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Decomposition of in vivo skin Raman spectra using multivariate curve resolution method

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Motivation

It is known that during the development of the disease, metabolic changes in the patient's body occur, which leads to changes in the biochemical composition of biological tissues and fluids. In recent years, Raman spectroscopy has been increasingly used to investigate these changes. However, Raman spectra of most biological tissue components overlap significantly, and it is difficult to separate individual components from the analysed Raman spectrum. Besides, most methods for analysing Raman spectra have an impossibility of physical interpretation of the components. The aim of our study is to investigate the possibilities of the multivariate curve resolution method [1] for the analysis of *in vivo* skin Raman spectra using a portable pectroscopy setup [2].

Raman spectra of skin

We used 1000 Raman spectra: 540 of normal skin (NS), 113 of keratosis (K), 122 of basal cell carcinoma (BCC), 67 of malignant melanoma (MM), and 158 of pigmented nevus (PN). *In vivo* Raman spectra of skin are recorded using a portable spectroscopic setup (see Fig.1) [2]. The spectra were cut in the range from 860 to 920 nm that corresponds to 1114-1874 cm-1. Then the spectra were preprocessed with baseline removal and smoothing by the Savitzky-Golay method [3].

Fig.1. Portable spectroscopic setup

MCR-ALS analysis

For unmixing spectra by Multivariate Curve Resolution–Alternating Least Squares (MCR-ALS) analysis we used a protocol by *Felten et al.* [4].
The main idea of MCR-ALS is to decompose the Raman spectra matrix D into smaller matrices C and ST (see Fig.2), where C represents the concentration profiles for each of the skin component, and ST is the matrix of Raman spectra of the components.
After initial estimation is given for C, it is optimized iteratively using an alternative least squares algorithm (ALS) until convergence is reached.

