CITAC
Cooperation on International Traceability in Analytical Chemistry

CITAC NEWS

2023

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Cooperation on International Traceability in Analytical Chemistry (CITAC)

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FOREWORD BY THE CHAIR

CITAC ACTIVITY IN 2022

Bernd Güttler // PTB, Germany

For many of us, this year will bring about the first instance since 2019 where we can meet with colleagues and friends for in person meetings and conferences. This will enable the "zoom free" exchange of thoughts and information and possibly even result in a drink together in different places around the world.

The CITAC/IUPAC workshop on Metrology, Quality and Conformity Assessment at Isranalytica in Tel Aviv held on the 17th - 19th January 2023 was such an event and from the many smiles that greeted me, it made it very clear that there is more to life than can be viewed through a computer screen. Many thanks to Ilya Kuselman for taking the risk to organize such a successful meeting. With contributions from industry, universities, research institutes, NMIs and CITAC members from all over the world, this was a Déjà vu of earlier days unaffected by a pandemic. A broad range of topics were presented from, the fundamental considerations of measurement uncertainty and traceability to the practical application of metrology in health (clinical and pharmaceutical), food and the environment (climate change) measurements. Whenever possible, I very much hope that we can now return to this form of essential exchange between people for good.

Of course, the pandemic has not yet disappeared and will still be in our minds for a long time to come. The interest in quantifying pathogens, such as viruses, is much more prominent now, as is also reflected by the results of the CITAC Best Paper Award (Andrea Briones et al., An SI-traceable reference material for virus-like particles, iScience 25, 104294, https://doi.org/10.1016/j.isci.2022.104294).

Nevertheless, we are now also able to return to more general and fundamental aspects of science and metrology and discuss this together. The skills that we have all developed during the pandemic for carrying out online meetings have helped to conduct a series of online-workshops on metrology in chemistry, organized by the BIPM. They provided a forum for the exchange of information between stakeholders interested in the topics in a comparatively easy way. Many current issues such as, microplastics, particles, viruses and, of course, infectious diseases were addressed. The latest in this series is a workshop on "The metrology of quantities which can be counted" 28 - 30 March 2023 and has been jointly organized by CCQM and CCU, with support from CITAC representatives on its steering committee. Information about this and other past and future workshops is available at https://www.bipm.org/en/committees/cc/ccqm/workshops. You can also register for these workshops under this link.

Have fun with metrology in chemistry!

ADDRESS OF THE VICE-CHAIR

MESSAGE FROM THE VICE CHAIR

Zoltan Mester // National Research Council (NRC), Canada

Dear friends and colleagues,

It is important to remember that CITAC is an international organization with members from all continents aiming to improve the worldwide comparability of chemical measurements through collaboration. We are doing this by observing the principles of mutual respect, peace, basic human rights, dignity and worth of every person as the foundation of our work.

One of the key theme of 2022, in measurement science, has been the digital transformation. In early 2022, standardization organizations banded together and issued a Joint Statement of intent on the digital transformation in the international scientific and quality infrastructure. The statement provides a platform for the signatories for the development, implementation, and promotion of the International System of Units (SI) Digital Framework as part of a wider digital transformation of the international scientific and quality infrastructure. The Joint Statement also supported the 2022 World Metrology Day theme, Metrology in the Digital Era. https://2022.worldmetrologyday.org/

In 2021, CCQM conducted a number of workshops to identify appropriate diagnostic technologies, platforms and data management approaches, and propose specific metrology interventions that could enable a more rapid response. The recommendations that resulted from this consultation will ensure that the metrology community is sufficiently prepared to support key measurements in future infectious disease outbreaks. The CCQM Roadmap to Metrology Readiness for Infectious Disease Pandemic Response was published in 2022:

https://www.bipm.org/documents/20126/74750777/Roadmap-to-Metrology-Readiness_050822_Final.pdf/c324192c-b145-1797-b29c-055b1b9044c1

Additionally a CCQM Task Group has been established to oversee the implementation of the recommendations over coming years.

In October 2022 the 27th meeting of the General Conference on Weights and Measures (CGPM) was held. One of the key outcomes of the meeting is the election of new CIPM members. Congratulations to newly elected members: Venu Gopal Achanta, India; Victoria Coleman, Australia; Jan-Theodoor Janssen, UK; Georgette Macdonald, Canada and Gustavo Ripper, Brazil!

Additionally, the CGPM has decided to expand the range of prefixes used within the International System of Units (SI).

This decision means that four new prefixes (two at the top end of the SI range and two at the bottom end of the SI range) can now be used to express measurements worldwide.

The proposal, championed by Richard Brown from NPL, member of CITAC, recommended four new names.

The new names for (very) large numbers are:

ronna (symbol R) for 1027 or 000 000 000 000 000 000	1 000 000 000
quetta (symbol Q) for 1030 or 000 000 000 000 000 000 000	1 000 000 000

And for very small numbers are:

ronto (symbol r) for 10−27 or 000 000 000 000 000 000 001	0.000 000
quecto (symbol q) for 10−30 or 000 000 000 000 000 000 000 001	0.000 000

These new prefixes are of particular interest for chemistry as we often traffic in these elementary particle number/concentration ranges dealing molar units.

In October 2023 the UNESCO Executive Board took the first step towards recognizing World Metrology Day following the proposal presented by Kazakhstan and supported by the BIPM and OIML. The decision will need to be ratified by the 42nd session of the UNESCO General Conference in November 2023. If all goes to plan, UNESCO will proclaim 20 May of each year as a UNESCO world day which will then be celebrated every year from 20 May 2024.

In my role as the coordinator of the CITAC Best Paper in Metrology Award I had the pleasure of facilitating the award process and announce three papers were voted by the CITAC constituency to be awarded:

Christine Brauckmann, Axel Pramann, Olaf Rienitz, Alexander Schulze, Pranee Phukphatthanachai and Jochen Vogl, Combining Isotope Dilution and Standard Addition – Elemental Analysis in Complex Samples, Molecules 26 (2021) 2649

https://www.mdpi.com/1420-3049/26/9/2649

Mojca Milavec, Megan H. Cleveland, Young-Kyung Bae, Robert I. Wielgosz, Maxim Vonsky, Jim F. Huggett, Metrological framework to support accurate, reliable, and reproducible nucleic acid measurements, Anal. Bioanal. Chem. 414 (2022) 791-806. (Accepted: 1 October 2021) (link)

https://link.springer.com/article/10.1007/s00216-021-03712-x

Akanksha Roberts, Subhasis Mahari, Deepshikha Shahdeo, Sonu Gandhi, Label-free detection of SARS-CoV-2 Spike S1 antigen triggered by electroactive gold nanoparticles on antibody coated fluorine-doped tin oxide (FTO) electrode, Anal. Chim. Acta 1188 (2021) 339207

https://www.sciencedirect.com/science/article/pii/S0003267021010333

Award Ceremony and Lectures of the CITAC Best Paper 2021, held on 2022/06/21

https://www.youtube.com/watch?v=GUcml8i2vHI&t=27s

Congratulations to the winners of 2022 and I would like to thank all the CITAC members for supporting the nomination and selections process.

I hope to see all of you, in person, in 2024!

Zoltan Mester

CITAC vice chair

MESSAGE FROM THE CITAC SECRETARY

BRIGHT METROLOGY!

Ricardo Bettencourt da Silva // University of Lisbon, Portugal

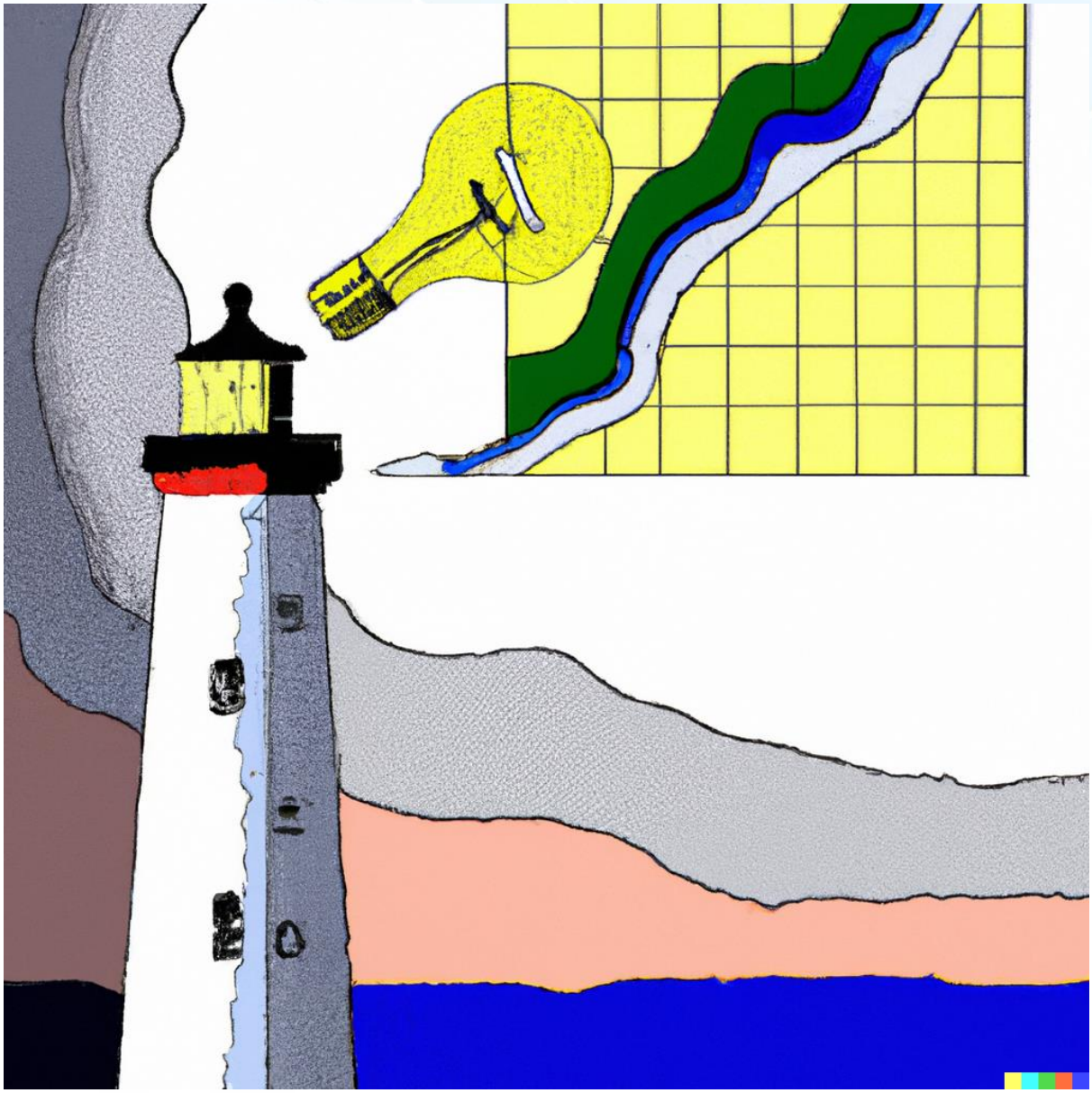
In an open world, people's interests are continuously managed by using tools developed internationally from multiple disciplines such as economics, law, politics, communication and many scientific and technological areas. Occasionally, competing or conflicting countries use the relevance of these areas for the well-being of people in disputes. We know several examples of the obscure use of economics, law, politics, communication, and scientific and technological preponderance to sponsor some interests frequently by weakening competing ones. Equivalent countermeasures are used to fight these endeavours, frequently with the motivation that go further than just keeping the initial balance. For their dark motivations, we know some dark economics, dark law, dark politics, dark communication and dark technology. The countermeasures with bright motivations would be a bright economy and so on. Unfortunately, it is difficult to have or distinguish actions with purely beneficial motivations. In most extreme cases, the conflict between counties drives to the most inhuman and anachronistic way of squeezing out conflicts: wars, the wars that kill young people that will never have the chance to understand or even contribute to a better world.

