Chemometrics Applied to Protein Process Analysis

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Protein processes, such as protein folding, dimerization processes, conformational transitions, protein-drug interactions, are very diverse in nature and require different experimental monitoring strategies. Some of them imply changes in one or more protein structural levels and, in many cases, this implies the use of several instrumental techniques, the proper fusion of the measurements acquired and the use of powerful chemometric tools to extract the maximum information of the protein processes.

Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS)[1,2] is proposed as a chemometric tool to resolve the conformations linked to the protein processes under study. MCR-ALS provides the concentration profiles associated with the different protein conformations occurring during the process and the related pure spectra. The concentration profiles describe the process mechanism and the structural information in the spectra characterizes the conformations involved.

To prove the quality of the experimental and theoretical methodology proposed, several real examples of protein processes are shown as case studies to illustrate how to select the appropriate experimental measurements and how to apply the data analysis tools according to the protein process of interest[3,4,5,6].

References

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