



## Differentiation of Bone Submitted to Single dose from fractional of Ionizing Radiation by ATR-FTIR Spectroscopy

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### 1. Introduction

Since the late 19th century, ionizing radiation has played an important role in the diagnosis and treatment of many diseases, particularly cancer. The transition from single dose (SD) to fractional dose (FD) delivery radiation administration was a major advancement in this discipline. This method has several benefits, including fewer side effects, improved tumor management, and preservation of normal tissues. In this work, we use the bone as a biomarker to differentiate single doses from fractional doses[1].

### 2. Methodology

The principal aim of this work was to differentiate SD from FD using a Fourier-transform infrared spectroscopy (Thermo Nicolet 6700, Waltham, MA, USA) system, combined with attenuated total reflectance (ATR-FTIR), which offers a nondestructive way to characterize samples. The sample fragments of bovine bone femur diaphysis cut into 1cm x 1cm x 1mm were irradiated with a multipurpose irradiator of Cobalt-60, separated into two groups: the first one containing these SD (1, 15, 60 kGy), and the second one containing these FD (1, 15, 75 kGy). the next step was to do the FTIR spectroscopy, all the ionizing samples, in the range of 4000 to 400cm<sup>-1</sup> Figure 1a, with 4 cm<sup>-1</sup> of spectral resolution, and 100 scans were co-added. Following, this in the data analysis, the spectra were subjected to the Savitzky-Golay filter to signal-to-noise ratio reduction (2nd polynomial in a 13 window 2nd derivative) and normalization [2]. After that, principal components analysis and linear discriminant analysis (PCA-LDA) models were performed, to segmentation of this model was evaluated by cross-validation and leave one out.

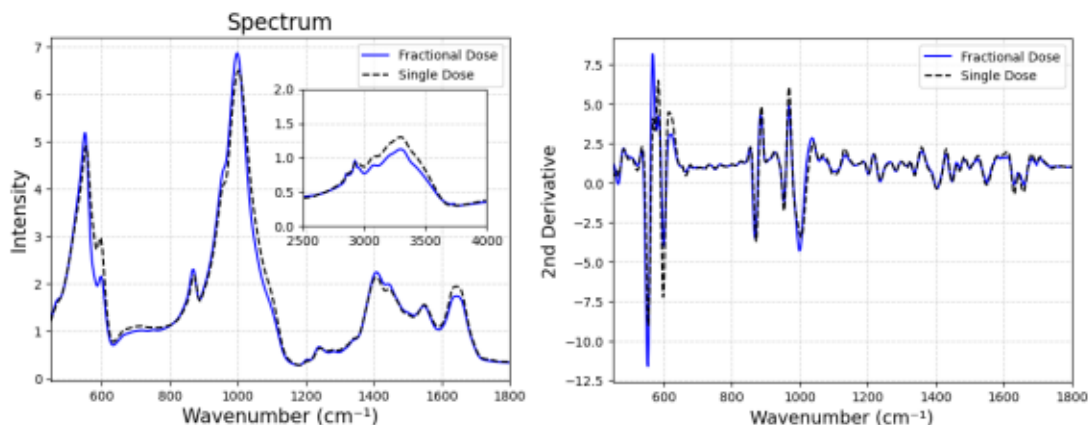


Figure 1: Difference to spectrum from Single Dose to Fractional Dose inserts high wavenumber b) Difference to second derivative from single Dose to fractional dose.

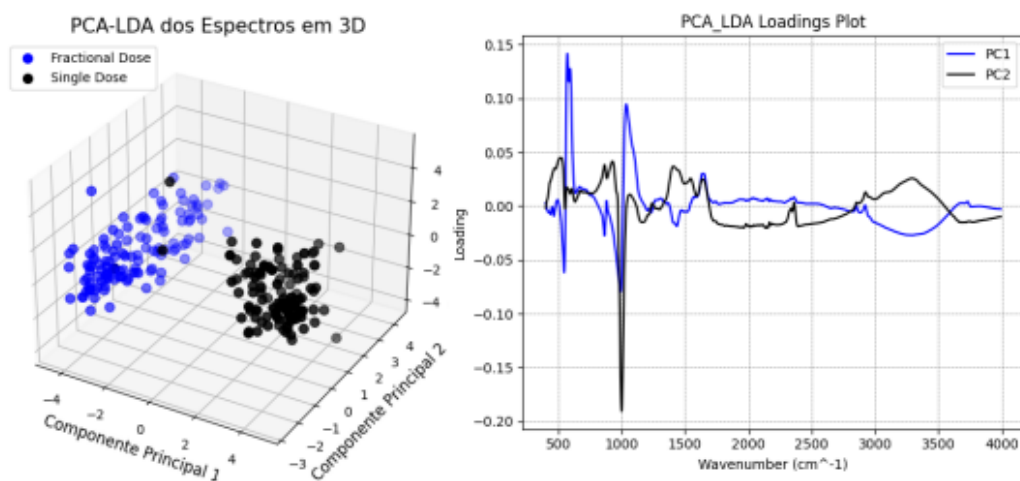


Figure 2: Figure 2: a) Model PCA-LDA b) Loadings Plot.

### 3. Results and Discussion

The biochemical composition of bone material may be detected by FTIR spectroscopy, regardless of small changes. The inherent complexity of spectra often makes it difficult to assess absorbance fluctuations directly from the raw data. To solve this issue, the preprocessing procedures were employed according to [2]. After that, was examine the commonalities and latent patterns between single and fractional ionizing doses using the PCA-LDA model, for this few metrics were employed for the analysis, like carbonate accumulation (CA), carbonate to mineral (CM), and mineral to the matrix (MM) are crucial spectral markers for assessing the distinctions between SD and FD, according to the chemometric analysis[1,3]. This model was evaluated by cross-validation leaving one out and achieving the accuracy of 0.9.

### 4. Conclusions

Multivariate PCA-LDA analysis and loading plot were performed and it was observed that the most discriminative spectral markers were Carbonate Accumulation, Carbonate to Mineral Mineral to Matrix,

Mineral Maturity, Crystallinity, Protein Secondary Structure; in addition it was obtained with this model an accuracy of 0.9.

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### **References**

- [1] P. Castro et al, Assessment of bone dose response using ATR-FTIR spectroscopy: A potential method for biodosimetry, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 273, pp.120900 (2022)).
- [2] M. Baker et al, Using Fourier transform IR spectroscopy to analyze biological materials *Nature protocols*, vol.9, pp.1771-91 (2014).
- [3] L. Bachmann et al, Infrared Absorption Bands of Enamel and Dentin Tissues from Human and Bovine Teeth *Applied Spectroscopy Reviews*, vol.38, pp.1 (2003).