



Online Workshop

# Assessment of Performance & Uncertainty in Qualitative Chemical Analysis

January 2022

ORGANISERS



**CITAC**  
Cooperation in International  
Traceability in Analytical Chemistry



**Eurachem**  
A focus for analytical chemistry in Europe



**HSA**  
Health Sciences Authority

# IMPORTANT INFORMATION

## REGISTRATION FOR WORKSHOP SESSIONS 1 TO 4

The registration is separate for each session and you may register for more than one session. You are kindly advised to register and sign-in early to secure your place for the workshop.

### Session 1: Terminology and Content of the Eurachem/CITAC Guide

[Click here to register](#)



### Session 2: Qualitative Chemical Analysis

[Click here to register](#)



### Session 3: Qualitative Forensic Analysis

[Click here to register](#)



### Session 4: Qualitative Analysis in Laboratory Medicine

[Click here to register](#)



## PRE-WORKSHOP ENGAGEMENT WITH PARTICIPANTS

The Speakers would like to invite you to post your questions in Pigeonhole before the event. You may cast your votes on questions posted by others in Pigeonhole if these interest you.

You may also post your questions live using the chatbox during the workshop.

The Pigeonhole closes on **5 January 2022**.

<https://pigeonhole.at/QUALI>



## 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.

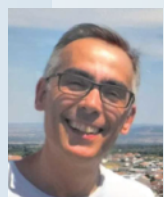
At the end of the three talks, a panel discussion is organised to reinforce the audiences' understanding on the advantages of quantifying the performance of qualitative chemical analysis, as well as to address challenges encountered. Questions and comments from the audience will be addressed to the Speakers.

### 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.

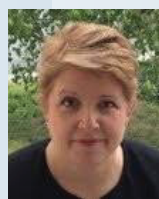
Professor Gary Edmond will provide the audience with a basic introduction to the terms in which legal systems, through especially common law systems, engage with scientific knowledge. The talk will explain what is required of experts, by way of evidence, if legal processes and decision-making are to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



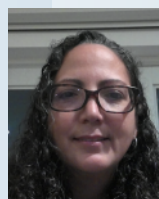
### Statistics of chemical matching in two murder cases – likelihood ratios may not tell the whole story

*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.*



# 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



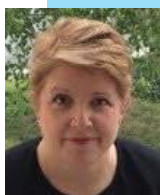
## **Emeritus Professor Brynn Hibbert**

- 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**

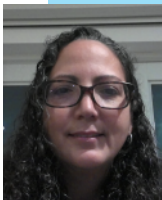
- *General Manager, National Serology Reference Laboratory, Australia*
- *Fellow, Royal College of Pathologists of Australasia*
- *Fellow, Australian Institute of Medical Scientists*





### **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](mailto:hsa_cml@hsa.gov.sg)