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## **MULTI-SCALE APPROACH FOR STATISTICAL BROAD ABSORPTION AND EMISSION SPECTRA OF ORGANIC COMPOUNDS AND BIOLOGIC OBJECTS**

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Growing importance on nanotechnology requires understanding and interpreting different types of spectra as one of the techniques for unravelling structural changing and various processes in molecular biology and chemistry, for the investigations or technological developments in energy research, electronics, medicine and pharmaceutical industry, environmental engineering and ecology. Spectroscopic analyses are powerful tools with high information contents to determine the spatial and chemical structures of molecular objects or to fingerprint even specific photo-physically (chemically) detected biological processes proceeding in and between those systems for controlling, testing, and monitoring biological polymers and drug compounds, their properties, physical and chemical reactions in the native environment.

The multi-scale Statistical Quantum-Mechanical/Molecular-Dynamical (SQMMD) methodology for generating electronic-vibrational (vibronic) spectral manifolds was developed and applied to provide detailed insight into the electron-nuclear processes that are involved into the interactions the molecular complexes with their environment in various thermo-dynamical (TD) conditions.

The statistical absorption spectra between 240–320 nm for estradiol in ethanol, hexane, or dimethyl sulfoxide (DMSO) solvents at the room temperature as well as a wide spectrum with including transitions to numerous excited states of tryptophan-cage mini protein (trp cage-mp) were produced. The thermal dependence of spectral width and intensity was established for a transition from first long-wavelength band of benzene surrounded by cyclohexane molecules which is forbidden for equilibrium planar structure. Both absorption and emission spectra of cyanoanthracene were generated under different TD condition that demonstrated temperature and pressure broadening and changing the spectral shape.

Human Serum Albumin (HSA) fluorescence absorption in the range of 240–280 nm originates from Trp, Tyr, and Phe residues but its fluorescence in the red wing of the spectrum longer than 300 nm is solely an intrinsic attribute of the Trp214 residue. Spectral shift and fluorescence quenching of Trp in the presence of drug molecules is a good marker to detect positions of small ligands bound to HSA and traveling through a living body. Spectral properties and charge transfer from excited states of Trp donor to microenvironmental acceptors such as drug ligands trapped near this residue into subdomain IIA of binding site I of HSA were computationally investigated with using SQMMD and the polarizable embedding approach (PE) for a surrounding model.

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## **INFLUENCE OF HUMIC SUBSTANCES ON THE PHOTOLYSIS OF ORGANIC CONTAMINANTS**

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Depending on their origin and structure, humic substances have a remarkable ability to absorb light and transfer this energy to other substrates and in some cases strongly affect photolysis of