CHanalysis 2023

7th Meeting of Swiss Analytical Scientists

29.-31. March 2023, Dorint Resort Blüemlisalp Beatenberg

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The Division Analytical Sciences (DAS) of the Swiss Chemical Society (SCS) is organizing *CH*analysis, a meeting of Swiss analytical scientists on a yearly basis.

The goal of this two-day conference series is to stimulate a stronger interaction among persons working in different areas of analytical sciences. Scientists from applied and fundamental research, from industry, education, and regulation are welcome.

The event starts on Wed, March 29, 2023, at 18.00h and ends on Fri, March 31, 2023, at 16.00h.

Sessions Topics

- Instrumentation
- Micro/Nano
- Methods
- Processes
- Data
- Omics

Confirmed Speakers

- Yury Tsybin, Spectroswiss
- Marc Pfeifer, HESSO
- Andreas Riedo, Uni Bern
- Simon Lobsiger, Metas
- Dorina Kotoni, Novartis
- Luc Patiny, Zakodium Sàrl
- Paolo Nanni, FGCZ

Panel Discussion"Didactics in Analytical Science"

- Prof. Dr Eric Bakker, (*DAS President*), University of Geneva
- Adrian Wichser, Empa
- Dr. Gunnar Schwarz, ETH Zurich
- Ahmad Jameel, Chemistry Student Union

Conference Location

Dorint Hotel Beatenberg
Hubel 114
3803 Beatenberg
Tel.: +41 33 841 41 11

http://hotel-interlaken.dorint.com/

Room reservation and allocation will be handled by the conference office.

Travel Information

Traveling by train:
Take the train to Interlaken West, then bus 101 to Beatenberg Hubel.
Swiss Railway timetable on www.sbb.ch

Traveling by car
Motorway 6 from Bern direction Interlaken, take exit 24, Interlaken-West, direction Beatenberg

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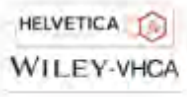

Exhibitors

Program

Wednesday March 29	
18.00	Welcome Apéro
18.45	Opening & DAS President Report by Eric Bakker
19.00	***Yury Tsybin***, Spectroswiss «Super-resolution mass spectrometry»
19.45	Get Together at the Hotelbar
Thursday March 30	
Instrumentation **Chair: Prof. F. Kalman, HES-SO Valais-Wallis**	
09.00	Keynote Lecture ***Marc Pfeifer***, HESSO «Analytical tools in diagnostics: Quo vadis ?»
09.30	***Yaotian Wu***, University of Geneva «Capacitive displays as direct signal transducers for potentiometric measurements»
09.50	***Ankit Jain***, ETH Zurich «A novel absorbance-activated droplet sorting platform for enzyme evolution»
10.10	***Tara Forrest***, University of Geneva «All Covalently Bound Ion-Selective Membranes for Increased Stability in Potentiometric Sensing»
10.30	Coffee Break
Micro/Nano **Chair: Prof. S. Schürch, University of Bern**	
11.00	Keynote Lecture ***Andreas Riedo***, University of Bern «In situ mass spectrometry on current and future space exploration missions for the detection of signatures of life»
11.30	***Naresh Kumar***, ETH Zurich «Surface Molecular Analysis at the Nanoscale using Tip-Enhanced Raman Spectroscopy»
11.50	***Chan Cao***, EPFL Lausanne «Biological nanopores for single-molecule sensing»
12.10	***Pascal Becker***, ETH Zurich «Reducing Sample Amount for the Forensic Analysis of Float Glass Fragments»
12.30	Lunch Break
Methods **Chair: Dr. H.P. Andres, METAS**	
14.00	Keynote Lecture ***Simon Lobsiger,*** METAS «Challenges of food contaminant analysis: key role of certified reference materials»
14.30	***Monique Kuonen***, ETH Zurich «Element Quantification of Water Reference Materials with N2 MICAP MS»
14.50	***Oscar Mendo Diaz***, Empa «Fingerprinting of Chlorinated Paraffins and their Transformation Products in Plastic Consumer Products»
15.15	***Alissa Agerova***, EPFL Lausanne «Identification of cyanotoxin oligopeptides with aerolysin nanopore»
15.30	Coffee Break

Processes
Chair: Dr. D. Kucina, Novartis

16.00 Keynote Lecture
Dorina Kotoni, Novartis
«Forced Degradation Studies: an overview on current best practices & regulatory environment»

16.30 ***Miloš Selaković***, Empa
«Analysis of Breath-related Volatile Organic Compounds with Laser Absorption Spectroscopy»

16.50 ***Selim Kazaz***, Empa
«Why Hydrogen Dissociation Catalysts do not work for Hydrogenation of p-Metals»

17.10 ***Alessia Cesarini***, ETH Zurich/Empa
«Analysis of alkane uptake over commercial C1-C4 coupling catalysts by combinatorial neutron imaging»

17.30 Poster Session

19.00 Dinner

20.30 Get Together at the Hotelbar

Friday March 31

Data
Chair: Prof. E. Pretsch, ETH Zurich and Prof. E. Bakker, University of Geneva

09.00 Keynote Lecture
Luc Patiny, Zakodium Sàrl
«Visualization and processing of analytical data in the browser»

09.30 ***Yousuf Hermani***, Empa
«Sparse Collection of XAFS data via Plasma X-rays»

09.50 ***Claudia Masucci***, University of Zurich/Empa
«Chlorinated Paraffins by Absorption Mode Fourier Transform via Atmospheric Pressure Glow Discharge Micro-Plasma Ionization»

10.10 ***METAS Award Lecture***
Dr. Michael Stravs, Eawag
«High-resolution mass spectrometry: from algorithms to the great outdoors»

10.30 Coffee Break

Omics Chair: Dr. D. Bleiner, Empa	
11.00	Keynote Lecture ***Paolo Nanni***, Functional Genomics Center Zurich (FGCZ) «Mass Spectrometry in Proteomics: Technologies, Methods, and Research Applications for the Life Sciences»
11.30	***Salome Püntener***, University of Zurich «Single-Molecule Peptide Identification using Fluorescence Blinking Fingerprints»
11.50	***Arya Agarwal***, EPFL Lausanne «Detection of oxytocin and vasopressin using biological nanopore»
12.10	***Bastian Duivelshof***, University of Geneva «Using protein-specific retention behavior to improve the characterization of therapeutic antibodies»
12.30	Lunch Break
14.00	***Analytical CHat*** **- Panel Discussion** **"Didactics of Analytical Science"** • Prof. Dr Eric Bakker, (*DAS President*), University of Geneva • Adrian Wichser, Empa • Dr Gunnar Schwarz, ETH Zurich • Dr Christoph Meyer, Lonza • Ahmad Jameel, Chemistry Student Union • **Moderation:** Dr. Davide Bleiner, Empa and University of Zurich
15.00	End of the SCS Symposium

TALKS

Super-Resolution Mass Spectrometry

Yury Tsybin

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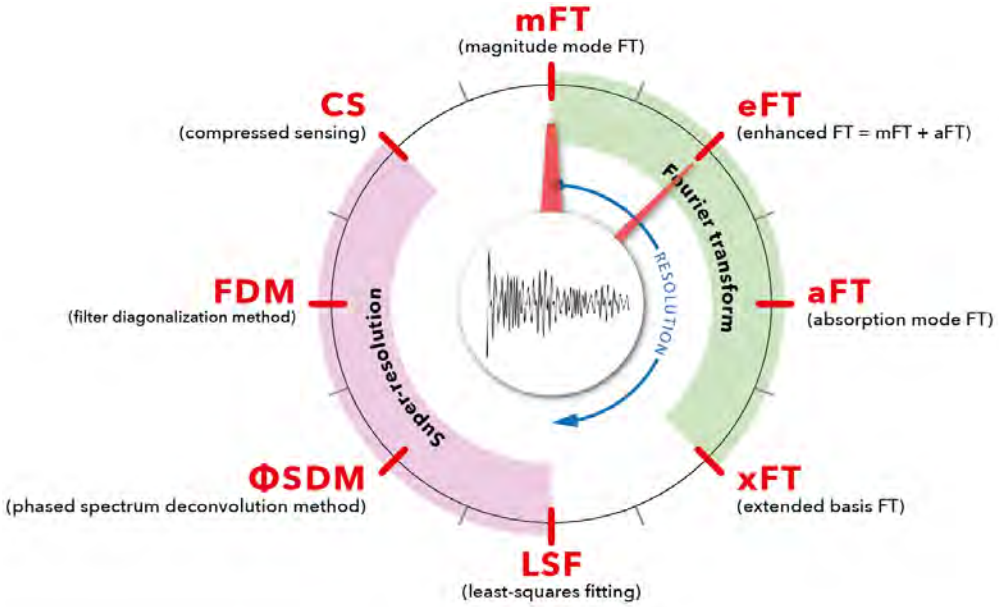
Resolution is one of the most important analytical characteristics in mass spectrometry. Fourier transform mass spectrometry (FTMS) offers the highest resolution performance among all mass spectrometers, Figure [1]. However, achieving high- and ultra-high-resolution in FTMS requires long ion detection times (time-domain transient length), up to 3-4 s and beyond [2]. Acquiring such long transients in FTMS is challenging and is not supported by the majority of FTMS instruments. In addition, the long transients are prohibitive for time-constraint experiments (omics and imaging).



Super-resolution mass spectrometry (SRMS) was thus introduced as an analytical technique to overcome the uncertainty principle in FT and provide a multiple-fold (2-10 times) increase in resolution compared to the conventional FT methods for the same length transients. To achieve this enhanced resolution performance, the SR algorithms are used, Figure [1]. Many SR algorithms, such as Filter Diagonalization Method (FDM), were initially developed and used in the NMR.

On a practical side, the SRMS implementation requires access to the time-domain transients. These are directly available from many NMR and FT-ICR MS instruments but not from the Orbitraps. To enable access to the Orbitrap transients, we developed an external high-performance data acquisition system (FTMS Booster) that acquires time-domain data in parallel to mass spectra [3].

We will introduce the basics of the SRMS and review the SRMS development and main methods from the early days to the most recent advances and applications [2]. Our group at EPFL and then at Spectroswiss has played a pioneering role in the SRMS development and coined the SRMS term.

[1] Y. O. Tsybin, *Chimia*, **2014**, *68*, 168-174.
[2] A. N. Kozhinov, A. Johnson, K. O. Nagornov *et al.*, DOI: 10.1021/acs.analchem.2c04742
[3] K. O. Nagornov, M. Zennegg, A. N. Kozhinov et al., *JASMS*, **2020**, *31*, 257-266

Analytical tools in diagnostics: Quo vadis?

Marc E. Pfeifer, Denis Prim, Milica Jović

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Physicians rely to a significant degree on *in vitro* diagnostic (IVD) tests and imaging modalities for diagnosis and therapeutic decision-making. An increasing number of accidents, infectious and particularly chronic diseases as well as other health problems have in recent decades given rise to sophisticated clinical laboratory automation solutions with high-throughput analyzers processing hundreds or even thousands of samples per day with high reliability and accuracy. Yet, the dynamic and magnitude of the Covid-19 pandemic brought even the larger laboratories to capacity limits. Throughout the world *drive-in* test centers were set up to primarily deal with the sample collection and a plethora of Point-Of-Care (POC) diagnostic devices – with to some extent questionable analytical performances – flooded the market in response to that extraordinary need for diagnostic testing. The pandemic has, no doubt, accelerated the roll-out of telemedicine and decentralization of diagnostic testing that was already occurring due to the progress being made for instance in information and communications technology (ICT), device miniaturization and integration as well as in molecular and engineering biology.

In this presentation, we will give an overview of the global market, of technological developments and milestones in IVD and more specifically in POC diagnostics. We will showcase examples how diagnostic testing is getting closer to patients and consumers, for instance with wearable sensors and at-home diagnostic instruments. To conclude, we will present a POC diagnostic system, aimed for the detection of mild traumatic brain injury (mTBI), that is currently in development [1], the challenges and the opportunities associated with increasing the technological readiness level (TRL) from a proof-of-concept demonstrator conceived in a research laboratory environment towards clinical evaluations and the possible future product development and regulatory approval.

[1] M. Jović, D. Prim, E. Saini, M. Pfeifer, *Biosensors*, **2022**, *12*, 172.

Capacitive displays as direct signal transducers for potentiometric measurements

Yaotian Wu, Eric Bakker*

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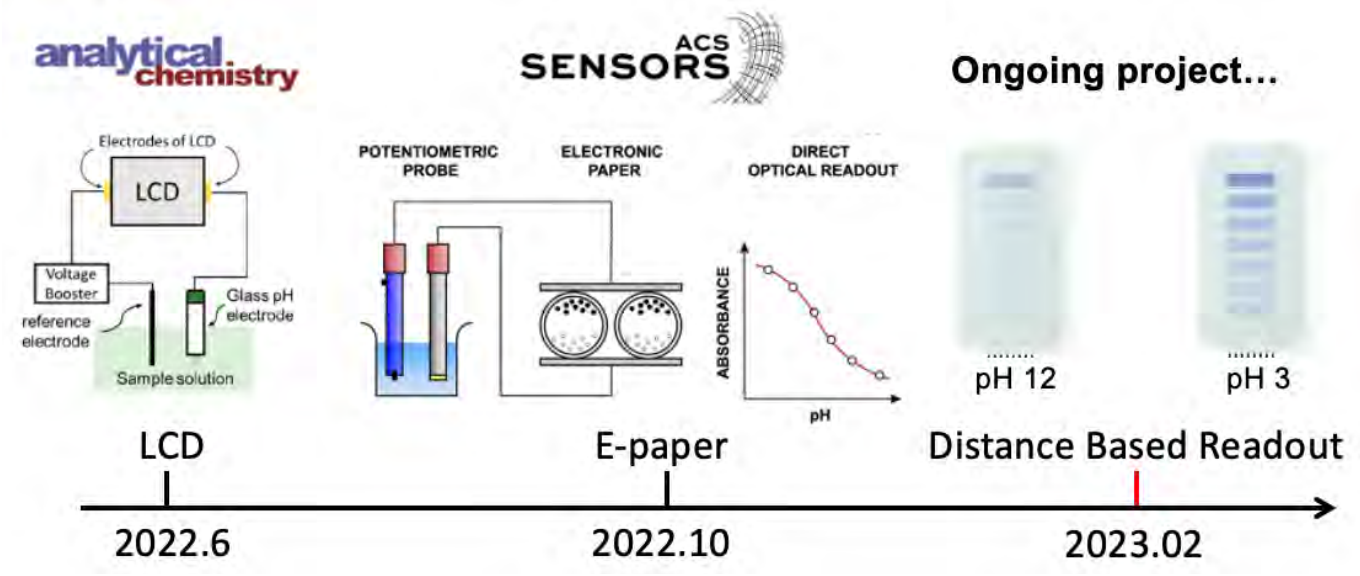
Fully self-powered chemical sensors are very attractive because they should be environmentally friendly and have the potential for miniaturization. Among all self-powered sensors, chemical sensors based on electrical-optical conversion seem attractive because of their precision and compatibility with wearable devices.

Our group reported on capacitive display elements, including liquid crystal displays and e-paper, as transducers to convert the potential signal to a readable color change for the first time. Capacitive displays may precisely tune their absorbance to the applied voltage, if possible with an uncertainty on the order of 0.5 mV.[1,2] Unlike traditional electrochromic materials that slowly change their color through chemical processes on a time scale of minutes, such display elements respond to the applied voltage physically, such as reorienting the liquid crystal in the pixel and migrating charged pigments in an electrical field.[3] This allows one to observe a much faster signal transaction with a few seconds and in a wide voltage range of about 1 V.

This contribution will demonstrate three self-powered sensors using capacitive displays to convert the potential signal directly to an optical readout, including the ability to achieve a direct distance-based readout without the need for a traditional power supply.



[1] Wu, Y. and E. Bakker, *ACS Sens.*, **2022**, *7(10)*, 3201-3207.
[2] Wu, Y. and E. Bakker, *Anal. Chem.*, **2022**, *94(29)*, 10408-10414.
[3] Jansod, S. and E. Bakker, *Anal. Chem.*, **2021**, *93(9)*, 4263-4269.

A novel absorbance-activated droplet sorting platform for enzyme evolution

Ankit Jain*[,a], Mariko Teshima*[,b], Tomas Buryska[a], Dennis Romeis[b], Magdalena Haslbeck[b], Manuel Döring[b], Volker Sieber[b], Stavros Stavrakis[a], Andrew deMello[a]

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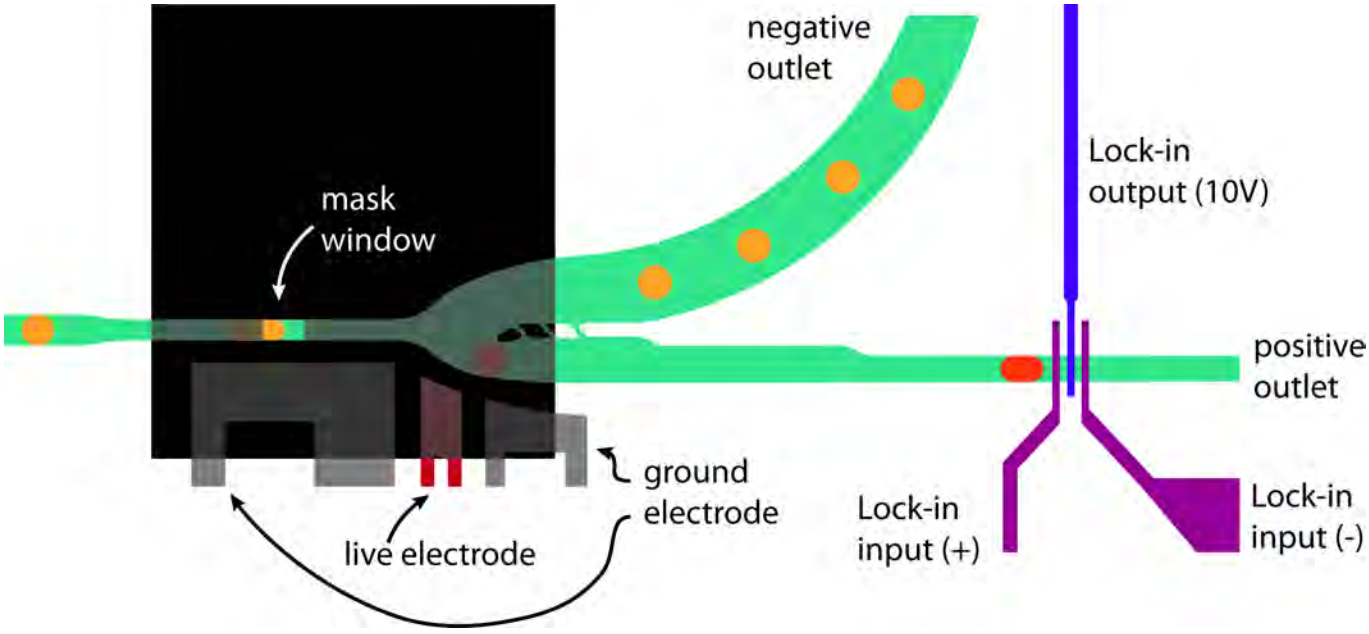
The past few decades have seen a dramatic increase in the use of biocatalysts in commercial chemical processes, shifting the emphasis from energy-intensive traditional chemistry to sustainable chemistry. Unsurprisingly, significant effort has gone into modifying and improving the characteristics of naturally occurring enzymes for use in specific biotechnological applications. Current enzyme engineering techniques, such as directed evolution, require the production and testing of large libraries of mutations to identify commercially valuable variants. Unfortunately, traditional screening approaches are unable to screen such large mutagenesis libraries in a robust and timely manner [1,2]. Droplet-based microfluidic systems are able to produce, process and sort picoliter droplets at kilohertz rates and have emerged as a potentially powerful and high-throughput tool for library screening. However, the reliance of these screening approaches on inline fluorescence detection either restricts their use to a limited number of natural substrates and enzyme classes or involves the use of surrogate substrates, which bias the enzyme optimization process [3,4]. Accordingly, enlarging the "detection toolbox" to include additional optical techniques is a recognized priority. Absorbance-detection, being the most widely used bulk detection method for bioanalytical measurements, is an obvious and potentially powerful option. However, unlike fluorescence, absorbance-based detection is compromised when optical pathlengths are small. This poses problems for it use in microfluidic devices, where optical pathlengths are on the order of tens or hundreds of microns. Moreover, in droplet-based microfluidic systems, scattering at the droplet and oil interface further complicates the detection, and reduces signal-to-noise ratios [5]. Consequently, the existing absorbance-activated droplet sorting platforms require a complicated optical assembly for absorbance detection and are often limited in throughput due to the use of droplet with large volumes [6-8].

