*CH*analysis 2026

March 18-19, 2026,

Dorint Resort Blüemlisalp Beatenberg

SCS Swiss Chemical Society

The **Division Analytical Sciences (DAS)** and the Section Chemistry and the Environment of the Swiss Chemical Society (SCS) are organizing CHanalysis, 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.

Invited Speakers

Prof. Davy Guillarme
University of Geneva

Prof. Koen Janssens
University of Antwerp

Dr. Corinne Jud
Agroscope

Dr. Pascal Miéville
EPFL Lausanne

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Program

Wed, March 18

12.15 Lunch

13.30 Welcome by DAS President

13.40 ***Prof. Davy Guillarme,*** University of Geneva and ***Dr. Pascal Miéville***, EPFL Lausanne
«The Centre de compétences Chimie et Toxicologie Analytiques (ccCTA), 30 years of analytical chemistry and toxicology in Suisse romande»

Session 1 Analytical Technologies
Chair: Davide Bleiner

14.00 ***Keynote by Prof. Koen Jannssens***, University of Antwerp
«Exploring the Chemistry of Artworks with X-ray eyes»

14.35 ***Naresh Kumar,*** ETH Zurich
«Nanoscale Visualization of Plasmon-Enhanced Hydrogen Activation on Pt(111) Surface using Tip-Enhanced Raman Spectroscopy»

14.50 ***Justine A. Rothen,*** University of Geneva
«Spatially Resolved Optical Ion Sensing with Voltammetric Ion Transfer Microscopy: Fundamentals and Applications»

15.05 Coffee Break and Networking

Session 2 Analytics for Life Science
Chair: Eric Bakker

16.05 ***Chan Cao***, University of Geneva
«Identification of glycosaminoglycans with different sulfation degrees with a biological nanopore»

16.30 ***Baptiste Clerc,*** METAS
«Large-scale biomonitoring of bisphenols in the Swiss population»

16.45 ***Kai Klopprogge,*** Roche
«Workflow Comparison of the Immunochemistry Analysers Snibe Maglumi X8 and Roche Cobas Pro e 801»

17.00 ***Yaotin Wu,*** University of Geneva
«Pulseometry: A Differential Readout to Compensate Signal Drift of Potentiometric Probes»

17.15 ***Poster Session & Poster Pitches***

20.00 ***Conference Dinner***

Program

Thu, March 19

Session 3 Quantitative Analytics
Chair: Hanspeter Andres

08.30 METAS Award Lecture 2026
Dr. Una Trivanovic*, METAS*
«Synthesis and dynamics of carbonaceous nanoparticles during enclosed spray combustion»

08.55 ***Laura Kronlachner,*** ETH Zurich
«A robust sample preparation and calibration strategy for nanoparticle analysis using laser ablation single particle-ICP-MS»

09.10 ***Gunnar Schwarz***, University of Bern
«From the Ordinary to the Exceptional: A Study of Quantitative Analyses in Lab Courses»

09.25 ***Dr. Christoph Jansen***, Metrohm Schweiz AG, Zofingen
«Automatic NIR Model Development»

09.45 Coffee Break and Networking

Session 4: Chemistry and the Environment
Chair: Thomas Bucheli

10.50 ***Davide Staedler,*** University of Lausanne
«Between concentration and effect, exposure is the key»

11.25 ***Keynote by Dr. Corinne Jud***, Agroscope
«The Role of Analytical Chemistry in Agricultural Research»

11.40 ***Ricardo Silvestre,*** HEIA Fribourg
«OctoChemDB: An Integrated Platform for HRMS-Based Small Molecule Dereplication»

11.55 ***Sergio Cirelli,*** University of Bern
«Airborne pesticide dynamics: a spatiotemporal analysis using passive air sampling»

12.15 Lunch Break

13.30 ***Panel Discussion «From Detection to Decision: Challenges in Nitrosamine Testing»***
Chair: Dr. Dennis Kucina, Novartis AG

14.30 Awards and Closing Remarks

14.45 End of the Meeting

TALKS

Identification of glycosaminoglycans with different sulfation degrees with a biological nanopore

Chan Cao, Xueqing Ma, Verena Rukes, Louis W. Perrin, Axel Camazzola, Ioan Iacovache, Romain R. Vivès

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Glycosaminoglycans (GAGs) are acidic polysaccharides that play crucial roles in various physiological and pathological processes. However, their high structural complexity has made comprehensive characterization difficult, often limiting analyses to short fragments. Nanopore technology offers a powerful single-molecule approach and has shown promise for monosaccharide and glycan analysis, yet distinguishing GAGs in complex mixtures remains challenging. In addition, the rapid translocation of GAGs through nanopores limits temporal resolution and hampers sequencing efforts. Here, we present a strategy that utilizes electrolyte-mediated, GAG-specific interactions within biological nanopores to overcome these limitations. The sulfate and carboxyl groups of GAGs interact with acidic residues within the aerolysin channel via divalent cations, thereby slowing GAG translocation by more than 100-fold. Mutating the interacting residues abolishes these effects, confirming their specificity. The interaction mechanism was further validated using all-atom molecular dynamics simulations and cryo-electron microscopy. Notably, similar sulfate-specific signatures were also observed in commonly used biological nanopores, inlcuding a-HL and MspA. Leveraging this mechanism, we successfully distinguished different GAG species within a mixed GAG sample, including long GAG polymers over 20 kDa. Furthermore, machine-learning analysis enabled high-accuracy identification of the regioselective desulfated HP variants. Together, these results represent a valuable step toward GAG identification and sequencing at the single-molecule level.

Airborne Pesticide Dynamics: A Spatiotemporal Analysis Using Passive Sampling.

S. Cirelli[1]*, K. Hornak[2], T.D. Bucheli[2] and A. C. Chiaia Hernández R[1].

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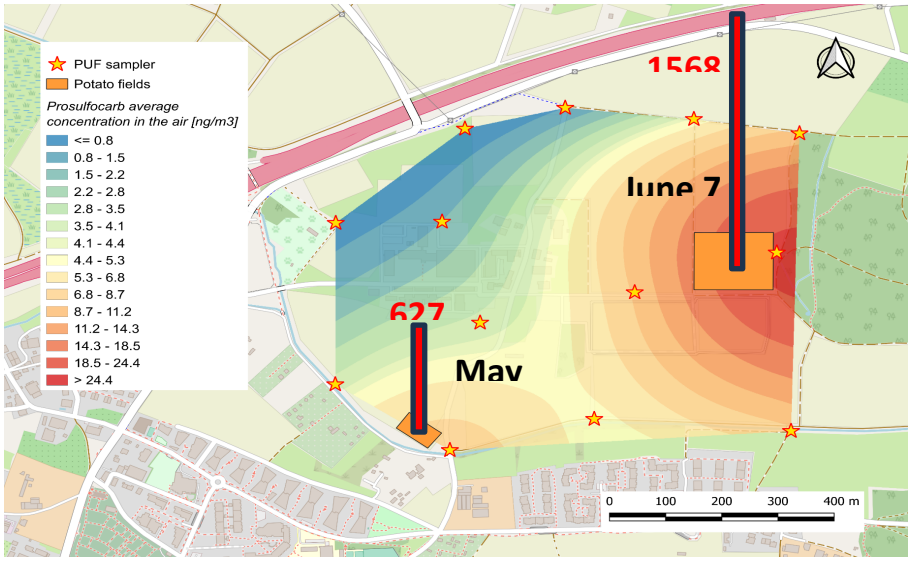
Current-use pesticides (CUPs) are crucial to modern agricultural practices, yet their off-target transport poses environmental and human health risks. Passive air sampling using polyurethane foam (PUF) disks is a practical method for monitoring CUP occurrence, transport, and temporal patterns [1]. In our study, 13 passive sampling stations were deployed around a controlled area of 39 agricultural fields (~600,000m^2) with detailed pesticide application records (compounds, quantities, locations). Samples were collected biweekly from late April to late October 2023 using in-house double-bowl samplers. Extracts were obtained using accelerated solvent extraction, and method recoveries were determined for 104 pesticides. A previously published effective sampling volume model [2] was adapted for CUPs and local meteorological conditions to estimate averaged airborne concentrations, enabling time-trend analyses. The high sampling frequency captured short-term application fluctuations and subsequent off-site transport. CUPs were detected at multiple locations, in some cases more than two kilometres from application sites, indicating substantial regional dispersion and potential risks to non-target areas.

Spatiotemporal distribution maps were generated by combining passive sampling data with pesticide application records (Figure 1), allowing systematic comparison of spatial extent, temporal persistence, and pattern stability among compounds.



