Use of advanced chemometrics for study of acidobasic and structural processes of bioligands

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The dissertation to be presented focuses on use of multivariate methods for data analyses (so called advanced chemometrics). The data in form of both spectral curves and combination of discrete points were obtained from various experiments monitored with optical spectroscopy methods. Use of soft model and hard model based curve resolution methods is demonstrated on analysis of experimental data of solution equilibria of two groups of oligonucleotides that are investigated in relation to oncologic disorders. Acid-base properties of adenine analogues were studied by the same means after we realized that there is scarce information about them despite their wide use in therapeutic and research applications.

Use of artificial neural networks for pattern recognition of sensor arrays is discussed as another approach to multivariate data analysis. Two arrays based on non specific cross-reactive sensors were designed for two different groups of analytes as first step of an attempt to develop high throughput sensor array for similar molecules. The feasibility of the concept is currently being assessed. As the work is on the very beginning only problems encountered during the development of data analysis procedure and steps taken towards their solution are described.