

“Profiling, Data Mining, Data Fusion – modern analytical strategies against food fraud of honeys and olive oils”



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Venue: Research Building Department
„Life, Light & Matter“ of the Interdisciplinary Faculty
of the University of Rostock,
seminar room 110, A.- Einstein-Str. 25, 18059 Rostock

Abstract

Drift time ion mobility spectrometry (DTIMS) is commonly associated with its use as a hyphenation technique in LC-HRMS and seldomly with its potential as a combined analyzer/detection system for gas chromatography. This study describes the application of Headspace-GC coupled to DTIMS in a non-targeted profiling approach for the authentication of the botanical origin of honey. This strategy is based on the analysis of the volatile organic carbons (VOC) and a data mining procedure of the resulting 3D data with suitable algorithms. The current gold standard in honey profiling is 1H-NMR, therefore, our HS-GC-IMS approach is directly compared to NMR profiling. While NMR spectroscopy has a number of advantages, it does also have significant disadvantages, such as pH influence and sensitivity. We were able to show that our fully automatable, cost-efficient and highly sensitive IMS-based methodology was not only able to keep up with the results from NMR profiling, but furthermore is much closer to sensory perception.

As most analytical techniques cover only one key aspect of the characteristics of a sample (e.g. NMR: solubles, GC-IMS: volatiles), we furthermore evaluated multivariate data fusion strategies, which combine data from different analytical techniques into a new data matrix. On the example of the geographic differentiation of extra virgin olive oils by FT-IR x GC-HS-IMS, it could be demonstrated, how powerful these fusion approaches can be compared to the singular interpretation of the techniques.

Speaker's Biography

Since 2011 Professor Weller is the head of the chair of instrumental analytical chemistry in the department of biotechnology of the University of Mannheim. His research focus deals with the authenticity and determination of origin via spectroscopic and spectrometric profiling techniques in combination with data mining approaches as well as in the field of phytoremediation and mobilization of polluted agricultural areas with organochlorine pesticides residues. He is the head of the interdisciplinary competence centre of “Chemometric based analysis and optimization of processes and materials” founded in 2018 at the University of Mannheim. He leads the group of chemometrics and multivariate data analysis within the group of food chemistry of the GdCh.

Professor Weller also researches in cooperation with partner universities, such as Hohenheim, Hamburg and Gießen and is also participating in more projects financed by public promoters, such as BMBF, AIF and BMWI, as well as the industry.

All interested are welcome

Team Viewer Link <http://go.teamviewer.com/v7/m19305426>

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