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A metabolomics approach to monitor the production of secondary metabolites in microbial symbionts and endophytes through automated dereplication of HRFTMS

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High resolution Fourier transform mass spectrometry (HRFTMS) was employed as complimentary metabolomic tool to dereplicate chemical profiles of sponge-associated microbes. Sponges act as hosts to a diverse population of symbiotic organisms including bacteria and fungi. These symbionts offer benefits to the host including protection, nutritional benefit and support to the sponge skeleton. They have also been recognised as an important source of secondary metabolites which may have bioactivity and therefore medicinal potential. The innovative strategy involved targeted cultivation and isolation of biologically active compounds. Principal Component (PCA), Hierarchical Clustering (HCA), and Orthogonal Partial Least Square-Discriminant (OPLS-DA) analyses were used to evaluate HRFT mass spectral data of culture extracts. The results of the statistical analysis identified and validated the best culture conditions and extraction procedure which optimized the isolation of novel bioactive metabolites. Production of secondary metabolites were investigated in several of the bacterial symbionts that were isolated from marine sponges. Novel secondary metabolites were screened using high resolution mass spectrometry-based metabolomics approaches. Metabolomic profiling using HR-ESI/FTMS-MS fragmentation were done at different stages of the growth phase for both solid and liquid culture media and subjected to molecular networking. Molecular networking the mass fragmentation data pinpoints functionalities that can be correlated to bioactivity and fermentation parameters as well as to predict and enhance the biosynthetic pathway involved in the production of the target secondary metabolite.

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Mass Spectrometric techniques for investigation of biodiesel potential of Microalgae biomass

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Microalgae oils have emerged as potential sources of nutrition, energy and oil besides useful bi-products, such as nutraceuticals, antioxidants and high performance lubricant additives. Microalgae are unicellular photosynthetic organisms with 5-50 µm in size that require primarily three components to produce biomass, i.e., water, CO₂ and sunlight with relatively higher photosynthetic efficiency against terrestrial plants. Microalgae biomass is comprised of neutral (triacylglycerides, TAG; free fatty acids, FFA) and polar lipids (glyceroglyco/phospholipids) besides specific molecules with high industrial potentials. Neutral lipids are important feedstocks of biodiesel due to their similarity with regular vegetable crops with regard to saturated and unsaturated fatty acid profile (C₁₄ to C₂₂) including C_{20:3}, C_{20:5} (EPA) and C_{22:6} (DHA). The presentation will highlight the role of Mass spectrometric techniques (ESI-MS; TOF, QMS; GC-MS) for determination of composition of microalgae oils generated from biomasses of *Dunaliella salina*, *Chlorella vulgaris*, *Spirulina platensis* and *Scenedesmus obliquus* species cultivated on a lab scales under different growth parameters in fresh and industrial waste water with an emphasis on exploring the biodiesel and PUFAs potential.

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