# Application of chemometrics in differentiation of synthesized and natural calcium phosphate

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## INTRODUCTION

Modern science has proven possibility to design and synthesize bone or tissue-like materials by imitating nature. These smart materials can be used to develop innovative third -generation biomaterials.

Research is based on Fourier transform infrared (FTIR) spectroscopy investigation of bone like apatites in conjunction with chemometric analyses. Combination of FTIR methods and chemometrics was used to investigate particle size of material and to evaluate the surface of amorphous calcium phosphate. Pearson Correlation Coefficients (PKK), Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA) were used in this work.

## AIMS OF WORK

To develop, assess and analyse the statistical model of the main components (PCA), which allows to evaluate the degree of crystallinity and particle size of unknown calcium phosphate.

## METHODS

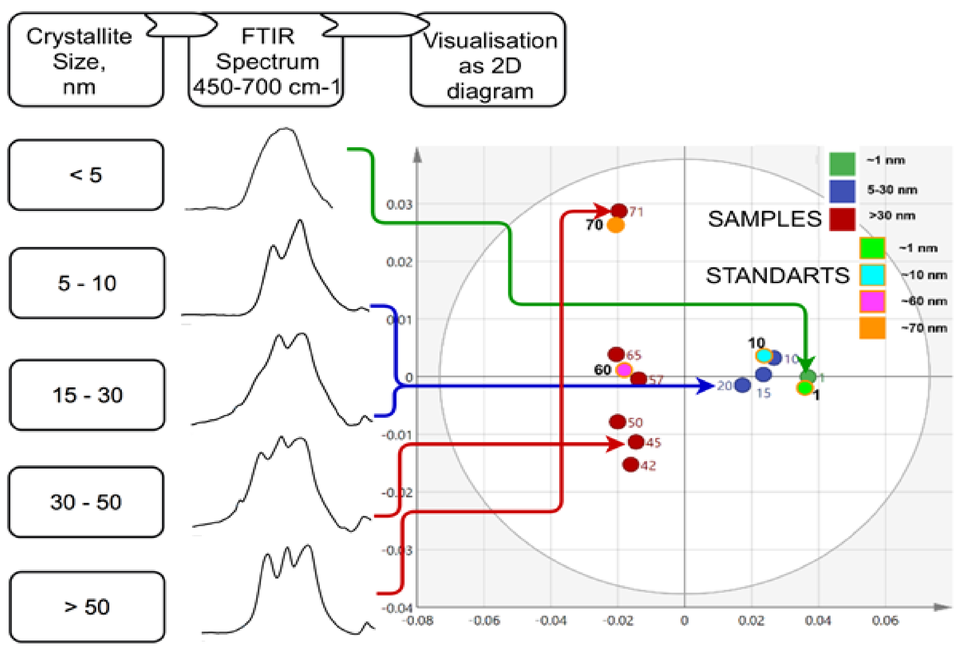
Chemometrics. *SIMCA 14 software* — the Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA) was performed by using Savitzky—Golay and 2nd derivative filter. For the HCA, Ward's algorithm was used.

Vibrational spectroscopy. FTIR PAS and DRIFT (PerkinElmer Spectrum One) 450– 4000 $cm^{-1}$, resolution of 4 $cm^{-1}$, average made from 10 scans.

