## Contents

**Preface** ................................................................. v

**Contributors** .......................................................... ix

1 Bryophytes: Liverworts, Mosses, and Hornworts: Extraction and Isolation Procedures ........................................... 1

   *Yoshinori Asakawa and Agnieszka Ludwiczuk*

2 Plant Tissue Extraction for Metabolomics ........................................ 21

   *Ute Roessner and Daniel Anthony Dias*

3 Detection of Polar Metabolites Through the Use of Gas Chromatography–Mass Spectrometry ......................................... 29

   *David P. De Souza*

4 A Robust GC-MS Method for the Quantitation of Fatty Acids in Biological Systems ........................................ 39

   *Nirupama Samanmalie Jayasinghe and Daniel Anthony Dias*

5 A Workflow from Untargeted LC-MS Profiling to Targeted Natural Product Isolation ........................................... 57

   *Damien L. Callahan and Candace E. Elliott*

6 Lipidomics: Extraction Protocols for Biological Matrices ........................................ 71

   *Thusitha Wasantha Thilaka Rupasinghe*

7 Metabolite Analysis of Biological Fluids and Tissues by Proton Nuclear Magnetic Resonance Spectroscopy ......................... 81

   *John Robert Sheedy*

8 NMR Spectroscopy: Structure Elucidation of Cycloelatanene A: A Natural Product Case Study ........................................ 99

   *Sylvia Urban and Daniel Anthony Dias*

9 NMR-Based Metabolomics: A Probe to Utilize Biodiversity .......... 117

   *Lucía P. Santos Pimenta, Hye Kyong Kim, Robert Verpoorte, and Young Hae Choi*

10 Extraction Protocol for Nontargeted NMR and LC-MS Metabolomics-Based Analysis of Hard Coral and Their Algal Symbionts ........................................... 129

    *Benjamin R. Gordon, William Leggat, and Cherie A. Motti*

11 Determination of Absolute Configuration Using Single Crystal X-Ray Diffraction ........................................... 149

    *Abigail L. Albright and Jonathan M. White*

12 Natural Product Chemistry in Action: The Synthesis of Melatonin Metabolites K₁ and K₂ ........................................ 163

    *Helmut M. Hügel and Oliver A.H. Jones*
13 Discovery, Biosynthesis, and Rational Engineering of Novel Enterocin and Wailupemycin Polyketide Analogues .................................................. 171
John A. Kalaitzis
14 Bioassays for Anticancer Activities ................................................................. 191
Janice McCauley, Ana Zivanovic, and Danielle Skropeta
15 Screening for Antidiabetic Activities ............................................................... 207
Rima Caccetta and Hani Al Salami
16 Screening for Antibacterial, Antifungal, and Anti quorum Sensing Activity .... 219
Elisa J. Hayhoe and Enzo A. Palombo
17 Metabolomics and Dereplication Strategies in Natural Products ...................... 227
Ahmed Fares Tawfike, Christina Viegelmann, and RuAngelie Edrada-Ebel
18 Bridging the Gap: Basic Metabolomics Methods for Natural Product Chemistry .................................................. 245
Oliver A.H. Jones and Helmut M. Hügel
19 Strategies in Biomarker Discovery. Peak Annotation by MS and Targeted LC-MS Micro-Fractionation for De Novo Structure Identification by Micro-NMR .............................................................. 267
Philippe J. Eugster, Gaëtan Glauser, and Jean-Luc Wolfender
20 Statistical Analysis of Metabolomics Data ......................................................... 291
Alysha M. De Livera, Moshe Olshansky, and Terence P. Speed

Index .................................................................................................................. 309