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. Caprication 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. cryn- gi* 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 Bârbulescu 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 rckd 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.

**Acknowledgments**

The authors thank Prof. Dr. Eng. Habil. Cristiana Rădulescu for her contribution in promoting the special issue.

Alina Bârbulescu
Lucia Barbeș

**References**

[1] A. A. Georgescu, A. Danet, C. Radulescu, I. D. Dulama, and D. Elena, “Determination of several elements in edible mushrooms using ICP-MS,” *Romanian Journal of Physics*, vol. 61, no. 5–6, pp. 1087–1097, 2016.

[2] A. Chilian, O. Bancuta, I. Bancuta et al., “Study of the influence of Zn concentration on the absorption and transport of Fe in maize by AAS and EDXRF analysis techniques,” *Romanian Reports in Physics*, vol. 67, no. 3, pp. 1138–1151, 2015.

[3] A. Bârbulescu and C. Ş. Dumitriu, “Assessing water quality by statistical methods,” *Water*, vol. 13, no. 8, p. 1026, 2021.

[4] A. Al-Taani, Y. Nazzal, F. Howari et al., “Contamination assessment of heavy metals in agricultural soil, in the Liwa Area (UAE),” *Toxics*, vol. 9, no. 3, p. 53, 2021.

[5] I. Manea, L. Manea, C. Radulescu et al., “Assessment of metals level in several meat products obtained through conventional and traditional methods,” *Romanian Report in Physics*, vol. 69, no. 4, p. 711, 2017.

[6] N. M. Tanase, I. V. Popescu, C. Radulescu et al., “Occurrence, toxicological risks of heavy metals and possible agricultural consequences of sewage sludge from urban treatment plants,” *Romanian Journal of Physics*, vol. 65, p. 812, 2020.

[7] A. Bârbulescu, L. Barbeș, and C. Ş. Dumitriu, “Assessing the water pollution of the Brahmaputra River using water quality indexes,” *Toxics*, vol. 9, no. 11, p. 297, 2021.

[8] C. Costa, C. Taiti, M. C. Strano et al., “Chapter 8- multivariate approaches to electronic nose and PTR–TOF–MS technologies in agro-food products,” in *Electronic Noses and Tongues in Food Science*, M. L. Rodríguez Méndez, Ed., pp. 73–82, Academic Press, 2016.

[9] S. L. C. Ferreira, M. M. Silva Junior, C. S. A. Felix et al., “Multivariate optimization techniques in food analysis - a review,” *Food Chemistry*, vol. 273, pp. 3–8, 2019.

[10] A. Valdés, A. Beltrán, C. Mellinas, A. Jiménez, and M. C. Gar- gíos, “Analytical methods combined with multivariate analysis for authentication of animal and vegetable food products with high fat content,” *Trends in Food Science & Technology*, vol. 77, pp. 120–130, 2018.

[11] L. Hsaini, R. Rouzouk, A. Irchad, R. Aboutayeb, and R. Ouaboub, “Do pollination and pollen sources affect fig seed
set and quality? First attempt using chemical and vibrational fingerprints coupled with chemometrics,” *Journal of Chemistry*, vol. 2022, Article ID 3969165, 13 pages, 2022.

[12] M. Rahemi and M. Jafari, “Effect of caprifig type on quality and quality of Estabhan dried fig Ficus carica cv. Sabz,” *Acta Horticulurae*, vol. 798, no. 798, pp. 249–252, 2008.

[13] B. Gaaliche, M. Trad, and M. Mars, “Effect of pollination intensity, frequency and pollen source on fig (Ficus carica L.) productivity and fruit quality,” *Scientia Horticulurae*, vol. 130, no. 4, pp. 737–742, 2011.

[14] M. Trad, C. Le Bourvellec, B. Gaaliche, C. Ginies, C. M. G. C. Renard, and M. Mars, “Caprification modifies polyphenols but not cell wall concentrations in ripe figs,” *Scientia Horticulurae*, vol. 160, pp. 115–122, 2013.

[15] Y. Rosianski, Z. E. Freiman, S. M. Cochavi, Z. Yablovitz, Z. Kerem, and M. A. Flaishman, “Advanced analysis of developmental and ripening characteristics of pollinated common-type fig (Ficus carica L.),” *Scientia Horticulurae*, vol. 198, pp. 98–106, 2016.

[16] J.-Y. Park, J. Ha, Y. Choi, P.-S. Chang, and K.-M. Park, “Optimization of spectrophotometric and fluorometric assays using alternative substrates for the high-throughput screening of lipase activity,” *Journal of Chemistry*, vol. 2021, Article ID 3688124, 10 pages.

[17] O. Buriac, M. Ciocpec, N. Duteanu, A. Negrea, P. Negrea, and I. Grozav, “Platinum (IV) recovery from waste solutions by adsorption onto Dibenzo-30-crown-10 Ether Immobilized on Amberlite XAD7 Resin-Factorial Design Analysis,” *Molecules*, vol. 25, no. 16, p. 3692, 2020.

