

1. Record Nr.	UNINA9910644087903321
Titolo	Capillary electrophoresis -- mass spectrometry for proteomics and metabolomics : principles and applications // edited by Rawi Ramautar and David D. Y. Chen
Pubbl/distr/stampa	Hoboken, New Jersey : , : John Wiley & Sons, , [2023] ©2023
ISBN	3-527-83309-9 3-527-83308-0
Descrizione fisica	1 online resource (403 pages)
Disciplina	541.372
Soggetti	Capillary electrophoresis
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Cover -- Title Page -- Copyright -- Contents -- Preface -- Chapter 1 Capillary Electrophoresis-Mass Spectrometry Interfacing: Principles and Recent Developments -- 1.1 Introduction -- 1.2 General Considerations of CE-ESI-MS -- 1.2.1 Electrospray Ionization -- 1.2.2 Electrical Circuit in CE-ESI-MS -- 1.2.3 CE Modes and Conditions in CE-MS -- 1.3 Sheath Liquid Interfaces -- 1.3.1 Coaxial SheathFlow ESI-MS Interface -- 1.3.2 Nanoflow Sheath Liquid ESI-MS Interface -- 1.4 Sheathless Interfaces -- 1.4.1 PorousTip Interface -- 1.4.2 Other Sheathless Interfaces -- 1.5 Other CE-ESI-MS Interfaces -- 1.5.1 Liquid Junction -- 1.5.2 InterfaceFree CE-MS -- 1.6 Microchip Electrophoresis-MS Interfaces -- 1.7 Alternative Ionization Techniques for CE-MS -- 1.7.1 CE and MCE Combined with MALDI-MS -- 1.7.2 CE-ICP-MS -- 1.8 Concluding Remarks and Outlook -- List of Abbreviations -- References -- Chapter 2 Data Analysis Strategies in CE-MS for Metabolomics -- 2.1 Introduction -- 2.2 The Annotation Challenge in CE-MSBased Untargeted Metabolomics -- 2.2.1 Peak Picking in CE-MS Metabolomics -- 2.2.2 Alignment Approaches -- 2.2.3 eff Transformation -- 2.2.3.1 Historical Evolution and Current State -- 2.2.3.2 Quantitative Aspects of the Use of Mobilograms -- 2.2.3.3 Technical Considerations of the eff Transformation -- 2.2.4 Reproducibility and Exchange of eff Information Using Libraries --

2.2.5 Interlaboratory Reproducibility -- 2.2.6 ROMANCE -- 2.2.7 Ion Mobility -- 2.3 Data Pretreatment -- 2.3.1 Area Normalization -- 2.3.2 Analytical Quality Monitoring -- 2.3.3 Data Filtering -- 2.4 Data Treatment -- 2.5 Concluding Remarks -- Acknowledgment -- References -- Chapter 3 DataProcessing Workflow for Relative Quantification from LabelFree and Isobaric LabelingBased Untargeted Shotgun Proteomics: From Database Search to Differential Expression Analysis.

