Eurachem
Dublin 2018

Eurachem Scientific Workshop

Data - Quality, Analysis and Integrity

14th & 15th May 2018
Dublin Castle, Ireland

DELEGATE NAME

The State Laboratory
An tSaotharlann Stáit

Supported by

DCU

ROYAL SOCIETY OF CHEMISTRY | ANALYTICAL DIVISION

ANALYTICAL CHEMISTRY TRUST FUND

Science Foundation Ireland sfi For what's next

Gold Sponsors

Agilent

quo data *QUALITY & STATISTICS!

Silver Sponsors

Anton Paar

BIPEA

Contents

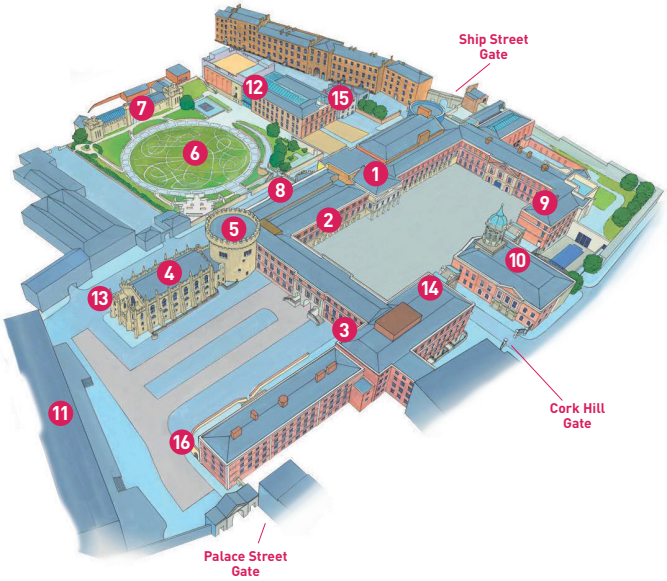
Get Social on Twitter

Follow the event on twitter using **@eurachem2018**. During the event join the discussions using the hashtag **#Eurachem2018**

FREE Wi-Fi

There is free Wi-Fi throughout the venue. Username **DC_Conference** and password **May-2018**

Conference Information



1. Dublin Castle Ticket Office
2. State Apartments
3. Viking & Medieval Excavation
4. Chapel Royal
5. Medieval Tower
6. Dubhlinn Gardens
7. Coach House Gallery
8. Terrace Café
9. Hibernia Conference Centre
10. Bedford Hall
11. Printworks Conference Centre
12. Chester Beatty Library
13. Revenue Museum
14. Revenue Commissioner
15. Assay Office
16. Garda Museum

Conference Venue
The conference will take place in the Hibernia Conference Centre located within Dublin Castle. There are three entrances to Dublin Castle. The Ship Street Gate entrance or the Cork Hill Gate entrance are the closest to the conference centre (please see the map above). Once inside the courtyard of Dublin Castle the Hibernia Conference Centre is located in the Upper Yard of the Castle (No 9 on the map).
Address: Dame Street, Dublin 2, Ireland

Find Dublin Castle
By Bus
Buses stopping on nearby George's Street: 9, 14, 15, 15A, 15B, 16, 65, 68, 83, 122, 140
Buses stopping on nearby Dame Street: 13, 27, 40, 49, 54A, 56A, 77A, 123, 150, 151, 747

By Tram (Luas)
The closest Luas stops are Westmoreland and Trinity. The next stops are St Stephen's Green on the Green Line and Jervis on the Red Line.

By Car
Please note there is no visitor parking available on site. The nearest public car parks are Q-Park Christchurch and Park Rite Drury Street.

At the Conference

Registration
The Registration desk will be located on the ground floor level and will be open during the conference from 8.30am on Monday 14th May. When you arrive at Dublin Castle Conference Centre, please ensure that you go to the registration desk to check in and collect your name badge.

Conference Information

Poster Set-Up
All posters need to be displayed by 10.00 on Monday 14th May in the designated area near the registration desk. Poster presenters will be required to be at their posters for the reception and poster session on Monday 14th May from 17.00 - 18.00.

Poster Pack-Down
All posters need to be removed from the poster boards by 17.00 on Tuesday 15th May. All posters must be removed by this time otherwise they will be disposed of.

Poster Session
Delegates are encouraged to attend the poster session on Monday 14th May at 17.00 - 18.00. Refreshments will be provided.

Exhibition
The exhibition will be open during the morning and afternoon coffee breaks and lunchtimes. We ask that you take the time to visit the stands.

Refreshments
Coffee breaks will be served each day on the lower ground floor outside the main conference hall. Lunch will be provided each day and will be served in Castle Hall.

Mobile Phones
We kindly ask all delegates to keep their mobile devices turned off or on 'silent' mode during all presentations.

Twitter:
You can join the Twitter conversation: @eurachem2018

Wi-Fi:
There is complimentary Wi-Fi available to delegates throughout the conference centre. Username **DC_Conference** and password **May-2018**

Conference Dinner
The conference dinner will be held in the renowned Guinness Storehouse, located in the heart of the legendary St. James's Gate Brewery in Dublin on Monday 14th May. Please arrive between 19.15 and 19.45 to allow time to follow the story of Guinness. This self-guided tour can take up to 20 minutes.

Visitors are asked to enter the building from the cobbled entrance situated on Market Street (in through the large black Guinness Gates). Once you have been through the tour you will then be guided to the Arrol Suite on the 2nd floor where you can learn to pull the perfect pint of Guinness. Dinner will commence at 20.00. (This event is included in the Eurachem Scientific Workshop registration fee).

All delegates who have booked to attend the conference dinner are required to arrange their own way to and from the dinner venue. Please see options below.

Options on how to get to the Guinness Storehouse:

Walk with the group, departing from Palace Street Gate (marked on the map) at 19.00 sharp, walking time 25 minutes.

or **Make your own way** there (a map & trail will be provided at the workshop).

or **Take the bus**. From Dame Street (outside Dublin Castle) the following buses will take you to the venue, 13, 40 & 123.

or **Take a taxi** which can be flagged in the street, collected at a rank or ordered using the MyTaxi app. The fare from Dublin Castle to the Guinness Storehouse should be less than 10euro.

Welcome Message

Dear Colleagues,
Welcome to Dublin Castle!

Eurachem Ireland, in conjunction with the Eurachem Education and Training Working Group (ETWG), are delighted to be hosting the 2018 Eurachem Workshop, exploring topics around Data – Quality, Analysis and Integrity, here in Dublin. This workshop takes place in conjunction with the General Assembly, the flagship annual meeting of Eurachem. Our Cypriot colleagues hosted a successful and insightful workshop in 2017, and we are delighted to build on this success in Dublin 2018. It is a great honour for us to welcome Eurachem back to Dublin, 21 years since we last hosted the General Assembly, back in 1997.

The programme for Eurachem 2018 is packed full with oral, flash and poster presentations around a diverse range of topics. Given the short time we have for this meeting, we have tried to maximise the number of presentation slots, making a fairly intense and hopefully rich programme. However, as importantly, we hope that this meeting will afford you the time to get to know the great community of people you are working alongside across Europe. Please make use of the times during lunch, coffees, the poster session and the conference dinner which are dedicated to networking and scientific discussion.

We would like to thank both the local organising and the scientific committees who have been particularly supportive. We would also like to acknowledge the help and support of Happenings, our conference organisers, who have pulled together the wonderful event you are participating in this week, and Fáilte Ireland, who supported our bid to bring Eurachem 2018 to Dublin.

Finally, we'll leave you with some relevant trivia - A Guinness brewer developed the famous statistical analysis tool, the students t-test. Who was this? Enjoy the tour on the way to the conference dinner to find out! Enjoy the meeting and many thanks for your support,

Blánaid White

Assoc. Prof. Blánaid White,
Scientific Workshop Chair

Vicki Barwick,
Education & Training Working Group Chair

Hugh G Fay

Dr. Hugh Fay,
Eurachem Ireland Vice-Chair

Barbara O'Leary

Barbara O'Leary,
Eurachem Ireland Chair

Conference Committee

Scientific Committee

Vicki Barwick UK
Patrice Behan Ireland
Oktay Cankur Turkey
Helen Cantwell Ireland
Eugenia Eftimie Totu Romania
Hugh Fay Ireland
Rosemary Hayden Ireland
Michael Koch Germany
Ted McGowan Ireland
David Milde Czech Republic
Brian Murphy Ireland
Michele O'Connor Ireland
Barbara O'Leary Ireland
Elizabeth Prichard UK
Alessandra Rachetti Austria
Lorens Sibbesen Denmark
Kyriacos Tsimillis Cyprus
Wolfhard Wegsheider Austria
Blánaid White, Chair Ireland
Alex Williams UK
Perihan Yolci Ömeroğlu Turkey

Local Organising Committee

Vicki Barwick UK
Patrice Behan Ireland
Helen Cantwell Ireland
Hugh Fay Ireland
Rosemary Hayden Ireland
Sean Hyland Ireland
Sean McGowan Ireland
Ted McGowan Ireland
Colmán Ó'Ríordáin Ireland
Barbara O'Leary Ireland
Blánaid White, Chair Ireland

Workshop Programme

Day 1 - Monday May 14th Theme "Current best practice/Where are we now?"	
9:00 - 10:00	Aoife Morrin, Insight Centre, DCU, Ireland and Vicki Barwick, LGC, UK: **'(Re)introduction to statistics: dusting off the cobwebs'**
8:30 - 10:00	Registration, Coffee & Exhibition
10:00 - 10:15	Welcome and Opening Address Ita Kinahan, The State Laboratory, Ireland
Session 1: Data Quality - Chaired by: Helen Cantwell	
10:15 - 11:00	Stefano Cappe, Data Management Team Leader, DATA Unit, European Food Safety, Italy: **'Can we quantify the quality of the data?'**
11:00 - 11:40	Ricardo Bettencourt da Silva, FCUL - University of Lisbon: **'Setting data requirements'**
11:40 - 12:00	David Milde, Palacky University, Czech Republic: Traceability, validation and measurement uncertainty - 3 pillars for quality of measurement results
12:00 - 13:00	**Lunch & Exhibition**
Session 2: Data Analysis - Chaired by: Hugh Fay	
13:00 - 13:40	Bertrand Colson, QuoData, Germany: **'Valid machine learning algorithms for multiparameter methods'**
13:40 - 14:00	Perihan Yolci Ömeroğlu, Uludag University, Turkey: Importance of sampling step to interpret analytical results in food safety analysis
14:00 - 14:20	Stephen Ellison, LGC, UK: Applications of robust estimators of covariance in examination of inter-laboratory study data
14:20 - 14:40	**Coffee & Exhibition**
Session 3: Data Integrity - Chaired by: Seán Hyland	
14:40 - 15:20	Kyriacos C. Tsimillis, Division of Quality Assurance, Pancyprian Union of Chemists, Cyprus: **'Requirements of the accreditation standards'**
15:20 - 15:40	Janine Arvizu, United States: A process for assessment of forensic data integrity
15:40 - 16:20	Freek Varossieau, Senior Product Specialist, Lab Informatics at Agilent Technologies: **'Data Integrity in CDS'**
16:20 - 16:40	Laura Gonzales-Macia, Osasen Sensores SL, Spain: Validation steps for a Point-of-Care (POC) diagnostic device: from prototype to market
16:40 - 17:00	Flash Presentations
17:00 - 18:00	**Poster and Networking Session**
19:30	**Conference Dinner at the Guinness Storehouse**