Based on these spatial and temporal patterns, compounds were clustered according to their dominant atmospheric behaviour. While some pesticides exhibited strong local concentration peaks with sustained temporal persistence, others showed broader spatial dispersion but limited temporal persistence,

Figure 1: Spatial distribution of averaged airborne concentrations during the period 26 May–9 June 2023 for the herbicide prosulfocarb. Two application events are indicated by red bars, representing the total amount applied in the treated field.

suggesting distinct transport and redistribution mechanisms. Linking the observed patterns to physicochemical properties (e.g., volatility and partitioning behaviour) improved our understanding of pesticide fate in air. This pattern-based classification approach enhances understanding of CUP distribution processes and provides a stronger basis for risk assessment and mitigation planning.

[1] Estellano V. H. et al. (**2015**) Assessing levels and seasonal variations of current-use pesticides (CUPs) in the Tuscan atmosphere, Italy, using polyurethane foam disks (PUF) passive air samplers, *Environmental*, Volume 205, Pages 52-59
[2] Herkert N. J. et al. (**2016**) A Model Using Local Weather Data to Determine the Effective Sampling Volume for PCB Congeners Collected on Passive Air Samplers, *Environmental Science & Technology* 2016 50 (13), 6690-6697

Large-scale biomonitoring of bisphenols in the Swiss population

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2022 and 2023, the Swiss Federal Food Safety and Veterinary Office (FSVO) conducted a study about salt intake in Switzerland. The study included a representative sample of adults from different regions, age groups, and genders across Switzerland. Beside the determination of some cardiometabolic indicators, 863 Participants completed detailed questionnaires about their dietary habits, knowledge about salt consumption and other lifestyle factors [1]. The participants were also asked to provide 24-hour urine samples. In this elaborate framework, the FSVO mandated METAS to determine in these urine samples the amount of some bisphenols, phthalate metabolites, and iodine.

Bisphenols (BPs) are used as monomer for the production of polycarbonates, epoxy resins and thermal paper. Due to their presence in common consumer products as well as their chemical structure, they can migrate into food, beverages, water, dust and soil, leading to human exposure by a variety of routes. Dietary ingestion is the most significant route of exposure [2]. BPs can leach into food and drinks from containers, especially when they are scratched, heated or washed repeatedly. BPs are suspected to have disrupting effects on the endocrine system of humans and animals. Endocrine-disrupting chemicals may mimic, block or interfere with the body's hormones and are associated with health issues [3]. Glucuronidation of BPs in the intestine and liver is considered the main metabolic pathway for most BPs while other metabolites only result when the glucuronidation pathway is saturated. These metabolites are mainly excreted through urine [4]. Therefore, human biomonitoring in urine is a crucial method to assess the possible presence of these chemicals in various body fluids to determine the overall extent of exposure in both a qualitative and quantitative manner.

Sample preparation was optimized for high-throughput. During the sample preparation, enzymatic hydrolysis is performed to cleave the glucuronides in urine, followed by protein precipitation. Eleven bisphenols were selected and analysed with ultra-high pressure liquid chromatography–mass spectrometry in a 13-minute run. The mass spectrometer was operated in negative ionization mode, using a scheduled multiple reaction method with three transitions per substance (one quantifying and two qualifying transitions) to ensure selectivity. Corresponding isotopically-labelled standards were added in equal amounts to all samples to ensure robustness. The Method Accuracy Profile associated with the β-expectation tolerance intervals was selected to assess and validate the quantitative performance of the newly developed analytical method. Measurement uncertainties were estimated based on the validation measurements.

We will present the results of this extensive biomonitoring study of bisphenols in Switzerland.

[1] https://www.blv.admin.ch/blv/en/home/lebensmittel-und-ernaehrung/forschung/gesundheitliche-risiken/ernaehrungsrisiken/salzstudie.html (29.01.2026).
[2] Vandenberg *et al.*, Reprod Toxicol, **2007**, *24*, 139-177.
[3] Teng *et al.*, Chem-Biol Interact, **2013**, *203*, 556-564.
[4] Trdan Lusin *et al.,* Toxicology, **2012,** *292*, 33–41.

Automatic NIR Model Development

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Near-infrared (NIR) spectroscopy offers clear advantages for routine analytical applications. It is fast, sustainable, easy to perform, requires no sample preparation, and generates no typical analytical waste. In addition, multiple parameters can be quantified simultaneously within seconds.

The development of identification models for raw materials is generally less effort and will not be addressed in this contribution.

In contrast, quantitative NIR methods still face several practical bottlenecks. For many applications, the main challenge is the effort required to develop models that allow the determination of all desired parameters. As a secondary analytical method, NIR analysers must be trained with spectra covering relevant concentration ranges and require reference values from primary analytical techniques. Collecting sufficient samples and reliable reference data generates cost and is often time-consuming.

For frequently used standard applications, instrument manufacturers often provide pre-calibrated systems. This represents the simplest way for end users to benefit from NIR spectroscopy and is widely established in markets such as food, fuels, polymers, and related industries.

The methods for creation of calibration models can be considered an early form of artificial intelligence. Compared to modern AI approaches, chemometrics typically achieves accurate results with relatively small data sets. Chemometrics is a statistical method that has been established since the 1960s.

One of the main challenges in model development is obtaining enough samples across the desired concentration range, as well as generating accurate reference values. While these steps remain demanding, the mathematical processing involved in building chemometric models can already be largely automated. This represents an important step toward automated method development.

If the final product is manufactured by mixing defined components, it is possible to artificially generate samples covering the required concentration range. This approach often results in surprisingly precise calibration models for liquid mixtures.

Using titration equipment, small amounts of concentrated components can be automatically added to the original matrix or diluted in a controlled manner. This enables the simulation of concentration distributions within the manufacturing tolerance range. If the final product is produced from the same components, matrix effects are minimal and do not limit model performance.

With this concept, high-quality NIR calibration models with low standard errors can be generated automatically, often within a single overnight run.

Exploring the Chemistry of Artworks with X-ray eyes

Koen Janssens and collaborators

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X-ray based methods of analysis are eminently suited for material characterization and chemical imaging of painted works of art and related cultural heritage (CH) artefacts. This can be realized by using X-rays generated in compact, laboratory sources and by means of powerful X-ray beams produced at synchrotron facilities. A comprehensive review of the possibilities of these methods for studying the chemical compounds present in painted works of art was recently published [1]. These can be employed for various purposes, e.g.,
- revisualization of overpainted representations, revealing early stages of the creative process or intentional alterations of the composition done during the lifetime of the artwork;
- (highly specific) identification of the pigment types used and the pigment subtypes present, providing opportunities to study the provenance and authenticity of works of art; and
- identification of the nature and distribution of secondary products, formed on the paint surface by spontaneous degradation of the original painting materials.

In this contribution, amongst others, the following recent case studies will be discussed:
(a) multiscale XRPD imaging of the spontaneous degradation of the pigments of the 13th vault paintings by Cimabue and Giotto in the Basilica of St. Francis in Assisi, IT [2];
(b) 3D elemental analysis by XRF tomography of minute paint samples from Rembrandt's 17th c. masterpiece The Nightwatch (NL) to better understand his paint formulation [3] and
(c) investigating of the exact nature of innovative purple pigments in works by Robert Delaunay, a prominent Parisian (F) early 20th C. fauvist artist [4].

[1] L. Monico, K. Janssens et al., Advanced X-ray techniques to study the alteration of pigments in paintings. Il Nuovo Cimento 2025; La Revista del Nuovo Cimento 48 (2025) 315-434.
[2] E. Avranovich et al., Multi-Scale X-ray Imaging of the Pigment Discoloration Processes Triggered by Chlorine Compounds in the Upper Basilica of Saint Francis of Assisi. Molecules 2023; 28: 6106.
[3] F.T.H. Broers et al. Correlated x-ray fluorescence and ptychographic nanotomography on Rembrandt's The Night Watch reveals unknown lead "layer", Sci. Adv. 2023; 9: eadj9394.
[4] V. Gonzalez et al., Structure−Optical Properties Relationships in Cobalt-Based Purple Pigments Used by Robert Delaunay. J. Am. Chem. Soc. 2025; 147: 2587–2596.

The Role of Analytical Chemistry in Agricultural Research

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Agricultural research, as conducted by Agroscope, covers the entire value chain from crop cultivation, and animal production to final consumer products. It contributes to a competitive and multifunctional agricultural sector and to the production of high-quality food for healthy nutrition within the framework of a resilient and healthy environment. Analytical chemistry is an essential pillar and in many respects a prerequisite for these activities. It ranges from the establishment of reference methods and the execution of standardized methodologies under accreditation to support legal tasks to dedicated method development and application for specific research questions. The mode of collaboration with internal and external partners includes everything from full support, over user lab guided method applications to both collaborative and own research projects for method development. Essential advantages of a fully fletched "inhouse" analytical chemical competence center include cost-efficient services owing to a critical mass and scaling factor, knowledge gains and securance, short ways between customers, partners and experts, and superior quality assurance/quality control due to standardized and harmonized procedures. Twenty-four years after the last such overview [1], we will provide several recent examples illustrating the withs and breaths of analytical chemical activities at Agroscope.

[1] H.J. Bachmann, T. Bucheli, J. Paul, N. Stünzi, H.R. Bossard, Chimia 2002, 56, 304-305.

