



ERASMUS MUNDUS MASTER IN QUALITY IN ANALYTICAL LABORATORIES (EMQAL)

MODULE DESCRIPTORS 2021 11th EMQAL EDITION

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Quality Management

Module Title:

Introduction to Quality Management

Module Code: QM01

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

No pre-requisites are necessary for this module.

Notional Learning Hours

(a) Contact time: 10

(b) Private study: 40

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Formal lectures in 60 / 90 min timetable

Convener:

The name of the member of permanent staff responsible for the module

Isabel Cavaco

University:

The name of the University and Department responsible for the module

University of Algarve / Department of Chemistry and Pharmacy

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

1. To motivate students for the importance of the implementation of Quality Systems in laboratories of analysis, considering the advantages and the costs involved.
2. To introduce the concepts of Quality Management, Quality Assurance and Quality Control
3. To introduce the concepts of certification and accreditation, and the ISO standards for Quality Systems
4. To introduce general aspects of Laboratory Quality Management

General learning outcomes (to which this module is contributing)

1. Design, implement and manage a quality system in an analytical laboratory

Specific learning outcomes expected from students at the end of this module and contributing to General Learning Outcome 1:

1. To recognize the necessary elements in the structure of a Quality System
2. To propose and design (in broad lines) a new Quality Management System, applied to a given organization.
3. To understand and justify clearly the importance of Quality Systems in analytical laboratories, in the context of both local and international economies
3. Analyze in detail the costs involved in Quality System implementation in routine analytical laboratories

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

This module aims to motivate students for Quality Management, and to introduce the fundamental concepts which will be applied throughout the program.

Part 1 – “Quality”: the module starts with a discussion on what is the meaning of “Quality”, how the concept has evolved along human History and the complexity of its modern definition. The concepts of product specifications, production variability and process are introduced. The Quality Policy Statement is introduced, as the foundation stone of the Quality Management System (QMS). The concept of quality is further explored and applied to Analytical Laboratories.

Part 2 – Quality Management Principles: The concepts of Quality System, Quality Management and Quality Control are distinguished and explained. The 8 principles of Quality Management are discussed: Customer Focus, and how it relates to the Quality policy; Leadership: what it means and how it affects the organization; the Involvement of People and how it can be pursued; the Process Approach and how to apply it to any activity; the importance of a Systematic Approach to Management, factual approach to decisions and the need for statistics, mutually beneficial relationships and Continual Improvement.

Part 3 – “Quality Management Implementation” – The steps towards implementing a QMS are described and exemplified. The concept of process approach to organize activities is developed. The concept of indicators is introduced, together with guidelines for defining and interpreting them. The most critical aspects of implementing a QMS are considered and discussed: the role and involvement of the Top Management, preparing Documentation, Assessing the QMS and implementing a Continual Improvement Cycle.

Part 3 – “Costs (and benefits) of Quality” – A brief analysis of the costs of implementing quality and a comparison with its benefits. This may provide EMQAL students with powerful arguments for future discussions convincing others to implement QMSs.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Students are asked to choose between two assessment modes:

- 1) Final Assignment (90%) + Homework Assignments (10%)

Or

- 2) Final Assignment (100%)

The Final Assignment typically consists in designing a Quality Management System applied to an organization. The detailed assignment structure will be described during the first class. The Homework Assignments are submitted daily and consist in developing the parts of the System which correspond to the topics taught each day. The Homework Assignments may receive feedback and can be used as part of the Final Assignment.

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Lecture notes will be available for students.

E. Pritchard, V. Barwick, “Quality Assurance in Analytical Chemistry”, Wiley, 2007

Recommended reading: ISO Quality system standards: ISO 9000, ISO 9001, ISO 14000, EN ISO/ICE 17025

Module Title:

Laboratory Quality Systems: ISO/IEC 17025

Module Code:

QM02

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Notional Learning Hours

(c) Contact time: 10h

(d) Private study: 40h

Format of Teaching:

Lectures and seminars: 8 h

Practical exercises: 2 h

Others (specify): 0 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Formal lectures in 60/90 min timetable

Real and practical examples

Convener:

The name of the member of permanent staff responsible for the module

Carmen Navarro

University:

The name of the University and Department responsible for the module

University of Barcelona, Quality Research Service

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

- 1.To introduce the structure and the content of the ISO/IEC 17025 standard.
- 2.To explain how this standard is implemented in analytical laboratories.
- 3.To teach how this standard is applied to the accreditation process of analytical laboratories.

General learning outcomes (to which this module is contributing)

1. Design, implement and manage a quality system in an analytical laboratory;
2. Implement suitable internal and external quality control activities in an analytical laboratory

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

The module will start with general view about ISO 17025 standard, emphasizing its scope in analytical laboratories, highlighting the differences with the scope of GLP and GMP regulations.

Then the requirements of the ISO/IEC 17025 standard will be presented, with real examples of its implementation in analytical laboratories.

Finally, the accreditation process will be explained emphasizing this assessment step (audit), the analysis of the causes of nonconformities, and the corrective actions taken. The main documents of the process will be studied. Sources of information about the accreditation bodies and accredited laboratories will be analyzed.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Homework and participation in the classroom discussion (40%)
Group Written Work assignment (60%)

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

- ISO/IEC 17025 standard (<https://www.iso.org/standard/66912.html>)
- UK's National Accreditation Board (<https://www.ukas.com/>)
- International Laboratory Accreditation Cooperation, ILAC (<https://ilac.org/>)
- European Accreditation (<https://european-accreditation.org/>)
- United States Accreditation Services (<http://usaaccreditation.com/laboratory-accreditation.html>)

Module Title:

Good Laboratory and Manufacturing Practices

Module Code:

QM03

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Notional Learning Hours

(e) Contact time: 10h

(f) Private study: 40h

Format of Teaching:

Lectures and seminars: 7.5 h

Practical exercises: 2.5 h

Others (specify): 0 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Formal lectures in 60/90 min timetable

Real and practical examples

Convener:

The name of the member of permanent staff responsible for the module

Carmen Navarro

University:

The name of the University and Department responsible for the module

University of Barcelona, Quality Research Service

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

1. To introduce the background, objective and scope of Good Laboratory Practice (GLP) and Good Manufacturing Practice (GMP).
2. To explain the legal basis and main aspects to take into account for GLP and GMP compliance
3. To explain how GLP can be implemented in the analytical laboratories and give some general ideas about specific aspects of GMP applied to quality control laboratories.
4. To explain the process of GLP and GMP certification and some aspects about international mutual acceptance

General learning outcomes (to which this module is contributing)

1. Design, implement and manage a quality system in an analytical laboratory;
2. Implement suitable internal and external quality control activities in an analytical laboratory

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

The module will start with a general overview about the background, objective and scope of GLP and GMP, highlighting the differences in the scope between both regulations. Then some information about the available documents at international level to support the implementation and compliance with GLP and GMP (USA Federal Register, European Union Directives, OECD documents,...) will be provided.

