

secrets of science

magazine

03/2023



Closing the loop on emissions

TOC analysis in the quest to achieve carbon neutrality

Why do batteries age?

GC-MS analysis of fluorophosphates as possible early-stage quality indicators for batteries

A guardian of purity

Determining trace amounts of sulfur compounds in Hydrogen fuel with SCD



Closing the loop on emissions
TOC analysis in the quest to achieve carbon neutrality **Page 20**

The five categories in the Secrets of Science

SWITCH ON
Discover more about our products and applications as well as current topics of interest.

MOVE ON
Explore the frontiers of science: new applications and fields of use for our systems and new configurations for applications.

ON SHOW
Accompany Shimadzu in action, with reports on events, exhibitions and seminars.

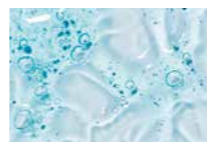
VOICES
Hear what our customers have to say about their work in interviews and guest-written articles and commentaries.

HANDS-ON
Learn more about tips and tricks for getting the most out of our devices (functions, maintenance, etc.) as well as service topics.



A guardian of purity
Determining trace amounts of sulfur compounds in Hydrogen fuel with SCD

04



Environmentally friendly and human-safe materials for regenerative medicine
Treating infected wounds with stretchable and anti-bacterial dressing

08



Metal-free for better results – inert LC columns
New solution for the analysis of critical components

12



Three new top performers
AIRsight FTIR/ Raman Microscope, Brevis GC-2050 and AIMsight Infrared Microscope

17



Why do batteries age?
GC-MS analysis of fluorophosphates as possible early-stage quality indicators for batteries

26



Critical mass: Studying treatments for age-related muscle loss
How researchers are using LC-MS/MS to investigate amino acids in blood plasma

31



Copper bottles: (un)healthy trend?
Determination of the concentration of the trace element copper with the Shimadzu AA-7800

36



Events

40



Taste the difference you can make.
Put your science skills to work where they matter.

www.shimadzu.eu/career



Newsletter
Latest news from Shimadzu straight to your inbox with Shimadzu Europe updates.

Subscribe now!



A guardian of purity

Determining trace amounts of sulfur compounds in hydrogen fuel with SCD



Omar Mayorga, Shimadzu Europa GmbH

By keeping the aim of carbon neutrality for 2050, hydrogen as fuel seems to have a big potential as it does not emit CO₂ when burned. It is well known that if impurities of sulfur components are present in hydrogen, the catalyst of the fuel cell could be damaged. In case of sulfur compounds, the ISO 14687-2 norm defines a quantification limit of 4 ppb total sulfur. In this article, it is explained how it was possible to effectively measure sulfur compounds at a low ppb level by means of a Nexis GC-2030 with sulfur chemiluminescence detector (SCD) and a gas sampling valve. In addition, a MicroJet Cryo-Trap system allows to get excellent chromatograms, even considering the big amount of sample injected to the detector.

Hydrogen plays a key role as fuel in different fields of industry for the transformation from fossil energy towards green energy. It is considered a clean fuel when consumed in a fuel cell since it produces only water. Hydrogen can be produced from a variety of domestic resources, such as natural gas, nuclear power, biomass and renewable power like solar and wind energy. These qualities make it an attractive fuel option for transportation and electricity generation applications. It can be used in cars, in houses, for portable power and in many more applications.[1]

The different shades of hydrogen: grey, blue and green

Depending on the industrial production method, hydrogen can be categorized in three different groups: grey hydrogen, the most widely produced type of hydrogen which is derived from natural gas, the high ratio of CO₂ being responsible for the "grey" designation to this hydrogen; blue hydrogen has a lower carbon dioxide impact on the environment because the carbon dioxide created in its manufacture is captured and stored; green hydrogen is produced in a completely different way: by electrolysis powered by renewable energies. This means that no harmful gases are created at any point in the production cycle. One of the most exciting things about green hydrogen is that it can be produced from water. Due to the abundance of water on planet Earth, it seems likely that green hydrogen could become a nearly limitless source of energy for all of us in the future.[2] →



Figure 1: Nexis GC-2030 equipped with SCD-2030 detector, LVO-2030 valve box and Microjet Cryo-Trap

How to keep hydrogen clear of contamination

Independent of the production route, contamination of hydrogen with various substances may occur that show degradation effects on the catalysts used in fuel cells, affecting the performance and limiting the lifetime. Among these are e.g. CO, CO₂ and hydrocarbons but also organic sulfur species. While many of the adverse effects are reversible, sulfur compounds pose a special risk, being catalyst poisons leading to irreversible damage, as they form strong metal-sulfur bonds.[3] Using the Nexis SCD-2030 from Shimadzu, a next-generation sulfur chemiluminescence detection system, this risk is being reduced thanks to its enhanced sensitivity reliability. The highest stability in its class and excellent equimolar response yields truly reliable results and improved laboratory productivity.

In this study, a valve system connected to a gas chromatograph (GC) with sulfur chemiluminescence detection (SCD) is presented. To reach the quantification limit, sample focusing prior to detection was done with a cryogenic cold trap by using liquid nitrogen cooling (Figure 1).

Results

Carbonyl sulfide (COS) at different concentrations was analyzed. It was possible to create a calibration curve with the lowest concentration of 1.3 ppb which is much lower than the 4 ppb indicated in the ISO norm. This calibration curve showed a very good linearity within the range up to 12.9 ppb as can be seen in Figure 2.

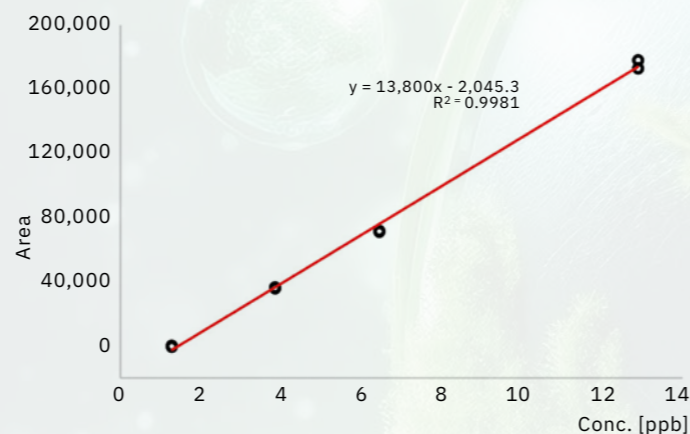


Figure 2: Calibration curve for carbonyl sulfide

To determine reproducibility of the analytical method, a 3.9-ppb COS standard was injected ten times. Calculation of the relative standard deviation (%RSD) for peak areas and concentrations can be seen and revealed the reliability of the setup (Table 1). Both area and concentration reproducibility were below 2 %, ensuring reliable detection and quantitation of the sulfur compounds at low concentrations.

#	Area	Conc. [ppb]
1	51,151	3.879
2	50,914	3.861
3	52,193	3.958
4	51,838	3.931
5	51,800	3.928
6	50,768	3.850
7	50,815	3.854
8	50,716	3.846
9	50,557	3.834
10	50,300	3.814
Average	51,105	3.876
%RSD	1.23	1.23

Table 1: Reproducibility of ten consecutive measurements of a 3.9-ppb COS standard

To guarantee long-term stability, an internal standard addition was implemented to the system by using tert-butyl mercaptan (TBM). In this case, the same compound was analyzed as target. As observed in the chromatogram of Figure 3, TBM could be successfully quantified with a concentration of 1.07 ppb (first peak at around 6 min) as well as effectively used as internal standard (second peak at around 10 min).

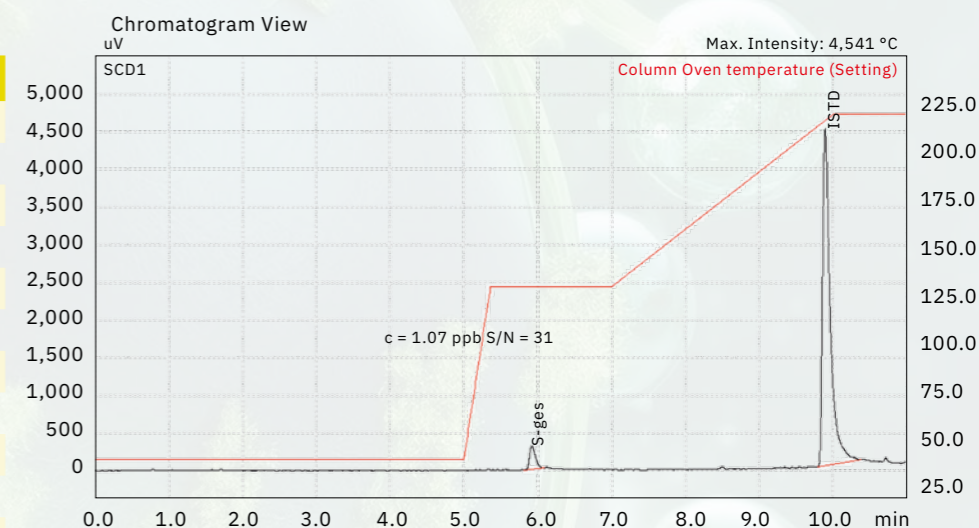


Figure 3: Analysis of TBM with internal standard

Paving the way for total sulfur compound quantification in hydrogen

The sulfur chemiluminescence detection using the Nexis SCD-2030 allows to selectively detect the total sulfur content in gases without the effect of hydrogen as matrix of the sample. Sulfur compounds can be determined with a quantification limit of less than 4 ppb, exceeding the requirements of ISO/DIS 14687 and DIN EN 17124. In the near future, the analysis of samples with more than one compound is planned and will corroborate the big potential of the system for total sulfur compound quantification in hydrogen fuel.

Note

For more information and references, please refer to the digital version of this edition.



Environmentally friendly and human-safe materials for regenerative medicine

Treating infected wounds with stretchable and antibacterial dressing



Anna Michalicha, Prof. Dr. Anna Belcarz, Medical University of Lublin

Despite the intense development of the biomaterials sector, wound management is a great challenge worldwide, laying a huge financial burden in all countries. One of the significant challenges that medicine has to face up until the 21st century is that conventional wound dressings facilitate the wound healing but not as efficiently as expected. Smart hydrogel wound dressings, such as stimuli-responsive and self-healing materials, may help to solve this problem. The development of a dressing prototype with antimicrobial potential that is able to respond to changes in the pH of the environment and is flexible and time-efficient when changing may be a great milestone in this field.