We present a novel absorbance-activated droplet sorting platform (iAADS) that allows the direct measurement of absorbance signals from pL-volume droplets using a lithographic mask and refractive index matched fluids, avoiding the use of complicated optical-fibers and external light sources, and allowing the sensitive interrogation and sorting of droplets at kilohertz rates. Additionally, we use an impedance-based detection to identify sorted droplets, which obviates the need for optical monitoring of the microfluidic system. Utilizing this platform, we show a rapid screening of a 10^5-member aldehyde dehydrogenase library towards D-glyceraldehyde using a NADH mediated coupled assay that results in the formation of WST-1 formazan. In a 2x coverage of the library, we successfully obtained four mutant variants with increased V_{max} and two with improved K_m. The most successful variant showed a 51% improvement in catalytic efficiency for the conversion of D-glyceraldehyde, and a notable increase in overall activity was observed for a broad substrate spectrum.

[1] L. Ye, C. Yang, H. Yu, *Applied Microbiology and Biotechnology* **2018**, *102* (2), 559–567
[2] L. Alejaldre, J. N. Pelletier, D. Quaglia, *BioEssays* **2021**, *43* (8), 2100052.
[3] P. Mair, F. Gielen, F. Hollfelder, *Current Opinion in Chemical Biology* **2017**, *37*, 137–144
[4] G. Kolaitis; A. Jain, D. Romeis, T. Buryska, M. Steiger, L. Wuerstl, M. Doering, B. Beer, S. Stavrakis, A. deMello, V. Sieber, *Chemrxiv* **2022**
[5] J. Probst, P. Howes, P. Arosio, S. Stavrakis, A. deMello, *Anal. Chem.* **2021**, 93 (21), 7673–7681

[6] F. Gielen, R. Hours, S. Emond, M. Fischlechner, U. Schell, F. Hollfelder, *PNAS* **2016**, 113 (47), E7383–E7389
[7] E. S.Richter, A. Link, J. S. McGrath, R. W.Sparrow, M. Gantz, E. J. Medcalf, F. Hollfelder, T. Franke, *Lab Chip* **2023**, 10.1039.D2LC00871H
[8] E. J. Medcalf, M. Gantz, T. S. Kaminski, F. Hollfelder, *bioRxiv* 2022.09.13.507731



All Covalently Bound Ion-Selective Membranes for Increased Stability in Potentiometric Sensing

Tara Forrest, Eric Bakker

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Solid-contact ion-selective electrodes have gained significant interest over the last decade due to their ease-of-use, miniaturisation possibilities and low maintenance. They can now be routinely found in the bioanalytical field where they are used to measure a range of blood electrolytes or in environmental monitoring where they enable the continuous measurement of a wide range of relevant ions, such as nitrate, pH or carbonate. Solid contact ion-selective electrodes include an electron conducting material, such as glassy carbon or gold, covered by a transducing material that is known to improve the stability of the signal and suppress undesired ion transport. The last component is a poly(vinyl chloride) (PVC)-based plasticised membrane loaded with ion-exchanger and ionophore that enable selective and sensitive sensing of the target analyte. Unfortunately, this system may suffer from leaching of membrane components that over time causes drift and loss of sensitivity[1], especially when their thickness is reduced to the nanoscale.

We present here a new strategy for creating leak-free ion-selective plasticised membranes. Drawing inspiration from previous work on single membrane component covalent attachment based on a plasticiser-free cross-linked poly(decyl methacrylate matrix)[2-3], we decided here to take advantage of "click" chemistry, also known as azide alkyne cycloaddition, to safely anchor membrane components. Chlorine groups naturally present on PVC can be replaced by azide groups, thus generating an appropriate platform to perform "click" reactions. A similar strategy was already previously developed in our group where "click" chemistry was used to attach a ferrocene molecule to PVC in order to create a transducer-free ion-selective electrode[4]. In our case, the aim is to modify membrane components, and the transducing element in a second step, to include an alkyne group, needed for the final covalent attachment. Taking advantage of the high yield of "click" reactions, alkyne-modified membrane components can then be covalently attached in a quantitative manner by controlling the stoichiometry to achieve a leak-free ion-selective membrane. These new electrodes will be tested using thin-layer membranes[5] to accelerate the leaching process and confirm their improved performances compared to conventional membranes that only rely on lipophilicity.

[1] E. Bakker, P. Bühlmann, E. Pretsch, *Chemical Reviews* **1997**, *97*, 3083-3132.
[2] K.R. Choi, X.V. Chen, J. Hu, P. Bühlmann, *Analytical Chemistry* **2021**, *93*, 16899-16905.
[3] Y. Qin, E. Bakker, *Analytical Chemistry* **2003**, *75*, 6002-6010.
[4] M. Pawlak, E. Grygolowicz-Pawlak, E. Bakker, *Analytical Chemistry* **2010**, *82*, 6887-6894.
[5] T. Forrest, E. Zdrachek, E. Bakker, *Electroanalysis* **2020**, *32*, 799-804.

In situ mass spectrometry on current and future space exploration missions for the detection of signatures of life

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For decades, the detection and identification of signatures of life, past or present, has been one of the key topics in space research and planetary exploration. Its detection is, however, extremely challenging, involving highly demanding aspects ranging from the operation of sophisticated instruments on Solar System bodies other than Earth to the definition of which bio-signature(s) the instruments should be looked for [1]. Since the first Viking mission in the 1970s on Mars, which represents one of the most promising targets in our Solar System, space agencies aim to find traces of life. Unfortunately, no conclusive answer has been found as of yet. Since the detection of liquid oceans underneath a several km thick ice crust, the icy moons of Jupiter and Saturn, e.g., Europa and Enceladus, are considered as high priority targets in current space exploration. Their liquid oceans might harbour life since the basic requirements for life are supported there. Consequently, space agencies, foremost ESA and NASA, are planning to explore these moons.

In this contribution, the most promising classes of signatures of life and the payload of the first Viking lander are briefly presented. This discussion is followed by an introduction of the Sample Analysis for Mars (SAM) instrument, part of the analytical payload of NASAs Curiosity rover, which represents the most sophisticated GC-MS system designed to find biologically relevant organic molecules to this date. Laser Ablation Ionisation Mass Spectrometry, operated in ablation or desorption mode, represents the next generation instrumentation for the detection and identification of traces of life on future missions. This measurement technique allows the detection of several classes of bio-signatures, using one instrument only. The performance of this measurement technique will be demonstrated based on recent studies conducted in laboratories of the University of Bern using a miniature space-prototype LIMS system. These studies cover microbes inoculated in Martian mudstone analogues [2], amino acids [3], and lipids [4].

[1] L.E. Hays, H.V. Graham, D.J.D. Marais, E.M. Hausrath, B. Horgan, T.M. McCollom, M.N. Parenteau, S.L. Potter-McIntyre, A.J. Williams, K.L. Lynch, *Astrobiol.*, **2017**, 17, 363-400.
[2] A. Riedo, C. de Koning, A.H. Stevens, C.S. Cockell, A. McDonald, A. Cedeño López, V. Grimaudo, M. Tulej, P. Wurz and P. Ehrenfreund, *Astrobiol.*, **2020**, 20, 1224-1235.
[3] N.F.W. Ligterink, V. Grimaudo, P. Moreno-García, R. Lukmanov, M. Tulej, I. Leya, R. Lindner, P. Wurz, C.S. Cockell, P. Ehrenfreund, A. Riedo, *Nature Sci. Rep.*, **2020**, *10*, 9641.
[4] N.J. Boeren, S. Gruchola, C.P. de Koning, P. Keresztes Schmidt, K.A. Kipfer, N.F.W. Ligterink, M. Tulej, P. Wurz, Andreas Riedo, *Planet. Sci. J.*, **2022**, *3*, 1-12.

Surface Molecular Analysis at the Nanoscale using Tip-Enhanced Raman Spectroscopy

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Label-free and non-destructive surface molecular analysis at the nanoscale under ambient conditions is essential in several areas of chemical, material and biological sciences including heterogenous catalysis, biomembranes, polymeric materials etc. However, conventional analytical techniques often lack the required sensitivity and/or spatial resolution to achieve this goal. In this talk, I will introduce a rather recent nanoanalytical technique called tip-enhanced Raman spectroscopy (TERS), which combines the molecular specificity and sensitivity of surface-enhanced Raman spectroscopy (SERS) and high spatial resolution of scanning probe microscopy (SPM) to provide correlative topographical and chemical surface characterization at the nanometer length-scales [1]. I will first present an overview of the fundamental principle of TERS and then demonstrate its application with the following three studies recently published by our laboratory:

1. Nanoscale Chemical Imaging of Supported Lipid Monolayers using TERS [2]
2. Molecular-Level Insights on Reactive Arrangement in On-Surface Photocatalytic Coupling Reactions Using TERS [3]
3. Visualizing Surface Phase Separation in PS-PMMA Polymer Blends at the Nanoscale [4]

Through these studies, I will show that TERS can provide unique molecular information which cannot be obtained by any other nanoanalytical techniques.

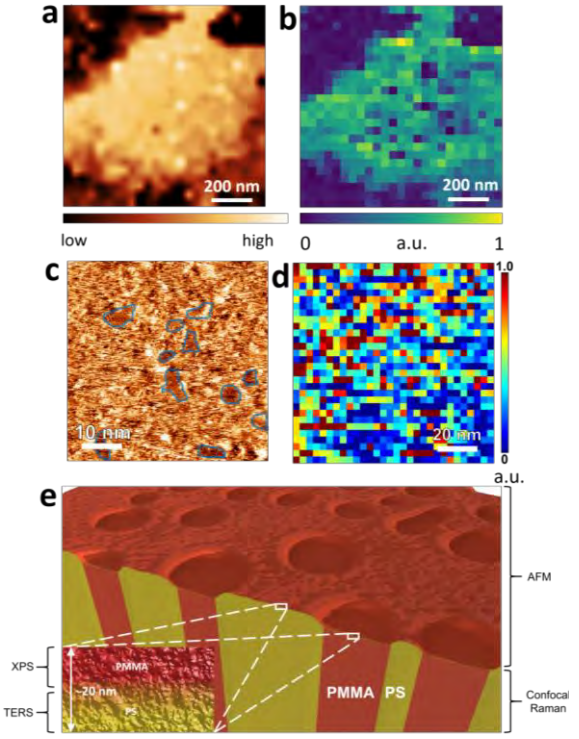

Figure 1. (a) STM topogrphy and (b) TERS images of a DPPC lipid monolayer on Au(111) surface [2]. (c) High-resolution STM topogrphy and (d) TERS images of 4NTP→DMAB photocatalytic conversion on Au(111) surface [3]. (e) Schematic illustration of the 3D structure of phase separation at PS-PMMA polymer blend surface determined using combined AFM, confocal Raman, XPS and TERS measurements [4].

References:

[1] D. Mrđenović, Z.-F. Cai, Y. Pandey, G. L. Bartolomeo, R. Zenobi, N. Kumar, *Nanoscale*, **2023**, *15*, 963-974.
[2] Y. Pandey, N. Kumar, G. Goubert, R. Zenobi, *Angew. Chem. Int. Ed.*, **2021**, *133*, 19189-19194.
[3] Z.-F. Cai, J. P. Merino, W. Fang, N. Kumar, J. O. Richardson, S. D. Feyter, R. Zenobi, *J. Am. Chem. Soc.*, **2022**, *144*, 538-546.
[4] D. Mrđenović, D. Abbott, V. Mougel, W. Su, N. Kumar, R. Zenobi, *ACS Appl. Mater. Interfaces,* **2022**, 14, 24938–24945

Single-Molecule Peptide Identification using Fluorescence Blinking Fingerprints

Salome Püntener[1,2] and Pablo Rivera-Fuentes[1,2]

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2) Department of Chemistry, University of Zurich, CH-8057, Zurich, Switzerland.
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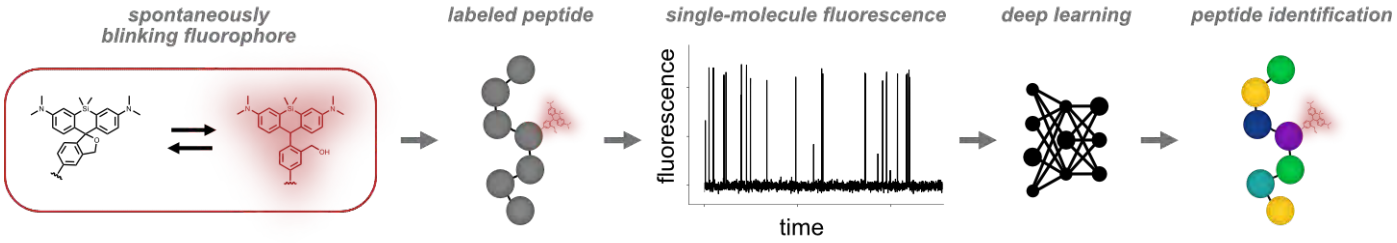
The analysis of the proteome is complicated by the presence of isoforms, post-translational modification (PTM), and the insufficient correlation between the abundance of protein and the transcriptomic or genomic information. As the current state-of-the-art, mass spectrometry-based proteomics methods remain limited in their sensitivity and dynamic range compared to the established single-molecule approaches in genomics and transcriptomics.[1,2] In particular, single-molecule identification of peptides and proteins would enable the analysis of biomarkers that are present in very small quantities, for example in diluted clinical samples, single cells, or isolated organelles.[3]



In this work, we provide a proof-of-concept of a fundamentally new approach to identify single peptide molecules, including subtle PTMs, that does not rely on sequencing.[4] Although this method is presently constrained to targeted studies, it holds potential as a widely applicable, rapid, and accurate single-molecule proteomics technology. Our approach exploits the emission of a spontaneously blinking fluorophore to capture information on the chemical environment of the probe.[5] We use single-molecule fluorescence measurements and a deep learning model based on convolutional, gated-recurrent unit layers to identify the peptide of interest in a targeted manner. By implementing Monte Carlo dropout, we obtain an uncertainty measure for classification which we use for filtering out low-quality traces. We first validate our method on a small set of unnatural peptides of the same length but varying amino acid sequences, which allows us to classify single peptide molecules with overall accuracies > 90 %.[4] Furthermore, the method can be applied to differentiate between peptides with a variable number and position of PTMs. The applicability of the analysis is demonstrated for two PTMs, including the epimerization of an amino acid which would be very difficult to analyze by mass spectrometry. We envision that the technology is adaptable to molecules beyond peptides and proteins depending on available conjugation strategies. Moreover, the method has the potential for further refinement in experimental and analysis aspects to improve the accuracy and extend the applicability to real biological samples.

[1] R. Aebersold, M. Mann, *Nature* **2016**, *537*, 347–355.
[2] B. Domon, R. Aebersold, *Nat Biotechnol* **2010**, *28*, 710–721.
[3] J. A. Alfaro, P. Bohländer, M. Dai *et al.*, *Nat Methods* **2021**, *18*, 604–617.
[4] S. Püntener, P. Rivera-Fuentes, **2023**, *manuscript in revision*. European Patent Application No. 22210671.8
[5] S. N. Uno, M. Kamiya, T. Yoshihara *et al.*, *Nat Chem* **2014**, *6*, 681–689.