A general overview of GLP requirements will be presented, emphasizing the aspects related to the responsibilities of the personnel working in analytical laboratories. After this, the process of implementation of GLP in an analytical laboratory will be carefully explained, using real and practical examples. The explanations will be focused on the features of GLP that make them different from the other quality management systems applied to laboratories.

In the case of GMP, the explanations will be focused on the activities of quality control laboratories, highlighting the similarities and differences with GLP.

The process for GLP certification will be explained and the impact, at national and international level for a laboratory included in its national program of GLP compliance, will be analyzed in terms of mutual agreement of results between countries. In the case of GMP, a general overview about certification in different countries will be explained.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Practical exercises and participation in the classroom discussions (40%)

Group Written Work assignment (60%)

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

- OECD Series on Principles of Good Laboratory Practice (GLP) and Compliance Monitoring (<http://www.oecd.org/chemicalsafety/testing/oecdseriesonprinciplesofgoodlaboratorypracticeglpandcompliancemonitoring.htm>)
- European Union GLP (https://ec.europa.eu/growth/sectors/chemicals/good-laboratory-practice_en)
- FDA GLP (<https://www.accessdata.fda.gov/scripts/cdrh/cfdocs/cfcfr/CFRSearch.cfm?CFRPart=58>)
- FDA Current Good Manufacturing Practice (CGMP) regulations (<https://www.fda.gov/drugs/pharmaceutical-quality-resources/current-good-manufacturing-practice-cgmp-regulations>)
- European Union Current Good Manufacturing Practice (CGMP) regulations (https://ec.europa.eu/health/documents/eudralex/vol-4_en)
- International Council for Harmonisation quality guidelines (<https://www.ich.org/page/quality-guidelines>)

Module Title:

Quality Systems Documentation

Module Code:

QM04

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

No pre-requisites are required.

Notional Learning Hours

(g) Contact time: 10 h

(h) Private study: 30 h

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Formal lectures combined with examples and exercises

Convener:

The name of the member of permanent staff responsible for the module

Rosa Vilanova

University:

The name of the University and Department responsible for the module

University of Barcelona / Agency for Policies and Quality

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

To present the different categories of documents, their structure and the relationship between them.

At the end of the module the learner is expected to be able to:

A1. To know the different categories of documents in a Quality System

A2. To know the structure and contents of different documents

A3. To know the documentation management

General learning outcomes (to which this module is contributing)

1. Design, implement and manage a quality system in an analytical laboratory;

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

This module explores the fundamental aspects of the quality system documentation, focusing on the different types of documents, their structure and contents, and how to manage the documentation. Topics that will be discussed include:

-Type of documents:

- Quality Policy, Quality Manual and related documentation
- Procedures, Work Instructions and Forms
- External and others documents
- Records

-Structure of each type of documentation.

-Documentation Management.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

1. Class activities (20 %). Evaluation of A1– A2
2. Work assignment (80 %). Evaluation of A1- A3.

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Recommended reading:

Quality standards and guidelines systems:

ISO 9001, ISO 17025, ISO 15189, OECD Series on Principles of Good Laboratory Practice (GLP), ICH Q10

MHRA GXP Data Integrity Guidance and Definitions

Management system documents:

ISO 15489, ISO 30301, ISO/TR 15801

Lecture presentation will be available for students.

Module Title:

Risk assessment in analytical laboratories

Module Code:

QM05

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

None

Notional Learning Hours

(i) Contact time: 10h

(j) Private study: 40h

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Lectures and resolution of practical cases in sessions of 120 or 150 minutes

Convener:

The name of the member of permanent staff responsible for the module

Anna Soler

University:

The name of the University and Department responsible for the module

Biomedical Diagnostic Center (BDC). Hospital Clínic de Barcelona

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

This course is an introduction to the study of key concepts and methodologies of risk assessment in analytical laboratories. It introduces the theory and the practice of standardization of risk assessment process and risk management, regarding the quality of data produced by an analytical laboratory. The course explores the most frequent tools and methodologies used in risk assessment and management in order to improve the processes of the laboratory.

General learning outcomes (to which this module is contributing)

1. Design, implement and manage a quality system in an analytical laboratory

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

1. Processes in the analytical laboratory
2. Basic concepts of risk assessment and risk management
3. Tools for risk management
4. Risk management applied to the processes of an analytical laboratory
5. Application and implementation of risk management strategy in an analytical laboratory

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Written assessment work: 70%.

Class activities: 30%.

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

1. ISO 31000:2018 Risk management. Guidelines
2. ICH Q9: Quality risk management
3. ISO 9001:2015 Quality management systems — Requirements
4. ISO 17025:2017 General requirements for the competence of testing and calibration laboratories

Module Title:

Calibration and verification

Module Code:

QM06

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Notional Learning Hours

(k) Contact time: 10 h

(l) Private study: 40 h

Format of Teaching:

Lectures and seminars: 10 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Formal lectures and seminars in 60/90 min timetable

Convener:

The name of the member of permanent staff responsible for the module

Oscar Núñez / Elisabet Fuguet

University:

The name of the University and Department responsible for the module

University of Barcelona, Department of Chemical Engineering and Analytical Chemistry

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

- The aim of this module is to address all the activities related to the verification and calibration of the instruments and equipment in an analytical laboratory.

General learning outcomes (to which this module is contributing)

2. Implement suitable internal and external quality control activities in an analytical laboratory
4. Develop and validate new methods of analysis;
5. Plan a validation program for a given method of analysis;
6. Critically analyze and evaluate data using statistical tools and software

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

This module explores the fundamental aspects of the quality system related with equipment calibration and verification. Topics that will be discussed include:

- Calibration and verification information
- Calibration and verification frequency
- Calibration methods
- Records/Documentation
- Contents and responsibilities

Documentation Management

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

1. Written assessment (70 %). Evaluation of learning outcomes 2-6
2. Seminar activities (30 %). Evaluation of learning outcomes 2-6

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Lecture notes will be available for students.

