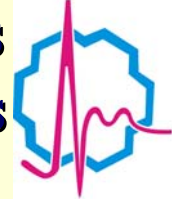




Spectral Properties of Indole Derivatives as Parts of New Pi-Electron-Containing Drugs

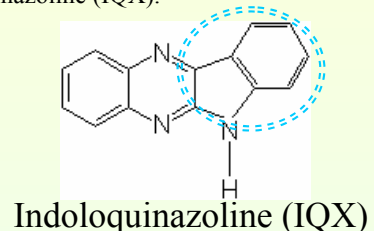
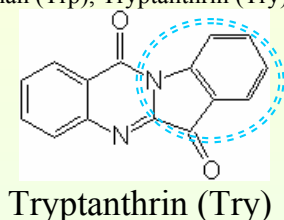
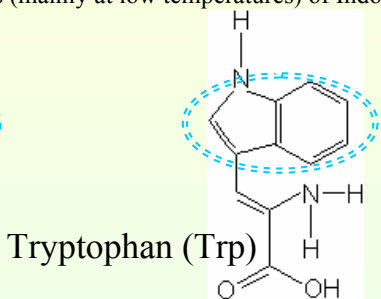
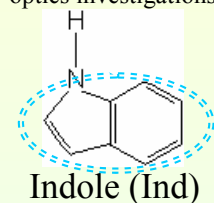


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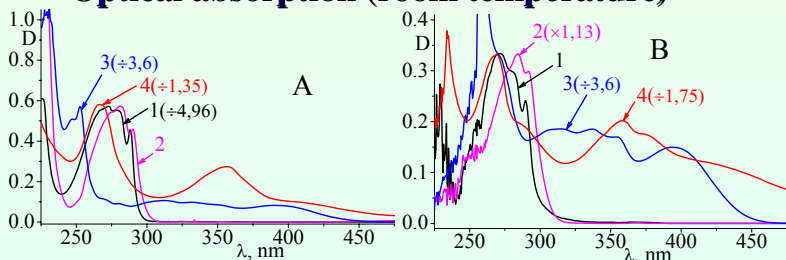
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Abstract. The majority of Indole derivatives are the class of biologically active pi-electron-containing compounds that possess broad "spectrum" of bio-medical activities. For example, Tryptophan is a well-known pi-electron-containing amino acid, the structure unit of high-molecular proteins that together with DNA/RNA are the smallest building blocks of any living creature. Tryptanthrin is a naturally occurring yellow alkaloid, that can easily bind to telomeric G4 DNA and stabilize it. Due to this unique feature Tryptanthrin possesses anti-pathogenic, anticancer, anti-inflammatory, etc activities [1,2]. At the moment scientists paid their attention on the investigations of optical absorption and fluorescence of this class of compounds mainly at room temperature [2]. We have an experience in the investigations of such class of compounds [3], and now our study is aimed at the comparative spectral investigations (mainly at low temperatures) of Indole (Ind), Tryptophan (Trp), Tryptanthrin (Try) and Indoloquinazoline (IQX).



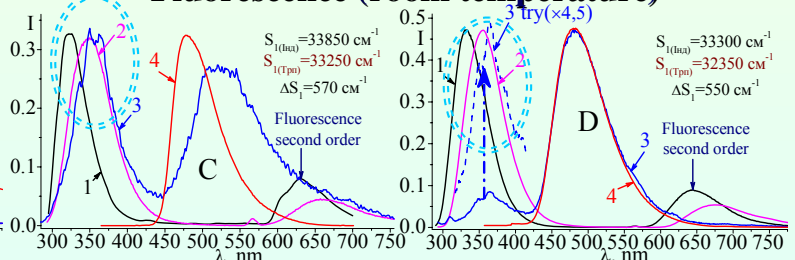
Comparative spectral investigations of optical absorption (at room temperature), fluorescence (at room temperature and $T = 78\text{ K}$) and phosphorescence (at $T = 78\text{ K}$) of solutions of Ind, Trp, Try and IQX (in different solvents) under different excitation wavelengths were carried out. The positions of the first excited singlet (S_1) and triplet (T_1) energy levels of these compounds were obtained. The effect of solvents on spectral properties of the investigated compounds is fixed.

