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EVALUATION OF THE ANTIOXIDANT, PHOTOPROTECTIVE AND PHOTOCHEMOPREVENTIVE POTENTIAL IN VITRO OF Tithonia diversifolia EXTRACTS BY AN ENVIRONMENTAL METABOLOMICS APPROACH

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Introduction: Tithonia diversifolia (Hemls.) A. Gray (Asteraceae) is an invasive plant popularly used for the treatment of several health problems. Despite of be a species rich in phenolics, there are few works describing its antioxidant properties and virtually none describing its photoprotective and photochemopreventive potential. Purpose of Study: The main aim of this work was to select extracts of T. diversifolia with photoprotective and photochemopreventive potential using an environmental metabolomics approach. Methods: A total of 170 samples of T. diversifolia were collected throughout a 24 months period at states of Goiás and São Paulo. Climate and soil data were obtained to the period. UHPLC-DAD-(ESI)-HRMS and NMR (J-resolved) analysis were used to obtain the metabolic profiles and the data from both techniques were concatenated to perform the multivariate analyses (HCA and PCA). The antioxidant assay by DPPH was used to selection of the more active samples [1]. The in vitro photoprotective and photochemopreventive activities were performed by cell culture (fibroblasts L929 and keratinocytes HaCaT) exposed to UVA (formation of intracellular ROS) [2] and UVB radiation (cell viability and lipid peroxidation) [3]. Results and Conclusions: The multivariate analyses and the dereplication step enabled to propose groups according to the discriminant classes of metabolites. The DPPH assay was performed with 24 samples from the proposed groups and the lesser EC_{50} values (7.21 and 6.36 µg/mL) were obtained, respectively, by a leaf sample collected from Goiás in December 2013 (LG1213) and a root sample collected from São Paulo in September 2013 (RS913). These two samples, rich in flavonoids and caffeoyl esters, showed photoprotective activity in vitro against damage induced by UVA and UVB radiation, and the leaf sample LG1213 showed photochemopreventive activity also. These results have shown that the environmental metabolomics can be a useful and fast approach to screen plant samples in order to find their interesting biological properties, using the plant chemical and environmental information, without the need to perform several *in vitro* assays.

Keywords: UHPLC-DAD-(ESI)-HRMS. J-resolved. Cell culture. **Financial support:** FAPESP (n° 2011/13361-6) and CAPES (n° 99999.003967/2014-00).

References:

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