Recommended reading:

E. Prichard, V. Barwick. Quality Assurance in Analytical Chemistry. Wiley 2007.

E. Prichard. Quality in the Analytical Chemistry Laboratory. ACOL Series. John Wiley & sons, 1995.

M. Parkany. Quality Assurance and TQM for Analytical Laboratories. The Royal Society of Chemistry, 1995.

B. W. Wenclawiak, M. Koch, E. Hadjicostas (Eds.). Quality Assurance in Analytical Chemistry. Springer 2003.

Module Title:

Proficiency Testing Schemes and Reference Materials

Module Code:

QM07

Pre-requisites (if any)

No pre-requisites are required

Notional Learning Hours

(m) Contact time: 10 h

(n) Private study: 40 h

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Formal lectures and practical seminars in the classroom in 60/120 min timetable

Convener:

Susana Amézqueta

University:

University of Barcelona, Department of Chemical Engineering and Analytical Chemistry

Module Description - The Purpose or Aims:

1. To show the role of certified reference materials for assuring traceability of analytical measurements.
2. To introduce the types and uses of reference materials (certified reference materials (CRMs) and quality control materials (QCMs) in analytical laboratories.
3. To introduce the preparation steps involved in the production of reference materials.
4. To provide guidelines for selecting suitable RMs for a specific purpose.
5. To introduce different types of intercomparison exercises and their aims.
6. To introduce the statistical concepts allowing the correct evaluation of the participation of an analytical laboratory in a proficiency test (PT).
7. To provide guidelines for establishing the participation program of an analytical laboratory in PTs and for evaluating laboratory participation.

General learning outcomes (to which this module is contributing)

2. Implement suitable internal and external quality control activities in an analytical laboratory
4. Develop and validate new methods of analysis
5. Plan a validation program for a given method of analysis
6. Critically analyze and evaluate data using statistical tools and software

Summary of Course Content:

The module aims to show to the students the different types of reference materials available and to introduce its proper use in an analytical laboratory, both in the validation step of an analytical method and in different steps of the laboratory quality control system (internal and external quality control). The preparation steps involved in production of RMs will be introduced, as well as all the analytical work required for homogeneity and stability tests. Different types of intercomparison exercises will be described and the different steps involved in the organization of a PT scheme will be detailed. The minimum statistical tools for the evaluation of the technical competence of a laboratory participating in a PT will be introduced. Guidelines for selecting suitable RMs and PTs for an analytical laboratory will be provided.

Assessment Methods:

Class activity (30 %)

Written assessment work (70 %)

Relevant literature:

1. Proficiency Testing in Analytical Chemistry. R.E. Lawn, M. Thompson, R. F. Walker. Royal Society of Chemistry. LGC (Teddington), 1997. ISBN: 0-85404-432-9
2. Practical statistics for the analytical scientist. A bench guide. T. Farrant. Royal Society of Chemistry. LGC (Teddington), 1997. ISBN: 0-85404-442-6

Module Title:

Method Validation

Module Code:
QM08

Pre-requisites (if any)

General orientation and knowledge in basic statistics (definitions, statistical test), and basic knowledge in Excel software is required.

Notional Learning Hours

- (o) Contact time: 15 h
- (p) Private study: 10 h

Format of Teaching:

Lectures and seminars: 10 h
Laboratory practices: 0 h
Others (specify): 0 h

Teaching Strategy:

Lectures will cover the theoretical part concerning definitions of validation and validation parameters and the method for calculating and determining them.

Exercises will cover a number of examples of calculating validation parameters. Creation of a validation report as the final conclusion of validation parameters determination will also be covered.

Convener:

Piotr Konieczka

University:

Gdańsk University of Technology / Faculty of Chemistry / Department of Analytical Chemistry

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

The principal aim of this module is to provide students with basic orientation in the field of method validation and determination of validation parameters.

Specifically the following aims should be achieved:

1. Provide insight in to basic theory – definition of validation parameters.
2. Provide skills permitting the effective usage of standard programs for the determination of validation parameters.
3. Provide students with abilities for proper understanding and interpretation of basic statistics for the determination of validation parameters

General learning outcomes (to which this module is contributing)

At the end of the module the student is expected to:

1. Getting general orientation in the role and place of method validation in the analytical process.
2. Learning usage of standard programs applied for validation parameters calculations.
3. Learning by examples validation parameter determination.

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

Lectures: Basic definition concerning with method validation and validation parameters. Tools used for validation parameters calculation. Basic statistical test. Method for determining selectivity, linearity, limit of detection, limit of quantitation, range, precision, accuracy, uncertainty.

Practical: Usage of standard computer program (MS Excel) for validation parameter calculations.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Assessment will be done on the basis of the preparation of a validation report on the basis of a set of data measurements. The solution of the latter part may be sent by the students for the evaluation by e-mail after the course.

Threshold:

Correct calculation of 50% of validation parameters and its presentation in the final validation report.

Good:

Correct calculation of 80% of validation parameters and its presentation in the final validation report.

Excellent:

Almost perfect calculation of all validation parameters and excellent preparation of the final validation report.

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Handouts of the lecture presentations will be prepared and sent to the students in advance (2 weeks before the course starts).

Recommended textbooks (in order of preference):

1. L. Huber, "Validation and Qualification in Analytical Laboratories", www.labcompliance.com, 1998.
2. A. Ambrus, "Practical Approach to Validation of Methods for Analysis of Residues", FAO/IAEA Training and Reference Centre for Food and Pesticide Control, Draft 1, <http://www.iaea.or.at/programmes/nafa/d5/trcfpc/d5-trcfpc.html>, 1999.
3. International Conference on Harmonization (ICH) of Technical Requirements for the Registration of Pharmaceuticals for Human Use: Text on Validation of Analytical Procedures, ICH-Q2A, Geneva 1994.
4. International Conference on Harmonization (ICH) of Technical Requirements for the Registration of Pharmaceuticals for Human Use: Validation of Analytical Procedures: Metrology, ICH-Q2B, Geneva 1996.
5. United States Pharmacopeial Convention, United States Pharmacopeia 23, US Rockville, 1995.
6. B. W. Wenclawiak, M. Koch, E. Hadjicostas, "Quality Assurance in Analytical Chemistry", Springer Verlag, Berlin Heidelberg 2004.
7. P. Konieczka, J. Namieśnik, "Quality Assurance and Quality Control in the Analytical Chemical Laboratory: A Practical Approach", CRC Press, Taylor and Francis Group, 2018.

Module Title:

Internal Quality Control

Module Code:

QM09

Pre-requisites (if any)

The modules QM01 and QM08, DA01 and DA02 must have been previously taken.

Notional Learning Hours

(q) Contact time: 15 h

(r) Private study: 20 h

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Formal lectures in 60/90 min timetable.