Workshop Programme

Day 2 - Tuesday May 15th Theme "Risks and emerging challenges/Where to go from here?"			
Session 1: Data Quality - Chaired by: Ted McGowan			
9:30 - 10:10	Bertil Magnusson, RISE (Research Institute of Sweden) and Trollboken AB: **'Revised internal QC from NORDTEST'**		
10:10 - 10: 30	Dinesh Kapu, Athlone Institue of Technology, Ireland: A correlation of the physical attributes of a potent anti-onychomycotic dosage form with microbiological performance.		
10:30 - 11:00	**Coffee & Exhibition**		
Session 2: Data Analysis - Chaired by: Patrice Behan			
11:00 - 11:40	Wolfhard Wegscheider, University of Leoben, General and Analytical Chemistry, Austria: **'Multivariate analysis (chemometrics) - quality of multivariate calibration'**		
11:40 - 12:00	Saorla Kavanagh, Dublin City University, Ireland: Assessing the relationship between honey chemistry and landscape composition		
12:00 - 13:00	**Lunch & Exhibition**		
Session 3: Data Integrity - Chaired by: Colmán Ó'Ríordáin			
13:00 - 13:40	Ilya Kuselman, Independent Consultant on Metrology, Israel: **'Risks of a false decision on conformity of a multicomponent material and quality of chemical analytical results'**		
13:40 - 14:00	Alessandra Rachetti, Montanuniversität Loeben, Loeben, Austria: Fake Data-Rationale, Detection and Implications		
Session 4: Breakout Sessions			
14:00 - 15:20	Parallel Breakout Sessions		
	Data Quality	Data Analysis	Data Integrity
15:20 - 15:40	**Coffee & Exhibition**		
15:40 - 16:00	Feedback from Breakout Sessions		
Session 5: Closing Session			
16:00 - 16:40	Ruth Morgan, UCL, UK: **'Future challenges for data: interpretation, application, communication'**		
16.40 - 16.50	Closing Address		

Conference Chair

Blánaid White

Blánaid White is an Associate Professor in the School of Chemical Sciences in DCU and is Associate Dean for Teaching and Learning in the Faculty of Science and Health.

Her research interests focus on the development of intelligent analysis tools and the application of analytical chemistry for the investigation of chemical and biochemical processes in the world around us. A primary focus of her research is the elucidation of molecular mechanisms which initiate and propagate oxidative stress, particularly that which leads to DNA damage.

A further research focus is the development of analytical platforms. She coordinates the Interreg-funded project Monitool, which seeks to develop new tools for monitoring the chemical status in transitional and coastal waters under the Water Framework Directive.

Blánaid White

Invited Speakers

Aoife Morrin

Associate Professor, School of Chemical Sciences, INSIGHT Centre for Data Analytics, National Centre for Sensor Research

Aoife Morrin obtained her PhD in electroanalytical chemistry in 2004 at Dublin City University (DCU) under Prof. Malcolm Smyth. Following her PhD she gained post-doctoral experience at the National Centre for Sensor Research at DCU. She took up an academic position in the School of Chemical Sciences at DCU as lecturer in Analytical Science in 2008.

She has an active research group where a lot of her focus has been on responsive materials for low-cost sensing. She is funded by Science Foundation Ireland for a work programme on wearables and epidermal sensing as a means to collect health diagnostic data. She, in collaboration with Prof. Dermot Diamond, has co-authored the book 'Advanced Data Processing using Microsoft Excel'. Their book gives an overview of how basic and advanced statistical methods can be used in the teaching and practice of the analytical sciences.

Vicki Barwick

Head of Commercial Training, Science & Innovation Division, LGC, UK

Vicki graduated with a degree in chemistry from the University of Nottingham in 1990. She began her career as an analytical chemist at LGC (formerly the Laboratory of the Government Chemist) working in the area of consumer product safety. She is currently the head of commercial training at LGC with responsibility for the development and delivery of quality assurance training.

She has worked in education and training in relation to analytical measurement for almost 20 years. Vicki is actively involved in the Eurachem network and is currently Chair of the Education and Training Working Group and a member of the Method Validation Working Group.

Invited Speakers

Ita Kinahan

State Chemist, The State Laboratory, Ireland

The State Laboratory is a scheduled office under the aegis of the Department of Public Expenditure and Reform which provides a comprehensive analytical and advisory service to Government departments and offices, thereby enabling them to implement and formulate the technical aspects of national and EU legislation.

The State Laboratory undertakes chemical analyses for a variety of different purposes which include monitoring the quality and safety of Irish food and prosecuting fraud e.g. illegal use or laundering of marked diesel, sale of counterfeit spirits or possession of illegal medicines.

Analyses for the presence of alcohol and drugs assist the Coroners to determine the cause of deaths, e.g. in cases of alcohol / drug overdoses, while, in the Customs area, analysis can show whether additional duties or fines may be payable. Staff are actively involved in EU and international analytical affairs and the State Chemist has enforcement and referee status under various Acts of the Oireachtas and their implementing regulations. The Laboratory provides representation for client Government Departments at EU meetings.

The State Laboratory is a designated EU National Reference Laboratory for residues of a wide range of veterinary medicines in food of animal origin; for additives for use in animal nutrition; for dioxins and polychlorinated biphenyls (PCBs); and for mycotoxins and heavy metals in animal feed. It has also been designated as the responsible Irish body for traceability of measurement in chemical metrology and bio-analysis.

Stefano Cappe

Data Management Team Leader, DATA Unit, European Food Safety

S. Cappe is responsible for the team "Data management" in the "Evidence management" unit of EFSA. The team is in charge of the data collections of chemical contaminants, additives, pesticide and veterinary medicinal products residues, zoonoses and antimicrobial resistance, molecular typing. The collected data provide the basis for many EFSA risk assessment works in the above areas.

His main work is around data collection, data integration, data quality, data warehouses and business intelligence to support data analysis and risk assessment. From 2001 to 2007 he worked in EMA (European Medicines Agency) in the development of the European pharmacovigilance system.

Invited Speakers

Alex Williams

Alex Williams, formerly the UK Government Chemist. Alex is a proposer and founder member of Eurachem. He is a member of the Eurachem working group on Uncertainty Evaluation and Traceability and is joint editor of the Eurachem guides on, Uncertainty, Traceability, Compliance and Setting Target Uncertainty.

Ricardo Bettencourt da Silva

Environmental Biogeochemistry Group - Centro de Química Estrutural (CQE@FCUL), University of Lisbon

After working in accredited laboratories as analyst and consultant for 15 years, Ricardo started a research and teaching career at the University of Lisbon. Since 2002 he has collaborated with the Portuguese Accreditation Body, as technical assessor,

and in training staff of laboratories. Ricardo is currently the secretary of CITAC, a member of the executive board, chair of the Eurachem working group on Qualitative Analysis and a member of the Eurachem working group on Measurement Uncertainty and Traceability of Eurachem.

He is co-editor of the Eurachem/CITAC guide for Setting the Target Measurement Uncertainty. His research interests are Metrology and Examinology in chemistry which are the sciences of measurements and qualitative analysis in chemistry, respectively (http://webpages.fc.ul.pt/~rjsilva/).

Invited Speakers

Bertrand Colson

QuoData, Germany

Bertrand Colson is an experienced data scientist involved in a variety of projects focusing on analytical quality assurance in the fields of food safety, process validation, forensics, and diagnostics.

He develops and validates novel approaches for data analysis and interpretation by

applying machine learning techniques to realize tailored solutions and powerful web applications.

As an expert in method development and validation, he contributes to several projects in international standardization e.g., to ISO/TC 34/SC 9/WG 2, a working group developing an international standard for validation of methods in the field of food safety.

Kyriacos C. Tsimillis

Division of Quality Assurance, Pancyprian Union of Chemists.

Kyriacos Tsimillis holds a BSc and a PhD in chemistry from the University of Athens where he was later a lecturer of physical chemistry.

Since 1982 he has been involved in standardization and certification activities in Cyprus and for twelve years in accreditation activities

(Director 2009-2013). He participated in the activities of EA, among others as a member of peer evaluation teams.

Since 1997 he represents the Pancyprian Union of Chemists (PUC) in Eurachem, including a two-year period as its Chair and for many years as a member of the Executive Committee; he is the author of research papers and review articles and a co-author of books on Quality. Since 2014 he is a member of the Division of Quality Assurance of the PUC.

Invited Speakers

Freek Varossieau

Senior Product Specialist: Lab Informatics at Agilent Technologies

Freek graduated in 1977 as a clinical chemist and worked for 10 years at the Netherlands Cancer Institute in New Drug Development for the EORTC, focusing on pre-clinical

Phase-I and II studies and Phase-I studies in patients.

In 1990 Freek joined Perkin-Elmer responsible for support contracts and expanded this to LIMS and networked CDS. At Agilent Technologies Freek currently holds a network specialist position for CDS, SDMS and ELN in Europe.

Bertil Magnusson

RISE (Research Institute of Sweden) and Trollboken AB.

Bertil started as a marine chemist looking for traces of metals in the Oceans in the 70's. After his PhD he joined a chemical company, AKZO-NOBEL, and worked there as a specialist in analytical chemistry mainly with spectroscopy (XRF, XRD, ICP) and wet chemistry. In 2002 Bertil joined SP, now

RISE (Research Institutes of Sweden), he is working with analysis and quality in measurements including accreditation, quality control, validation, measurement uncertainty and decision making.

A major part is teaching and taking part in writing guidelines from e.g. Nordtest and Eurachem. In 2016 he started a small company supporting labs with quality in measurement, www.trollboken.se.

Invited Speakers

Wolfhard Wegscheider

Professor of General and Analytical Chemistry at the Montanuniversitaet Leoben, Austria.

W. W. received his education from the Graz University of Technology majoring in technical chemistry with a specialisation in biochemistry and food chemistry. His diploma thesis and doctoral thesis were in analytical chemistry with an emphasis on trace analysis and environmental analysis.

W.W. is a member of several learned societies such as GDCh, GOECh, Co-operation on International Traceability in Analytical Chemistry (CITAC) and Eurachem where he is also a founding member of the Working Group on Education and Training and of the Working Group on Measurement Uncertainty and Traceability. He is currently is a Member of the Board of Directors of the Austrian Society of Analytical Chemistry - ASAC. In 2010 he was appointed a Fellow of the International Union of Pure and Applied Chemistry (IUPAC).

He is a consultant to the Austrian Federal Ministry for Agriculture, Forestry, Environment and Water Management and a lead auditor in the Austrian Accreditation of Laboratories System. Presently he is chair of the Board of Trustees of OeAD GmbH, the Austrian Agency for International Cooperation in Education and Research. W.W. is a member of the Statistics Committee of AOAC International for the period 2016-2019.

