## The Prospects of Aquaphotomics in Biomedical Science and Engineering

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**Introduction:** Newly developed scientific discipline Aquaphotomics [1], which is based on near infrared spectroscopy (NIRS) introduced water near infrared spectra as a valuable source of information on aqueous systems, most importantly biological [2]. Giving the rapid growth of this discipline and better understanding of the role of water in biological systems, we can expect in the years to come major developments and applications of Aquaphotomics within the following three areas: 1) Characterization of biomaterials, 2) Biomedical measurements and monitoring and 3) Early diagnosis and screening.

**Soft contact lenses characterization:** Hydrogels are commonly used for the manufacture of soft contact lenses, but they have numerous other applications in biomedicine. The functionality of hydrogels strongly depend on the water content and water-transporting ability, therefore they seem as ideal candidates for Aquaphotomics studies.

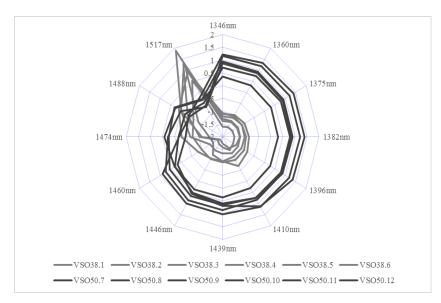


Figure 1. Aquagrams of the contact lenses calculated at selected wavelengths. The averaged spectra of lenses across all experiments show differences in water spectral pattern for different hydrogel materials VSO38 (nominal water content 38%) and VSO50 (nominal water content 48%) [3]

Our findings about the state of water in soft contact lenses with low and medium water content (Figure 1) [3] is in agreement with the scientific literature that water in lenses exists in generally three states: strongly bound, loosely bound and free water [4], but our subsequent study on new and worn (spoiled) contact lenses [5] provided further clarification on the roles of different water types – strongly bound water (absorbing at 1517nm) provides stability of the polymer network while other types are involved in the transport (especially oxygen) and hydration of other solutes such as proteins on the surface of worn lenses.

**Improving Dialysis Efficacy through Monitoring of Spent Dialysate:** The NIRS method has already been proposed to measure urea in spent dialysate, the most commonly used representative marker for accumulated waste solutes, in dialysis patients, since urea absorbs in this region [6]. Our proposition is not to monitor urea removal, or other waste materials in spent dialysate, but to monitor water cleanliness. In a pilot study we collected spent dialysate of 18 patients during 3 sessions of haemodialysis after 5min, 45min, 90min and 135min of treatment. The NIR absorbance spectra of dialysate samples were acquired and studied using multivariate analysis and Aquaphotomics approach. Our results (Figure 2) showed that the absorbance spectra of spent dialysate could be classified well according to the duration of therapy even by monitoring just absorbance of water at 1410nm (free water molecules [1]).

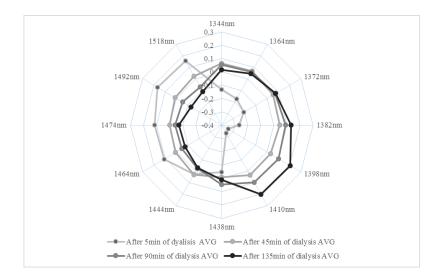


Figure 2. Averaged aquagrams of spent dialysate for all patients after 5min, 45min, 90min and 135min of haemodialysis treatment

Continuous measurement using online monitoring devices could provide new tools for more efficient dialysis treatment [5].

**Early screening of colorectal cancer:** Current improvement strategies in cancer screening and diagnostic based on body fluids are focused on searching for better biomarkers or improving levels of detection. Again, our approach is opposite to the current trend - why not focus on cumulative effects of all biomarkers of disease on biological water – in that case an absorption spectra of water could be used as a biomarker of disease [2]. In an ongoing pilot study which so far included 70 patients - 33 with benign colon lesions and 37 with confirmed malignant lesions, we performed acquisition of near infrared spectra of urine and serum samples. Various preprocessing and analytic approaches were utilized in the analysis of serum and urine absorbance spectral data. Developed PLS-DA models were assessed based on the criteria generally used for assessing the preliminary NIR models. Both NIR models could discriminate between sera and urine from patients with benign and those with malignant lesions indicating the usefulness of the method for the colon cancer screening ( $\mathbb{R}^2 > 0.70$ ). Our results show better accuracy of discrimination for serum spectral model (86,63%) comparing to urine spectral model (overall accuracy 78,48%).

## **Future directions:**

Translation of these progresses into clinical outcomes improvements will take time. In the talk, the three examples of utilization of Aquaphotomics in biomedicine will be presented and more elaborated.

## **References:**

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