Workflow Comparison of the Immunochemistry Analysers Snibe Maglumi X8 and Roche Cobas Pro e 801

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Multiple analysers are available for use in central processing laboratories that measure similar panels of tests. We conducted a throughput and performance stress test to compare operational performance, usability and efficiency of two analysers, the Snibe Maglumi X8 [1] and Roche Cobas® Pro e 801 [2] in a routine laboratory setting. This prospective, observational study used anonymised left-over serum samples from individuals undergoing health checks. For each analyser, a batch of 100 samples was created, barcoded and analysed to measure a panel of six assays (triiodothyronine [T3], thyroxine [T4], thyroid-stimulating hormone [TSH], carcinoembryonic antigen [CEA], Vitamin B12 and Vitamin D total), to mirror different assay protocols and indications. Test runs were completed on three different days, using the same serum sample for all six tests; tests commenced at the same time each day and all analyses were conducted by the same researcher. The metrics recorded for each test run included the time taken: from registration to first test pipetting, to pipette 100 samples, and to the first and last result. Initial pipetting times were quicker with Maglumi X8, while processing of samples and analysis times were quicker with Cobas Pro e 801 (see table; further results to be reported in the poster).

	Day 1		Day 2		Day 3	
	Maglumi X8	**Cobas Pro e 801**	**Maglumi X8**	**Cobas Pro e 801**	**Maglumi X8**	**Cobas Pro e 801**
Time to pipette first test (post registration)	**30s**	2m 18s	**30s**	3m 18s	**30s**	3m 18s
Time to pipette first sample (all six tests)	**15s**	48s	**15s**	48s	**15s**	48s
Time to provide first sample result	37m 14s	**27m 45s**	37m 14s	**27m 45s**	37m 14s	**27m 45s**
Time to pipette 100 samples	3h 38m	**2h 13m**	3h 33m	**2h 10m**	2h 42m*	**2h 10m**
Time to provide last sample result	4h 15m	**2h 30m**	4h 5m	**2h 28m**	3h 19m	**2h 28m**

h, hours, m, minutes; s, seconds. *Based on 58 samples due to analyser breakdown

[1] Snibe Co., Ltd. (2021). MAGLUMI® X8 Fully Automatic Chemiluminescence Immunoassay System Technical Specification. https://mse-group.co/assets/images/MAGLUMI-X8-M1012E01-210202.pdf (accessed 16 Jan 2026).

[2] Roche Diagnostics International Ltd. cobas® pro integrated solutions – Product Brochure. 2023. https://diagnostics.roche.com/content/dam/diagnostics/Blueprint/en/pdf/cps/cobas-pro/MC--05530-External-cobas%20pro%20integrated%20solutions%20-%20Product%20Brochure.pdf (accessed 16 Jan 2026).

A robust sample preparation and calibration strategy for nanoparticle analysis using laser ablation single particle-ICP-MS

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Nanoparticles are widely used in technological and biomedical applications due to the unique physicochemical properties that emerge at the nanoscale [1,2]. Therefore, robust analytical strategies for nanoparticle characterization are required, both for quality control in material production and for evaluating potential environmental and human health impacts. Single-particle inductively coupled plasma mass spectrometry (SP-ICP-MS) is a well-established analytical technique for determining particle sizes and number concentrations [1]. However, conventional implementations relying on liquid suspensions can be affected by suspension stability, transport efficiency, and spectral interferences from the suspension medium.

To mitigate these limitations, solid sampling can be implemented using laser ablation combined with SP-ICP-MS (LA-SP-ICP-MS) [2,3], allowing direct analysis of nanoparticles embedded in solid matrices. Furthermore, embedded nanoparticles are preserved in the solid polymer film without requiring resuspension. As in conventional liquid-based analysis of nanoparticles, a key requirement for quantitative LA-SP-ICP-MS is the availability of suitable calibration standards.

Here, we report a sample preparation and calibration strategy based on spin-coated polymer thin films containing dispersed nanoparticles [4]. Spin coating was used to reproducibly produce homogeneous thin films with isolated particles while minimizing agglomeration. Spin-coated polymer thin films are also used as calibration standards by incorporating a defined amount of dissolved elemental standard and ablating a well-defined area of the film with known thickness.

Nanoparticles composed of single elements were analysed using quadrupole ICP-MS, whereas multi-element nanoparticles were characterized using time-of-flight ICP-MS. Further developments focus on strategies enabling the use of ICP-Q-MS/MS for multi-element particles, relying on reaction gases for temporal broadening of the transient particle signals. The proposed polymer thin-film strategy provides a promising approach toward standardized, reproducible calibration materials and, by that, supports ongoing development of LA-SP-ICP-MS for nanoparticle sizing and counting in solids.

[1] D. Mozhayeva and C. Engelhard, *J. Anal. At. Spectrom.*, 2020, **35**, 1740–1783.
[2] S. Yamashita, Y. Yoshikuni, H. Obayashi, T. Suzuki, D. Green and T. Hirata, *Anal. Chem.*, 2019, **91**, 4544–4551.
[3] D. Metarapi, M. Šala, K. Vogel-Mikuš, V. S. Šelih and J. T. Van Elteren, *Anal. Chem.*, 2019, **91**, 6200–6205.
[4] L. Kronlachner, Z. Gajarska, P. Becker, D. Gunther and A. Limbeck, *J. Anal. At. Spectrom.*, 2025, **40**, 467–477.

Nanoscale Visualization of Plasmon-Enhanced Hydrogen Activation on Pt(111) Surface using Tip-Enhanced Raman Spectroscopy

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Understanding and controlling molecular hydrogen activation at solid surfaces is a central challenge in heterogeneous catalysis and energy-efficient chemical transformations [1]. Despite extensive studies on plasmon-assisted catalysis, direct nanoscale visualization of light-enhanced H_2 activation on well-defined catalytic surfaces and clear discrimination between electronic and thermal mechanisms has remained elusive. Here, we address this challenge by developing a nanoanalytical strategy enabling *in situ*, spatially resolved interrogation of plasmon-enhanced H_2 activation on Pt(111) under ambient conditions.

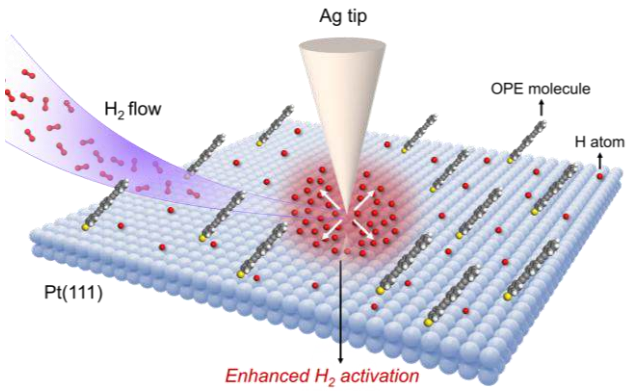

Figure 1. Scheme of the STM-TERS setup used to monitor plasmonically-enhanced H_2 activation on Pt(111) using reductive desoprtion of OPE moelcules.

Using tip-enhanced Raman spectroscopy (TERS) with nanometric spatial resolution and molecular specificity [2], we directly visualize H_2 activation through the reductive desorption of a self-assembled oligomeric phenylene–ethynylene (OPE) thiol monolayer serving as a molecular reporter (Figure 1). Time-resolved TERS measurements reveal accelerated desorption dynamics under visible-light illumination, while hyperspectral TERS imaging uncovers circular regions of enhanced reactivity extending 180–300 nm around the plasmonic near-field [3]. Quantitative analysis shows a ~20% increase in H_2 activation relative to the surrounding surface, providing the first real-space visualization of plasmon-enhanced H_2 dissociation at the nanoscale on a non-plasmonic catalyst.

To elucidate the underlying mechanism, the experimental nanoanalytical data are combined with finite element (FE) electromagnetic simulations, density functional theory (DFT), and quantum mechanical modeling. FE analysis demonstrates that plasmonic heating in the TERS junction is limited to the millikelvin range, which is orders of magnitude too small to account for the observed enhancement, thereby excluding photothermal effects. In contrast, quantum calculations reveal that localized surface plasmon resonance generates hot electrons on Pt(111) with energies sufficient to overcome H_2 dissociation barriers via an indirect hot-electron transfer mechanism. Furthermore, DFT modeling shows that the dissociated hydrogen atoms propagate far beyond the near-field through a collective surface "crowd effect," leading to long-range amplification of reactivity.

This work establishes TERS as a powerful nanoanalytical platform for disentangling electronic and thermal contributions in plasmon-enhanced catalysis and for directly mapping reactive intermediates and surface dynamics with nanometer precision. The mechanistic insights gained here open new avenues for the rational design of light-assisted catalytic systems capable of operating efficiently under mild conditions, with broad implications for hydrogenation chemistry and sustainable catalysis.