Ilya Kuselman

Independent Consultant on Metrology, Israel.

Ilya Kuselman received his Ph.D. in inorganic chemistry from Kalinin State University, and his D.Sc. in analytical chemistry - from the R&D Institute for Rare Metal Industry, Moscow, Russia.

From 1971 to 1990 Ilya was firstly a researcher before becoming Head of Metrology in the Chemistry Division of All-Union R&D Institute of Non-ferrous Secondary Metals, Donetsk, Ukraine, USSR.

From 1991 to 2014 he was a Director of the National Physical Laboratory of Israel. Now Ilya is an independent consultant on metrology in Israel.

He has published more than 200 papers on metrology and quality in analytical chemistry. Ilya is a member of CITAC, ISO/REMCO and IUPAC Analytical Chemistry Division.

Invited Speakers

Ruth Morgan

Professor Ruth Morgan is the Founder and Director of the UCL Centre for the Forensic Sciences and Professor of Crime and Forensic Science at UCL.

The Centre facilitates a network of researchers from a wide range of different disciplines, to enable a strategic and multidisciplinary research programme in collaboration with external partners and forensic science stakeholders. Her

research group is focussed on developing the field of forensic science evidence interpretation. Professor Morgan has received the PW Allen Award from the Chartered Society of Forensic Sciences for best publication in the Chartered Society of Forensic Science journal 'Science and Justice' in 2006 and 2017.

She sits on a number of advisory bodies including groups at the Home Office and the Knowledge Transfer Network, and is the Vice Chair of the London Geological Society Forensic Geoscience Group.

Gold Sponsors

Agilent

Agilent is a leader in Pharmaceutical, Life Sciences, Diagnostics, and applied markets. The company provides laboratories worldwide with instruments, services, consumables, applications and expertise, enabling customers to gain the insights they seek. Agilent has about 13500 employees globally and had revenues of $4.47 billion in fiscal year 2017.

Agilent
Tel.: 01 605 8324
customercare_ireland@agilent.com
www.agilent.com

Agilent Technologies Ireland Ltd
Unit 3 Euro House, Euro Business Park, Little Island
Cork, Ireland

QuoData

QuoData is based in Dresden and Berlin and provides statistical expertise and consulting services to support industry, research and government in quality assurance and process optimization.

They specialize in proficiency testing, validation of measurement methods, experimental and sampling design. Utilizing state-of-the-art data science methods and novel approaches for data analysis and determination of measurement uncertainties, QuoData develops software solutions, online platforms and provides expertise to an international clientele.

The interdisciplinary Data Science team of QuoData has been involved in the design and the evolution of proficiency tests and validation studies for more than 20 years in the fields of environmental issues, food safety, diagnostics, material research and more.

QuoData
Tel.: +49 351 40 28 867 0
info@quodata.de
www.quodata.de/en

QuoData GmbH, Quality & Statistics, Prellerstraße 14
01309 Dresden, Germany

Silver Sponsors

Anton Paar

Anton Paar produces high-end measuring and laboratory instruments for industry and research. It is the world leader in the measurement of density, concentration and CO_2 and in the field of rheometry.

Other areas of specialty are: petroleum testing, microwave synthesis, viscometry, polarimetry, refractometry, x-ray scattering, sample preparation and surface characterization.

The core competence of Anton Paar - high-precision production - and close contact to the scientific community form the basis for the quality of Anton Paar's instruments.

Anton Paar's strong sales network in more than 110 countries guarantees customers rapid support and answers to their application and service queries.

Anton Paar GmbH
Anton-Paar-Str. 20
A-8054 Graz
Austria

Tel.: +43 (0) 316 257-0
Fax: +43 (0) 316 257-257
info@anton-paar.com
www.anton-paar.com

Anton Paar Ltd
Unit F, The Courtyard
St Albans, AL4 0LA
UK

Tel: +44(0)1992514730
info.gb@anton-paar.com
www.anton-paar.com

BIPEA

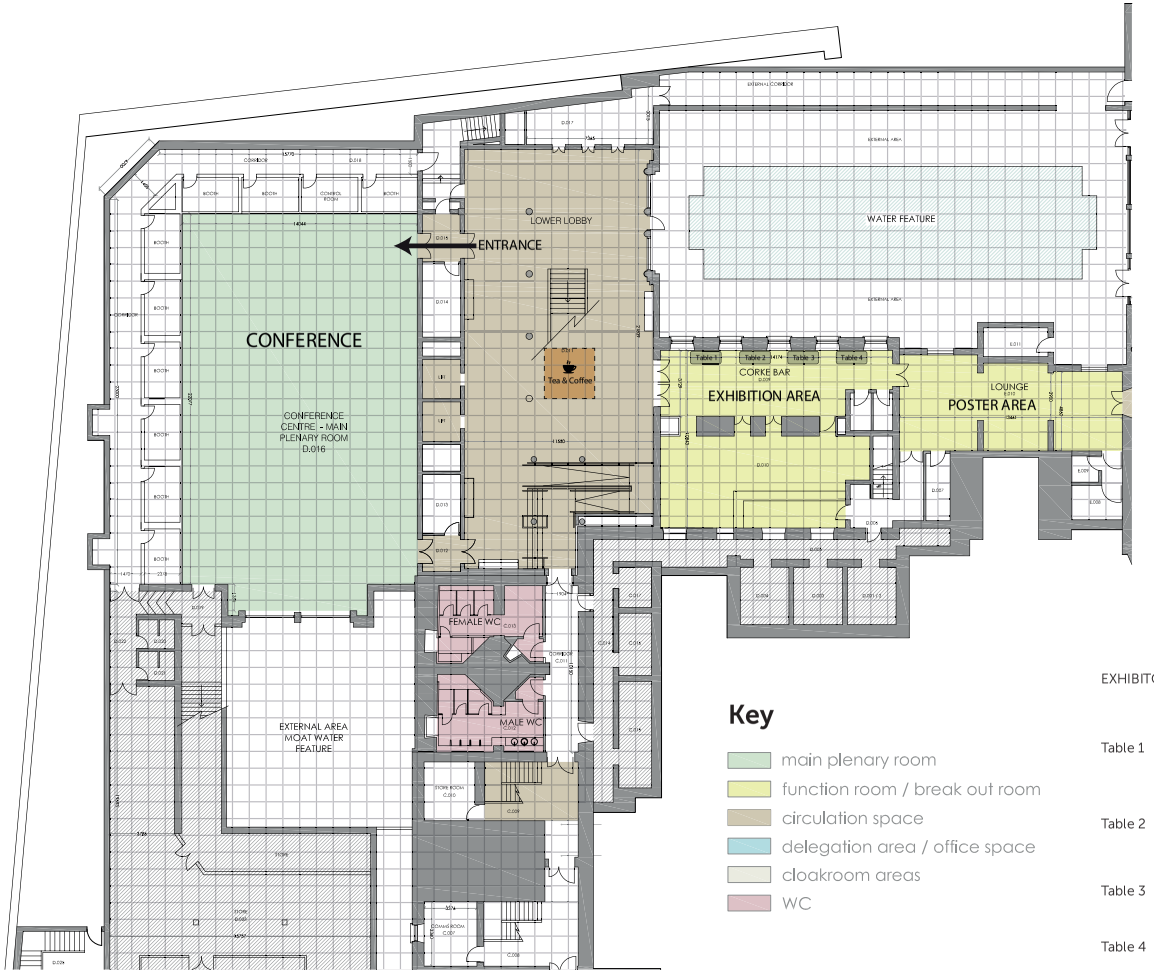
Provider of proficiency testing programmes in microbiology, chemistry and physics.

Created in 1970, BIPEA is a nonprofit organization providing proficiency testing programmes and reference materials for laboratories concerned by quality control and analytical accuracy. Present in more than 120 countries, services cover different fields like food, feed, drinks, waters, soils and cosmetics.

BIPEA is certified to ISO 9001 by the Lloyd's Register Quality Assurance and accredited by COFRAC according to the ISO/IEC 17043 standard for the organization of proficiency testing programmes (scope 1-1495 available on www.cofrac.fr). Today BIPEA provide a service to over 2000 laboratories.

Feel free to contact BIPEA - www.bipea.org

Floor Plan



Key

- main plenary room
- function room / break out room
- circulation space
- delegation area / office space
- cloakroom areas
- WC

EXHIBITORS

Table 1 Agilent

Table 2 quodata *QUALITY & STATISTICS

Table 3 Anton Paar

Table 4 BIPEA

Abstract Index

Lecture (L)

Contributed Communication (CC)

Poster (P)

L02
Can we quantify the quality of the data?

Cappè S[1]
[1]*Evidence Management Unit (EFSA)*

EFSA is mandated[1] to collect data to support risk assessment activities. The Evidence Management Unit is responsible for collecting data in several areas (contaminants, additives, zoonoses, pesticide and veterinary medicines residues) from Member States' competent authorities, academia and industry. This information is used by the unit to assess dietary exposure to chemicals and deliver annual reports. The availability of data has been placed at centre of EFSA 2020 strategy[2], setting up strategic objectives to widen and open the data at the basis of EFSA's scientific advice process. Within this effort, data quality is a fundamental component, guaranteeing the "fitness for purpose" of the collected data for the risk assessment process, as also clarified in the outcome of EFSA Prometheus project[3].

We often define data as of "good" or "poor" in quality. In the past years EFSA and MSs were fully engaged on data quality, improvements were obtained through the use of data standardisation with Standard Sample Description[4], grants to support electronic transmission, automatic validation rules, training of data providers, annually revised guidance documents, and the constant update of standard terminologies. Based on this experience EFSA decided to adopt a quantitative approach on quality in order to better focus its investments and initiate a process of continuous improvement.

As for quality in general, the process starts with the definition of the data quality objectives as defined by the data users and complemented by in-depth analysis of the data (data quality profiling). Once the objectives are clarified, it is essential to define measurable Key Performance Indicators (KPIs) and the expected targets. The KPIs are regularly acquired and results are shared with the user community (the data providers) and with governance bodies responsible for the data quality. The setting up of a governance process is essential to guide the investment on data quality in a sounding and cost-effective manner. They control the specific investments to improve data quality: e.g. new validation rules, training for data providers change to data quality objectives and KPIs. This approach is currently piloted in EFSA to quantify the quality of the data received from the domains describe above. The case of analytical data on contaminants is here used as an example to show how to define data quality objectives and the related KPIs. The development of these indicators was developed in strong collaboration with the national organizations providing this data to EFSA and was piloted through a grant agreement including five Member States institutions. The data quality measures have been integrated in the EFSA Scientific Data Warehouse. With this example it is also possible to highlight the limitations of the current approach and the lessons learnt.

