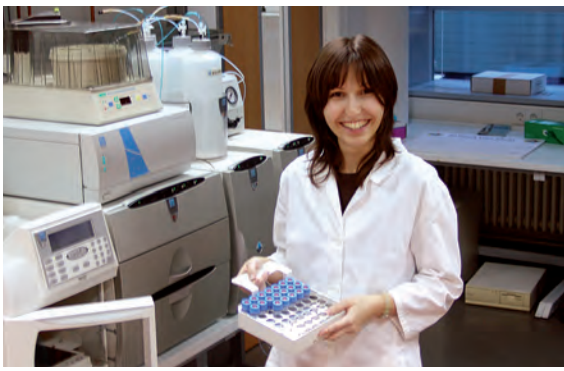

Research Service Facility
Laboratory for Spectrometry

Spectroscopic methods are essential to analysing biogeochemical samples and determining their chemical composition including minerals, metals, and heavy metals. Chromatographic methods are used to identify carbohydrates in water samples and in plant extracts. The Laboratory for Spectrometry (SpecLab), headed by Michael Raessler, performs both of these techniques, and works to address the growing need for method development in the analytical sciences.

In 2005, the Laboratory for Spectrometry (SpecLab) was launched as an offshoot of "ChemLab", the former central service facility for inorganic chemical analyses. SpecLab now focuses on spectroscopic and chromatographic analyses of water, plant, and soil samples, as well as soil extracts. Routine analyses implement methods ensuring the sensitive and reliable determination of carbohydrates in plant extracts and water samples. The methods implemented by SpecLab were successfully presented at national and international conferences in locations ranging from Israel and Japan to the US, and have been published in high-impact scientific journals.

Spectroscopy

Spectroscopic analyses base upon the interactions of electromagnetic radiation with atoms, ions, or molecules to identify chemical compounds. The liquid sample is pumped via capillary tubing to a nebulizer, where an aerosol is produced using pneumatic force. This aerosol is then transported to argon plasma, where the solvent is removed. The aerosol is then vaporized, atomized, and ionized at temperatures of about 6000 – 8000 K. The light emitted by the excited atoms and ions in the plasma is measured to obtain information about the sample. As the excited material in the plasma emits light at several different wavelengths, the emissions from the plasma are polychromatic. This polychromatic radiation is then separated into individual wavelengths. The emissions from each excited compound can thus be identified, and the intensity can be measured without interference from emissions of other wavelengths. Finally, the separated emission lines of each element present in the sample reach the detector. Quantification of the analyte in the sample is based upon the intensity of the measured emission after appropriate calibration.

Portrait of the Leader

Michael Raessler studied chemistry in Munich and Kiel. After completing his undergraduate work he joined the GSF Research Centre for Environment and Health, Institute of Ecological Chemistry, at Neuherberg, and obtained his PhD in analytical chemistry and environmental analytics from Technical University of Munich (TUM). In 1997, he built up the service facility of Inorganic Analytics at MPI-BGC, serving as its head until 2005. Since 2006 he has served as the head of the SpecLab service facility; he also teaches at the FSU Jena.

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Spectroscopic Instrumentation
The following equipment is used for spectroscopic measurements and analyses:

- ICP atomic emission spectrometer, 'Optima 3300 DV', Perkin-Elmer
- GF atomic absorption spectrometer, 'Zeman 3030', Perkin-Elmer
- UV/VIS spectrometer, 'Lambda2', Perkin Elmer
- Microwave-assisted high pressure digestion unit, 'Multiwave', Perkin-Elmer

Spectroscopic Measurement Record
In 2010 and 2011, approximately 3,000 spectroscopic analyses were carried out, including about 1,900 water samples. These analyses detected the following elements: aluminium (Al), boron (B), calcium (Ca), cadmium (Cd), copper (Cu), iron (Fe), potassium (K), magnesium (Mg), manganese (Mn), sodium (Na), nickel (Ni), phosphorus (P), sulphur (S), silicon (Si), strontium (Sr), and zinc (Zn). Of the approximately 1,000 soil extracts that were analysed, roughly 200 extracted ammonium chloride, 500 extracted dithionite, 230 extracted oxalate, and 72 extracted ammonium acetate. Elements detected in the ammonium chloride and ammonium acetate extracts were Al, Ca, Fe, K, Mg, Mn, Na, and P. Elements detected in the dithionite and oxalate extracts were Al and Fe. Additionally, about 40 plant samples were digested and analysed for phosphorus, as well as an additional 20 coal/lignite samples that were analysed for heavy metals in accordance with the German sewage directive ('Klärschlammverordnung', DIN EN ISO 11885). To guarantee high-quality analytical data, SpecLab has a rigid quality control protocol; wherever possible, analyses employ standard reference materials issued by the National Institute of Standards and Technology (NIST).

Chromatography
Carbohydrates are one of the major components of plants; the composition of these carbohydrates varies with season, light availability, and vegetative stage. Additionally, the composition of non-structural carbohydrates (NSC) reflects growth and variations in photosynthesis, as well as abiotic stress phenomena such as hyperosmosis. In addition to studying the biological properties of carbohydrates, their exact identification and quantification in plant material is also of vital importance to establishing more precise and reliable carbon balances to more accurately understand biogeochemical cycles and create more realistic models.

Speclab's method for analysing these carbohydrates is based on High Performance Anion Exchange Chromatography coupled with Pulsed Amperometric Detection (HPAEC-PAD). A Dionex ICS 3000 ion chromatographic system equipped with a SP gradient pump, a column oven, an AS 40 autosampler, and an ED amperometric detector with a gold working electrode are used for this process. Analyses are carried out using a CarboPac PA 10 column with 18 mMol NaOH as the eluent, at a flow rate of 1 mL/min. Overall analysis time, including column regeneration, is 30 min.

More than 1,000 plant samples of different origin (*e.g.*, perennial rye grass, deciduous trees such as ash, oak, and wild cherry; and evergreens such as larch and pine) have been analysed for compounds such as sugar alcohols, glucose, sucrose, fructose, arabinose, galactose, raffinose salicin, polyfructans, inulin, and starch.

Atomic emission spectrometer with inductive couped plasma (ICP) ‚Optima 3300DV' from Perkin Elmer

Ion chromatography system with amperometric detector, ‚ICS-3000' from Dionex