

## ANTHROPIC INFLUENCE IN THE METABOLIC COMPOSITION OF MANGROVE ESPECIES

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**Abstract:** Mangrove forest, composed by salt tolerant trees that live in rough coastal conditions, is one of the most diverse biomes on planet. A total of 349 secondary metabolites have been reported so far from mangrove species worldwide, including triterpenes, diterpenes, steroids, flavonoids, naphthoquinones and iridoid glucosides.[1] Despite its importance, human activities as aquaculture, agriculture, and urban land have threatened its survival.[1] In order to stimulate its conservation, this work aim to evaluate the anthropic influence in metabolic composition of mangrove species (*Rhizophora mangle*, *Laguncularia racemosa* and *Avicennia schaueriana*) from Pernambuco State -Brazil. Stems and leaves of *A. schaueriana* (Black mangrove), *L. racemosa* (White mangrove) and *R. mangle* (Red mangrove), were collected at three regions of Pernambuco-Brazil during 2014 and extracted by maceration using MeOH and MeOH:H<sub>2</sub>O (3:7, v/v). The extracts were analyzed by HPLC-DAD-TOF and HPLC-DAD-IT in both ESI positive and negative modes. MS-based dereplication was performed by on-flow detection of high resolution molecular formula of the molecules and collision induced MS/MS technique for fragmentation of molecular ions, assisted by molecular networking workflow, according to figure 1.[2] DAD detector was set to record between 200 and 800 nm. Preliminary results led to the in situ identification of mono, di, tri-*O*-glucosyl flavonoids, methoxy-flavonoids, and proanthocyanidins, previously described in mangrove forest. The metabolites were distributed among all three collected plant species. Molecular networking organized MS/MS data based on chemical similarity and allowed dereplication of known molecules and detection of related analogues. HPLC-MS data will also be employed in multivariate data analyses as hierarchical clustering analysis (HCA) and principal component analysis (PCA) to identify the anthropic influence in terms of metabolic variation.

[1] Wu, J., Xiao, Q., Xu, J., Li, M. Y., Pan, J. Y. and Yang, M. H. 2008. Natural products from true mangrove flora: source, chemistry and bioactivities. *Natural Product Reports*, 25(5): 955-981.

[2] Watrous, J., Roach, P., Alexandrov, T., Heath, B. S., Yang, J. Y., Kersten, R. D., van der Voort, M Pogliano, K., Gross, H., Raaijmakers, J.M., Moore, B.S., Laskin, J., Bandeira, N. and Dorrestein, P. C. 2012. Mass spectral molecular networking of living microbial colonies. *Proc. Natl. Acad. Sci. USA* 109: 1743-1752.

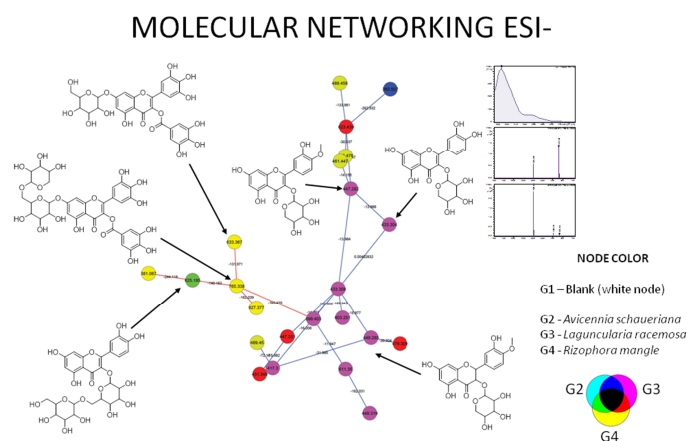


Figure 1. Detection of flavonoids based on molecular networking workflow and MS/MS spectra similarity.