1. Article 33 of Regulation (EC) No 178/2002
2. EFSA 2020 Strategy, available at https://www.efsa.europa.eu/sites/default/files/151008.pdf
3. Prometheus (Promoting Methods for Evidence Use in scientific assessment described in EFSA (European Food Safety Authority), 2015. Scientific report on Principles and process for dealing with data and evidence in scientific assessments. EFSA Journal 2015;13(5):4121, 35 pp. doi:10.2903/j.efsa.2015.4121
4. EFSA (European Food Safety Authority), 2013. Standard Sample Description ver. 2.0. EFSA Journal 2013;11(10):3424, 114 pp., doi:10.2903/j.efsa.2013.3424

L03
Setting data requirements

da Silva R[1], Williams A[2]
[1]Centro de Química Estrutural (CQE@FCUL) University of Lisbon, Lisbon, Portugal, [2]Eurachem

A prime requirement is the reliable and accurate collection of all the data associated with the sample from its arrival in the laboratory, through the measurement process, to the final report to the customer. A Laboratory Information Management System (LIMS) provides a facility for doing this and, if well designed, eliminates the need for any manual transcription of data and by using, for example, barcoding reduces the possibility of errors when manually entering information. However, it is still necessary to determine what data is required particularly for the measurement process.

This presentation concentrates on the measurement data required to ensure that the measurement result is fit for purpose, a requirement that is addressed during measurement procedure validation but should also be checked in routine measurements.

As an example, setting the data requirements to achieve the target measurement uncertainty will be discussed. This includes determining the number of replicate signals or analytical portions, the number of points on the calibration curve, and the uncertainty of used reference materials. Also discussed are the requirements for the traceability of the values of the reference materials used and how the data is processed to check that the required uncertainty has been achieved.

Additionally, the issue of structuring the data, not only to meet the management needs associated with a particular sample or similar samples, but also to meet possible future needs is discussed.

The above is dealing with specifying the data required by the laboratory to produce a satisfactory result and report. A much wider problem is how to structure this data so that not only can data from a specific sample be retrieved but the data can be used for much wider applications, for example.

- What percentage of samples showed non-compliance, subdivided by types of samples e.g. food, environment and even subdivided further types of food, environment contaminants. This information can be useful, for example, to redefine the target measurement uncertainty.

- Comparison of the uncertainty achieved as a function of the procedure, type of sample, approach used for uncertainty evaluation, cost of analysis et cetera.

Structuring the data to be able to carry out such analysis is quite a problem for just a single laboratory, since it is not known what future applications might be desirable. In addition, it is wider issue if such analyses want to be carried out for example across accredited laboratories or any other group laboratories such as within Eurachem.

L04

Data integrity: Requirements of the accreditation standards

Tsimillis K[1]
[1]*Division Of Quality Assurance, Pancyprian Union Of Chemists, Nicosia, Cyprus*

The requirements for the competence of laboratories are described in two standards, namely ISO/IEC 17025:2017 [1] and ISO 15189:2012 [2]. The former applies to all laboratories except to medical laboratories where the latter is the most appropriate. After the new standard ISO/IEC 17025 [1], laboratory activities may include, further to testing and calibration, sampling associated with subsequent testing or calibration. These standards are the ones used by accreditation bodies in the assessment of laboratories for their accreditation. This is why the term "accreditation standards" is used throughout this presentation. The requirements of these standards include specific references to data, their protection and integrity. This presentation refers to the requirements of the accreditation standards for laboratories in a comparative way. According to ISO 9000 [3], data is defined as facts about an object i.e. an entity, an item, anything perceivable or conceivable. This may include among others a product, a service, a process, a person, an organization, a system, a resource. Data is also the primary product of laboratory work and represents the basis on which results, reports and certificates can be issued and opinions and interpretations and statements of compliance can be reported. The recently published ISO/IEC 17025:2017 [1] introduces additional provisions compared to the 2005 edition for the control of data and information management. According to this standard, "laboratory information management system(s)" includes the management of data and information contained in both computerised and non-computerized systems. Similar is the definition given in ISO 15189 [2] for "information systems". Both standards provide for the laboratory information management system(s) used for the collection, processing, recording, reporting, storage or retrieval of data; the standards also provide for the need for validation for functionality of these systems including the proper functioning of interfaces within the laboratory information system(s) before introduction as well as whenever changes are made. The standards specify certain requirements with regard to the protection from unauthorized access, against tampering and loss, inappropriate environmental conditions and other factors which may affect the integrity of data and information. Particular requirements are also set regarding documentation and personnel for the management of the information system(s). Particular requirements are set for cases when a laboratory information management system is managed and maintained off-site or through an external provider. In general, the two standards set requirements for data integrity in a similar way; however, ISO 15189 [2] addresses these issues in a way that reflects the particular needs of the sector dealing with personal data of the patients.

1. ISO/IEC 17025 (2017) General requirements for the competence of testing and calibration laboratories.

2. ISO 15189 (2012) Medical laboratories – Requirements for quality and competence

3. ISO 9000 (2015) Quality management systems – Fundamentals and vocabulary.

L06
Revised internal QC from 'NORDTEST'

Magnusson B[1]
[1]*RISE, Research Institutes of Sweden and Trollboken AB*

The aim of the "Trollbook1" is to give good and practical guidance on internal quality control for the analysts in their daily work with the analytical methods. This 5th version of the handbook is a minor revision. The main updates are:

- more focus on target control limits. In cases where the clients demand is lower than the performance of the method wider control limits can be set. Since this will results in fewer out of control values we recommend laboratories to consider this option,
- long-term evaluation (chapter 10) now discusses changing of control limits and central line in separate paragraphs,
- pooled standard deviation is recommended to obtain the standard deviation for setting the control limits in a range chart,
- combined standard deviation is now more correctly called pooled standard deviation
- a detailed example (10) of pooling standard deviation for the repeatability, sr and the within-la reproducibility, sRw from an internal control measuring three replicates in every analytical run is added. If all results would be used to calculate sRw a too low estimate will be obtained resulting in too narrow control limits.

About the Trollbook - The handbook starts, after an introduction, with two chapters (Chapters 2 and 3) on general issues of analytical quality, described with specific reference to internal quality control. They are followed by an introduction to control charting (Chapter 4). The tools of control charting are described in the following chapters: control charts (Chapter 5), control samples (Chapter 6) and control limits (Chapter 7). Chapter 8 summarises the tools in a description of how to start a quality control program.

How the data of internal quality control are used is described in the following two chapters. Chapter 9 explains the interpretation of quality control data to be performed after every analytical run, whereas Chapter 10 explains how the quality control programme should be reviewed periodically to investigate if the program is still optimal to control the quality of the analysis.

The last chapter contains nine examples illustrating how control charts can be started as well as practical application of the control rules and the yearly review.

1. B. Magnusson, H. Hovind, M. Krysell, U. Lund and I. Mäkinen, Handbook of internal control, Nordtest Report TR 569 (ed. 5) 2018. Available from www.nordtest.info.

L07

Multivariate analysis (chemometrics) - quality of multivariate calibration

Wegscheider W[1]
[1]*Department of General, Analytical and Physical Chemistry, Montanuniversitaet Leoben, Austria*

The observation of multiple signals for one and the same sample simultaneously or within short time intervals has paved the way for many measurement systems that are lacking selectivity for producing meaningful data. The introduction of fast recording instruments has driven the development of equally fast and efficient data reduction strategies in the analytical laboratory, in process monitoring and in modern sensing in general. This has not just made available procedures that take much less time than classical ones, but also made possible the measurement of completely new quantities so far not accessible to analytical chemical laboratories.

In practice, there are frequently measured multiple signals on representative samples that for the purpose of calibration have been characterized with respect to the analyte(s) by independent, often time consuming methods of analysis.

These advances, however, have a couple of consequences that require special attention in optimization and validation of these multivariate measurements. One of the consequences is that there is not direct way to visualize or plot the signals vs. concentration due to the multidimensionality of the signals and/or concentrations. It also follows that the classical approach to monitor the stability of a measurement process over time by Shewhart control charts is not viable.

Over the years, however, there has been established a number of alternative procedures - multivariate themselves - that aid in giving insight in the internal structure of the multivariate calibration processes. These can be used to identify particularly influential calibration samples, the distinction between useful and less useful, or even confusing, signals/wavelengths, and unknowns for which a particular calibration can or cannot be applied to.

Some recent examples of multivariate calibration that have been incorporated into modern commercial instrumentation will be provided to stress the growing impact of this type of analytical measurement.

L08

Risks of a false decision on conformity of a multicomponent material and quality of chemical analytical results

Kuselman I[1], Pennecchi F[2], da Silva R[3], Hibbert B[4]
[1]Independent Consultant on Metrology, Modiin, Israel, [2]Istituto Nazionale di Ricerca Metrologica (INRIM), Turin, Italy, [3]Faculdade de Ciências da Universidade de Lisboa, Lisboa, Portugal, [4]School of Chemistry, UNSW Sydney, Sydney, Australia

Comparing chemical analytical (test) results with the material specification, regulatory or acceptance limits of the component content, one should decide whether the tested sample (batch/lot) conforms or not. It is known that measurement uncertainty, which characterizes the quality of a result, leads to risks of false decisions. Evaluation of such risks for a multicomponent material or object involves calculation of probabilities of false decisions for the different components of the material or object (particular consumer's and/or producer's risks). At the same time, even when conformity assessment for each component of a sample is successful, the total probability of a false decision (total consumer's risk or producer's risk) on the conformity of the sample as a whole may still be significant. The total risk due to measurement uncertainty can be evaluated as a combination of the particular risks of conformity assessment of the sample components, whenever there is independence among their test results. Possible correlation can be viewed as a further quality parameter of the results, influencing the total risk of false decisions. It should be also taken into account at the risk evaluation.

L09

Future challenges for data: interpretation, application, communication

Morgan RM[1,2]
[1]*UCL Department of Security and Crime Science, London, UK,* [2]*UCL Centre for the Forensic Sciences, London, UK*

The innovations and developments in data analysis in the last 10 years have been phenomenal. The capacity for accuracy, precision and reliability in measurements, combined with the ability to interrogate larger datasets than ever before has created significant opportunities to identify and understand trends, relationships and networks.

This talk will draw out the importance of not only ensuring good data quality, analysis integrity and compliance, but also addressing the importance of ensuring this foundation is the basis for robust and transparent inferences about the meaning of the data in different contexts. Examples will be presented from the field of forensic science, a field where these trends have led to transformation, but also produced significant challenges in a complex interdisciplinary space. A specific challenge for many applied disciplines is understanding the decision-making processes that are integral to establishing robust inferences from data. Examples of the importance of using data to understand the significance of the data itself, and also the decision making that occurs in drawing conclusions will be presented.

The value of both good data for making robust and accurate classifications but also for demonstrating the significance of conclusions that are reached from that data will be discussed.

Abstracts

CC01
Traceability, validation and measurement uncertainty - 3 pillars for quality of measurement results

Milde D[1]
[1]*Palacky University in Olomouc, Olomouc, Czech Republic*

This presentation will provide an overview of establishing so called 3 pillars (metrological traceability, validation of measurement procedure and measurement uncertainty) for quality of measurement results in chemical laboratory. The brief introduction of each concept based on International vocabulary of metrology will be provided as well as approaches how to establish and demonstrate them in practice. This will be linked to Eurachem guidance that is freely available on www.eurachem.org website [1-3].