[1] Zhou *et al.*, *J. Am. Chem. Soc.*, **2006**, *128*, 1780-1781.
[2] Cai and Kumar *et al. J. Am. Chem. Soc.*, **2025**, *147*, 39838–39845.
[3] Cai and Kumar *et al.*, ChemRxiv preprint, **2025**, DOI: 10.26434/chemrxiv-2025-w41qh.

Spatially Resolved Optical Ion Sensing with Voltammetric Ion Transfer Microscopy: Fundamentals and Applications

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Ion concentration gradients are fundamental for numerous chemical, biological and environmental processes and techniques capable of spatially resolved ion detection are essential to obtain a deeper understanding of such heterogeneous systems. However, well-established methodologies of chemical imaging typically suffer from long acquisition times, limiting their applicability to dynamic systems. To address this limitation, our group has recently developed a new approach, termed Voltammetric Ion Transfer Microscopy (VITM), enabling the acquisitions of millions of spatially resolved concentration within seconds.[1] The imaging platform consists of a planar electrode coated with a thin ion-selective membrane (ISM) incorporating a redox probe, a lipophilic derivative of the stable radical TEMPO, and a lipophilic rhodamine fluorophore as optical reporter.[2,3] The radical form of TEMPO may quench the fluorescence of the dye, allowing for a direct correlation between electrochemical and optical signals.[4] The conversion of lip-TEMPO between its radical and cationic forms using dynamic electrochemistry induces ion transfer between the aqueous and organic phases to preserve membrane electroneutrality while simultaneously modulating the fluorescence intensity (Figure 1a). This contribution considers some limitations of the system and extends its scope of applicability. Specifically, we report on the incorporation of a new ammonium ionophore in the membrane, which enables the selective imaging of ammonium ions in chemical and biochemical gradients.

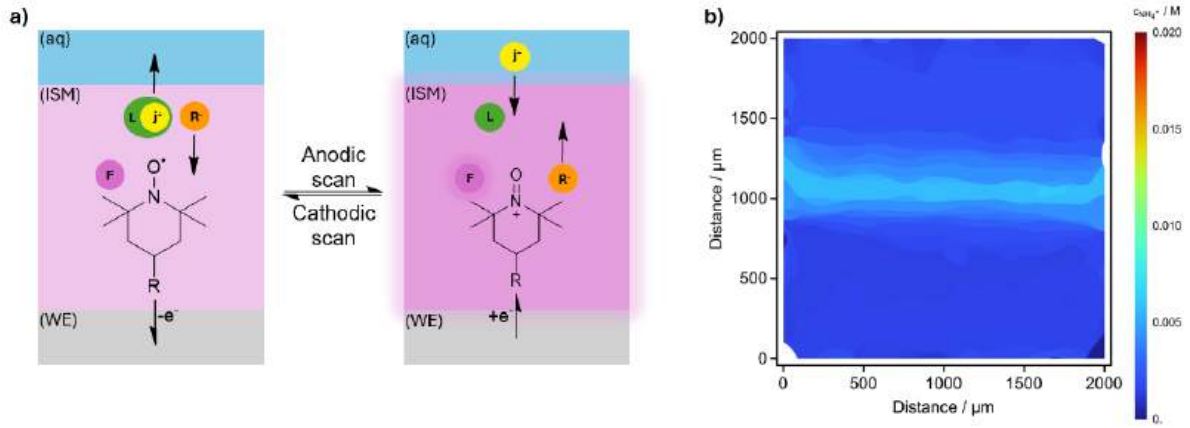

Figure 1. a) Ion transfer mechanism and related fluorescence intensity change of the fluorophore (F). R- represents a cation exchanger, j^+ a generic cation and L an ionophore. **b)** Ammonium concentration density plot. Solutions of urease (top) and urea (bottom) flow over the membrane from left to right. Ammonium is produced along the central portion of the image where the two solutions meet and enzyme turnover occurs.

[1] G. Junquetti Mattos, J.A. Rothen, T. J. Cherubini, E. Bakker, *JACS Au*, **2025**, *5*, 5538-5546.
[2] G. Junquetti Mattos, N. Yu. Tiuftiakov, E. Bakker, *Electrochem. Commun.*, **2023**, *157*, 107603.
[3] G. Junquetti Mattos, J. A. Rothen, N. Yu. Tiuftiakov, E. Bakker, *Anal. Chim. Acta*, **2024**, *1299*, 342388.
[4] P. Zhu, J.-P. Clamme, A. A. Deniz, *Biophys. J.*, **2005**, *89*, L37-L39.

From the Ordinary to the Exceptional: A Study of Quantitative Analyses in Lab Courses

Gunnar Schwarz

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The purpose and value of laboratory courses remain subjects of an ongoing debate, [1] and while general recommendations exist,[2] little is known about similarities and differences in approaches. Quantitative analytical experiments are a common feature of student laboratory courses across institutions and disciplines. Yet, discussions have often focused on instrumentation[3] rather than broader analytical or pedagogical aspects.
This contribution presents the results of a comprehensive literature survey[4] of 160 articles published between 2014 and 2024 in the Journal of Chemical Education that describe hands-on experiments for students involving quantitative analyses. Each experiment was categorized according to analytical and pedagogical criteria. The resulting compilation serves as a valuable resource for instructors seeking inspiration for experiments.
Beyond providing an overview of available experiments, the analysis offers additional insights, e.g. conveying the range of quantified analytes, utilized sample types, and employed quantification approaches as well as instrumentation. Pedagogical practices such as provided instruction, group work, and assessment strategies were also examined. While the surveyed experiments cover a broad spectrum of topics and methods, several potential gaps were identified. Based on these findings, specific recommendations for quantitative analytical experiments in student laboratory courses are proposed.

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OctoChemDB: An Integrated Platform for HRMS-Based Small Molecule Dereplication

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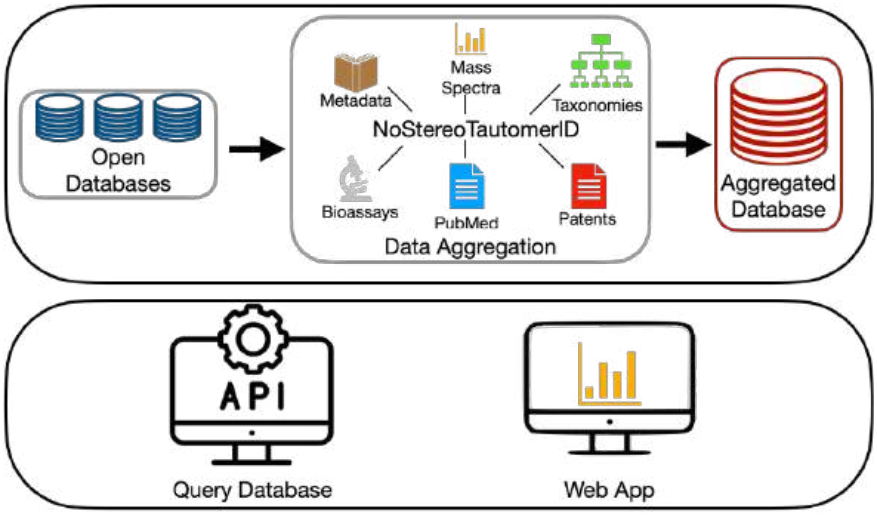
High-resolution mass spectrometry (HRMS) is routinely applied to small molecule identification and dereplication, but the interpretation of MS and MS/MS data is often hindered by the dispersion of reference information across multiple resources. We present OctoChemDB (octochemdb.cheminfo.org), a web-based tool supporting HRMS-based identification through accurate mass calculations and MS/MS data analysis with integrated access to chemical, spectral, and literature-based reference information within a single environment. The OctoChemDB platform is described in detail in a manuscript accepted for publication in Analytical Chemistry.

OctoChemDB enables monoisotopic mass–based searches with defined mass accuracy, molecular formula generation, isotopic pattern comparison, MS/MS fragment analysis, and spectral similarity matching against literature-reported spectra. Reference data accessed through the application include chemical structures, PubMed abstracts, patent information, bioactivity records, and taxonomic annotations.



OctoChemDB relies on an automated framework that aggregates chemical, spectral, and associated reference data from open resources and exposes them through a web-based application. The approach is demonstrated through the identification of known compounds, including widely used reference molecules such as caffeine and MDMA, from HRMS and MS/MS data, highlighting its utility for rapid and informed dereplication in analytical chemistry workflows.

