

High resolution tailored metabolomics in health related and environmental research

Philippe Schmitt-Kopplin

1. Helmholtz Zentrum München, Analytical BioGeoChemistry, Oberschleißheim, Germany

Email: schmitt-kopplin@helmholtz-muenchen.de

2. Technische Universität München, Analytical Food Chemistry, Freising/Weihenstephan, Germany



Prof. Ph. Schmitt-Kopplin's team performs tailored and comprehensive metabolomics in food, health and geosciences. He has a strong profile in analytical chemistry with integrated approaches combining (ultra)high resolution mass spectrometry, separation sciences, NMR-spectroscopy with (bio)informatics for the description of complex organic systems on a molecular level. A focus in the last decade was to implement magnetic resonance mass spectrometry into applications for a rapid and robust tool for deep metabotyping and small molecules profiling. One focus is on the chemical understanding of microbiomes in health and environments and integrating these information with existing biological, metaproteome or metagenome data. His interdisciplinary studies are related to relevant geochemical questions (C and S-cycling, halogens, origin of life) and important biology/health issues related to environmental factors (allergies, nutrition, metabolic diseases) at the interface of chemistry and biology. He is director of the research unit analytical BioGeoChemistry of the Helmholtz Zentrum München, Germany and is member of the Technische University Munich and heads the Comprehensive Foodomics Platform of the Institute of analytical Food Chemistry.

Abstract:

From a traditional definition in the field of human health, metabolomics measures the concentrations of the large number of naturally occurring small molecules (called metabolites), that are produced as intermediates and end-products of all metabolic processes. They are analyzed from biological samples and body fluids such as urine, saliva, blood plasma, tissue sample; even the simple breath (exhaled breath condensates) can carry the information about the state of health. The total number of different metabolites is still unknown; some estimation ranges from few ten thousands to about one million, but even this latter estimate may be conservative; including plant and bacterial metabolites that are not necessary to keep the organism alive, also referred to as secondary metabolites, the number is enormously larger. The probable number of metabolites is also considerably larger than the number of corresponding genes, so it seems that the currently available databases cover at best 5% of the total number of existing metabolites. With our integrated analytical approaches (LC-MS, NMR and ICR-FT/MS) data we annotate from databases around 10% of the experimental signals.

Metabolomic, as the comprehensive study of metabolic reactions is growing very rapidly and integrates the knowledge of earlier developed Omics-branches. Especially ICR-FT/MS describes highly complex mixtures in complex systems on the level of the elementary composition distribution and is shown in this presentation as an dedicated and innovative mass spectrometry tool to understand the composition and processes on a molecular level in various study fields from food chemistry, biology, microbiomes towards the discovery of new bioactives.