3.1 Introduction -- 3.2 Spectra Acquisition and Database Search -- 3.2.1 Parameters Affecting Sequence Database Search -- 3.2.1.1 Database Selection -- 3.2.1.2 Enzyme Specificity and Missed Cleavages -- 3.2.1.3 Posttranslational Modifications -- 3.2.1.4 Precursor Mass Tolerance -- 3.2.2 Target-Decoy Search Strategy for False Discovery Rate Estimation -- 3.2.3 Database Search Engines -- 3.2.3.1 SEQUEST -- 3.2.3.2 Mascot -- 3.2.3.3 Multiple Search Engines -- 3.2.4 Protein Inference -- 3.3 Relative Protein Quantification -- 3.3.1 Filtering -- 3.3.2 Missing Value Imputation -- 3.3.2.1 Imputation Methods -- 3.3.2.2 Comparative Studies -- 3.3.2.3 Normalization -- 3.3.3 Summarization -- 3.3.4 Differential Expression Analysis -- 3.4 Conclusions -- References -- Chapter 4 Data Processing in Metabolomics Capillary Electrophoresis-Mass Spectrometry -- 4.1 Data Extraction and the Interpretation of the Extracted Data -- 4.2 Data Preprocessing -- 4.2.1 Handling Missing Values -- 4.2.2 Normalization -- 4.2.3 Transformation -- 4.2.4 Scaling -- 4.3 Statistical Analysis -- 4.3.1 TwoSample TTest -- 4.3.2 Principal Component Analysis (PCA) -- 4.3.3 Partial LeastSquares Discriminant Analysis (PLS-DA) -- 4.3.4 Support Vector Machine -- 4.3.5 Logistic Regression -- 4.3.6 Random Forest Model -- 4.3.7 Evaluation of Classification Models -- 4.4 Metabolite Identification -- References -- Chapter 5 Utility and Advances of Capillary Electrophoresis-Mass Spectrometry for Metabolomics -- 5.1 Introduction -- 5.2 Technological Developments -- 5.2.1 Improving Sensitivity -- 5.2.2 Increasing Metabolome Coverage -- 5.2.3 Increasing Annotation Capacity -- 5.2.4 Tackling Anionic Profiling -- 5.2.5 Increasing Sample Throughput -- 5.3 Applications -- 5.3.1 Biomedical Samples -- 5.3.2 Microbial Extracts -- 5.3.3 Plants -- 5.4 Concluding Remarks -- Acknowledgment -- Conflict of Interest.

References -- Chapter 6 Comprehensive Lipid Profiling by Multisegment Injection-Nonaqueous Capillary Electrophoresis-Mass Spectrometry: Expanding Coverage Beyond Hydrophilic Metabolites -- 6.1 The Early Origins of Lipidomics -- 6.2 Major Instrumental Platforms in Lipidomics: The Role of Separation Science -- 6.3 NACE-MS: An Emerging Separation Platform for Lipidomics? -- 6.4 Multiplexed Separations for Fatty Acids by MSI-NACE-MS -- 6.5 Comprehensive Lipid Profiling Strategies by MSI-NACE-MS -- 6.6 Future Perspectives and Summary -- References -- Chapter 7 Strategies for Identification of Modified Amino Acids with CE-MS in Metabolomics -- 7.1 Introduction -- 7.1.1 PostTranslational Modifications and Modified Amino Acids -- 7.1.2 Modified Amino Acids as Biomarkers of Pathologies -- 7.2 Methods for the Detection of Modified Amino Acids -- 7.3 Capillary Electrophoresis Coupled to Mass Spectrometry to Analyze Modified Amino Acids -- 7.3.1 Applications of CE-MS for Analysis of Modified Amino Acids -- 7.4 Recent Developments to Enhance and Facilitate the Annotation Process in CE-MS -- Acknowledgments -- References -- Chapter 8 CE-MS Approaches for SingleCell Metabolomics -- 8.1 Introduction -- 8.2 Techniques for SingleCell Metabolome Analysis -- 8.2.1 Highly Sensitive CE-MS Interfacing -- 8.2.2 Online Sample Preconcentration Techniques --

