EFFECT OF INFRARED LIGHT ON PROTEIN INTERFACIAL WATER. CONSEQUENCES FOR PROTEIN SELF-ASSEMBLY AND PROTEIN-SURFACE INTERACTION.

[1, 2] M. Kowacz, [2] M. Marchel[b], [3] L. Juknaité, [2] J. M. S. S. Esperança, [3] M. J. Romão, [3] A. L. Carvalho, [2] L. P. N. Rebelo, [1] P. Warszyński

[1] Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, Niezapominajek 8, 30-239 Krakow, Poland; [2] Instituto de Tecnologia Química e Biológica António Xavier, Universidade Nova de Lisboa, Av. da República, 2780-157 Oeiras, Portugal; [3] UCIBIO - REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal; e-mail: nckowacz@cyf-kr.edu.pl

We demonstrate that a physical trigger, a non-ionizing infrared (IR) radiation at wavelengths strongly absorbed by liquid water, can be used to induce and kinetically control protein self-assembly in solution [1] and to modulate protein-surface interactions.

We measured FTIR spectra of aqueous solutions of proteins exposed to infrared radiation (emitted by light emitting diodes) and we observed increased correlation of protein interfacial water molecules. In order to verify the effect of this enhanced ordering of interfacial water on protein crystallization, we have subjected our crystallization drops to IR radiation. As the result we could induce crystal nucleation at protein concentration much lower than that needed to obtain crystals under control conditions. Furthermore, we were able to prevent non-specific protein aggregation (a process involved in many disease conditions) and to favor periodic self-assembly in IR-irradiated samples. We have also performed experiments on the effect of IR-exposure on protein adsorption at silica nanoparticles. For highly charged proteins, hydrophilicity of protein-decorated solids (expressed by changes in sediment volume in aqueous solution) would increase in response to IR. This is consistent with suggested IR-induced enhanced hydration of proteins. However, for proteins with larger fraction of solvent-exposed apolar surface, IR radiation would result in reduced hydrophilicity of the solid with adsorbed proteins (more compact sediment in aqueous solution). This effect can be interpreted as a result of the IR-enhanced hydration of ions that would make them less prone to adsorb at the protein surface and thus, would attenuate their effect on reduction of protein-water interfacial tension.

Owing to many important implications of the protein hydration, the IR radiation can be explored as a new tool to control bio-inspired processes. For example, it has been shown that protein physiological activity is inherently bound to its ability to induce structuring of adjacent water layers and that functional motions of proteins are associated with breaking and subsequent restoration of this water structure. On the other hand, protein ability to fold (for many proteins necessary to perform their function) is recognized to depend on entropy gain on dehydration of hydrophobic compartments. Our results suggests that both hydration of polar regions and dehydration of apolar ones can be influenced by the remote physical trigger - the infrared radiation.

This work was finantially supported by National Science Centre trough grant FUGA number DEC-2015/16/S/ST4/00465

[1] M. Kowacz et al. *J. Crystal Growth* 2016, doi:10.1016/j.jcrysgro.2016.01.003