

Aspects of recent developments of smart multi-way calibration methods coupled with LC-MS and LC-DAD in analytical chemistry

Multi-way calibration methods having second-order or extended advantages are gaining more and more attentions in the field of analytical sciences. It is a smart and green quantitative analysis strategy based on mathematical separation of complicated chemical systems when combined with advanced analytical instruments capable of generating multidimensional arrays, e.g. HPLC-DAD, LC-MS and EEMs. It enables one to quantify directly and rapidly the component(s) of analytical interest even in the presence of unknown interferences not included in the calibration samples and makes the final goal of analytical chemistry achievable even without the aid of complicated separation procedures. These multi-way calibration methods could be applied to resolve different problems of qualitative and quantitative analysis in complicated chemical systems by combining with the advanced analytical instruments. The performances of these algorithms have been evaluated by using simulated and real experimental datasets. They have been utilized to simultaneous or direct determinations of multiple component(s) of analytical interest in many fields such as pharmaceutical, biomedical, environmental, food sciences. The main points on successful applications of these chemometric methods combined with advanced analytical instruments have been also summarized. Some recent developments on the theories and their applications of multi-way calibration methodologies including second- and third-order calibration are also reviewed in detail.

Biography

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