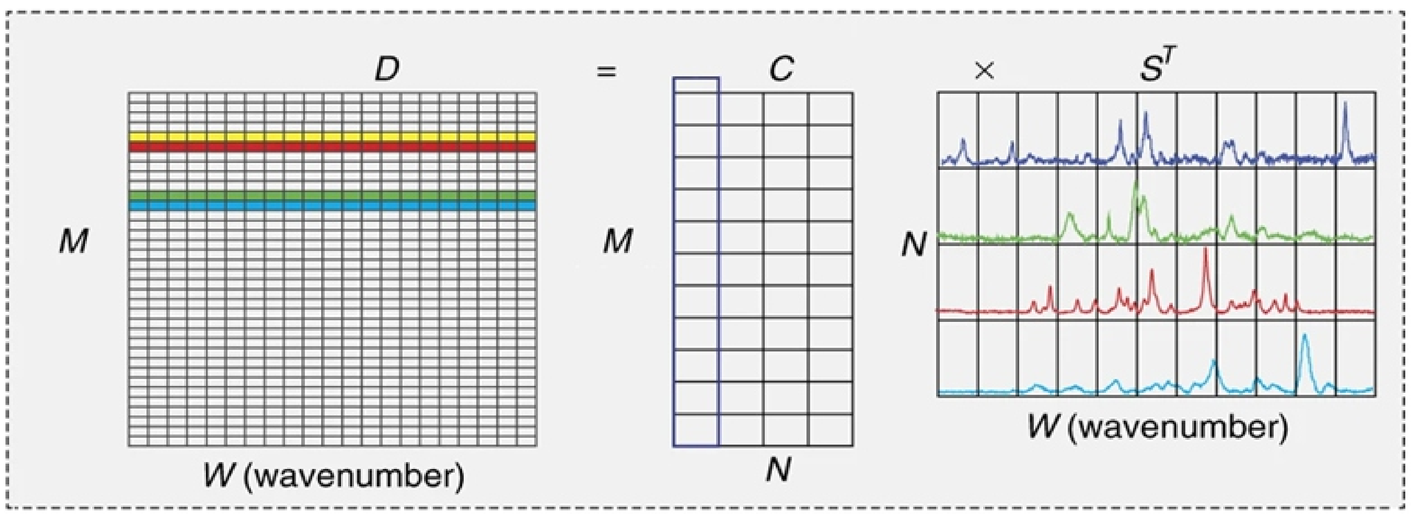

Fig.2. Illustration of the MCR-ALS method

Results

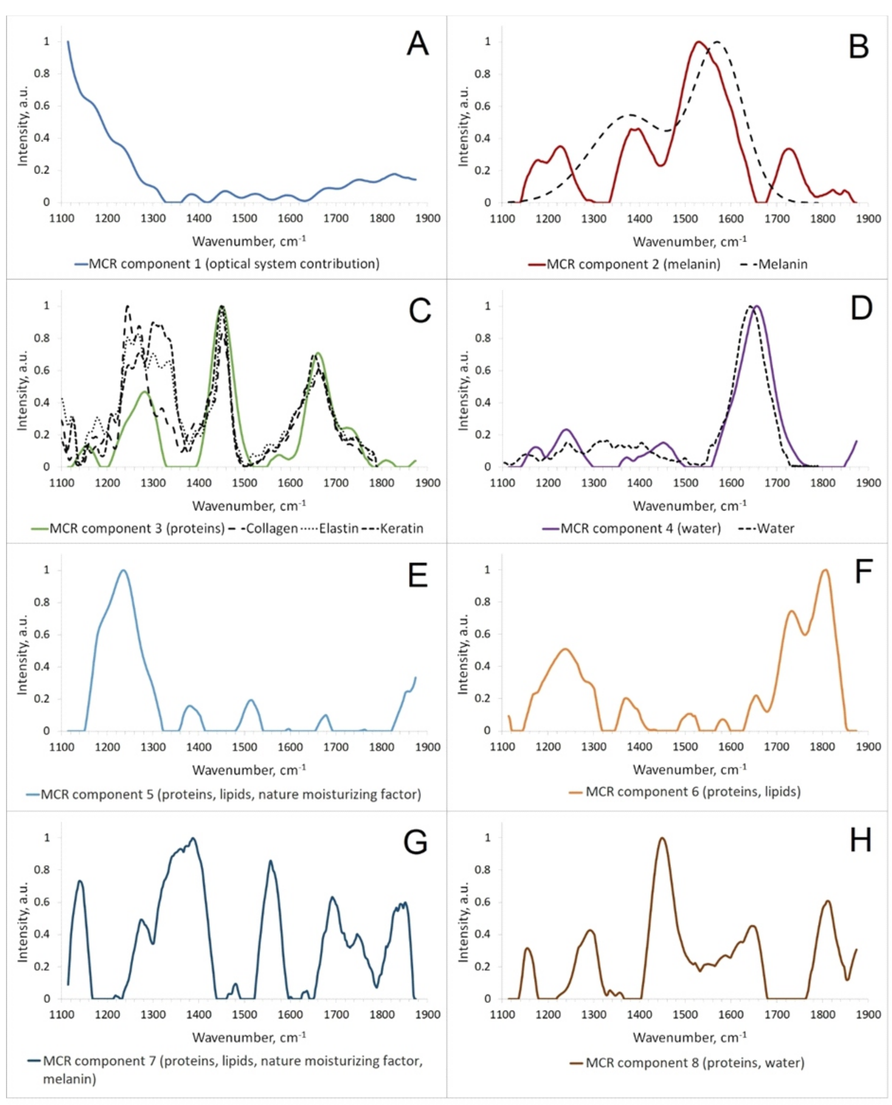

Fig.3. Raman spectra obtained by MCR-ALS analysis of in vivo Raman spectra of skin (solid lines – spectra obtained in our study, dashed lines – obtained in [6])

The component 1 (Fig. 3, A) corresponds to the contribution of the optical system [5]. In the spectrum of the component 2 (Fig. 3, B), the peaks at 1390 and 1520 cm-1 correspond to melanin [5, 6]. In the spectrum of the component 3 (Fig. 3, C), the peak at 1280 cm-1 is amide III, at 1450 cm-1 – is keratin, collagen and elastin, at 1660 cm-1 – is collagen [6]. In the spectrum of component 4 (Fig. 3, D), the most intense peak at 1650 cm-1 corresponds to water [6].The spectrum of the component 5 (Fig. 3, E) may correspond to the contribution of lipids and natural moisturizing factor [5, 6]. Besides, in the spectra of components 5 and 6 (Fig. 3, E, F) we can see an intense peak at 1240 cm-1 of proteins. The spectrum of the component 6 (Fig. 3, F) may also correspond to the contribution of lipids [6]. In the spectrum of the component 7 (Fig. 3, G), we can note peaks of natural moisturizing factor, lipids, melanin, and collagen [5, 6]. In the spectrum of the component 8 (Fig. 3, H) one can see intense peaks at 1450 and 1650 cm-1, which is contribution of proteins and water.
Further, we applied logistic regression for two cases (see Fig. 4). In the case of malignant (MM, BCC; n = 189) vs benign (K, PN; n = 271) neoplasms classification, ROC AUC is 0.698 (0.650–0.746, 95% CI), and in the case of MM (n = 67) vs pigmented neoplasms (n = 271) classification, ROC AUC is 0.702 (0.629–0.776, 95% CI).

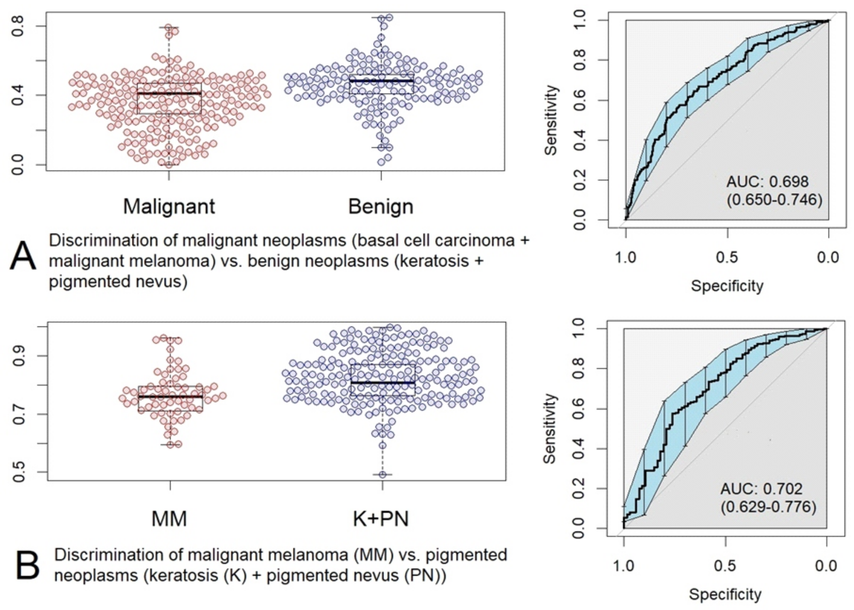

Fig.4. Box-plots and ROC-curves of predicted values of logistic regression: A – malignant (BCC + MM) vs benign (K + PN), B – MM vs pigmented (K + PN)

Conclusion

The obtained results show that the multivariate curve resolution analysis can provide new information about the biochemical profiles of the skin tissues. Such information may be used in medical diagnostics and screening of the population for the analysis of Raman spectra with a low signal-to-noise ratio.

Acknowledgements

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See References