In the middle of all this darkness, let us believe there are activities managed positively, even in the darkest scenarios, since they interest everyone. Probably naifly, we can believe that some achievements from metrologists are protected even between countries at war. At least the reliability of some determinations is important to preserve, such as the quantity and quality of cereals that are being exported to African populations from the centre of the ongoing war in Europe.

The past has some lessons for us about how measurement capabilities need to be preserved regardless of our first instinct to break all links between conflicting positions.

The history of "General Conference on Weights and Measures" (CGPM), the supreme authority of the International Bureau of Weights and Measures (BIPM), that act on matters related to measurement science and measurement standards proves the particularities of international metrology in the middle of conflicts between countries. Although formal liaison between the various organisations of the meter convention is handled by the member state's ambassador to France, requiring diplomatic relations with France, during both world wars, nations at war with France retained their CGPM membership.

In these dark times, let's look at some bright lighthouse and believe that the future will be better and not just a continuous repetition of the same mistakes from people that do not know or do not understand the consequences of past dramatic events.



Picture generated by DALL·E: “Create a painting, in Dali style, where a lighthouse illuminates a graph with values reported with error bars”

Ricardo Bettencourt da Silva

EDITORIAL

RELATION BETWEEN QbD, AQbD AND MEASUREMENT UNCERTAINTY

Felipe Rebello Lourenço

Quality by Design (QbD) is a systematic approach to drug development that focuses on understanding and controlling the critical quality attributes (CQAs) of a product. Analytical Quality by Design (AQbD) is an extension of QbD, specifically focused on analytical method development and validation.

Measurement uncertainty is a critical component of both QbD and AQbD. The measurement uncertainty of analytical methods must be understood and controlled to ensure accurate and precise measurements of CQAs. The AQbD approach involves systematically identifying the sources of measurement uncertainty and optimizing the analytical method to reduce the impact of these uncertainties on the results.

Measurement uncertainty is also important in the QbD approach to drug development. QbD requires a thorough understanding of the manufacturing process, and accurate measurement of CQAs is critical to this understanding. Measurement uncertainty must be evaluated to ensure that CQAs are measured with sufficient accuracy and precision, and to determine the acceptable range of CQAs.

In both QbD and AQbD, measurement uncertainty is evaluated by estimating the sources of variation in the measurement process and quantifying the impact of each source on the measurement result. The sources of variation may include the equipment used for the measurement, the environmental conditions in which the measurement is made, and the skill of the analyst performing the measurement.

By controlling the sources of variation, manufacturers can optimize their processes and ensure consistent product quality. AQbD provides a structured approach to method development and validation that includes the evaluation and control of measurement uncertainty. QbD provides a broader framework for drug development that includes the optimization of the manufacturing process and the control of CQAs.

In conclusion, measurement uncertainty is a critical component of both QbD and AQbD in the pharmaceutical industry. Accurate measurement of CQAs is essential to both approaches, and measurement uncertainty must be evaluated to ensure that CQAs are measured with sufficient

accuracy and precision. AQbD provides a structured approach to method development and validation that includes the evaluation and control of measurement uncertainty, while QbD provides a broader framework for drug development that includes the optimization of the manufacturing process and the control of CQAs.

Felipe Rebello Lourenço

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Angelique Botha // NMISA, South Africa

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IMEKO REPORT

Michela Sega // INRIM, Italy, IMEKO TC8 Chair

REPORT FROM ISO/REMCO

Angelique Botha // NMISA, South Africa, ISO/REMCO Chair

IUPAC REPORT

Zoltan Mester // NRC, Canada, President of the IUPAC ACD

LIAISON REPORTS

AFRIMETS REPORT

Angelique Botha // NMISA, South Africa

SUMMARY OF GENERAL ISSUES

AFRIMETS (the African regional metrology organisation) held its 15th General Assembly and related meetings during July 2022. Most of the technical committees including the Technical Committee for Quality Systems (TC-QS) met online before the General Assembly. The AFRIMETS TCQM meeting to discuss activities in metrology for chemistry and biology took place in conjunction with the 2nd Africa Food Safety Workshop hosted by the NMISA in Johannesburg, South Africa with the support of the FAO-IAEA Joint Technical Centre and the Africa Food Safety Network on Friday, 1 July 2022.

In terms of the election of executive officers, Dr Henry Rotich from KEBS in Kenya was elected as the Chairperson of AFRIMETS for the next period (2 years). Mr John Paul Musimami from UNBS in Uganda was elected as Vice-chair responsible for Legal Metrology and Mr Matthew Ranganai from SIRDC-NMI in Zimbabwe was elected as Vice-chair for Scientific Metrology.

Some good progress has been made with the development of the AFRIMETS Services Database. The first concept draft of the database was developed by the contractor. It mimics the Key Comparison Database of the BIPM (KCDB), but is designed to capture the quality confirmed (3rd party accredited or peer reviewed) calibration and measurement capabilities (CMCs) of the national metrology institutes (NMIs) in Africa (and later the Legal Metrology Bodies). Testing of the database commenced in October 2022 to check the operability of the system and to correct bugs. Data entry is anticipated to start during the first half of 2023. The AFRIMETS Capabilities and Services Database (ACSD) will support the mutual recognition of metrology capabilities for the African Continental Free Trade Agreement (AfCFTA). The African States that are party to the Metre Convention and the Associates of the CGPM will continue to publish their CMCs in the KCDB, for international recognition of their services.

The quality systems of NIS in Egypt, KEBS in Kenya, DEFNAT in Tunisia and NMISA in South Africa were re-confirmed as fit-for-purpose for the CIPM MRA. The quality system of LPEE-Morocco was confirmed, and they published their first CMCs. The review of the AFRIMETS quality systems by the AFRIMETS TC-QS confirmed that the calibration and measurement capabilities published in the international key comparison database (KCDB) are supported by total quality managements systems implemented in accordance with ISO/IEC 17025 and ISO 17034 as required. The review or re-review of the quality systems of NMIE in Ethiopia, GSA in Ghana, SIRDC-NMI in Zimbabwe, INRAP in Tunisia, and NSI in Namibia are underway.

The General Assembly decided that a minimal membership fee will be implemented per country from 2023 onwards. AFRIMETS will be registered as a non-profit company with a bank account. The next General Assembly will be held in July 2023 in Egypt, hosted by NIS.

CURRENT TC AND WORKING GROUP CHAIRS AND CONTACT DETAILS

The AFRIMETS structure includes working groups to mirror the international consultative committee working groups (CC-WGs) and are identified as TC-(parameter).

The contact details of the TC-Chairs important to Chemistry are listed below:

Function	Name	Details
TC-QM Vice-Chair (Bio analysis)	Dr Angelique Botha Mrs Désirée Prevoo-Franszen	National Metrology Institute of South Africa (NMISA), Private Bag X34, Lynnwood Ridge, 0040, RSA Tel: +27 12 947 2705 e-mail: abotha@nmisa.org Tel: +27 12 947 2738 e-mail: dprevoo@nmisa.org
TC-Mass and Related Quantities	Mr Thomas Mautjana	National Metrology Institute of South Africa, Private Bag X34, Lynnwood Ridge, 0040, RSA Tel: +27 12 947 2880 e-mail: tmautjana@nmisa.org
TC-QS Vice-Chair (CMCs)	Dr Noha Emad Khaled Dr Wynand Louw	National Institute for Standards (NIS), Tersa Street, El Haram, Giza, 12211 Egypt Tel: ++(202)33862322 e-mail: nemadnis@yahoo.co.uk or nemadnis@netscape.net National Metrology Institute of South Africa (NMISA), Private Bag X34, Lynnwood Ridge, 0040, RSA Tel: +27 12 947 2895 e-mail: wlouw@nmisa.org

AFRIMETS CMCs

As of 8 February 2023, there were a total of 736 AFRIMETS CMCs accepted in Appendix C of the KCDB.

The CMCs originate from:

South Africa (NMISA) = 534
(123 CMCs in Chemistry and Biology)

Egypt (NIS) = 99
(2 CMCs in Chemistry)

Zimbabwe (SIRDC) = 19

Kenya (KEBS) = 27
(2 CMCs in Chemistry)

Tunisia (DEFNAT) = 21

Zambia (ZMA) = 11

Namibia (NSI) = 7

Morocco (LPEE) = 15

Botswana (BOBS) = 3

DEVELOPMENT WORK IN CHEMISTRY AND BIOLOGY

INRAP, who is the designated institute for metrology in chemistry in Tunisia, is currently in the process of implementing a national strategy in Metrology in Chemistry to achieve comparability of measurement results to meet the national needs in terms of production of certified reference materials (CRMs) and organisation of proficiency testing (PT) schemes. INRAP has developed a roadmap for the implementation of the national strategy in metrology in chemistry with the support of BIPM and AFRIMETS experts.

The commissioning of the Gravimetric Unit for CRM production at INRAP with the support of the PTB under a bilateral project has progressed well. The laboratory participated in a capacity building comparison of the BIPM (CCQM-K148.d) for patulin in acetonitrile in October 2022 and participated in a bilateral comparison with the BIPM for aflatoxin B1 in acetonitrile. The training in ISO 17034:2016 and ISO Guide 35 (supported by the PTB) for the competent production of reference materials, has supported INRAP with their participation in the abovementioned comparisons using their newly established capability in the gravimetric preparation of calibration solutions.

NIS in Egypt has submitted new CMC claims in the field of Chemistry and Biology for 2023 that includes their measurement capabilities for poly aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs) and endosulfanes in food.

In June 2022, the National Metrology Institute of South Africa (NMISA) hosted the 2nd Africa Food Safety Workshop (AFSW) in collaboration with the FAO-IAEA Joint Technical Centre, the IAEA Technical Cooperation Department, and the Africa Food Safety Network to promote standards, reliable methods of analysis and inter-institutional cooperation for better public health and trade. The workshop was attended by more than 250 representatives from national, regional, and international institutions from over 35 countries in the chemistry and microbiological field as well as prominent industry experts, academia, and regulators. Participation in the workshop has allowed organisations to engage with influential scientists across the globe and key role players from Africa and the international community.

The purpose of the event was to enhance networking opportunities among food safety stakeholders in Africa; to facilitate the sharing of analytical knowledge and transfer of developed technologies related to a range of food hazards, and to encourage continent-wide discussions on how to best improve national/regional food safety control systems to safeguard consumers and facilitate trade. Through diverse discussion panels, the event explored how to best align laboratories to address challenges of setting food safety standards for both trade and public health; fitting food safety control systems into the African Continental Free Trade Agreement (AfCFTA) arrangements and reducing trade rejections.

