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### **<sup>13</sup>C Solid-State NMR associated with multivariate analysis to study degradation of natural. organic matter**

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The identification of the organic components involved in the degradation of natural organic matter is crucial for understanding degradation mechanisms. Solid-state <sup>13</sup>C nuclear magnetic resonance spectroscopy (ssNMR) has been widely used for analyzing organic compounds, including those related to environmental sensitive systems. However, interpreting <sup>13</sup>C NMR spectra can be challenging due to sample complexity, with strong line superposition being a common problem. Thus, the use of multivariate analysis has become almost mandatory, not only to identify organic components, but also to separate samples according to their composition, origin or other physical chemical properties. Recently, an approach that combines pulse sequence induced T<sub>1</sub> spectral modulation with spectral separation based on Multivariate Curve Resolution (PSIM-MCR) was successfully applied to help elucidating the composition of pretreated sugarcane bagasse (1) and constructing polymers. (2) The approach explores the sensitivity of solid state NMR to spin interaction and relaxation times, so, in principle, different type of spectral modulation provide by a specific pulse sequences can also be used. In this presentation an analysis of the spectral separation capability of MCR will be discussed based on the degree of line superposition, line width and signal to noise ratio. The possible extension of the PSIM-MCR approach to decompose solid-state <sup>13</sup>C NMR spectra based on properties such C-H coupling, chemical shift anisotropy, T<sub>1ρ</sub> relaxation times is also considered. The approaches are tested in model samples, such semicrystalline polymer, micro crystalline cellulose and applied to assist the interpretation of solid-state <sup>13</sup>C NMR spectra used for characterizing the degradation of organic matter in colonies of fungus growing ants.

**Palavras-chave:** <sup>13</sup>C NMR. Multivariate statistics. Organic matter.

**Agência de fomento:** Sem auxílio

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