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Laser-Induced Breakdown Spectroscopy (LIBS) has been successfully applied to analyze several molecular compounds used in pharmaceutical manufacturing. However, the LIBS technique for pharmaceutical application was traditionally limited to target a molecular compound by tagging an atom characteristic of this ingredient, which is absent from the bulk formulation. Therefore, this approach has been utilized for the analysis of many active pharmaceutical ingredients or excipient in pharmaceutical preparation. In our laboratory, we have highlighted that the emission signal originating from small diatomic fragments like C_2 can be correlated to the presence of aromatic ring in the formulation [1,2]. In the present work, we carried out a chemometric study of the plasma emission from different pharmaceutical formulation, in comparison to the conventional approach. From the different multivariate calibration, Partial Least Square regression showed the most accurate prediction over Principal Component Regression and Multi-Linear Regression. With the traditional approach, the analysis of molecular compound without an atom different of C, H, O or N was nearly impossible. However, our recent results, combining LIBS and chemometrics enable the quantitative analysis of this "category" of molecules that was not thinkable to be analyzed with the traditional approach.

1. L. St-Onge, R. Sing, S. Béchard, M. Sabsabi, Appl. Phys. A 69, (1999), S913.

2. L. St-Onge, M. Tourigny, M. Sabsabi, Poster presentation at AAPS (2004), Poster T3040