

Introduction to Natural Product Metabolomics and to Efficient Isolation Strategies for Biomarker Identification

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Friday 28 August 2015

METABOLOMICS - DATA MINING & BIOMARKER ID

09h00 - 10h30 (90') - Wolfender

1. Introduction to metabolomics: general principles

BREAK 10h30 - 10h45

10h45 - 12h15 (90') - Wolfender

2. Non-separative spectral methods for metabolomics (MS, NMR, IR)

LUNCH BREAK 12h15 - 13h30

13h30 - 15h00 (90') - Wolfender

3. Separative techniques: HPLC, UHPLC and GC

4. MS hyphenation with separation techniques (LC-MS, GC-MS)

BREAK 15h00 - 15h15

15h15 - 16h45 (90') - Wolfender

5. Introduction to *Arabidopsis thaliana*: a case study for metabolomics

6. Rapid analysis in HPLC for Fingerprinting

7. Multivariate data analysis (PCA, HCA)

Saturday 29 August 2015

METABOLOMICS - DATA MINING & BIOMARKER ID

09h00 - 10h30 (90') - Wolfender

8. Advanced multivariate data analysis (Supervised methods)

9. Biomarkers identification (HRMS, MS/MS microNMR)

BREAK 10h.30 - 10h.45

10h45 - 12h15 (90') - Wolfender

10. Generation of biological Knowledge

11 . Examples of metabolomics in natural product research and discussion

LUNCH BREAK 12h.15 - 13h.30

Saturday 29 August 2015

PREPARATIVE METHODS FOR BIOACTIVE NATURAL PRODUCT ISOLATION

13h30 - 15h00 (90') - Queiroz

1. Generalities on natural product matrices and sample preparation

2. Preparative LC methods (FLASH, MPLC, semi prep. HPLC)

BREAK 15h.00 - 15h.15

15h15 - 16h45 (90') - Queiroz

3. Liquid preparative chromatography methods (CPC, HSCCC)

4. Strategies for bioactivity guided isolation

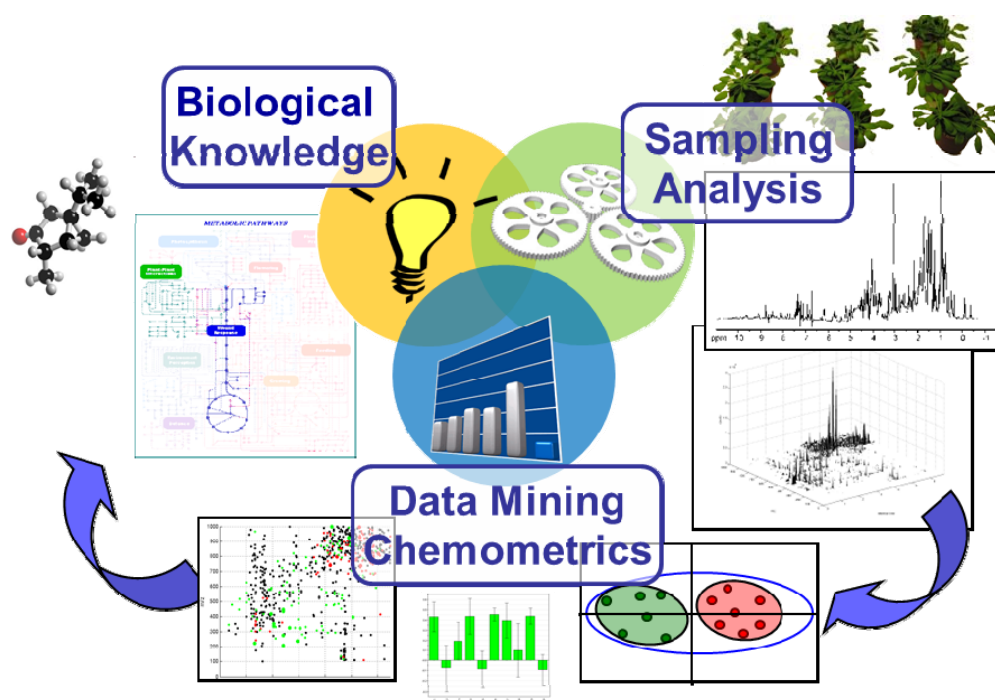
5. Final Discussion

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Plants produce over 200,000 different metabolites/natural products, many of which play important functions in plant growth, development and defense. Recent developments in mass spectrometry (MS) nuclear magnetic resonance (NMR) [1] have enabled metabolite analysis at the metabolomic level [2]. This workshop will introduce all methods for studying plant metabolomes. Metabolomics experimental design, sample preparation, statistics and bioinformatics tools and biomarker identification will be discussed and illustrated by several applications in the field of natural product research.



Summary of typical plant metabolomics workflow

In addition a section will be entirely dedicated to natural products isolation at the preparative scale. Various modern and efficient strategies will be discussed including chromatography gradient transfer methods, MS-targeted isolation integration of the fractionations strategies with miniaturized bioassays [3].

1. Wolfender J-L, Marti G, Thomas A, Bertrand S (2015). Current approaches and challenges for the metabolite profiling of complex natural extracts. *J Chromatogr A* 1382: 136-164.
2. Wolfender J-L, Rudaz S, Choi YH, Kim HK (2013). Plant metabolomics: from holistic data to relevant biomarkers. *Curr. Med. Chem.* 20: 1056-90.
3. Queiroz EF, Wolfender J-L. 2014. Innovative Strategies in the Search for Bioactive Plant Constituents. In *Handbook of Chemical and Biological Plant Analytical Methods*, First Edition. Hostettmann K, Stuppner H, Marston A, Chen S (Ed.). John Wiley & Sons, Ltd.