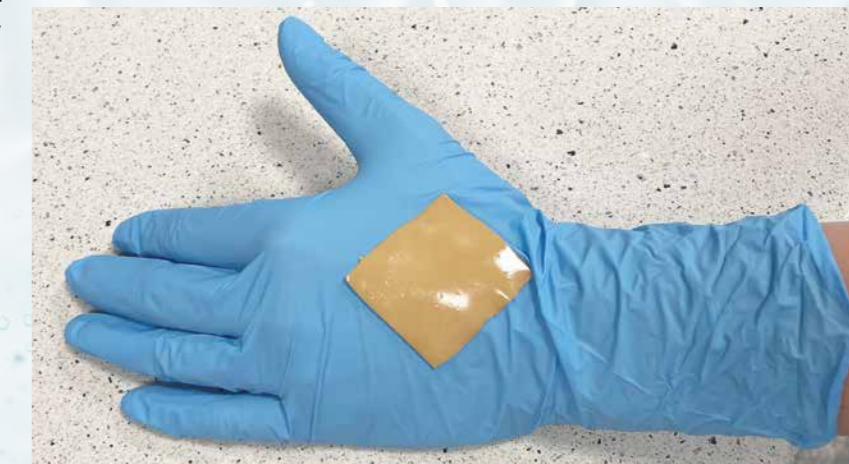
Dressings for difficult wounds – enhancing old solutions with natural components

Each of us, at least once in our lives, secured a wound with a bandage. Such products are well known and have accompanied us since childhood. Dressings are designed to treat a variety of wounds, from very harmless to infected and deadly ones. One of the significant challenges that medicine has to face up until the 21st century is that conventional wound dressings (e.g. bandages, foams, hydrogels) facilitate wound healing but not as efficiently as expected. Another significant challenge in the area of wound dressing design and improvement is the increasing problem of bacterial resistance to conventional drugs (mainly antibiotics) used in the treatment of infections.

Wound treatment difficulties are caused by acute wounds turning into chronic wounds as a consequence of extended healing. Infections often hinder the formation of blood vessels and thus the entire process of wound healing. Wound dressings, as of right now, demand the addition of extra antibacterial agents to act effectively against bacterial infection during the wound healing process. Nanosilver is

one of the currently used alternatives to antibiotics when it comes to antibacterial protection of the wound healing area. Besides, some polymers (for example chitosan) show low antimicrobial properties themselves due to their cationic nature but low mechanical resistance. Therefore, it seems to be crucial to develop wound dressings with strong antibacterial properties toward a wide spectrum of bacteria without further supplementation. Moreover, the actual gold standard for new-generation biomaterials is their ease of biodegradation. It's particularly useful for patients with chronic wounds or wounds that require extended healing times. →

Figure 1: The prototype of an intelligent hydrogel



Smart hydrogel wound dressings (SHWDs), such as stimuli-responsive and self-healing materials, may help to solve this problem. Hydrogel-based formula wound dressing materials have gained popularity in the last decades. Actually, there have been many wound dressing materials based on natural polymers. However, they are characterized by many limitations. Scientists worldwide are working on inventing new SHWDs (also called intelligent wound dressings) that address the issues of infection, exudate and bleeding in skin wounds with self-healing properties.

A potential solution to this problem is a two-component hydrogel composed of polysaccharide and tannic acid (a phenolic derivative). Both ingredients are widely used: as food additives, anti-corrosive agents, in the dyeing process, in alcoholic and non-alcoholic beverages, frozen dairy products, soft and hard candy or meat products. Tannic acid was used in the 1920s as an antibacterial agent in burn wound treatment. In some studies, the use of tannic acid in severe burn cases has been found to reduce burn mortality from approximately 35 to 11 %. After World War II, the use of tannic acid was abandoned due to the widespread use of antibiotics. However, more recently, there has been a resurgence of research on this interesting natural compound.

Two-compound hydrogel with antibacterial properties and hemostatic effect

As a team focused on designing new biomaterials and modifying existing ones, Dr. Anna Belcarz, professor at the Medical University of Lublin, and Anna Michalicha, Ph.D. student at the Medical University of Lublin's Doctoral School, created such a two-compound hydrogel. It can be shaped into a thin dressing with a thickness of 2–3 mm and high elasticity. The dressing adheres to the skin spontaneously, releases (in a pH-dependent manner) tannic acid as an astringent and antibacterial agent and absorbs a significant amount of exudate from the wound. It is worth noting that the antibacterial activity of tannic acid is non-specific, so it acts against all bacteria, including those that are antibiotic-resistant ones. Additionally, the invented hydrogel inhibits bleeding from the wound (hemostatic effect). This combination of properties makes it a promising candidate for the treatment of open, exuding and bleeding wounds that are susceptible to bacterial infections.

However, these are not the only important features for potential wound dressings. According to the co-author of the invention, Dr. Anna Belcarz, professor at the Medical University of Lublin, "Dressings applied to wounds located in different parts of the body are subjected to crushing and squeezing. Additionally, when applied to the neck, elbows, knees, knuckles and other moving parts of the body, they must also withstand repeated stretching without damaging the structure. Therefore, one of the most important characteristics of dressings is their adequate mechanical strength, including compression and stretching." To determine the values of these parameters, an appropriate tool should be used. For this purpose, the Shimadzu texture analyzer is used in the Department of Biochemistry and Biotechnology at the Medical University of Lublin.

"The EZ-SX texture analyzer is the ideal tool for determining these important parameters," says Anna Michalicha, Ph.D. student at the Medical University of Lublin's Doctoral School. "This device is relatively small and adjustable. Its operation is simple and intuitive, it can be quickly learned, and working with it is a pleasure. The data obtained during the measurement can then be subjected to multiple analyses depending on the required information."

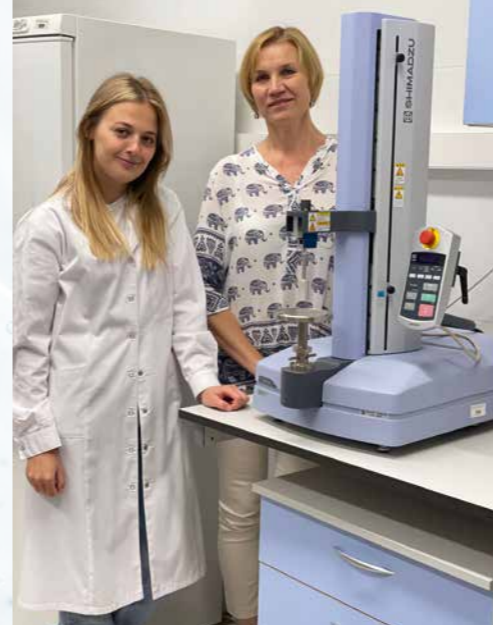


Figure 2: The authors of the smart dressing, Anna Michalicha (left) and Prof. Dr. Anna Belcarz (right)

A collaboration with many benefits

The scientific team chose to collaborate with Shimadzu precisely because they understand that working with top-notch specialists can bring numerous benefits to everyone, especially to the scientists who are involved in the advancement of medicine. This partnership offers the opportunity to leverage the expertise of esteemed professionals and opens the door to a wide array of benefits for everyone involved. Their advanced equipment has played a pivotal role, and without it these outcomes would not have been possible. It allows to continuously expand their knowledge and skills to contribute to the advancement of medicine and innovative solutions in the field of biomaterials.

The research revealed that the dressing can be compressed with a force of 100 N (equivalent to 10 kg pressure) to around 10 % of its initial thickness without losing the coherence of its structure. Additionally, after the force is released, it returns to its original dimensions. It also withstands reversible stretching, even by several hundred percent. "One could say that a patient can even lie and stand on the attached dressing without damaging it," claim the inventors of the innovation.

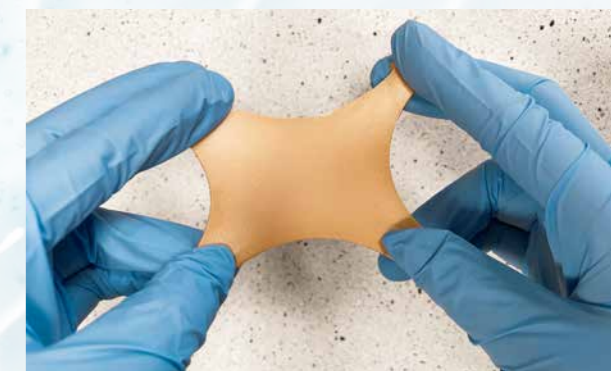
A promising hydrogel dressing is the subject of research funded by the National Science Center in Poland. Since 2023, its composition and synthesis method is protected by patent in the Polish Patent Office.

A step towards the next generation of healing devices

Curdlan-tannic acid hydrogel allows to create a pH-responsive wound dressing of high flexibility and stretchability. It is highly adhesive to skin, of enhanced wound healing potential and an increased antimicrobial activity (based on the general mechanism of protein denaturation (thus acting also on drug-resistant bacterial strains). It could be used for the treatment of chronic and burn wounds.

Note

For more information and references, please refer to the digital version of this edition.



Metal-free for better results – inert LC columns

New solution for the analysis of critical components

Dr. Martin Meyer, Shimadzu Europa GmbH

In recent years, increasing demands in the analysis of biological material, particularly in medical research, have resulted in more and more liquid chromatography columns (LC columns) being marketed as bioinert. The main objective is to reduce the metal interaction between the target molecule and the column hardware. This should lead to better sensitivity and reproducibility. This article describes the principle of adsorption, how inert columns can prevent it and which solutions Shimadzu offers.



A large number of LC-column providers who have included inert columns in their portfolios advertise that there are no interactions between the metal of the column and the analytes and that the results of analysis are therefore more precise. In comparison, in standard stainless steel columns interactions between column metal and analytes are possible. Depending on the analytes, the difference between a standard and a bioinert column can be considerable (Figure 1).

The processes that lead to adsorption effects on the metal of the column can be differentiated into two phenomena. On the one hand, the release of metal ions from the column or the system, which then accumulate, for example, in the stationary phase can lead to ionic interactions there. The second effect is the coordinated action of the positive metal surface on electron-rich analytes. Both effects result in a portion of certain analytes remaining on the column longer or not breaking away from the column at all. This results in losses of sensitivity or a degradation of peak form.

Molecules that carry phosphate groups, such as oligonucleotides and phosphopeptides, are affected. However, tetracyclines and mycotoxins and other molecules can also suffer significantly from the consequences of metal interaction.[1, 2] Furthermore, proteins and peptides can be susceptible to metal ion catalyzed decomposition, which is also prevented by the use of bioinert columns. →

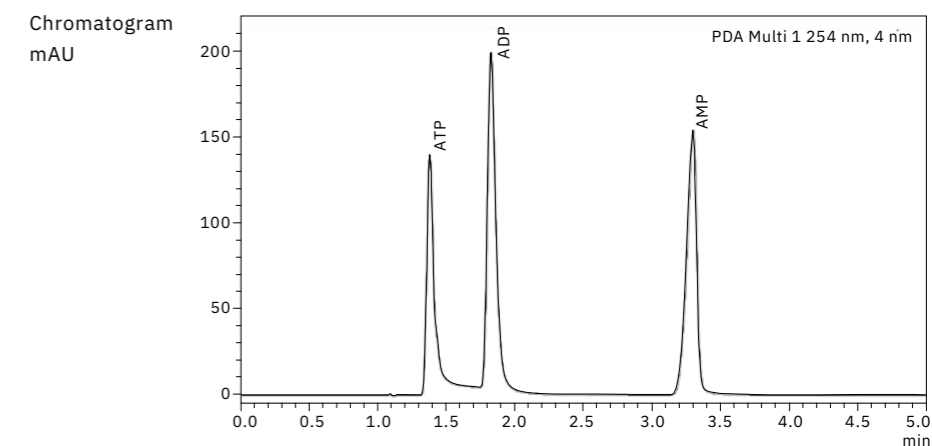
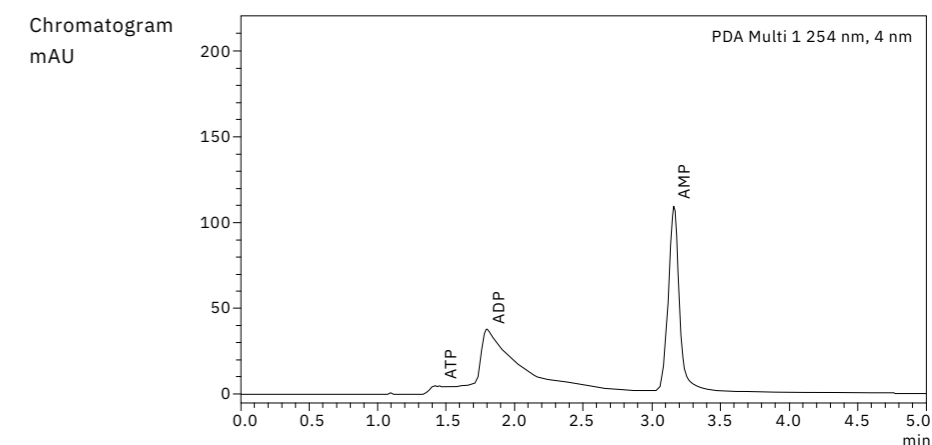


