NBP-2025
9th International Conference
NanoBioPhysics: Fundamentals and Applied Aspects
6–9 October 2025, Kharkiv, Ukraine

SOME ASPECTS OF OPTICAL SPECTROSCOPY OF DRUGS BASED ON INDOLE DERIVATIVES

Kudrya V.Y. [1], Tkach N.V. [1*], Karpenko O.S. [2], Dubey I.Y. [3], and Naumenko A.P. [1]

1 - Faculty of Physics, Taras Shevchenko National University of Kyiv, 64/13 Volodymyrs'ka str., 01601, Kyiv, Ukraine;
2 - Department of Medical Chemistry and Chemoinformatics, A.V.Bogatsky Physico-Chemical Institute of the NAS of Ukraine, 86, Lyustdorfs'ka doroha str., 65080, Odesa, Ukraine;
3 - Institute of Molecular Biology and Genetics of the NAS of Ukraine, 150 Zabolotnogo str., 03143, Kyiv, Ukraine

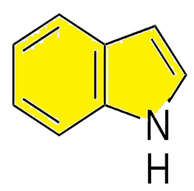
ANNOTATION

Indole is a well-known heteroaromatic compound consisting of the fused benzene and pyrrole rings. Compounds containing the indole fragment form the great class of biologically active substances that possess a broad range of bio-medical activities (such as anti-pathogenic, anticancer, anti-inflammatory, etc). One of the natural amino acids – tryptophan – is an indole derivative. The naturally occurring alkaloid – Tryptanthrin – can easily bind and stabilize the telomeric G-quadruplex (G4) DNA. Due to this unique feature Tryptanthrin and its metal complexes demonstrate antitumor properties and other types of biological activity [1,2]. As we have shown [3], the attachment of some groups to heteroaromatic π-electron system could cause dramatic changes of optical spectra. Now our presentation is aimed to highlight some aspects of optical spectroscopy investigations (mainly at low temperatures) of indole (Ind), tryptophan (Trp) and tetracyclic drugs Tryptanthrin (Try) and Indolo[2,1-b]quinazoline-6,12-dione (IQX).

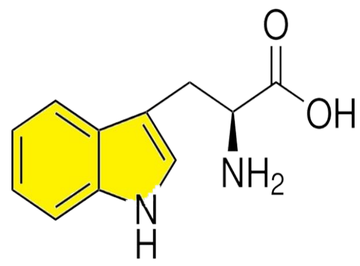
METHODS

Optical absorption (at room temperature), fluorescence (at room temperature and T=78K) and phosphorescence (at T=78K) of the solutions of Ind, Trp, Try and IQX in different solvents were investigated under different excitation wavelengths. Positions of the first excited singlet (S_1) and triplet (T_1) energy levels of these compounds were estimated. The spectral manifestation of solvent effects on the studied compounds properties was obtained.

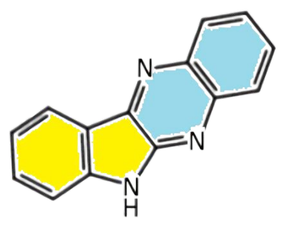
OBJECTS



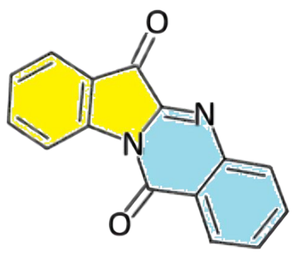
Indole (Ind)



Tryptophan (Trp)



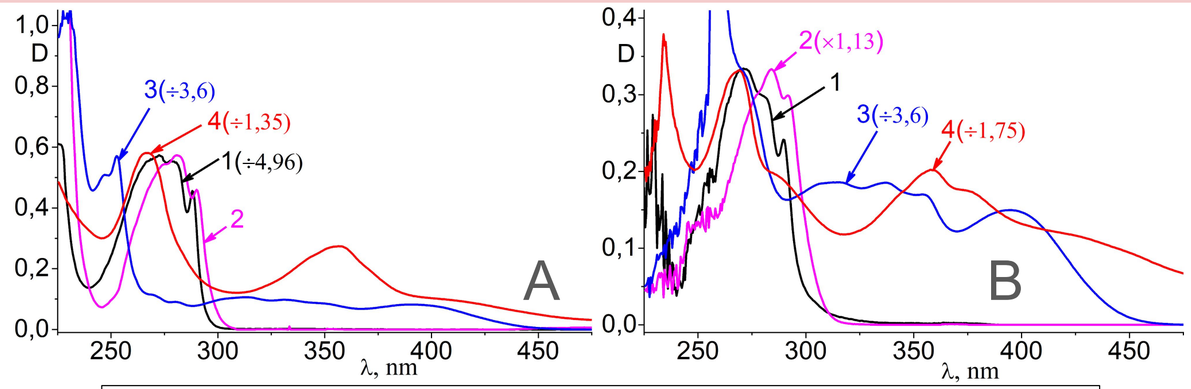
Tryptanthrin (Try)