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Between concentration and effect, exposure is the key

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Analytical chemistry is central to the study of chemical pollutants, yet the interpretation of analytical data often remains disconnected from real exposure and effect. The detection of contaminants at ultra-trace levels has reached an unprecedented degree of sensitivity, particularly through advanced mass spectrometry and non-targeted screening approaches. However, analytical performance alone does not define relevance. Concentration values are bounded by instrumental limits, target selection, and matrix effects, and they provide only a partial view of chemical risk. What ultimately determines toxicological and environmental significance is exposure: its duration, frequency, routes, and bioaccessible fraction [1,2]. Emerging pollutants such as bisphenols, PFAS, and rubber-related additives illustrate this gap between analytical detection and meaningful interpretation [1,3,4]. Transformation products, mixture effects, and cumulative low-dose exposure challenge traditional concentration-centric paradigms [1,3-5]. By integrating analytical chemistry with exposure-oriented tools - such as migration studies, passive and continuous sampling, and human biomonitoring - chemical data acquire contextual depth [1,6,7] . The exposome concept offers a unifying analytical framework to connect chemical fingerprints with realistic exposure scenarios and downstream effects. Reframing analytical results through the lens of exposure allows analytical chemistry to move from compound detection toward actionable knowledge, supporting more robust risk assessment and evidence-based environmental and regulatory decisions.

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Synthesis and dynamics of carbonaceous nanoparticles during enclosed spray combustion

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Aviation is a growing source of carbonaceous nanoparticle pollution, also referred to as soot, which is unique due to the particularly small size of the particles and the emission of particles at high altitudes. Currently, there are no commercially available soot generators on the market which can produce aircraft-like particles in the laboratory which limits our ability to calibrate instruments meant to measure aviation emissions [1], conduct research on the health impacts of such small soot particles, and to understand their roll in contrail formation. Here, enclosed spray combustion (ESC) is developed as a method for the synthesis of aircraft like particles, filling this gap in the market. ESC particles with median mobility diameters, d_m, between 15 and 180 nm were produced covering the range in which aircraft emissions typically fall while still matching the organic carbon to total carbon ratio observed in soot from aircraft at high thrust [2]. This system was then used to elucidate the dynamics of soot during ESC [3] comparing in-flame measurements to discrete element modelling simulations. This showed that the primary particles of soot reached their final diameter very early on in the flame and then particles grew primarily through agglomeration. Finally, the trade-offs between soot elimination through oxidation and emissions of nitrogen oxides (NOx) were investigated [4] using a strategy similar to the rich-quench-lean (RQL) jet engine design. At lower heights above the burner, injecting oxygen (quenching) resulted in a larger reduction in soot emissions but simultaneously more NOx emissions. Inversely, late injection of oxygen resulted in the lowest NOx emissions but the highest soot emissions. In this way, ESC is demonstrated as a versatile method for generating aircraft-like soot in the laboratory both for calibration purposes and fundamental research on soot.

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Pulseometry: A Differential Readout to Compensate Signal Drift of Potentiometric Probes

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Ion selective electrodes are widely used sensors in POCT devices to assay electrolytes in whole blood samples. With single-use systems the first solution contact normally results in an important signal drift that negatively affects measurement accuracy. In this work, a novel approach coined pulseometry is proposed to compensate for signal drift. The potentiometric signal is processed through a differential circuit incorporating RC components of different time constants. The differential potential will remain constant for a slowly drifting baseline while a rapid potential change will result in a peak-shaped difference signal that may be baseline subtracted and integrated to extract the components information. The method was successfully integrated into mass fabricated, microfluidic test cards used in commercial blood gas electrolyte analyzers. Blood calcium levels from three individuals were measured, giving standard deviations of 0.008-0.024 mM, improving precision by 36-67 % compared to potentiometry. These results showcase the potential of pulseometry for improving the performance of electrochemical sensing in clinical diagnostics.

POSTERS

Self-calibrated potentiometric sensors for ion analysis

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Potentiometric ion selective electrodes (ISEs) have shown significant potential in a wide range of applications, allowing rapid analysis with exceptional selectivity. Being highly suitable for healthcare and environmental monitoring, the development of these sensing devices is having a massive commercial impact [1]. The emerging interest in ISE development is bringing important advancements, but further drastic simplification goes unfortunately at the expense of accuracy, which is not acceptable. A major drawback of potentiometry is that every interface of the electrochemical cell can generate differences in potential, promoting unpredictable electromotive force (EMF) drifts and affecting accuracy. Thus, ISEs require to be calibrated using standard solutions before and/or after each measurement. This task can be time-consuming and requires complex instrumentation, which is undesired [2].

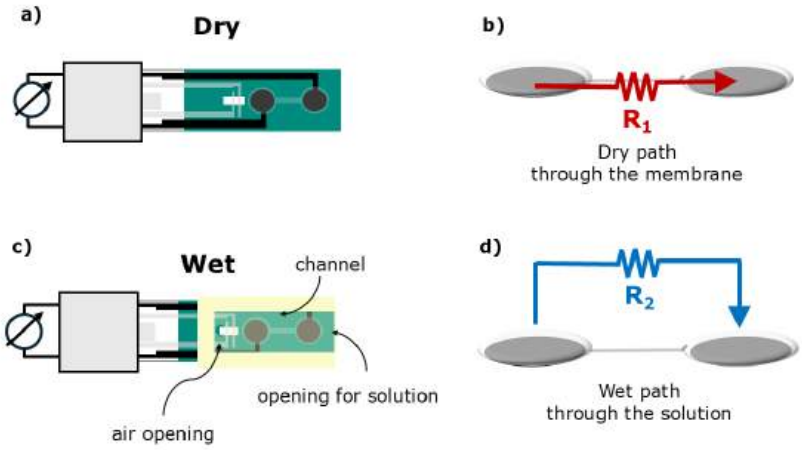

Figure 1. assembled setup for dry a) and b) wet measurements; current pathway in dry c) and wet b) measurements.

To overcome these limitations, we propose a novel self-calibrated potentiometric sensor that aims to eliminate the need of any fluid-handling and calibration process, enhancing data reproducibility and accuracy. To attain this goal a membrane bridge is cast between two electrodes and a dry measurement is performed, allowing one to measure the potential between the two membranes in a dry state, before exposure to sample (Fig. 1a-b). The device is then wetted with the sample through capillarity, and a new measurement is carried out. The current path through the solution is now dominant as the resistance of the solution is significantly smaller (<1000 x) than the resistance of the membrane bridge (Fig. 1c-d). With this strategy it is possible to subtract the EMF baseline of the dry measurement from that of the final measurement, thereby correcting potential variations at the membrane/electrode interface. As a proof of concept, we explore the application of this new approach in the development of pH sensing devices.

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Urinary volatilomics for biomarker discovery in kidney stone patients and healthy controls

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Nephrolithiasis is a common and recurrent disease with increasing incidence worldwide, partly driven by modifiable lifestyle factors such as diet [1-3]. Non-invasive biomarkers are needed to improve risk stratification and prevention strategies [4]. This study aimed to identify urinary volatile organic compounds (VOCs) that differentiate kidney stone formers from healthy individuals and to explore their associations with fermented food intake.

In this case–control study, 24-h urine samples from 232 recurrent kidney stone patients and 168 healthy controls from the Swiss Kidney Stone Cohort were analyzed using untargeted volatilomic profiling by dynamic headspace gas chromatography–mass spectrometry. Data were quality-filtered, normalized, and adjusted for relevant confounders including age, sex, body mass index, smoking status, diabetes, and study center. Uni- and multivariate statistical analyses were used to identify discriminant metabolites.
Seventy-seven urinary VOCs differed significantly between kidney stone formers and controls. Octane, 1,1'-oxybis- and 6-methyl-5-hepten-2-one were more abundant in controls, whereas acetic acid and propanoic acid were higher in stone formers. Three VOCs were associated with fermented food intake. Notably, 3-nonen-2-one emerged as a potential mediator of the inverse association between coffee consumption and kidney stone risk.

Distinct urinary VOC signatures differentiate kidney stone formers from healthy controls. These findings highlight the potential of urinary VOCs as non-invasive biomarkers and suggest a possible metabolic pathway linking coffee consumption to reduced kidney stone risk.

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Leaching resistant ion-selective membranes based on self-plasticized poly(vinyl chloride) (PVC) membranes

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Ion-selective electrodes (ISEs) are an important type of electrochemical sensors routinely used in analytical measurements across fields such as environmental analysis, clinical and pharmaceutical analysis. The core part of these ISEs is the ion-selective membranes, which contains important sensing components such as an ionophore and ion-exchanger that impart selectivity and permselectvity, as well as a plasticizer which increases flexibility and malleability of the polymer (typically PVC). This increases the glass transition temperature and forms a blend in which all sensing components are dissolved. A significant challenge with these PVC-plasticizer based matrices in component leaching, by which membrane components diffuse out, resulting in a decline of selectivity and sensitivity, and hence overall lifetime[1]. This also increases risk of cytotoxiticy, particularly with sensors intended for in-vivo use[2].

Several strategies have been explored to characterize and prevent this leaching of membrane components. Lewenstam et al. studied the leakage of ion-exchangers from polymeric membranes using stripping voltammetry[3]. A common method to overcome plasticizer leaching in recent times involves creating internally plasticized polymers by grafting the plasticizer onto the PVC backbone, as shown by Navarro et al. where they covalently link a thiol-modified DEHP plasticizer onto PVC[4]. Similarly, click chemistry has been recently reported for retaining membrane components on azide-modified PVC chains[5].

