
Preface

Estimation of the metabolite complement of plant material involves a wide range of techniques and technologies and that breadth continues to increase. The plant metabolome is both highly complex and highly dynamic and its measurement requires very careful control of “noise”, since biological, experimental, and technical variability at all stages of the experimental workflow threaten to overwhelm the biological signals. The workflow must start with detailed and statistically justified experimental design leading to careful identification and preparation of study material followed by harvest and quenching of metabolism. Metabolomics research typically involves multiple sites for material preparation and analysis and most investigations are “high throughput”, meaning that chemical analysis of sample sets are inevitably carried out over an extended period of time. These factors mean that well-validated procedures for shipping and storage of biological materials are required prior to application of one or more of the wide range of chemical analysis techniques which yield highly multivariate metabolomic data. A range of data analyses procedures must be applied to these data, starting with data cleaning and alignment (pre-processing), proceeding possibly to chemical identification and finally to statistical modelling designed to produce justifiable and biologically relevant results. Across all stages of this workflow, up to and including the statistical analysis, accurate and detailed collection of meta-data are also essential for good process management, to satisfy reporting requirements and to ensure wider interpretability and reuse (durability) of results. This volume therefore presents methods for all the stages of the plant metabolomics workflow.

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