Indoloquinazoline (IQX)

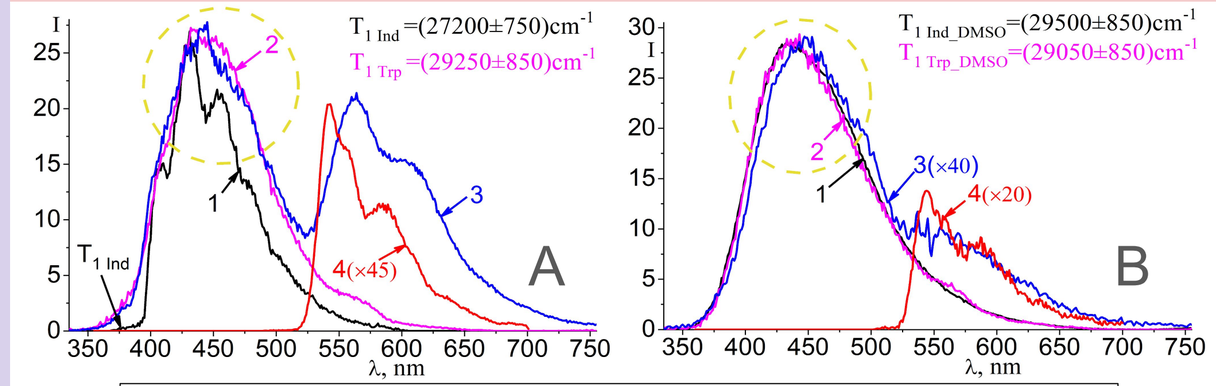
RESULTS

OPTICAL ABSORPTION (ROOM TEMPERATURE)



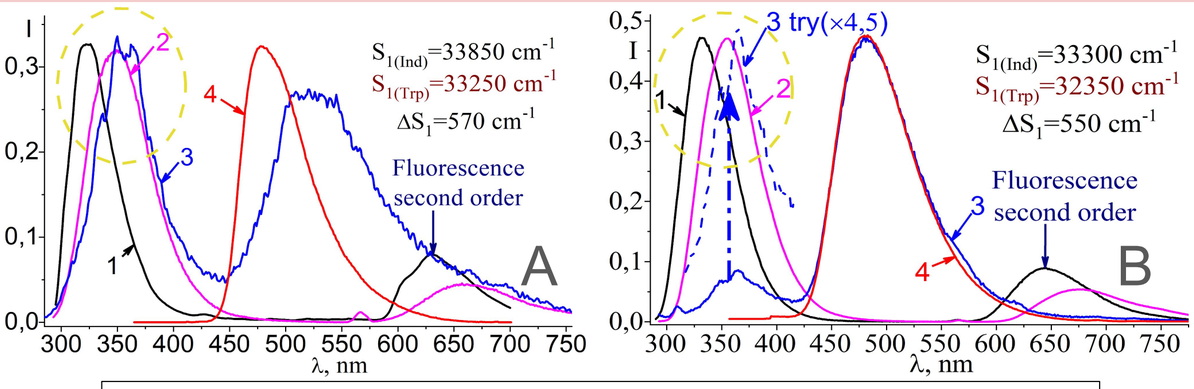
Optical absorption spectra: 1-Ind, 2-Trp, 3-Try, 4-IQX (solutions in A-ethanol, B-DMSO, C=10⁻⁵M).

PHOSPHORESCENCE (T=78K)