Convener:

Piotr Konieczka

University:

Gdańsk University of Technology / Faculty of Chemistry / Department of Analytical Chemistry

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

4. To introduce the concept and the activities of internal quality control in analytical laboratories.
5. To explain the requirements of ISO 17025 standard concerning internal quality control.
6. To explain the statistical tools used in quality control.
7. To teach the types, preparation and use of control charts.
8. To enable students to assess the results of the quality control activities.

General learning outcomes (to which this module is contributing)

At the end of the module the student is expected to:

4. Understand the concept and get to know the activities of internal quality control in analytical laboratories.
5. Become familiar with the requirements of ISO 17025 standard concerning internal quality control.
6. Understand and be able to properly apply the statistical tools used in quality control.
7. Acquire experience in the preparation and use of the different types of control charts.
8. Become familiar with the interpretation of the results of the internal quality control activities and propose preventive and corrective actions if they are necessary.

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

The module will start reviewing the processes of method development, validation, routine implementation and quality control (internal and external). The relationship among these activities will be clarified and reinforced. Then, the requirements of the ISO 17025 and ISO 15189 standards concerning internal quality control will be revisited and compared. Next, by means of selected examples of sets of analytical data, the statistical tools used in quality control will be reviewed. Then the preparation and use of Shewhart charts for the assessment of trueness and precision will be explained. Subsequently, the less used CUSUM and multivariate charts will be briefly introduced. Next, several case studies will be proposed in order to practice the interpretation of quality control results and to propose changes in the analytical methods so as to correct their malfunctioning.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

1. SLO1 to SLO5 – Homework and participation in the classroom discussions (50%)
2. SLO3 to SLO5 – Written exam (50%) Almost perfect calculation of all validation parameters and excellent preparation of the final validation report.

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Lectures notes and a copy of the ISO/IEC 17025 standard will be available for students.

Recommended reading:

1. D.L.Massart, B.G.M. Vandeginste, L.M.C. Buydens, S. de Jong, P.J. Lewi, J. Smeyers-Verbeque. *Handbook of Chemometrics and Qualimetrics*. Elsevier. 1997.
2. E. Mullins. *Statistics for the quality control chemistry laboratory*. The Royal Society of Chemistry 2003.
3. W. Funk, V. Dammann, G. Donnevert. *Quality Assurance in Analytical Chemistry*. Second Edition. VCH. 2007.

Module Title:

Laboratory Audits (EN ISO 19011)

Module Code:

QM10

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Modules QM01 to QM09

Notional Learning Hours

(s) Contact time: 10 h

(t) Private study: 40 h

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Lectures and resolution of practical case studies in sessions of 2-2,5 h

Convener:

The name of the member of permanent staff responsible for the module

Àngels Sahuquillo

University:

The name of the University and Department responsible for the module

University of Barcelona. Department of Chemical Engineering and Analytical Chemistry.

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

The aim of the module is to provide basic tools to be able to:

- Know the key concepts related to analytical laboratory audits.
- Understand the process of an audit and the requirements to guarantee the evaluation of a quality management system (mainly based on ISO 17025).
- Identify and prepare the documents needed in the different steps of an audit process.
- Develop an audit in practice from the point of view of the two involved parts: analytical laboratories and auditors.

General learning outcomes (to which this module is contributing)

2. Implement suitable internal and external quality control activities in an analytical laboratory
4. Develop and validate new methods of analysis;
5. Plan a validation program for a given method of analysis;
6. Critically analyse and evaluate data using statistical tools and software

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

The contents of the module are the following:

1. Introduction: Concept of auditing and defined criteria. Types of audits and aims. Elements of the audit process: audit team and evaluation of evidences. Steps of an audit.
2. Documents related to all steps of the audit process: initial preparation, schedule of meetings, questionnaires; audit reports.
3. Case studies: audit process in practice in simulated or real scenarios (when possible) where students will practice the preparation of an audit from an analytical laboratory, and the development of an audit from the point of view of the auditors.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Class activities (resolution of proposed situations): 30 %

Written assignment: 70 %

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

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

ISO/IEC 19011:2018. Guidelines for auditing management systems.

Professional Skills

Module Title: <i>Technical writing and scientific communication</i>
Module Code: PS01
Pre-requisites (if any) <i>Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.</i>
Students will be assumed to have, at least, the minimum level of English for acceptance onto the EMQAL program.
Notional Learning Hours (u) Contact time: 10 h (v) Private study: 40 h
Format of Teaching: Workshop: 10 h
Teaching Strategy: <i>Please show how the contact hours are to be allocated in terms of the type of class involved.</i> The workshops will be organised into four two-and-a-half-hour sessions and will adopt a task-based, genre approach to the processes and products of technical writing (specifically, research papers and scientific posters) and scientific communication (specifically, conference papers).
Convener: <i>The name of the member of permanent staff responsible for the module</i> Iain Robinson
University: <i>The name of the University and Department responsible for the module</i> University of Barcelona (External – UB Language Services)
Module Description - Purpose or Aims: <i>This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the aims in numerical order.</i> <ol style="list-style-type: none">1. To provide an insight into the requirements of both written and oral communication in science, in general, and the communication needs of Analytical Chemists, in particular.2. To provide students with experience of the processes of undertaking research and writing research papers in Analytical Chemistry.3. To provide students with experience of the processes of undertaking research and writing and designing scientific posters and delivering a conference paper in Analytical Chemistry.4. To familiarise students with standard formats and conventions in the research papers, scientific posters and conference papers of Analytical Chemists.5. To enable students to develop their own voice in both written and oral communication and to acquire a sense of audience.6. To provide students with the writing skills to produce clear, well-structured and concise documents (both research papers and posters).7. To provide students with the oral presentation skills to produce clear, well-structured conference papers in Analytical Chemistry.
General learning outcomes (to which this module is contributing) <ol style="list-style-type: none">7. Prepare and compile a scientific report and communicate the findings orally.8. Seek employment and be a valuable asset in a professional environment.

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

The course aims to provide students with the necessary **oral and writing skills** to document their findings **accurately** and to communicate their significance **persuasively** to specific discourse communities. To this end, the course focuses on describing the format and basic components of research papers, scientific posters and conference papers in Analytical Chemistry (and other products of scientific discourse, as appropriate) to familiarise students with standard formats and conventions. Particular attention is given, in a **scaffolding approach**, to examining and drafting research paper **abstracts, introductions, methods, procedures, results, discussions and conclusions**; writing and designing scientific posters, **presenting information** and **graphics** appropriately and determining the most appropriate **layout** for a poster; and, writing and presenting a conference paper, focusing on **skills of delivery and audience interaction**.