8.2.3 Isolation of Single Cells -- 8.3 Application to SingleCell
Metabolome Analysis -- 8.3.1 Metabolome Analysis of Large Single
Cells with Highly Sensitive Interface -- 8.3.2 SingleCell Metabolome
Analysis with Highly Sensitive Interface and OSP Method -- 8.3.3
SingleCell Metabolome Analysis by Online Sampling and Highly
Sensitive Interface -- 8.4 Conclusions -- References -- Chapter 9 CE-
MS Approaches for Peptidomics -- 9.1 Introduction -- 9.2 Sample
Preparation -- 9.3 CE-MS -- 9.3.1 Basic Characterization.
9.3.2 Peptide Identification -- 9.3.3 Peptide Quantitation -- 9.4
Applications -- 9.4.1 Search, Identification, and Determination of
Biomarkers -- 9.4.2 Food Peptidomics -- 9.4.3 Other Applications --
9.5 Conclusions -- Acknowledgments -- List of Abbreviations --
References -- Chapter 10 Capillary Zone Electrophoresis-Mass
Spectrometry for TopDown Proteomics: Technological Development
and Biological Applications -- 10.1 Introduction -- 10.2 Technological
Development -- 10.2.1 CE-MS Interface -- 10.2.2 Capillary Coating --
10.2.3 Sample Loading Capacity and Separation Window -- 10.2.4
Coupling Novel GasPhase Fragmentation Techniques to CZE-MS/MS for
TDP -- 10.2.5 Electrophoretic Mobility Prediction of Proteoforms --
10.3 Applications of CZE-MSBased TDP -- 10.3.1 Delineation of
Proteoforms of Complex Proteomes, Disease Biomarkers, and
Biopharmaceuticals -- 10.3.2 CZE-MS for Native TDP -- 10.4
Conclusions and Perspectives -- Acknowledgments -- References --
Chapter 11 CE-MS Methods for the Characterization of Monoclonal
Antibodies -- 11.1 Introduction -- 11.2 mAb Characterization
Approaches -- 11.3 Applications -- 11.3.1 Primary Structure
Characterization of Monoclonal Antibodies -- 11.3.1.1 Analytical
Workflow -- 11.3.1.2 Amino Acid Sequence Characterization Using CE-
MS(/MS) -- 11.3.1.3 PTMs Characterization and Relative Quantification
Using CE-MS(/MS) -- 11.3.1.4 Glycosylation Determination Using CE-
MS(/MS) -- 11.3.2 MiddleUp/MiddleDown Analysis -- 11.3.2.1
Analytical Workflow -- 11.3.2.2 mAb Analysis Using MiddleUp Strategy
-- 11.3.2.3 mAb Analysis Using Middle-Down Strategy -- 11.3.3 Intact
Analysis -- 11.3.3.1 Analytical Workflow -- 11.3.3.2 mAb Analysis in
Denaturing Conditions Using CE-MS -- 11.3.3.3 mAb Analysis in Native
Conditions Using CE-MS -- 11.3.4 Automation: Future of CE-MS for
mAb Analysis -- 11.4 Conclusion -- References.
Chapter 12 CE and CE-MS Approaches for Glycan Analysis -- 12.1 The
Importance of Glycosylation -- 12.2 Capillary Electrophoresis in
Analytical Glycomics -- 12.2.1 Sample Preparation for CEBased Glycan
Analysis -- 12.2.2 Analysis of Oligosaccharides from Biological
Samples -- 12.2.3 Structural Elucidation of Carbohydrates: The GU
Value Approach -- 12.2.4 LIF Sensitivity and Quantification -- 12.3 CE-
MS of Oligosaccharides -- 12.3.1 Major Parameters to Set the ESI for
CE-MS of Derivatized Oligosaccharides -- 12.3.2 CE-MS for
Quantitative Carbohydrate Analysis -- 12.3.3 CE-MS for Glycomic
Studies -- 12.4 Conclusions and Future Prospective --
Acknowledgment -- References -- Chapter 13 CE-MS Approaches for
Glyco(proteo)mic Analysis -- 13.1 Introduction -- 13.1.1 NLinked
Glycosylation -- 13.1.2 OLinked Glycosylation -- 13.1.3 Glycosylation
Workflows -- 13.1.4 Analytical Approaches -- 13.1.5 CE-MS Interfaces
-- 13.2 Glycan Analysis by CE-MS -- 13.2.1 Glycan Derivatization
Strategies -- 13.3 Glycopeptide Analysis -- 13.3.1 Sample Treatment
-- 13.3.2 Separation Conditions -- 13.3.3 Applications -- 13.4 Protein
Analysis -- 13.4.1 Sample Treatment -- 13.4.2 Separation Conditions
-- 13.4.3 Applications -- 13.5 Conclusions and Outlook --
Acknowledgments -- List of Abbreviations -- References -- Index --
EULA.
