Near infrared spectroscopy and aquaphotomics – a possible tool for cancer diagnostics?

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Introduction

Late cancer diagnosis is one of the causes of high mortality rate. Biopsy and histopathology, being a gold standard in cancer diagnosis, are complex, invasive and expensive. The development of new low-cost and rapid methods for mass screening of patients and early cancer diagnosis is an urgent need in modern medicine. The detection of compositional changes in a patient's biological fluids (blood and urine) caused by cancer distribution is a perspective direction of the research in this field [1].

Optical spectroscopy has great potential in cancer diagnostics. Using fiber optic probes in cost-effective NIR region is a very powerful and flexible method for non-invasive *in vivo* and *in vitro* diagnostics [2-3]. NIR-spectra of biological fluids presumably contain information about the molecular changes in the normal and abnormal conditions of the cells and the patient's condition. Therefore, they can be used to predict the response to a particular treatment protocol [4]. However, NIR spectroscopy has not been yet widely used in clinical practice because of the lack of a unified strategy for spectral data analysis.

Intensive water absorption in the 700–1900 nm region usually complicates the analysis of the obtained data and reduces their informative value. Nevertheless, water absorption bands themselves contain information about different conformations of water molecules in cells. Water molecules form hydrogen bonds between each other and with their surroundings, which makes water absorption bands very sensitive to the sample composition [5].

In the present work, aquaphotomics combined with multivariate data analysis was used to study NIR spectra of plasma and serum of blood and urine, obtained from patients before and after cancer surgery. The difference in the water molecular structure in body fluids before and after surgery was investigated.

Materials and Methods

The biological body fluids (urine, plasma and serum) were collected from 14 patients before and after different cancer surgeries at the Charité—Universitätsmedizin Berlin (Germany). NIR measurements were performed in the region 900–1700 nm using a portable fibre-optic NIRQuest512 spectrometer (Ocean Optics, Inc., Orlando, FL, USA). Principal component analysis (PCA) was used to describe the basic multidimensional characteristics of the NIR data matrix. PCA-loadings were analyzed in order to find the characteristic water bands and water matrix coordinates (WAMACs), showing changes in biological fluids before and after surgery.

Results

The mean spectrum of samples before surgery was subtracted from the samples after surgery and the difference is plotted (Fig. 1) to show the highest spectral variation between them. It is clearly seen that spectral shape for all of the fluids is very similar. Subtracted peaks with assignments are presented in Table 1.

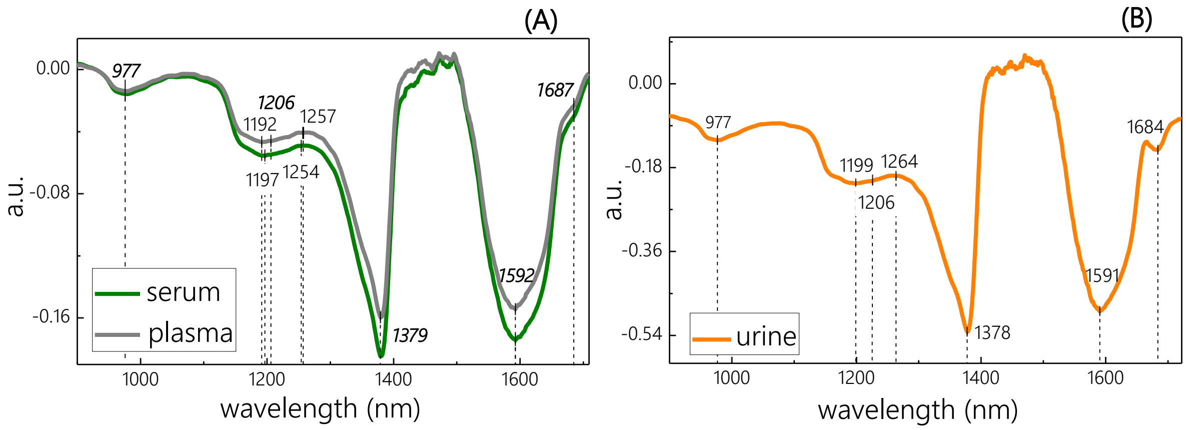

Fig. 1. Subtracted average spectra of samples before and after surgery for (A) – serum, plasma, and (B) – urine.

Table 1. Assignment of the characteristic water absorbance bands.

Urine, nm	Plasma, nm	Serum, nm	Assignment
977	977	977	**976** nm - bulk water, strong correlation with water activity
1199	1192	1196	**1194.67** nm - $H+(H_2O)_4$, 2nd overt. 2nd overtone Superoxide Tetrahydrate O_2-.$(H_2O)_3$
1205	1206	1206	**1210.3** nm - 2nd overtone IHB stretch (OH-$(H_2O)_3$)
1264	1257	1254	**1250.8** nm '-OH strech in fully hydrated hydronium, 2nd overt. **1268** nm - 'singlet oxygen
1378	1379	1379	**1379** nm - H_2O - v_1+v_3
1591	1592	1592	**1590.8** nm - aqueous proton $[H+\cdot(H_2O)_6]$ - H_2O in H_5O_2+ asymmetric stretch, 1st overt.
1684	1687	1687	**1682.9** nm - aqueous proton $[H+\cdot(H_2O)_5]$ - H_3O+ symmetric stretch, 1st overt.

PCA was also performed and provided further insights which will be presented.

Aknowledgment

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