ADLERSHOFER KOLLOQUIUM Analytik

Topic: **Water and wastewater through the magnifying glass of mass spectrometry**

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Chair: Dr. Rudolf Schneider (BAM)

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Branch Adlershof, Richard-Willstätter-Str. 11, 12489 Berlin
Building 8.05 / Lecture Hall

Summary: The increasing availability and sensitivity of LC-MS systems has widely opened the analytical window for polar analytes, the so-called new emerging contaminants. These are increasing numbers of compounds from pharmaceuticals and personal care products, herbicides, fungicides and industrial chemicals as well as their transformation products in water treatment and in the environment. LC with high resolution mass spectrometry (HiRes-MS) enables to perform screening approaches to detect a considerable number of known and unknown analytes in complex samples.
In this work we will show the possibilities and limits of applications of target and non-target screening with LC-electrospray ionization-quadrupole-time-of-flight-mass spectrometry (LC-ESI-Q-TOF-MS) combined with computer based data evaluation based on statistical analysis and on tools of computational mass spectrometry. This will be demonstrated for samples from a river Rhine campaign, from electrochemical and microcosm experiments, and from a pilot ozonation plant. In all cases HiRes-MS enables to get a more comprehensive overview on sample composition and identities of so far unknown compounds and their transformation products.