Several practical examples from analytical laboratory will be also presented. Firstly examples dealing with determination of elemental impurities in pharmaceutical products (US Pharmacopeia 232, ICH Q3D) by ICP-MS in the laboratory working under good manufacturing practice will be shown. The second group of examples origination from a research analytical laboratory with focus on a metrological part and three mentioned pillars [4, 5].

Acknowledgements
This work was supported by Ministry of Education, Youth and Sports of the Czech Republic (LTV 17015, LO 1305).

References

1. EURACHEM/CITAC Guide: Traceability in Chemical Measurement (2003). Available from www.eurachem.org and www.citac.cc.

2. B. Magnusson and U. Örnemark (eds.) Eurachem Guide: The Fitness for Purpose of Analytical Methods – A Laboratory Guide to Method Validation and Related Topics, 2nd ed. 2014. www.eurachem.org. ISBN 978-91-87461-59-0.

3. S. L. R. Ellison and A. Williams (eds). Eurachem/CITAC guide: Quantifying Uncertainty in Analytical Measurement, 3rd edition, 2012, www.eurachem.org. ISBN 978-0-948926-30-3.

4. M. Jarošová, D. Milde, M. Kuba: Comparison of ICP-MS and AAS – Elemental analysis of coffee. Czech J. Food Sci. 32, 354-359 (2014).

5. L. Veverková, Š. Hradilová, D. Milde, A. Panáček, J. Skopalová, L. Kvítek, K. Petrželová, R. Zbořil: Accurate determination of silver nanoparticles in animal tissues by inductively coupled plasma mass spectrometry. Spectrochim. Acta, part B 102, 7-11 (2014).

CC02

Valid machine learning algorithms for multiparameter methods

Colson B[1], Gowik P[2], Hettwer K[1], Simon K[1], Stoyke M[2], Uhlig S[1]
[1]QuoData GmbH Quality & Statistics, Dresden, Germany, [2]BVL, Berlin, Germany

In the light of recent food fraud cases, the issue of food authenticity is receiving increasing attention. New analytical methods and evaluation approaches are currently being proposed in order to address this issue. In this framework, the evaluation of mass spectral profiles constitutes a promising avenue, e.g. for the determination of food origin. Relevant evaluation approaches include PCA, cluster analysis, discriminant analysis, etc. The aim is to derive criteria for the assignation of unknown samples to subpopulations. These criteria are derived on the basis of samples whose origin is known – the training set. A reliable evaluation requires that the number of samples must be *considerably* larger than the number of parameters. However, in the framework of multiparameter mass spectrometry methods, the required ratio between sample and parameter numbers is inverted, with e.g. 100 samples versus over 10 000 parameters. In this presentation, approaches for a reliable specification of criteria in spite of insufficient sample numbers are discussed.

Consider the example that, on the basis of a batch of 100 fish, the task is to decide which come from origin A and which from origin B. In the case of the training set, each sample is allocated to one of the two subpopulations. Once the measurements have been performed, the resulting multiparameter spectral dataset is so large and manifold that it will always be possible to identify criteria which will result in satisfactory levels of discriminatory power – in the sense that test decisions after application of the criteria agree with the "true answers". However, the question is whether the application of the criteria to a test set will yield reliable test decisions.

One possible approach consists in developing a function which measures the "distance" between a particular sample's spectrum and the spectra of all the samples belonging to the subpopulation under consideration. The reliability of the criteria depends on an appropriate consideration of the measurement uncertainty of the multiparameter method.

CC03

Importance of sampling step to interpret analytical results in food safety analysis

Yolci Ömeroğlu P[1]
[1]*Uludag University Faculty of Agriculture Food Engineering Department, Bursa, Turkey*

The European Commission aims to assure a high level of food safety within the EU from farm-to-fork by effective monitoring the market. To facilitate the international food trade and to protect consumers' health, European Union, and National Authorities set legal limits for the analyte being into consideration. For those purposes, each year more than thousands of food samples are analyzed worldwide.

Food safety testing methods include two main steps: sampling performed outside of the laboratory, and laboratory operations comprising of sample preparation, sample size reduction, sample processing, extraction, clean-up, and determination. Sample is defined as one or more units selected from a population of units, or a portion of material selected from a larger quantity of material. Reliable analytical results can only be reported to customer if a representative sample reflecting the properties of lot being sampled can be provided. The primary samples from a lot must be taken randomly and should consist of sufficient material to provide laboratory samples required from a single lot. Variations, caused by heterogeneity, contamination, loss of analyte or use of an incorrect sampling plan, may be observed between the compositions of random samples taken from a lot. These variations can lead to uncertainty in sampling step and should be taken into account. It was reported that sampling uncertainty is the biggest contributor in major food testing including aflatoxin and pesticide residue analysis. In this presentation, various sampling plans in food testing, contribution of sampling uncertainty to overall measurement uncertainty, interpretation of analytical results taking into account sampling uncertainty are aimed to be explained and discussed in detail.

CC04/P05

Applications of robust estimators of covariance in examination of inter-laboratory study data

Ellison S[1]
[1]*LGC, Teddington, United Kingdom*

Many inter-laboratory studies involve the collection of results for more than one measurand from each participant. For example, in a collaborative study aimed at validation of a new standard measurement procedure, results for more than one test material are usually collected, either to obtain information on precision at different levels or as part of a split-level design. In reference material certification by inter-laboratory study, results for multiple analytes in the same candidate reference material may be obtained, or a separate quality control material of known properties may be included for assessing laboratory performance. Proficiency testing rounds also frequently collect data for multiple measurands, on multiple test items, or both. In these circumstances, the identification of anomalous results can be challenging, as it is possible for a laboratory to have results with an acceptable range for each individual measurand on each test item but nonetheless differ substantially from the remainder of the population in terms of the general pattern of results. Identifying such anomalies is an important step in initial data inspection and 'clean-up'.

Several approaches for outlier identification in multivariate data are available. For bivariate data, Youden plots can be effective. For multivariate data, principal component analysis and measures such as Mahalanobis distance can be valuable aids. However, while visual inspection is always useful for inspection, it is often useful to include criteria for declaring an observation as anomalous; for example, for univariate outlier detection, critical values for common statistical outlier tests are used to decide whether follow-up action is appropriate. For multivariate data, such criteria will commonly require information on covariance between different measurands. Since most interlaboratory data sets show at least some outliers, however, the usual measures, such as covariance and Pearson correlation, can badly overestimate the covariance of the underlying distribution.

There are, however, a number of outlier-resistant procedures for obtaining estimates of covariance or correlation. These include, for example, a simple pairwise procedure due to Gnanadesikan and Kettenring, and more complex iterative procedures such as the minimum covariance determinant method. Rank correlation is also relatively resistant to extreme values compared to the usual Pearson correlation.

This short paper illustrates the use of selected robust estimators of covariance or correlation in the identification on anomalous laboratory results in inter-laboratory data. It is shown that robust estimators can substantially reduce the impact of outlying values on multivariate confidence regions and consequently lead to sharper identification of anomalies even where traditional univariate outlier detection may fail to locate anomalous results.

Abstracts

CC05
A process for assessment of forensic data integrity

Arvizu J[1]
[1]*Independent, Tijeras, United States*

In recent years, reports of invalid forensic methods (e.g., bullet lead analysis; microscopic hair analysis) and analyst misconduct (e.g., dry labbing; falsified credentials) have rocked the legal community and led to numerous exonerations. Forensic laboratories throughout the United States have been plagued by instances of blatant fraud, analyst incompetence, and procedural deficiencies. Though the legal community relies on forensic results, it often lacks scientific training and remains ignorant of data integrity problems, resulting in case outcomes that are based on invalid scientific conclusions.

Hundreds of forensic laboratories have developed quality systems and been accredited to ISO/IEC 17025, but accreditation does not ensure that a laboratory's reported results have integrity. While the scientists who work in forensic laboratories are generally aware of the importance of quality assurance, operational pressures and pragmatic considerations may limit their focus to those aspects of forensic science that are within their direct control inside the laboratory. Forensic analysts responsible for production testing may have little, if any, direct knowledge of the theoretical principles or practical constraints that influence the quality of the evidentiary samples that are delivered to the laboratory for testing. Yet analysts may testify based on the unverified assumption that the evidence tested in the laboratory was representative of the evidence in the field. Similarly, a validation study that effectively characterizes the qualitative and quantitative performance of an analytical method may nevertheless be insufficient for forensic use.

This presentation draws from decades of experience conducting audits of analytical laboratories and their work product. A summary of forensic integrity problems will be provided, including the most common problems (widely distributed and frequently identified) and the most serious problems (those with the highest risk of false incrimination).

This presentation will also introduce a process for objectively evaluating the integrity of forensic results based on a practical and universally applicable definition of forensic data integrity. The principle behind this process is that an analytical result has integrity and can be reliably used as the basis for consequential forensic decisions *if records demonstrate*:

1. the sample(s) is(are) unambiguously representative of the original evidence;
2. the analytical method has been empirically validated and found to be appropriate for its intended forensic use; and
3. the analysis was reliably conducted and reported in accordance with relevant standards.

This process for evaluating forensic integrity is applicable to the full scope of test methods conducted by forensic laboratories—from DNA and toxicology to gunshot residue and controlled substances—and addresses the problems that adversely affect the integrity of forensic results, including fraud, sampling errors, metrological failures, and invalid methods. The efficacy of this assessment process will be demonstrated, using examples drawn from criminal cases in the United States.

CC06

Validation steps for a Point-of-Care (POC) diagnostic device; from prototype to market

Gonzales-Macia L[1], Urien-Berrio M[1], Jaureguibeitia A[2]
[1]Osasen Sensores SL, Derio, Spain, [2]Biolan Microbiosensores SL, Zamudio, Spain

The development of self-testing devices has revolutionized the health monitoring and diagnosis areas by providing patients with reliable home-based analysis. Point-of-care (POC) biosensors are miniaturized portable devices that integrate all the functions of centralized laboratory testing without the need for trained staff. However, in order to be considered as real alternatives to the pharmacy or GP visits, the devices should prove their feasibility for a specific intended use by fulfilling a series of particular requirements.

Analytical and clinical validation, CE marking and accreditation are some of the steps to follow before a POC device reaches the market. At the same time, internal quality control and external quality assessments are also necessary to ensure the good operation of POC devices. Despite the promising characteristics of a new technology, no market opportunity is viable if the prototype fails to demonstrate its reliability and reproducibility for the intended use. Several institutions (FDA, EMA) are responsible for the regulation and approval of novel devices. They are essential to ensure good practice and maintaining compliance and they normally provide guidelines to assist the users through the validation method. However, the route to obtain the final certifications and device commercialization is long and not always clear.

At OSASEN, we apply innovative tools to the fabrication of robust POC biosensor systems for rapid in vitro diagnostics. Our researchers have a broad expertise in the areas of material printing techniques and electrochemical determination, working to provide rapid and affordable solutions to healthcare. Recently, we have developed a low-cost disposable electrochemical biosensor for hypolactasia diagnostics that will reduce current test time and improve patient test tolerance. Hypolactasia affects over half of the world population and is related to lactase deficiency, preventing digestion of ingested lactose. The number of validation steps followed to bring the biosensor device to the market will be here discussed. Further advices in the preparation of similar processes will be also provided.