***Figure 1**: Delegation to the 2nd Africa Food Safety Workshop hosted by the NMISA in South Africa in June 2022.*

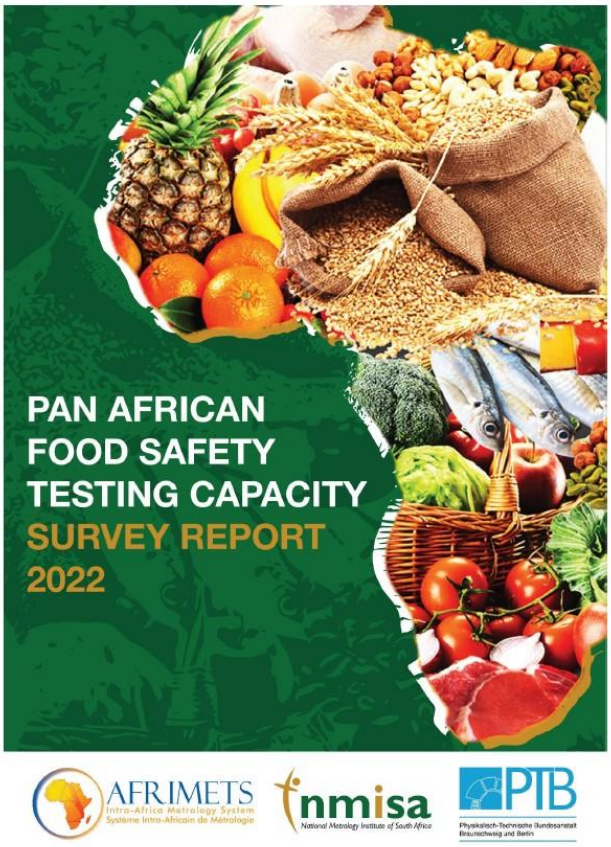
In 2022, a survey was initiated on behalf of AFRIMETS to consolidate information on the laboratory food testing capabilities on the African continent. The purpose of the survey was to identify gaps to help inform future food testing capacity building activities within the Africa Continental Free Trade Area (AfCFTA) in support of the African Union's Food Safety Strategy for Africa (FSSA). Survey responses (113) were received from 60% of the countries in Africa and were supplemented with additional ISO/IEC 17025 laboratory accreditation information to reflect the food testing capabilities of 76% of the countries in Africa.

Several laboratories develop their own in-house methods, where method validation using appropriate matrix certified reference materials (CRMs) and proficiency testing (PT) schemes are critical for demonstrating methods are fit-for-purpose. The survey identified training needs in areas such as sample preparation; method validation and analytical techniques, including gas chromatography (GC), liquid chromatography (LC), etc. Other needs include, how to set up specific methods for heavy metals, pesticides, and veterinary drug residue analysis, establishment of metrological traceability and the estimation of uncertainty of measurement. Another laboratory challenge is the maintenance and troubleshooting of analytical instruments, for which training should be prioritised.

Due to COVID-19, the implementation of the planned AFRIMETS supplementary comparison for pesticides in fruit was delayed to 2022/23. The comparison would enable AFRIMETS NMIs, such as INRAP in Tunisia, who has an advanced capability in this area, to claim new CMCs. Much interest has also been shown by developing NMIs from the SIM region, such as Columbia, Bolivia, and Argentina as well as from other NMIs active in the Organic Analysis Working Group (OAWG) of the CCQM. The comparison protocol was presented to the CCQM Organic Analysis Working Group (OAWG) in November 2022. Currently, the protocol is being updated for final approval by the OAWG.

AFRIMETS is also supporting Phase 2 of the Pan African Quality Infrastructure (PAQI) project Harnessing quality infrastructure in the cassava

value chain with the organisation of a proficiency testing (PT) scheme for cassava. The PT scheme is planned for four (4) PT rounds. The first round for the determination of protein and moisture in cassava flour was completed in the beginning of 2023 and round 2 for the analysis of toxic and nutritional elements in cassava is currently underway. The third round of the PT for the analysis of pesticides in cassava will start in June 2023 and the final round for the analysis of hydrogen cyanide (HCN) in cassava will commence in November 2023. The PT scheme will also include a virtual workshop in October 2023 where the results of the completed PT rounds will be discussed by the participants to identify opportunities for improvement and standardisation of measurement methods.



FUTURE ACTIVITIES

In response to the training needs identified during the Pan African Food Testing Capability Survey in 2022, AFRIMETS, with the support of PTB, is planning a range of summer schools for the African food testing laboratories in 2023 and 2024. The summer schools will involve dedicated training in several measurement techniques, such as gas and liquid chromatography for organic analysis as well as plasma spectrometry for elemental analysis. The hands-on training in instrument operation, maintenance and troubleshooting will be followed by training on the practicalities of food analysis for a range of analytes, including pesticides, mycotoxins, heavy metals and nutritional elements. The training will comprise of two-week sessions for the trainees where they will attend lectures on the theory of the techniques and the sample analysis approaches during the first week and then have practical sessions where they will be working on the instruments, prepare samples and perform sample analysis during the second week.

For any further information on the activities in AFRIMETS or the activities of the TC-QM for Chemistry, please contact:

AFRIMETS Chair: Prof. Dr Mohamed Amer (NIS, Egypt): amer_nis@yahoo.com

Head of the Secretariat: Dr Wynand Louw (NMISA, South Africa): wlouw@nmisa.org

TC-QM Chair; Dr Angelique Botha (NMISA, South Africa): abotha@nmisa.org

TC-QM Vice-Chair; Ms Désirée Prevoo-Franszen (NMISA, South Africa): dprevoo@nmisa.org

LIAISON REPORTS

EURAMET ACTIVIES IN 2022

Michela Sega // INRIM, Italy

EURAMET is the Regional Metrology Organization (RMO) of Europe. It coordinates the cooperation of National Metrology Institutes (NMI) in Europe in different fields of metrology, such as traceability of measurements to the SI units, international recognition of national measurement standards and related Calibration and Measurement Capabilities (CMC), research projects, etc. Through the knowledge transfer and cooperation among its members, EURAMET facilitates the development of the national metrology infrastructures.

EURAMET is currently chaired by Jörn Stenger (PTB, Germany) who succeeded to Hans Arne Frøystein (JV, Norway); the two Vice-Chairpersons are Miruna Dobre (SMD, Belgium) for the General Assembly (GA), who replaced Maria Luisa Rastello (INRiM, Italy) and Maguelonne Chambon (LNE, France) for the European Metrology Programme for Innovation and Research (EMPIR) related matters. Due to Covid-19 pandemic, the EURAMET 16th GA took place as a hybrid meeting from 30th May to 2nd June 2022, in Vienna, Austria, hosted by BEV, the Austrian NMI. The EURAMET 17th GA will take place from 30th May to 2nd June 2023, in Tallin, Estonia, hosted by Metrosert, the Estonian NMI. An extraordinary GA was held on 17th January 2023, as an online meeting.

European Partnerships are a key implementation tool of the European Commission's Horizon Europe; an ambitious research and innovation programme, running from 2021 to 2027. Among these, the European Partnership on Metrology (Metrology Partnership) aims at bringing together the measurement science community and stakeholders to deliver on global challenges including health and climate, support the European Green Deal, and underpin innovation in industry through collaborative research. The European Partnership on Metrology is co-funded by the Member States and the European Union with an expected budget of around 690 million euro. The expected impact of the European Partnership on Metrology is manifold, as it will support a wide range of policies, commerce and advancement of key European challenges. It will comprise seven call cycles between 2021 to 2027, covering topics such as Green Deal, Health, Digital Transformation, Fundamental Metrology, Integrated European Metrology, Industry needs, Pre-normative and Knowledge transfer and capacity building measures. The Partnership builds on the progress achieved under the previous European Metrology Research Programmes, and aims to break new ground by contributing to the development of self-sustaining, coordinated metrology infrastructures, with the capacity to continue joint research and innovation after 2030.

In 2023 a call within the European Partnership on Metrology framework was launched, via the usual two stage process, on the following major topics, addressing specific challenges: fundamental metrology, industry, normative, research potential, capacity building coordination. Stage 1, opening on the 11th January, aims at offering stakeholders from any country the opportunity to influence the

projects undertaken by the European Community by identifying potential research topics. The highest priority topics received at Stage 1 will provide the basis for Stage 2 which will open on 23rd June 2023. Major information on the calls can be found at https://www.metpart.eu/.

One of the most important initiatives undertaken by EURAMET for the promotion of cooperation conceived in a broader scope towards better partnership, communication, and harmonization is the European Metrology Networks (EMNs). These are collaborative structures which go beyond joint research to increase the coordination of measurement science across Europe, addressing scientific and societal challenges, infrastructure and services in response to European and global metrology needs. Currently there are eleven EMNs: Advanced Manufacturing, Climate and Ocean Observation, Energy Gases, Mathematics and Statistics, Pollution Monitoring, Quantum Technologies, Radiation Protection, Safe and Sustainable Food, Smart Electricity Grids, Smart Specialisation in Northern Europe, and Traceability in Laboratory Medicine. Each EMN, by providing a single point of contact, aims at underpinning regulation and standardization by establishing a comprehensive and longer-term infrastructure, promoting best practice and disseminating knowledge in its respective fields. Further EMNs are in preparation or under consideration. More information on EMNs can be found at https://www.euramet.org/european-metrology-networks/.

Technical collaboration in EURAMET is organized within ten Technical Committees (TCs), focusing on specific areas which represent the forum for scientific and technical cooperation in the respective fields. In addition, two Committees deal with the overall topics Quality and Interdisciplinary Metrology. The TCs are responsible for the execution of the activities required by EURAMET as RMO for the fulfilment of the Mutual Recognition Arrangement of the International Committee of Weights and Measures (CIPM-MRA). The types of technical cooperation carried out within the TCs are: cooperation in research, comparison of measurement standards, metrological traceability, and consultation on facilities.

One of the ten TCs is devoted to Metrology in Chemistry (Technical Committee for Metrology in Chemistry, TC-MC), which is concerned with primary methods and reference materials for chemical measurements and research in metrology to support different sectors in the amount of substance fields.

NEWS FROM EURAMET TECHNICAL COMMITTEE IN METROLOGY IN CHEMISTRY (TC-MC)

TC-MC is chaired by Teemu Näykki (SYKE, FI) who took over from Sophie Vaslin-Reimann (LNE, France). 31 EURAMET member countries are represented in TC-MC plus the European Commission. BIPM has the status of observers.

The technical activities are carried out within the four technical Sub-committees dealing with gas analysis (SC-GA), inorganic analysis (SC-IA), electrochemical analysis (SC-EA), bio and organic analysis (SC-BOA). The convenors of the subcommittees are: Janneke van Wjik (VSL, NL) for SC-GA, Rainer Stosch (PTB, DE) for SC-IA, Mine Bilsel (UME, TR) for SC-BOA and Matilda Roziková (CMI, CZ) for SC-EA who took over from Daniela Stoica (LNE, FR). In addition, a strategy working group, chaired by the TC-Chair, is also active on the following tasks: advice to TC-Chair and subcommittee convenors, strategic planning of comparisons, support actions, coordination, organization of workshops.