Reducing Sample Amount for the Forensic Analysis of Float Glass Fragments

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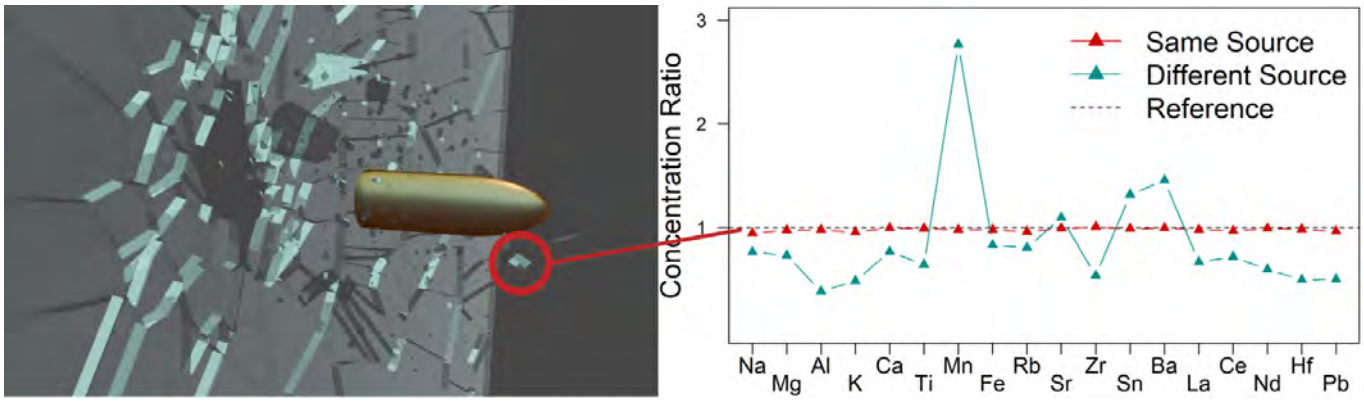
Float glass is a common piece of evidence in burglaries, car crashes and violent crime. The matching of a fragment found in a suspect's clothes or skin to broken glass at the crime scene can be a strong link between the two.[1] Currently, refractive index measurements and elemental fingerprint matching are used to determine the source of a glass fragment. While refractive index measurements suffer from a high rate of errors, elemental fingerprint determination requires a sample volume that is often larger than the common pieces of evidence. Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) for the determination of elemental fingerprints has proven to be the most efficient analytical method for glass fragments, requiring fragments that are approx. 400 x 200 x 100 µm in size.[2] However, half of the recovered samples are smaller than that, limiting the application of the method.[3]



In this work, a new LA-ICP-MS method was developed using a low dispersion ablation cell allowing for a resolved laser pulse analysis of fragments. Due to the fast aerosol washout, multi-elemental analysis with sequential mass analysers was no longer possible. As such, a time of flight mass spectrometer was used for quasi-simultaneous detection of multiple elements. This layer-by-layer approach provides more information from small samples and decreases the required sample volume significantly (approx. 20 µg to 0.8 µg). Furthermore, the increased amount of data points allows the use of new statistical treatments such as multivariate statistical tests. This work investigated different matching procedures, achieving comparable error rates to the established method, while requiring 25x less sample material. Additionally, the effect of aerosol transport on the matching of glass fragments was investigated, with a focus on the effect of uneven samples in low dispersion laser ablation. As a result, the low dispersion ablation cell was modified to allow better aerosol transport for large spot sizes and uneven samples.

[1] R. J. Watling, B. F. Lynch and D. Herring, *J. Anal. At. Spectrom.*, **1997**, *12*, 195–203.
[2] P. Weis, M. Dücking, P. Watzke, S. Menges and S. Becker, *J. Anal. At. Spectrom.*, **2011**, *26*, 1273–1284.
[3] P. Becker, C. Neff, S. Hess, P. Weis and D. Günther, *J. Anal. At. Spectrom.*, **2020**, *35*, 2248–2254.

Challenges of food contaminant analysis: key role of certified reference materials

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Food contaminants are chemical substances (e.g. polycyclic aromatic hydrocarbons, pesticides, dioxins, PCBs, heavy metals) or biological materials (e.g. viruses, bacteria, fungi) that can be harmful to humans. These contaminants can enter the food or form in it during production, processing, storage or transportation, through contact with packaging materials and manufacturing devices, as well as through contamination from the environment. In addition, they can also have their origin from natural sources (natural toxins) or can even be added intentionally (food fraud).

The large number of possible contaminants and the presence of these contaminants in a wide variety of food matrices over a wide range of concentrations pose significant challenges to analytical methods. To address these challenges, a national competence center for chemical and biological analyses in the field of food safety and nutrition is being established at METAS. We currently operate a total of four national reference laboratories (NRLs) in the area of food analysis and perform chemical and biological analyses in food monitoring and population biomonitoring studies. We ensure, through traceable measurement procedures and certified reference materials, that the results of potential hazards from contaminants in food are valid and comparable worldwide.

In this talk, an overview of challenges in the analytics of food contaminants based on current projects at METAS is given. A concrete example for the analysis of polycyclic aromatic hydrocarbons (PAHs) is used to show that the availability of certified reference materials is of central importance in food analysis in order to guarantee the validity of measurement results.

Element Quantification of Water Reference Materials with N_2 MICAP MS

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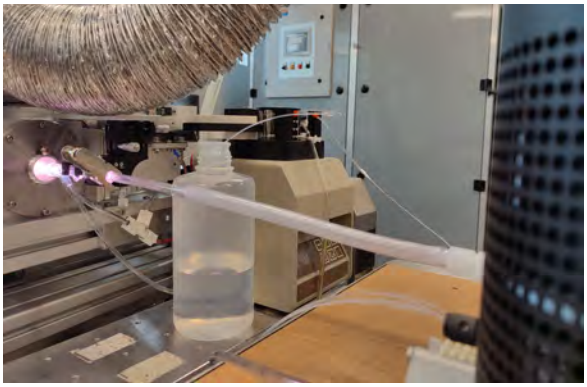
The nitrogen sustained high-power microwave inductively coupled atmospheric pressure plasma (N_2 MICAP)[1] has gained increasing attention in recent years as an alternative ion source for inorganic mass spectrometry (MS) due to its comparable performance to the conventional argon based inductively coupled plasma (Ar ICP).[2,3] In addition to its more cost-effective operation, the nitrogen plasma reduces argon-based plasma species, which enables the analysis of more abundant isotopes of the elements K, Ca, Cr, Fe, and Se in particular. In this study, the N_2 MICAP was combined with a quadrupole mass spectrometer to investigate its quantification capabilities and possible spectral interferences in aqueous solutions with different sample introduction setups.



Two certified water reference materials were analysed with solution nebulization and their main and trace elements were quantified by means of external calibration as well as standard addition. Since wet sample introduction results in a lower plasma temperature due to mass load effects caused by the solvent, additional measurements were made in which a desolvator was used to reduce the water content of the aerosols. With solution nebulization, a high abundance of NO is observed, which is suspected to suppress elements with high ionization energies.[4] Since using desolvation decreases such oxygen-based species, higher sensitivities of these elements are expected. A comparison between quantification using wet and desolvated sample introduction is made in terms of detection limits, trueness and precision of the determined element concentrations as well as possible spectral interferences.

[1] J. Jevtic, A. Menon, V. Pikelja, Patent No.: PCT/US2014/024306, **2014.**
[2] M. Schild, A. Gundlach-Graham, A. Menon, J. Jevtic, V. Pikelja, M. Tanner, B. Hattendorf, D. Günther, *Anal. Chem.* **2018**, *90*, 13443-13450.
[3] C. Neff, P. Becker, B. Hattendorf, D. Günther, *J. Anal. At. Spectrom.* **2021**, *36*, 1750-1757.
[4] M. Kuonen, G. Niu, B. Hattendorf, D. Günther, *J. Anal. At. Spectrom* **2023**, Accepted Manuscript

Fingerprinting of Chlorinated Paraffins and their Transformation Products in Plastic Consumer Products

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Chlorinated paraffins (CPs) are high production volume chemicals (1 million t/y) commonly used as plasticizers and flame retardants in plastic materials and as coolant fluids in metalwork [1]. Technical CP mixtures can contain a broad range of carbon (C, n_C=9–30) and chlorine (Cl, n_{Cl}=2–20) homologues with millions of constitutional isomers and stereoisomers. Therefore, CP-containing plastics used in our daily life can contain up to 400 C-Cl-homologues and a detailed mass spectrometric analysis provides complete homologue distributions and with it, fingerprints of such materials.

Exposing CPs to heat leads to the formation of unsaturated compounds such as chlorinated mono- (COs), di (CdiOs) and tri-olefins (CtriOs) [2]. These transformations can occur at different stages of plastic manipulations altering homologue distributions of initial CP mixtures providing new patterns. These patterns can be interpreted as specific fingerprints, motifs that can be distinguished and tracked. Such fingerprints may lead to manufacturers, production processes or specific applications of CP-containing materials. Therefore, CP fingerprinting can develop to a promising tool for future source apportionment studies to identify polluting sources and with it, to reduce environmental burden of CPs and hazards to humans.

We have developed an LC-APCI-Orbitrap-MS method to analyze plastic consumer products. The formation of $[M+Cl]^-$ ions by a soft-ionization technique and the high resolution of the Orbitrap-MS are required in the analysis of CPs and their transformation products. Moreover, an R-based automatic spectra evaluation routine (RASER) was used to evaluate thousands of ions of the various isotope clusters corresponding to 1600 homologues of CPs, COs, CdiOs and CtriOs [3].

We will demonstrate the potential of the new method on several CP-containing plastic materials. Five unique patterns were deduced per item from C- and Cl-homologue distributions, carbon and chlorine numbers, and saturation degrees, which collectively created the fingerprint of each plastic material.

[1] Glüge, J. et al., Sci. Total Environ., 89 (**2016**) 1123–1146.

[2] Schinkel, L. et al., Chemosphere, 194 (**2018**) 803–811.

[3] Knobloch, M. et al., Anal. Chem., 94 (**2022**) 13777–13784.

Identification of cyanotoxin oligopeptides with aerolysin nanopore

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Microcystins (MCs) are cyanotoxin oligopeptides produced by cyanobacteria, which compromise water quality. Directly monitoring cyanotoxin concentrations in water is challenging, due to the low concentration and high structural diversity of these toxins. The limitations of the present analytical methods can be overcome by the development of a single-molecule nanopore-based sensing platform allowing for portable, real-time, standard-free measurements for cyanotoxins in lake water. This approach would optimize cyanotoxin detection and quantification by accelerating the process, which is crucial for preserving water quality and protecting public health. Experiments have demonstrated the possibility to discriminate 3 most common microcystin variants only differing by a single amino acid.

«Forced Degradation Studies: an overview on current best practices & regulatory environment»

Dorina Kotoni

Novartis Pharma AG

Stress testing (also known as forced degradation) of pharmaceutical products has long been recognized as a critical part of the drug development process, providing foundational information related to intrinsic stability characteristics and to the development of stability-indicating analytical methods. The presentation will cover an overview of current best practices and regulatory environment with a focus on special requirements of ANVISA (Brazilian Health regulatory Agency). A benchmarking study undertaken by nine pharmaceutical companies and ANVISA with a goal of understanding the utility of various stress testing conditions for producing pharmaceutically-relevant chemical degradation of drugs will be presented.

Main focus of the study was to determine whether solution phase stress testing of solid drug products produced degradation products that were both unique when compared to other stress conditions and relevant to the formal drug product stability data. The results from studies of 62 solid dosage form drug products were compiled. A total of 387 degradation products were reported as being observed in stress testing studies, along with 173 degradation products observed in accelerated and/or long-term stability studies for the 62 drug products. Among these, 25 of the stress testing degradation products were unique to the solution phase stress testing of the drug products; however, none of these unique degradation products were relevant to the formal stability data. The relevant degradation productswere sufficiently accounted for by stress testing studies that included only drug substance stressing (in solution and in the solid state) and drug product stressing (in the solid state). Based on these results, it is the opinion of the authors that for solid dosage form drug products, well-designed stress testing studies need not include solution phase stress testing of the drug product in order to be comprehensive.

[1] John M. Campbell, Chris Foti, Chloe Wang, Neal Adams, Leonardo R. Allain, Gabriela Araujo, Renan Azevedo, Jucara Ribeiro Franca, Simon R. Hicks, Steven Hostyn, Patrick J. Jansen, Dorina Kotoni, Andreas Kuemmell, Stacey Marden, Gregory Rullo, Ana Claudia O. Santos, Gregory W. Sluggett, Todd Zelesky, Steven W. Baertschi, *Journal of Pharmaceutical Sciences*, **2022**, 111 (2), 298-305

Analysis of Breath-related Volatile Organic Compounds with Laser Absorption Spectroscopy

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Analysis of volatile organic compounds (VOCs) in breath has the potential for non-invasive and inexpensive medical diagnostics. This requires, however, highly sensitive and selective analytical techniques. Laser-absorption spectroscopy (LAS) is a promising candidate for future point-of-care diagnostics and health status monitoring. This method is already established for selective quantification of inorganic molecules in the mid-infrared (mid-IR) spectral range, providing a fast and accurate response, and having the potential for compact, easy-to-use and cost-effective instrumentation.

We expanded the application of LAS for the detection of VOCs by using a novel extended-tuning quantum-cascade (QC-XT) laser [1], coupled to a 76-m-optical-path multipass cell (MPC), and that covers the spectral range between 1063–1102 cm^{-1}[2]. By means of a gas calibration unit (HovaCAL) single and multi-compound gas standards of breath-relevant VOCs at ppm (or ppb) level with variable water content were generated. Several VOCs, containing up to four carbon atoms (C4), reveal significant fine structure in their ro-vibrational spectrum. Such distinct narrow features were also observed for larger rigid or symmetrical molecules (~C6).

Currently, we are adopting the spectrometer for in-situ breath analysis by designing an inlet system that minimises gas-exchange times and VOC adsorption, prevents water condensation, and allows for constant gas pressure in the MPC. Spiking of the breath samples either with a deuterated internal standard or with the analyte of interest was used for method validation. Excellent precision (typically ~1 ppb for 25 s averaging time) and high accuracy was achieved with a time resolution of 360 ms. Typical relative expanded uncertainty (k=2) of <2% has been found in the spiking experiments. The outstanding selectivity and accuracy of the method are a result of the broad measuring spectral range, high spectral resolution, and the unique spectral fingerprints of the investigated VOCs.

We acknowledge support from Zürich Exhalomics [3] and Evi Diethelm-Winteler-Stiftung.

[1] Yves Bidaux, Alfredo Bismuto, Camille Tardy, Romain Terazzi, Tobias Gresch, Stéphane Blaser, Antoine Muller, Jerome Faist, *Applied Physics Letters*, **2015**, *107*, 221108.
[2] Raphael Brechbühler, Miloš Selaković, Philipp Scheidegger, Herbert Looser, André Kupferschmid, Stéphane Blaser, Jérémy Butet, Lukas Emmenegger, Béla Tuzson, *Analitical Chemistry*, **2023**, *95*, 5, 2857–2864
[3] https://www.exhalomics.ch/ (Accessed: 11.02.2023)

Why Hydrogen Dissociation Catalysts do not work for Hydrogenation of p-Metals

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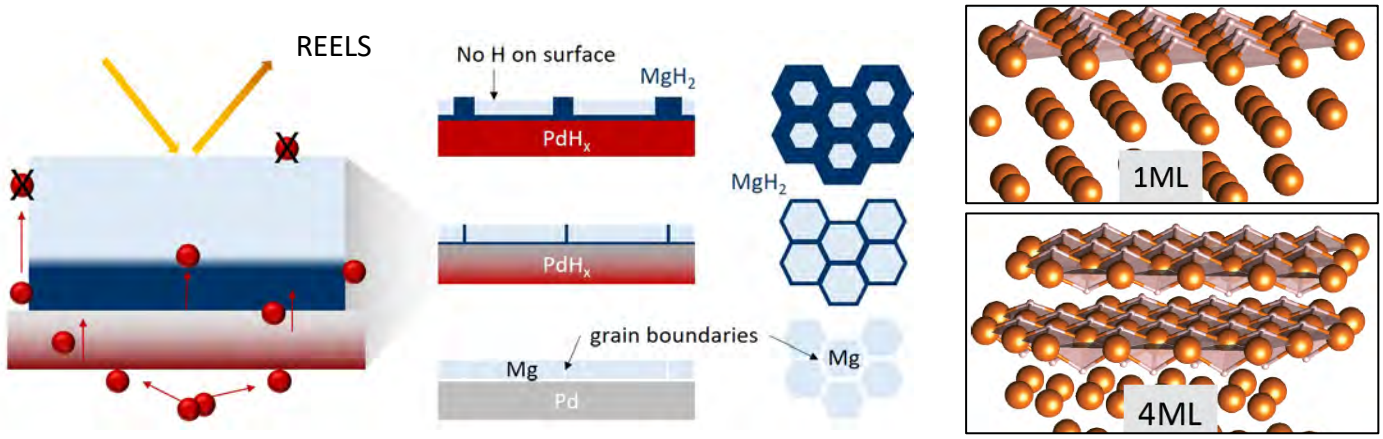
The Magnesium – Hydrogen system is a model system for understanding key processes in hydrogen storage based on p-metal hydrides. Considerable effort has been spent to improve its sluggish sorption kinetics, creating a huge empirical database[1]. In short, the dissociation of H_2 on the Mg surface is highly activated [2]. In contrast to the obvious assumption, overlayers/nanoparticles catalyzing hydrogen dissociation only marginally improve the kinetics.

In this study, in situ time-resolved reflecting electron energy loss spectroscopy (REELS) measurements are used to follow the hydrogen sorption behaviour in magnesium thin films under working conditions enabled by a custom-built setup [3]. The energies of the surface and bulk plasmons are interlinked allowing absolute statements [4]. The measurements, corroborated by electronic structure calculations, demonstrate the hydrogen uptake via growth of magnesium hydride without the presence of chemisorbed hydrogen on the metallic magnesium surface. The observation of the formation of a charge fluctuation layer at the Mg – MgH_2 interface prompts implications of new methods for improving the hydrogen sorption kinetics in p-Metals.



[1] M. Kappes, M. Iannuzzi, and R. M. Carranza, *J. Electrochem. Society*, **2013**, *160*, C168.
[2] M. Johansson, C. W. Ostenfeld, and I. Chorkendorff, *Phys. Rev. B*, **2006**, *74*, 193408.
[3] R. Delmelle, B. Probst, R. Alberto, A. Züttel, D. Bleiner, and A. Borgschulte, *Rev. Sci. Instrum.*, **2015**, *86*, 053104.
[4] W. S. M. Werner, *Journal of Surface Analysis*, **2005**, *12*, 127.

Analysis of alkane uptake over commercial C_1-C_4 coupling catalysts by combinatorial neutron imaging

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Today's reliance on fossil source-derived long-chain hydrocarbons, key commodity chemicals used in various end-user applications such as jet fuels, puts pressure on environmental and sustainability targets. Current promising routes for the sustainable production of these chemicals rely on the coupling of small molecules (C_1-C_4), but the catalysts employed in these transformations suffer from poor selectivity towards a single target product,[1] as well as rapid deactivation.[2] Herein, neutron imaging is utilized to gain understanding on the adsorption kinetics of two probe molecules, n-hexane (C_6) and n-dodecane (C_{12}), over several commercially available catalysts. The large cross section of neutron with hydrogen gives rise to strong contrast changes when H-containing molecules are adsorbed on the materials, therefore allowing the quantification of such species under *operando* conditions.[3] Furthermore, the custom-made combinatorial setup employed for the experiments allows the simultaneous investigation of up to 69 samples under identical conditions. The results showed a strong diffusion limitation for n-dodecane over most porous materials in comparison with n-hexane, indicating that the diffusion of long chain products out of the pore network under typical reaction temperatures (473-623 K) is a crucial parameter for catalyst deactivation. These findings provide key insights on the adsorption of hydrocarbons with different lengths over systems with varying porosity and pore connectivity, enabling the future design of optimized catalysts for coupling reactions.