The course undertakes an analysis of the scientific discourse of Analytical Chemists and so helps students participate in the **socio-cultural practices of their discipline** enabling them to become rhetorically flexible and genre aware. Drawing on experimental work previously undertaken by the students, the writing and scientific communication workshop will provide an opportunity for students to **draft a research paper** and to adapt its findings for **presentation in a scientific poster and conference paper**. Specific oral communication and writing support is anticipated in terms of the use of **rhetorical patterns** (general-specific, problem-solution, etc.), the enhancement of **textual coherence** through a focus on cohesive devices, **accurate citation** and referencing, an introduction to **corpus tools** to promote writer autonomy, and exercises raising student **awareness** of the metadiscourse of **textual organisation, reader and listener engagement** and the **expressing of stance**.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

- Students will be assessed on the successful application of a range of rhetorical devices and genre patterns in the reporting of their own experimental work following each of the workshop sessions.
- Students will also be assessed on their ability to present their findings accurately and persuasively in a simulated conference setting.
- On completion of the course, students should have written a full research paper and designed a corresponding scientific poster demonstrating their ability to write accurately and persuasively.

Relevant literature:

Details on any resources required should be included (e.g. core texts; recommended reading material, etc.)

Students will be provided with specific course materials in each workshop.

Module Title:

IT Tools

Module Code:

PS02

Pre-requisites (if any)

None

Notional Learning Hours

- (a) Contact time: 10
- (b) Private study: 40

Format of Teaching:

Lectures and seminars: 10 h
Laboratory practices: 40 h

Teaching Strategy:

Through a combination of lectures and exercises students are introduced to MATLAB. Students perform the exercises individually on their own computers.

Convener:

Bjørn Grung, UiB

University:

UiB

Module Description - The Purpose or Aims:

1. To learn basic commands in MATLAB
2. To learn how to use MATLAB for mathematical calculations and graphical representation of numerical data.
3. To learn about data import from analytical equipment

At the end of the module the student is expected to be able to

1. Use MATLAB in command line modus to perform simple calculations
2. present data in two and three dimensional graphs
3. create functions and scripts to handle analytical data

General learning outcomes (to which this module is contributing)

6: To critically analyse and evaluate data using statistical tools and software

8: seek employment and be a valuable asset in a professional environment

Summary of Course Content:

The module is designed to be taught using MATLAB. The course contains traditional classes, but the exercises are the heart of the course. These are done individually on their own computer, using the MATLAB license from UiB. Topics covered will be operators, scripts, functions, conditional statements, loops, data structures, plotting tools and data import. It is expected that the students spend time outside of class to solve the daily exercises.

Assessment Methods:

A computer exercise devoting to the import of data, simple data treatment and plotting of the data. A working program is necessary to pass.

Relevant literature:

Lecture notes will be made available.

Recommended reading:

Jim Sizemore & John Paul Mueller: MATLAB for Dummies. John Wiley & Sons, 2014. ISBN: 978-1-118-82010-0.

Module Title:

Project Management

Module Code: PS03

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

No pre-requisites needed.

Notional Learning Hours

- (a) Contact time: 15h
- (b) Private study: 35h

Format of Teaching:

Lectures and seminars: 15 h
Laboratory practices: h
Others (specify): h

Teaching Strategy:

Formal classes in 120/150 minutes timetable

Convener:

The name of the member of permanent staff responsible for the module

Maria de Belém Costa Freitas

University:

The name of the University and Department responsible for the module

Algarve University/Department of Earth, Sea and Environmental Sciences

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

This module aims to explain students the fundamentals of projects management, which are directly linked to the project execution and control and the management of unexpected changes. The student should understand that the crucial role of a project manager is to guarantee the project will end up within the estimated resources, achieving the estimated outcomes.

General learning outcomes (to which this module is contributing)

8. Seek employment and be a valuable asset in a professional environment

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

1. Introduction: all relevant activities in a company having specific objectives, deadlines and use of scarce resources need project management. We will deepen the most relevant basic soft-skills in project management: resources allocation, team building, discipline, holistic vision, communication and leadership.
2. Project strategy: definition of a project background and foreground potential analysis and the protection or valorisation of project results.
3. Implementation: budget appropriation, eligibilities, achievement of estimated outcomes and legal concerns.
4. Outcomes and communication

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

The assessment will be based in paper reviews by groups of students that will present their final critical overview to the class.

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Lecture notes will be accessible to students.

In each class, specific bibliography will be presented for the concerning subject.

Module Title:

Job search strategies

Module Code:

PS04

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Personal account of LinkedIn already opened

Notional Learning Hours

(w) Contact time: 10 h

(x) Private study: 40 h

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Formal lectures and practical seminars in the classroom in 60/120 min timetable.

Convener:

The name of the member of permanent staff responsible for the module

M^a Amparo Díaz Llairo

University:

The name of the University and Department responsible for the module

University of Barcelona, Department of Psychology

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

Main goals achieved:

Despite current economic uncertainties, many companies are still recruiting, but in doing so they are seeking the best they can find. In the digital age, finding the right kind of talent through online, and from social networks in particular, is becoming increasingly important.

This course examined what the key success factors are behind hiring through social networks and other web networks. Moreover, how can companies present themselves and attract the best candidates through the web? This course provided valuable insight into how companies recruit through the web and the new trends of recruitment in a digital era.

Specific goals achieved:

- To know and learn the process to find a job through social media
- To understand if all social media are appropriated in all recruitment processes and if this apply or not for all business
- To know the advantages of social media versus the traditional recruitment methods
- To know the most common mistakes when using social media in job search and how to avoid these mistakes.
- To know the most effective social media in recruitment 3.0.
- To know how to apply job postings in social media
- To know how to use hootsuite in the job search process.
- To know the process to control the personal branding reputation
- To know the new trends of job search in a digital era: Big data, mobile recruitment and robotics.

Competences achieved:

- Innovation and Technology
- Analytical and critical thinking
- Active learning strategies
- Creativity, Originality and initiative
- Resilience
- Flexibility
- Leadership and social influence
- Service orientation

General learning outcomes (to which this module is contributing)

Prepare and compile a scientific report and communicate the findings orally
Seek employment and be a valuable asset in a professional environment

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

The sharply increased importance of skills such as Technology competency is identified by most of worldwide employers, however, other skills such as creativity, originality and initiative, critical thinking, persuasion, will likewise retain or increase their value, as will resilience, flexibility and complex problem-solving. Leadership and social influence as well as service orientation also see an outsized increase in demand of worldwide employers. The students are prepared for new challenges in finding Jobs worldwide with the new technologies and social media strategies.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Methodology:

Practical and Interactive: this course was highly interactive, typically taking a case study approach that we have found to be an effective method of fostering discussions and transferring knowledge.