CC07

A correlation of the physical attributes of a potent anti-onychomycotic dosage form with microbiological performance

Kapu D[1]
[1]*Athlone Institute of Technology, Athlone, Ireland*

Introduction
Onychomycosis is a clinical fungal nail infection caused by *Trichophyton rubrum*. It is one of the prominent concurrent diseases among diabetic and HIV afflicted populations. Prognosis of this condition results in severe pain and sometimes a disabling of the infected region. Growing concerns about antimicrobial resistance and prolonged therapeutic durations demand development of novel and rapid formulation approaches to cure onychomycosis. Among those alternatives to overcome antimicrobial resistance, active compounds derived from natural resources have been increasingly adopted due to high biocompatibility and low toxicity. In pursuit of this goal, researchers at Athlone Institute of Technology have invented a potent, antimicrobial modified oil (MO) towards various bacterial and fungal infections thereby challenging the commercialized products.

Quality-by-design (QbD) is the *c*GMP prescribed by the regulatory agencies. Establishing patient oriented quality targeted product profile (QTPP) and developing the dosage forms within the constructed design space by correlating critical quality attributes (CQA) with product performance and risk assessment is the key principle of QbD. In this research, QbD principles according to ICHQ8 (R2) have been adopted to formulate MO in a topical dosage form.

Objectives
- Antifungal enhancement of a novel derivative of modified oil (MO) with promising potency towards *Trichophyton rubrum*.
- Adoption of an integrated pharmaceutics and analytical strategy to guide our MO into a superior ungual dosage form.

Materials and Methods
To meet the challenging pre-requisites in correlating CQA towards a superior QTPP, multiple combinations of MO with compendial excipients were formulated. Chemical compatibility was assessed by infrared spectroscopy, differential scanning calorimetry and augmented using anti-fungal testing in the presence of interfering anatomical derivatives. These experiments have guided the discrimination of best-in-class mixtures from potentially sub-optimal selections, based on the CQA of MO. Next, the physical aspects affecting product performance were established using texture analysis, particle size distribution and conductivity as profiling tools.

Conclusions
A superior (versus marketed OTC dosage form) and potent dosage form has been identified from trial mixtures through these analytical techniques. The formulation developed through the application of this strategic approach has proven stable over 90 days in terms of ongoing physical attributes and biological performance.

CC08

Assessing the relationship between honey chemistry and landscape composition

Kavanagh S[1], Stout J[2], White B[1]
[1]Dublin City University, Dublin, Ireland, [2]Trinity College Dublin, Dublin, Ireland

The relationship between landscape composition and honey chemistry has not yet been explored. Honey contains biologically active compounds with potential antioxidative, antibacterial and anticarcinogenic effects. These compounds are beneficial not only to human health but also to bee health.

The aim of this research is to investigate the relationship between landscape composition and honey chemistry.

A total of 131 honey samples were obtained from beekeepers across the island of Ireland. The landscape composition around each hive site was determined using the CORINE Land Cover 2012 database and quantified to a 5 km radius. The phenolic composition of each honey sample was identified and quantified using HPLC-UV.

An analysis of bioactive compounds in Irish honey comparing profiles among geographical regions and harvest times using univariate and multivariate techniques was carried out and the results will be presented and discussed.

Preliminary results suggest that the composition of the surrounding landscape impacts the composition and concentration of phenols in honey. This study has shown that there is a significant difference in the phenolic composition between honeys from predominantly rural areas compared to honeys from predominantly urban areas.

CC09
Fake data – Rationale, detection and implications

Rachetti A[1], Wegscheider W[1]
[1]*Montanuniversität Leoben, Leoben, Austria*

The purpose of this contribution is to review the status of literature on an ugly side of science, tampering with data, and to present some thoughts on the consequences of reporting only "good" data.

In December 2000, the US office of Science and Technology Policy (OSTP) defined research misconduct as "fabrication, falsification or plagiarism (FFP) in proposing, performing or reviewing research or in reporting research results.

A number of spectacular cases of grave misconduct has received wide attention but it may be safely said that only a very narrow number of scientists engage in downright fraud. Real fraud only occurs if the procedures needed to replicate the results of the work or the results themselves are in some way knowingly misrepresented. D. Goldstein is of the opinion that outright fraud is only to be found in the biomedical sciences and never in fields like physics or astronomy or geology.

The reasons for any questionable behaviour by scientists are widespread. J. Antonakis in his position paper identifies five serious diseases that plague the scientific community:

- Significosis, an inordinate focus on statistically significant results
- Neophilia, an excessive appreciation for novelty
- Theorrea, a mania for new theory
- Arigorium, a deficiency of rigor in theoretical and empirical work
- Disjunctivitis, a proclivity to produce large quantities of redundant, trivial and incoherent works

How to spot data fabrication? It has been suggested that statisticians should not publish too much on the methods to detect fraud, since then those wishing to pervert science without being caught will learn how to avoid detection.

S. Evans states that the features of false data will not be the same as ordinary errors. A skilled manipulator might be able to produce convincing data in one dimension, but it is much more difficult to retain the nature of real data when viewed in more dimensions. And wherever there is human intervention, there will often be a digit preference.

There are several methods to detect invented or manipulated data that. Less grave forms of misconduct, like omitting data and keeping inadequate records are almost impossible to detect. The scientific community has to be aware that by not accepting data that do not support a hypothesis or by reporting the "better" values only one relies a questionable "prior" in a Bayesian sense and conclusions will be questionable or incorrect.

We have to accept, in D. Goldstein's words that scientists are not disinterested truth-seekers, they are more like players in an intense, winner-take-all competition for scientific prestige, or perhaps merchants in a noholds barred market-place of ideas.

Abstracts

P01

Using ICP scan analysis as a powerful diagnostic and troubleshooting tool in analytical laboratories

Loucaides A[1], Wilkinson N[1], Papageorgiou G[1], Stylianou C[1], Christodoulou L[1]
[1]*Aristos Loucaides Chemical Laboratory Ltd, Aglanjia, Cyprus*

Contemporary market requirements pose an ever-increasing demand on testing laboratories to cope with more and more non-standard investigations. These may relate to a wide spectrum of materials and matrices, ranging from simple-matrix aqueous samples (e.g. surface, ground & drinking waters, wastewaters) to very complex matrices of different samples sizes and textures like solid deposits, semi-solid residues, soils, sediments, sludge & biological samples etc.

Modern laboratory instrumentation has been providing laboratories with cutting-edge technology to help them engage efficiently and effectively in *forensic* type of investigations, which in small countries, like Cyprus, form a substantial part of our workload, not relating to routine and standardized laboratory activities.

Our laboratory, as being one of the most long- standing private testing laboratories on the island, is frequently engaged in projects that demand investigations on unknown materials. These can be as part of process troubleshooting or even as part of enquiries received from governmental and/or private institutions in the context of anomalies directly associated with or indirectly relating to public health and safety.

Laboratory instrumentation like XRF, XRD, FTIR, GC MS, LC MS/MS and ICP, are all at our disposal for the above kind of *forensic* type investigations. These normally come as very demanding enquiries, on behalf of customers, both in terms of fast TAT's as well as accurate and helpful interpretations.

ICP scanning, provides a qualitative/semi-quantitative analysis covering the entire spectrum of metals, metalloids, alkalies & alkaline earth elements of the periodic table (over 70 elements), in a fraction of the time required by other techniques (anodic stripping voltametry, FAAS etc.). As such, it can be applied in problem solving enquiries as an extremely efficient diagnostic tool, either on its own or complementing other analytical techniques.

However, deciding whether to select ICP scanning over other analytical techniques or in combination with them, selecting the most appropriate sample preparation technique, and most importantly interpreting the results in an appropriate manner that will be of real value to the customer, requires extensive analytical experience, excellent customer feedback, a solid scientific background and the ability to handle and present data in a statistically sound and scientifically justified manner. Therefore, the ability to assess the overall quality and integrity of the produced data, forms an integral part and indispensable requirement of adopting this analytical technique, including the ability to decide whether to reject outliers and/or provide additional instrumental justification/verification.

A number of laboratory projects over the last 15 years, that have employed the ICP scan technique, will be presented, together with detailed reference to data produced and the relevant interpretation provided to end customers.

P02

A new metrological treatment of the calibration data of the cumulative standard addition method

Dadamos T[1], Damaceno A[1], Fertonani F[1], Bettencourt da Silva R[2]
[1]Universidade Estadual Paulista, São José do Rio Preto, São Paulo, Brazil, [2]Faculdade de Ciências, Universidade de Lisboa, Lisbon, Portugal

This work presents methodologies for the development, optimization and validation of procedures for the electrochemical measurement of biochemical parameters in biological fluids. The developed methodology was applied to the voltammetric measurement of uric acid in human serum. The measurements were performed using a cumulative standard addition method (SAM-C), involving a new statistical treatment of the calibration data, which allows the calibration of the instrumentation in a small volume of serum. If the instrumental method of analysis does not consume analysed item volume in the signal collection process, such as molecular spectroscopy, potentiometry and voltammetry, the need for a large volume of the analysed item can be overcome by performing consecutive additions of known quantities of the analyte to the same analytical portion as signal is being collected. Typically, analyte is added through a volume of analyte stock solution. However, since native analyte is diluted as a new volume of analyte stock solution is added, the construction of the calibration curve should take the added analyte mass, *m*, has the independent variable (i.e. the stock solution concentration times the added cumulative volume) and the total sample volume, *v*, (i.e. sample volume plus cumulative added stock solution volume) times the observed signal, *I*, (i.e. *v*I*) has the dependent variable. The ratio between the intercept and the slope of the calibration curve (*v*I* vs. *m*) represents the estimated analyte mass in the item, m_s, and this value divided by the analytical portion volume, V_s, the analyte concentration, Y_s, in the item ($Y_s = m_s / V_s$). If the native analyte dilution as stock solution volume is added is not considered, measurements can be affected by a large error. This error is larger if stock solution concentration used in standard additions is similar to native analyte concentration. The measurement uncertainty was estimated using developed *bottom-up* approaches and using pragmatic *top-down* approaches presented in the literature. The uncertainty components were combined using the Uncertainty Propagation Law or the numerical Kragten and Monte Carlo methods. The *bottom-up* assessments of measurements uncertainty involve the estimation of the extrapolation uncertainty from the regression model or using Monte Carlo simulations applicable to when the assumptions of the regression model are not valid. The cumulative standard addition method was successfully applied to the analysis of human serum by adding 1.0, 3.0, 5.0, 7.0 and 9.0 mg dL^{-1} of AU to 5 mL of serum. The tools developed for the construction and optimization of working electrodes are applicable to the measurement of other analytes and matrices. The developed cumulative standard addition method and respective measurement models, are applicable to any kind of non-destructive chemical measurement of a solution.

