Spectro-Luminescent Manifestation of Heavy Atoms Effect on π -Electron System of Molecular Complex Based on Tryptanthrin as a Part of New Effective Drug



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INTRODUCTION

Tryptanthrin is a naturally occurring yellow well-known alkaloid, the indologuinazoline π -electron-containing compound. Tryptanthrin and its derivatives possess broad "spectrum" of health-care activities including anti-pathogenic, antibacterial, anticancer and anti-inflammatory due to its unique feature of binding to telomeric G4 DNA and stabilizing it. In particular, complexes based on iodotryptanthrin and bromo-tryptanthrin possess the higher anticancer activity than other tryptanthrin derivatives. The feature of tryptanthrin binding to G4 DNA can be used in nanobiotechnology for the development of new antitumor drugs.

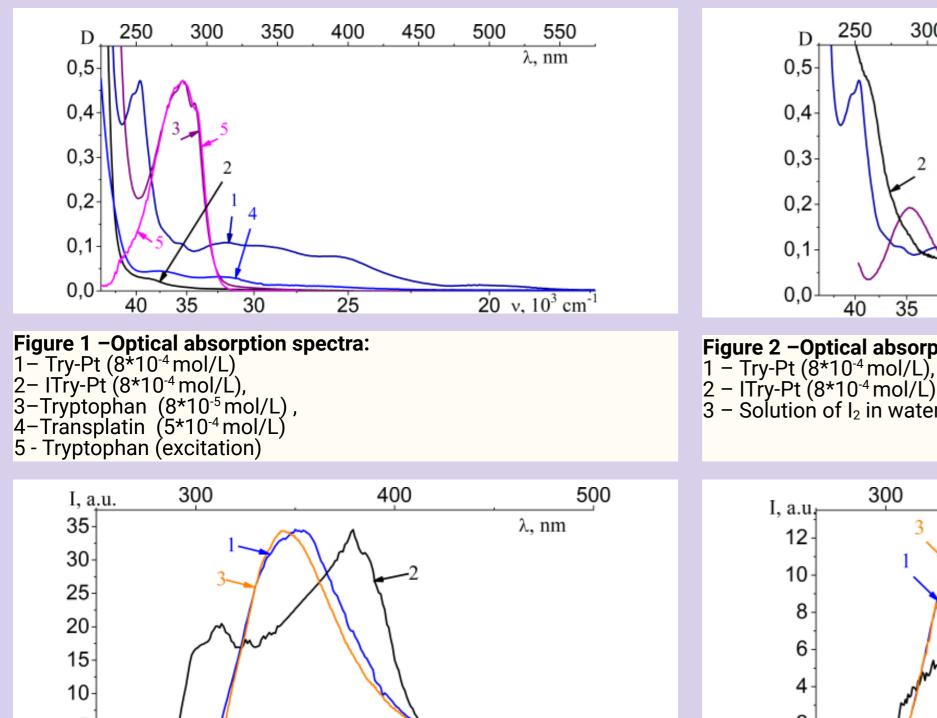
OBJECTIVE

Our study is devoted to the comparative opticsspectral investigations (especially fluorescence and phosphorescence at low temperatures under different excitation wavelengths) of the tryptanthrin-based (Try-Pt) and 8-iodotryptanthrine (ITry-Pt) molecular complexes with platinum formed in different types of solvents, obtaining the position of the first excited electronic levels using optical absorption spectra, fluorescence, and phosphorescence spectra, determination of the effect of iodine in this structure.

METHODS

Optical absorption spectra were recorded on Cary 60 (Agilent) UV-Vis spectrophotometer at room temperature. Fluorescence and phosphorescence spectra (emission and excitation) were recorded on Cary Eclipse (Varian) and Horiba FluoroMax Plus fluorescent spectrophotometers (fluorescence - at room temperature and T=78K, phosphorescence at T=78K). Spectra were excited by Xenon lamp. All measurements carried out using standard quartz cuvettes with 10 mm pathlength. Fluorescence and phosphorescence spectra were corrected for the wavelength response of the system. The excitation wavelengths were chosen using optical absorption spectra maxima. The errors of optical density, fluorescence/ phosphorescence intensities and wavelengths were standard for these equipments.





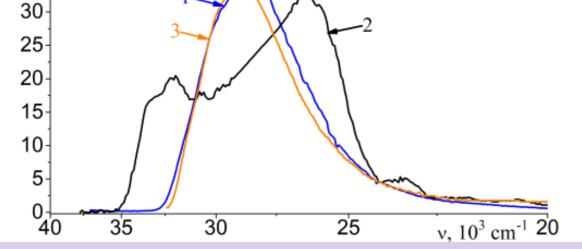
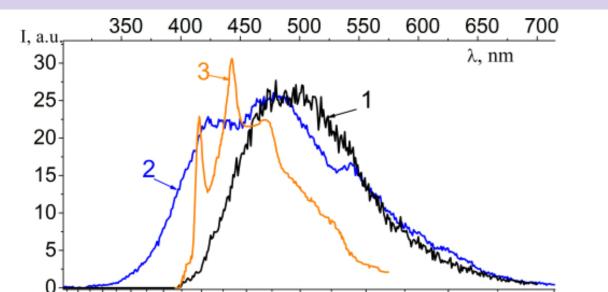


Figure 4 – Fluorescence spectra of complexes with tryptanthrin: 1 – Try-Pt (÷6.37), 2 – IŤry-Pť;

3 – Tryptophan. λ_{excitation}=255 нм. T=78K.