Class activity with a short oral presentation (30 %)

Written assessment work (70 %)

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Lectures notes will be available to the students.

Bibliography for consultancy:

- Talent 3.0. Díaz-Llairó, Amparo (Lid Publishing) 2018

Module Title:

Entrepreneurship and leadership skills

Module Code:

PS05

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

No prerequisites needed

Notional Learning Hours

(a) Contact time: 10h

(b) Private study: 20h

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Practice-oriented seminars

Convener:

The name of the member of permanent staff responsible for the module

Miquel Nadal

University:

The name of the University and Department responsible for the module

University of Barcelona, Department of Social Psychology and Quantitative Psychology

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

1. Leadership fundamentals: understanding the leader's role in a fast-paced environment
2. Self-leadership as a key performance indicator: learn how to take control of your own personal development
3. Find out the relationship between leadership and entrepreneurship
4. Entrepreneurship basics: how to start your own business from scratch
5. Science-based entrepreneurship: personality traits that will make you a good leader

General learning outcomes (to which this module is contributing)

7. Prepare and compile a scientific report and communicate the findings orally
8. Seek employment and be a valuable asset in a professional environment

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

This module aims to dig deep to the psychology principles of entrepreneurship. In addition to this, we will also find out how being a good leader and self-leadership pave the way to become a successful entrepreneur. The main goal of this module is to put the leadership basic principles into practice as well as to start your own business project (and make it profitable).

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Classroom Participation (10%)

Written assessment work (90%)

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

No required literature

Analytical Methods

Module Title:

Water Analysis

Module Code:

AM01

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Basic analytical chemistry, Environmental chemistry

Notional Learning Hours

- (a) Contact time: 10 h
- (b) Private study: 20h

Format of Teaching:

Lectures and seminars: 10 h
Laboratory practices: 0 h
Others (specify): consultation hours 5 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.
Formal lectures in 60 - 120 min. timetable

Convener:

The name of the member of permanent staff responsible for the module
Paweł Kubica

University:

The name of the University and Department responsible for the module
Gdańsk University of Technology / Faculty of Chemistry / Department of Analytical Chemistry

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

1. To familiarize Students with properties of water, sampling and general characterization and classification. 1.To demonstrate the importance to sampling as a part of analytical process.
2. To familiarize Students with inorganic analysis of components of natural/drinking/waste water. To introduce fundamentals of the most important techniques for inorganic analysis in water.
3. To familiarize Students with water analysis for organic components
4. To provide the principles of techniques (and modern instrumentation) used in final determination of organics in water, mainly gas and liquid chromatography and hyphenated techniques (GC-MS, LC-MS)
5. To provide the students with the skills to develop the methods of determination of organic pollutants in water

General learning outcomes (to which this module is contributing)

1. The Students will learn the importance of sampling for obtaining reliable and meaningful analytical results. Strategy, techniques and devices for water sampling will be taught, especially to make the students capable to evaluate whether sampling for a given purpose was properly planned and executed
2. The Students will learn the basic determination of water properties with simple techniques and more advanced one including instrumental analysis. After completion of this module Students will be able to choose the specific sample collection and sample treatment for specific analyte determination depending on their nature and origin.
3. After completion of this module the student will know the problems of trace organic pollutants determination in water, the respective techniques and principles of sample preparation and final determination and the skills to select and develop the methods of sample preparation and final determination of organic compounds in water

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

1. Properties of water as a chemical compound and type of waters and classification of ground and surface waters with respect to their quality
2. General comments on sampling importance and types of samples; sampling points arrangement, strategy of sampling (where, when, what, how, and how many samples)
3. Techniques and corresponding devices to collect ground and surface water including advantages and disadvantages of manual and automated sampling, also future trends in sampling
4. The significance and determination of inorganic components of water in different types of water at macro, micro and trace concentrations. Their origin, distribution, different chemical forms and types of chemical interaction among metals species in water will be considered.
5. Common organic water pollutants and problems of determination of organic trace pollutants with overview of sample preparation methods
6. Principles of extraction of semi-volatile and non-volatile organic pollutants, extraction of volatile organic compounds (static headspace, dynamic headspace, steam and vacuum distillation)
6. Separation techniques (gas and liquid chromatography, capillary electrophoresis, hyphenated techniques) in environmental analysis with exemplary analytical procedures for selected organics in water
7. Future trends in determination of trace organics in water and green methods/techniques of organic pollutants determination

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

The assessment will be in form of written test with open and closed questions. 60% of total points required to pass. Additional activity during classes will provide extra points for the Student

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

1. J. Namieśnik, P. Szefer. "Analytical Measurements in Aquatic Environments". Taylor & Francis Group. 2010.
2. APHA-AWWA-WPCF. "Standard Methods for the Examination of Water and Wastewater", 21 ed., 2005.
3. Chunlong Zhang, Fundamentals of Environmental Sampling and Analysis, Wiley Interscience, John Wiley and Sons, Inc., Hoboken, New Jersey, 2007
4. D. S. Hage, J. D. Carr, Analytical Chemistry and Quantitative Analysis, Pearson, Upper Saddle River, 2011
5. J. Pawliszyn, H.L. Lord, Handbook of Sample Preparation, Wiley, 2010
6. Frank R. Spellman; The Science of Water, Concepts and Applications; CRC Press, Taylor & Francis Group; second Edition; 2008
7. M.de la Guardia, S. Garrigues, Challenges in Green Analytical Chemistry, RSC Publishing 2011
8. Zygmunt B., Banel A., Chapter 1: Strategy of collecting samples from aquatic environment, Analytical measurements in aquatic environments, Namieśnik J., Szefer P., eds., CRC Press Edition Office, 2010

Module Title:

Food Analysis

Module Code:

AM02

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Notional Learning Hours

(y) Contact time: 10 h

(z) Private study: 25 h

Format of Teaching:

Lectures and seminars: 9 h

Laboratory practices: 0 h

Others (specify): 1 h (on line connection to analytical systems: UPLC, GC, NIR or HS-IMS working with food samples)

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Formal lectures in 100/120 min timetable, with some practical exercises and discussion.

