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Nota di contenuto	Intro -- Contents -- Preface -- Chapter 1 -- Commonly Used Chemometrics for Spectral Modeling Transfer -- Abstract -- Challenges and Solutions of Spectral Analysis -- Classic Algorithms -- Spectral Substration Correction -- Shenk's Algorithm -- Direct Standardization -- Piecewise Direct Standardization -- Procrustes Analysis -- Target Transformation Factor Analysis -- Maximum Likelihood Principal Component Analysis -- Slope/Bias Correction -- Improvement of Classic Algorithms -- New Developments in Algorithms -- Canonical Correlation Analysis -- Spectral Space Transformation -- Alternating Trilinear Decomposition -- Multi-Task Learning -- Generalized Least Squares -- Other Algorithms -- Global Calibration, Robust Calibration and Model Update -- Progress of Applications -- SBC Method -- SSC Method -- Shenk's Method -- DS Method -- PDS Method -- CCA Method -- Establishment of Global Model -- Other Applications -- References -- Biographical Sketch -- Chapter 2 -- 1H-NMR Fingerprinting and Pattern Recognition Stepwise Strategy for Quality and Authenticity Control of Olive Oil -- Abstract -- Introduction -- 1H-NMR Spectra of Vegetable Oils -- Adulteration of Olive Oil with Vegetable Oils -- PLS-DA Models to Confirm the Presence of Virgin Olive Oil or Olive Oil in Blends with Vegetable Oils -- PLS-DA Models to Discriminate Blends of Virgin Olive Oil with Vegetable Oils -- PLS-DA Models to Discriminate Blends of Olive Oil with Vegetable Oils

-- PLS-R Models to Determine the Percentage of Vegetable Oil in the Blend with Virgin Olive Oil or Olive Oil -- PLS-DA Models to Discriminate Between 'Legal' and 'Illegal' Blends of Virgin Olive Oil or Olive Oil with Vegetable Oils -- PLS-DA Models to Discriminate between Blends of Virgin Olive Oil or Olive Oil with Different Compositions of Vegetable Oils.
 Prediction of Blends of Olive Oil with other Vegetable Oils --
 Conclusion -- Acknowledgments -- References -- Chapter 3 -- A Metabolomics Approach Based on ¹H-NMR Fingerprinting and Multivariate Data Analysis for Virgin Olive Oil Stability Assessment --
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Sommario/riassunto

"Chemometrics is a discipline of chemistry that finds correlation between specific data using mathematical and statistical methods. During any thorough research, the scientists are handling vast amounts of data related to the samples which are being researched. In this type of research, finding the correlation (similarities or differences) between analyzed samples and data is of great importance. In the first chapter, commonly used chemometrics for spectral modeling transfer is examined. The second chapter provides an analytical tool to detect fraud when olive oil is illegally blended with VOs or a 'legal' blend is falsely labelled with respect to the botanical nature of the oils mixed and/or the percentage of each oil in the declared mixture. H-NMR spectral data of olive and virgin olive oils and their mixtures with the VOs most commonly used to make blends was analysed by pattern recognition techniques to develop multivariate classification and regression models, which were organised in a decision tree to afford a stepwise strategy for the aimed purposes. The next chapter focuses on a metabolomics approach based on H-NMR fingerprinting and multivariate data analysis for virgin olive oil stability assessments. In the fourth chapter, the authors review unsupervised methods using both principal component analysis (PCA) and hierarchical cluster analysis (HCA). Using these methods, they were able to spot the correlation between the samples and underlying data structures without the potential bias of scientists about the previous knowledge of data samples"--