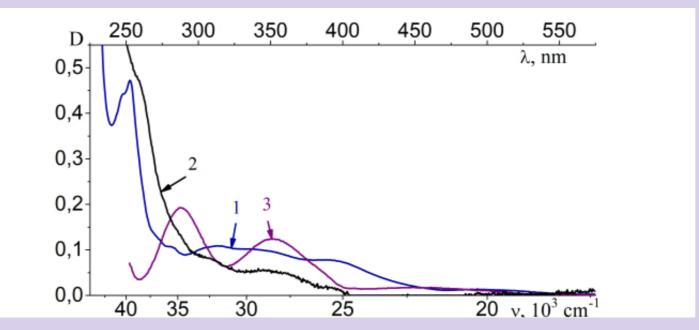
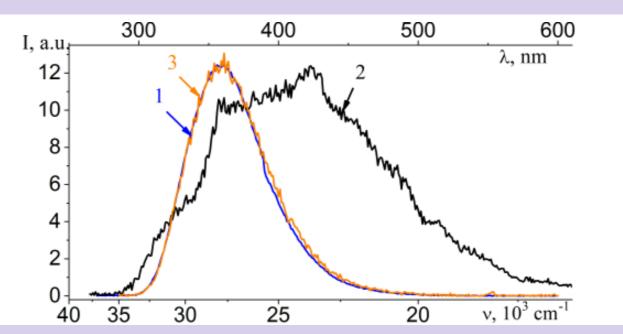
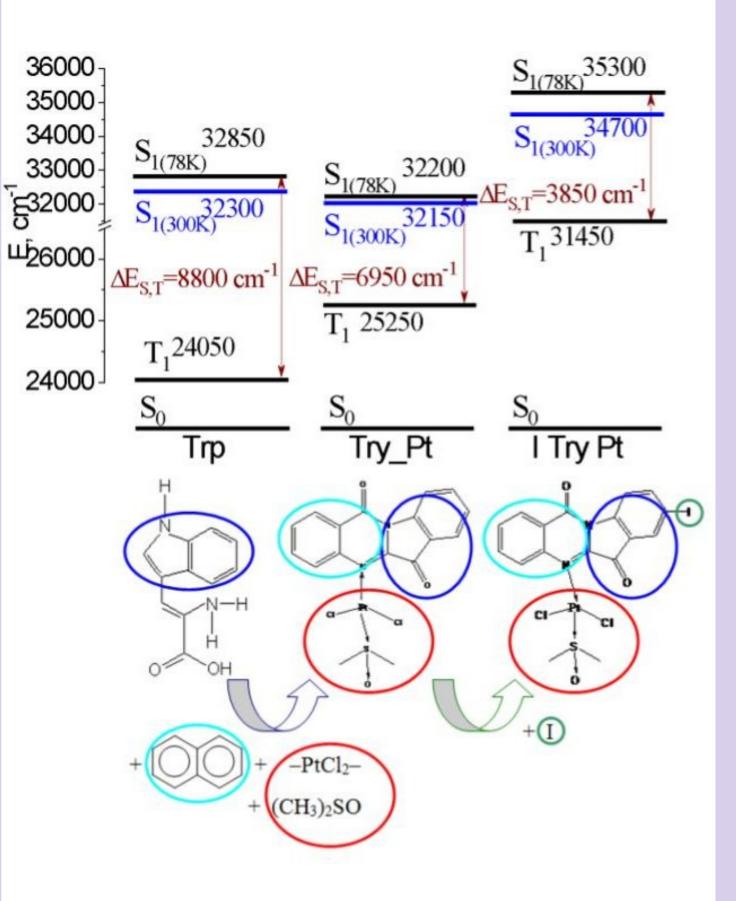


Figure 2 – Optical absorption spectra:

- 2 ITry-Pt (8*10⁻⁴ mol/L) (17 times enlarged);
- 3 Solution of I_2 in water (C=2,5.10⁵ mol/L)



- Figure 3 Fluorescence spectra of complexes with tryptanthrin: 1 – Try-Pt, 2 – IŤry-Pt;
- 3 Tryptophan, λ_{excittion}=255 нм. Т=300К.



3230 28 26 24 22 20 18 $16 v, 10^3 cm^{-1} 14$

Figure 5 – Phosphorescence spectra of complexes with tryptanthrin: 1 – Try-Pt(÷1.75), 2 – ITry-Pt; 3 – Tryptophan. T=78K.

Figure 6 Energy diagram of the position of the first excited electronic levels S₁ and T₁ of Try-Pt, ITry-Pt and tryptophan (Trp)

CONCLUSION

1. The existence of two optical absorption centers in the Try-Pt molecule has confirmed.

2. Blue shift and a decrease in the value of the optical density of the short-wave bands (related with the absorption of the π -electron system) of the optical absorption spectrum of ITry-Pt in comparison with the corresponding spectrum of Try-Pt, as well as the appearance of new bands with maxima at wavelengths of 288 and 350 nm (related with the iodine atom absorption) is a spectral manifestation in the optical absorption of the influence of the iodine atom on the π -electron system of tryptanthrin.

3. A significant decrease in the fluorescence intensity of ITry-Pt (~25 times) in relation to the corresponding fluorescence intensity of Try-Pt and a blue shift of the short-wavelength edge of the fluorescence spectrum of ITry-Pt relative to the corresponding spectrum of Try-Pt is a fluorescent manifestation of the known influence effect of a "heavy atom" of iodine on the π -electron system of tryptanthrin.

4. An increase in the ratio of phosphorescence intensity to fluorescence intensity when an iodine atom is attached to the π -electron system and a blue shift of the short-wavelength edge of the phosphorescence spectrum of the ITry-Pt complex comparing to the short-wavelength edge of the corresponding Try-Pt spectrum (as a result of a decrease in the energy) difference between the singlet (S) and triplet (T) levels and an increase in the probability of the S-T transition) is a phosphorescent manifestation of the effect of the iodine atom on the π -electron system of tryptanthrin.