Figure 1: Chromatograms of nucleotides on conventional column + LC (top) and on inert column and LC (bottom)

Method	Disadvantage
Surface passivation with acids	Temporary Time-consuming
Surface passivation with sample or matrix	Not stable Time-consuming
Chelating agent	Ion suppression
Other metals such as titanium and MP35N (a nickel-cobalt alloy)	Interaction/washout of metals still possible
Pure PEEK columns	Low pressure stability
Glass-covered	Frit made of another material -> PEEK or coating
PEEK-lined	Limited solvent compatibility
Coatings	-

Table 1: Methods for passivation of LC systems

The effects of metals on chromatography have been known for more than 20 years.[4] To date, various methods have been applied to solve the problems of metal interactions (Table 1).

There are a range of temporary solutions such as passivation with acid or with the sample itself, but these passivations must be renewed after some time and make the method itself less robust. Alternative solutions, such as the use of metals other than steel, can reduce some of the adsorption effects, but ultimately metal is still used, which can still cause interactions.

The two most commonly used techniques by inert column manufacturers are lining the metal column with a polyetheretherketone (PEEK) polymer layer and coating the metal surface of the column. Shimadzu offers both variants: the coated columns under the name Shim-pack Scepter Claris ("CL" for short) and the PEEK-lined columns with the addition "metal-free" or "MF" for short.

Effects of inert components

The phenomena that lead to adsorption are shown in Figure 2 as well as the use of inert column material to prevent interactions. To investigate the effects of these inert components, the applicability of the inert Shimadzu Nexera XS system and the metal-free Shim-pack Scepter columns for the analysis of nucleotides and phosphopeptides was tested. Both substances are relevant for medical research.

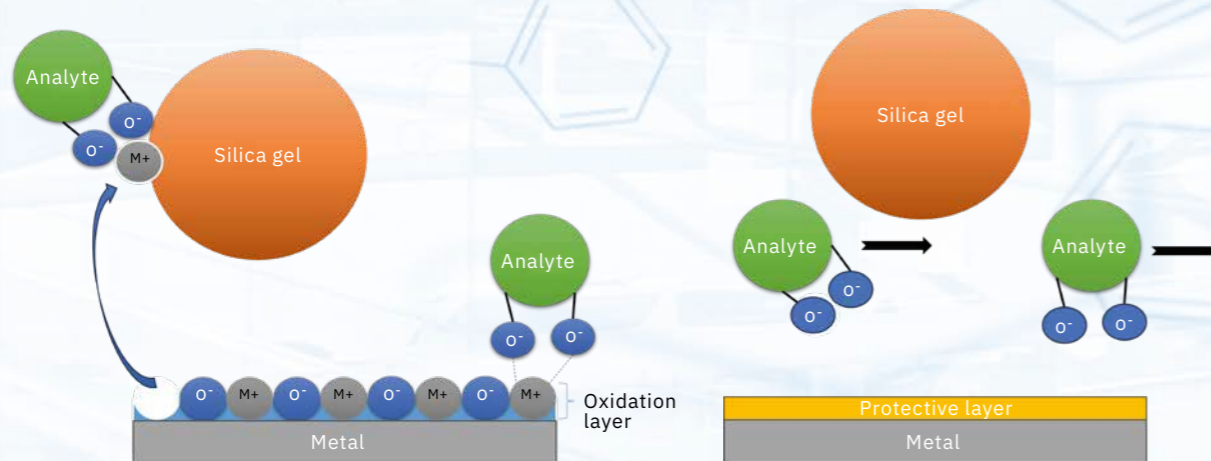


Figure 2: Mechanisms of adsorption of analytes on the metal surface

For sample preparation no standard glass vials are to be used to store samples because these also have metals on the glass surface and adsorptions can occur. The Nexera XS inert system, in which the entire flow path is inertly lined, was used for all analyses. As a result, the system is ideally coordinated for the inert column hardware.

Results

Nucleotides

The adsorption of metals can be recognized by a poor recovery and a strong peak broadening of the adsorbed components due to an intensified interaction. In fact, the peak forms and the sensitivity of adenosine triphosphate (ATP) and adenosine diphosphate (ADP) are poor if a conventional column is combined with a standard UHPLC system. The use of an inert column and an inert system provides the best results, with very symmetrical peak forms and the highest signal intensity (Figure 1).

When working with conventional columns and systems, an especially important factor is the influence of the injection number on sensitivity and peak form. The reason for this is that the analyte forms a passivation layer on the metal surface as the number of injections increases. This is illustrated in Figure 3, in which the tailing factor serves as a function of the number of injections. Values that fluctuate greatly over the course of the injections indicate poor reproducibility. Some users intentionally utilize the passivation effect of the sample or other substances to condition their system, but this passivation layer is not permanent and dissipates over time. Therefore, the completely inert configuration offers the best conditions for the analyzed nucleotides. →

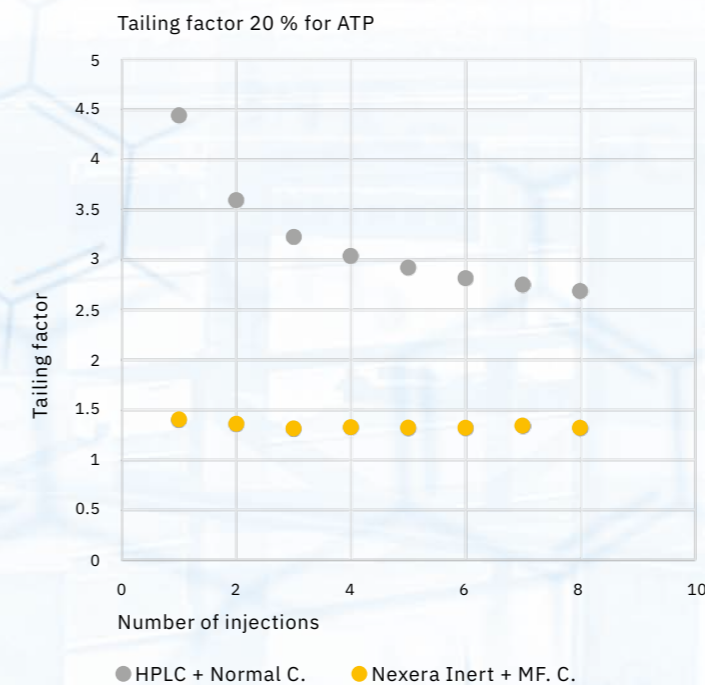


Figure 3: Tailing factor for adenosine triphosphate as a function of the number of injections

Phosphopeptides

The standard column with metal material performed poorly in the analysis of the phosphopeptide mixture. Several compounds were not detectable, and the available compounds showed small, wide peaks. A considerable increase in performance was achieved by using the bioinert columns. Not only was it possible to detect all compounds present in the standard mixture, but this occurred with at least 50 % higher sensitivity compared to the non-inert column (Figure 4).

Furthermore, the quantity or position of the phosphate group influences the degree of adsorption. Thus, some compounds can also be detected on the metal column, while others are no longer detectable at all.

More sensitivity in the analysis

The use of metal-free components both in the LC device and in the LC column substantially improved the sensitivity of the nucleotide analysis. Additionally, the reproducibility is better compared to conventional systems. All phosphopeptide components could be detected with the coated columns and with PEEK-lined columns. Compared to this, when using a metal column, some compounds were adsorbed to such a great extent that they were no longer detectable. The sensitivity of both bioinert modified columns was similar, making Shimadzu columns a very good option for the analysis of phosphopeptides.

Note

For more information and references, please refer to the digital version of this edition.

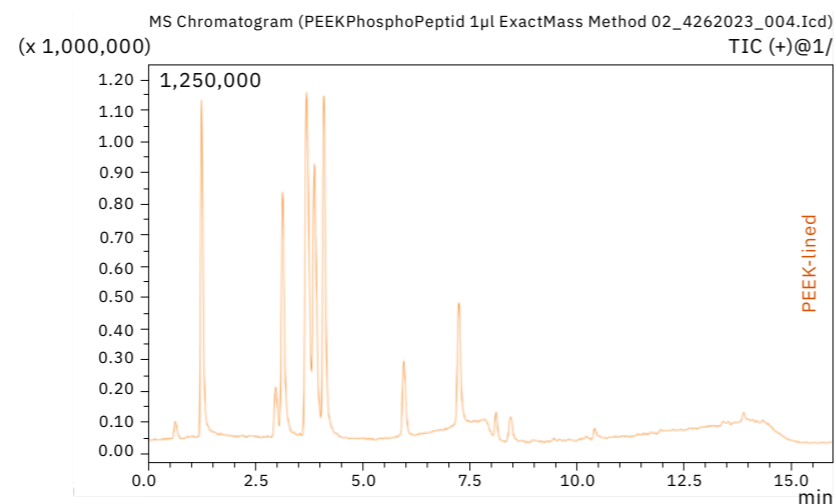
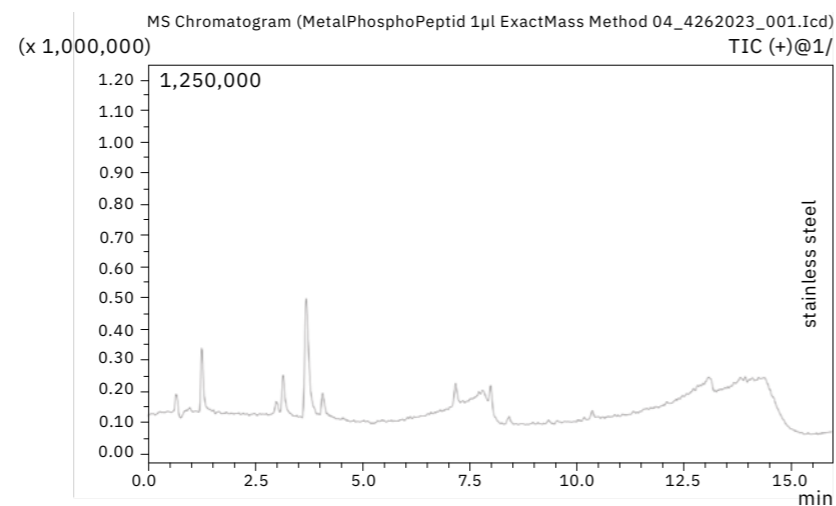
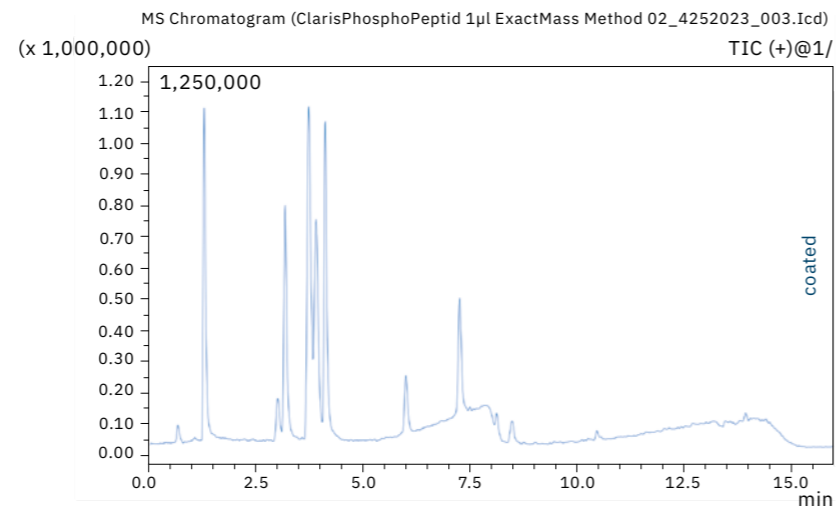


