Determination of inflamed and non-inflamed patients with FTIR supervised by C-reactive protein

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Introduction: C-reactive protein (CRP) is produced in the liver due to inflammatory processes resulting from infection or necrosis and chronic pathologies. Fourier transform infrared spectroscopy (FT-IR) is a fast, eficiente and inexpensive technique that can be used to analyze the global biochemistry of blood based on the vibrational energy of biomolecules. In this study, FT-IR and chemometry were used to differentiate inflamed and non-inflamed patients. This allows to correlate with anthropometric and biochemical predictive factors for atherosclerotic diseases, cerebrovascular accident, obesity implications and general chronic inflammatory pathologies. **Methods:** blood samples from patients considered normal (n=72) by hemogram were collected to obtain plasma by centrifugation (3500 rpm, 15 min). For FT-IR analysis, plasma aliquots were deposited on the crystal and dehydrated in air current (60-65 ºC, 1.5 min). Reading were taken (in triplicate) in a spectromer (Spectrum™ 400 FT-IR/FT-NIR – PerkinElmer) in the attenuated total reflectance mode (ATR-FTIR) in the range of 650-4000 cm^{-1} with a spectral resolution of 4 cm^{-1} and 4 scan pulses. For chemometric data processing, the interval principal component analysis method (iPCA) was used. The spectrum was split into 30, 40, 50 and 60 in order to look for the best visual graphic separation. For data treatment, normalization (0-1), Multiple Scatter Correction, first derivative (5-point window) and mean-center were used. hypothesis tests (t teste or U test) were applied to analyze differences in anthropometric parameters (body mass index (BMI) and abdominal circumference (AC)) and biochemical parameters (glucose, cholesterol, HDL, LDL, VLDL, triacylglycerols (TG), leptin and cfDNA) in patients inflamed (n=25) and non-inflamed (n=47). The reference value of 2 mg/L was used as the limit between inflamed and non-inflamed. Study approved by CEP UNISC (4,278.678). **Results:** PCA with spectral fragmentation = 30 in the range of 1093-983 cm^{-1} showed the best visual separation for inflamed and non-inflamed. PC1 (40.21%) provided $p = 0.014$ and PC5 (2.77%) provided $p = 0.001$. The parameters that obtained significant p-values (< 0.05) for inflamed and non-inflamed were: BMI ($p < 0.001$), AC ($p < 0.001$), glucose ($p = 0.007$), VLDL ($p = 0.01$), TG ($p = 0.01$), leptin ($p < 0.001$) and cfDNA ($p = 0.013$). Highlights for $p = 0.013$ (U test) of cfDNA, which is known to be increased in chronic or necrotic cases. The median cfDNA (ng/mL) was 29.3 for non-inflamed with 25th percentiles = 21.3 and 75th = 43.95 and median of 42.4 for inflamed with percentiles of 25th = 28.3 and 75th = 53.65. **Conclusion:** FT-IR coupled with chemometric techniques proved to be an efficient screening method for inflamed and non-inflamed individuals. This allows for correlation with various anthropometric and biochemical parameters that are useful as preclinical indicative screening, assisting in early diagnosis and treatment.

Keywords: PCR, FTIR, PCA