The TC-MC members are actively participating in the European Programmes on Metrology, being involved in all the targeted programmes; in addition, they cooperate within various EMN, among which Climate and Ocean Observation, Energy Gases, Mathematics and Statistics, Pollution Monitoring, Safe and Sustainable Food, Traceability in Laboratory Medicine, thus indicating the cross-disciplinary nature of the TC itself.

TC-MC MEETING IN 2022

The annual meeting of the TC-MC was held online from 31st January to 2nd February 2022, due to the persistence of the emergency related

to Covid-19 pandemic. The first day was reserved for the Strategy WG meeting. Sophie Vaslin – Reimann (LNE) will end her second chairperson mandate in June 2022; Teemu Näykki (FMI – SYKE, FI) will officially take over during the next EURAMET GA.

The four technical subcommittees reconvened, as usual, ahead of the annual TC-MC plenary meeting on 1st February 2022. A review of new claims as well as the obligatory re-review of a range of existing claims were carried out. Running and new projects and comparisons in the framework of EURAMET and EMPIR and also proposals for the upcoming EMP call were discussed in detail in all sub-committees. Janneke Van Wijk (SC-GA) and Rainer Stosch (SC-IA) will end their mandate by the end of the year; the TC chair asked for their availability to remain in office for an additional mandate. The voting will be carried out within each SC.

On 1st February a specific workshop in preparation for the 2022 EMP call was held, with the presence of about 75 participants. The proposals addressed all the different targeted programmes, i.e. digital transformation, health, integrated European metrology, normative, with a particular focus on health, due also to the activities carried out within the various NMIs and DIs.

The plenary meeting took place on the 2nd February 2022. Some highlights on EURAMET, BIPM/CIPM, CCQM strategy and activities within its main working groups were given. The convenors of the subcommittees gave an overview of the activities of each subcommittee and of the main outcomes of the meetings carried out in the previous day. A section of the meeting was devoted to EMNs dealing with topics related to the amount of substance field dealing with topics related to the amount of substance field. An overview was given on the EMN for Climate and Ocean Observation (coordinated by NPL), EMN for Energy Gases (coordinated by VSL), EMN for Laboratory Medicine (coordinated by PTB). The following potential future EMNs were also presented: EMN for Environment (LNE) and EMN for Safe and Sustainable Food (INRIM).

TC-MC MEETING IN 2023

The annual meeting of the TC-MC was held in Paris, France, hosted by LNE online from 31st January to 2nd February 2023. It was the first meeting in presence, after three years of Covid-19 pandemic. The Strategy WG meeting had an online meeting on 27th January.

The four technical subcommittees reconvened, as usual, ahead of the annual TC-MC plenary meeting on 31st January 2023. A review of new claims as well as the obligatory re-review of a range of existing claims were carried out. Running and new projects and comparisons in the framework of EURAMET, EMPIR, EMP and also proposals for the upcoming EMP call were discussed in detail in all sub-committees.

The plenary meeting took place on 1st and 2nd February 2023. Some highlights on EURAMET, BIPM/CIPM, CCQM strategy and activities within its main working groups were given. The conveners of the subcommittees gave an overview of the activities of each subcommittee and of the main outcomes of the meetings carried out in the previous day. A section of the meeting was devoted to EMNs dealing with topics related to the amount of substance field. An overview was given on the EMN for Climate and Ocean Observation (coordinated by NPL), EMN for Energy Gases (coordinated by VSL), EMN for Laboratory Medicine (coordinated by LNE), EMN for Environment Pollution (coordinated by LNE) and EMN for Safe and Sustainable Food (coordinated by INRiM). On 1st February a specific workshop in preparation for the 2023 EMP call was held, addressing all the different targeted programmes.

The next TC-MC meeting will be held at the beginning of February 2024, hosted by VSL, Netherlands.

LIAISON REPORTS

IMEKO REPORT

Michela Sega // INRIM, Italy, IMEKO TC8 Chair

IMEKO, the International Measurement Confederation, founded in 1958, is a non-governmental federation of 42 Member Organizations individually concerned with the advancement of measurement technology. It has a consultative status with UNESCO and UNIDO. Its fundamental objectives are the promotion of international interchange of scientific and technical information in the field of measurement and instrumentation and the enhancement of international co-operation among scientists and engineers from research and industry. Prof. Frank Härtig (Germany) is the current President of IMEKO, Prof. Paolo Carbone (Italy) is the President Elect and Chair of the Technical Board, Prof. Masatoshi Ishikawa (Japan), as past President, is the Advisory President and Chair of the Advisory Board.

IMEKO Secretariat is located in Budapest (Hungary). More information about IMEKO and its structure can be found on the IMEKO website (www.imeko.org).

In 2022, due to the improvement to the Covid-19 pandemic, many IMEKO events were organized in hybrid form, including the Presidential Board and the General Council meetings. The IMEKO 2022 General Council Sessions took place on 27-28 August in Berlin, hosted by PTB. The hybrid mode organization allowed an excellent representation of the Technical Committees and Member Organisations with over 70 participants. IMBIH (Bosnia and Herzegovina) and EMI (United Arab Emirates), were warmly welcomed as new official members. 65 new members within IMEKO Technical Committees and 12 new TC officers were approved. The recommendations of the four working groups, i.e. "TC functioning", "TC events", "IMEKO publishing activity", "TB functioning", aiming at revising the existing IMEKO documents, were part of the Technical Board report. The working groups are continuing their activities. Some statistics on the continuously increasing success of the IMEKO Journals were presented.

In 2022, many TC events were organized, among which:

- TC4 Symposium 2022, 25th IMEKO TC4 Symposium and 23rd International Workshop on ADC and DAC Modelling and Testing (IWADC), Brescia, ITALY, 12 - 14 September 2022;
- M4Dconf2022, First International IMEKO TC6 Conference on Metrology and Digital Transformation, Berlin, GERMANY, 19 - 21 September 2022
- TC4 MetroArchaeo 2022, IMEKO TC4 International Conference on Metrology for Archaeology and Cultural Heritage, Cosenza, ITALY, 19 - 21 September 2022
- 24th TC3 Conference on the Measurement of Force, Mass and Torque, 14th TC5 Conference on the Measurement of Hardness, 6th TC16 Conference on Pressure and Vacuum Measurement, and 5th TC22 Conference on Vibration Measurement, Cavtat-Dubrovnik, CROATIA, 11 - 13 October 2022
- Joint IMEKO TC11 & TC24 hybrid conference, TC 11 Measurement for a better life, TC24 Chemical measurements towards a sustainable future, Dubrovnik, CROATIA, 16 - 20 October 2022

- 6th IMEKOFOODS Conference (HYBRID), Food on a global market – opportunities or threats, Dubrovnik, CROATIA, 07 - 09 November 2022

- TC 8 online workshop, Traceability the backbone of metrology, 8 November 2022.

The TCs can select best contributions to IMEKO events to be published, as enhanced versions of the corresponding papers, in Measurement, the official journal of IMEKO, after the events. Additional contributions to IMEKO events can be also published in the IMEKO Online Journal ACTA IMEKO, which published its four issues in 2022 (https://acta.imeko.org/index.php/acta-imeko). In addition, two more specific journals are also available: Measurement: Sensors, in line with the increasing demand for sensor-related publications and for open-access publishing model, and Measurement: Food, in line with the rapid growth of studies on food and nutrition measurements. The launch of a new journal Measurement: Energy is planned. Periodic newsletters are prepared by IMEKO Secretariat and can be accessed through IMEKO webpage.

The preparation for the XXIV IMEKO World Congress is ongoing. It will take place at the new Congress Center of Hamburg (Germany) on 26th-29th August 2024, hosted by PTB, the German Member Organization of IMEKO. More information and updates can be found on the dedicated website (https://www.imeko2024.org/).

LIAISON REPORTS

REPORT FROM ISO/REMCO

Angelique Botha // NMISA, South Africa, ISO/REMCO Chair

ANNUAL MEETING OF ISO/TC 334 I JUNE 2022

The third meeting of ISO/TC 334 was held as an on-line meeting during the second week of June 2022. A total of 79 participants joined the meeting with representatives from 43 member bodies (59% of the P-members) and for the first time also 3 O-members participated in the meeting. Representatives from 5 international organisations attended the meeting representing 38% of the external liaisons, but none of the internal ISO liaisons (other technical committees) attended the meeting. Currently, ISO/TC 334 has 12 internal (ISO) liaisons in force, 13 category A liaisons and 4 category C liaisons with external organisations and three liaisons managed at ISO level (JCGM/WG1 responsible for the Guide to the Expression of Uncertainty in Measurement (GUM), JCGM/WG2 responsible for the International Vocabulary for Metrology (VIM) and JCTLM responsible for measurement traceability in laboratory medicine).

Some specific liaison activities of ISO/TC 334 during 2022 included working with ISO/TC 212 (Clinical Laboratory testing and in vitro diagnostic test systems) on the revision of ISO 15193-5 for the requirements of RMs in clinical applications. In ISO/CASCO (the ISO Committee for Conformity Assessment), the systematic review of ISO 17034 on the competent production of reference materials was completed in 2022. During the systematic review, more comments on the standard were submitted by ISO/TC 334 members compared to their counterparts in ISO/CASCO. In consultation with ISO/TC 334, the decision was taken in ISO/CASCO to confirm ISO 17034 and to only consider the revision of ISO 17034 again when the new ISO 33400 series of standards for reference materials have been published. ISO/TC 334 members also provided input and comments on the revision of ISO 17043 for the competence of proficiency testing providers to ensure that materials used for proficiency testing meet the basic requirements of reference materials (RMs).

PROGRAM OF WORK OF ISO/TC 334

The program of work of ISO/TC 334 have now been updated based on the decisions taken at the third annual meeting of the committee and are listed below. The program includes the transformation of the existing ISO/REMCO Guides as well as the new work items of the committee that will also be transformed into international standards. ISO/TC 334 currently has eight (8) projects in hand for the development of the ISO 33400 series of standards. During the third meeting of the committee, it was noted that there was no immediate need to consider revision or transformation of the technical reports developed by the committee.

Figure 1 below depicts the relationships between the different documents previously developed by ISO/REMCO and currently being developed by ISO/TC 334.