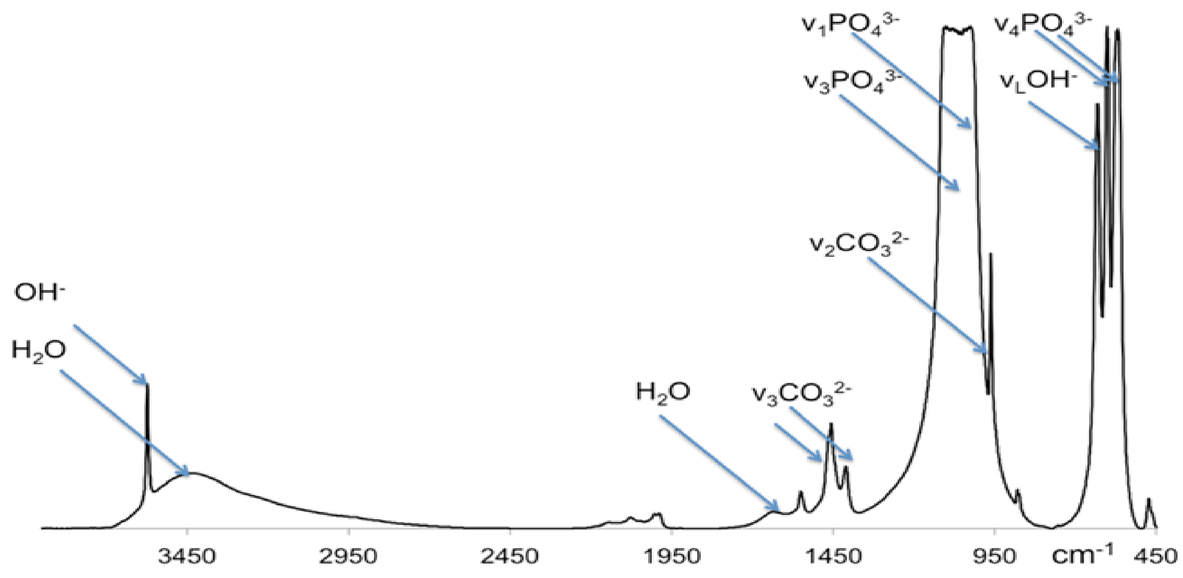
Spectral pre-processing. *SpectraGryph 1.2.14*— spectra viewing, smoothing, baseline correction, and normalization.

## RESULTS

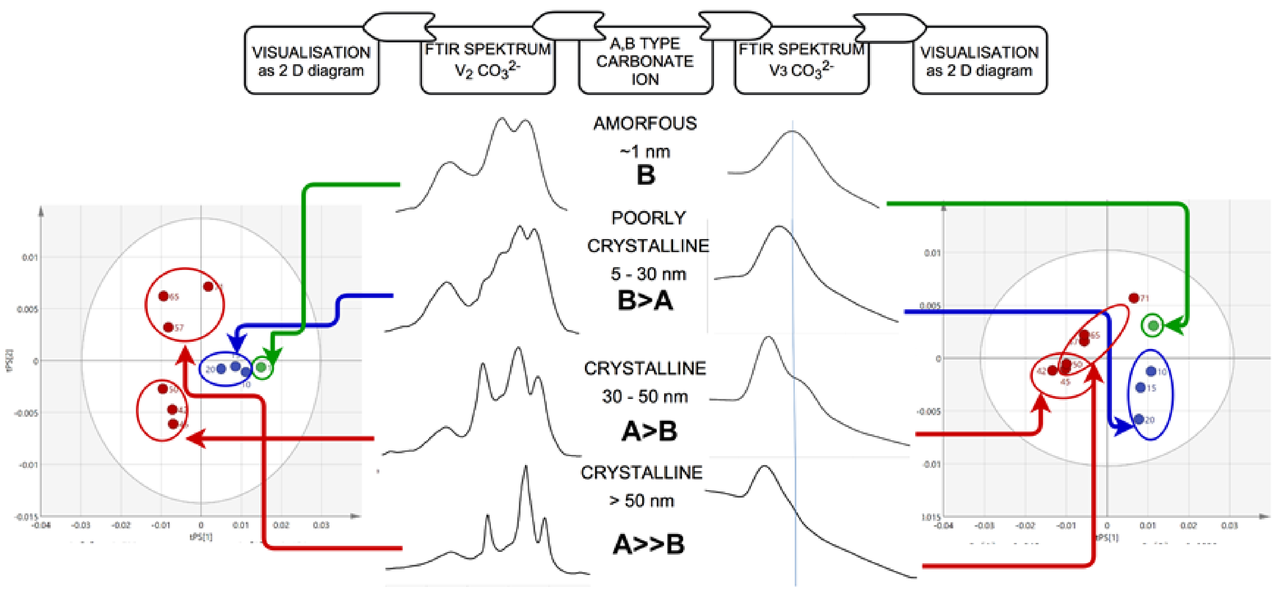
### *Differentiation of FTIR PAS and DRIFT spectra Relationships of FTIR visual interpretation and statistical analysis for determining the crystallinity and particle size of calcium phosphate*




