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## **RESEARCH AREA**

The determinant role of the weak molecular interactions in the transport of bioactive molecules is associated either to their moderated adsorption onto the macromolecule's surface or also to the solubility of bioactive molecules moderated by the formation of inclusion complexes. The latter process offers too the selective and sensitive detection of bioactive molecules. Further the stereo-chemical and structural facts, the weak molecular interactions and the resulted chemical equilibria are also affected by the temperature and the molecular environment. During the last few years we described the effect of the bulk properties of the molecular environment onto the stabilities of the above mentioned inclusion complexes and also the effect of the solvent water structures have been investigated accordingly in our lab. Some cases the antioxidant, scavenging effect has been investigated regarding to the target-specific therapeutic applications. Our overall goal is to perform investigations to determine the effect of the molecular packing in the stability of drugs, to clarify the role of micro-solvation and to describe the related overall mechanisms.

## **TECHNIQUES AVAILABLE IN THE LAB**

Investigation (measurement and data-evaluation) of weak molecular interactions by fluorescence (steady-state, anisotropy, lifetime, anisotropy decay, solvent-relaxation) methods. Protein dynamics by scanning and isotherm calorimetry. Vibrational analysis by Raman-spectroscopy, surface and tip-enhanced Raman spectroscopy. Theoretical molecular modelling by the HyperChem and Gaussian codes using personal and supercomputers.

## **SELECTED PUBLICATIONS**

Preisz, Zs., Kunsági-Máté, S. (2021) Effect of methotrexate and its photodegradation products on the temperature induced denaturation of human serum albumin. Spectrochim Acta A 245:118898.

Kovács, F., Yan, H., Li, H., **Kunsági-Máté, S.** (2021) Temperature-Induced Change of Water Structure in Aqueous Solutions of Some Kosmotropic and Chaotropic Salts. **Int J Mol Sci 22:** 12896.

Preisz, Zs., Hartvig, N., Bognár, B., Kálai, T., **Kunsági-Máté**, **S.** (2021) Comparative EPR Study on the Scavenging Effect of Methotrexate with the Isomers of Its Photoswitchable Derivative. **Pharmaceuticals 14:** 665.

Preisz, Zs., Nagymihály, Z., Lemli, B., Kollár, L., **Kunsági-Máté, S.** (2020) Weak interaction of the antimetabolite drug methotrexate with a cavitand derivative. **Int J Mol Sci 21:** 4345.

Kovács, F., **Kunsági-Máté, S.** (2020) Change of liquid water structure under the presence of phosphate anion during changing its kosmotropic character to chaotropic along its deprotonation route. **Chem Phys Lett 756:** 137827.