- ISO/WD 33400 (previously ISO Guide 30) – Reference materials – Selected terms and definitions
- ISO/DIS 33401 (previously ISO Guide 31) – Reference materials – Contents of certificates, labels and accompanying documentation

- ISO/CD 33402 (previously ISO Guide 80) – Guidance for the in-house preparation of quality control materials (QCMs)
- ISO/DIS 33403 (previously ISO Guide 33) – Reference materials – Good practice in using reference materials
- ISO/DIS 33405 (previously ISO Guide 35) – Reference materials – Guidance for the characterization and assessment of homogeneity and stability
- ISO/DIS 33406 (previously WD/ISO Guide 85) – Guidance for the production of reference materials having one or more assigned qualitative property values
- ISO/DIS 33407 (previously WD/ISO Guide 86) – Guidance for the production of pure organic certified reference materials
- ISO/AWI 33408 (previously AWI/ISO Guide 87) – Guidance for 'pure' reference materials for metals and metalloids

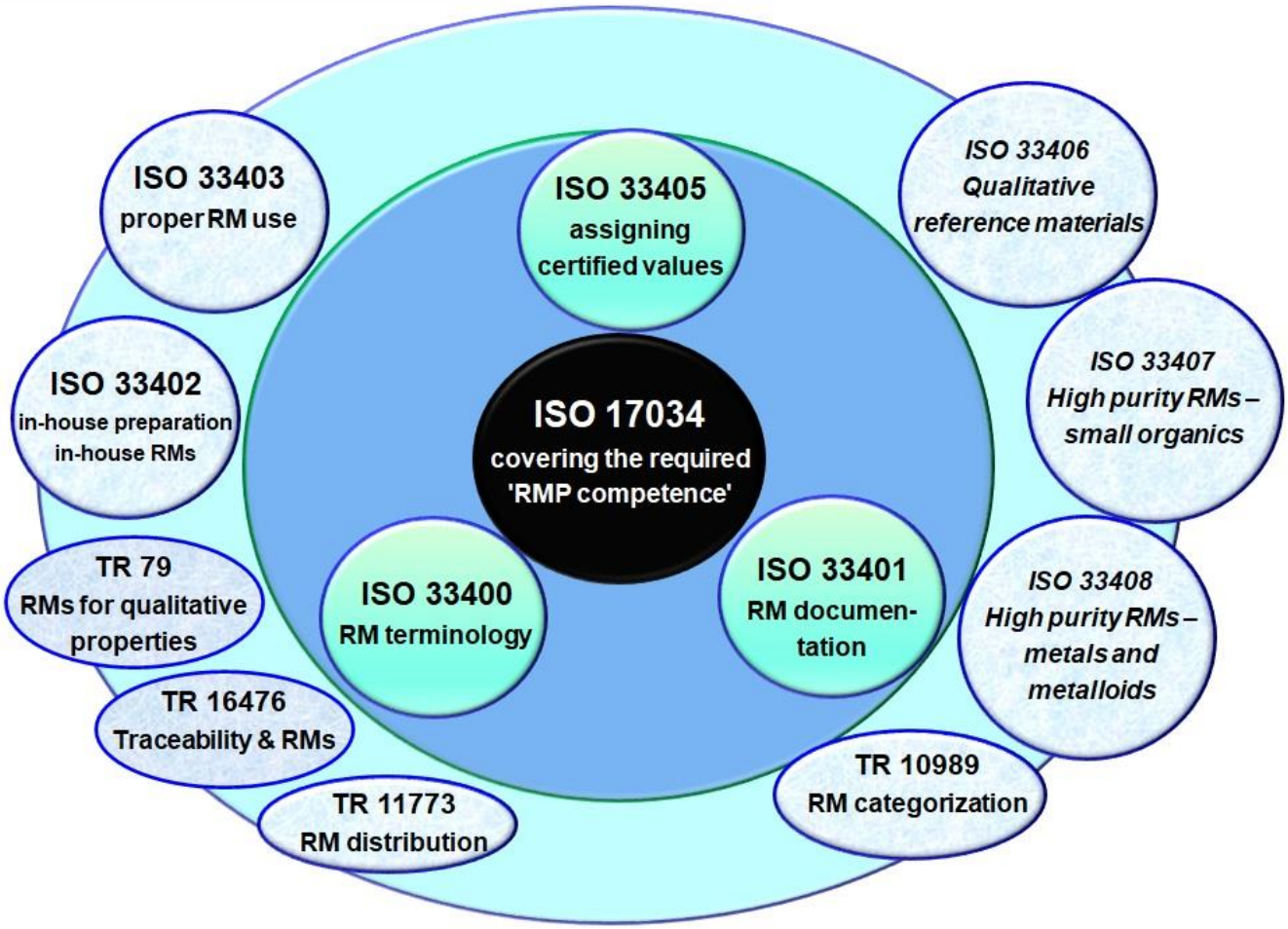


***Figure 2**: Schematic diagram of the planned ISO 33400 series standards for the transformation of the ISO/REMCO Guides 30 to 35 to international standards as well as the other projects of ISO/TC 334*

UPDATE ON THE PROGRESS WITH THE TRANSFORMATION OF THE ISO/REMCO GUIDES INTO THE ISO 33400 SERIES OF STANDARDS

The development of several of the new standards of the ISO 33400 series has progressed well and have recently been submitted for the draft international standard (DIS)-ballot. These include ISO 33401 on the accompanying documents for reference materials, ISO 33403 for guidance on good practice in the use of reference materials, ISO 33405 for the characterization of reference materials including the assessment of homogeneity and stability. The new standard ISO 33407 being developed for the production of high purity reference materials for organic molecules with a defined structure as well as ISO 33406 for the production of reference materials with qualitative properties have also advanced to the DIS-ballot stage.

ISO 33400 for the terms and definitions related to reference materials is still at the working draft (WD)-stage. Within the working group there has been some discussions about including new terms and definitions in the standard, such as the term operationally defined measurand. The strong liaison relationship between ISO/TC 334 and JCGM/WG2 working on the revision of the International Vocabulary for Metrology (VIM) also continues. There is also strong support in the working group to refer to a certified reference material as a reference material with one or more certified property value. The term certified value will then be defined to include all the required characteristics of such a value, including the associated reported uncertainty and established metrological traceability.

The drafting of ISO 33406 for the production of qualitative reference materials are also progressing well. Some decisions that was taken on the drafting of the document at the third ISO/TC 334 meeting included: the use of 'qualitative property' as superordinate term for 'nominal' and 'ordinal'; as well as 'categorical' as a synonym for 'qualitative' but the term 'categorical' is not used in the standard. No provisions of ISO 33405 will be repeated in ISO 33406; the standard will only contain the additional provisions required for qualitative RMs. The provision of uncertainty statements will be considered as optional for qualitative properties but guidance on the topic will be included in the standard. Content from the collection of examples in the technical report on reference materials with qualitative property values (TR 79) will be included in the new standard, where relevant. The committee draft (CD)-ballot for ISO 33406 was completed in the middle of 2022. The working group completed the discussions on the comments received during the CD-ballot in February 2023.

ISO 33408 for the production of high purity reference materials of metals and metalloids is at the working draft (WD)-stage. The working draft still needs more information on purity determination by indirect, rather than direct methods. The convenor of the working group, Dr Zoltan Mester, invited ISO/TC 334 members to nominate experts from commercial and industrial reference material producers to ensure wider representation and inputs from the community in the working group.

The next meeting of ISO/TC 334 will be a virtual meeting during the week of 5 to 9 June 2023.

Angelique Botha

ISO/TC 334 Chair

LIAISON REPORTS

IUPAC REPORT

Zoltan Mester // NRC, Canada, President of the IUPAC ACD

EVENTS OF INTEREST IN 2023-2025

1, IUPAC General Assembly and World Chemistry Congress, 2023 - IUPAC | CHAINS 2023 – Chains beyond the molecular frontier (iupac2023.org)

2, IUPAC Analytical Chemistry Award(s) nomination deadline – January 2025.

PROJECTS OF INTEREST

IUPAC GLOBAL WOMEN'S BREAKFAST "BREAKING BARRIERS IN SCIENCE"

On February 14, 2023 the IUPAC Global Women's Breakfast (#GWB2023) was held in conjunction with the U.N. Day of Women and Girls in Science. The goal of the GWB series is to establish an active network of people of all genders to overcome the barriers to gender equality in science.

The theme of #GWB2023 was "Breaking Barriers in Science". Groups from all types of science organizations from high schools, to science societies, universities, companies, governments and non-governmental organizations are invited to host events. GWB is also a flagship event of the International Year of Basic Sciences for Sustainable Development bringing together people from all science disciplines.

Look for announcement for #GWB2024

Global Women's Breakfast - IUPAC | International Union of Pure and Applied Chemistry

2019-001-2-100 - PREPARATION OF THE 5TH EDITION OF THE IUPAC GREEN BOOK

Review of Green Book content

The contents of the 4th Edition of the Green Book will be reviewed by the Task Group in consultation with the IUPAC divisions and committees, to identify which aspects should be retained (e.g. should all the data tables be retained), what areas need to be revised, enhanced or deleted, and which topics needed to be added (e.g. perhaps less emphasis on data tables, and more information on NMR, nanoscience, computational chemistry and simulations, non-equilibrium thermodynamics and statistical mechanics etc.)

We will also review the biophysical areas represented by Div I and generate such materials as needed to be included in the Green Book or as a supplement to the Green Book specifically Bio-Physical materials.

Digitally Native Book

We plan to carefully evaluate the methodology used with the preparation of the Portuguese version of the 3rd Edition which created an XML version of the Green Book and tested the software infrastructure to use this XML version to derive the print versions. This would in principle enable the production of more versatile Web based versions of the Green Book in addition to the printed book.

This would also facilitate semantically marked up content very suitable to link to the evolving Gold Book and provide and online resource to be used by others in generating correct text for other

publications which use the material in the Green Book (i.e. symbols and units).

This work links to the project supported by CPCDS on the Gold Book and work by CODATA & IUPAC on representation of Units.

2021-015-2-500 - GREENNESS OF OFFICIAL STANDARD METHODS

1. Evaluate the current status of greenness of the sample preparation methods used in official standard methods;

2. Provide metric tools to assess the greenness of sample preparation methods;

3. Proposing events and publications for up-to-date discussion related to the official standard methods based on their greenness degree;

4. Develop a roadmap for greener alternative analytical methods, emphasizing in sample preparation;

5. Contribute to the permanent establishment of a network of specialists as well as interested representatives and institutions involved in this topic to promote a common understanding of greenness degree;

6. Linking universities, industries, and governmental/non-governmental sectors to better approach relevant themes and contents in the topic.

2021-017-2-500 - HARMONIZATION OF APPROACHES TO INTERLABORATORY COMPARISON OF QUALITATIVE AND RELATED PROPERTY VALUES OF A SUBSTANCE OR MATERIAL

Qualitative property values of a substance or material are nominal values. A nominal property value is a word or alphanumerical code given for identification reasons, where the property (variable) has no magnitude (JCGM 200:2012 – VIM clause 1.30). Nominal variables are coded by exhaustive and disjoint classes or categories with no natural ordering. For example, imperfections of welds are coded by the following five classes/categories: cracks, cavities, inclusions, lack of fusion/penetration, and geometrical shape errors.

If a quantity has a clear ordering, then it is an 'ordinal quantity' (VIM clause 1.26). For example, the ordinal Mohs scale of mineral hardness is based on the ability of one mineral natural sample to scratch another: corundum (Al_2O_3) is harder than topaz ($Al_2SiO_4(OH^-,F^-)_2$), but diamond (C) is harder than corundum, etc. Such ordinal property values are categorical, as nominal data, but are not entirely qualitative. They are not quantitative also and could be named as semi-quantitative values. Moreover, some products are characterized by combined quantitative and qualitative property values. For example, the property values of dry sausages include mass fractions of fat, protein, moisture and salt (quantitative values), as well as color of the sausage cross section, smell and taste (qualitative values). A comprehensive (universal) scale of property values is necessary for comparison of complete test results of the sausage in different laboratories.