P03

Select appropriate data analysis method for evaluation of non-isothermal kinetic parameters

Eftimie Totu E[1], Buga R[1], Totu T[1], Agir I[2], Yildirim R[2]
[1]University Politehnica of Bucharest, Bucharest, Romania, [2]Yildiz Technical University, Istanbul, Turkey

This work presents a critical analysis of some results obtained by applying three different methods to determine non-isothermal kinetic parameters for thermal decomposition of biopolymers for dental medicine. The methods assessed are integral methods – Coats – Redfern and modified Coats-Redfern, and an iterative method. To calculate the integral from the Coats-Redfern modified method it has been used the trapezoidal method for unequal distances. There have been taken in study four different polymeric nanocomposites used for 3D printed dental devices. From the data calculated for each kinetically workable decomposition stage it was easily noticed that there are significant and variable differences between the values of the non-isothermal kinetic parameters (activation energy-E_a, pre-exponential factor-*A*). However, the rate constant calculated using the obtained parameters from the two integral methods applied, lead to similar values despite the recorded differences. Much more, for the iterative method there has been recorded a lack of convergence. Even if significant differences between particular values of kinetic parameters have been obtained the value of the constant rate (k) was similar. In such conditions, when despite the differences between the non-isothermal kinetic parameters calculated by help of the mentioned three methods the thermogravimetric data could be correctly described, a question rise: which method is most appropriate to be applied? The data analysis of all involved parameters has been performed. Subsequently it was developed an assessment program based on linear regression in order to decide which of the mentioned methods is the most appropriate to describe the non-isothermal chemical processes. The program developed allow the selection of the reaction order, *n*, corresponding to the best linearity of

$$\left[log \frac{d\alpha}{(1-\alpha)^n T^2}, \frac{1}{T} \right]$$

where α is the conversion factor and *T* - the absolute temperature. The maximum number of experimental points which could be used is 30. Also, the solution proposed by us overpass the difficulties related to the linearization for the correct reaction order, *n*, of the specific Coats-Redfern equations.

Acknowledgements: This work was supported by a grant of the Romanian National Authority for Scientific Research and Innovation, CCDI- UEFISCDI, project number 30/2016, within PNCDI III. In addition, the research was partially supported by the scientific and technological research council of Turkey, TUBITAK, project number 9150165, MANUNET ERA-NET.

P04
Multivariate data analysis in analytical chemistry

Majek P[1], Majekova M[2]
[1]*Institute of Analytical Chemistry STU in Bratislava, Bratislava, Slovakia,* [2]*Center of Experimental Medicine, Institute of Experimental Pharmacology and Toxicology, Slovak Academy of Sciences, Bratislava, Slovakia*

Multivariate data analysis (MVA) is the investigation of many variables, simultaneously, in order to understand the relationships that may exist between them. MVA methods have been known around for decades, but until recently, have primarily been used in laboratories and rarely being applied to production processes. Analytical chemistry and chemical analysis in the laboratories are mainly associated with the development of chemistry as a scientific discipline and with the progress in techniques and instrumentation because even a simple analyte often represents a multi-component system. Modern automatic analysis methods provide opportunities to collect large amounts of data very easily. For example, in clinical chemistry it is routine to determine many analytes for each specimen of blood, urine, etc. A number of chromatographic and spectroscopic methods can provide analytical data on many components of a single specimen. The widespread use of multi-channel array detectors in spectroscopy and the development of miniature sensor arrays based on solid state or biospecific detection methods have further encouraged the use of multi-analyte measurements, and extended their applications to areas such as process analysis. The result of the analysis is a huge data set and its structure is described by a number of variables that contribute to the overall information about the object being investigated. Data handling of this set is performed by chemometrics, where multidimensional statistical analysis and graphic visualization represent one of its most important parts.

There are several classifications of multidimensional statistical methods – the most common division splits multidimensional statistical methods following: (i) multivariate statistical analysis of multivariate distributions, determination of their fundamental characteristics and hypothesis testing, (ii) analysis of relationship between variables – regression and correlation analysis, analysis of variance and analysis of covariance, canonical correlation analysis, (iii) methods of reducing the number of variables – principal component analysis and factor analysis, (iv) multidimensional classification methods – cluster analysis and discrimination analysis.

This work provides a (non-exhaustive) overview with a brief description of each method in order to help user to decide which specified statistical approach is suitable for a real type of data evaluation.

Acknowledgement: This work was supported by the Scientific Grant Agency of the Ministry of Education of Slovak Republic and the Slovak Academy of Sciences VEGA 2/0127/18 and the Slovak Research and Development Agency under the contract No. APVV-15-0455.

P06
Evaluation of matrix effects

Palma C[1], Morgado V[1], Bettencourt da Silva R[2]
[1]Instituto Hidrográfico, Lisboa, Portugal, [2]CQE - Faculdade de Ciências da Universidade de Lisboa, Lisboa, Portugal

The measurement of trace levels of analytes in complex matrices, such as heavy metals in sediments or pesticide residues in foodstuffs, is frequently affected by matrix effects that vary with the analysed item. In some cases, the determination of the analyte in items of the same class, such as sediments with equivalent organic matter contents or the same fruit, are affected by different matrix effects due to the type of organic matter of the sediment or the maturation of the fruit.

During the development and validation of the measurement procedure, it is necessary to take the variability of matrix effects into account and it can be extremely useful to quantify these effects separately in order to know if it is necessary to improve the robustness of the procedure to matrix effects to increase measurement quality (i.e. to reduce measurement uncertainty).

The standard addition method is the most popular tool used to eliminate matrix effects that vary with the analysed item. However, since its use involves additional analytical work, it should only be used whenever strictly necessary.

This work, presents a methodology to separately quantify the variability of matrix effects in complex measurements in order to decide about the need to improve measurements robustness to these effects. This methodology is based on the comparison of the mean recovery estimated from the analysis of various reference materials and was applied to measurements of heavy metals in sediments by atomic spectrometry where measurements trueness was assessed from the participation in proficiency tests.

P07

Twenty rounds of proficiency test activity organized by the European Union Reference Laboratory for *Escherichia coli* (EURL-VTEC)

Ferreri C[1], Tozzoli R[1], Maugliani A[1], Chiani P[1], Arancia S[1], Michelacci V[1], Minelli F[1], Babsa S[1], Galati F[1], Patriarca M[1], Morabito S[1]
[1]*Istituto Superiore Di Sanità, Rome, Italy*

The EU Reference Laboratory for *E. coli* (EURL-VTEC) was established at the Istituto Superiore di Sanità in 2006, according to the Regulation (EC) No. 882/2004. The EURL coordinates a network of 34 EU National Reference Laboratories (NRLs) plus many non-EU NRLs and the main objective of its mandate is to ensure that the methods used by the NRLs for the identification and typing of pathogenic *E. coli* strains and their detection in food and animal samples are harmonized.

The EURL accomplishes its mandate by developing and evaluating methods, distributing reference materials, organizing proficiency tests (PT), hosting scientists from NRLs for training stages and also collaborating with other EU structures (EFSA, ECDC).

Since 2006, the EURL has developed and evaluated standard operating procedures for the identification and typing of STEC and for their detection in food, mainly based on PCR detection of virulence genes. In particular, it coordinated the development of the ISO/TS 13136:2012 on the detection of STEC in food and animal feed, based on the Real Time PCR screening of food enrichment cultures.

To evaluate both the methods and the performance of the NRL network in their application, the EURL organized so far 20 rounds of proficiency tests (PT) conducted in compliance with the International Standard ISO/IEC 17043:2010.

Eight PTs were dedicated to bacterial typing and included the detection of STEC virulence genes by PCR and the identification of the serogroups most involved in human disease in Europe. Twelve PTs were dedicated to the detection of STEC in different matrices (carcass swabs, milk, spinach, water, seeds, sprouts, spent irrigation water, ground beef meat and rocket salad) using the ISO/TS 13136:2012.

A positive trend was observed in both the number of participating laboratories (from 21 in 2007 up to 40 in 2017) and their performance (up to 97.2 % of labs that correctly identified the presence of virulence genes in the test samples). The overall evaluation highlighted that an excellent preparedness has been built in the EU towards the ability to identify the main virulence genes of STEC, while the capacity to detect other *E. coli* pathotypes and their most represented serogroups, although to a lesser extent, is also present with a good performance.

The control of pathogenic *E. coli* in food and animals represents a challenge for the development of specific detection methods and requires a network of skilled and trained laboratories throughout the EU for their detection in the vehicles of infection. The EURL-VTEC is working to consolidate such a network, in order: i) to contribute to the knowledge of the epidemiology of STEC infections in Europe; ii) to gather harmonized data on the prevalence of these pathogens in the food samples finalized to the definition of microbiological criteria for STEC; iii) to provide the EC with a network of laboratories operating with standardized operative procedures and tools to ensure a harmonized monitoring of these microorganisms and to face possible emergencies.

P08

Exploring data quality of multivariate HRMS data in food authenticity research

Kostakis M[1], Dasenaki M[1], Aalizadez R[1], Thomaidis N[1]
[1]*National and Kapodistrian University of Athens, Zographou, Greece*

The rapid development of HRMS-based metabolomics boosted the research and the development of new approaches in food authenticity studies. The large amount of data produced with HRMS techniques can be used to determine the molecular fingerprint of food and to detect food fraud, using both targeted and untargeted metabolomics approaches. However, this technique has not been widely used so far by official authorities in EU for food adulteration control, with the main drawback being the difficulty of data treatment and integrity assessment by the end user. Moreover, most of the times the results of multivariate statistical processing are binary, and there is not always a clear compliance with parameters characterizing an adulterated product. The aim of this study is to investigate the development of validation protocols to assess the data quality of multivariate statistical processing. Juice-to juice adulteration of pomegranate juice with apple juice was used as a case study in order to produce and validate a statistical model that can reliably assess food adulteration.

