(Bio) Analytical Studies in Complex Matrices: Combination of Experimental and Computational Methodologies

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Abstract

The combination of chromatographic analysis with computational methodologies represents a powerful approach in the context of method development as well as in the rationalization of the experimental data. This is valid both in Academia and in industrial settings for the study of matrices with different complexity in (bio)pharmaceutical, omics, nutraceutical applications, to cite but a few [1]. As a result of technological advancements in terms of computational power and related facilities, the integration between chromatographic techniques to computational systems is progressively experiencing a wide expansion towards new domains as in a green analytical chemistry perspective. In the last decades, the above combination has crossed over the board of achiral chromatography towards the ever-increasing domain of chiral chromatography applications [1]. Special focus is given to MDs and *ab-initio* simulations, both representing valid tools to deeper insight into the enantiorecognition mechanisms of specific materials; to establish the absolute configuration of the chiral compounds [2-4]. Parallel to the contribution of computational science in improving the quality and accelerating the achievement of accurate results, enormous advancements in the (bio)pharmaceutical and nutraceutical sciences have been fuelled by the advent and the late diffusion of mass spectrometry (MS) detectors. Because of this extreme sensitivity, these instruments have become widely employed in the pharmaceutical and food supplement industries, as well as in research-oriented institutions, and – more recently – in clinical and forensic laboratories. Mass spectrometry is indeed a powerful unrivalled technique for increasing quantitative capability, providing peak identification, and elucidating the structure of unknown compounds.
The coupling of HPLC- or U(H)PLC-UV system to a MS detector has become almost routine also in the field of chiral analysis as it allows sensitive and selective measurements as well as the identification of multiple chiral analytes in complex biological matrices or synthetic sample mixtures.
Along this line, the development and application of environmentally friendly and MS fully compatible HPLC and UHPLC methods for either the achiral or chiral analysis (or both) of different compounds (i) in commercially available dietary supplements [2], (ii) of forensic and intelligence relevance [3] and (iii) of pharmaceutical interest [4].Experimental protocols have been successfully coupled to *in silico* simulations [2-4], while the utility of advanced microsampling devices has been plainly demonstrated [3].

References

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