In this work, we characterize and quantify plasticizer leaching by GC-MS after exposing plasticized membranes to methanol solution to understand its effect on membrane properties. As a potential solution, inspired work by Braslau et al.[6], we also present synthesis of a self-plasticized poly(vinyl chloride) (PVC) derivative for ion selective membranes. A DEHP plasticizer - like analogue was “clicked’ onto an azide-modified PVC backbone using the simple, high-yielding, copper-catalyzed azide-alkyne cycloaddition reaction. The resultant polymer creates a flexible and stretchable film, overcoming the need for an additional plasticizer and is tested to detect a library of ions, working as a leak-free, operational sensor.

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Development of Reference Electrodes Based on Lipophilic Organic Electrolytes Integrated with Solid-Contact Ion-Selective Electrodes

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Recently, considerable effort in both research and industry has been devoted to the development of electrochemical sensing platforms and analytical devices for non-invasive, rapid and continuous monitoring of biomarkers [1]. In this context, the design of reliable, miniaturized reference electrodes (REs) remains an often overlooked yet critical challenge. In the previous two decades, REs based on organic electrolytes have emerged as a viable alternative to conventional double-junction REs. The potential of these REs is stabilized via the partitioning of an organic salt between a water-immiscible salt bridge and an aqueous sample. Various salt bridge implementations using free-flowing ionic liquids or polymeric membranes open vast opportunities for miniaturization [2]. It has been shown recently, however, that the potential stability of such REs often comes at the cost of their lifetime owing to rapid leaching of the reference salt, which remains a major obstacle for their use in real-world applications [3].

In this work, we systematically investigate reference electrodes based on lipophilic organic electrolytes embedded in polymeric membranes, with particular emphasis on the electrolyte lipophilicity and electrode lifetime. Bis(trifluoromethanesulfonyl)imide [$C_1C_1N^-$] was selected as the anionic component due to its highly delocalized charge, which promotes efficient ionic transport within the membrane. The influence of the overall electrolyte lipophilicity on ion partitioning was examined by varying the cationic species, which are more lipophilic than [$C_1C_1N^-$]. The results provide design guidelines for optimizing organic electrolyte lipophilicity for use in REs and demonstrate their potential integration with solid-contact ion-selective electrodes (SC-ISEs), paving the way toward robust all-solid-state electrochemical sensors with improved stability and analytical precision.

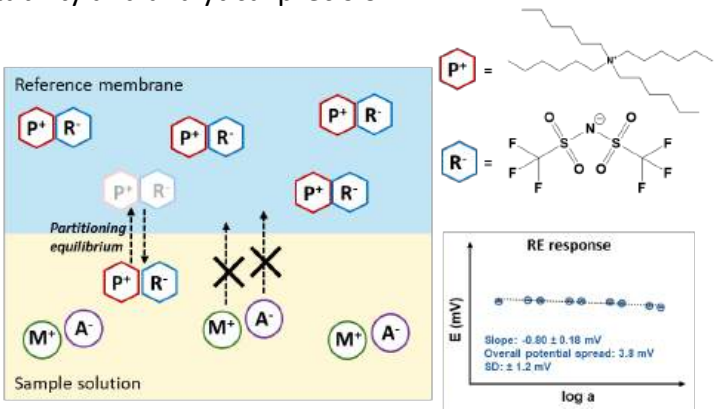

Figure 1. Partitioning of P^+R^- between the membrane and solution interface results in a concentration-independent potential. Most other sample ions are excluded from the membrane owing to their lower lipophilicity.

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Multimodal tomographic approach for studying Iron Age mineralised textiles

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Textile remains from ancient times are rare because they are perishable in most sedimentary environments and are often found in a fragmented state. However, their study provides extremely precious information on the social and cultural life of past societies, such as textile production and funerary practices. In some cases, the preservation of their morphology can be exceptional when they are found in close association with corroded metal artefacts. This phenomenon is known as mineralisation, and the study of mineralised textiles provides extremely valuable archaeological information [1-3]. It relies on the diffusion of inorganic ions produced by the corrosion of metals into the fibres and followed by the precipitation of minerals on the fibre surface [4]. In earlier work using Synchrotron X-ray microtomography (SR-µCT) we have shown a detailed, non-invasive study of mineralised textiles (6th–5th, Creney-le-Paradis, France) by giving access to the microscopic characteristics of their internal morphology [1-3]. However, the underlying physico-chemical mechanism responsible for the nucleation and growth of corrosion products has yet to be elucidated and it is essential to be able to distinguish between organic and inorganic phases, which is not straightforward with X-rays. Neutron tomography is hereby complementary to X-ray tomography and has been successfully applied in the field of cultural heritage [5-6]. Contrary to X-rays, neutrons show a high capacity to penetrate metals, while presenting a high contrast for light elements, which facilitates their identification [5-6]. It is therefore well suited to study the presence of organic materials and their distribution in metallic archaeological objects [5-6].

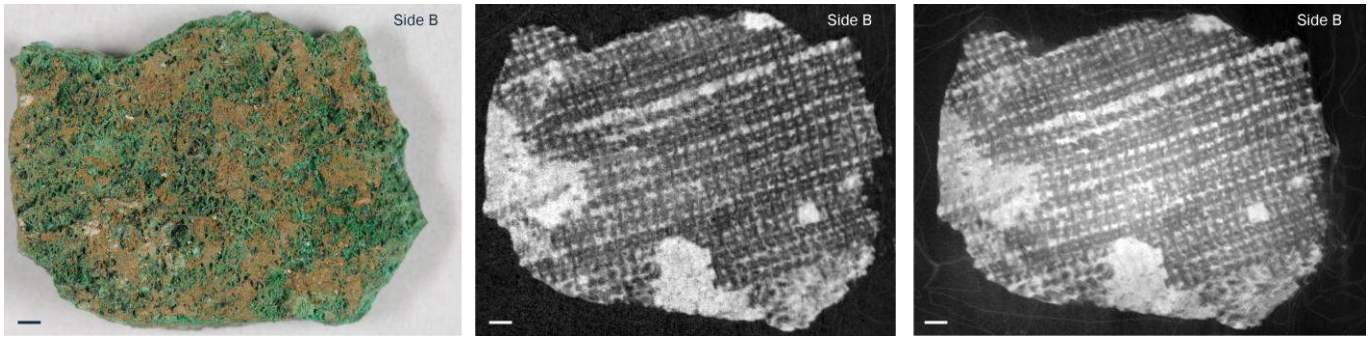

Fig. 1: Left: macrophotography of side B of mineralised textile fragment A1_7 from Creney-le-Paradis (France, 6th-5th BC), its corresponding Neutron µCT virtual section (middle) and X-rays µCT virtual section (right). All scale bars: 1 mm.

We will present here the preliminary results obtained from a combined X-ray and neutron microtomography study of mineralised textile fragments from the exceptional site Creney-le-Paradis, which is one of the most significant elite burials discovered in France. These data will help to discriminate between mineral and organic phases and thus elucidate the successive chemical steps involved in the mineralisation process responsible for their preservation.

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Revealing Nanocluster Surface Charge by Titrimetric Permselectivity Change

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In 2010, our group introduced a potentiometric titration method to assess the purity of lipophilic electrolyte salts in an organic phase [1]. The method is based on a change of the permselectivity of an organic phase by titrating a lipophilic salt with it corresponding lipophilic counter ion and measuring the potential difference between two aqueous phase electrodes immersed in the same organic phase. Before the end point, the system will have a permselectivity dictated by the lipophilic salt which will act as an ion exchanger and exhibit a potential difference corresponding to:

$$\Delta E = \frac{RT}{z_i F} ln \frac{a_i(aq1)}{a_i(aq2)} \qquad (1)$$

Where a_i correspond to the activity of the common ion in organic solution and the internal solutions of the two pipette electrodes. After the end point an excess of the titrating salt of opposite sign will act as new ion exchanger and change the permselectivity of the organic phase. This will result in an abrupt potential change, giving the same potential amplitude dictated by Eq. 1 but of opposite sign. Tiuftiakov et al. recently used the same method to assess salt impurity of highly lipophilic electrolytes used in liquid junction-free reference electrodes [2].

In this work we use the potentiometric titration approach described above in a DCE : EtOAc (1:1) organic solution to attempt the titration of atomically precise gold and copper nanoclusters to assess their net charge. The approach displaces the more hydrophilic counter ion of the nanocluster with the more lipophilic tetrakis(4-chlorophenyl)borate. This simple and precise technique should allow for the direct assessment of nanomaterial charge without requiring electrophoretic or spectroscopic methods.

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Uncovering the Chemistry of 19th-Century Swiss Postage Stamps

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Despite their small size, postage stamps are culturally significant artifacts that reflect the artistic, technological, and political contexts of their production. Nowadays, they are an integral part of the world's cultural heritage due to their historical and social significance. They constitute a unique form of art, in some cases selling for high prices. Although the material composition of stamps from several countries, including Italy, Portugal, and the Ottoman Empire, has been studied,[1–3] Swiss postage stamps remain largely unexplored. In particular, the pigments used in their production are unknown, as printers jealously guarded their know-how to prevent counterfeiting.