Figure 1. Schematic representation of the study.

[1] R. Handler, D. Shonnard, *Biofuels for Aviation*, **2016**, Chapter 6.
[2] J. Ihli, R. R. Jacob, M. Holler, M. Guizar-Sicairos, A. Diaz, J. C. da Silva, D. Ferreira Sanchez, F. Krumeich, D. Grolimund, M. Taddei, W. -C. Cheng, Y. Shu, A. Menzel, J. A. van Bokhoven, *Nat. Commun*., **2017**, 8, 809.
[3] J. Terreni, E. Billeter, O. Sambalova, X. Liu, M. Trottmann, A. Sterzi, H. Geerlings, P. Trtik, A. Kaestner, A. Borgschulte, *Phys. Chem. Chem. Phys.*, **2020**, 22, 22979-22988.

Visualization and processing of chemical information in the browser

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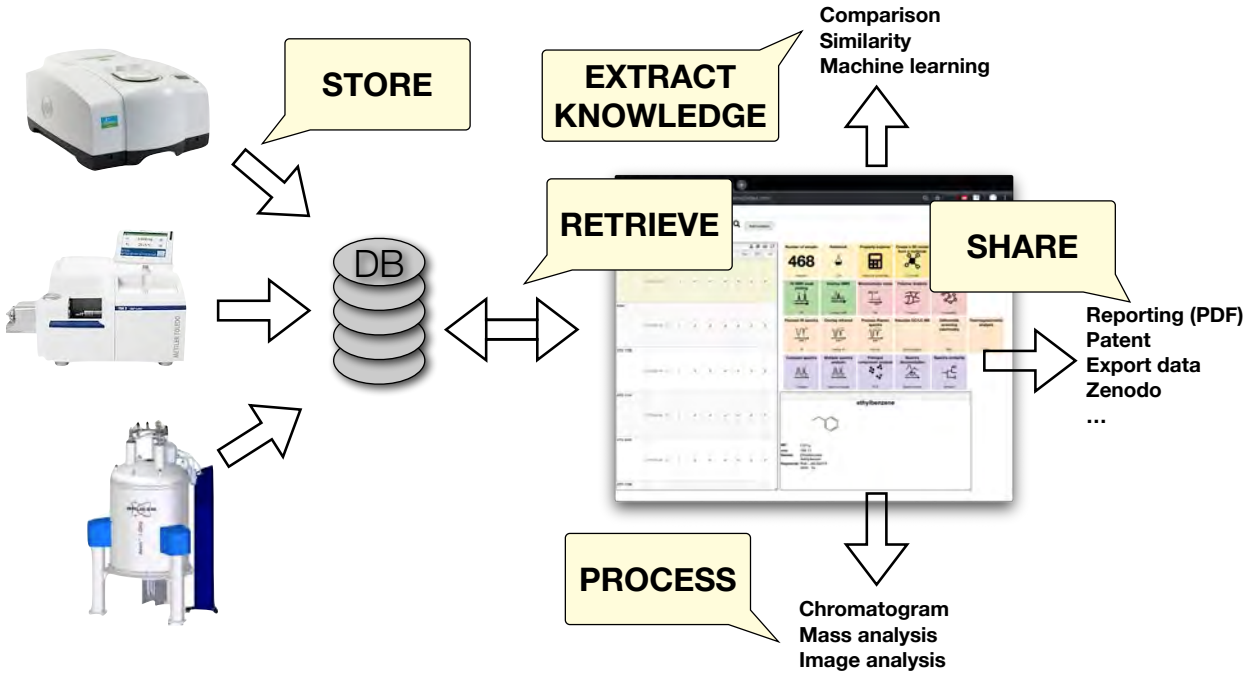
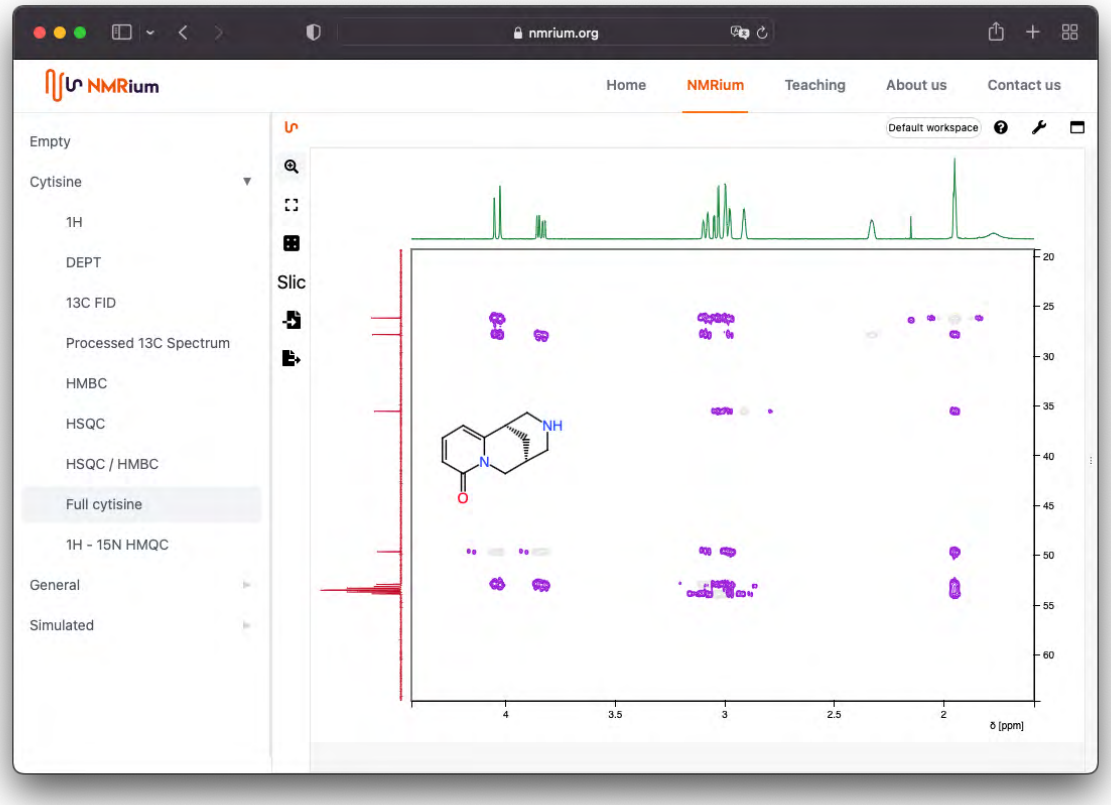
Nowadays, computers come with a browser pre-installed, and many web applications have been developed to perform everyday tasks such as webmail, maps, document editing, etc. The main advantage is that no software needs to be installed and updating is done by simply reloading the web page. Moreover, this approach is cross-platform and the data can be accessed from anywhere.

For over 20 years we have been dealing with data workflow and the idea of storing data in a database as quickly as possible and processing it directly in the browser. This is done with the help of over 150 JavaScript libraries that have been developed over the years.



Analytical data workflow

In this presentation, we will show how data can be stored, retrieved, processed, and eventually knowledge can be extracted from it [1], using **www.c6h6.org** as an example [2]. We will present an advanced application of mass spectra analysis of polymers (**www.polycalc.org**) performed directly in the browser [3]. Finally, we will present **www.NMRium.org**, a freely accessible website that allows to visualize, compare and process NMR spectra [4].



Example of browser web application for NMR data processing

[1] Jablonka, K. M., Patiny, L., & Smit, B. (2022). Making the collective knowledge of chemistry open and machine actionable. *Nature Chemistry*, *14*(4), 365–376.

[2] Patiny, L., Zasso, M., Kostro, D., Bernal, A., Castillo, A. M. M., Bolaños, A., Asencio, M. A. A., Pellet, N., Todd, M., Schloerer, N., Kuhn, S., Holmes, E., Javor, S., & Wist, J. (2018). The C6H6 NMR repository: An integral solution to control the flow of your data from the magnet to the public. *Magnetic Resonance in Chemistry*, *56*(6), 520–528. https://doi.org/10.1002/mrc.4669

[3] Desport, J. S., Frache, G., & Patiny, L. (2019). MSPolyCalc: a web-based App for polymer mass spectrometry data interpretation. The case study of a pharmaceutical excipient. *Rapid Communications in Mass Spectrometry*. **https://doi.org/10.1002/rcm.8652**

[4] Patiny, L., Musallam, H., Zasso, M., Bolaños, A., Kostro, D., Wenk, M., Ahkrin, S., Jeannerat, D., Ziegler, E., Liermann, J., Schloerer, N., & Wist, J.. (2022). NMRium: ReactJS component to display and process NMR spectra (v0.33.0). Zenodo. https://doi.org/10.5281/zenodo.7258284

Sparse Collection of XAFS data via Plasma X-rays

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X-ray absorption spectroscopy (XAFS) is used to fingerprint materials via the detection of absorption edges as well as structure, even in amorphous materials. XAFS is readily used to study catalysts, soil samples, metals and various chemical processes. Most of the XAFS experiments are performed at synchrotron beamlines, which are large facilities with a limited access based on proposal acceptance. Therefore, tabletop setups are useful, as they can provide an experimental access 24/7, for in-situ chemical analysis. One such facility (EMPULSE) is under development at EMPA in Switzerland.

EMPULSE is a terawatt laser facility developed to generate coherent/incoherent X-rays for the purpose X-ray spectroscopy and X-ray imaging by means of chirped pulse amplification [1]. X-rays are generated by shooting a high intensity, short laser pulse on a solid target, to induce a plasma. The output wavelength and energy of the emitted X-rays depends on the drive pulse characteristics and the target material. The characterization is done by a useful set of optical diagnostics.

A unique approach to quick noise-free XAFS measurements on tabletop based on the principle of Bayesian Compressed sensing is proposed. The technique relies on sparsely acquiring the raw data and using optimization algorithms to reconstruct the final signal. XAFS signals are sparse in discrete cosine transform domain and if the data is collected randomly, mathematical optimization techniques such as L1 normalization can be used to reconstruct the raw data. This can shorten the acquisition time to a few minutes without sacrificing the resolution. The proof of concept is presented, as implemented by a python code and a post-processing analysis of a case study on a Co foil. The results demonstrate that a 75% rate of compression for NEXAFS region and a 50% compression rate for EXAFS region, is possible, from which signals are accurately reconstructed to study the chemical information.

References:

[1]Hemani, Y., Galimberti, M. and Bleiner, D., "EMPULSE: a compact terawatt chirped pulse amplification laser for generating coherent x-rays," International Conference on X-Ray Lasers 2020, D. Bleiner, Ed. (2021).

Chlorinated Paraffins Analysis by High-Resolution Mass Spectrometry Coupled with an Atmospheric Pressure Glow Discharge Micro-Plasma Ionization

Claudia Masucci[1,2], Kevin Kraft[1,2], Marco Knloboch[1,2], Konstantin Nagornov[3], Anton Kozhinov[3], Yury Tsybin[3], Davide Bleiner[1,2]

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CPs mixtures contain hundreds of thousands of homologues. The single-chain CP-materials also contain a small amount of chlorinated olefins (COs), which are their transformation product that can interfere. Monitoring CPs currently requires a chromatographic method coupled to a MS and induction of chlorine adduct formation by adding dichlorometane to a methanol: water solution.

The liquid sampling - atmospheric pressure glow discharge (LS-APGD) micro-plasma ionization source is a proven method to obtain atomic and molecular (CAM) information from a variety of analytes[1]. To further extend upon the already versatile capabilities of the LS-APGD ionization source, it was coupled to a high-resolution Orbitrap MS as a new technique for the challenging analysis of Chlorinated Paraffins (CPs) materials.

As the complexity of CP mixtures requires both high resolution (e.g. R ≈ 120'000 at m/z …)[2] and high sensitivity, we coupled the CAM-Orbitrap LTQ XL system to an external high-performance data acquisition (DAQ) system (FTMS Booster X2). The employed DAQ system enables mass spectra representation in the absorption mode Fourier transform helping to improve mass spectral resolution and dynamic range[3].

Synthetized C18-chloroparaffin material of low, medium and high chlorination degrees of different concentrations was analysed and detected for the first time as nitrate adduct in a methanol: water solution. We will present the ability to resolve CPs from the COs interferences (separated by 18 mDa) already with a resolution of 30'000 at m/z …. The DAQ proved to be able to double the resolution, provide the spectral dynamic range of 3.5 orders of magnitude, and improve the sensitivity.

[1] Tyler J. Williams, R.Kenneth Marcus, *J. Anal. At. Spectrom*, **2020**, *35*, 1910
[2] Knobloch M.C. et al., *Chemosphere*, **2021**, 283, 131199
[3] Jacob R. Bills et al., J. Am. Soc. Mass Spectrom, **2021**, 32, 1224-1236

High-resolution mass spectrometry: from algorithms to the great outdoors

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High-resolution mass spectrometry has become indispensable as a core technology in environmental analytics and metabolomics, providing broad chemical coverage and the potential to identify new compounds. I highlight contributions in diverse aspects of the field, from computational mass spectrometry to environmental applications. First, *RMassBank* [1], an automated workflow to generate high-quality MS^2 spectral library records including automatic recalibration, to support data contributions to the community-driven mass spectral database *MassBank*. Second, *MSNovelist* [2], a novel algorithm to propose chemical structures from MS^2 spectra based on chemical fingerprint prediction with *CSI:FingerID* and *de novo* structure generation with a recurrent neural network, making it possible to discover completely new structures not yet recorded in any chemical database. Third is *MS^2field* [3], a transportable lab-in-the-field equipped with an Orbitrap mass spectrometer, a fully automated water sampling system, and live quantification, to monitor micropollutant contamination in near real-time and to acquire highly time-resolved time profiles with broad chemical coverage.

[1] M.A. Stravs, E.L. Schymanski, H.P.Singer, J. Hollender, *J Mass Spec*, **2013**, *48*, 89-99
[2] M.A. Stravs, K. Dührkop, S. Böcker, N. Zamboni, *Nat Meth*, **2022**, *19*, 865-870
[3] M.A. Stravs, C. Stamm, C. Ort, H. Singer, *Environ Sci Technol Lett*, **2021**, *8(5)*, 373-380

Mass Spectrometry in Proteomics: Technologies, Methods, and Research Applications for the Life Sciences

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Mass spectrometry (MS) has evolved from a technology to characterize small chemical molecules to an indispensable tool in the hands of researchers in all life sciences. Thanks to their analytical power and versatility, MS-based methods enable the investigation of proteins, peptides, metabolites, lipids, glycans, and biomolecules in general. Many life science studies involve MS at some step, either to check the quality of molecules (i.e., identity of a protein), to characterize them in detail (i.e., glycan profiling of an antibody), to discover new markers for biological processes (i.e., metabolites involved in a specific disease), or to validate findings obtained by other analytical means (i.e., increased level of specific protein post-translational modifications). Mass spectrometry is increasingly relevant also in the biopharmaceutical sector, where the filing of new biotechnological products follows detailed characterization procedures.

Given its broad range of applications, MS is a field of research and technology development on its own, with branches concentrating on different life science disciplines, and more specifically on distinct types of biomolecules and applications. Examples of these disciplines are proteomics, metabolomics, lipidomics and glycomics, which focus on the large-scale studies of proteins, metabolites, lipids and glycans, respectively. The analysis of these classes of biomolecules requires different analytical workflows and instrument capabilities, but also distinct technical and scientific expertise.

In this lecture[1], we will discuss the most important technological and analytical developments that shaped the field of life science mass spectrometry, with a particular focus on the field of proteomics. We will provide examples on how proteomics is applied to unravel cellular mechanisms, to analyze protein interaction networks, or to characterize protein structures. We will also comment on the importance of data analysis and bioinformatics.

[1] P. Nanni, P. Gehrig, R. Schlapbach *Chimia*, **2022**, *76*, 73

Biological nanopores for single-molecule sensing

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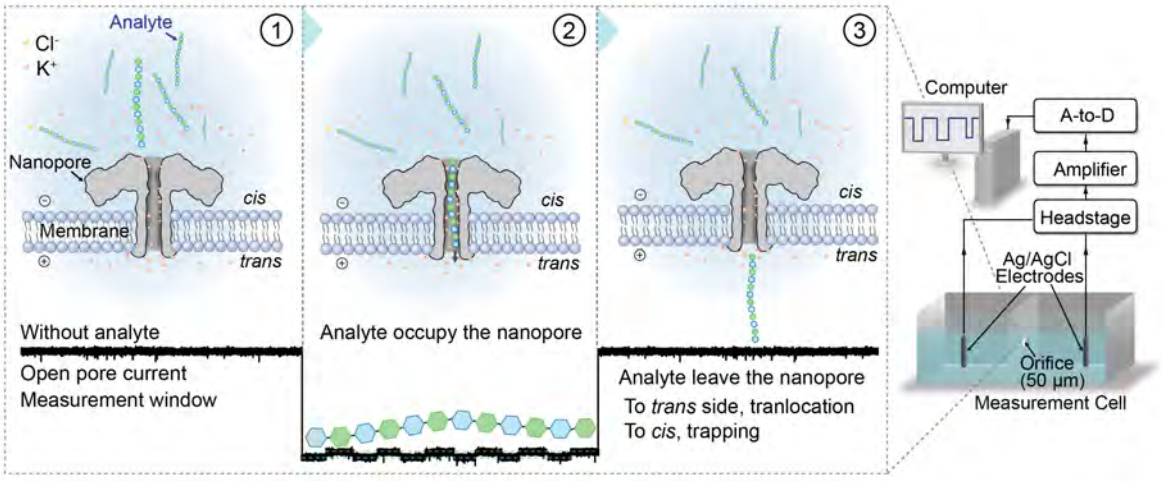
Single molecule nanopore technique has revolutionized DNA sequencing which advanced the development of precision medicine, and recently is making significant impacts on proteomics research [1]. By measuring the ionic current induced as a single molecule passes through a nanopore detector, the chemical and physical properties of the detected molecule can be obtained, including the size, mass, composition, structure, sequence and conformation. As an analytical tool, the nanopore technique highlights several unique advantages: (i) no requirement of additional labelling and amplification; (ii) the cheap electric readout, which can be easily miniaturized and massively parallelized for a high-throughput analysis; (iii) measuring a fundamentally different property of the analyte compared to other techniques, the ionic current difference induced by the target molecule; (iv) direct detection of mixture samples without the need for additional separation steps.