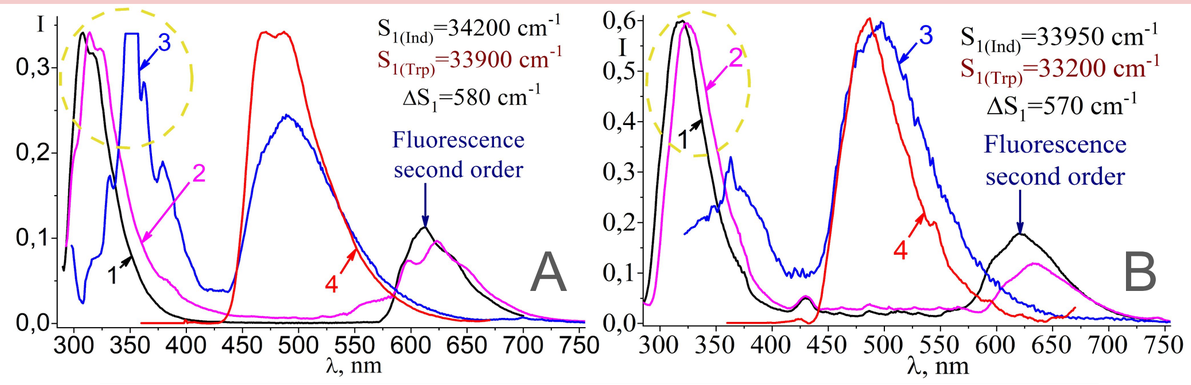
Normalized phosphorescence spectra (T = 78K): 1-Ind, 2-Trp, 3-Try, 4-IQX (solutions in A-ethanol, B-DMSO, C=10⁻⁵M, λ_{exc}(1-3) = 270nm, λ_{exc}(4) = 340nm).

FLUORESCENCE (ROOM TEMPERATURE)



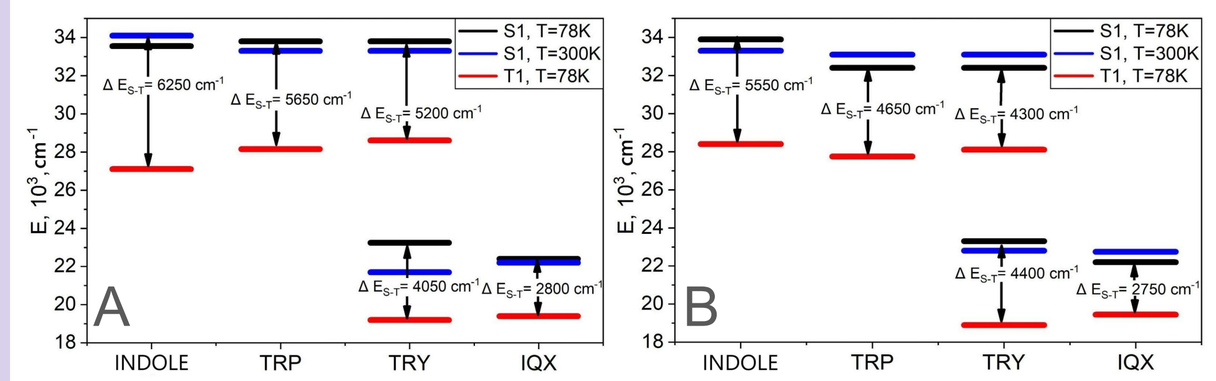
Normalized fluorescence spectrum (room temperature): 1-Ind, 2-Trp, 3-Try, 4-IQX (solutions in A-ethanol, B-DMSO, C=10⁻⁵M, λ_{exc}(1-3) = 270nm, λ_{exc}(4) = 340nm).

FLUORESCENCE (T=78K)



Normalized fluorescence spectrum (T = 78K): 1-Ind, 2-Trp, 3-Try, 4-IQX (solutions in A-ethanol, B-DMSO, C=10⁻⁵M, λ_{exc}(1-3) = 270nm, λ_{exc}(4) = 340nm).

ENERGY LEVELS



The general scheme of S_1 and T_1 energy levels positions of Indole, Tryptophan, Tryptanthrin, and IQX (solutions in A-ethanol, B-DMSO). The diagram shows the data at 78 K (red and dark line) and 300 K (blue line).

CONCLUSIONS

The main centre of optical absorption, fluorescence, and phosphorescence of Trp is the **Indole π-electron system**. The optical absorption spectra of Try and IQX are complex, but they contain a band associated with the absorption of the **Indole π-electron system**. In the fluorescence (at both temperatures) and phosphorescence of Try, two optical centers have been observed, one of them is associated with emission from the **Indole segment** of Try π-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 an emission from the **Indole π-electron system.**

REFERENCES

1. B.Pedro, M.Pineiro, A.J.Burke, Synthesis, 54(19), 4235 (2022).
2. Q.-P.Qin, B.-Q.Zou, F.-L.Hu, G.-B.Huang, S.-L.Wang, Y.-Q.Gu, M.-X.Tan, Med. Chem. Commun., 9, 1639 (2018).
3. V.Yu.Kudrya, T.-Y.Zhang, M.-X.Tan, A.P.Naumenko, J.Luminescence, 266, 120242 (2024).

naz.tkach2001@gmail.com