Figure 4: Chromatograms of the phosphopeptide sample on the coated column (top), the stainless steel column (middle) and the PEEK-lined column (bottom)

Three new top performers

AIRsight FTIR/Raman Microscope, Brevis GC-2050 and AIMsight Infrared Microscope



Dr. Franz Kramp, Dr. Johannes Hesper, Shimadzu Europa GmbH

They are high-performance, compact and user friendly: With three new products, including one that is the first of its kind, Shimadzu proves its innovative strength for the laboratory of the future.

A world first: AIRsight FTIR/Raman Microscope

Shimadzu has dedicated itself to developing better and better devices for use in industry, laboratories and science. With the AIRsight, Shimadzu replaces two separate devices with one. The AIRsight is the only microscope in the world that can perform both FTIR and Raman spectroscopy.

In the process, two types of analyses complement each other: While infrared spectroscopy is often used in conjunction with a spectra database to detect organic compounds, Raman spectroscopy is particularly suited for the analysis of aqueous solutions, inorganic substances and microscopic samples.

It is the only microscope that is able to record FTIR and Raman spectra from an extremely small sample in the same place. As a result, this combination provides important additional information and leads to a more thorough analysis.

Thanks to the combined technologies, a single AIRsight instrument requires much less space than a classic combination of two devices, an infrared and a Raman microscope. And since both technologies are controlled by the same high-performance AMsolution software, overall usability is simplified and improved considerably.

The AIRsight Infrared/Raman microscope improves analytical efficiency by making it easier to perform all process steps, from sample observation to data analysis. The devices also increase accuracy, as the user can obtain qualitative infrared and Raman spectra in the same position without having to move the samples to the next device. →



Nice to have two features in one





Small but mighty

High performance with a small footprint: Brevis GC-2050 gas chromatograph

As a more compact version of the popular Nexis GC-2030, the Brevis GC-2050 combines a low space requirement with high analytical performance. Small enough that a typical lab table can accommodate multiple units, the GC-2050 allows for the simultaneous operation of two analysis lines with standard capillary columns. The GC-2050 can be operated and maintained compatibly with its larger brother GC-2030, as it uses the same techniques for sample injection and detection as well as the control of carrier and detector gases.

In addition to helium, the GC-2050 can optionally be operated with hydrogen, nitrogen or argon. Therefore, if the price of helium rises, it is possible to switch to alternative gases at any time. If the user is committed to expensive helium for GC analysis, various techniques allow for significantly reduced gas consumption. For example, a complete split flow is required only during sample injection. During the remaining analysis time, the GC-2050 reduces consumption and avoids unnecessary use of the carrier gas.

Furthermore, during standby times it can switch to nitrogen, which is more economical. When a new sample measurement starts, the GC-2050 will then revert automatically to helium as the carrier gas.

At night or during longer rest times, the system can switch off automatically after all ongoing processes have ended. At a freely selectable time, it will switch back on to continue with new measurements.

Leaky connections within an analytical line can adversely affect the analytical result. After maintenance work, the GC-2050 performs an automatic leak check and warns the operator if there is a leak. Changing the separating column is made easier by the user-friendly ClickTek technology, as no tools are needed and leaks due to insufficient or excess tightening are eliminated.

The GC-2050 can be used flexibly with a variety of CDS software platforms (chromatography data software), including: LabSolutions (Shimadzu), Chromeleon 7 (Thermo Fisher Scientific), OpenLab (Agilent Technologies) and beginning next year, also Empower 3 (Waters Corporation).



Environmentally and user friendly: AIMsight infrared microscope

With the new AIMsight, Shimadzu presents the successor to the AIM-9000. With it, Shimadzu meets both the increasing requirements for infrared microscopes and the growing demand for highly sensitive instruments that allow for rapid, easy and trouble-free measurements of microsamples.

AIMsight builds on the high sensitivity of the well-known AIM-9000 and offers an improved operator experience thanks to greater automation. The infrared microscope is also connected to an IRTracer-100, IRXross or IRAffinity-1S so that it is possible to analyze microranges with maximum sensitivity. In addition, numerous accessories are available to analyze a wide variety of different samples.

Besides trace analysis of impurities and quality control in areas such as chemistry, electrical devices and electronics, machines and transportation, this instrument will play a role in the study of microplastics, tiny plastic particles that have a negative effect on the environment.

The device supports laboratories not only in simplifying their employees' workflows, but also in protecting the environment. The AIMsight uses the new T2SL detector (Type-II Super Lattice), which is referred to as a next-generation quantum infrared detector. It uses neither mercury (Hg) nor cadmium (Cd), which are forbidden in electrical and electronic devices according to the European Directive for the Restriction of Hazardous Substances (RoHS).

This means that the AIMsight is not only an environmentally friendly instrument, but also an invaluable tool for analyzing contaminant traces and for quality control.



Discovers even the most minimal traces

Note

For more information and references, please refer to the digital version of this edition.





Closing the loop on emissions

TOC analysis in the quest to achieve carbon neutrality

Markus Janssen,
Shimadzu Europa GmbH

Carbon neutrality, a key goal in the fight against climate change, requires a delicate balance between carbon emissions and removals. Disruptions to the natural carbon cycle intensify climate challenges. Cleaner technologies and innovative Negative Emission Technologies (NETs) are critical to achieving carbon neutrality. TOC analysis plays an important role in quantifying carbon dynamics, evaluating carbon-sequestering materials such as concrete and advancing sustainability. By using TOC analysis to “close the loop on emissions”, effective carbon management becomes a pathway to a greener future.

In the quest to combat climate change and promote a sustainable future, the concept of carbon neutrality has gained significant prominence. Carbon neutrality, often synonymous with net-zero emissions, refers to the state in which the release of carbon dioxide (CO₂) and other greenhouse gases into the atmosphere is balanced or offset by the removal or reduction of an equivalent amount.

The pressing issue is that the excessive release of carbon dioxide (CO₂) into the atmosphere is largely man-made and is disrupting the natural carbon cycle with alarming consequences. The carbon cycle, a delicate natural process that regulates the flow of carbon between the atmosphere, oceans, land and living organisms, is being disrupted on an unprecedented scale. In a world where this balance is out of control, the consequences of anthropogenic emissions exacerbate the challenges of climate change.

Two complementary ways to achieve carbon neutrality

First, emissions must be reduced at the source through the adoption of cleaner technologies and sustainable practices. The second critical aspect could be the implementation of negative emission technologies (NETs). These innovative approaches focus on removing carbon dioxide from the atmosphere and actively work to offset any remaining emissions. A remarkable feature of NETs is that they mimic natural dynamics in their carbon sequestration mechanisms.





Understanding carbon complexity is key

In order to pursue carbon neutrality, carbon in its various forms must be studied. CO₂ is an essential natural component and is not inherently problematic. The oceans, for example, act as vast carbon sinks, absorbing approximately 25 % of CO₂ emissions and contributing to dissolved inorganic carbon (DIC), total inorganic carbon (TIC) and total organic carbon (TOC). When CO₂ dissolves in water, it forms carbonic acid (H₂CO₃), which further dissociates into bicarbonate (HCO₃⁻) and carbonate (CO₃²⁻) ions. This equilibrium depends on the pH of the water (Figure 1).

TIC includes these inorganic forms of carbon which together represent the sum of carbon for potential gaseous CO₂ release under certain conditions. Some carbon remains in the oceans as marine organisms use it to build shells. Over time, these remains can become sedimentary rocks, effectively storing carbon for millions of years. Algae and phytoplankton convert CO₂ into biomass, a form of total organic carbon (TOC). As they are consumed by other organisms, organic carbon moves up the food chain, increasing TOC levels in the broader ecosphere. Both TIC and TOC cycles facilitate forms of carbon sequestration.

The NET worth: taking climate change head-on with these methods

Negative emission technologies (NETs) are man-made carbon sequestration methods designed to remove CO₂ from the atmosphere or from emission sources. To develop effective NETs, measurement of both total organic carbon (TOC) and total inorganic carbon (TIC) is critical. TOC analyzers, such as the TOC-L and TOC-4200 systems, play an important role in this process because they operate on the principle of the inner carbon cycle. High temperature oxidation converts organic carbon compounds to carbon dioxide (CO₂), which can then be quantified using non-dispersive infrared (NDIR) detectors. Next, the pH of the sample is changed to release dissolved carbon dioxide (CO₂) from inorganic carbon sources, which can also be quantified by NDIR.

Microorganisms as a solution for a large-scale problem

Just like in the book “The War of the Worlds” by H.G. Wells, bacteria might hold the key to preserve our planet and our species. Though it is widely acknowledged that plants and microalgae can use CO₂ in photosynthesis to produce their own nutrients, the primitive life form of bacteria could hold distinct advantages over these organisms. They exhibit a significantly accelerated growth rate and life cycle, thrive in densely populated cultures and are readily amenable to genetic manipulation. Moreover, like other microorganisms, bacteria show remarkable potential in producing a diverse range of bio-alcohols and fatty acids essential for various industrial applications, including oil production.

