



Screening Program of Aqueous and Organic Extracts from Marine-Derived Fungi to Discover New *Plasmodium falciparum* Inhibitors

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The World Health Organization (WHO) has reported that in 2019, 229 million new cases and 409,000 deaths of malaria, even though these numbers indicated a reduction of approximately 41% of cases between 2000-2015 and 67% of mortality [1]. The discovery of new bioactive natural products is an important approach to identify novel antimalarial agents [2].

In the present investigation we assessed the biological and chemical profile of the aqueous and organic extracts obtained from cultures of marine-derived fungi. Twenty-seven fungi strains were isolated from marine organisms collected of Espírito Santo state coastline (Brazil). Fungal cultures were grown with nutrients and artificial sea water. After the growth, both aqueous and organic extracts were obtained [3]. In total, 135 samples were screened and evaluated for their antiplasmodial activity against *Plasmodium falciparum* 3D7 strain [4]. In addition, the samples were analyzed by UPLC-QToF-MS/MS and the Feature-Based Molecular Networking was constructed using the Global Natural Product Social Molecular Networking (GNPS) web-platform.

Considerable antiplasmodial activities (Inhibition > 80% at 50 µg/mL) were observed for eight fungi strains (M3, M13, M15, M16, M20, M23, M28 and M30). Molecular networking analysis of all samples was used to quickly organize the data and investigate the secondary metabolite diversity. The integration of Feature-Based Molecular Networking and biological assays is an attractive strategy for selection of promising natural products as candidates for isolation and identification of new antiplasmodial agents.

1. WHO, **World Malaria Report**, 2020. World Health Organization, 2020.
2. Yang, B. et al. **Current Medicinal Chemistry**, v. 25, p. 3796–3825, 2018.
3. Rodriguez, Julie P. G. et al. **Journal of Natural Products**, v. 83, n. 1, p. 55–65, 2020.
4. Smilkstein, M. et al. **Antimicrobial Agents and Chemotherapy**, v. 48, p. 1803–1806, 2004.

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