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Metabolomics as a tool for anticancer lead-finding from natural products

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Natural products have been the source of many drugs, particularly anticancer agents, of which more than 50% originated from natural sources. However, due to the slow and painstaking methods of conventional lead finding, new strategies for the detection of active compounds are necessary. Metabolomics has the potential for this approach since it provides an integrated view of the composition of therapeutic agents, such as plant extracts, and their biological effects on organisms and especially their disease states. In this work we developed a method for the *in situ* identification of the bioactive compounds from six Brazilian Chrysobalanaceae plant species with cytotoxic potential. Also we propose a method to monitoring metabolic changes in biological systems, such as cell lines and tumors, in response to external of pharmacological stimuli of the therapeutic agent based on spectroscopic analysis and chemometric modeling. *In situ* identification of Chrysobalanaceae plant metabolites were performed by combination of the Interval Multivariate Curve Resolution (MCR) algorithm with on-line HPLC-DAD-ESI-QToF-MS/MS. Interval MCR-ALS was employed on deconvoluting the LC-UV fingerprint by using alternating least square and additional constraints based on non-linear combination to discriminate between ambiguous MS molecular ions. The online HPLC-DAD-ESI-QToF-MS/MS method led to the identification of 40 known compounds, especially flavonoids glycosides, proanthocyanidins and kaurane diterpenes, that have been previously described for Chrysobalanaceae. According to the literature, kaurane diterpenes demonstrated cytotoxic activity in different bioassays. For determination of the cytotoxic compounds of Chrysobalanaceae plant extracts, the metabolic profiles obtained by LC-MS and NMR should be correlated with the results of *in vitro* cytotoxic activity through the use of bioinformatics, as well as inferences on the possible synergistic and/or antagonistic interactions. Additionally, metabolic changes of tumor cell lines in response to external or pharmacological stimuli of the plant extracts should be monitored by LC-MS and ^{1}H NMR to determine the mechanism of action, that may be identified by metabolic changes in the biological systems.

Biography

Fausto Carnevale Neto has a graduation degree in pharmacy (2008) from Sao Paulo State University, Brazil, and a master degree in Organic Chemistry (2010) from Chemistry Institute at Sao Paulo State University, Araraquara, Brazil. He is a Ph.D. student at Chemistry Institute , Sao Paulo State University, Araraquara, Brazil, and is currently in an visiting Ph.D. scholar at UW South Lake Union Medicine School, at Seattle, US.

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