Here, we rationally designed a set of mutated pores and evaluated them *in silico* by molecular simulations and *in vitro* by single-channel recording and molecular translocation experiments to study the pore structural variation, ion selectivity, ionic conductance and capabilities for sensing several biomolecules, including DNA and peptides [2]. Our results show that the ion selectivity and sensing ability of aerolysin are mostly controlled by electrostatics and the narrow diameter of the double β-barrel cap. By engineering single-site mutants, a more accurate molecular detection of nucleic acids and peptides has been achieved. These findings open avenues for developing aerolysin nanopores into powerful sensing devices.



[1] S.F. Mayer, C. Cao, M. Dal Peraro, Biological nanopores for single-molecule sensing *Iscience*, **2022**, *25*, 104145.
[2] C. Cao, N. Cirauqui, M.J. Marcaida, et al. Single-molecule sensing of peptides and nucleic acids by engineered aerolysin nanopores. *Nat Commun.,* **2019**, *10*, 4918.

Detection of oxytocin and vasopressin using biological nanopore

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Oxytocin and vasopressin are neuropeptides that are synthesized in the hypothalamus region of the brain. These peptides play a pivotal role in various physiological processes, including uterine contraction during childbirth, lactation, social bonding, regulation of peripheral fluid balance and blood pressure etc., as well as responsible for a plethora of neuropsychiatric functions [1]. This makes oxytocin and vasopressin highly promising targets for medical research and clinical diagnosis[2]. The levels of oxytocin in body fluids such as blood or cerebrospinal fluid are mostly measured using Enzyme-Linked ImmunoSorbent Assay (ELISA), which has high sensitivity but may induce cross-reactivity with other molecules. Recently, single-molecule nanopore sensing is emerging as a powerful tool for detecting biomolecules, including DNA and peptides[3]. In our research, we use a biological protein pore, aerolysin, to identify and quantify the oxytocin and vasopressin neuropeptides. By tuning the buffer condition, a strong electroosmotic flow was generated to capture these non-charged peptides. Our nanopore results showed that, oxytocin and vasopressin interact with the aerolysin nanopore differently which led to characteristic ionic current signatures. In the future, we expect to use such method for monitoring the level of certain neuropeptides in the body fluids.

[1] Gruber, C.W. *Physiology of invertebrate oxytocin and vasopressin neuropeptides.* Exp Physiol. **2014**; 99(1):55-61

[2] Voinsky, I., Bennuri, S.C., Svigals, J. et al. *Peripheral Blood Mononuclear Cell Oxytocin and Vasopressin Receptor Expression Positively Correlates with Social and Behavioral Function in Children with Autism*. Sci Rep 9. **2019**; 13443

[3] Mayer, S.F., Cao, C., Peraro, M.D. *Biological nanopores for single-molecule sensing,* iScience, Volume 25, Issue 4, **2022**, 104145, ISSN 2589-0042

Using protein-specific retention behavior to improve the characterization of therapeutic antibodies

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Therapeutic monoclonal antibodies (mAbs) have grown significantly in popularity over the last 30 years as a class of human therapeutics, leading to an interesting alternative to small molecule drugs in the pharmaceutical industry. The characterization of mAbs is complex but of utmost importance, due to the occurrence of post-translational modifications (PTMs) that could hamper the drug safety and efficacy. Liquid chromatography has emerged as a key technique in the characterization of size, charge, hydrophobic, and hydrophilic protein variants. Coupled to mass spectrometry, chromatographic techniques provide well-established strategies to characterize the aforementioned structural protein variants. Moreover, the functional characterization of therapeutic antibodies using affinity liquid chromatography has become increasingly important to relate the observed PTMs to distinct pharmacodynamic and pharmacokinetic (PK/PD) properties *in vivo*. Together, this provide vital information on the critical quality attributes (CQAs) of therapeutic antibodies.

In this work, we took a closer look into how recently discovered protein-specific retention behavior can improve the current characterization techniques for therapeutic antibodies. We focused specifically on the use of ultra-short column formats (i.e., 10-15 mm), retention modelling software[1] and the use of special multi-isocratic and negative gradient types in affinity chromatography[2]. This could help to further improve the speed and/or selectivity of these state-of-the-art characterization techniques and prepare them for the next-generation of antibody-based products such as, antibody-drug conjugates (ADCs), fusion proteins, and bi-specific antibodies.

[1] B.L. Duivelshof, A. Zöldhegyi, D. Guillarme, M.A. Lauber, S. Fekete; J Pharm Biomed Anal., 221 (2022); https://doi.org/10.1016/j.jpba.2022.115039

[2] T. Bouvarel, B.L. Duivelshof, J. Camperi, T. Schlothauer, A. Knaupp, C. Stella, D. Guillarme; J Chromatogr A, 1682 (2022); https://doi.org/10.1016/j.chroma.2022.463518

POSTERS

Self-powered Potentiometric Sensor Based on Self-powered Amplifier with Dual Electronic Paper Display

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Developing self-powered potentiometric sensors are attractive because of their simple operation, low cost, fast response, and ability to be integrated with other technologies. Self-powered potentiometric sensors that give a direct colorimetric output are especially attractive because no power supply is needed, which dramatically reduces waste[1]. The current approach using an electronic paper display, however, still has limitations because the visualization of small pH changes is difficult.

A self-powered ion-selective potentiometric sensor is introduced here that may amplify the epaper pixel sensitivity by improving the self-powered circuit. The potential of three pH electrodes with different inner filling solutions (pH 6, pH 9 and pH 12) are directly read out optically. In this way the electronic paper display responds to a wide range of pH values. Subsequently, the voltage is amplified by changing the circuit from parallel to serial capacitors. As a result, the voltage is amplified 3-fold and a greatly improved sensitivity is observed in another electronic paper display, with a precision better than 0.1 pH units.

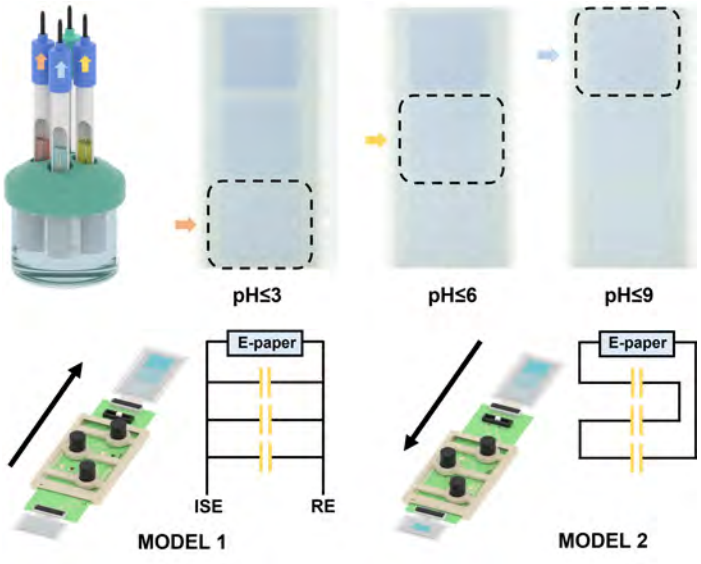

Figure 1. The response of epaper pixel to pH by a coupled pH probe in two different configurations and the scheme of a portable device.

[1] Y. Wu, E. Bakker, *ACS sensors*, **2022**, *7(10)*, 3201-3207.

Paper-based laser-pyrolyzed electrofluidics for capillary-driven electrochemical biosensing

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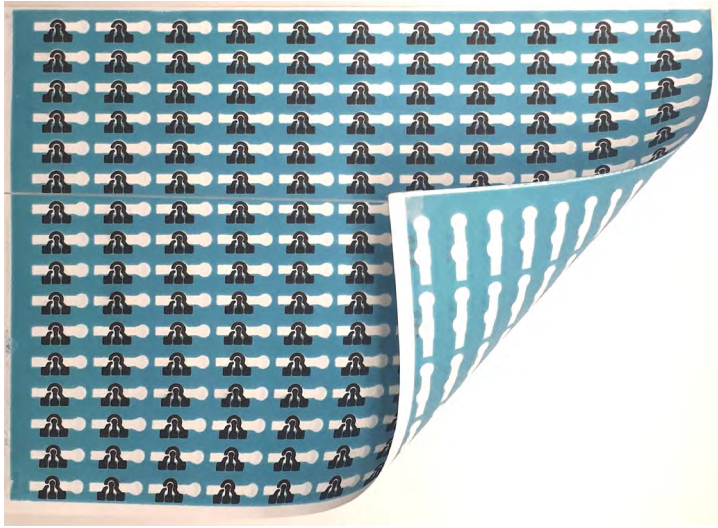
Microfluidic paper-based analytical devices (µPADs), such as lateral flow assays, have become indispensable tools for disease diagnostics, owing to their low cost and simple operation via passive capillary-driven flow. While most contemporary tests rely on qualitative colorimetric readouts, electrochemical signal transduction provides an attractive and potentially more powerful route towards device miniaturization and quantitative signal outputs. Unfortunately, electrode fabrication on cellulose paper is challenging due to the inhomogeneous nature of this fibrous material, and the cost and complexity of current fabrication techniques are often prohibitive for single-use applications. Furthermore, the integration of non-porous electrodes in capillary-driven assays may hinder capillary flow and pose limitations to device architecture. Here, we present a method for fabricating electrodes embedded into paper using laser-induced pyrolysis of the cellulose itself [1]. In this way, cellulose serves not only as a flow-driving substrate but also as a precursor for the electrodes. The graphenic electrodes display high conductivity, porous electroactive structures and fast capillary wicking. Combined with wax patterning of fluidic channels, we fabricate and assemble these functional electrofluidic layers into devices for in vitro diagnostics We showcase the potential of our approach by developing two capillary-driven bioassays of clinical relevance. (i) In a lateral flow format, we demonstrate a flow injection device for the continuous analysis of alkaline phosphatase in serum. (ii) We present a vertical flow device with flow-through electrodes for CRISPR-assisted molecular diagnostics of HPV16 down to 1 copy / µl. Importantly, these proof-of-concept devices maintain the operational simplicity of lateral flow immunoassays. To conclude, this platform offers a rapid prototyping environment coupled with computer-aided design and does not rely on specialized equipment for fabrication. Moreover, the unique morphology of the electrodes opens doors to novel device architectures for a broad scope of applications in the analytical sciences.

[1] L. Bezinge, J. M. Lesinski, A. Suea-Ngam, D. A. Richards, A. J. deMello, C.-J. Shih, *ChemRxiv*. 2023, doi: 10.26434/chemrxiv-2023-4gqxm.



Label-Free and Non-Destructive Nanoscale Chemical Analysis using Tip-enhanced Optical Spectroscopy

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Analytical tools for high-resolution chemical analysis are essential to study nanoscale properties of materials such as biological membranes, 2D materials including graphene, 1D materials including carbon nanotubes (CNTs), polymers or heterogenous catalysts [1]. However, conventional analytical tools such as confocal optical (Raman and fluorescence) spectroscopy often lack the required sensitivity and spatial resolution to obtain nanoscale information. Tip-enhanced optical spectroscopy (TEOS) overcomes this challenge by confining light to a nanoscopic volume and enhancing the intensity of the local electromagnetic (EM) field by orders of magnitude *via* a combination of localized surface plasmon resonance and lightning rod effect [2]. The enhancement of the local EM field dramatically improves the sensitivity of the optical spectroscopy. Furthermore, the confinement of light overcomes the optical diffraction limit pushing the spatial resolution down to the nanoscale that can reveal new structural and chemical properties together with the correlative topographical information. Due to its non-destructive and label-free nature and the ability to apply in both air and liquid environments, the application field of TEOS is constantly growing. In this work, we demonstrate that hyperspectral tip-enhanced optical microscopy is a sensitive analytical tool to investigate nanoscale properties and can be applied to a variety of samples in diverse areas of scientific research including heterogenous catalysis [3], 1D materials (CNTs) and 2D materials (GO) as illustrated in Fig. 1.

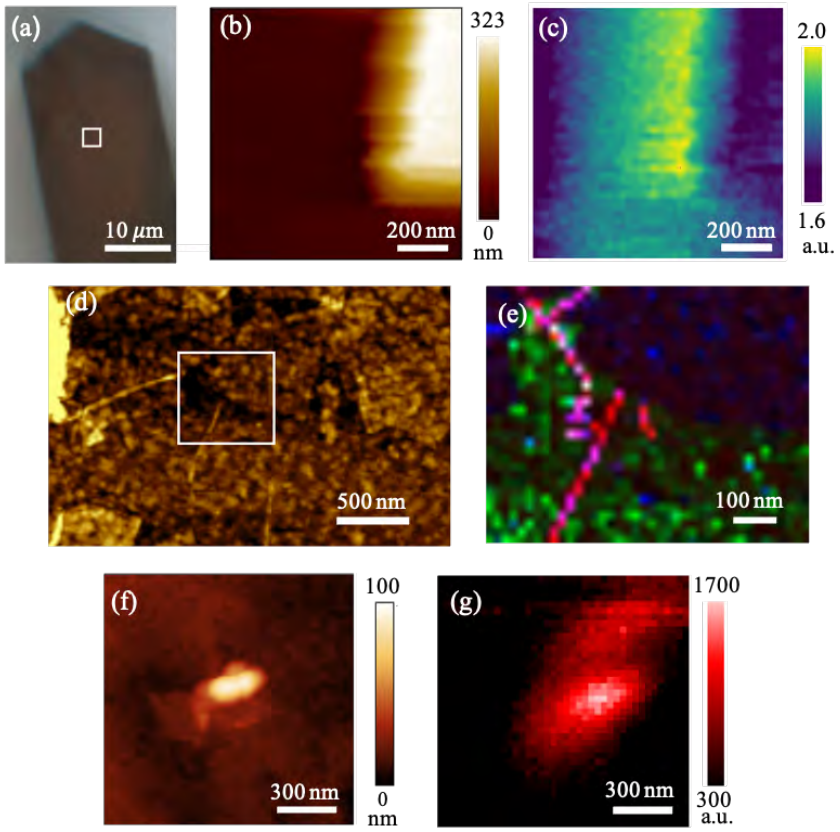

Fig. 1. (a) Optical image of a ZSM-5 catalyst subjected to 90 minutes of methanol to hydrocarbon reaction. (b) AFM height image of the region marked in Panel a. (c) Tip-enhanced fluorescence (TEFL) image of the coke species formed in the region shown in Panel b. (d) AFM height image of single-wall CNTs and graphene oxide (GO) on Au surface. (e) Tip-enhanced Raman spectroscopy (TERS) image of the CNTs (red) and GO (blue) on Au measured in the region marked in Panel d. (f) AFM height and (g) TERS images of a GO flake on Si. Panels d-g contain unpublished data.

[1] Kumar et al., *EPJ Techniques and Instrumentation*, **2015**, 2:9
[2] M. Asghari-Khiavi et al., *J. Raman Spectrosc.*, **2012**, *43*, 173-180.
[3] Bienz et al., *Catal. Sci. Technol.*, **2022**, *12*, 5795-5801.

A novel time-dependent potentiometric glucose biosensor

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Glucose sensing has been on the frontline of biosensors for more than six decades, when the first glucose monitoring system was reported by Clark & Lyons in 1962. [1] Since then, thousands of such sensors have been reported, invasive or non-invasive, enzymatic or non-enzymatic, disposable or not, targeting blood or other bodily fluids, like sweat and urine. Considering the plethora of glucose studies reported in the literature, the remaining question is whether there is still room for improvement in the field. A considerable number of the reported sensors are enzymatic and based on electroanalytical techniques, like amperometry. Among them, the ones that have been commercialised use a mediator acting as an electron carrier (e.g. ferricyanide) between the electrode and enzyme. Also, they are typically screen-printed, which gives them the advantage of low cost to the detriment of accuracy. [2]

We report here a novel method for monitoring glucose based on a time-dependent response. The principle of measuring is based on a two-step process that involves the oxidation of a mediator and the subsequent monitoring of the open-circuit potential over time. This process enables one to record a time-dependent response that is a function of the level of glucose in contact with the sensor. As glucose is oxidised by the enzyme, the generated electrons gradually reduce the oxidised mediator manifesting a change in the open-circuit potential, the rate of which depends on the glucose levels. The readout is similar to that of chronopotentiometry where a transition time, rather than an electrochemical signal -like current- is monitored. The sensing membrane employed is based on ferrocene-modified poly(ethylenimine) used as mediator and glucose oxidase. In addition, a diffusion limiting membrane enables the steady-state diffusion of glucose towards the electrode and can be used to fine tune the selectivity, which is currently under examination.

This simple monitoring protocol requires low-power consumption and results in better reproducibility compared to the classic amperometric approach used for glucose sensing. The additional advantage of the specific approach lies in its universality, which makes possible the development of similar time-depended sensors for other analytes.

[1] L. C. Clark, C. Lyons, *Ann. N. Y. Acad. Sci.*, **1962**, *102 (1)*, 29– 45.
[2] E. Witkowska Nery, M. Kundys, P. S. Jeleń, M. Jönsson-Niedziółka, *Anal. Chem.*, **2016,** *88*, 11271–11282.

Development of an Extraction Method for Nanoparticles in Sludge Using an In-House Reference Material

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Rare earth elements (REEs) are technologically critical and increasingly widespread in a broad range of applications[1]. Throughout the life cycle, from mining to disposal of REE-containing products, REEs are released into air, soil and water. They are therefore of environmental concern, and their impact and fate once released is an active research field.[2] As the interface between anthropogenic REEs in wastewater and their release into the environment, wastewater treatment plants (WWTPs) are especially interesting to study the behavior of REEs. Comparison of the REE concentrations in the influent to and in the effluent from WWTPs allows an assessment of the REE removal efficiency, with the removed REEs being accumulated in the sewage sludge.[3] Digested sludge, with a typical sludge age of around 30 days, therefore, can be regarded as an effective passive sampling system for REEs, with considerably less temporal fluctuations of the REE contents compared to the wastewater streams. The total content of REEs in sewage sludge in Switzerland was determined previously,[4] but information regarding the state in which REEs are occurring is still missing: REEs are expected to be present as REE nanoparticles, but knowledge about their elemental composition, size distribution and concentration compared to dissolved REEs is currently limited.

