Discrimination of ionizing radiation effects on bone using Fourier Transform Infrared Spectroscopy using K-means

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Abstract: We demonstrated the feasibility of using ATR-FTIR spectroscopy associated with k-means clustering to evaluate the recognition of different doses. Our results open up new possibilities for protein monitoring relating to dose responses.
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1. Introduction

Ionizing radiation works with gamma ray sources or X-ray generators. The majority of the practices which ionizing radiations demonstrate a broad range of applications such as medicine, radiography, and food safety. Bones are living material that requires controlled radiation-dose for their biological stabilization. Other works indicated biochemical alterations in the bone material [1].The characterization of the irradiated bone tissue can be a tool in understanding which components are affected and how certain doses of ionizing radiation alter its molecular structure and mechanical properties. In the clinical diagnostic context, alternative techniques have been employed to promote an accurate bioanalysis.

Fourier-transform infrared spectroscopy coupled with attenuated total reflectance (ATR-FTIR) is an optical technique which reports variations of vibrational bonds and their fundamental feature in biological material.

In the article reported here, specific characteristics of the bone chemical alteration with different doses were investigated to improve understanding of the role of organic modification.

2. Materials and Methods

2.1 Sample preparation

In this work, we use 30 fragments of bone were obtained from bovine femur diaphysis. Samples were cut into 1 cm x 1 cm x 1 mm, which were polished and stored properly in the refrigerated environment.Irradiation of samples was performed with a Cobalt-60 Gammacell Irradiator source at doses of 0,1 kGy, 1 kGy, whereas the fragments exposed to a dose of 15 kGy was irradiated in a multipurpose irradiator of Cobalt-60.

2.2 ATR-FTIR Spectroscopy

Bones samples were pressed into the diamond crystal of ATR. The FTIR spectrometer was equipped with a deuterated triglycine sulfate (DTGS) detector (Thermo Scientific). For each group, 100 scans were co-added, and the spectrum obtained represents the averaged from 10 replicates.

2.3 K-means clustering

Raw ATR-FTIR spectra were truncated to a range of 1200-1800 cm^{-1}, vector normalized. In sequence, k-means clustering are applied to doses-responses recognition. All data were performed using MATLAB R2017a software (The Mathworks Inc., Natick, MA, USA).

3. Results and Discussion

For the ATR-FTIR spectra, the differences at the vector normalized are not noticeable. This fact is demonstrated in Figure 1.

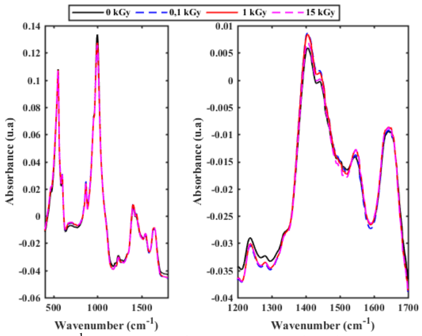

Fig. 1: Typical bone ATR-FTIR region (400-1800 cm-[1]) of averaged vector-normalized raw FTIR spectra (A) Organic vibration region of bone spectra (1200-1800 cm^{-1}) (B)

The spectra from non-irradiated (0 kGy) are compared with other groups (0,1 kGy, 1 kGy and 15 kGy) to obtain the spectral differences. To enhance classification of the proper characteristics, which remark the dose-response effect, we use the K-means clustering in the organic vibration region.

K-means clustering is a chemometric methodology which centroids plot are used to classify the class-specific information of all observed class grouping [3].

The centroids results of K-means clustering were selected in Figure 2 showed the performance of non-irradiated and irradiated bone samples and correspondent spectral differences.

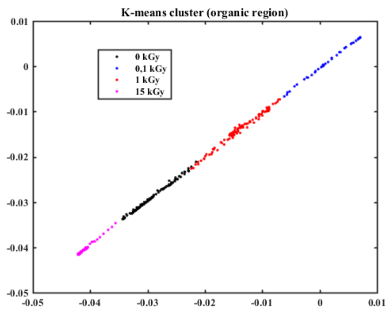

Fig. 2: K-means clustering of organic region

Regarding potential modifications of the composition that will influence the molecular dynamics of material bonding, the most prominent spectral alterations are in the organic molecules[4], reported in Figure 2.

3. Conclusion

We have presented the results of ATR-FTIR associated to k-means clustering efficiency to recognize irradiated samples. The differences expressed between these dose-response categories can be thought of as corresponding to organic region alterations. This could potentially allow identification of biomarkers conserved or not across the dose-response in bone material.

4. Acknowledgements

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5. References

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