In the controlled environment of a laboratory, the use of a TOC-L analyzer makes it possible to evaluate the uptake of carbon dioxide by microbial metabolism. The initial amount of CO₂ introduced into the closed bacterial culture medium was precisely measured by TIC analysis. →

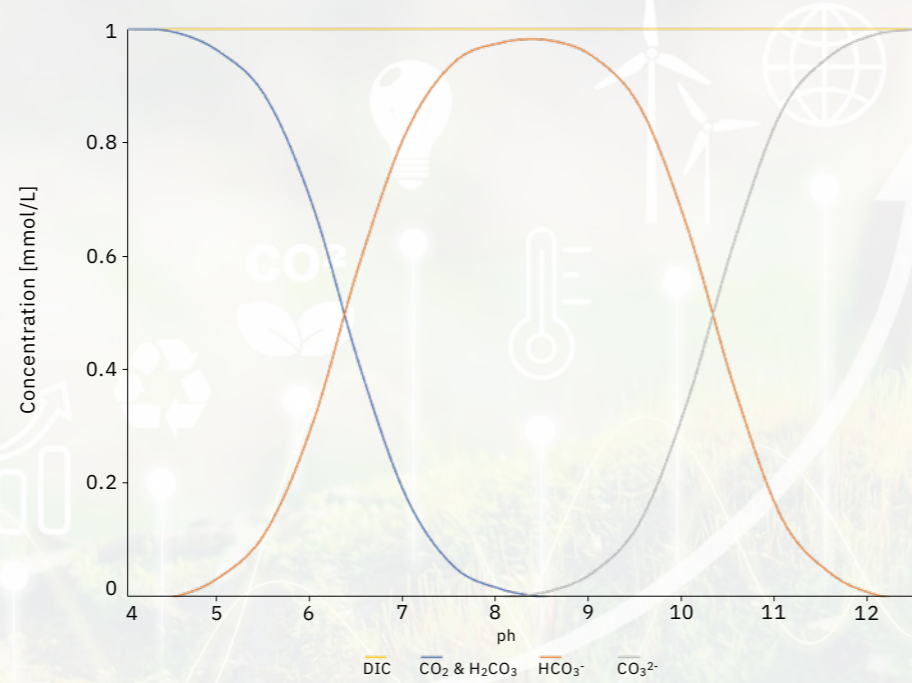


Figure 1: Carbonic acid equilibrium in water



The experiment was then meticulously replicated after 3 and 24 hours, allowing accurate quantification of the carbon used to increase microbial biomass (Table 1). This detailed approach provides valuable insights into the dynamics of microbial carbon utilization.

Notably, this natural process showcases the inherent ability of microorganisms to actively capture and utilize carbon dioxide. Within a span of 24 hours, an amount of approximately 5 g CO₂ per liter of medium could be effectively bound, all the while producing valuable biomass that could be processed into biofuel or other valuable feedstock. The biomass produced can be accurately measured as well using TOC analysis. This allows researchers to precisely quantify the organic carbon content, providing a comprehensive understanding of the microbial biomass generated during the process.

Building materials against climate change: carbon-sequestering concrete

Cement production is a significant source of CO₂ emissions (approximately 4.5 % of global emissions [1]), contributing to the greenhouse effect and global warming.

Carbon-sequestering concrete is a specialized form of concrete that actively captures and stores CO₂ during its curing process. This innovative approach involves incorporating materials that react with CO₂, such as certain mineral additives, into the concrete mix. As the concrete cures, these materials react with atmospheric CO₂ and convert it into a mineral form, effectively storing the carbon within the concrete structure.

TIC analysis is used to evaluate the carbon sequestration capabilities of this concrete. While other methods such as thermal analysis or titration of a hydrochloric acid solution can also be used, they require significant time and effort and can only measure small sample quantities, leading to biased results due to uneven sample distribution. Using the TOC-L with the solid sample measurement system SSM-5000A, milled and dried concrete samples can be analyzed quickly, easily and accurately by simply weighing them into a sample boat for analysis.

In an experiment (Table 2), two types of concrete samples were examined: ordinary concrete and CO₂-sequestering concrete. The CO₂-sequestering concrete showed about up to five times higher CO₂ absorbing potential than the ordinary concrete, highlighting its effective CO₂ absorption capability.

Time passed	TIC conc. [mg C/L]	Coefficient of variation [%]	Total CO ₂ bound by microbiology [mg/L]
0 hours	1,694	0.45	0.00
3 hours	1,163	0.95	1,943.46
24 hours	288.3	1.26	5,144.86

[CO₂/C]: 44.01 g/mol / 12.01 g/mol = 3.66

Table 1: CO₂ fixation by microbial metabolism

Sample	TIC result [wt-% C]	Coefficient of variation [%]	CO ₂ Potential [wt-%]
Ordinary concrete	1.41	2.96	5.16
CO ₂ -sequestering concrete	6.76	2.01	24.74

[CO₂/C]: 44.01 g/mol / 12.01 g/mol = 3.66

Table 2: Evaluation of carbon-sequestering concrete

DACCS: Direct Air Carbon Capture

While efforts to reduce emissions by binding CO₂ in products are commendable, they alone may not achieve negative emissions. Direct air carbon capture and sequestration (DACCS) technology, which is still in development, may offer an innovative way to actively remove carbon from the atmosphere and safely store it as stable carbonate rock. The integration of an online total organic carbon (TOC) analyzer provides valuable information on various process steps. It continuously monitors the TOC and TIC content of the DAC fluid before injection into an underground storage site, ensuring that any organic or inorganic impurities are accounted for.

The process begins with direct air capture (DAC) technology, which uses specialized equipment to extract CO₂ directly from the air. After purification to meet storage standards, the compressed gas is transported to the designated site. There, it is injected into underground rock formations using pumped-up groundwater or seawater. The CO₂ is dissolved in the carbonated water, recombines with minerals and over months forms pockets of carbonate rock within the porous basalt that are stable for geologic timespans. Subsurface injection with water eliminates the risk of gas leakage and provides safe long-term carbon storage. Other methods under development involve injecting gaseous CO₂ or supercritical fluid into suitable storage sites, such as saline aquifers or depleted oil and gas reservoirs.

With the ability to quantify both organic and inorganic carbon sources, TOC analyzers facilitate the advancement of effective negative emission technologies (NETs) that mimic natural carbon sequestration mechanisms. They provide invaluable insight into carbon dynamics and play a key role in achieving carbon neutrality by evaluating the efficiency of carbon-sequestering materials like concrete. Analyzers with TIC analysis capability, like the TOC-L and TOC-4200, are important in the development and implementation of carbon sequestration and emerging technologies like direct air carbon capture and sequestration (DACCS). By enabling complete accounting of the flow of carbon through TOC/TIC analysis, these analyzers contribute significantly to the creation of a sustainable future. They provide a comprehensive understanding and quantification of carbon dynamics in these processes, thus paving the way for effective carbon management and a greener planet.

The realignment of humanity with nature

The climate is like a big puzzle messed up by human influence. Recently, the UN has changed the term “global warming” to “global boiling”, redefining the urgency we confront. But this challenge also sparks human creativity, driving us to find answers. By implementing NETs that mimic natural mechanisms, we achieve complete accountability of carbon in sequestration processes (CO₂ gas to liquid/solid or CO₂ to biomass). This transformation allows us not only to realign our products and our way of life but also ourselves with nature, our essential ally, and natural NET.

Note

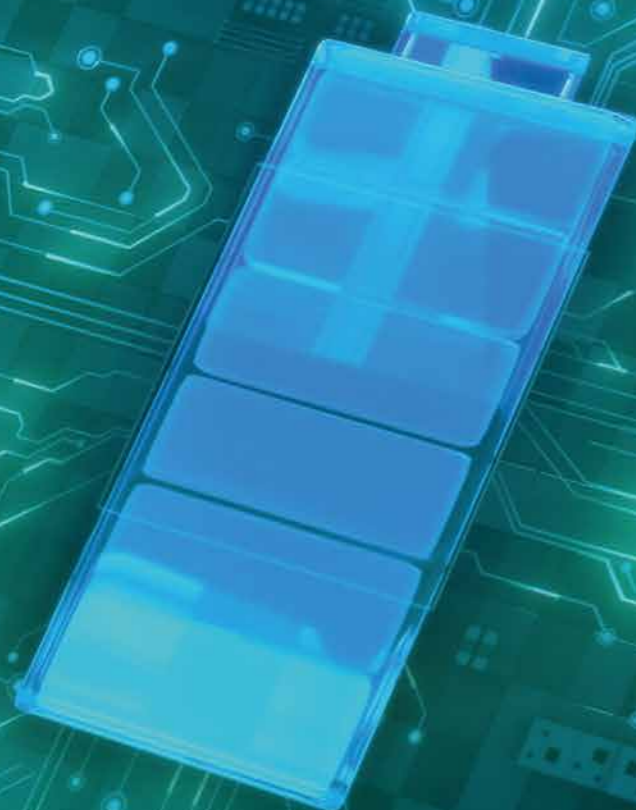
For more information and references, please refer to the digital version of this edition.



Why do batteries age?

GC-MS analysis of fluorophosphates as possible early-stage quality indicators for batteries

Dr. Waldemar Weber, Shimadzu Europa GmbH



A significant part of battery aging can be considered as a result of the decomposition of the electrolyte. The electrolyte solution is a crucial part of a typical lithium-ion battery (LIB), consisting of Li salt (e.g. LiPF_6), organic carbonates and additives to ensure a stable transport of Li ions during charging and discharging processes.

Especially fluor-containing organophosphates are of interest due to their potential neurotoxicity.[4, 5, 6] While the electrochemical aging takes place in the battery itself, the chemical aging starts already during manufacturing, storage and transport of the electrolyte. Typical factors that influence this are: exposure to air and moisture, too high temperature during manufacturing/storage, long-term storage in general. Wrong materials in the production pipeline like glass are problematic as well due to a catalytic reaction of the fluoric acid traces with SiO_2 as follows: $\text{SiO}_2 + 6\text{HF} \rightarrow \text{H}_2[\text{SiF}_6] + 2\text{H}_2\text{O}$. This application is an example for the analysis of an electrolyte solution for the qualitative determination of fluorophosphates as a possibility for an early-stage quality control.

Sample preparation and measurement

25 μl LIB electrolyte consisting of ethyl methyl carbonate and ethylene carbonate (1:1) with 1M LiPF_6 has been diluted with 1 mL dichloromethane and centrifuged for 5 min at 8,500 rpm to remove the solid LiPF_6 . The centrifuged solution was transferred into a 2-mL GC glass vial and stored at 7 °C until it was measured by a GCMS-QP2020 NX (Figure 1). →

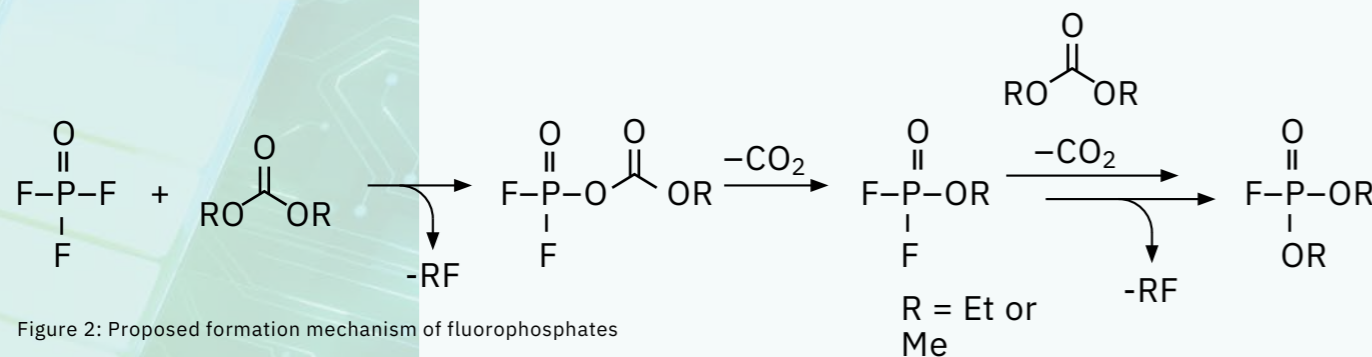


Figure 1: Shimadzu GCMS-QP2020 NX with AOC-30i liquid sampler

Decomposition mechanism of LIB electrolyte

The electrolyte used for this experiment was stored for around one year at $-30\text{ }^{\circ}\text{C}$ in a refrigerator, any aging processes under such conditions should be extremely slowed down. Nevertheless, such a long storage already has an influence on decomposition a chemical rearrangement of ethyl methyl carbonate (EMC) to dimethyl carbonate (DMC) and diethyl carbonate (DEC) could be observed. The decomposition of LiPF_6 salt under reaction with traces of water and the corresponding electrolyte solvent can be influenced by electrochemical and chemical processes. The reaction mechanisms are basically identical, the content of the produced organophosphates is strongly dependent on the aging stage of the electrolyte/LIB.[2, 3] For the dissolved LiPF_6 salt, a thermodynamic equilibrium $\text{LiPF}_6 \leftrightarrow \text{LiF} + \text{PF}_5$ is considered as a starting point for its destruction, where the PF_5 is forming POF_3 under reaction with traces of water followed by a chain of reactions of POF_3 with organic carbonate solvents.

