

The primary exploratory objective of the doctoral dissertation entitled “Studies on interactions of methyl benzoate and biphenyl derivatives with selected complex chemical and biological macromolecules” was to investigate the mechanisms of interactions between molecules exhibiting photoinduced intramolecular charge transfer (electron and/or proton) and selected macrocyclic carriers and to elucidate the mechanisms of interactions between two methyl benzoate derivatives and animal proteins (BSA).

Analysis of experimental data obtained using steady-state and time-resolved spectroscopy and nuclear magnetic resonance spectroscopy methods provided information on possible deactivation pathways of electronically excited molecules within selected supramolecular carriers and determined the effect of geometry, both of the „guest” and „host” molecules, on the persistence of the resulting complexes. The stoichiometry of the tested inclusion complexes, their formation constants and the orientation of the molecule inside the macrocyclic carrier were also determined.

From a purely scientific point of view, it was extremely interesting to explore and elucidate the influence of the spatial structure of various macrocyclic carriers (cyclodextrins (CD), cucurbit[7]uriles (CB[7]) and sulfonic calix[6]arene (SCA[6]) on the phenomenon of photoinduced intramolecular proton and electron transfer, as well as understanding what role universal (dipole-dipole) and specific (intermolecular hydrogen bonding) intermolecular interactions play in the coordination process.

Analysis of the time-dependent fluorescence spectra recorded with the streak camera also provided very valuable information on the relaxation of the molecules of the medium around the excited state luminescent compound under study. In aqueous solutions containing SCA[6] and CB[7], the solvation relaxation process was found to be at least two (SCA[6]) or three (CB[7]) orders slower than the situation when the luminescent molecule is in a homogeneous medium (pure solvent). It was also found that the average solvation relaxation time in the molecule-protein system is about an order of magnitude longer than in the system with macrocyclic carriers (CB[7] and SCA[6]).

Investigations of the interactions of a biphenyl derivative — a donor-acceptor compound which, due to its ability to rotate around a single bond between donor and acceptor, already forms a spectrally heterogeneous system in the ground state — with γ -CDs demonstrated that in both investigated environments (DMSO and DMSO-water), stable complexes of stoichiometry 1: 1, with the values of the equilibrium constants depending on both the concentration of the molecule and the wavelength of the excitation light.

As the study of drug interactions with various biomolecules is of unflagging interest among numerous groups of pharmacists, biochemists or medical scientists, the present study also sought to understand the interaction processes between two methyl benzoate derivatives and three key amino acids (tryptophan (Trp), tyrosine (Tyr) and phenylalanine (Phe)) and bovine serum albumin (BSA). Quantitative analysis of the spectroscopic data showed that both I-Trp, II-Trp and I-BSA, II-BSA form complexes that demonstrate a 1:1 stoichiometry. Moreover, the specific interaction between II and Trp as well as II and BSA involves the OH and/or -COOCH₃ groups of the II molecule (no photoinduced intramolecular proton transfer process can occur).