and fluorescence. We have analyzed complex mixtures of water and fat-soluble vitamins B6, B9, B12, PP, C, E, D, A as well.

Application of ICA decomposition algorithms on the data from real objects is of great practical interest, especially where the mixture composition is not known exactly. We have applied ICA and ALS to the analysis of vitamins and metals in ten complex multivitamin drugs. Spectra of individual vitamins were extracted and compound concentrations in the initial drug were obtained with 10% relative error. We also examined different fuels (gasoline, diesel fuel) and carried out quantitative and qualitative analysis of five aromatic compounds and three sulfur-containing organic substances. Their detection limits were comparable to the chromatographic determination.

The study has shown that the nature and the number of components present in mixtures, as well as selected spectral region and other instrumental factors, like noise, step, and speed of scan, severely influenced the results. In most cases, however, MILCA, SNICA and ALS provided superior results than other techniques used.