The problem of analysis of qualitative data is recognized by international groups, such as ISO TC 334 (former ISO/REMCO), ISO TC69 SC6 and Eurachem/CITAC WG, working on development of guidelines for different applications of metrological concepts to qualitative data. There are also publications on intensive development of statistical methods CATANOVA for nominal values and ORDANOVA for ordinal values, e.g., papers of Tamar Gadrich et al. https://doi.org/10.1007/s42452-020-03907-4 and https://doi.org/10.1016/j.jspi.2021.04.005, respectively. These methods are analogous to ANOVA (analysis of variance) for quantitative values.

IUPAC has contributed terminology efforts in this field, starting from Rene Dybkaer's "Ontology on Property" (https://ontology.iupac.org/ or https://doi.org/10.1351/978-87-990010-1-9), the IUPAC Silver Book (https://iupac.org/what-we-do/books/silverbook/) and Nominal Properties 2017 Recommendations (https://doi.org/10.1515/pac-2011-0613), and as a member organization of JCGM developing the forthcoming International Vocabulary of Metrology (VIM4).

Harmonization of approaches to interlaboratory comparisons of nominal and ordinal values, alone and together with quantitative values, will be helpful for characterization of examination methods and reference materials with qualitative and related properties, for proficiency testing of chemical laboratories involved in qualitative analysis, and will contribute to world-wide conformity assessment.

2019-039-3-500 - A REVIEW OF CURRENT STATUS OF ANALYTICAL CHEMISTRY EDUCATION.

There is plenty of anecdotal evidence for the erosion of analytical chemistry as a discipline. This is impacted by faculty appointments, funding structures and perception of the field as being a service function. Additionally, as instruments become easier to use there is a mistaken belief in some industrial organisations that there is a reduced need for highly trained analytical specialists. There have been warning signs that the current, university chemistry curriculum, often with a does not address the needs of chemistry graduates and future employers and does not enable analytical practitioners to maximise the value of their work. The project will reflect on the interdisciplinary curriculum development efforts which has been the trend in many universities worldwide. This is a significant economic cost, considering that in many economies the most used practical skills of graduates is actually related to chemical analysis. A deep and fundamental understanding of analytical chemistry is required to foster the next generation of analytical scientists who have the insight and capacity to contribute to fundamental new developments in this field as well as the generation of new disruptive technologies. The project will document the status quo in various regions of the world regarding the health of the discipline, proportion of professorships, funding and quality of analytical chemistry education. It will examine current attempts to address these shortcomings and offer some ways forward. The findings will be published in the form of white paper to support future curriculum development, funding and hiring decision.

2012-005-1-500 - VOCABULARY OF CONCEPTS AND TERMS IN ANALYTICAL CHEMISTRY

The revised Orange Book project. The Orange Book (present title "Compendium of Analytical Nomenclature" 3rd Edition) was published in 1998, and now is in the process of revision. The new Orange Book will be in a consistent glossary style format with definitions of concepts in different fields of analytical chemistry. The nineteen chapters of the 3rd edition will become eleven in the present revision. We have taken the decision to concentrate on methods and not attempt to venture into the ocean of applications. The first chapter will set the metrological scene with definitions from the Green Book, the International Vocabulary of Concepts and Associated Terms in Metrology (VIM) and selected chemometrics and statistical terms. The project is nearing completing, publication is expected in 2023.

https://doi.org/10.1039/9781788012881

2020. 2017-005-3-500 - ANALYTICAL CHEMISTRY OF NANOMATERIALS.

The impact of materials structured at the nanometer scale becomes enormous and continues to increase. Analytical chemistry of nanomaterials belongs to emerging issues in this field. Together with physical and physicochemical characterization of shape, size, and structure nanoparticles, analytical chemistry research considers isolation/purification and detection- CITAC News // April 2020 39 identification/ quantification/ spatial composition characterization of nanomaterials in bulk materials, special nanotechnology products, complex matrices of environmental, biological and food samples, and others. The project intends to produce a guidance document on best analytical chemistry practices for the characterization of such materials. 2016-007-1-500 Risks of conformity assessment of a multicomponent material or object in relation to measurement uncertainty of its test results. To develop an approach for evaluation of the probability of false decisions in conformity assessment of a multicomponent material or object in relation to measurement uncertainty of test (chemical analytical) results of a sample of the

material or object. This probability, combining probabilities of false decisions concerning different components of the material or object, will characterize the sample conformity as a whole. The solution to this problem is important for understanding conformity assessment risks in customs control, clinical analysis, pharmaceutical industry, environmental control, and other fields.

ANALYTICAL CHEMISTRY DIVISION

Division Details - IUPAC | International Union of Pure and Applied Chemistry

ANALYTICAL CHEMISTRY AWARDS

The Analytical Chemistry Division of IUPAC has established two awards, including:

– The Emerging Innovator Award in Analytical Chemistry – an award to recognize outstanding work undertaken by an emerging analytical scientist that corresponds to the aims of the Analytical Chemistry Division.

– The IUPAC Analytical Chemistry Medal – an award to recognize significant lifetime contribution to the aims of the Analytical Chemistry Division.

The awards are open worldwide to researchers working in the field of analytical chemistry. The Emerging Innovator Award is for researchers who are at an early stage of their independent career, as measured by the completion of a PhD within the last ten years. Appropriate consideration will be given to those who have taken a career break or followed a different study path. Nominations must be based on published works in the field of analytical chemistry. The Analytical Chemistry Medal is for researchers who have a substantial record of achievements demonstrated by the number and quality of their publications, by being actively involved in international partnerships as well as by their commitment in the training of the next generation of analytical chemists.

The Award will be presented every two years during the IUPAC General Assembly/World Chemistry Congress. The awardees will be invited to the meeting of the Analytical Chemistry Division to receive their award and to present a lecture.

Nomination package must include a letter of nomination and a curriculum vitae of the nominee. See specific details in the application forms.

IUPAC Awards in Analytical Chemistry – Call for nominations - IUPAC | International Union of Pure and Applied Chemistry

DIVISION MEMBERSHIP

As results of the 2021 election of Analytical Chemistry division membership the composition of the division for the 2022-2023 biennium is as follows:

Division President - David Shaw;

Division Past President - Zoltán Mester,

Division Secretary – Luisa Torsi

Division Vice President - Derek Craston,

Titular Members – Resat Apak; Vasilisa B. Baranovskaia; Jiri Barek; Ilya Kuselman; Takae Takeuchi; Susanne Kristina Wiedmer

Associate Members – Franziska Emmerling; Erico Marlon de Moraes Flores; Ivo Leito; Hongmei Li; Aura Tintaru ; Winfield Earle Waghorne

National Representatives - Maria Filomena Camoes, Orawon Chailapakul, Attila Felinger, D. Brynn Hibbert, Serigne Amadou Ndiaye, Mariela Pistón, Rufus H. Sha'Ato, Luisa Torsi, Frank Vanhaecke.

COUNCIL

The IUPAC Council will has met virtually as part of virtual World Chemistry Congress in August 2021. Next Council Meeting will take place, face to face in The Hague. Technical details and program is currently being developed to account for the virtual meeting. It is expected that large part of the IUPAC meetings will be publically accessible capitalizing on the remote conferencing features.

IUPAC ANALYTICAL CHEMISTRY PUBLICATIONS IN 2021

Westwood, Steven, Lippa, Katrice, Shimuzu, Yoshitaka, Lalerle, Beatrice, Saito, Takeshi, Duewer, David, Dai, Xinhua, Davies, Stephen, Ricci, Marina, Baldan, Annarita, Lang, Brian, Sarge, Stefan, Wang, Haifeng, Pratt, Ken, Josephs, Ralf, Mariassy, Mikael, Pfeifer, Dietmar, Warren, John, Bremser, Wolfram, Ellison, Stephen, Toman, Blaza, Nelson, Michael, Huang, Ting, Fajgelj, Ales, Gören, Ahmet, Mackay, Lindsey and Wielgosz, Robert. "Methods for the SI-traceable value assignment of the purity of organic compounds (IUPAC Technical Report)" Pure and Applied Chemistry, vol. 95, no. 1, 2023, pp. 1-77. https://doi.org/10.1515/pac-2020-0804

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Villa, Igor M., Holden, Norman E., Possolo, Antonio, Ickert, Ryan Ben, Hibbert, David Brynn, Renne, Paul R., Bonardi, Mauro L. and De Bièvre, Paul. "IUGS–IUPAC recommendations and status reports on the half-lives of 87Rb, 146Sm, 147Sm, 234U, 235U, and 238U (IUPAC Technical Report)" Pure and Applied Chemistry, vol. 94, no. 9, 2022, pp. 1085-1092. https://doi.org/10.1515/pac-2021-1202

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Apak, Reşat, Calokerinos, Antony, Gorinstein, Shela, Segundo, Marcela Alves, Hibbert, David Brynn, Gülçin, İlhami, Demirci Çekiç, Sema, Güçlü, Kubilay, Özyürek, Mustafa, Çelik, Saliha Esin, Magalhães, Luís M. and Arancibia-Avila, Patricia. "Methods to evaluate the scavenging activity of antioxidants toward reactive oxygen and nitrogen species (IUPAC Technical Report)" Pure and Applied Chemistry, vol. 94, no. 1, 2022, pp. 87-144. https://doi.org/10.1515/pac-2020-0902

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Strömert, Philip, Hunold, Johannes, Castro, André, Neumann, Steffen and Koepler, Oliver. "Ontologies4Chem: the landscape of ontologies in chemistry" Pure and Applied Chemistry, vol. 94, no. 6, 2022, pp. 605-622. https://doi.org/10.1515/pac-2021-2007

CITAC BEST PAPER AWARD 2022

SUMMARY OF "ABSOLUTE QUANTIFICATION OF TOTAL HAEMOGLOBIN IN WHOLE BLOOD BY HPLC ISOTOPE DILUTION INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY"

Mengyun Pan, Yanli Lu, Liuxing Feng, Xirui Zhou, Jinping Xiong, Hongmei Li

SUMMARY OF "PRIMARY MEASUREMENT OF GASEOUS ELEMENTAL MERCURY CONCENTRATION WITH A DYNAMIC RANGE OF SIX DECADES''

Abneesh Srivastava, Joseph T. Hodg

CITAC BEST PAPER AWARD 2022

SUMMARY OF "ABSOLUTE QUANTIFICATION OF TOTAL HAEMOGLOBIN IN WHOLE BLOOD BY HPLC ISOTOPE DILUTION INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY"

Analytical Chemistry. 2022, 94, 11753−11759

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INTRODUCTION

Hemoglobin (HGB) is a Fe-containing protein responsible for oxygen transport in vertebrates, which consists of four isoforms, each contains 4 iron atoms and 8 sulfur atoms. HGB is an important bio-maker,[1-3] and accurate determination of HGB could provide very important clinical information in clinical laboratory.[4] For total HGB measurement, the International Committee for Standardization in Haematology (ICSH) has recommended a reference method which was based on the photometric determination of cyanmet haemoglobin (HiCN method).[5] However, because the calibration is based on a reference preparation which is specified by WHO but not linked to a SI-traceable pure protein standard, its results can't be traceable to International System of Units (SI).[6] Moreover, highly toxic potassium cyanide need to be used for derivatization and stabilization in the HiCN method. Several emerging approaches, including cell tracking velocimetry,[7] biocatalytic precipitation atom transfer radical polymerization,[8] and microfluidic-based integrated solutions[9] for HGB detection have been proposed, and the results would be more reliable provided that the methods were validated by SI-traceable high order reference procedure. HGB molecular contains 4 iron atoms and 8 sulfur atoms, so it is possible to develop a HPLC isotope dilution Inductively coupled plasma mass spectrometry (HPLC ID-ICP-MS) method for HGB determination.