In order to reliably quantify REE nanoparticles in sludge, an effective extraction method is necessary. However, evaluating the efficiency of different extraction methods requires a material with a similar matrix to sewage sludge and a known nanoparticle content. Since there is no such reference material commercially available, an in-house reference material was produced and then used to evaluate different extraction methods. As a first proof of concept, this reference material was prepared by spiking sewage sludge with a known concentration of 60 nm gold nanoparticles. Different protocols for oxidative digestion were investigated, and the extracts were measured by single-particle ICP-MS. The gold recovery was determined based on the total digestion of the spiked sludge, and the efficiency of the different extraction methods was quantified.

[1] A. Cobelo-García, M. Filella, P. Croot, C. Frazzoli, G. Du Laing, N. Ospina-Alvarez, S. Rauch, P. Salaun, J. Schäfer and S. Zimmermann, *Environ. Sci. Pollut. Res.*, **2015**, *22*, 15188–15194.
[2] W. Gwenzi, L. Mangori, C. Danha, N. Chaukura, N. Dunjana and E. Sanganyado, *Sci. Tot. Env.*, **2018**, *636*, 299–313.
[3] B. Vriens, A. Voegelin, S. J. Hug, R. Kaegi, L. H. E. Winkel, A. M. Buser and M. Berg*, Environ. Sci. Technol.*, **2017**, *51*, 10943–10953.
[3] Kaegi, R.; Gogos, A.; Voegelin, A.; Hug, S. J.; Winkel, L. H. E.; Buser, A. M.; Berg, M *Water Research X*, **2021**, *11*, 100092.

Developing nanopore for the detection of protein post-translational modifications

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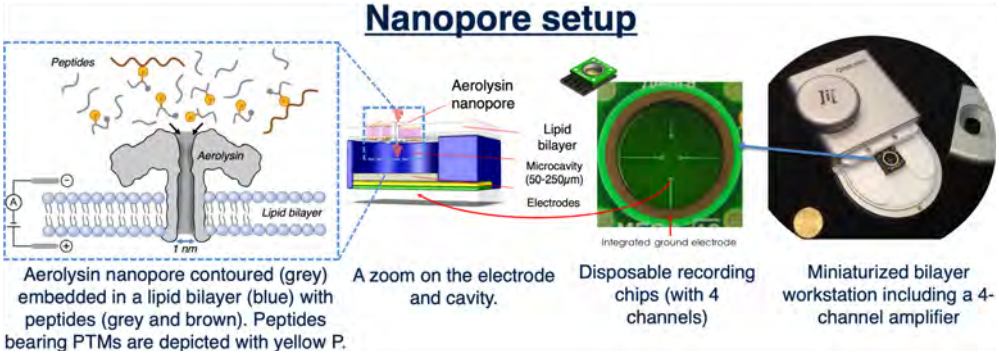
Protein post-translational modifications (PTMs) play a crucial role in many biological processes, by modulating the protein properties both on the chemical and biological aspects and at different spatial and temporal scales[1,2]. Protein PTMs are not only important for key cellular functions, but they can also be used as reliable biomarkers for several diseases[3,4]. However, only a few techniques are available to accurately detect and measure their levels, capture their complexity at a single-molecule level and characterize their versatile roles in health and disease[4]. Nanopore sensing provides high sensitivity for the detection of low-abundance proteins, holding the potential to impact single-molecule proteomics and especially PTMs detection[5,6].



Here, we show the ability of a biological nanopore, the pore-forming toxin aerolysin[7], to detect and distinguish peptides derived from proteins involved in neurodegenerative diseases bearing single or multiple PTMs (mainly phosphorylation, nitration, and oxidation) at different positions and in various combinations. The characteristic current signatures of these peptides and their PTM variants could be confidently identified using a deep learning approach. We further demonstrate that nanopore can quantify low levels of these peptides in red blood cells (up to picomolar concentration), showing promising prospects for developing nanopore-based diagnostic strategies for neurodegenerative diseases. Our work highlights the unique advantage of using nanopores as tools for the simultaneous detection of multiple PTMs and paves the way for their use for biomarker discovery and diagnostics.

1 Ramazi, S. *et al. Database* 2021, baab012 (2021)
2 Wang, Y.-C. *et al. Cell Res.* 24, 143–160 (2014)
3 Gupta, R. *et al. Ageing Res. Rev.* 68, 101336 (2021)
4 Pagel, O. *et al. Expert Rev. Proteomics* 12, 235–253 (2015)
5 Cao, C. *et al. Acc. Chem. Res.* 51, 331–341 (2018)
6 Alfaro, J. A. *et al. Nat. Methods* 18, 604–617 (2021)
7 Cao, C. *et al. Nat. Commun.* 10, 4918 (2019)

Investigation of Different Ablation Environments for LA-N_2-MICAP-MS

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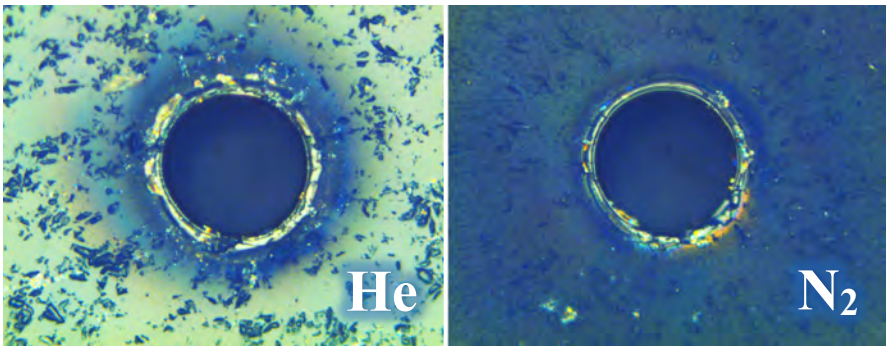
Inductively Coupled Plasma Mass Spectrometry (ICP-MS) has been established as a routine method for qualitative and quantitative element analysis. However, the method has potential for improvements including the consumption of argon gas and limited tolerance to gases other than helium or argon as carrier gas for laser aerosols.[1] Other plasma configurations and other plasma gases have been reported.[2-4] However, none of these approaches have been commercialized in ICP-MS. A novel high power nitrogen microwave inductively coupled atmospheric-pressure plasma (MICAP) design was recently introduced and first results indicate a performance comparable to Ar-ICPs.[4] Additionally, the use of nitrogen as plasma gas allows a reduction of running costs by 70 %.[1] Furthermore, this design has proven to be stable towards air introduction.[1,4] Recently, the established laser ablation (LA) procedure under helium environment was employed in combination with a MICAP-MS, showing comparable performance to the Ar-ICP method much like the solution-based method.[5]



Based on the extended gas tolerance of the nitrogen plasma source, various laser generated aerosols produced within different gas environments were directly introduced into the MICAP. Since most LA procedures are based on helium ablation,[6] the results obtained within nitrogen and air were directly comparable (without the use of a gas exchange device (GED) required previously)[7]. Figures of merit for the different ablation environments were investigated using different standard reference materials and will be discussed. Furthermore, SEM studies of the sample surface and particle size distribution measurements were carried out to explain the results obtained in helium, argon, nitrogen and air.

[1] M. Schild, A. Gundlach-Graham, A. Menon, J. Jevtic, V. Pikelja, M. Tanner, B. Hattendorf, D. Günther, *Anal. Chem.* **2018**, *90*, 13443-13450.
[2] Okamoto, Y. *J. Anal. At. Spectrom.* **1994**, *9*, 745-749.
[3] Hammer, M. R. *Spectrochim. Acta - Part B At. Spectrosc.* **2008**, *63*, 456-464.
[4] A.J. Schwartz, Y. Cheung, J. Jevtic, V. Pikelja, A. Menon, S.J. Ray, G.M. Hieftje, *J. Anal. At. Spectrom.* **2016**, *31*, 440-449.
[5] C. Neff, P. Becker, B. Hattendorf, D. Günther, *J. Anal. At. Spectrom.* **2021**, *36*, 1750-1757.
[6] S.M. Eggins, L.P.J. Kinsley, J.M.G. Shelley, *Appl. Surf. Sci.* **1998**, *127-129*, 278-286.
[7] R. Kovacs, K. Nishiguchi, K. Utanib, D. Günther, *J. Anal. At. Spectrom.*, **2010**, *25*, 142-147

Deep-learning unfolded algorithm for XAS signal reconstruction

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X-ray absorption spectroscopy (XAS) is a powerful analytical technique, which can be used for obtaining chemical and elemental information. XAS works with most sample environments, and is widely used in material sciences, catalysis, physical chemistry and biosciences.

The sequential measurement of samples is mostly performed at synchrotron beamlines where the beam time is dependent on proposal acceptance. Additionally, time-resolved analysis need complex optical setups and fast signal processing electronics as the scanning should be faster than the chemical reaction being investigated.

An ideal setup would allow researchers to acquire the entire spectrum in a single shot with low sample damage intensity, without sacrificing information, in their own laboratory.

Compressive sensing (CS) is a mathematical approach used to overcome the Shannon-Nyquist theorem which states that the sampling rate must be higher than the highest frequency divided by two in order to reconstruct a signal without loss. CS is readily used in signal processing to reconstruct under sampled signals without losing any important information by taking advantage of the sparsity of the said signal in a fixed basis. On the condition that the measurement matrix is incoherent with the signal in its sparse basis, we can solve the underdetermined linear system $y = Ax$ using the L_1-norm minimization of the solution vector y, giving a good approximation of the original signal.

In the recent years, there has been extensive research in the area of combining CS with deep-learning techniques for efficient results. In 2018, Zhang et al. proposed a deep-learning unfolded iterative soft thresholding algorithm (ISTA-Net) for CS-reconstruction of images [1]. In our research, the structure was adapted to work with XAS spectral signals. It is trained on 212'108 simulated XAS spectra from the Materials Project. The proof of concept is done by using 588 reference XAS spectra in the validation set. The results show an accuracy of 95% (with error threshold at 1%) when reconstructing from 25% of the original data set; compared to the classical approach with an accuracy of 83% at 50% of the original data size.

[1] J. Zhang and B. Ghanem, „ISTA-Net: Interpretable Optimization-Inspired Deep Network for Image Compressive Sensing“, **2018** IEEE/CVF Conference on Computer Vision and Pattern Recognition, S. 1828–1837

Laser-induced XUV spectroscopy (LIXS) for fluorine detection

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Laser-induced breakdown spectroscopy (LIBS) is a widely used elemental analysis method for solid samples. However, for some elements like halogens, the detection is difficult. In LIBS, the signal can vary significantly, due to flicker noise leading to poor precision. As established in a previous publication [1] a new method was developed called laser-induced XUV spectroscopy (LIXS) that makes use of shorter wavelength signals in the range of several nm, originating from the earlier hotter stage of the plasma. This gives several advantages. As the plasma is more stable in the earlier stages, the ionization process is more consistent, leading to a higher stability of the signal. In particular, halogens can be detected more easily due to the strong emission lines in the XUV range.

In this study, we used several reference materials to test the capabilities of the LIXS setup to measure F in different samples ranging from LiF to PTFE and show the difference between LIXS and LIBS for its detection and reproducibility. In addition, geological samples were analyzed to see the application of the system in fields ranging from geology to space exploration. The system consists of a Nd:YAG laser operated at 532nm, focused on the sample in a vacuum chamber with a fluence of 20J/cm^2. The emissions are separated through a variable-line-spacing grating and collected with a back-illuminated X-ray CCD detector and calibrated with a calibration sample to get the spectra in the range of 4 to 22nm.

The results showed that the F lines of the LIXS setup can be detected for all samples where as in the LIBS spectra detection was difficult and in the case of PTFE not detectable at all. Additionally the fluctuation of the signal from LIBS was much greater than from the LIXS setup showing the stability gained by using the LIXS setup. The Geological samples also showed lines for most element contained in the sample, showing that it could be a promising analysis tool for space exploration.

References:

[1] Qu, D., Ohannessian, N., Wyder, C., Trottmann, M., Wichser, A., Lippert, T., Bleiner, D., "High-precision mapping of fluorine and lithium in energy materials by means of laser-induced XUV spectroscopy (LIXS), Spectrochimica Acta Part B: Atomic Spectroscopy 181 (2021) 106214

Investigation of NiFe alloy for water splitting by XPS/HAXPES and EIS

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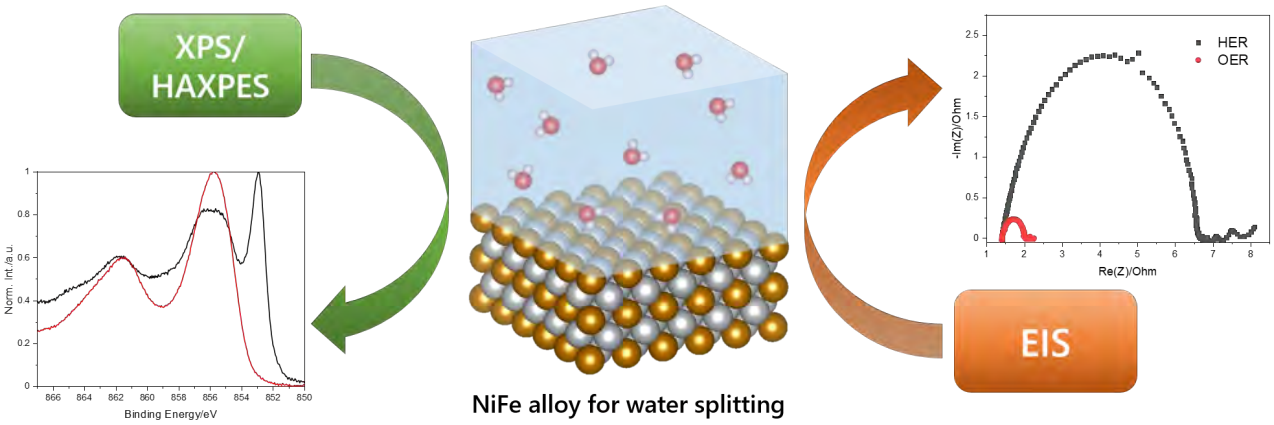
Alkaline water electrolysis is one of the simplest methods used for renewable hydrogen production [1]. In contrast to electrolyzers relying on acidic electrolytes, alkaline electrolyzers reach high con-version efficiency with abundant metals such as Ni-Fe alloys [2]. The outstanding properties can be mainly traced back to the host material Ni, which is both stable and electro-catalytically active in alkaline media. This peculiarity can be related to its ability to form various compounds with hydrogen and oxygen (NiO, $Ni(OH)_2$, NiOOH), which are known to stabilize Ni when in contact with electrolyte solutions as categorized in equilibrium Pourbaix diagrams. Moreover, it is widely accepted that the interaction between Ni and Fe is significant for enhancing the OER activity [3]. Here we investigate the surface and bulk modifications of the NiFe alloy, as well as the electrochemical properties, combining soft- and hard X-ray photoelectron spectroscopy (XPS/HAXPES) with electrochemical impedance spectroscopy (EIS).



[1] D. M. F. Santos and C. A. C. Sequeira, Quim. Nova, **2013**, 36, 1176.
[2] L. Trotochaud, S. L., et al., Journal of the American Chemical Society, **2014**, 136, 6744.
[3] H. Xiao, et. al., Proc. Natl. Acad. Sci. U.S.A. **2018**, 115, 5872−5877.

Driving charged probes on the surface of ion-selective membranes: a new perspective for reversible bioassays

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Redox probes have been frequently used in aptamer-based devices for separation-free bioassays [1]. The redox reporter can be replaced by a charged nanoparticle, which can strongly affect the ions distribution in ion-selective membranes (ISMs), resulting in an electrochemical signal with better selectivity. A glassy carbon electrode modified with a conducting polymer (*i.e.* PEDOT-C_{14}) can be used to drive the charged nanoparticles on the surface of the ISM by reducing and oxidizing the transducing layer. In this case, the ISM serves as a permselective barrier to avoid interference from redox species in the aqueous phase.

We report here the use of mercaptoundecanoic acid-capped gold nanoparticles (Au@MUA NPs) attached to the surface of a PEDOT-C14 modified glassy carbon electrode covered with an ISM. Depending on the redox state of the transducing layer, Au@MUA NPs are either attracted (oxidation) or repelled (reduction) at the ISM (Figure 1A, left panel). Since the Au@MUA NPs have fluorescence properties [2], the electrochemical experiments were coupled to a confocal microscopy system to visualize this process better (Figure 1A, right panel). Such approach is promising for a biosensing system, where those probes are attached to the surface of the electrode through a biorecognition element. The binding of a specific target affects the interaction of this probe with the ISM, resulting in a measurable electrochemical output during cycles of ion transfer that can be used to measure molecular concentrations in real time (Figure 1B).

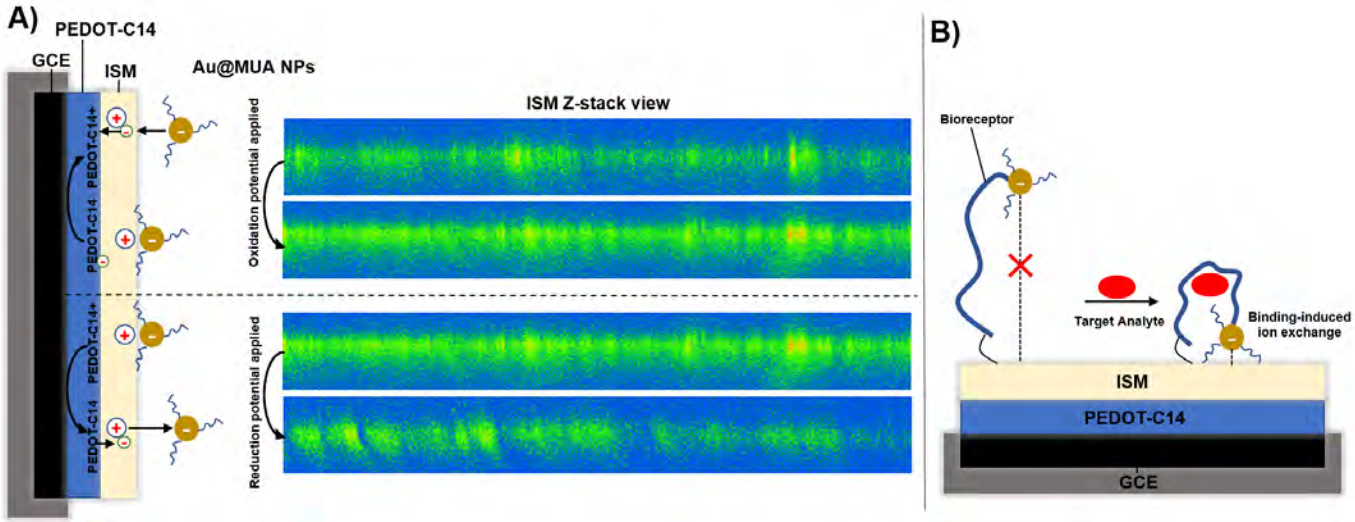

Figure 1. A) Scheme of the sensing mechanism and confocal microscopy images **B)** Biosensing principle.

