

## Optical Properties of Films of Thiochrome Dye with Tryptophan Amino Acid

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Despite the significant achievements of biophysical science, many mechanisms of interaction between biological molecules and external agents (medicines) are not explained. There are many different approaches to the study of the interaction of proteins with drugs. One of them is a study of the spectral properties of  $\pi$ -conjugated amino acids (tyrosine, tryptophan, phenylalanine), which absorb and emit in the UV-Vis region, and provide information about the conformational states of biopolymers in the initial state and when changing the external environment. More significant studies can be detected by adding fluorescent dyes that have high-intensity absorption and photoluminescence. In the presence of third agents, such as drugs, fluorescent dyes can change their structure, electronic properties, etc.

Thiochrome ( $CH_{14}N_4N_4OS$ ) is a natural dye formed by the oxidation of thiamine (vitamin B). Thiochrome in the study plays the role of the detector of complex formation. It has freely solubility in water, is not toxic to biological systems, and has intense fluorescence at 443 nm. The dye contains two aromatic rings. Also, tryptophan has an aromatic ring. Both molecules, with the help of aromatic rings, can create the non-covalent,  $\pi$ - $\pi$  stacking bond.

**Spectral studies make it possible to determine the availability of complex formation of a thiochrome with a tryptophan. And the distribution of charge, electronic and oscillatory structure, forms of molecular orbitals of individual molecules, and their complexes can be characterized by quantum-chemical calculations: semi-empirical and DFT method. The purpose of this work is to study the spectra of absorption of composite films of tryptophan with the thiochrome and to establish the mechanisms of their interaction in the formation of complexes in the case of  $\pi$ - $\pi$  stacking.**

### Topics

Session D. Biomedical optics and sensors technology

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