[18] A. Gabor, C. M. Davidescu, A. Negrea et al., “Optimizing the lanthanum adsorption process onto chemically modified biomaterials using factorial and response surface design,” *Journal of Environmental Management*, vol. 204, pp. 839–844, 2017.

[19] S. Al-Asheh, R. Jumah, F. Banat, and S. Hammad, “The use of experimental factorial design for analysing the effect of spray dryer operating variables on the production of tomato powder,” *Food and Bioproducts Processing*, vol. 81, no. 2, pp. 81–88, 2003.

[20] A. Mihailescu, M. Negrea, M. Ciocpec et al., “Full factorial design for gold recovery from industrial solutions,” *Toxics*, vol. 9, no. 5, p. 111, 2021.

[21] N. Ngamkhae, O. Monthakantarit, Y. Chulikhit et al., “Optimized extraction method for Kleeb Bua Daeng formula with the aid of the experimental design,” *Journal of Chemistry*, vol. 2021, Article ID 1457729, 10 pages, 2021.

[22] Y. Deng, S. Sriviriyajan, A. Tedasen, P. Hiransai, and P. Graident, “Anti-cancer effects of Piper nigrum via inducing multiple molecular signaling in vivo and in vitro,” *Journal of Ethnopharmacology*, vol. 188, pp. 87–95, 2016.

[23] Z. Zarai, E. Boujebene, N. Ben Salem, Y. Gargouri, and A. Sayari, “Antioxidant and antimicrobial activities of various solvent extracts, piperine and piperic acid from Piper nigrum,” *Lebensmittel-Wissenschaft und-Technologie-Food Science and Technology*, vol. 50, no. 2, pp. 634–641, 2013.

[24] J. H. Park, J. Y. Choi, D. J. Son et al., “Anti-Inflammatory effect of titrated extract of Centella asiatica in phthalic anhydride-induced allergic dermatitis animal model,” *International Journal of Molecular Sciences*, vol. 18, no. 4, p. 738, 2017.

[25] F. Pittella, R. Dutra, D. Junior, M. T. Lopes, and N. Barbosa, “Antioxidant and cytotoxic activities of Centella asiatica (L) urb,” *International Journal of Molecular Sciences*, vol. 10, no. 9, pp. 3713–3721, 2009.

[26] H. A. Alhazmi, W. Ahsan, M. Al Bratty et al., “Chemo-profiling of illicit amphetamine tablets seized from Jazan, Saudi Arabia, using gas chromatography-mass spectrometry and chemometric techniques,” *Journal of Chemistry*, vol. 2021, 10 pages, 2021.

[27] A. Bárbolescu, L. Barbeș, and C. Ş. Dumitriu, “Computer-aided classification of new psychoactive substances,” *Journal of Chemistry*, vol. 2021, Article ID 4816970, 11 pages, 2021.

[28] A. Voicu, N. Duteanu, M. Voicu, D. Vlad, and V. Dumitrascu, “The rcdd and cluster R packages applied to drug candidate selection,” *Journal of Cheminformatics*, vol. 12, no. 1, p. 3, 2020.

[29] S. Mente and M. Kuhn, “The use of the R language for medicinal chemistry applications,” *Current Topics in Medicinal Chemistry*, vol. 12, no. 18, pp. 1957–1964, 2012.

[30] R. Guha, “Chemical informatics functionality in R,” *Journal of Statistical Software*, vol. 18, no. 6, 2007.

[31] H. A. Alhazmi, A. Khalid, S. Sultana et al., “Determination of phytocomponents of twenty-one varieties of smokeless tobacco using gas chromatography-mass spectroscopy (GC-MS),” *South African Journal of Chemistry*, vol. 72, no. 1, pp. 47–54, 2019.

[32] M. Al Bratty, W. Ahsan, H. A. Alhazmi, I. M. Attafi, I. A. Khardali, and S. I. Abdelwahab, “Determination of trace metal concentrations in different parts of the khat varieties (Catha edulis) using inductively coupled plasma-mass spectroscopy technique and their human exposure assessment,” *Pharmacognosy Magazine*, vol. 15, no. 63, pp. 449–458, 2019.

[33] A. Khalid, H. A. Alhazmi, A. N. Abdalla et al., “GC-MS analysis and cytotoxicity evaluation of shammah (smokeless tobacco) samples of Jazan region of Saudi Arabia as promoter of cancer cell proliferation,” *Journal of Chemistry*, vol. 2019, Article ID 3254836, 8 pages, 2019.

[34] A. Bárbolescu, L. Barbeș, and C. Ş. Dumitriu, “Computer-aided methods for molecular classification,” *Mathematics*, vol. 10, no. 9, p. 1543, 2022.