Combining biophysical and multivariate statistical approaches in the analysis of plasma to discriminates multiple sclerosis disease

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Multiple sclerosis (MS) is one of the most common neurodegenerative diseases showing various symptoms both of physical and cognitive type. In this work, differential scanning calorimetry (DSC) and attenuated total reflection Fourier transformed infrared (ATR-FTIR) spectroscopy are used to analyze plasma samples for discriminating MS patients (n 45) from healthy control (n 40) individuals, and identifying potential spectral biomarkers helping the diagnosis through a quick non-invasive blood test. DSC data were combined in a single diagnostic index (thermal liquid biopsy score) and provides information about overall real-time alterations in plasma proteome that may be indicative of MS. Similarly, the differences in the spectral features both in the fingerprint region (1800-900 cm -1) and in the high region (3050-2800 cm -1) of the infrared spectra were highlighted also with the support of different chemometric methods, to capture the most significant wavenumbers for the differentiation. The results show an increase in the lipid/protein ratio in MS patients, indicating changes in the level (metabolism) of these molecular components in the plasma. Moreover, the multivariate tools provided a promising rate of success in the diagnosis. The highest level of performance, in terms of sensitivity (78%) and specificity (83%), was obtained through the random forest model applied in the fingerprint IR region. The overall results suggest that both biophysical approaches on plasma samples, requiring minimal or no manipulation, coupled with statistical multivariate approaches, are promising analytical tools to support MS diagnosis through the identification of spectral biomarkers.