



On the use of NIR Spectroscopy Coupled to Chemometrics for Relative Dating of Human Fossil Bones

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Abstract

The possibility of using near infrared spectroscopy (NIR) coupled to chemometric exploratory data processing in order to obtain a fast, cheap and non-destructive dating of human fossil bones is presented and discussed. The proposed approach has been applied to the differentiation of human fossil bones from two necropolises in the Middle Nile (Saggai and Geili).

Principal component analysis of the spectral data after suitable pretreatment (standard normal variate + first derivative) allowed to evidence cluster of bones corresponding to the different antiquity of the samples, thus indicating that the proposed approach can lead to an accurate (although relative) dating of the fossil samples.

Analysis of the PCA loading suggested that the spectral region which are most relevant for the observed differentiation are 5000–5700 cm⁻¹ and 7000–7500 cm⁻¹.

Introduction

The dating of fossil remains, in particular, human bones, is of capital importance not only for the correct attribution of the sample, per se, but also as the characterization of different antiquity of the specimens found in tombs or necropolises can be coupled with additional palaeontological information to provide insight social and cultural evolution, population migrations, habits and lifestyle [1]. In this framework, it has to be stressed that the "traditional" approaches for dating fossils (and, in particular, bones) suffer from many drawbacks: they are often rather cumbersome, requiring extensive pretreatment of the sample (hence, being destructive), they involve long/time-consuming analytical procedures, and they are rather expensive – just to cite the main ones [2]. Based on this considerations, in the last years we have proposed different approaches based on coupling chemometric exploratory data analysis to thermal analysis which allowed a reliable relative dating of fossil bone samples in a rapid and relatively economic fashion [3-5]. However, this approach was still (micro-)destructive. Accordingly, in the present communication the possibility of using a rapid, cheap and non-invasive/non-destructive technique, namely near infrared (NIR) spectroscopy, coupled with chemometric processing of the recorded spectra, in order to achieve a relative dating of fossil bone samples is addressed. The approach has been applied to characterize human fossil bone samples from the Middle Nile.

Materials & Methods

Samples. All fossil bone samples come from skeletons unburied from the Saggai and Geili necropolises (Sudan). In particular, NIR analysis was conducted on femur and humerus fragments belonging to 6 different skeletons (two from the Mesolithic, two from the Meroitic and two from the Christian periods).

NIR analysis. NIR analysis was carried out on a Thermo Nicolet FT-NIR 6700 spectrometer, equipped with an integrating sphere and an InGaAs detector (Thermo Scientific, Walton, MA). The

spectra were acquired at a nominal resolution of 4 cm^{-1} in the range $4000\text{--}10000\text{ cm}^{-1}$, averaging 82 scans; at least three replicate measurements were carried out on each fossil bone samples after changing its orientation on the sampling hole of the sphere. Prior to the chemometric analysis, the spectra were pretreated by SNV, first derivative (2nd order polynomial, 15 points window) and mean centering.

Results

The pretreated NIR spectral data were analysed by Principal component analysis in order to verify whether this approach could provide a differentiation based on the different antiquity of the samples, irrespectively of the specific bone fragment used in the analysis. Figure 1 shows the scores of the different samples onto the first three principal components extracted.

The scores plot reported in Fig. 1 shows a clear separation among the samples from the three different epochs. In particular, the most ancient samples (the Mesolithic samples from Saggai) are well separated from the other four skeletons, already on PC1. On the other hand, PC2 and PC3 contribute to the separation of the Meroitic from the Christian samples.

Inspection of the plot reported in Fig.1 shows also how it is possible to observe sub-clustering related to the different skeletons.

Inspection of the loadings provides the support for interpreting the observed different in terms of spectral regions contributing the most: it was found that the most relevant bands to account for the observed differentiation are $5000\text{--}5700\text{ cm}^{-1}$ and $7000\text{--}7500\text{ cm}^{-1}$.

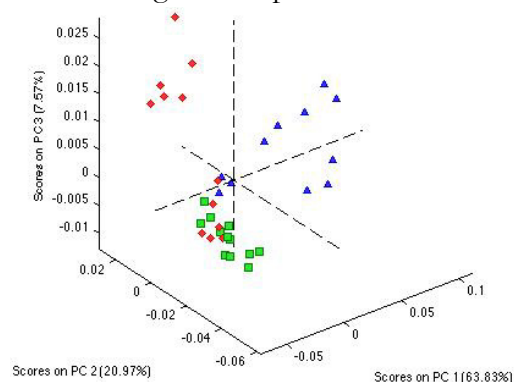


Fig. 1; PCA on NIR data: scores plot. Legend: blue – Mesolithic (Saggai), green – Meroitic (Geili), red – Christian (Geili)

Conclusions

The result show that the proposed approach, i.e. coupling NIR spectroscopy to chemometric data processing, is absolutely promising in the light of achieving a rapid, fast and non-destructive dating (although only a relative one) of human fossil bone samples. This approach is generally applicable and it can be easily extended to the analysis of other fossil samples and to a wider range of specimens in general.

References

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