

Different Interaction Models for Explanation of Optical Properties of Ligand-Polynucleotides Systems

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Spectrophotometry in visible region was used to investigate the processes of complexation in a system of ligand-polynucleotide. These investigations were developed in large area of wavelengths and polynucleotide concentrations. But usually not whole set of obtained data is used simultaneously at binding parameters determination especially for Scatchard plot construction and other simple methods.

Many ligands can bind to double stranded matrix forming several types of complexes with different optical parameters. Those binding parameters for each type of complex can be calculated via using optimization programs of optical titration data. So, the influence of different complexes on total optical properties of mixtures at multimodal binding can be found.

Using two kinds of competitive binding models, describing ligands interaction with polyelectrolyte, the equilibrium composition (association constants, stoichiometry and molar extinction coefficients) was calculated by the DALSMOD optimization program of spectrophotometric concentration dependences for Actinomycin D derivatives in the presence of native and denatured DNA samples.

Two binding models for competitive binding with different values of parameters were considered. The first model provides for accounting cooperative effects at interaction on adjacent sites of external binding molecules. And the second model describes the differences in spectral and thermodynamic parameters between monomeric bound intercalated ligands and molecules bound to neighbour site sizes.

Spatially unlocalized monovalent ions added to the system can be competitive ligands at drugs (cations) binding. In consideration of monovalent ions (Na^+ , K^+) influence of as competitors for both external and intercalating binding types and using both models, the accounting of different types of complexes contribution in observable optical absorption were found for different concentration of added ions.