



Online Workshop

Assessment of Performance & Uncertainty in Qualitative Chemical Analysis

January 2022

ORGANISERS



Session 1



Terminology and Content of the Eurachem/CITAC Guide

Date: 19 January 2022

Time: 07:00 to 10:00 UTC

Abstract

The first session of the workshop starts with an introduction of terminology for the management of qualitative analysis reliability. Afterwards, the content of the Eurachem/CITAC Guide "Assessment of Performance and Uncertainty in Qualitative Chemical Analysis" is presented and discussed. Selected examples from the Guide will be explained to aid the audience in its implementation. Questions and comments from the audience will be addressed to the Speakers.

References

1. G. Nordin, R. Dybkaer, U. Forsum, X. Fuentes-Arderiu, F. Pontet, "Vocabulary on nominal property, examination, and related concepts for clinical laboratory sciences (IFCC-IUPAC Recommendations 2017)", *Pure Appl. Chem.* 90 (2018) 913–935.
2. Eurachem/CITAC guide on "Assessment of performance and uncertainty in qualitative chemical analysis"
(<https://www.eurachem.org/index.php/publications/guides/performance-and-uncertainty-in-qualitative-analysis>)

Talks & Speakers' Information



The VIM4 approach to nominal properties

Dr Gunnar Nordin



Topic 1: Objective, structure and background of the EURACHEM/CITAC Guide

Topic 2: Application examples of the Guide to the identification of compounds by GC-MS

Dr Ricardo Bettencourt da Silva



Topic 1: Expressions of confidence in qualitative analysis

Topic 2: Application example of the Guide to enzyme multiplied immunoassay technique

Dr Stephen R. Ellison

Session 2



Qualitative Chemical Analysis

Date: 20 January 2022

Time: 07:00 to 10:00 UTC

Abstract

At the second session of the workshop, the Speakers will present three talks covering examples on quantification and reporting of qualitative analysis performance and uncertainty in different fields of chemical analysis. The examples include assessing chance match probabilities when compounds are identified using IR spectroscopy and identifying microplastics in sediments using ATR-FTIR.

The Bayesian approach to obtain overall probabilities for situations with multiple qualitative inputs will be explained using examples with different hydrocarbons measured in a contaminated environment. In this example, the combination of information to determine from which of a number of candidate sources the spill is most likely to have come will be demonstrated.

At the end of the three talks, a panel discussion is organised to reinforce the audiences' understanding on the advantages of quantifying the performance of qualitative chemical analysis, as well as to address challenges encountered. Questions and comments from the audience will be addressed to the Speakers.

Talks & Speakers' Information



Identification of compounds using IR spectroscopy - Assessing infrared chance match probabilities

Dr Stephen R. Ellison



Identification of microplastics in sediments by ATR-FTIR

Dr Ricardo Bettencourt da Silva



Environmental spills – Assessing uncertainty of decisions of source of pollution based on combined data

Emeritus Professor Brynn Hibbert

Session 3



Qualitative Forensic Analysis

Date: 24 January 2022

Time: 07:00 to 10:00 UTC

Abstract

At the third session of the workshop, the speakers will present different viewpoints related to the topic of forensic reporting.

Professor Gary Edmond will provide the audience with a basic introduction to the terms in which legal systems, through especially common law systems, engage with scientific knowledge. The talk will explain what is required of experts, by way of evidence, if legal processes and decision-making are to fulfil their primary aim of doing justice in the pursuit of truth.

Emeritus Professor Brynn Hibbert will review two murder investigations in which likelihood ratios were relevant to the outcome of the case.

Dr. Michael Coble will discuss the evolution and use of statistics for conveying DNA results in forensic cases. The use of statistics in DNA reports has widespread acceptance in courtrooms but continues to evolve as additional data is collected.

And lastly Agnes Winokur will discuss the current status of consensus-based standard development efforts in statistical reporting for qualitative seized drug analysis. While Seized Drugs typically uses statistical evaluations for sampling and quantitative measurements, it is a newer approach for qualitative analysis. Ms. Winokur will discuss the challenges that drive the data gathering stage and lessons learned.

Talks & Speakers' Information



Validation and Accreditation

Melissa Kennedy, M.S.



Helping with fact-finding: What courts need from scientific experts (and why)

Professor Gary Edmond



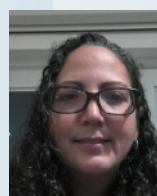
Statistics of chemical matching in two murder cases – likelihood ratios may not tell the whole story

Emeritus Professor Brynn Hibbert



The evolution and use of statistics providing the strength of evidence in forensic DNA cases

Dr Michael Coble



Challenges associated with statistical reporting in qualitative seized drug analysis

Agnes D. Winokur, M.S.

Session 4



Qualitative Analysis in Laboratory Medicine

Date: 27 January 2022

Time: 07:00 to 10:00 UTC

Abstract

At the fourth session of the workshop, practical cases and topics critical for measuring the trueness and uncertainty of binary results in medical laboratories will be presented.

A measurement uncertainty program for qualitative tests using quality control data is presented. Further, topics on traceability and validation of qualitative results in the medical laboratory will be covered.