The exact reaction mechanisms are still a point of intensive research. One of the proposed mechanisms from POF_3 to fluorophosphates is shown in Figure 2. Summarizing, the destruction process can be divided in four steps, 1: creation of POF_3 , 2: creation of difluorophosphate, 3: creation of monofluorophosphates, 4: creation of trialkyl phosphates.



A simple and reliable method to identify early signs of destruction using liquid injection for GC-MS

To analyze the highly volatile destruction products of step 1 and 2, a headspace-based injection for GC-MS is required due to a coalition with the solvent. The liquid-based injection used for this application allows the analysis of the products in step 3 and 4. The used electrolyte consists of ethyl methyl carbonate, therefore methylated, ethylated and mixed ethyl methyl phosphate species can be expected. A SCAN/SIM mode for detection allows a clear identification of compounds by a mass spectrum and a sensitive and selective detection using SIM traces. The applied m/z values for SIM detection are collected in Table 1. For the analyzed electrolyte, only dialkylated species could be detected (Table 1) but no trialkylated ones. The reason is a decomposition at the very early stage as just long-term stored electrolyte was used, where the creation of trialkylated species has not started yet. The obtained mass spectrum is shown in Figure 3 and the corresponding chromatograms in Figure 4. The general problem for identifying such compounds is the absence of $M+$ peak

in the spectra (except DMFP) and their absence in typical GC-MS libraries (except DEFP). To identify the spectrum, researchers used synthesized standards and for more complicated species NCI with CI GC-MS detections in addition.[3] →

Compound	Chemical structure	m/z for SIM	Ret. Time [min]
Dimethyl fluorophosphate (DMFP)		97, 98, 128	4.44
Ethyl methyl fluorophosphate (EMFP)		97, 115, 127, 141	6.3
Diethyl fluorophosphate (DEFP)		101, 113, 129	9.0

Table 1: Chemical structures and the used m/z SIM traces for detection

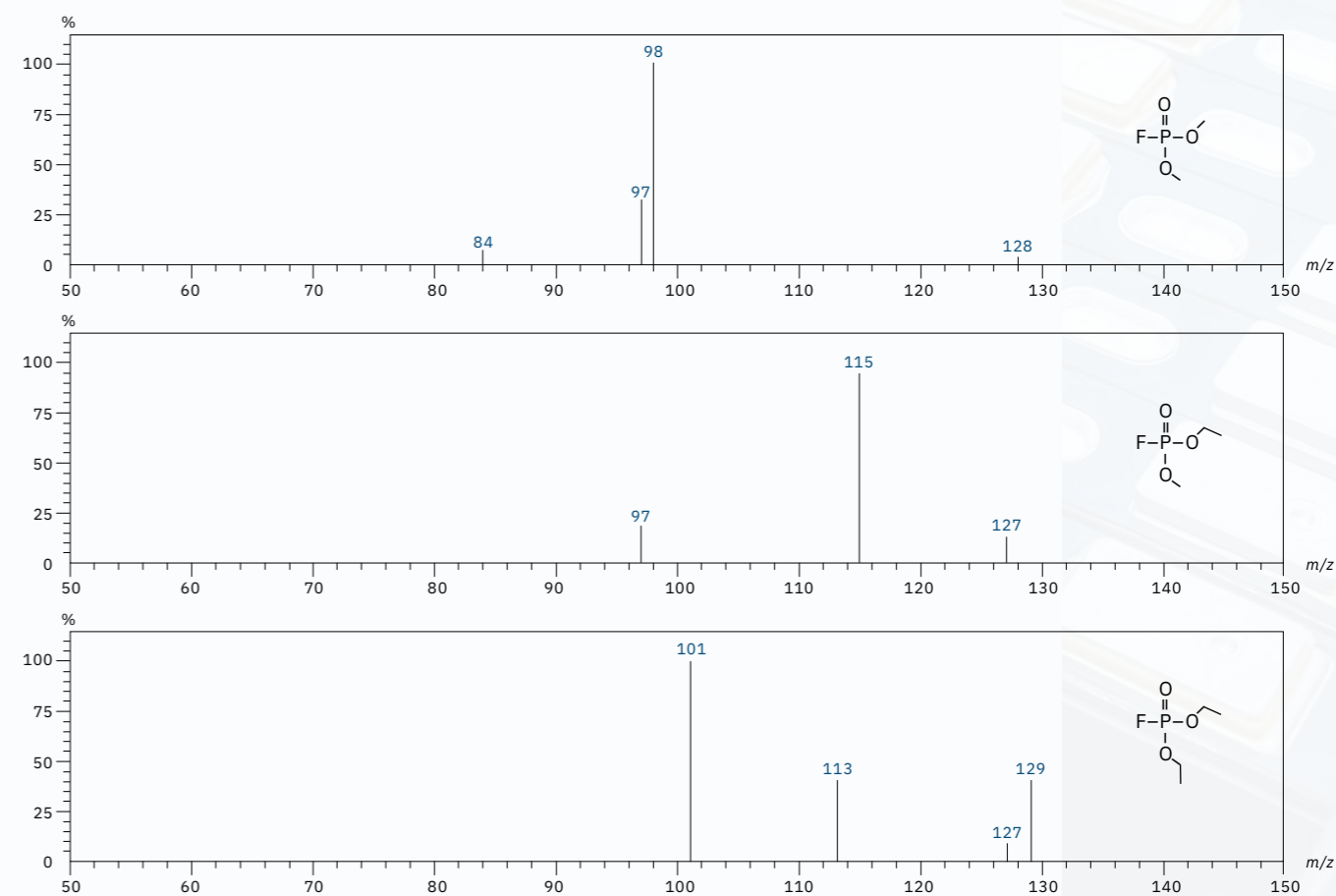


Figure 3: Mass spectra of the detected fluorophosphates, DMFP (top), EMFP (middle), DEFP (bottom)

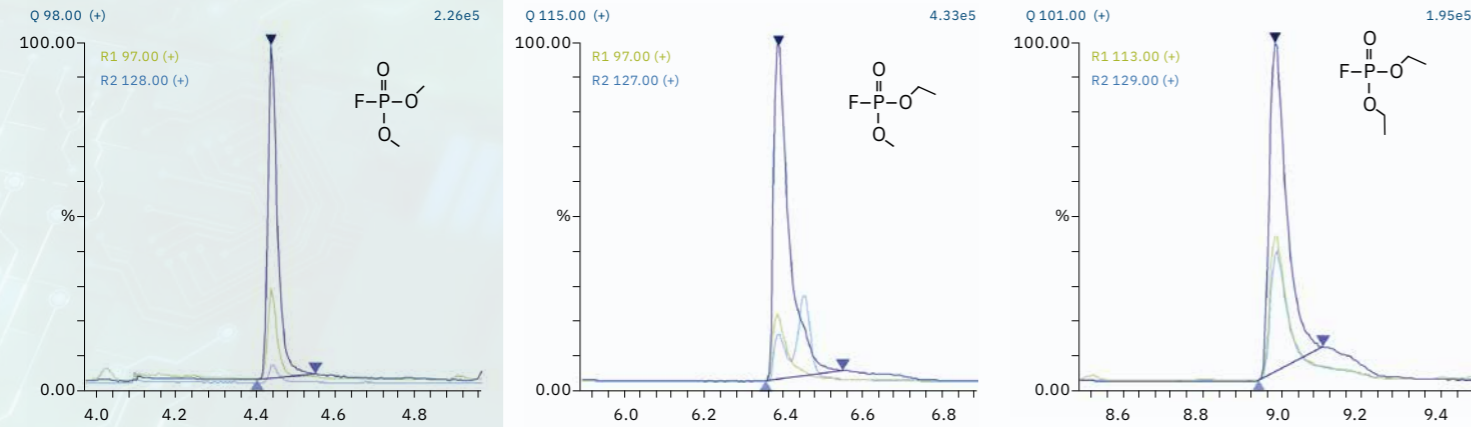


Figure 4: GC-MS chromatogram of DMFP, EMFP and DEFP in LIB electrolyte

Aiming for a prolonged battery life

LiPF₆-based LIB electrolyte degrades during chemical and electrochemical processes. With the GC-MS-based analysis method a clear identification of three fluorinated alkyl phosphates has been successfully accomplished in a long-term stored electrolyte. It shows the suitability of the GCMS-QP2020 NX to offer a reliable and simple way of analysis even at early stages of electrolyte decomposition in order to make battery life more predictable and sustainable.

Note

For more information and references, please refer to the digital version of this edition.



Critical mass: Studying treatments for age-related muscle loss

How researchers are using LC-MS/MS to investigate amino acids in blood plasma

Dr. Theocharis Ispoglou, Luke Aldrich, Leeds Beckett University

Loss of muscle mass and strength, known as sarcopenia, is a significant cause of hospitalization and loss of independence in older people. Researchers at Leeds Beckett University's Carnegie School of Sport are on a mission to understand the effect of amino acid supplements and steroid hormones on muscle mass. We talk to them about how the adoption of Shimadzu's LC-MS equipment has revolutionized their ability to examine levels of these small molecules in blood plasma and to monitor how they change during efforts to prevent and better manage sarcopenia. →



The challenge of muscle loss (sarcopenia)

Sarcopenia is the medical term for the progressive (and often rapid) loss of muscle mass and strength. It is typically associated with aging, physical inactivity and inadequate nutrition as the key causative factors and is estimated to affect about 10 % of those aged 60 or over, a proportion increasing further with advancing age. The reductions in muscle mass and strength make it difficult to perform everyday tasks.

A key factor underlying the disease is a reduction in the body’s ability to synthesize protein (often due to lack of muscle use), which leads to a reduced mass of skeletal muscles. One way of boosting muscle mass is to increase consumption of high-quality proteins, namely the branched chain amino acids or BCAAs, and taking protein and amino acid supplements is also recommended by many authorities. However, optimizing interventions using amino acid supplements is difficult because of a lack of understanding about what happens to them in the body and the limited number of well-controlled trials assessing their efficacy.

Using LC-MS to monitor amino acids in the body

One of the many research groups tackling this challenge is a team led by **Dr. Theocharis Ispoglou** at the Carnegie School of Sport. Part of Leeds Beckett University, the school is one of the largest UK providers of higher education sports courses, but also undertakes research programs, including several focused on improving human health.

The work of Dr. Ispoglou is firmly aligned with that objective, and over his 17 years at the Carnegie School of Sport, he has increasingly focused on the role of nutritional and exercise interventions in optimizing muscle health across the lifespan. “In my current research, I’m focusing on how nutritional supplements, alongside a balanced diet and exercise, can help us age more healthily, considering the clinical setting and not just the sports side,” he explains.