Optical absorption (room temperature)



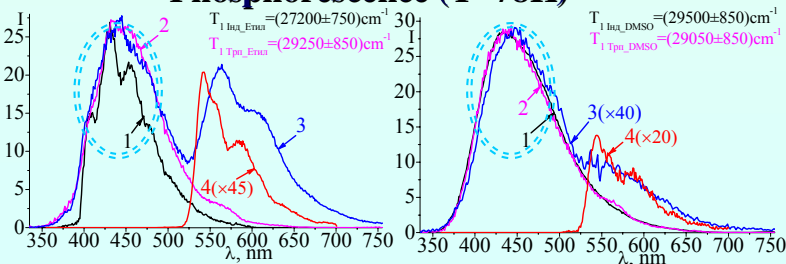
Optical absorption spectra: 1-Ind, 2-Trp, 3-Try, 4-IQX (solutions in A-ethanol, B-DMSO, $C=10^{-5}\text{ M}$).

Fluorescence (room temperature)



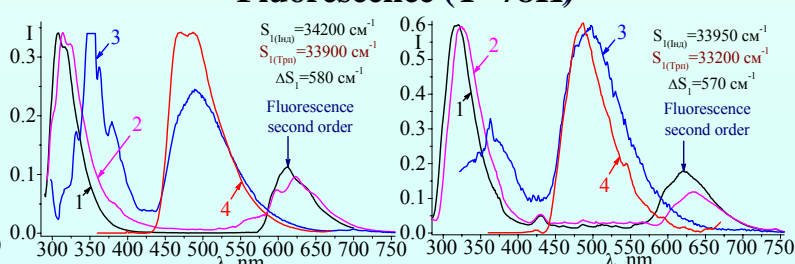
Normalized fluorescence spectra (room temperature): 1-Ind, 2-Trp, 3-Try, 4-IQX (solutions in C-ethanol, D-DMSO, $C=10^{-5}\text{ M}$, $\lambda_{\text{ex}}(1-3)=270\text{ nm}$, $\lambda_{\text{ex}}(4)=340\text{ nm}$).

Phosphorescence ($T=78\text{ K}$)



Normalized phosphorescence spectra ($T=78\text{ K}$): 1-Ind, 2-Trp, 3-Try, 4-IQX (solutions in C-ethanol, D-DMSO, $C=10^{-5}\text{ M}$, $\lambda_{\text{ex}}(1-3)=270\text{ nm}$, $\lambda_{\text{ex}}(4)=340\text{ nm}$).

Fluorescence ($T=78\text{ K}$)



Normalized fluorescence spectra ($T=78\text{ K}$): 1-Ind, 2-Trp, 3-Try, 4-IQX (solutions in C-ethanol, D-DMSO, $C=10^{-5}\text{ M}$, $\lambda_{\text{ex}}(1-3)=270\text{ nm}$, $\lambda_{\text{ex}}(4)=340\text{ nm}$).

Conclusions

The main centre of optical absorption, fluorescence and phosphorescence of Trp is **Ind pi-electron system**. Optical absorption spectra of Try and IQX are complex, but they contain the band associated with absorption of **Ind pi-electron system**. In fluorescence (under both temperatures) and phosphorescence of Try two optical centers have been fixed, one of them is associated with emission of **Ind-segment** of Try pi-electron system. In contrast to Try, in fluorescence (under both temperatures) and phosphorescence of IQX only one optical center has been fixed, **it is not** emission of **Ind pi-electron system**.

References

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- [3] V. Yu. Kudrya, T.-Y. Zhang, M.-X. Tan, A. P. Naumenko, *J. Luminescence*, **2024**, 266, 120242.