Phd Thesis Defense: Development of computational tools and pipelines for enhanced interpretation of Raman spectroscopy in biomedical applications

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Raman spectroscopy has gained increasing attention over the last few decades due to its ability to non-destructively extract chemical information from samples. However, despite advances in instrumentation, it has not yet become standard practice in the biomedical field. One of the main reasons is the difficulty in interpreting and extracting the chemical information encoded in Raman signal, so as to validate the technique using complementary, well established techniques.
Considering this, the aim of this Thesis is to develop tools and analytical pipelines that

enhance the biochemical interpretation of Raman spectra, and to demonstrate its usefulness in two relevant biomedical research lines: breast cancer resistance to neoadjuvant treatments and the diagnosis of choroidal melanoma.
Firstly, we developed and validated RamanBiolib, an open-source Raman spectral library accompanied by search algorithms, aimed at providing rapid and objective identification of biomolecules. Secondly, we used RamanBiolib after spectral unmixing to identify and quantify cytochrome c molecule in breast cancer cells resistant to neoadjuvant treatments. This revealed a shift towards its reduced state to avoid apoptosis and acquire drug resistance. Then we also characterized lipid droplets in triple-negative breast cancer cells, highlighting the relevance of variable importance analysis in classification models. This approach allows for the biochemical interpretation of their classification performance and assessing possible background contributions to their accuracy. By doing so, significant changes in lipid unsaturation were detected. Furthermore, we developed RamanTF, a transformer-based algorithm that automatically quantifies key biomolecules from raw spectra.
Finally, to study melanin-rich samples, we defined a pre-processing and analysis workflow to correct instrumental interferences that were observed in previous studies, but not corrected yet. With this established workflow, key melanin properties were identified, such as melanin structural disorder or defects abundance, which can be used as biomarkers to diagnose choroidal melanomas. Overall, the tools, discussions, and results presented in this Thesis advance Raman spectroscopy towards clinical application and provide a basis for its widespread adoption as a routine technique in biomedical and diagnostic research.

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