References

1. King B. The practical realization of the traceability of chemical measurements standards. *Accredit Qual Assur.* 2000;5(10-11):429-36.
2. Armbruster D. Metrological Traceability of Assays and Comparability of Patient Test Results. *Clinics in laboratory medicine.* 2017;37(1):119-135.
3. Sturgeon C, Butler SA, Gould F, Johnson S, Rowlands S, Stenman UH, et al. Recommendations for validation testing of home pregnancy tests (HPTs) in Europe. *Clinical Chemistry and Laboratory Medicine* 2021;59(5):823-835
4. P. Pereira, Quality control of qualitative tests for medical laboratories, Lisbon: Author-edition, 2019.
5. P. Pereira, B. Magnusson, E. Theodorsson, J. O. Westgard and P. Encarnação, "Measurement uncertainty as a tool for evaluating the 'grey zone' to reduce the false negatives in immunochemical screening of blood donors for infectious diseases," *Accred. Qual. Assur.* 2016;21:25-32.

Talks & Speakers' Information



Traceability in qualitative analysis

Professor Elvar Theodorsson



Assessment of performance and uncertainty in qualitative tests in the medical laboratory

Dr Paulo Pereira



An overview of a national Uncertainty of Measurement programme for infectious disease testing using quality control data

Wayne Dimech

Speakers' Profile



Dr Gunnar Nordin

- Senior Advisor at EQUALIS AB, Sweden
- Member of Joint Committee for Guides in Metrology Working Group on the International Vocabulary on Metrology
- Author of International Union of Pure and Applied Chemistry (IUPAC)'s Vocabulary For Nominal Properties And Nominal Examinations — Basic And General Concepts and Associated Terms



Dr Ricardo Bettencourt da Silva

- Researcher at University of Lisbon, Portugal
- Secretary of Cooperation on International Traceability in Analytical Chemistry (CITAC)
- Co-Editor of the EURACHEM/CITAC Guide "Assessment of Performance and Uncertainty in Qualitative Chemical Analysis"
- Chair of EURACHEM's Qualitative Analysis Working Group



Dr Stephen R. Ellison

- Science Fellow, LGC Limited, United Kingdom
- Co-Editor of the EURACHEM/CITAC Guide "Assessment of Performance and Uncertainty in Qualitative Chemical Analysis"
- Secretary of EURACHEM's Qualitative Analysis Working Group
- Member, CITAC



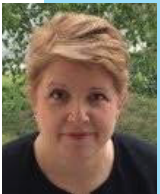
Emeritus Professor Brynn Hibbert

- Emeritus Professor, University of New South Wales (UNSW), Australia
- Member of the Order of Australia (AM) for "significant service to science in the discipline of chemistry, to professional societies, and to sport through illicit drug profiling"
- Secretary of the Interdivisional Committee for Terminology, Nomenclature and Symbols of IUPAC
- Past Chair of the IUPAC Analytical Division
- Past Chair of the Analytical Division of the Royal Australian Chemical Institute - Past President of the Royal Society of New South Wales



Professor Gary Edmond

• *Law Professor, Faculty of Law and Justice, UNSW Sydney, Australia*



Melissa Kennedy, M.S.

• *Director of Accreditation, ANSI National Accreditation Board/ANAB, United States*



Professor Elvar Theodorsson

• *Professor, Department of Biomedical and Clinical Sciences, Linköping University, Sweden*

• *Member, EURACHEM*

• *Chair, Working Group for Traceability Education and Promotion, Joint Committee for Traceability in Laboratory Medicine (JCTLM)*



Dr Paulo Pereira

• *Senior Postdoc Researcher, Coordinator of R&D Department, Portuguese Institute of Blood and Transplantation, Lisbon, Portugal*

• *Member of EURACHEM's Qualitative Analysis Working Group*



Wayne Dimech

• *General Manager, National Serology Reference Laboratory, Australia*

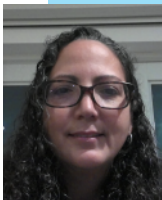
• *Fellow, Royal College of Pathologists of Australasia*

• *Fellow, Australian Institute of Medical Scientists*



Dr Michael Coble

- Associate Professor and the Associate Director of the Center for Human Identification, University of North Texas Health Science Center in Fort Worth, Texas
- Fellow, American Academy of Forensic Sciences
- Member, International Society for Forensic Genetics
- Commissioner, Texas Forensic Science Commission
- Member, North Carolina Forensic Science Advisory Board
- Invited guest, Scientific Working Group on DNA Analysis Methods (SWGDM)
- Co-editor of the Forensic Biology subject area of WIREs Forensic Science journal and is a member of the editorial board of Forensic Science International: Genetics and The Journal of Forensic Sciences.



Agnes D. Winokur, M.S.

- Associate Laboratory Director, Drug Enforcement Administration (DEA)
- Chair, National Institute of Standards and Technology (NIST) Organization of Scientific Area Committees for Forensic Science (OSAC) Seized Drugs Sub-committee
- Member, International Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG)
- Member, American Academy of Forensic Sciences and Chair of the Academy's Opioids and Emerging Drugs Ad-Hoc Committee
- Vice-chair and technical contact for numerous forensic drug related standards at the ASTM International E30 Forensic Sciences Committee

Facilitator's Profile



Dr Teo Tang Lin

- Division Director, Chemical Metrology Division, Health Sciences Authority, Singapore
- Member, CITAC



For enquiries, please send us your email at: hsa_cml@hsa.gov.sg