NMR and chemometrics in the study of bipolar disorder

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Abstract
The Bipolar Disorder (BD) is a psychiatric illness that affects 1% of the global population. Furthermore, it has been one of the ten biggest incapacitating disorders that affect adults during their productive age. Having in mind that diagnostics of the BD is difficult and based on clinical evaluation, our current research has for aim the comparison of the metabolic profiles among control group and the patients with BD. To enlarge results obtained in previous studies on BD biomarkers, the blood serum samples were analyzed using $^1$H Nuclear Resonance Magnetic (NMR) spectroscopy and chemometrics methods in the data analysis. As result, the most important regions in the $^1$H NMR spectra responsible for the samples classification into two groups have been identified to be from 0.0 to 4.0 ppm and confirmed some of our previous results.

Key words: Bipolar Disorder, Metabolomics, Chemometrics.

Introduction
The bipolar disorder (BD) is a chronic psychiatric illness that affects around 1% of the world population.¹ Today, the bipolar disorder, like many other mental illnesses, is being evaluated only by interview with patient, his familiars and close friends. However, possible errors in the diagnostic may prejudice the drug treatment of patients. This may be an indicative to the elevated rate from 73 to 90% of the desistance among the patients during treatment²,³. For this, the metabolomics, the newest "omic" platform applied in the chemical and biochemical studies of organisms, can permit us to identify changes in the metabolism and characterize them through the quantification and identification of metabolites inside and out of cell. This way, it is almost becoming possible to profile metabolic differences for any situation. Thereby, the current research has as the objective to compare the metabolic profiles among patients from the control group and the patients with BD. In order to achieve this, blood serum sample, collected and prepared by our collaborators (UNIFESP, Sao Paulo, Brazil), were analyzed using $^1$H Nuclear Resonance Magnetic (NMR) spectroscopy and chemometrics methods in data understanding.

Results and Discussion
Ten and twenty-eight blood serum samples of people with BD and from control group, respectively, were analyzed. All data were recorded in triplicate. For this, the NMR Bruker spectrometer equipment (Avance III 600 MHz) and D$_2$O as solvent for samples dilution had been used. The data obtained in $^1$H NMR spectra were then analyzed applying the Principal Component Analysis (PCA) and during this analysis, outliers were excluded.

Conclusions
The most important $^1$H NMR spectral region (0.0 to 4.0 ppm) for two groups separation has been identified. Thus, the expectation is that our next studies may enable the identification the biomarkers for this mental illness.

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¹Young, A. H. BSpych. 2011, 198, 336-337.

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