Session 7 - NMR Spectroscopy / MS imaging (Co-chairs: Deborde/Schneider)

07-01: NMR in plant science –methods and selected examples

Bernd Schneider

Max Planck Institute for Chemical Ecology, Beutenberg Campus, Hans Knöll Str. 8, 07745 Jena, Germany

Nuclear magnetic resonance (NMR) techniques have expanded into various sciences such as chemistry, biochemistry, medicine, and material science. Nowadays NMR is one of the most powerful analytical techniques to study chemical structures, including low-molecular weight compounds and macromolecules as well as their dynamics and their interaction with the chemical environment. Therefore, NMR spectroscopy and related techniques, such as magnetic resonance imaging (MRI) and magnetic resonance microscopy (MRM), are still gaining increasing attention in natural product chemistry, chemical ecology and many disciplines of plant sciences. Although of intrinsically moderate sensitivity, the unique possibilities to directly determine linkages between atoms of a molecule, to distinguish isomers, to analyse molecules of any polarity without derivatization, the ease of quantification of compounds in a mixture, as well as the non-destructiveness and other advantages of NMR justify the purchase of the relatively expensive spectrometer hardware.

After providing an overview on the different magnetic resonance techniques, including coupling methods (e.g. LC-NMR) and combinations of NMR with other analytical tools (e.g. laser-assisted microdissection), this presentation will focus on applications of NMR in plant natural product chemistry and chemical ecology. In particular, this presentation aims to illustrate how NMR can be used to deepen our understanding of the role of natural compounds in the complexity of inter- and intra-species interactions that occur in nature. Selected examples will demonstrate how NMR can be used to examine the chemical and enantiomeric purity of compounds, to elucidate new natural products, to identify the structures of enzyme products, as well as how to study spatio-temporal distribution of natural products within special plant cells and tissue. Recent developments, e.g. retrobiosynthetic approaches demonstrating the capabilities of NMR to elucidate biosynthetic and metabolic pathways by means of using stable isotope labelling, are also subject of the presentation.