

***In situ* Chemical Diversity Characterization of *Sextonia rubra* fruits by MALDI-CID-FT-ICR Imaging and Molecular Networks**

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Sextonia rubra is a tropical tree endemic to the Guiana Shield and the Brazilian Amazon. It is known for its heartwood natural durability that comprises numerous lactone derivatives [1]. However its fruits have not been studied chemically. Here we propose analytical methods to explore the chemical diversity of these fruits using imaging MS and chemoinformatics analysis.

We analyzed fruit sections by MALDI-CID-FT-ICR. All MS² spectra were aggregated and analyzed using the MetGem software [2]. This metabolomic tool allows the annotation of the detected ions by querying fragmentation spectra databases.

Thus, lactone derivatives were detected in all tissues, flavonoids in internal tissues and alkaloids in external tissues. These results suggest a distribution of specialized metabolites according to their ecological role. Our methodology proves to be relevant for annotating the structures of the molecules while preserving the information of their spatial distribution.

References

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