Fig. 1: Selection of several stamps analyzed in this work, highlighting the diversity of colors and compositions found on Swiss postage stamps

In this study, we present the first systematic material characterization of 98 Swiss stamps issued between 1850 and 1908 using a combination of non-invasive analytical techniques including Raman Spectroscopy, Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR) together with Scanning Electron Microscopy with Energy Dispersive X-ray spectroscopy (SEM-EDX). In specific cases where the presence of organic dyes was suspected, High Performance Liquid Chromatography coupled with Diode Array Detection (HPLC-DAD) was also applied. This multianalytical approach allowed to identify most of the inorganic pigments present, whereas the use of HPLC-DAD was decisive in identifying the organic red dyes. Our results highlight pigment choices between Swiss stamps and those reported for other European countries during the 19th century.This study sheds new light on the material history of Swiss postage stamps and stresses the value of combining spectroscopy, imaging, and chromatography techniques in philatelic research and, more broadly, in heritage science.

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Characterization of a downward-oriented nitrogen microwave inductively coupled atmospheric-pressure plasma TOF-MS for multielement analysis using microdroplets

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In this fundamental investigation, we evaluate and characterize the analytical performance of a recently built, downward-oriented, nitrogen-sustained microwave inductively coupled atmospheric-pressure plasma time-of-flight mass spectrometer (DW-N_2-MICAP-TOFMS), tailored for single-entity detection using a piezoelectrically actuated microdroplet generator. Principal objectives that drive these studies are: i) to improve sample introduction systems for larger micron-scale droplets by leveraging gravity-assisted transport – extending the conceptual framework introduced by Vonderach et al. for downward-pointing argon-based ICP-TOFMS, which mitigates limitations inherent to conventional horizontal ICP geometries; and ii) broadening the mechanistic understanding of ionization dynamics in nitrogen plasmas, while optimizing instrument parameters for improved sensitivity and cost-efficiency [1]. The initial results achieved with DW-N_2-MICAP-TOFMS yielded detection efficiencies (DE) and sensitivities that, for the majority of trace elements, are commensurable to those of downward-pointing argon-based ICP-TOFMS. Systematic variation of auxiliary gas flow rates (0.9–1.25 L min^{-1}) and plasma power (850–1450 W) revealed distinct ionization behaviours of analyte ions. Notably, elements with low first ionization energies exhibited a marked decline in DEs when the plasma power was reduced to 1250 W, beyond which further reductions had minimal additional impact. In contrast, elements possessing higher ionization energies demonstrated a progressive and pronounced decrease in DEs with diminishing plasma power. Increasing the auxiliary gas flow improved the DEs for elements with low first ionization energy, yet concurrently diminished the DEs for analytes with high ionization energies and superior oxygen bond strength—likely a consequence of localized plasma cooling, which impairs efficient atomization and ionization, ultimately compromising sampling efficiency. Furthermore, the absence of argon-derived polyatomic interferences in DW-N_2-MICAP-TOFMS enabled more accurate and simplified quantification of isotopes such as ^{39}K, ^{75}As, and ^{80}Se, which are typically challenging to measure in standard ICP-MS instrument [2-3]. We could also demonstrate consistent and reproducible introduction of 65 µm droplets at high dispensing frequencies (600 kHz), facilitated by a minimal helium flow rate (0.15 L min^{-1}) for effective desolvation. At frequencies up to 400 kHz, CeO^+/Ce^+ ratios remained below 0.1%; however, a notable rise to 2% was observed at 600 kHz, attributed to increased solvent load in the plasma [4]. Importantly, preheating the helium carrier gas to 100 °C reduced the CeO^+/Ce^+ ratio to ~1% at dispensing frequencies exceeding 400 kHz, possibly by enhancing the rate of evaporation, thereby aiding in rapid and uniform microdroplet desolvation. Taken together, these results underscore the analytical robustness of the DW-N_2-MICAP-TOFMS. By eliminating the reliance on argon, this configuration not only minimizes plasma gas costs but is also emerging as a compelling alternative to conventional argon-based ICP-TOFMS systems for multielement analysis of single entities (droplets, cells, and particles) across the microscopic regime.

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A Molecularly Imprinted Membrane for High-Density Lipoprotein Extraction in Point-of-Care Testing

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Cholesterol is transported in the body within micellar assemblies called lipoproteins. Among these, Low Density Lipoproteins (LDL) are colloquially called “bad cholesterol” because they distribute cholesterol from the liver to the body and tend to accumulate on blood vessels’ interior walls causing arteriosclerosis.

The determination of LDL cholesterol (LDL-C) levels in blood is therefore a key parameter to prevent cardiovascular diseases. Nowadays, LDL-C is quantified indirectly by assessing the quantity of total cholesterol and subtracting the amount in non-LDL lipoproteins, in particular in High Density Lipoproteins (HDL). The analytical performance of this method is limited as the uncertainties of the individual measurements accumulate. The direct and specific determination of LDL-C using a dedicated assay would be a more accurate strategy. To develop such a specific assay, Molecularly Imprinted Polymers (MIPs) are an interesting class of polymer-based molecular recognition reagents engineered to bind to one single target compound. Selectivity is introduced during MIP synthesis thanks to a template molecule that guides the formation of specific imprints that are sterically and chemically complementary to the target analyte.

We will present the results of a project aiming at the development of a novel point-of-care test of LDL-C using MIP [1]. A molecularly imprinted membrane (MIM) was used for the solid-phase affinity extraction (SPAE) of HDL in a paper-based lateral flow test. Samples travelled by capillarity through the MIM before reaching a detection zone where LDL cholesterol was quantified enzymatically. MIMs were produced by impregnation of the membrane with a dispersion of MIPs selective for HDL. The MIM enabled the removal of HDL with an efficiency of typically 68%. However, quantification of LDL cholesterol suffered from strong non-specific binding of LDL, likely due to its inherent colloidal instability. Overall, our results highlight the challenges associated with SPAE of colloidal particles. Furthermore, our study demonstrates a novel, efficient, and potentially generic modality to integrate SPAE into paper-based POC diagnostic tests.

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Amperometric and Colorimetric Evaluation of a Platinum-Decorated Multi-Walled Carbon Nanotube/Graphene Oxide Nanoribbon Nanozyme

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We report a platinum-incorporated multi-walled carbon nanotube/graphene oxide nanoribbon composite (Pt/MWCNT-GONR) as a peroxidase-mimicking nanozyme for analytical sensing applications. Nanoribbon formation induced by microwave-assisted oxidation increased the accessible surface area and electroactive sites of MWCNTs, enabling efficient platinum loading via a self-reduction process. The peroxidase-like activity of Pt/MWCNT-GONR was evaluated using the oxidation of 3,3',5,5'-tetramethylbenzidine (TMB) in the presence of hydrogen peroxide as a model analytical reaction. Catalytic activity was quantified by analyzing initial reaction rates from time-dependent absorbance measurements. In addition, chronoamperometric measurements at the reduction potential of oxidized TMB provided an electrochemical readout of the catalytic process. Under constant substrate concentrations, the steady-state current change (ΔI) increased systematically with increasing nanozyme loading, demonstrating a quantitative relationship between catalytic activity and electrochemical response. These results indicate that Pt/MWCNT-GONR enables dual-mode signal transduction and is a promising nanozyme-based platform for quantitative colorimetric and electrochemical biosensing.

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Nanopore-based Identification of Histone 3 Post-Translational Modifications

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Post-Translational Modifications (PTMs) of proteins play crucial roles in modulating the function of proteins, which are key players in cellular function and diseases [1]. Specifically, dysregulation of the PTMs on Histone 3 have been linked to disease; for instance, depletion of H3K18-acetylation (H3K18ac) was associated with aggressive cancers, as well as poor patient prognosis with higher chance of tumor recurrence [2-3], and H3K36-acetylation (H3K36ac) reduces DNA damage signaling [4]. With many additional histone PTMs under active investigation, there is a growing demand for detection techniques that offer high sensitivity, reproducibility, and lower costs, compared to traditional mass spectrometry [5]. Here, we address this need with the use of nanopore technology, a single-molecule detection method that is already successful for DNA-sequencing and increasingly explored for protein analysis [5]. Using this approach, we target discrimination of the Histone 3 wild-type (H3wt) from its variants with three PTMs: H3K18ac, H3K36ac and H3K18 with a decanoyl (H3K18dec). The optimization of the experimental process was completed through testing of multiple genetically engineered nanopores by comparing their interaction with the H3wt. This allowed characterization of our different analytes individually, analyzing their dwell times, signal frequencies, and current blockages. We enabled label-free measurements of the H3 protein and discriminated it from its PTMs.