In this study, we proposed an absolute quantitative strategy for total HGB in whole blood sample based on the determination of natural Fe and S by HPLC ID-ICP-MS. And transferrin (Tf), another Fe-containing biomarker in whole blood, was also simultaneous quantified by adjusting the flow rate of ^{54}Fe spike. The HPLC-ID-ICP-MS approach showed good correlation with the traditional HiCN method in the assays of 21 whole blood specimens. This proposed strategy does not require toxic reagent and is less influenced by different haemoglobin forms, which has the potential to be a SI-traceable high order reference procedure in clinical assay.

EXPERIMENTAL SECTION

HPLC-ID-ICP-MS Procedure. HGB and its protein impurities were separated by size exclusion chromatography (SEC). The peak of target proteins were identified by retention time matching with their corresponding standard proteins. In the online HPLC-ID-ICP-MS approach, the enriched isotope solution was continuously introduced to the eluate from the outlet of the SEC column through a Y-formed three-way connection. To realize simultaneous quantification of Tf and HGB by determining Fe, the flow rate of 54Fe spike solution was adjusted over the elution time in consideration of the significant Fe difference in Tf and HGB. The procedure via S is similar to that of Fe, except that it's not necessary to change the flow rate of 34S spike solution.

Method Validation and Comparison. For accuracy control, a CRM of IRMM/IFCC-467 was used for method validation. Moreover, for method comparison, the proposed HPLC-ID-ICP-MS assay was performed on 21 blinded whole blood specimens that were tested with HiCN method.7 Linear regression model of the HPLC-ID-ICP-MS and HiCN results were employed to investigate the correlation between the two approaches.

RESULTS AND DISCUSSION

Quantification of Total HGB and Tf in Whole Blood via Iron. The HPLC-ID-ICP-MS mass spectrum of Tf and HGB in whole blood was shown in **Figure 1**. The flow rate of the post-column ^{54}Fe spike was adjusted to achieve optimal $^{56}Fe/^{54}Fe$ ratio of the protein peak. The flow rate of ^{54}Fe spike solution was set at 0.05 mL min^{-1} in the first 24 min to fit for the Fe concentration in Tf, and adjusted to 0.4 mL min^{-1} to fit for the significant different HGB iron concentration. In **Figure 1A**, the signals of 54Fe quickly changed and achieved stability after the flow rate was altered. **Figure 1B** showed the ratio of $^{56}Fe/^{54}Fe$ obtained from integration of the intensities of ^{56}Fe and ^{54}Fe. According to IDMS equation and the iron stoichiometry in HGB and Tf, the concentrations of the two proteins in whole blood could be calculated.

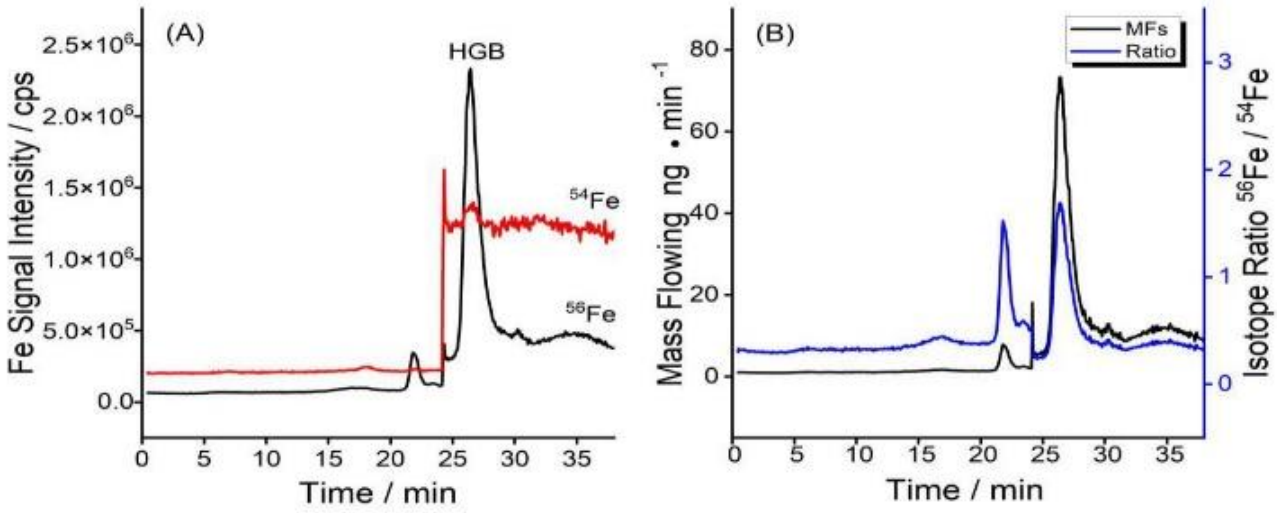

Figure 1. Mass spectrum of Fe of whole blood sample. (A) Fe intensity in HPLC-ID-ICP-MS. (B) Mass flow chromatogram of iron and $^{56}Fe/^{54}Fe$.

Quantification of Total HGB in Whole Blood via Sulfur. Figure 2A showed the sulfur mass spectrum of the whole blood sample, and the flow rate of the 34S spike solution flow speed need not change. In **Figure 2A**, the peak of sulfur at the retention time of 22 min was much higher than that of the iron mass spectrum (**Figure 1A**). It was inferred that other sulfur-containing proteins and Tf overlapped each other in the SEC chromatogram, which may be derived from Alb. Because the molecular weight of Tf was similar with that of Alb, the retention time of them were

very close and the two proteins could not be fully separated with the present SEC condition. As a result, the Tf could not be simulteneously quantified by this HPLC-ID-ICP-MS method via the determination of sulfur with SEC. In order to figure out this problem, we used the ion exchange column (IEC) to separate the HGB, Tf, Alb standard proteins and the whole blood sample. The Fe and S mass spectrum of HPLC-ICP-MS (IEC) in **Figure 3** confirmed the sulfur contribution at 22 min (**Figure 2A**) was mainly from Alb.

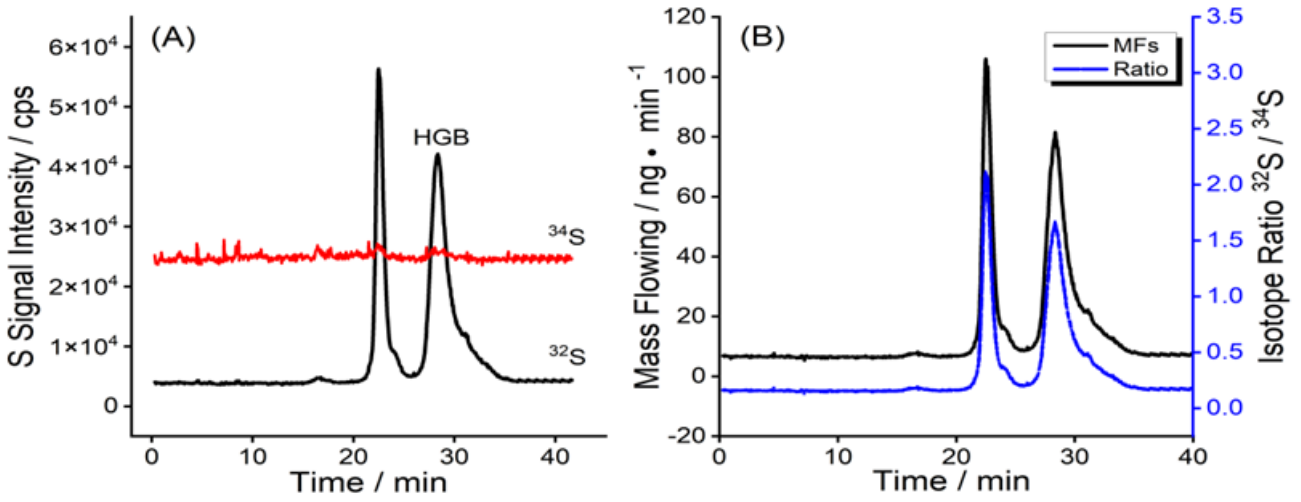

Figure 2. Mass spectrum of of S of whole blood. (A) S intensity in HPLC-ID-ICP-MS. (B) Mass flow chromatogram of sulfur and ^{32}S/^{34}S.

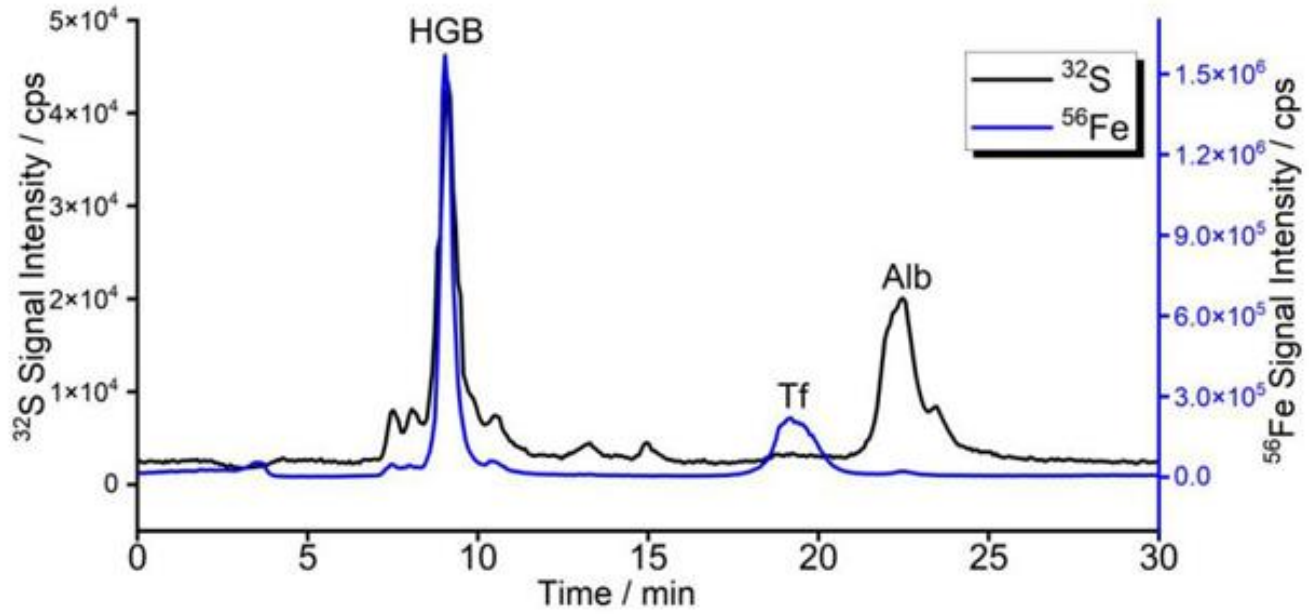

Figure 3. Mass spectrum of HGB in whole blood using online HPLC-ICP-M (IEC).

