

Investigation of the NMR parameters analyses, by a made-up MATLAB® GUI (guide user interface), on an in-house database

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One of the goals of the metabolomics is to study the fluctuation on chemical composition from biological systems, in response to various factors such as genetics, age, pathology, development, environment and stress. Currently, the two main analytical techniques used to measure and detect those variations are NMR spectroscopy and mass spectrometry. These two techniques have their advantages and limitations and, are often used complementary. However, as a tool for metabolomics, NMR has some unique characteristic. It is a universal detector for all molecules containing NMR-active nuclei, it has a very high reproducibility for its based on the physical characteristics of compounds, can provide a detailed analysis on the biomolecular composition very quickly, with a relatively simple sample preparation and, for all hydrogen-bearing molecules, the intensity of all of those nuclei are proportional to their molar concentration which allows the calculation of the real metabolite concentration. The objective of this work is to investigate the NMR parameters analyses of 35000 FIDs presented in a natural products database created by NMR experiments acquired in the past 10 years at NuBBE UNESP, Araraquara. The parameters were identified using a made-up MATLAB® GUI interface. The results showed variations between the data, which requires standardization through chemometric tools, as well as the creation of a protocol for future analysis by NMR experiments.

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Biography

Rafael Teixeira Freire has a undergrad in chemistry and has completed his Master degree in organic chemistry in 2008 at the age of 26 years. He is doing his Ph.D. at the Institute of Chemistry University of São Paulo State, Araraquara-Brazil with a sandwich program at University of Florida, Gainesville-USA.

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