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# **ENHANCING THE USE OF CHEMOMETRICS TOOLS FOR CHROMATOGRAPHERS: TOWARDS AUTOMATED DATA-PROCESSING IN MULTIDIMENSIONAL SEPARATIONS**

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In separation sciences, we are witnessing a major increase in the amount of data generated by chromatographic instruments. This is mainly due to the advent of comprehensive chromatography and the use of multichannel detectors. The combination of both elements (e.g., LCxLC-MS or GCxGC-MS) gives an extra order of magnitude in the amount of data generated.

The conversion of this enormous quantity of data in information constitutes a tremendous task. Within the chemometrics discipline, a major effort has been made to develop multivariate tools aimed at interpreting and calibrating the data obtained by such methods. However, the use of these methods becomes most of times especially troublesome. In practice, the main bottleneck to solve is the number of man-hours (and sometimes experienced man-hours) to process the data. One way to overcome this problem is by increasing the level of automation in data-processing algorithms.

In this communication, a methodology is presented aimed to apply multivariate methods in a more unsupervised fashion. From the raw data to peak table, the focus is to decrease the demand of user intervention and user expertise. The methodology is intended to scan automatically an entire (one-dimensional or two-dimensional) chromatogram obtained using a multi-channel detector, gaining the benefits of multivariate peak resolution techniques. The methodology is illustrated with different examples and techniques (including LCxLC-MS and GCxGC-MS).