One of the team’s current projects is directly related to sarcopenia and is being carried out by Ph.D. research student **Luke Aldrich**, who is jointly supervised by Dr. Ispoglou and by Dr. Antonis Stavropoulos (also at the Carnegie School of

Sport). For the last 18 months, he has been using Shimadzu’s LCMS-8045 system to undertake investigations into how the composition of amino acid supplements affects the blood plasma concentrations of a range of essential amino acids. To enable solid conclusions to be drawn, Luke explains, the work has involved an intensive sampling regime: “Recently, we completed a study involving 10 adults over the age of 60, which consisted of three trials. Each of these involved collecting blood samples at eight time points over a period of four hours, with a total of 240 samples being collected in the study as a whole.”

Increased sample number enables more precise results

The number of samples in itself breaks new ground for the group, which in the past had to outsource their analyses: “There was no way we could have done something like that previously because of the cost,” says Dr. Ispoglou. “But now, with the sampling limitation removed, we can take as many time points as we need and so generate more detailed and informative concentration curves for amino acids in the blood plasma.” →

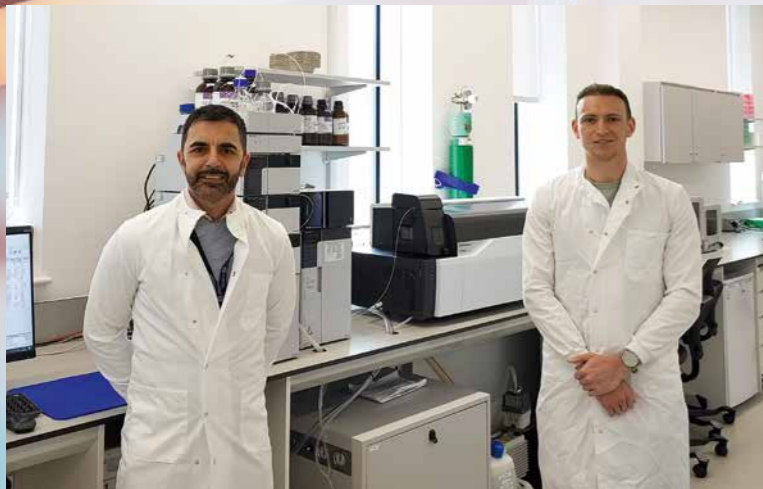


Figure 1: Dr. Theocharis Ispoglou (left) and Ph.D. student Luke Aldrich (right) with their Shimadzu LCMS-8045 system in the Carnegie School of Sport at Leeds Beckett University

Amino acid	Retention time (min)
1 Tryptophan	1.073
2 Phenylalanine	1.100
3 Tyrosine	1.195
4 Leucine	1.213
5 Methionine	1.280
6 Isoleucine	1.296
7 Valine	1.530
8 Threonine	1.830
9 Alanine	1.975
10 Serine	2.000
11 Proline	2.064
12 Asparagine	2.226
13 Glutamine	2.312
14 Arginine	3.877
15 Glutamic acid	4.857
16 Lysine	4.861
17 Aspartic acid	5.060

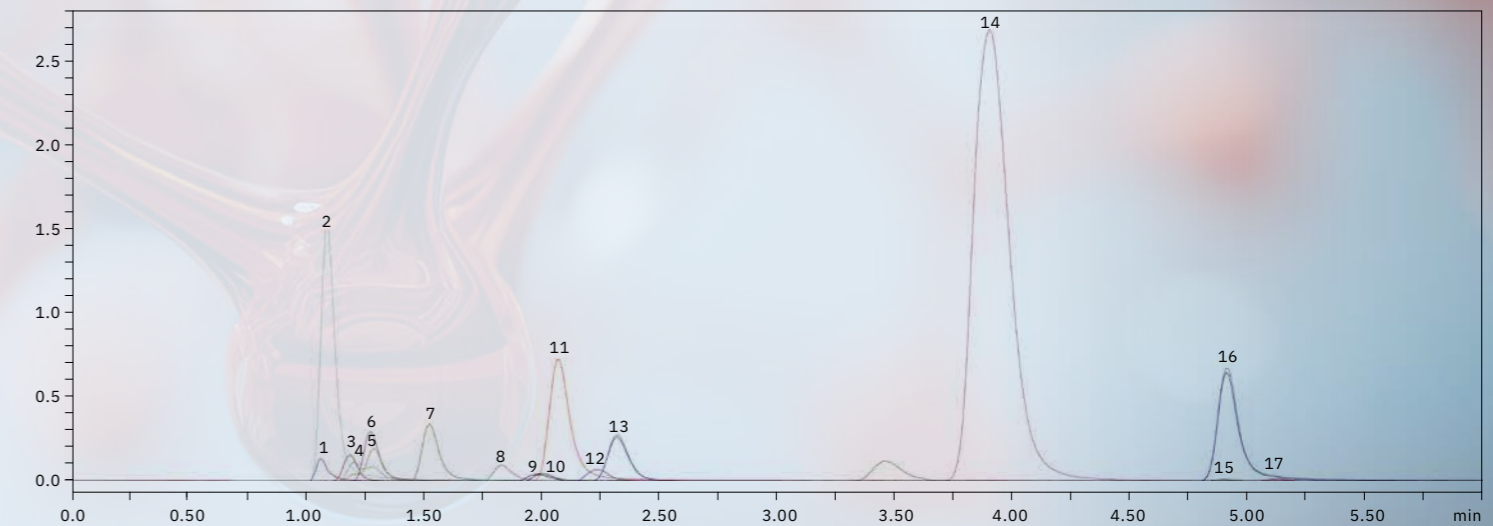
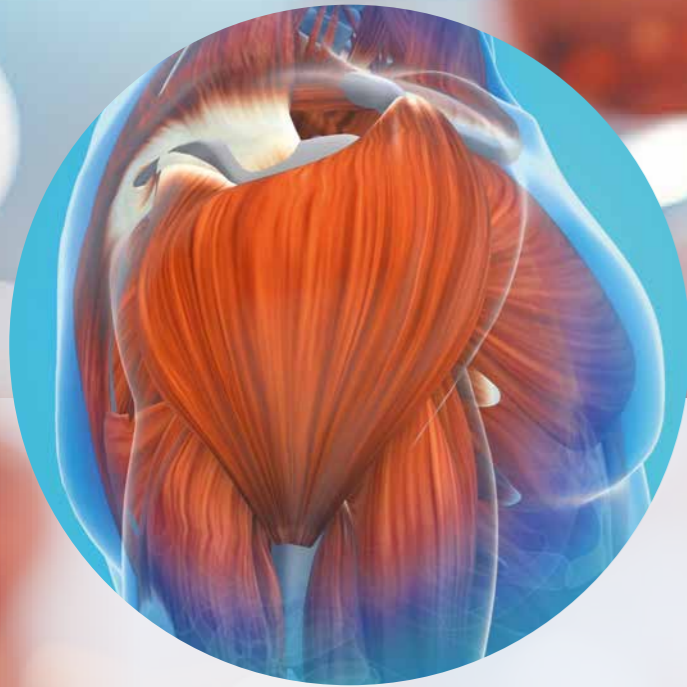


Figure 2: A typical LC-MS chromatogram obtained by Dr. Ispoglou’s team using the Shimadzu LCMS-8045, showing 17 amino acids analyzed within 10 minutes. Note the separation of several groups of amino acids despite their close elution.



Understanding causative links thanks to new capabilities provided by LC-MS

But it is not just the study design that is proving fruitful – the analytical methodology also marks a milestone, simply because LC-MS is not widely used in the fields of sports nutrition and exercise science. With analytical targets commonly being proteins or hormones, it is normal for researchers to use immunoassays for analysis, and they tend not to have in-house access to chromatographic techniques for smaller molecules or the experience to use them effectively.

But by having easy access to an LC-MS system, Dr. Ispoglou's team has been able to make significant progress: "All the data we get from LC-MS helps us obtain a fuller and more accurate picture of what's happening, meaning that we're now in a much better position to look at potential causative and mechanistic links. These are things that we certainly couldn't have done before!"

Thorough training and on-the-spot support

This change in capability only came about because of a major investment by Leeds Beckett University in the Carnegie School of Sport. Opened in 2020, the new building brought together previously separate facilities under one roof – and importantly for Dr. Ispoglou, it was a unique opportunity to expand the laboratory facilities available to his group. "We had done some preliminary research about the sensitivity and specificity of LC-MS, and we knew it would be perfect for our research. I was delighted that the Shimadzu team made a very competitive offer, and their system came out on top – for me, it was a dream that I'd been chasing for years!"

But because no-one in the group had prior experience of LC-MS, with their new equipment came a need for training. Luke Aldrich picks up the story: "We received the LC-MS in November 2021, and shortly after that we had our first training session from Shimadzu. We were starting from scratch, but our Shimadzu trainers were great, going through the theoretical side of the chromatography first, followed by an introduction to operating the system as well as training on data analysis, sample preparation and standard preparation – the whole lot!"

The Shimadzu team has also been really responsive, says Luke, providing rapid support by email or phone any time they need it: "They're straight on to it and really helpful. In the last six months, we have often benefitted from same-day on-site support from Shimadzu technical specialists. Not many manufacturers offer that level of service."

Future steps already in the making

At the time of writing (June 2023), a 30-adult study has recently been completed, with preliminary results showing clear differences in amino acid levels between a control group versus those undertaking either an exercise regime or a program of nutritional supplements. The results are yet to be published, but Dr. Ispoglou says that the work seems to support the findings of an earlier case study carried out by the team with a 57-year-old with sarcopenia:[1] "In this early work, we showed that the sum total of 17 amino acids increased by 19.1 % after 24 weeks of an exercise and dietary intervention – in line with the literature in this area. So, we're really looking forward to publishing the results of our new much larger study!"

Two further projects that the team are developing, and which will also use LC-MS, involve the School of Health at Leeds Beckett. The lead researcher will be Dr. John George, who says that the first study will use LC-MS to reveal the biochemical pathways involved in regulating the biogenesis of the cell envelope of Gram-negative bacteria, which could be important for understanding how these cells grow or achieve homeostasis as well as aiding potential drug discovery attempts. The second project, he says, will involve challenging bacteria with a number of antibiotics and monitoring their cellular response by LC-MS, potentially aiding the discovery of new drugs targeting antibiotic-resistant bacteria.

LC-MS is helping sarcopenia research get to the next level

Dr. Ispoglou concludes that the availability of the Shimadzu LC-MS equipment within the new laboratory facilities at the Carnegie School of Sport has been a game-changer for the team's ambitions. "To continually advance your research, you need to invest in equipment and people, and our new instrumentation has absolutely enabled us to take our research to the next level," he says. "LC-MS certainly has the potential to foster the development of novel insights in the field of sport, exercise science and nutrition."

And through it all, it is clear that the Shimadzu team has been central to helping the team get started with LC-MS, says Dr. Ispoglou: "They've been incredible, and our experience has been highly positive. It's clear to me that they genuinely care about what we're doing, and they want us to do the best with the data we have." Luke agrees: "We can't fault Shimadzu at all – the equipment is reliable, and the service has been brilliant!"

Note

For more information and references, please refer to the digital version of this edition.



Copper bottles: (un)healthy trend?