[1] Idili et. al, *Anal. Chem.*, **2021**, *8*, 4023-4032.
[2] Zhu et. al, *ACS Appl. Nano Mater.*, **2021**, *4*, 3197-3203.

Improved Reproducibility of Constant Potential Coulometry for Environmental Applications: B) Detection of Fluoride

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The levels of fluoride ions in unpolluted water are around 0.01-0.3 mg/L in fresh water and 1.2-1.5 mg/L in seawater.[1] With such low levels of F^-, the need for analytical methods that can sense small changes that often remain undetected using established potentiometric probes is essential. Bobacka and co-workers have introduced solid contact electrodes with transducing materials acting as a capacitive layer to perform constant-potential coulometry with ion selective electrodes (ISEs).[2] By setting a fixed reference potential, any ion activity changes at the electrode surface will result in a potential difference that generates a transient current between the counter (CE) and working electrode (WE), giving a capacitive current readout. Our group coupled the WE with an electronic capacitor, allowing one to use ISEs with inner solutions and avoid non-ideal behavior of the capacitive layer for better performance.[3,4] However, flowing even a residual current across an ISE membrane results in concentration polarizations in the membrane, which introduce potential drift. This can be overcome by switching the WE and the reference electrode (RE) positions, treating the ISE as RE.[5,6]

In this work we use a LaF_3 single crystal-based F^- ISE as RE and an Ag/AgCl reference element as WE for constant potential coulometry. Treating the ISE as working electrode would increase the RC time constant by more than 10-fold and generate noise owing to the forcing of ions through the crystal. An electronic capacitor is placed in series of the WE by the means of circuit printed device (CapaBox) allowing us to place different capacitors and resistances in series and to electronically discharge them by short circuiting. This system is implemented in a flow cell to assess 0.01 and 0.001 logarithmic changes in fluoride activity, with outstanding reproducibility. The average standards deviation founds are 7.8×10^{-10} C and 1.4×10^{-9} C corresponding to an average relative error of 0.013 % and 0.084 % respectively. The principle will be implemented in a field deployable device for aquatic measurements.

[1] Camargo, J. A. *Chemosphere* **2003**, *50* (3), 251–264.
[2] Hupa, E.; Vanamo, U.; Bobacka, J. *Electroanalysis* **2015**, *27* (3), 591–594.
[3] Kraikaew, P.; Sailapu, S. K.; Bakker, E. *Anal. Chem.* **2020**, *92* (20), 14174–14180.
[4] Kraikaew, P.; Jeanneret, S.; Soda, Y.; Cherubini, T.; Bakker, E. *ACS Sens.* **2020**, *5* (3), 650–654.
[5] Kraikaew, P.; Soda, Y.; Nussbaum, R.; Jeanneret, S.; Bakker, E. *Sens. Actuators B Chem.* **2023**, *379*, 133220.
[6] Delmo, N.; Mousavi, Z.; Sokalski, T.; Bobacka, J. *Membranes* **2022**, *12* (12), 1221.

Improved Reproducibility of Constant-Potential Coulometry for Environmental Applications: A) Measurement of pH

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Constant-potential coulometry has recently emerged as a promising readout for solid-contact ion-selective electrodes. It takes advantage of the capacitive behavior of the ion-to-electron transducing layer and results in an increased precision [1]. With the application of a reference potential, any potential variation at the sample and ion-selective electrode (ISE) interface resulting from an analyte activity change induces an opposite potential variation at the transducing layer, giving a transient current. Our group replaced the latter layer by an electronic capacitor to take advantage of its ideal behavior and to achieve automated electronic control of the circuit [2].
However, flowing current through the ion-selective membrane was recently demonstrated to be a source of potential drift due to forced diffusion inside the membrane phase [3]. Bobacka and co-workers proposed to invert the classical conformation on using the ISE as reference electrode (RE) and a modified membrane-based electrode as working electrode (WE) [4].
In this work, we improved the latter idea using an Ag/AgCl electrode as WE together with a membrane-based pH sensing electrode as RE. We built an electronic circuit to control automatically the capacitor and demonstrated that the charge drift was much less significant when flowing current through the AgCl layer, which resulted in an improved precision. This principle is applied to ultra-sensitive pH sensing in environmental samples and will be applied to field campaigns.

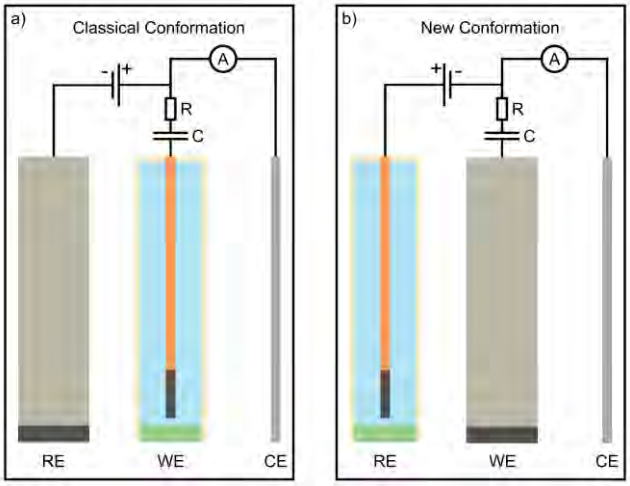

Figure 1. Three electrodes setup for constant-potential coulometry with a) the ISE as WE and b) as RE.

[1] Hupa, E.; Vanamo, U.; Bobacka, J. *Electroanalysis*, **2015**, *27* (3), 591–594.
[2] Kraikaew, P.; Sailapu, S. K.; Bakker, E. *Sensors and Actuators B: Chemical*, **2021**, *344*, 130282.
[3] Kraikaew, P.; Soda, Y.; Nussbaum, R.; Jeanneret, S.; Bakker, E. *Sensors and Actuators B: Chemical* **2023**, *379*, 133220.
[4] Delmo, N.; Mousavi, Z.; Sokalski, T.; Bobacka, J. *Membranes* **2022**, *12* (12), 1221.

Distributed-Feedback in "Röntgen Materials" for Coherent X-ray Spectroscopy

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About 50 years ago, Yariv [1] theoretically proposed distributed feedback as a way to realize x-ray amplification. In this project, the experimental realization is the main objective, using pulsed laser deposition (PLD), to realize a structured material suitable for x-ray distributed feedback. Such compact coherent x-ray source would permit spatially resolved and high-resolution x-ray spectroscopy in the home lab.

We have performed the calculation of the gain co-efficient for the various röntgen materials that includes alkaline earth metal oxide, p-block compound semiconductor, 3-d transition metal oxide, carbide, nitrides and finally lanthanide series oxide, carbide and nitride. Our theoretical analysis showed that the alkaline earth metal oxide are promising materials with higher gain co-efficient of about $7.74*10^8$ cm^{-1} for 0.001 um^3 crystal and the highest of the all materials considered for calculation. Except the alkaline earth metal oxide, other oxide materials such as transition and lanthanide metal oxide shows the least gain value and this is due to their larger lattice parameter. Nitrides, carbides and compound semiconductor shows better gain value compared with oxide materials but they are one order in magnitude less than alkaline earth metal oxide. The gain value can be further increased by increasing the length of the gain medium and decreasing the volume of the crystal.

In order to realize the concept highlighted above, a methodology for suitable materials synthesis has to be developed. To realize such a small single crystal, we propose to use the PLD to grow such material as an epitaxial thin film. Later, it could be patterned using lithography and etching to get our final small single crystallite of required dimension on a substrate.

Reference:

1. Yariv, Amnon. "Analytical considerations of Bragg coupling coefficients and distributed-feedback x-ray lasers in single crystals." *Applied Physics Letters* 25, no. 2 (1974): 105-107.

Nanopore-based investigation of bacterial Hsp70 reveals entropic pulling as mechanism of function

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The Hsp70 family of ATP-dependent chaperons is an essential component in cellular networks. These molecular motors are involved in the prevention of protein aggregation, control of the activity of regulatory proteins, and membrane translocation of proteins[1]. Despite their crucial role in ensuring protein quality, the underlying physical mechanism of their functions has not been identified. Recently, nanopores have proven useful as a novel approach to analyzing the function of motor enzymes[2]. We designed a system that uses the biological nanopore, aerolysin, to observe DnaK (the Hsp70 isoform found in *E. Coli*) on the single molecule level as it interacts with a substrate protein. The nanopore measurements allow us to analyze the response of this system to defined voltage-induced forces. By comparing the behavior of the substrate in the presence and absence of DnaK we can for the first time identify the physical mechanism of the motor. Our results provide experimental proof that the bacterial Hsp70 uses the entropic pulling mechanism[3] to generate a force on its substrate and rule out other proposed models (Brownian ratchet or power-stroke mechanism).

[1.] Wickner, S., Camberg, J. L., Doyle, S. M. & Johnston, D. M. Molecular Chaperones☆. in Reference Module in Life Sciences (Elsevier, 2017). doi:10.1016/B978-0-12-809633-8.06723-6.
[2.] Laszlo, A. H., Derrington, I. M. & Gundlach, J. H. MspA nanopore as a single-molecule tool: From sequencing to SPRNT. Methods 105, 75–89 (2016).
[3.] Sousa, R. & Lafer, E. M. The Physics of Entropic Pulling: A Novel Model for the Hsp70 Motor Mechanism. Int J Mol Sci 20, E2334 (2019).

250+ Multiple-Choice and True-False Questions for Quantitative Element Analysis

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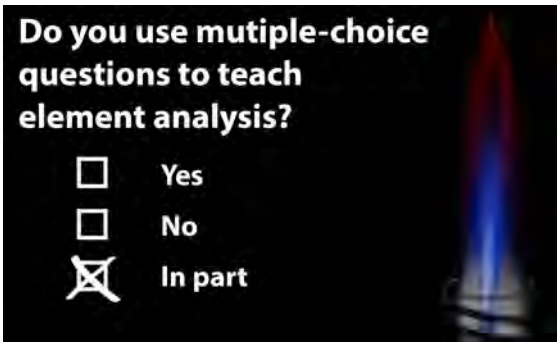
Whether for exams, exercises or classroom discussions, developing questions is often a tedious but necessary part of teaching. The goal should not be to ask as many questions as possible, but to ask as many learning-supporting questions as possible. Despite shortcomings, multiple-choice questions can be a valuable opportunity to engage students. Yet, due to the lack of tangible design models, their development requires much effort and there are not many specific multiple-choice questions available for advanced analytical chemistry [1-3]. Here, a collection of more than 250 multiple-choice and true-false items for quantitative instrumental element analysis, covering fundamentals of the analytical process, ICP-OES, AAS, ICP-MS and XRF, with keys and brief explanations are presented. Furthermore, guidelines for designing questions for summative assessments (exams) are revisited in formative contexts. To ease the development of multiple-choice questions, the generation of distractors based on responses to open-ended questions is investigated within a routine teaching context, whereas it is demonstrated that both elicit the same rate of correct responses.



[1] G. Kortemeyer, *Journal of Science Education Technology*, **2016**, *25*, 561-574.
[2] G. Schwarz, *Chimia*, **2021**, *75*, 33-38.
[3] G. Schwarz, *Journal of Chemical Education*, **2021**, *98*, 2122-2127.

Manufacturing Method for Solid-Contact Ion-Elective Electrodes using Fluid Dispenser

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Due to the possibility of miniaturization, Solid-Contact Ion-Selective Electrodes (SC-ISEs) are very powerful tools for medical diagnostics. SC-ISEs allow real-time and non-invasive analysis of ions in various biological samples such a blood, sweat, urine and interstitial fluid.

In its most simple form, a SC-ISE consists of at least two components; a transducer layer serving to maintain a high potential stability, and a polymeric membrane containing an ionophore to introduce selectivity for a specific ion. The potentiometric response associated with this membrane can then be correlated with the activity of the ion in solution.
More complex configurations involving enzymatic layer, blocking membrane or anti-fouling component may be added depending on the desired sensor configuration.

The deposition of the transducer layer as well as the membrane is generally performed by drop-casting with a micropipette, which may result in variations of the deposited volumes and introduces undesired uncertainties regarding the subsequent experimental data. For instance, it has been demonstrated by Zdrachek *et al.* that the amount of single-walled carbon nanotubes (SWCNTs) deposited correlates with the capacitance of the ion-to-electron transducing layer, which in turn affects the potential stability and reproducibility of SC-ISEs [1].

This work investigates the use of a fluid dispenser to manufacture SC-ISEs with increased speed, precision and reproducibility in the following configuration: Screen-printed electrode as substrate, SWCNTs as transducer layer, polymeric ion-selective membrane and optional agarose gel layer. The reproducibility of the deposited amount of transducer is assessed by a chronopotentiometry protocol proposed by Johan Bobacka [2] while the amounts of membrane and agarose gel is assessed by colorimetric absorbance [3].

[1] E. Zdrachek, E. Bakker, *Microchim Acta*, **2021**, *188*, 149.
[2] J. Bobacka, *Anal Chem*, **1999**, *71*, 4931-4937.
[3] Y. Soda, K. J. Robinson, T. J. Cherubini, E. Bakker, *Lab Chip*, **2020**, *20*, 1441-1448.

Origin of the magnetic effect on the electrochemical hydrogen evolution reaction

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Recently it was shown that applying a magnetic field increases the electrochemical efficiency of hydrogen production by water splitting.[1],[2] This is surprising since magnetic energies are orders of magnitudes lower than chemical free energies sparking controversial debates on the origin of the effect. Here we present a careful study on how magnetic fields influence the oxygen evolution and hydrogen evolution reaction (OER and HER) on Ni electrodes. For this, we utilized cyclic voltammetry together with in-situ reflectivity measurements. This allows us to follow the electro-chemical properties and the evolution of the electro-catalytically active Ni-oxide layer. The magnetic effect on the electrochemical properties is relatively small. However, we observe that the Ni-oxide layer growth depends significantly on the magnetic field. From this we conclude that at least in this case, the sought magnetically increased efficiency is due to a structural modification of the surface. The growth involves the motion of paramagnetic ions (Ni) strongly affected by magnetic fields. The new restructured surface enhances the electrochemical hydrogen production by formation of channels, providing pathways for the ions and a larger electro-catalytically active surface area.

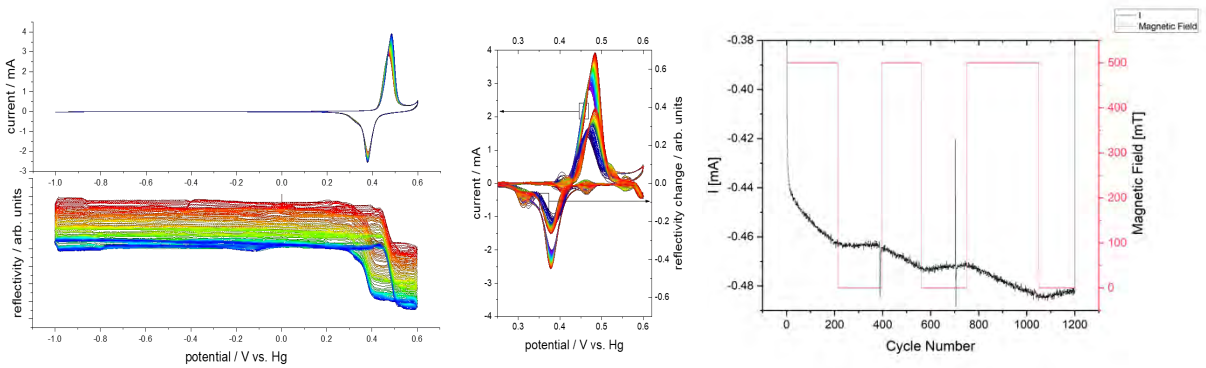

Figure 1: (left) cyclic voltammogram of Ni in KOH together with reflectivity measurements. (right) The change in strength of electric current over the cyclic numbers in dependence of the magnetic field.

References:

[1] Donghoon Kim et al, "Magnetoelectric effect in hydrogen harvesting: Magnetic field as a trigger of catalytic reactions ", *Adv. Mater. 34,* **(2022),** 2110612.

[2] Olga Sambalova et al, "Magnetic field enhancement of electrochemical hydrogen evolution reaction probed by magneto-optics", *International Journal of Hydrogen Energy 46,* **(2021),** 3346-3353.

From the Bulk to the Nanoscale: role of surface activity and hydrolysis of carbonate ionophore VII in the poor performance of carbonate-selective optical nanosensors

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Ionophore-based ion-selective sensors are well-established tools that are readily applicable for environmental analysis and medical diagnostics. The availability of a multitude of ionophores selective to various inorganic cations and anions allows a practically minded analyst to conveniently fine tune their sensor to respond to an ion of interest in the desired concentration range [1]. However, in the haste of the never-ending search for superior complexing agents with improved binding characteristics, fundamental aspects of their interaction with the analyte ion often receive limited attention.

Herein we showcase a more in-depth analysis of the response mechanism of carbonate-selective optical sensors based on carbonate ionophore VII. This carrier has been successfully applied for carbonate detection with bulk membranes [2], yet, its application in sensing nanospheres was complicated by the heightened surface activity of the ionophore and required additional facilitation of interphase transfer by the optical reporter [3]. Upon further investigation we found that this ionophore tends to undergo hydrolysis while on particle surface (Fig. 1). This is not only shown to diminish the robustness of the sensor response due to extraction of the ligand into the particle bulk without analyte, but also contradicted the results of previous studies conducted with bulk sensors [4]. This contribution presents research on the fundamental influence of ionophore hydrolysis on the structure of the ion-ionophore complex through acquisition of adduct crystal structures for the first time.