The measurable range for HGB via Fe and S were 10.0-240.0 g L^{-1}. The limits of detection (LOD) via Fe and S were 0.01 g L^{-1} and 0.07 g L^{-1}, respectively. The intraassay and interassay CVs were 0.89%-1.35% and 1.19%-2.15% via Fe. The intraassay and interassay CV was 0.99%-1.56% and 1.55%-2.55% via S.

Method Validation and Comparison. IRMM/IFCC-467, isolated from whole blood and certified by ICSH reference procedure (HiCN method), was used for method validation. The measured concentration and standard deviation (SD) of IRMM/IFCC-467 was 117.6 ± 0.7 g L^{-1} calculated via iron and 119.2 ± 1.1 g L^{-1} via sulfur, which were in good agreement with the certified value (119.7 ± 3.7 g L^{-1}). In the method comparison in **Figure 4**, significant correlations were also observed between the total HGB in whole blood measured using the HPLC-ID-ICP-MS and HiCN method. The regression equation via S was: y=0.9323x+9.1845 (r2=0.9697), and that via Fe was: y=0.9320x+5.1377 (r2=0.9909).

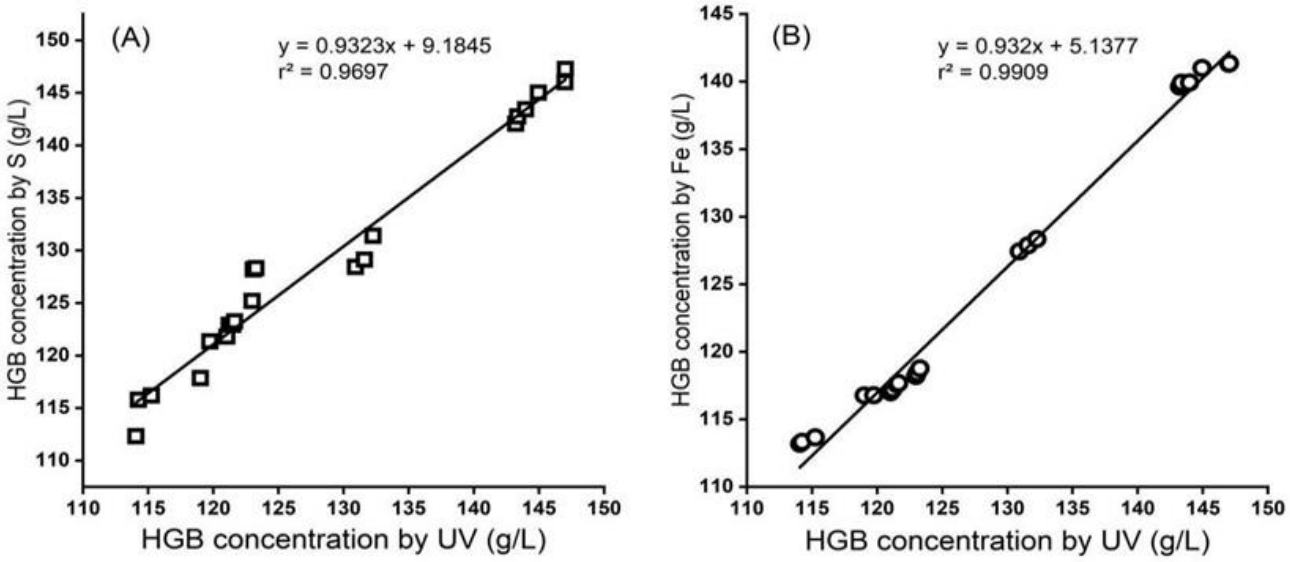

Figure 4. Relationship between HiCN method and HPLC-ID-ICP-MS. (A) via S; (B) via Fe for HGB in whole blood sample.

CONCLUSIONS

Reference measurement methods for HGB traceable to SI are very important in clinical diagnosis. In this study, a potential reference procedure for total HGB in whole blood by HPLC-ID-ICP-MS was conducted by determining iron and sulfur respectively. HGB and Tf in whole blood were absolutely quantified simultaneously in one elution procedure. The results via Fe and S were in good agreement, and the ICP-MS assay showed good correlation with the HiCN-based assay. This isotope dilution ICP-MS based strategy has enormous potential to serve as reference measurement procedure for total HGB and its variants in whole blood, which could be traceable to SI, and does not require toxic derivation reagent. Furthermore, this strategy can also be used for the quantitative analysis of other sulfur or iron-containing proteins in clinical area.

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CITAC BEST PAPER AWARD 2022

SUMMARY OF "PRIMARY MEASUREMENT OF GASEOUS ELEMENTAL MERCURY CONCENTRATION WITH A DYNAMIC RANGE OF SIX DECADES"

Analytical Chemistry 2022 94 (45), 15818-15826

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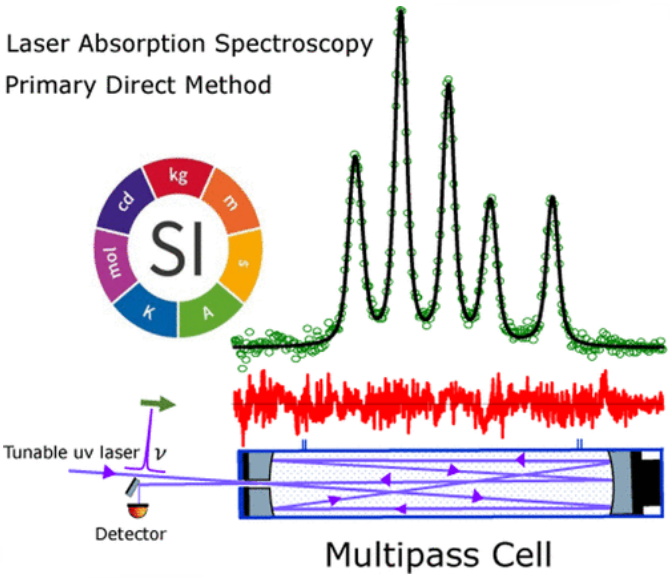
SUMMARY

The reduction of anthropogenic mercury emissions is a global effort, garnering commitment from nearly 137 countries in the 2017 Minamata convention. In the US the EPA-mandated Mercury and Air Toxics Standards regulates industrial emissions, thereby driving the requirement for accurate measurements of mercury. To establish industry compliance the National Institute of Standards and Technology (NIST) developed an SI-traceable certification program for vendor Hg-in-air generators, which are in turn used for certification of continuous emission monitoring systems in the field. Historically, in this program the mercury emitted by a NIST prime Hg generator was value-assigned on the SI using an SRM 3133® Hg standard combined with isotope dilution cold vapor inductively coupled mass spectrometry measurements. To circumvent issues related to throughput, sample processing, and dependence on a reference material, Srivastava and Hodges (2018) applied a linear laser absorption spectroscopy (LAS) method to measure the absolute number density of gaseous elemental mercury (GEM). With this approach, light absorption is described by the Beer-Lambert law and modelled in terms of the intrinsic atomic parameters of mercury and physical observables to obtain the analyte number density.



In this work, we describe a dual-cell approach to achieve a measurement range spanning six decades from 1 ng m-3 (representative of ambient levels) to an upper bound of 1000 gm-3 (representative of high anthropogenic source emission levels). The resulting relative standard uncertainties are 0.5% across the mass concentration range 0.25 μg m−3 to 1000 μg m−3. We present the spectroscopic model and

uncertainty analysis which are required for a primary direct measurement method. We also describe the multipass cell part of the dual cell (added in this study) and report high-precision measurements of pressure-broadening and -shifting parameters for air-broadened Hg lines required for enabling accurate spectroscopic retrievals of mass concentrations over a wide pressure range. We include assessments of the performance limits of the system, including spectrum fit quality, limits of detection, and residual bias in the integrated spectrum area. We conclude with LAS measurements of GEM in air produced by a commercial system commonly used as a transfer standard for emissions monitoring applications, and we discuss plans for a next-generation LAS system.

CITAC BEST PAPER AWARD 2022

SUMMARY OF "AN SI-TRACEABLE REFERENCE MATERIAL FOR VIRUS-LIKE PARTICLES"

iScience 25 (2022) 104294

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SUMMARY

A reference material for virus-like particles traceable to the International System of Units (Syste` me International d'Unite´ s – the SI) is reported. The material addresses the need for developing reference standards to benchmark virus-like gene delivery systems and help harmonize measurement approaches for characterization and testing. The material is a major component of synthetic polypeptide virus-like particles produced by the state-of-the-art synthetic and analytical chemistry methods used to generate gene delivery systems. The purity profile of the material is evaluated to the highest metrological order demonstrating traceability to the SI. The material adds to the emerging toolkit of reference standards for quantitative biology currently being developed at the National Physical laboratory, UK.

Virus-like particles (VLPs) are important tools for applications ranging from gene therapy and vaccine development to virus diagnostics. Of increasing interest are synthetic VLPs, which assemble from well characterized polypeptides, and demonstrate a proven ability to deliver the cargo of interest into human cells without cytotoxicity or a pathogenic bias. The interest is compounded by the need for SI-traceable reference materials based on VLPs to benchmark the performance of commercial products and technologies. Here we present the compositional analysis of a VLP constituent, C3-hub peptide, which was characterized using the mass balance method.

Karl Fischer (KF) titration was used to determine water content, whereas ion chromatography (IC) and fluorine qNMR (19F qNMR) were used to assign the values for trifluoroacetic acid (TFA) as the solid material is a salt with TFA as the counter-ion. In addition, elemental analysis confirmed the identity and amounts of the major elements present in the material. The sequence of the triskelion C3-hub arm was confirmed, and as peptide impurities in the highly charged peptide could not be separated chromatographically, these were identified as impurities by their mass to charge ratio and quantified by relative response to main component using the Thermo Fischer LTQ Orbitrap. The work continues into the field of biology, where methods are being optimised so that post-transfected samples can be analysed and quantified by LCMS.

ABOUT CITAC

CITAC – Cooperation on International Traceability in Analytical Chemistry – arose out of an international workshop held in association with the Pittsburgh Conference in Atlanta in March 1995. The aim of this workshop was to discuss how analytical activities could be developed to meet the needs of the 21st century, and it identified a wide variety of issues to be addressed to ensure that analytical measurements made in different countries or at different times are comparable. These range from the development of traceable reference materials and methods to the harmonisation of analytical quality practices.

The CITAC initiative aims to foster collaboration between existing organisation to improve the international comparability of chemical measurement. A Working Group takes matters forward and its initial activities have centred on a few specific high priority activities. The first tasks included the compilation of a directory of certified reference materials under development; preparation of quality system guidelines for the production of reference materials; preparation of a directory of international chemical metrology activities; defining criteria for establishing traceability to the mole; and the preparation of an international guide to quality in analytical chemistry.

Many of these activities are of a strategic nature, laying the ground for the improvement of international analytical measurement. This reflects the added geographical complexities associated with a world-wide organisation, such as greater diversity in culture and in technical approach, and frequently long timescales associated with its activities. Nevertheless, if the full benefits of improved analytical measurement are to be realised internationally, a truly global approach is needed, and there is a clear role for CITAC to play in this respect.

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