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MOLECULAR NETWORKING TO DEREPLICATE THE METABOLOME OF ZOANTHIDS ALONG BRAZILIAN COAST

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Abstract: Untargeted liquid chromatography-mass spectrometry (LC-MS) is used to rapidly profile crude natural product (NP) extracts; however, when the objective is to dereplicate known entities from complex biological extracts, specially whole systems or communities as zoanthids colonies, chemometric tools are required to fully access information from acquired data. In this work, the metabolome of *Palythoa* species were dereplicated by LC-MS combined with molecular networking method.[1,2] Molecular networking aid in situ detection of known molecules by clustering the complex data set of MS/MS spectra according to fragmentation pattern similarities.[1,2] Zoanthids *P. caribaeorum* and *P. variabilis*, collected in Ceará, Rio de Janeiro and Santa Catarina States, were extracted by maceration using methanol and analyzed by LC-DAD-IT and LC-DAD-TOF, in both ESI modes. Dereplication initiated with calculation of molecular formulae using TOF-MS data (accurate molecular weights < 5ppm). The resulting formulae were compared with different metabolic database (METLIN, MarinLit, DMNP), considering chemotaxonomic information, and the possible putative structures were proposed by MS/MS-based fragmentation pattern. Retention time (shift tolerance of ±0.05 min) and UV spectra were used as orthogonal information on peak annotation. Additionally, the dereplication workflow were assisted by molecular networking, i.e., MS/MS spectra clustering by cosine similarity. The method led to the dereplication of polyhydroxy-ecdysteroids, as shown in figure 1, and alkaloids (zoanthamine derivatives), previous described for *Palythoa*. It was also observed mycosporine and indole-diterpenes derivatives, probably produced by microbial association. Molecular networking demonstrated to be a powerful complement to accelerated dereplication strategies and can support studies in the metabolome of aquatic communities.

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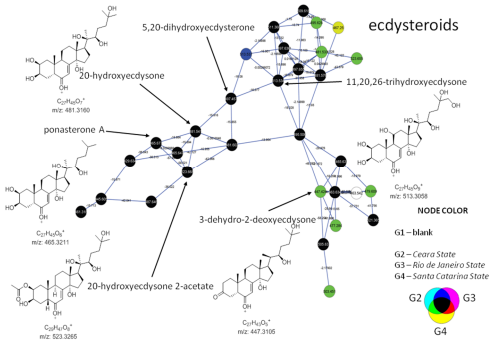

Figure 1. Dereplication of ecdysteroids based on molecular networking workflow and MS/MS spectra similarity.