Chemometrics in Analytical Chemistry-2014
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CHEMOMETRIC SOLUTIONS TO PROBLEMS IN COMPREHENSIVE TWO-DIMENSIONAL LIQUID CHROMATOGRAPHY

Title should be upper case, using Times New Roman 14 pt font

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Comprehensive two-dimensional liquid chromatography shows great promise for the analysis of complex metabolomic samples, but due to the higher complexity of this type of data, new chemometric approaches must be developed to be able to maximize the information yield from these data. Both multivariate curve resolution – alternating least squares (MCR-ALS) and parallel factor analysis (PARAFAC) have been shown to be quite useful in this regard. Some examples of useful strategies for data analysis, including combining the use of MCR-ALS and PARAFAC, correction for retention time shifts and background contributions, and a new unimodality constraint for MCR-ALS will be discussed in this presentation. Applications of these methods to urine samples as well as designed calibration experiments will be illustrated.

Except for the title, the abstract should be in Times New Roman 12 font. Body of abstract should be less than 250 words