### *The main functional groups of calcium phosphate in FTIR sectrum*

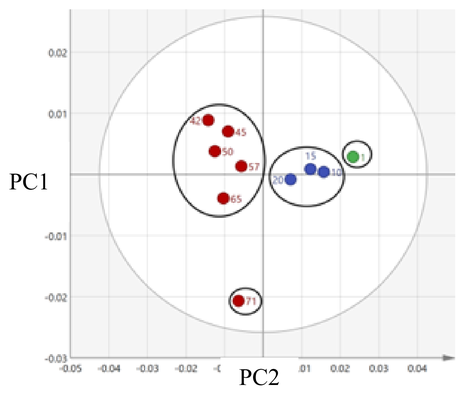



### *The relationships of FTIR visual interaction and statistical analysis for determination of degree of crystallinity and particle size of calcium phosphate and carbonate content*

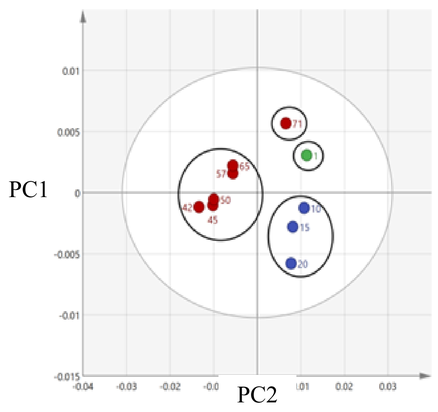



### *PCA formation in separate functional groups:*

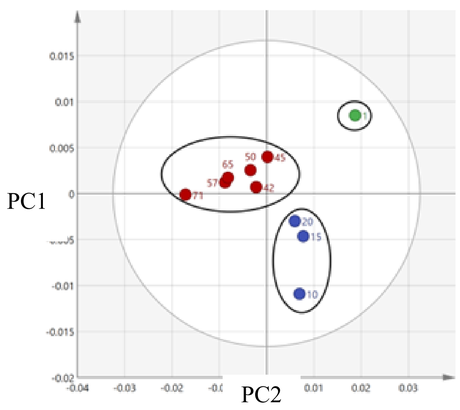
*a) 450–700 $cm^{-1}$ ($v_4PO_4^{3-}$,$OH^-$)*



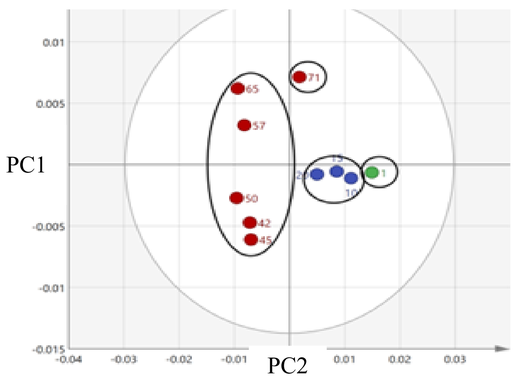

*b) 800–880 ($v_3$ $CO_3^{2-}$)*




*c) 900–1200 $cm^{-1}$ ($v_1$ $v_3$ $PO_4^{3-}$)*




*d) 1350–1800 $cm^{-1}$ ($v_3$ $CO_3^{2-}$ A, B, non-apatitic; $OH^-$*




## CONCLUSIONS

Research prove possibility to predict the position of the sample in the cluster and crystallite parameters (size and degree of crystallinity), A/B type carbonate formation and high effectivity of FTIR methods for fast and accurate bone like apatite description and analyses. The PC and HCA analysis helps to confirm or reject out assumptions and evaluate the effects of factors on cluster formation.

## ACKNOWLEDGEMENTS

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