Convener:

The name of the member of permanent staff responsible for the module

Miguel Palma Lovillo

University:

The name of the University and Department responsible for the module

University of Cadiz (Spain)

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

- To introduce the main properties of food samples that affects the analytical methods to be used
- To introduce the fundamentals of sample treatment in food analysis.
- To introduce extraction, clean-up and preconcentration techniques in the field of food analysis.
- To present the specific working conditions for specific foods, including beverages, juices, solid foods, functional foods and nutraceuticals
- To present several examples of food analysis, from the specific compounds (fats, proteins, carbohydrates, phenolics, minerals, antioxidant activity) to the separation (HPLC, GC) to the detections systems (MS, UV-Vis, IR and AAS)

General learning outcomes (to which this module is contributing)

At the end of the module the learner is expected to be able to:

1. To establish the right sampling conditions for foods
2. To correctly select the most adequate extraction, clean-up and preconcentration techniques for specific food samples.
3. To determine the most convenient analytical method of specific food samples
4. To select the between different analytical methods available for the food samples

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

First, the introduction to food analysis and requirements for sample treatment in this field will be provided. The principles of extraction will be presented, as well as, the clean-up and/or preconcentration of sample extracts will be discussed. Several analytical methodologies interesting in food analysis, including both chromatographic methods and spectrophotometric methods will be presented. Advantages and problems related to the food sample to be analyzed will be discussed to allow for the selection of the most convenient analytical method. Specific examples of analytical methods for foods will be used to illustrate the working conditions for food samples. Analytical methods for food authentication will be specifically discussed. Finally, basics of sensory analysis will be presented.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

LO1-LO4 – Assignment and critical exposition about the state-of-the-art of an food analytical problem solved (50%)

LO1-LO4 – Work assignment (50%)

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Lecture notes will be available for students.

Recommended reading:

1. Food Analysis. S. Suzanne Nielsen. Springer. 2017
2. Chemical Analysis of Food. Techniques and Applications. Yolanda Picó. Elsevier 2017.
3. Methods in Food Analysis: Applied to Plant Products. Maynard Joslyn. 2012.
4. Modern Techniques for Food Authentication. Da-Wen Sun. Academic Press. 2018.
5. Fast liquid chromatography-mass spectrometry methods in food and environmental analysis. Oscar Núñez, Héctor Gallart-Ayala. Imperial College Press, 2015
6. Sensory Analysis for Food and Beverage Quality Control. A Practical Guide. David Kilcast. Elsevier. 2010

Module Title:

Environmental Analysis

Module Code:

AM03

Pre-requisites (if any)

Basic analytical chemistry, Environmental chemistry

Notional Learning Hours

(aa) Contact time: 10 h

(bb) Private study: 10 h

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Formal lectures in 60/90 min timetable.

Convener:

Marek Tobiszewski

University:

Gdańsk University of Technology / Faculty of Chemistry / Department of Analytical Chemistry

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

9. To demonstrate sampling plans
10. To show sampling techniques for water, air, soil and sediments
11. To non-instrumental aspects of environmental analysis

General learning outcomes (to which this module is contributing)

At the end of the module the student is expected to:

9. Understanding the purpose, types of samples and basic rules of sample collection
10. Knowledge on typical problems during sampling
11. Knowledge on non-instrumental aspects of environmental analysis

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

1. Samples – basic characterization
2. Sampling plans
3. Sampling techniques for air
4. Sampling techniques for water, soil and sediments
5. Problems related to trace analysis at sampling, storage and sample preparation steps
6. Speciation and speciation analysis I
7. Speciation and speciation analysis II
8. Total parameters
9. Biomonitoring with bioindicators and biomonitors
10. Biological early warning systems

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

The assessment will be in form of written test with open questions. 60% of total points required to pass.

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Optional:

Handbooks on environmental sampling.

Tutorial reviews on the topics of lectures

Module Title:

Sampling and sample treatment

Module Code:

AM04

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

None.

Notional Learning Hours

(cc) Contact time: 10

(dd) Private study: 40

Format of Teaching:

Lectures and seminars: 7 h

Others (specify): case studies 3 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Formal lectures in 60/90m minutes sessions.

Case studies and group discussion based on sampling or sample treatment problems.

Convener:

The name of the member of permanent staff responsible for the module

Anna de Juan / Mercè Granados

University:

The name of the University and Department responsible for the module

Universitat de Barcelona. Chemical Engineering and Analytical Chemistry Department

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

1. To describe basic concepts, provide understanding and problem solving capabilities regarding the Theory of Sampling (TOS) by P. Gy.
2. To practice the design of sampling strategies and the quantitative estimation of sampling error in real sampling problems.
3. To describe the fundamentals of extraction techniques
4. To provide understanding of extraction and clean-up and/or preconcentration strategies
5. To practice the design of sample treatment schemes

General learning outcomes (to which this module is contributing)

3. Understand, select and apply a set of instrumental analytical techniques appropriate for a given problem

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

Sampling

1. Basic sampling concepts and TOS terminology. Lot dimensionality. Heterogeneity concept. Sampling Unit Operations (SUO).
2. Definition and estimation of sampling errors. Replication experiments. Sample mass reduction and sampling devices.

Sample treatment

3. Basic concepts related to extraction. Ultrasound assisted extraction. Microwave assisted extraction. Pressurized liquid extraction.
4. Clean-up and preconcentration. Liquid-liquid extraction. Solid phase extraction.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

- Work assignment (100%).

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Lectures will be mostly based on teaching material that the students will have beforehand (slides, research articles,...).

Recommended reading material)

1. Petersen, L, Minkinen, P. & Kim H. Esbensen (2005). Representative Sampling for reliable data analysis: Theory of Sampling. *Chemometrics and intelligent laboratory systems*, vol. 77, issue 1-2, p. 261-277.
2. Petersen, L, C. Dahl, K.H. Esbensen (2004). Representative mass reduction in sampling – a critical survey of techniques and hardware. *Chemometrics and Intelligent Laboratory Systems*, vol. 74, Issue 1, p. 95-114.
3. Petersen L. & K. H. Esbensen (2005). Representative Process Sampling for Reliable Data Analysis – a Tutorial. *Journal of Chemometrics*, vol. 19, Issue 11-12. p. 625-647.
4. Dean, John R. Extraction techniques in analytical sciences. Wiley, 2009

Module Title:

Advanced Instrumental Analysis in Practice

Module Code:

AM05

Pre-requisites (if any)

DA01, PS01

Notional Learning Hours

(ee) Contact time: 28 h

(ff) Private study: 22 h

Format of Teaching:

Laboratory practices: 28 h

Teaching Strategy:

Practical work in an analytical laboratory: 7 sessions of 4 h each.

Convener:

Egil Nodland

University:

University of Bergen

Module Description - The Purpose or Aims:

1. To revise some basic laboratory operations such as weighing, preparation of solutions, pH measurement, filtration, centrifugation and titration.
2. To learn about simple sample pretreatment in the laboratory such as digestions and extraction procedures.
3. To learn the use of basic spectroscopic techniques such as molecular absorption spectroscopy and atomic absorption spectroscopy and be familiar with the calibration methods used for these techniques.
4. To learn the use of separation techniques such as gas chromatography and liquid chromatography and the used calibration methods.
5. To critically discuss analytical results obtained in the laboratory and to prepare a report for an analytical service.