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Standardization of Collection and Qualitative Analysis of Exhaled Breath Condensate

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Introduction

Painless, non-invasive collection makes exhaled breath an attractive source of biomarkers for numerous diseases and medical conditions. As analytical instruments become more sensitive, low-abundance small molecules become easier to detect, paving the way for breath analysis to become a routine clinical tool. In addition to exhaled breath vapor (EBV), exhaled breath condensate (EBC) can be collected by cooling the exhaled air and collecting the condensate. However, variability in collection techniques and the lack of standardized sample collection protocols, including subject behaviour, hinder the comparison between studies and the establishment of clinical routines. A study was conducted to collect EBC from fourteen participants with three different collection devices to compare and optimize device handling, metabolite collection, and analytical detection.

Experimental Methods

A standardized pre-collection protocol was developed that outlines a twelve-hour abstinence from food, alcohol, coffee, and nicotine, a six-hour abstinence from scented personal care and all oral hygiene products, and avoidance of hand soap for at least one hour before collection. Three EBC collection devices, each equipped with a saliva trap-mouthpiece, were cooled to -78 °C with an isopropanol-dry ice mixture and connected to a flow meter allowing participants to maintain a constant 8 L/min exhalation flow. Exhalation was performed consecutively into a glass cold trap, a *Falcon* tube in a cyclone fashion [1], and the commercially available *RTube*^{TM} [2], with condensation achieved through cooling. Fourteen participants (gender-balanced) took part in the study.

The chemical analysis of EBC samples was performed using dynamic headspace vacuum in-tube extraction gas chromatography coupled to mass spectrometry (DHS-V-ITEX-GC-MS) [3]. The collected EBC was measured separately for each participant and collection method, and the peak identification was completed with the NIST23 spectral library. Another aliquot was pooled by method and gender, then analyzed with HiSorb thermal desorption GC-MS (HiSorb TD-GC-MS) [4].

Results and Discussions

On average, the cold trap requires about 32 L of exhaled air to obtain 1 mL of EBC, while the cyclone requires 45 L and the *RTube*^{TM} over 60 L to obtain the same amount. The amount is nearly identical between men and women. Potential factors influencing this ratio are the cooled surface area of the device, the airflow, and the degree of contact with this surface. The most consistent cooling was achieved for the cold trap by using a dewar flask, while the cyclone and *RTube*^{TM} used custom 3D-printed double-walled cooling containers.

While the cold trap and cyclone offer a similar experience for the participant, the collection from the cyclone is more convenient, as is the preparation and collection of blanks. The design of the *RTube*^{TM}

makes collection very easy; however, the cost is considerably high, and obtaining a blank that contains the *RTube™* plasticizers is extremely challenging.
A preliminary analysis of the detected compound names reveals approximately 100 relevant (identified, non-artefacts or background) peaks for each of the collection devices, with the *RTube™* detecting fewer hydrocarbons but more oxygen-and-nitrogen-containing compounds than the other two devices. Further analysis of the GC-MS data is ongoing.

Conclusions

The standardized pre-collection protocol for the participants proved effective, as prominent interfering peaks such as menthol from toothpaste were not observed. Among the three EBC collection devices – the cold trap, the cyclone, and the *RTube™* – the cyclone was most straightforward to operate and ranked highest in the participant rankings. Its slightly lower EBC yield compared to the cold trap probably lies in the smaller surface area of the *Falcon* tube and slightly less effective insulation of the cooling container. The cyclone is ideally suited for time-based measurements with several collection points.
Overall, the cyclone appears to be the best option from a usage perspective and the possibilities it offers. Whether it is also the top choice based on the collected and detected compounds remains to be fully assessed.

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Biomonitoring of phthalate metabolites in the Swiss population

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Phthalates are synthetic organic chemicals widely used as plasticizers in many consumer products. They raise significant concerns for human health due to their potential endocrine-disrupting and developmental effects, and in recent years the use of several phthalates has been restricted or limited [1]. Given their widespread use and associated health concerns, understanding which phthalates are present in the population and at what concentrations is essential for evaluating human exposure. In humans, phthalates undergo several biotransformation steps—including initial hydrolysis, oxidative modifications, and subsequent glucuronidation—before being eliminated in urine. Therefore, urinary phthalate metabolites represent reliable biomarkers of exposure [2, 3].

In our study, thirty metabolites originating from sixteen parent phthalates, as well as two alternative plasticizers, were quantified in more than 1000 urine samples collected from 863 adults in Switzerland. These samples were part of the large-scale, national Swiss Salt Study 2 (SS2), organized by the Federal Food Safety and Veterinary Office (FSVO) [4]. Urine samples were collected over a 24-hour period, and phthalate metabolites were analyzed after enzymatic hydrolysis (using β-glucuronidase from E. coli K12) to cleave glucuronides, followed by protein precipitation. Metabolites were quantified in a single 15-minute run using a newly optimized ultra-high-pressure liquid chromatography (UHPLC) method coupled to electrospray tandem mass spectrometry (ESI-MS/MS), incorporating 30 isotopically labelled internal standards. The method was thoroughly validated using in-house quality controls, successful proficiency tests, and quantitative performance assessment through the Method Accuracy Profile with β-expectation tolerance intervals [5].

In the poster, we present the optimized analytical method, its quantitative performance (including limits of quantification, trueness, and precision), and the results of the first biomonitoring study assessing phthalate exposure in the Swiss adult population.

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Flow amperometric sulfite sensor based on redox composite of nickel hexacyanoferrate decorated on 3D mesoporous graphene aerogel for food safety

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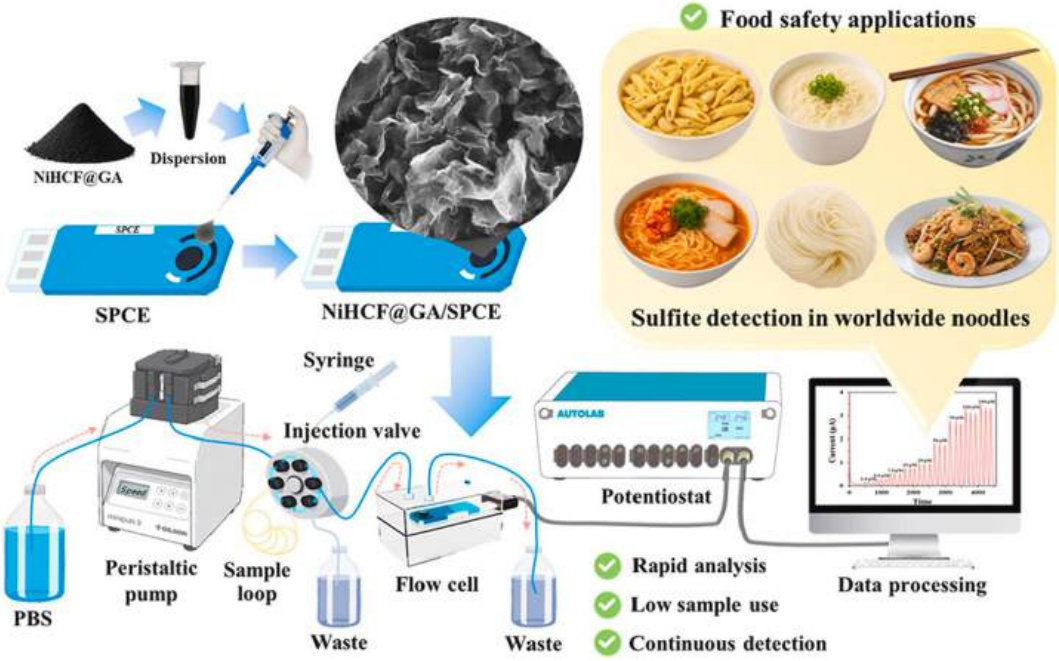
A novel redox composite of nickel hexacyanoferrate on 3D mesoporous graphene aerogel (NiHCF@GA) was developed as an electrocatalyst for amperometric sulfite (SO_3^{2-}) detection in food quality noodles. A graphene aerogel (GA) with a 3D mesoporous structure was synthesized from graphene oxide via hydrothermal and freeze-drying processes, providing a large surface area to support NiHCF, resulting in high stability. The NiHCF@GA-modified screen-printed carbon electrode (SPCE) offered high conductivity, fast electron transfer, and strong electrocatalytic activity toward SO_3^{2-} detection. Using a low constant applied potential of 0.45 V, the amperometric sensor minimized interference, resulting in enhanced selectivity. Coupled with flow injection analysis, it showed a linear range of 0.0025–27.50 mmol L^{-1} and a low detection limit of 2.50 µmol L^{-1} (S/N = 3). The sensor exhibited rapid response, excellent operational reusability (130 times) and long-term operational (9 days) and storage (4 weeks) stability with a high reproducibility (RSD = 1.11 %). SO_3^{2-} in global noodle products was accurately quantified with recoveries of 90.6–105.1 %, consistent with UV–Vis spectroscopy using Ellman's reagent.



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