Determination of the concentration of the trace element copper with the Shimadzu AA-7800

Dr. Johannes Hesper, Shimadzu Europa

The use of copper vessels for storing and consuming water has a long tradition in some cultures. In recent years, copper bottles or cups have also gained popularity in our part of the world. In addition to the material's antibacterial properties, manufacturers often mention the enrichment of the water with trace elements. Copper (Cu) is an essential trace element for the human body. The use of copper bottles causes small quantities of copper to be released into the water. The Shimadzu AA-7800 Atomic Absorption Spectrophotometer was used to analyze how large and how healthy these quantities actually are.

Copper bottles for drinking water are very trendy right now. Their use has increased in the past few years, and manufacturers often advertise their positive health effects, for example in the sense of Ayurveda. But how much of the essential trace element copper is actually released in a Cu bottle? And, in this case, does the drinking water still comply with the recommendations of the current German Drinking Water Ordinance?[1] It prescribes a maximum value of 2 mg/L (2 ppm) of copper, which should not be exceeded.

To determine the quantity of the copper migration, an uncoated, cleaned copper bottle (99.7 % copper, manufacturer's declared value) was filled with tap water and stored closed for six days at room temperature. On days zero, one, two and six, the copper content was determined using the new AA-7800 Atomic Absorption Spectrophotometer in flame mode (acetylene flame). →



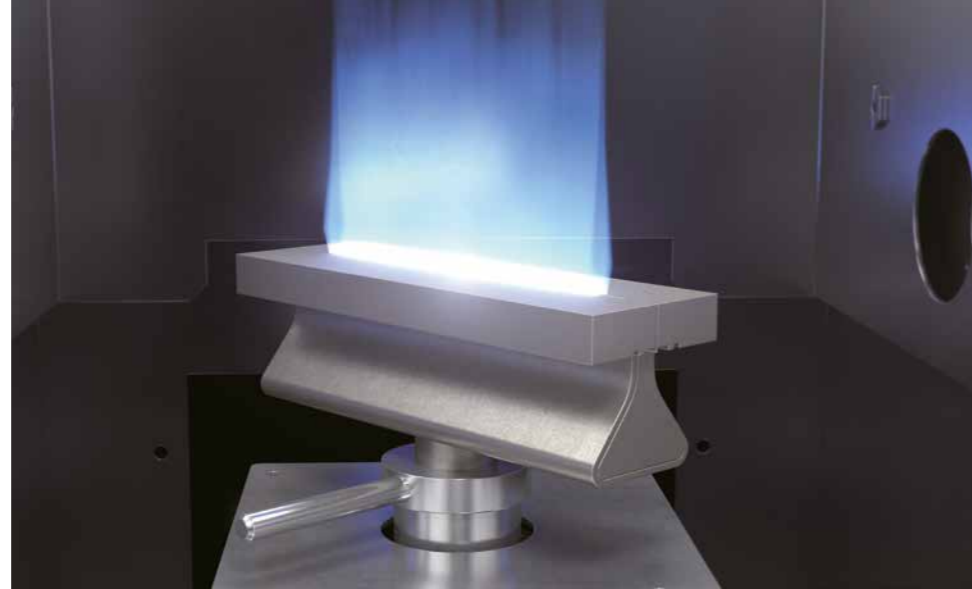


Figure 1: Acetylene flame (C₂H₂) of the AA-7800

On day zero, three samples (blind samples) were taken from the bottle and acidified with 1 % HNO₃ (nitric acid) to stabilize the copper in solution. On the next day, three more samples were drawn and acidified. The same procedure was repeated on day two and for a fourth and last time on the sixth day.

Finally, all the samples were measured against an external copper calibration. The calibration line obtained is illustrated in Figure 2 and shows a very high linearity in the measuring range of 0–3 ppm Cu with R² = 0.9998.

The proven standard measurement settings for copper from the Shimadzu cookbook (Flame AAS) were used. Using the copper (Cu) hollow-cathode lamp, the copper absorption was measured at 324.8 nm in the acetylene flame and determined against the calibration.

The measurement results are listed in Table 1.

Abs = 0.14053 Conc. + 0.0025703
r = 0.9999

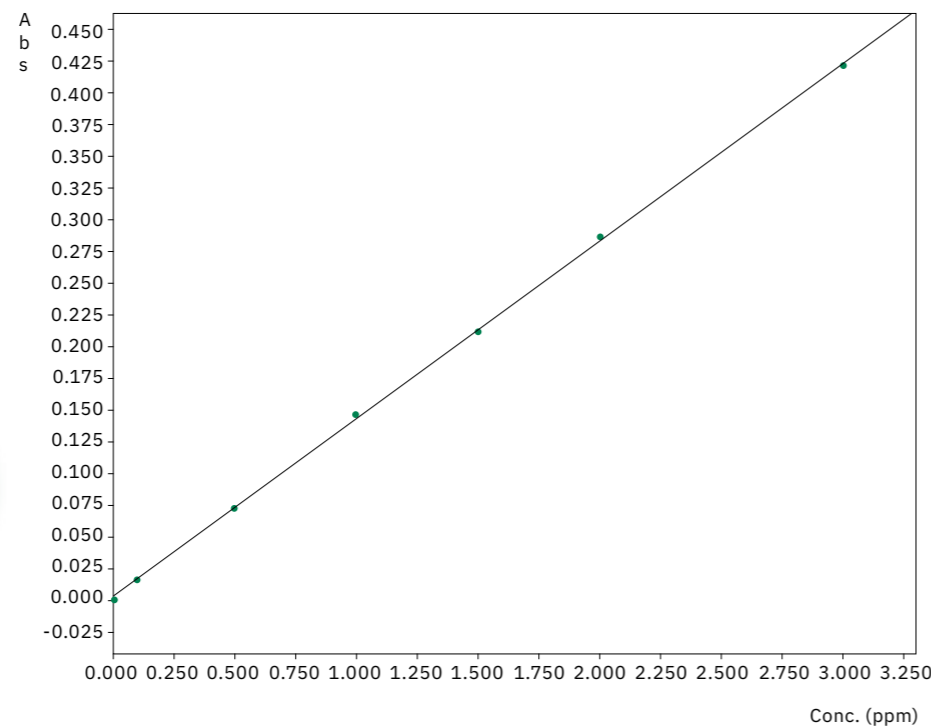


Figure 2: Cu calibration of the AA-7800F (C₂H₂ flame)

Day	#1	#2	#3	Mean	SD
0	0.0294	0.0265	0.0287	0.0	0.005
1	1.0405	1.0619	1.059	1.1	0.035
2	1.7692	1.7728	1.7934	1.8	0.039
6	3.6293	3.5389	3.8321	3.7	0.450

Table 1: Cu concentration (ppm) after 0, 1, 2 and 6 days of the three replicate measurements, their rounded mean values and standard deviations



While the measured value on the sixth day, at 3.7 ppm, was a little bit outside the working range of 0–3 ppm, it can nevertheless be assumed that the calibration retains its validity until then and that the absorption signal remains linearly dependent on the Cu concentration.

Effect of Cu bottle on Cu content in drinking water
Error bars reflect three times the standard deviation of three triplicates

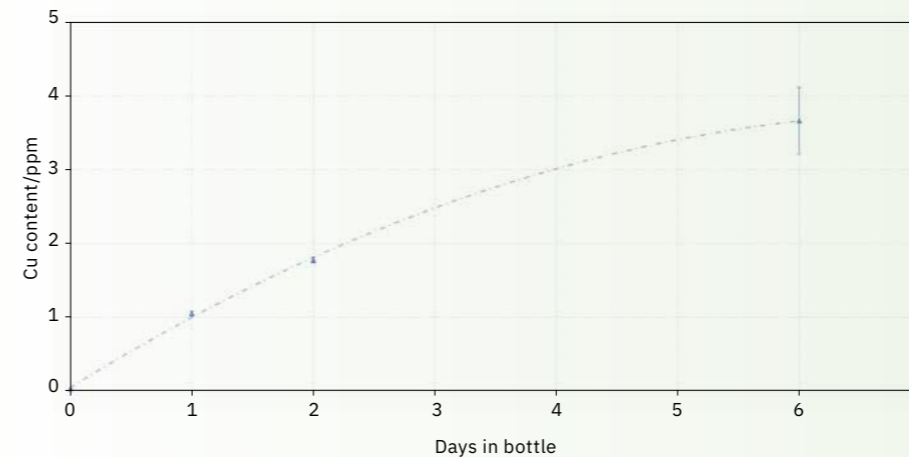


Figure 3: Influence of copper bottle on copper concentration in drinking water according to days

Therefore, the copper content of the drinking water increased daily from the original value of 0 ppm (approx. 30 ppb) to be above the limit value in the German Drinking Water Ordinance on the sixth day, at 3.6 ppm Cu. The limit value of 2 mg/L copper was probably already exceeded on the third day, but no samples were taken on this day.

The Shimadzu AA-7800 Atomic Absorption Spectrophotometer, with up to eight hollow-cathode lamps, offers two optimal background compensations for the correction of the sample matrix. The high-current pulse technology (SR method) and the deuterium (D₂) background compensation are available as standard for measurement with flame and graphite tube. Thanks to the optional

autosampler ASC-7800, up to 60 samples can be measured comfortably. The comprehensive safety functions also make the use of acetylene gas extremely safe, which makes it ideal for the analysis of trace elements even in difficult matrices.

Using copper bottles safely

Anyone who is considering using a copper bottle should make sure that it is made of high-quality copper in order to prevent possible health risks due to heavy metals. This is because copper can be toxic in large quantities and lead to copper poisoning. This expresses itself in symptoms including nausea, vomiting, abdominal pain and other health problems.

Based on the non-representative measuring results, drinking water should be stored in a copper bottle for a maximum of two days because otherwise the recommendations of the German Drinking Water Ordinance are exceeded. Drinks and fruit juices that contain acid should not be stored in a copper bottle because otherwise an accelerated release of copper is to be expected.

Note
For more information and references, please refer to the digital version of this edition.



**Lab Innovations**

Birmingham, UK

November 01–02, 2023

**EBF**

Barcelona, Spain

November 15–17, 2023

**ISEAC**

Amsterdam, Netherlands

November 20–24, 2023

**DYMAT**

Colmar, France

November 27–29, 2023

**JEC**

Paris, France

March 05–07, 2024

**AD/PD 2024**

Lisbon, Portugal

March 05–09, 2024

secrets of science
magazineCustomer Magazine of
Shimadzu Europa GmbH,
Duisburg**Publisher**Shimadzu Europa GmbH
Albert-Hahn-Str. 6–10
D-47269 Duisburg
Tel.: +49(0)203 7687-0
shimadzu@shimadzu.eu
www.shimadzu.eu**Editorial Team**Uta Steeger,
Sonja Wischnewsky,
Andrea Wagner-Neumann,
Christopher Brünn**Design**Bartenbach AG
Kaufmannshof 1
D-55120 Mainz**Circulation**German: 4,600
English: 3,885**©Copyright**Shimadzu Europa GmbH,
Duisburg, November 2023.
Reprint, also in extracts,
only with the permission
of the editors.

@ShimadzuEurope

Even more insight

Dive deeper into the topics covered in “Secrets of Science” magazine! The digital version offers even more information, including additional chromatograms, tables and content details. Go for it: and get to the bottom of these secrets of science.



Digital version
shimadzu-webapp.eu