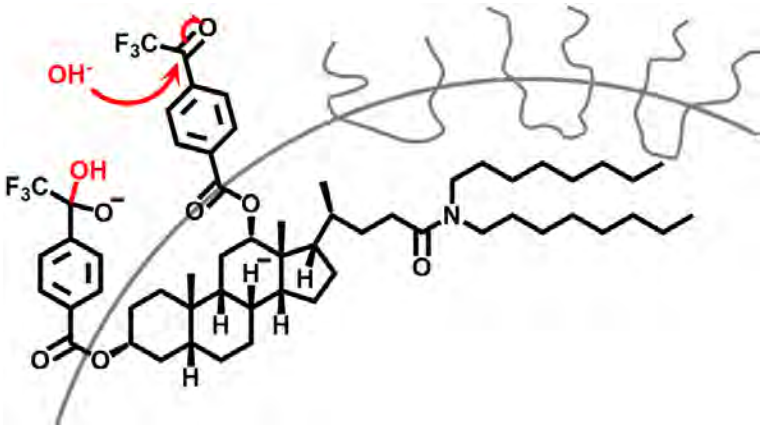

Figure 1. Carbonate ionophore VII hydrolysis on nanosphere surface.

[1] P. Bühlmann, E. Pretsch, E. Bakker, *Chem. Rev.*, **1998**, *98*, 1593-1687.
[2] X. Xie, M. Pawlak, M. Tercier-Waeber, E. Bakker, *Anal. Chem.*, **2012**, 84, 3163-3169.
[3] N.Y. Tiuftiakov, K.J. Robinson, E. Bakker, *Electroanalysis*, **2023**, 35, e202200507.
[4] M.E. Meyerhoff, E. Pretsch, D.H. Welti, W. Simon, *Anal.Chem.*, **1987**, 59, 144–150.

Inkjet printed electrochemical sensors for drug testing applications

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Cannabis (Marijuana, Hash) with its main psychoactive compound (-) Δ^9-Tetrahydrocannabinol **3** (Δ^9-THC) is with 209 Mio users one of the most consumed drugs world-wide. Its use is steadily increasing due to the ongoing global legalization.[1] Associated with the usage is an impairment of the ability to drive vehicles. Currently performed urine-based road-side tests do not provide sufficient information on quantity consumed, time of exposure and current impairment. The accurate determination of impairment-related blood-concentrations still requires bulky lab-based techniques. An alternative approach is electrochemical sensing based on disposable inkjet printed (IJP) electrodes. Such sensors have high sensitivity, allow miniaturization and processing on large scale at vanishingly low costs which are requirements for an auspicious road-side sensor.[2]

Here, we present an approach to use graphene-based IJP electrodes for indirect electrochemical detection of Δ^9-THC 3. Currently proposed systems are based on aminophenols **1** (AP) that are reversibly oxidized to quinoneimines **2** (QI) at the electrode (Fig. 1a) generating concentration depend AP/QI redox peaks in cyclic voltamograms (CVs) (Fig. 1b).[3] Phenolic species as Δ^9-THC **3** quench QI **2** reducing quantitatively its concentration (Fig. 1c). Consequently, the PA/QI redox peaks decay in intensity enabling indirect Δ^9-THC quantification (Fig. 1b). Our specifically modified graphene electrodes demonstrate an improved sensitivity towards the electrochemical reduction of quinone derivates (Fig. 2) and represent a promising road-side device for electrochemical Δ^9-THC determination.

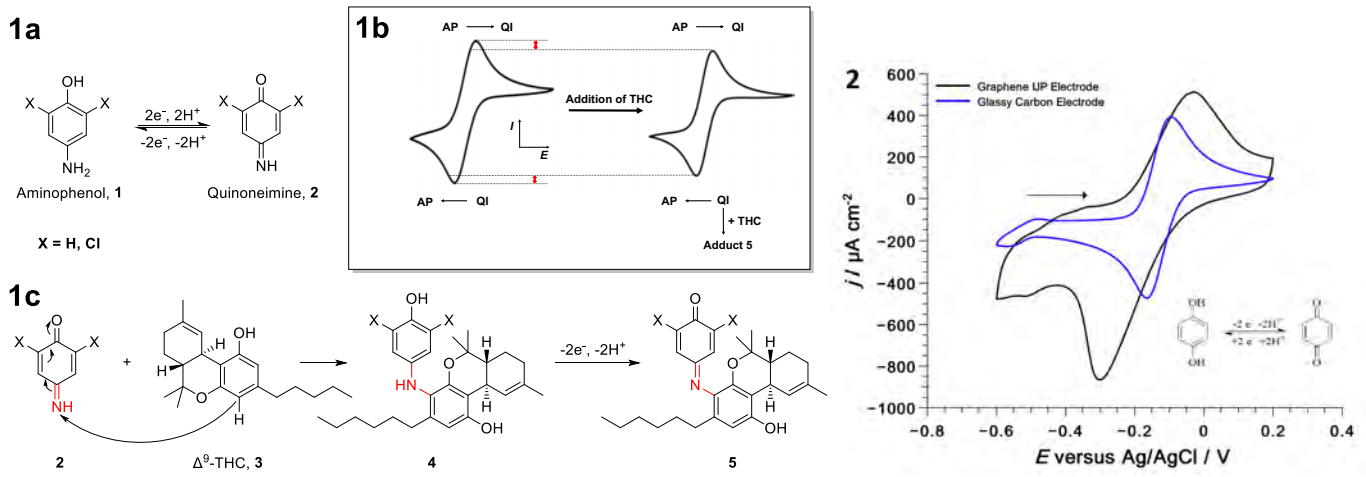

Fig. 1: Electrochemical redox reaction of aminophenol and quinoneimine (a), the irreversible chemical redox reaction in presence of Δ^9-THC (b) and the associated CVs (c).
Fig. 2: CVs of 1 mM benzoquinone in 0.1M KNO_3 at 100 mV s^{-1} recorded with an IJP graphene electrode (**black**) and a glassy carbon electrode (**blue**).

[1] United Nations Office on Drugs and Crime (UNODC). World Drug Report **2022**.
[2] B. Nagar, *et al.*, *ChemElectroChem*, **2020**, 7, 460-468.
[3] E. R. Lowe, C. E. Banks, R. G. Compton, *Anal. Bioanal. Chem.*, **2005**, 383, 523-531.

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Mass Spectrometry tools for confident discrimination of different qualities of post-consumer recycled plastics

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Plastic is ubiquitously present in every aspect of our modern lives and, consequently, it constitutes a big portion of household waste. Most of the plastic in use is made from fossil fuels. Due to its properties, fossil-fuel derived plastic can remain intact for decades or even centuries after use. To preserve our natural resources and reduce the environmental impact of plastic production and waste, plastic waste could become a valuable resource if re-used (recycled) to manufacture new products instead of ending up in landfill. By recycling, the dependence on fossil fuel for plastic production can be reduced, a major step towards tackling the plastic waste problem by keeping it in circulation as long as possible.

To successfully reintroduce or repurpose post-consumer recycled plastics (PCR), there is a need to characterize the recycled plastic pellets to ensure no harmful impurities are present that may hinder the end-product performance and most importantly, consumer safety.

In this presentation, an analytical workflow using state of the art high resolution mass spectrometry was used for the analysis of different batches of recycled low density polyethylene (rLDPE). By using analytical and statistical tools, chemical profiling of various PCR sample batches were performed and key marker compounds characteristic for various levels of quality PCR samples were detected and identified.

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Nanoparticle identification using single particle ICP-ToF-MS acquisition coupled to cluster analysis. From engineered to natural nanoparticles

Submitted by Jamie Royce (Nu Instruments) on behalf of

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spICP-MS where a single isotope signal can be acquired continuously at dwell times between 10-100µs is a particularly helpful technique when investigating the number and size of of individual elemental nanoparticles. The technique is improved upon when using an ICP-Time of Flight -MS as the multi-element compositions of each particle can be determined. The ICP-ToF-MS is further optimized for the single particle technique when able to continuously collect the ion beam at a few tens of µs per spectra with no interruption as it allows

i/ the complete evaluation of each NP signal
ii/ collecting all NP signals without loss
iii/ determining the (multi)-elemental composition of NPs individually

This makes the information on the NP population in the sample more thorough and reliable compare to information provided using a conventional single isotope ICP-MS method. Indeed, single particle composition is given simultaneously, and part of the interest of using a multi-elemental spICP-MS analysis is its potential for the identification / classification of natural or synthetic compounds for the determination of the risk assessment and of the possible health hazard. In this study, the signal of mono-, bi- and tri-metallic synthetic nanoparticles either alone or mixed will be analysed using a novel ICP-ToF-MS with the desired performance characteristics (Nu Instruments *Vitesse*) and multiple ways to examine the data produced will be explored.

In addition, natural particles including aluminium oxide, montmorillonite and kaolinite which are particles now dispersed in the environment due to the increase of anthropogenic activities (*ie*. soil erosion in the critical zone), will be investigated.

(Tharaud et *al., Journal of Analytical Atomic Spectrometry*, 2022)

Improved compound identification in GC-MS analysis using an EI&CI-TOFMS

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Introduction

Many non-target analysis (NTA) approaches using common GC-MS setups only identify about 50-60 % of the found compounds due to the lack of molecular ion information. To generate this information the use of a soft ionization e.g., chemical ionization (CI) in a second GC run seems to be constructive. Unfortunately, this is very time consuming and subsequent data alignment is highly complex. Here we present a Time-of-Flight (TOF) mass spectrometer operating an EI and a CI source simultaneously within one GC-run. Both ion sources are sampling the same GC effluent. By coupling both ionization sources directly to one single gas chromatograph (GC), structural as well as accurate mass molecular ion information is generated within one single chromatographic run to overcome known problems for NTA using GC-MS setups.

Methods

A GC (Agilent 6890A, Agilent Technologies Inc., Santa Clara, USA) was coupled to an ecTOF (TOFWERK AG, Thun, Switzerland), operating a 70 eV EI source and the newly developed HRP CI source [1,2]. Various GC methods and sampling procedures were employed depending on the analytical need of the study, including liquid injection of extracted samples, headspace sampling including SPME and thermal desorption using Tenax tubes. To generate the ideal molecular ion information for various compound classes, different reactant ions (e.g., N_2H^+, H_3O^+ and NH_4^+) were used for the chemical ionization process [3].

Results

Standard procedures employed by routine laboratories, e.g., target screening for material emissions or steroid screening, is shown to be feasible using the GC-ecTOF. It is demonstrated, that standard methods for target analysis and suspect screening are improved using the ecTOF. Especially when EI library hits are fair but with low corresponding probability, CI information can be used to increase compound identification confidence. False positives from an EI only approach can easily be identified and often correctly annotated. Using the accurate mass information generated by CI, molecular sum formula for not-listed unknowns can be derived. Combining this with the structural information generated by EI, tentative structure elucidation becomes feasible in many cases. Various experiments will be discussed, illustrating the potential of the GC-ecTOF for targeted, suspect screening and NTA approaches, including applications in fields such as environmental contaminants, material emissions, food flavour analysis and metabolomic research.

Acknowledgements

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References

[1] Bräkling, S. et al. Parallel Operation of Electron Ionization and Chemical Ionization for GC-MS Using a SingleTOF Mass Analyzer. Anal Chem., **2022**, 94 (15), 6057-6064.

[2] Bräkling, S. et al. Hydrogen Plasma-Based Medium Pressure Chemical Ionization Source for GC-TOFMS. J. Am. Soc. Mass Spectrom., **2022**, 33 (3), 499-509.

[3] Bräkling, S. et al. Gas chromatography coupled to time-of-flight mass spectrometry using parallel electron and chemical ionization with permeation tube facilitated reagent ion control for material emission analysis. Rapid Commun Mass Spectrom., **2023,** 37:e9461.

Recent improvements in Mpx/hr LA-ICP-TOFMS mapping

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Laser ablation ICPMS mapping is continuously striving for ever faster speeds and ever higher spatial resolution. The main physical limitations in this endeavour are 1) the wash-out time and dispersion of laser-produced aerosol being transported into the ICPMS, 2) the repetition rate at which the laser can fire, 3) the spatial precision at which individual laser shots can be placed at very high speeds and repetition rates, 4) the optical quality of the laser ablation system, and ultimately for smaller and smaller laser spot sizes, 5) the detection sensitivity of the ICPMS.

While point 2) could advance much beyond current state-of-art, 1) poses a physical limit on maximum repetition rates achievable. Both are fields of intensive technological development in the past decade. Points 3) and 4) are well understood technical challenges, and while ultimately the interplay of stage precision and laser spot size will also put a physical limit on feasibility, technological improvements can still be expected.

Here, we present current developments on the LA-ICPMS mapping capabilities of the icpTOF (TOFWERK AG, Switzerland) coupled to an imageGEO (ESL, USA). We demonstrate excellent spatial precision and reproducibility of the ablation at high repetition rates by encoder triggering on the laser system, as well as improved sensitivity under dry-plasma conditions and improved data acquisition speed on the ICP-TOFMS. In combination, this allows for routine sample mapping in the Mpx/hr range without compromising data quality or sensitivity.

Novel Time-of-Flight Residual Gas Analyzer (TOF-RGA) for in situ Real-time Process Monitoring

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Spacetek Technology's IonTamer™ instruments are compact time-of-flight residual gas analyzers (ToF-RGA) for monitoring the composition of gases in real time, at high resolution, and with high sensitivity. The ToF-RGA mass spectrometers detect species over a mass range up to 1200 u/e and with a mass resolution up to 1800 at full width at half maximum.

The capabilities of the IonTamer™ instruments are demonstrated through several application experiments [1]: (1) The FC5311 calibration liquid contains perfluorophenanthrene (C14F24, molecular weight of 624.1115 u), a well-known high molecular weight compound [2] used for calibration of mass spectrometers with extended mass range. Its fragmentation pattern covers a mass range from 12 u up to more than 624 u. (2) Helium, neon, argon, krypton, and xenon are noble gases found in the Earth's atmosphere with abundances relative to air ranging from about 1% (Ar) through to a few parts per million (ppm) (He, Kr) and a few tens of parts per billion (ppb) (Xe). (3) Quantitative detection of noble gases ranging over the pressure range from high vacuum conditions down to ultra-high vacuum. The isotopic ratios of noble gases in a calibration gas mixture were analyzed as a reference. (4) Real-time process monitoring of reaction products in an X-ray photoelectron spectroscopy (XPS) facility while the synthesis of graphene from ethene (C_2H_4) on a heated silver probe was ongoing.

References

[1] S. Gasc, L. Hofer, *Chimia*, **2022**, 76, 52-59.

[2] Hans-Joachim Hübschmann. Handbook of GC/MS: Fundamentals and Applications. WILEY-VCH Verlag GmbH & Co. KGaA Weinheim, Second Edition, 2009

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TECHNOLOGY

Analysis of automotive paint and glass samples by combined LIBS and Raman spectroscopy

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Two main goals in forensic analysis are the classification of samples present at the crime scene to obtain information on the origin and the discrimination from other samples found. The variety of possible samples is manifold and can range from organic and inorganic materials to samples of human origin. As diverse as the range of samples, the samples themselves contain much complexity. Another challenge in forensic analysis is that often only very small samples are available. Therefore, analytical techniques are required that exhibit high sensitivity and minimal sample destruction. Among other techniques like scanning electron microscopy-energy dispersive X-ray, X-ray fluorescence spectrometry and laser ablation ICP-MS, also Raman and Laser-induced Breakdown Spectroscopy (LIBS) have been established in forensic analysis.

Here we will show with two different examples, namely the analysis of glass and automotive paint samples, the benefits of the combination of LIBS and Raman spectroscopy with multivariate analysis for forensic analysis. With the combination it is possible to obtain complementary (elemental as well as molecular) information of a sample and this can lead to an improved classification and discrimination of the samples. The data were obtained with a newly developed instrument that allows subsequent measurements with both techniques at the same microscopic sample spot by sharing one high-resolution, wide-range Echelle spectrometer.

We measured sixteen different glass samples with LIBS and Raman. The results show that with LIBS and also the combination of LIBS and Raman fourteen of the sixteen samples could be differentiated. By using standardized integral values of selected LIBS lines instead of the whole spectrum we could significantly improve the differentiation. The combination with Raman leads to an improved stability of the differentiation due to the additional information.

Automotive paint samples consist of different layers with varying composition. By measuring cross sections of eight different samples with LIBS and Raman we obtained layer and sublayer-specific chemical information with a spatial resolution of about 10 micrometer. The elemental cross section profiles together with the characteristic Raman and fluorescence signatures turned out to be very unique for macro- and microscopically similar samples.

Literature:

[1] V. Merk, D. Huber, L. Pfeifer, S. Damaske, S. Merk, W. Werncke, M. Schuster, Spectrochim Acta B **2021**, *180*, 106198
[2] V. Merk, W. Werncke, L. Pfeifer, Analyst **2022**, *147*, 5470-5476

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Food Analysis Using Raman Microscopy

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Raman microscopy is a fantastic tool for the analysis food and drinks, an important task to keep the industry safe and legitimate. This poster will present several different approaches to analysing such samples using Raman microscopy.

Raman can be used to analyse liquids directly, with so sample damage, such as whisky and edible oils. Analysing drinking alcohol is important to ensure it is safe to drink, whilst the edible oil market frequently sees fraudulent sales where cheaper oils are passed off as higher quality products.

Raman spectroscopy's limit of detection can reach extremely low levels, in the order of parts per million, by using Surfaced Enhanced Raman Spectroscopy (SERS). One such industry requiring such low levels of detection is pesticide identification, limits of pesticide concentration are set to ensure that fresh produce, such as apples, are safe for human consumption. SERS can be used to detect pesticide concentrations lower than tolerance levels set by regulatory authorities.

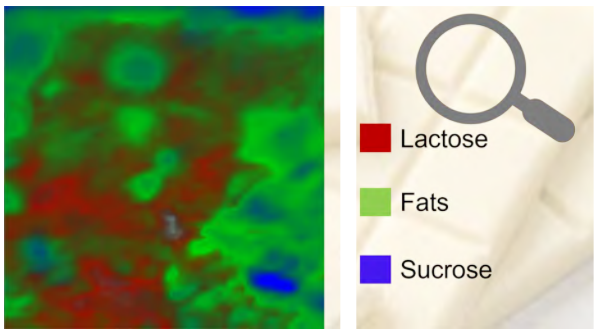

Figure 1: Raman map o white chocolate

A final way in which Raman microscopy ca be utilised in the food industry is by Raman mapping. Here information on sample constituents can be gathered, as well as their distribution within the sample. For exa ıple, Figure 1, shows a map of white chocolate revealing the location of the different sample components.

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