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FTIR Spectroscopy for the Differentiation of Nanosized Calcium Phosphates

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Infra-red spectroscopy is an invaluable method. Different Fourier transform infrared spectroscopy (FTIR) sampling methods are commonly used to identify functional groups in calcium phosphates [1]. This study compares four different FTIR characterization methods: cantilever-enhanced PAS, DRIFT, ATR, and transmission. An analysis of the spectra will be conducted by multivariate statistics (Principal component analysis (PCA), Pearson product-moment correlation coefficient (PPMCC) and Cluster Analysis (CA)) [2].

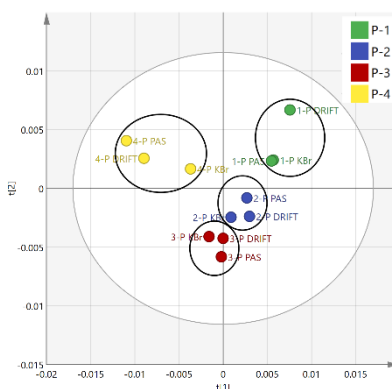


Fig. 1. PCA of FTIR spectra with different level of crystallinity

Using statistical methods, we found: 1. The importance of spectral analysis: normalization, baseline correction, Fourier self-deconvolution, selection of spectral regions; 2. A crystallinity degree of calcium phosphate affects the shape of FTIR spectra, independently from FTIR sampling method, what is proofed by PCA and shown by PCA biplot (Fig. 1).

Keywords: FTIR, PAS, DRIFT, nanosized calcium phosphate, Multivariate statistics.

References:

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2. D. Naumann et al., in *Modern Techniques for Rapid Microbiological Analysis* (Eds.) 43–96 (1991).