P09

Using measurement uncertainty to assess the fitness for purpose of analytical procedures used in pharmaceutical industries

Lourenço F[1], da Silva R[2]
[1]*Faculdade de Ciências Farmacêuticas, Universidade de São Paulo, São Paulo, Brazil,* [2]*Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal*

Analytical procedures used in the pharmaceutical industry are often subject to international validation protocols, however the estimation of the measurement uncertainty is rarely considered. In this paper, we estimated the uncertainty of measurements of linezolid and caspofungin, in pharmaceutical dosages, using eight analytical procedures, and determined the risk of the measurement uncertainty producing wrong compliance decisions. This risk was estimate from the Bayesian updating of a prior knowledge of the variability of pharmaceuticals composition from medicines production, with the measurement of this composition in a sample of a medicine using the measurement procedure. Several sources of uncertainty affecting performed measurements were considering in this study, including analytical instrument quantification, weighing and volumetric operations, chromatographic repeatability, microbiological variability, among others. The combined relative standard uncertainties of linezolid measurements were found to be 1.06 %, 1.26 %, 1.55 % and 4.10 % for UV spectrophotometric assays, ultrahigh-pressure liquid chromatographic (UPLC) method, agar diffusion and colorimetric bioassay, respectively. For caspofungin quantification, relative standard uncertainties were found to be 1.44 %, 2.45 %, 1.25 % and 0.85 % for UPLC, capillary electrophoresis (CE), CE with internal standardization, and agar diffusion microbiological assay, respectively. The content of the active substance of 50,000 lots were simulated from the expected variability of pharmaceuticals production (i.e. the *a priori* distribution), and for each simulated content it was simulated the measured quantity value by taking the measurement uncertainty. Sequential simulations were performed by the Monte Carlo Method, MCMC. Consumers' risk is defined as the probability of a lot not meeting the specification being considered compliant since the measured quantity value is within the specification limits. On the other hand, producers' risk is the probability of a complaint lot being wrongly rejected since the measured quantity value is outside the specification limits. It was assumed, based on previous knowledge about the industrial production of the studied pharmaceutical dosages, that the content of the active substance has a normal distribution centered in the middle of the specification interval and with a dispersion that guarantee that 99.73% (49,863/50,000) of produced lots are within the specification. Small consumers' risks, between 0.050 %, for caspofungin measurement by agar diffusion method, and 0.121 %, for the quantification of linezolid by colorimetric bioassay, were estimated. Producers' risks were found to be very high, between 41 %, for the quantification of caspofungin by agar diffusion method, and 97 %, for the quantification of linezolid by colorimetric bioassay. Consumers' and producers' risks can be reduced by decreasing the measurement uncertainty, achieved by increasing the number of repetitions, using internal standardization or reducing other major sources of uncertainty. All these analytical procedures were validated in our lab, however some of them are not fit for assessing products conformity. The impact of the measurement uncertainty in compliance assessment can be controlled if the measurement uncertainty is part of the compliance decision rule.

P10

Quality control procedures in food microbiological testing

Yolci Ömeroğlu P[1], Abbasova T[2], Babayeva N[2]
[1]Uludag University Faculty of Agriculture Food Engineering Department, Bursa, Turkey, [2]Azerbaijan Standardization Institute, Agriculture and food products testing laboratory

Microbiological food analyses are based on biological, biochemical, molecular methods for the detection, identification or enumeration of microorganisms in food. Each day many laboratories carry out thousands of microbiological analysis of food and water in order to control the critical control points in HACPP plan for the production, final and raw material quality and compliance with the legal requirements. Therefore, the laboratories should produce reliable measurement results. To meet those specific needs, a proper method should be selected, moreover if there is a standard test method on that area, it should be preferred. To comply with the fitness of the purposes, the methods should be validated or verified. Following verification of the method performance criteria, proper internal or external quality control tools should be selected to systematically monitor and to evaluate the daily work. Internal quality control consists of all the procedures undertaken by a laboratory for the continuous evaluation of its work in order to ensure the consistency of results day-to-day and their conformity with defined criteria. The quality control procedures in a food microbiological testing laboratories include use of spiked samples contaminated with reference culture, checking the linearity of dilutions, assessing repeatability and reproducibility of the method during routine analysis, checking replicate counting of the colonies in petri dishes by two analysts, positive and negative growing test for reference culture, checking water quality used in the analysis, sterility tests, calibration of equipment, quality assurance for temperature controlled equipments, monitoring sterilization process, participation proficiency tests, etc. In this presentation, it is aimed to explain the quality control tools for a food microbiological testing laboratory with given examples in addition to the statistical tools for the evaluation of the results.

P11
Data integrity in the Forensic Explosives Laboratory

Fenwick C[1], Sonden L[1]
[1]*Dstl, Forensic Explosives Laboratory, Fort Halstead, Sevenoaks, England*

The Forensic Explosives Laboratory (FEL) carries out forensic analysis of explosives and related materials in relation to suspected criminal and terrorist use. FEL's main output is expert witness statements for use in the Criminal Justice System. For expert witness statements to be used in court, FEL is required by the Forensic Science Regulator (FSR) to be accredited by the UK Accreditation Service (UKAS) to ISO17025 and the FSR's Codes of Practice and Conduct for Forensic Science Practitioners.

Within the last year, data integrity has become a hot topic within forensic science, and the FSR and UKAS have been applying pressure to forensic laboratories to provide more robust assurance of data integrity of forensic results and supporting information such as quality assurance and environmental monitoring. Poor data integrity could increase the risk of a miscarriage of justice, which could result in a criminal or terrorist walking free, or an innocent person being sent to prison.

FEL are in the process of improving data integrity by assessing the risks and putting proportionate measures in place to eliminate or mitigate them.

P12
Acetonitrile analysis in hydrocarbon (Crude C4) by gas chromatography

Demirlek Y B[1], Coşar T[1]
[1]*Petkim Petrochemical*

In the by-product extracted by steam naphtha cracking process Crude C4, consist of approximately 40-50 different components. Acetonitrile, one of these products, damages the process that C4 used as raw material. By this study a new chromatographic method has been developed to determine acetonitrile quantity in crude C4 mix which produced by steam naphtha cracking process. As conclusion, Acetonitrile as up to 3 ppm has detected in crude C4 with appropriate system configuration and right system parameters. Method validation studies made by a gas chromatograph with a suitable column and valid result had obtained.

P13

Eurachem: a focus for analytical chemistry in Europe

Eurachem Executive Committee: Barwick V[1], Bettencourt da Silva RJN[2], Brookman B[1], Bulska E[3], Ellison SL[1], Magnusson B[4], Milde D[5], Patriarca M[6], Ramsey MH[7], Sibbesen L[8], Eftimie Totu E[9], Tsimillis K[10], Vercruysse I[11], Wegscheider W[12]

[1]LGC, UK; [2]University of Lisbon, Portugal; [3]University of Warsaw, Poland; [4]Research Institutes of Sweden, Bioscience & Materials, Chemistry & Materials, Sweden; [5]Palacky University in Olomouc, Czech Republic; [6]Istituto Superiore di Sanità, Italy; [7]Sussex University, UK; [8]LAB Quality International, Denmark; [9]University "Politehnica" of Bucharest, Romania; [10]Pancyprian Union of Chemists, Cyprus; [11]BELAB, Belgium; [12]Montanuniversität Leoben, Leoben, Austria

Eurachem (www.eurachem.org) is a network of organisations within Europe designed to a) establish a system for the international traceability of chemical measurements and b) promote good quality practices in analytical sciences. Currently represented in 33 European countries, the aim is to provide a forum for analytical scientists, laboratory staff and those interested in using the results of analytical measurements to discuss common problems and develop informed and considered approaches to both technical and policy issues.

Members and stakeholders meet once a year at the Eurachem General Assembly. An Executive Committee and several topical Working Groups pursue the organisation's stated goals throughout the year, often in cooperation with other organisations. Participation is open and channeled through national representatives.

Eurachem's main output is authoritative guidance documents, promoted through dedicated events which are also designed to provide opportunities for collecting feedback. Beside the guides there are also information leaflets, i.e. short briefing documents on specific topics usually intended to inform a wide audience, including laboratory staff, managers and laboratory customers. This poster aims to summarise current Eurachem activities, inform readers about the available guidance and attract active participation.

P14
Eurachem Ireland

O'Leary B[1], Fay H[2], Cantwell H[1], Ó'Ríordáin C[1], McGowan S[1], Behan P[3], Hayden R[4], McGowan T[5], White B[6], Hyland S[7], O'Gorman M[8]
[1]The State Laboratory, [2]Henkel Ireland, [3]Dublin Institute of Technology, [4]HSE Public Analyst's Laboratory, [5]Sligo Institute of Technology, [6]Dublin City University, [7]Pesticides Laboratory DAFM, [8]Pfizer

Eurachem is an organisation within Europe which aims to promote excellence in analytical sciences. It is composed of a network of national and other organisations. In Ireland, the organization which promotes the objectives of Eurachem is Eurachem Ireland. Eurachem Ireland has members from industry, from regulatory laboratories and from educational institutes and provides a forum for the discussion of common interests. It operates a mailing list to keep members informed of new developments and to increase awareness of opportunities to participate in research.

The activities of Eurachem Ireland are varied. Eurachem Ireland holds regular workshops, annually facilitating a TrainMic workshop focussing on topics in metrology in chemistry. Each year, in conjunction with educational institutions, it runs the Eurachem Analytical Measurement Competition for undergraduate chemistry students. Articles are published in the Irish Chemical News under Eurachem Ireland's Focus on Analytical Chemistry and Irish representatives, recommended by Eurachem Ireland, now sit on many of the Eurachem Working Groups.

All are welcome to become involved in Eurachem Ireland whether by suggesting topics for workshops, joining a Eurachem Working Group or simply joining the mailing list to keep informed of activities.

Mailing list:	Send an email to eurachem@statelab.ie
Website:	www.statelab.ie/eurachem.html
LinkedIn:	Eurachem Ireland

Abstract

P15

Eurachem Method Validation Working Group

Eurachem Method Validation Working Group members ("C" denotes corresponding member): Vercruysse I[1], Lamon G[2], Sibbesen L[3], Robouch P[4], Dehouck P[4], Pohl B[5] (C), Bogan Y[6] (C), Christie É[7], Cantwell H[8], Clancy J[9], Gregori E[10], Patriarca M[10], Gjengedal ELF[11], Bulska E[12] (C), Hrastelj N[13], Morillas Bravo PP[14], Raposo F[15], Karlsson A[16], Örnemark U, Akçadağ F[17], Biniçi B[17], Yilmaz A[18], Yolci Ömeroglu P[19], Barwick V[20], Ellison S[20] (C), Boubetra A[21]

[1]BELAB, Belgium, [2]SGS, Belgium, [3]LAB Quality, Denmark, [4]IRMM, EU, [5]Merck KGaA, Germany, [6]The Marine Institute, Ireland, [7]EPA, Ireland, [8]State Laboratory, Ireland, [9]Henkel Ireland, [10]Istituto Superiore di Sanità, Italy, [11]Uni. f. Miljø- og Biovidenskab, Norway, [12]University of Warsaw, Poland, [13]EuCheMS, Slovenia, [14]Canal de Isabel II, Spain, [15]CSIC, Dept. of Food Biotechnology, Spain, [16]RISE, Sweden, [17]UME, Turkey, [18]Cevre Laboratory, Turkey, [19]Okan University, Turkey, [20]LGC, UK, [21]BIPEA, France

The Eurachem Method Validation Working Group (MVWG) aims to function as a centre of expertise in the field by assembling and promoting best practice in method validation. The working group has members from countries throughout Europe and meet twice a year to provide guidance on method validation which will be applicable to all chemical analytical laboratories, meet the requirements for accreditation and address new developments within analytical chemistry.

The group organizes and contributes to international seminars and workshops on issues related to method validation within analytical chemistry. They ran an international workshop entitled Method Validation - Current Practices and Future Challenges in Ghent in 2016 and will host a session on method validation in the 22nd International Mass Spectrometry Conference to be held in Florence in August, 2018.

The MVWG produce a guide to method validation entitled "The Fitness for Purpose of Analytical Methods: A Laboratory Guide to Method Validation and Related Topics". This is available to download at www.eurachem.org/index.php/publications/guides/mv.

Conference Notes

Head Office, Belfast
Tel: +44 (0)28 9066 4020

Dublin Office
Tel: +353 (0)1 5314118

www.happeningconferences.com

happening
conferences & events