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Editorial

Challenges and Opportunities in the Application of Chemometrics in the Pharmaceutical and Food Science Industries

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Nowadays, water, air, and soil pollution significantly impact the environment, the plants' growth, and food quality, given that many plants act as bioaccumulators. Therefore, consumers are concerned with food origin, authenticity, composition, and processing since its quality affects their health and lives [1–6].

Used for modeling problems from the environmental sciences, multivariate data analysis [4, 7–10], among which Principal Component Analysis and clustering became an important tool that, in combination with instrumental techniques, has a vital role in the control and monitoring of the various stages of the production chain. The most effective applications of chemometrics in the research and technology of functional foods and pharmaceuticals are those related to measuring compositional parameters based on instrumental analysis methods.

The advantages of the predictive capacity of multiple parameters have made significant contributions to the development of most applications currently used by the food and pharmaceutical industry and the emergence of new applications. With the development of new analysis tools and techniques, new analytical strategies, such as profiling and fingerprinting, contribute to obtaining a large data volume that characterizes the studied systems.

This special issue contains original research papers on developing multivariate and multidirectional methods, methodological aspects of chemometrics research were aimed at optimizing chemical systems, selection of process variables, and fusion of experimental data.

The article of Hssaini et al. [11] answers the question of whether pollination and pollen sources influence the fig seed set and their quality, using a combined approach of vibrational spectroscopy and ionomic fingerprinting. The topic treated is important since the pollination is required for fruit loading and has an important impact on fruit quality [12–15]. Results showed that pollination and pollen source significantly impacted seed set as it was higher in fertilized seeds than in control. Caprification displayed a significant effect on seeds' phenolic components. FTIR-ATR indicated that the fertilized sets have a high vibrational intensity than the control in all fingerprint regions.

Principal component analysis showed high throughput classification with similar patterns for FTIR-ATR fingerprinting and ionomic and biochemical analysis. The multivariate analysis provided identical samples' classification, indicating that vibrational spectroscopy may be accurate, fast, and cost-effective to investigate this effect on large samples further.

This study provides valuable information to understand better the impact of the mutualism between fig and its wasp on seed set.

The article of Park et al. [16] investigated the influence of the reaction conditions on the spectrophotometric and fluorometric assays using different substrates for optimizing for screening the lipase activity from *Chromobacterium viscosum*, *Pseudomonas fluorescens*, *Sus scrofa* pancreas, and *Triticum aestivum*. Different pH, temperature, and substrates have been considered. Experiments of 17 agricultural

products have confirmed the optimized conditions (pH = 7 and temperature = 30°C). The authors also proposed *P. eryngii* as a novel source of lipases. Factorial design is one of the most used methods for optimizing the extraction of different substances, applied to reduce the number of laboratory experiments or confirm the experimental findings [17–20].

In their article, Ngamkhae et al. [21] applied this method to optimize the Kleeb Bua Daeng extraction, one of the most used remedies used in Thailand. Its active components are *Centella asiatica* L., *Nelumbo nucifera* Gaertn., and *Piper nigrum* L, having mainly antioxidant, anti-inflammatory, analgesic, and antidepressant effects [22–25].

Seventeen laboratory experiments at three levels (−1, 0, +1) and three factors (type of solvent—ethyl acetate, ethanol, methanol—number of extraction times—1, 2, 4—and material-to-solvent ratio −1 : 3, 1 : 6, and 1 : 9) were used to evaluate the optimal conditions of the extraction process. In each experiment, different dependent variables were considered: percentage extraction yield, total phenolic content, total flavonoid content, total carotenoid content, and total anthocyanin content. The highest content of each total active compound was not obtained in the same conditions. Therefore, the optimal condition for each active content for product development should be chosen depending on the purpose because different types of active compounds express different biological activities.

Moreover, improving the variable factors from the study for the basic solvent extraction technique might be necessary to get the better suitable variable factors such as changing the type of organic solvent to the ratio of ethanol and water for the extraction.

The articles of Alhazmi et al. [26] and Bărbulescu et al. [27] employ chemometric methods [28–30] for analyzing new drugs. In [26], the amphetamine tables collected in some cities in Saudi Arabia have been studied to determine their content. The same techniques—GC-MS and ICP-MS—have been used by the authors to perform analysis of various other substances of abuse and determined a number of constituents [31–33] in the samples. Apart from the amphetamine, other psychoactive and nonpsychoactive additives were also identified (caffeine, lidocaine, diphenhydramine, and 8-chlorotheophylline), which may have been added to enhance the effects of amphetamine and to increase the dependence. The samples have finally been classified into six clusters, using hierarchical clustering with average linking, based on the percentage of different compounds found.

The appearance on the free market of synthetic cannabinoids raised the researchers' interest in establishing their molecular similarity. A rigorous criterion for classifying drugs is their chemical structure. In [27], the authors present their research on the structural similarity of two groups of drugs—benzoylindoles and phenylacetylindoles—using the facilities provided by rcdk and ChemmineR packages in R. Statistical analysis and clustering of the molecules are performed based on their numerical characteristics extracted using cheminformatics methods. Their similarities/dissimilarities have been emphasized using the Tanimoto index, dendrograms, and heat map. The highest discrepancies are found in the phenylacetylindoles group. Further practical studies should confirm the similarity of the actions and effects in the same cluster and the possible cure using the same inhibitors. The study is extended in [34] with the possible activities of the investigated drugs.

We hope that the readers will find new idea for their research in the related research fields.

Conflicts of Interest

The editors declare that they have no conflicts of interest regarding the publication of this special issue.

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