Research at the edge of interfacial bionanoscience and quantum biophysics: New perspectives for tuning of the stability and electron transfer patterns of globular proteins

<u>D.E. Khoshtariya</u>, M. Makharadze, T. Dolidze, M. Shushanyan, S. Uchaneishvili, T. Tretyakova, N. Shengelia, T. Partskhaladze, D. Waldeck, R. van Eldik dimitri.khoshtariya@tsu.ge

Institute for Biophysics and Bionanoscience, Department of Physics, I. Javakhishvili Tbilisi State University, Tbilisi, Chavchavadze Ave. 1

Department of Biophysics, I. Beritashvili Center of Experimental Biomedicine, Tbilisi Department of Chemistry and Biochemistry, University of Pittsburgh, Pennsylvania, USA Department of Chemistry and Pharmacy, University of Erlangen, Germany

The year of 2013 turned to be culminating in the research history of our faculty-based institution. There were summarized, analyzed and published fundamental results of essentially interdisciplinary character obtained during the previous years and in 2013, as well. In particular, we would like to mention the following outcome:

(a) We accomplished theoretical analysis of experimental results of the previous two years encompassing the electron-transfer mechanisms for a redox-active metalloenzyme azurin (Az), integrated within the "sandwich-like" interfacial nanodevices, in addition placed in contact with a glassy substance: hydrated protic ionic melt of choline dihydrogenphosphate ([ch][dhp]). The final results were published as an extended article [1].

(b) For another redox-active protein, myoglobin (Mb), integrated into a nanodevice that was analogous to the abovementioned one, the experimental studies of electron transfer patterns were performed within 2012-2013, and respective in-depth theoretical analysis was accomplished in 2013 as well. In contrast to other cases studied before by other authors, for extremely tightly immobilized Mb (the unique case that was disclosed in our studies) our analysis revealed rather restricted reorganization of "coupled" water molecule (instead of long-range diffusional translocation), in overall, leading to an essential acceleration of the electron transfer rate. The final results were published as an extended article [2].

(c) It has also been accomplished the analysis of results for an impact of the additive substance – dimethyl sulfoxide (DMSO) on the characteristics of functional activity and thermal stability for the protein that is well-known for its quantum catalytic mechanism, α -chymotrypsin (α -CT). It has conclusively been established the dualistic nature of the DMSO impact on α -CT The final results were also published as an extended article [3].

(d) In 2013 we have explored an impact of the added [ch][dhp] on athermal stability of the same protein - α -CT. What was discloses is a dramatic stabilizing effect of the protic ionic melt component: the 10 °C stabilization at 3 M [ch][dhp], the effect that seems very interesting from the standpoint of bionanotechnological developments. Respective paper currently is in preparation [4].

(e) The next paper which is in preparation, considers the proposed mechanism for an electron exchange between the Au-electrode and head groups of cystein that is self-assembled on this platform. This issue was studied jointly with the University of Erlangen during 2013 [5].

References:

D.E. Khoshtariya et al., <u>Phys. Chem. Chem. Phys.</u> 2013, *15*, 16515-16526; [2] D.E. Khoshtariya et al., <u>J. Phys. Chem. B</u>, 2014, *118*, 692-706; [3] T. Tretyakova et al. <u>Biophys. Chem.</u>, 2013, *175/176*, 17-27; [4] M. Makharadze et al., <u>Biophys. Chem.</u>, 2014, To be published; [5] T.D. Dolidze et al., <u>Biotechnol. Bioengin</u>, 2014, To be published.