Semi-quantitative analysis in FTIR: exploring and testing four methods for band area calculation in bone

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Semi-quantitative analysis are largely used in the Fourier Transform Infrared Spectroscopy (FTIR)[1]. This study analyzes amide I band for 50 bovine bone spectra[2,3]. For this purpose, we compared the results of four methods to provide the area under the curve: Integration, Gaussian, Lorentz, and Triangulation.

Bone fragments were obtained from bovine femur diaphysis. 50 bone fragments were cut 4 mm×4 mm×1 mm and polished. Spectra were taken from 4000 cm^{-1} to 550 cm^{-1}, with a resolution of 2 cm^{-1}, 32 scans per spectra with a diamond ATR coupled to a FTIR spectrometer (Nicolet 6700, Thermo, EUA). Each sample was analyzed ten times, being repositioned on the equipment.

The measured areas change due to instable condition in overlap between peaks and theirs noise signals and this represented a contrast point when it was compared to the other methods (Fig. 1).

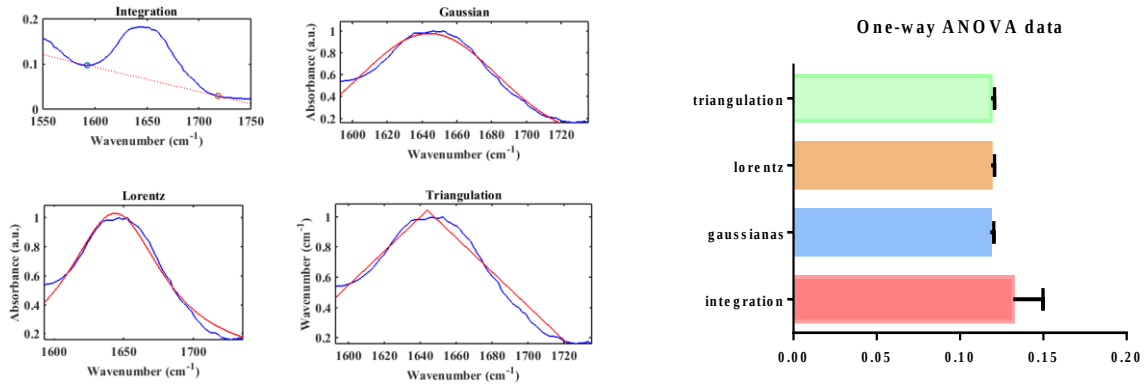

Fig. 1. Area under Amide I band for FTIR bone spectra and comparison among the methods tested.

Measurement value areas obtained using Lorentz, Triangulation, and Gaussian were statistically compared with one-way ANOVA providing no significantly differences. As a result, the method of Integration was more sensitive for instable bands which means overlapping and noise signals because of its high standard deviation.

Therefore, instable behavior bands affect the area values in different approaches because mathematical modeling is not yet consolidated. More models and tests will be applied in future works on this field before study laser cut bone spectra.

References

[1] A.B. Rodriguez-Navarro, C.S. Romanek, P. Alvarez-Lloret, K.F. Gaines. *Environmental Science and Technology*, 2006, **40**, 4936.
[2] D. Farlay, G. Panczer, C. Rey, P. Delmas, *Journal of Bone and Mineral Metabolism*, 2010, **28**, 433.
[3] C. Benetti, P. A. Ana, L. Bachmann, D. M. Zezell, *Applied Spectroscopy*, 2015, **69**, 1496.

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