At the end of the module the learner is expected to be able to:

1. Properly carry out the basic laboratory operations used in an analytical laboratory.
2. Select the most suitable sample treatment previous to an analytical measuring step.
3. Recognize the different elements of the instruments and how the instruments operate
4. Select and apply an analytical technique for the measurement of some analytes in pharmaceuticals, food or environmental samples.

Elaborate laboratory reports containing the results and the information related to the analytical method used.

General learning outcomes (to which this module is contributing)

3. understand, select and apply a set of instrumental analytical techniques appropriate for a given problem;

Summary of Course Content:

This is an on-hands module designed to be totally taught in teaching laboratories. The main steps included in the analytical process will be understood and followed: sample pretreatment, analytical measurement and data treatment. Different analytical techniques will be applied covering optical methods, electroanalytical techniques and separation techniques.

Assessment Methods:

Written lab report.

Relevant literature:

Reading material will be distributed

<p>Module Title:</p> <p><i>Biological Analysis</i></p>
<p>Module Code:</p> <p>AM06</p>
<p>Maximum Number of Students: 20</p>
<p>Total ECTS Credits</p> <p>2</p>
<p>Notional Learning Hours</p> <p>(a) Contact Time - 14h (b) Private Study - 32h</p> <p>Format of Teaching:</p> <p>Lectures 10 h Laboratories or Practicals 4 h Other 0 h</p> <p>Teaching Strategy: Formal lectures in 150 min timetable.</p>
<p>Convener:</p> <p>Leonor Faleiro</p>
<p>University:</p> <p>UAIG</p>
<p>Language of Tuition:</p> <p>English</p>
<p>Module Description - The Purpose or Aims:</p> <ol style="list-style-type: none"> 1. Introduce fundamental concepts on biological analysis including water and food microbiology. 2. Introduce standard operating procedures in microbiological quality of water and food and other biological analysis.
<p>Learning Outcomes:</p> <p>At the end of the module is expected that the student will be able to:</p> <ol style="list-style-type: none"> 1. Recognize and describe several microbial agents that can cause food spoilage, poisoning and foodborne and waterborne infection. 2. Be able to put in place standard operating procedures to examine food and water microbiological quality. 3. Apply the appropriate measures to prevent food poisoning and waterborne and foodborne infections.
<p>Summary of Course Content:</p> <p>This module introduces concepts of classical and molecular approaches to evaluate the microbiological quality of food and water. The microbial growth, intrinsic and extrinsic factors in food spoilage, poisoning and food and water infection are explored. Laboratory techniques to examine food and water microbiological quality are described and discussed.</p>
<p>Transferable Skills Taught:</p>

Assessment Methods:

LO1 – Written Examination (100%)

Assessment Criteria:

Threshold

LO1 – To recognize microorganisms that cause foodborne and waterborne diseases.

LO2 – To outline methods to assess water and food microbiological quality.

LO3 – To describe how to control microorganisms growth

Good

LO1 – To point out possible sources of microorganisms that cause waterborne and foodborne diseases.

LO2 – To be able to select the most appropriate technique to perform the analysis of one sample.

LO3 – Outline methods of food preservation and correlate each method with microbial growth.

Excellent

LO1 – To point out extrinsic and intrinsic factors that are responsible for specific microbial growth on foods.

LO2 – Given a set of samples, select the most appropriate techniques to analyze each sample.

LO3 – To describe advantages and disadvantages of food preservation technologies and their implications to microbial food safety and food quality.

Resource Implications of Proposal and Proposed Solutions:

Lecture notes will be accessible to students

Madigan, M.T., Bender, K.S., Buckley, D.H., Sattley, W.M., Stahl, (2018). D.A. Brock Biology of Microorganisms (15th Edition). Pearson, ISBN-13: 978-0134268668.

Black, J.G., Black, L.J. (2015). Microbiology, Principles and Explorations. 9 th Ed., Wiley

Forsythe, S.J., (2020) The Microbiology of Safe Food, 3rd Edition. ISBN: 978-1-119-40553-5

Pre-Requisites:

Module Title:

Molecular Spectroscopy

Module Code:

AM07

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Notional Learning Hours

- (a) Contact time: 10h
- (b) Private study: 40h

Format of Teaching:

Lectures and seminars: 10h

Laboratory practices: 0h

Others (specify):

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Due to Covid-19 all classes will be on-line. Therefore, there will be 5h of formal lectures, arranged in slots of 60 or 120 minutes, and 2 practical works that will be exemplified on-line by the lecturer.

Convener:

Luísa Barreira

University:

The name of the University and Department responsible for the module

Universidade do Algarve /Departamento de Química e Farmácia

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

To introduce the fundamentals of molecular spectroscopy techniques.

To understand the bases of the equipment used in molecular spectroscopy techniques.

Instrumentation of UV/vis molecular absorption spectroscopy, and emission spectroscopy.

Quantitative analysis by absorption and emission spectroscopy.

General learning outcomes (to which this module is contributing)

3. Understand, select and apply a set of instrumental analytical techniques appropriate for a given problem.

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

This module will discuss the fundamentals and applicability of some analytical techniques based on molecular spectroscopy. The theory implied in transmission, absorption and emission of electromagnetic radiation at the molecular level will be analyzed. The basis of the most common instrument components in the design of instrumentation for optical spectroscopy will be discussed. The module will focus on the theory, instrumentation and practice of molecular absorption (UV/vis) and emission spectroscopy analytical techniques. The importance of Lambert-Beer law in absorption and emission spectroscopic analysis will be discussed accordingly to its applicability limitations.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Written exam (100%).

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Lecture notes will be available to students

Recommended reading:

- D.A. Skoog, D.M. West and F.J. Holler: "Fundamentals of Analytical Chemistry". 7th ed. Chapters 22-25, Saunders College, 1996.

Module Title:

Vibrational Spectroscopy

Module Code:

AM08

Pre-requisites (if any)

None

Notional Learning Hours

(a) Contact time: 12 h

(b) Private study: 38 h

Format of Teaching:

Lectures and seminars: 8 h

Laboratory practices: 4 h

Teaching Strategy:

Formal lectures in 90 min timetable. Laboratory exercises

Convener:

Egil Nodland

University:

University of Bergen

Module Description - The Purpose or Aims:

To introduce infrared spectroscopy
Introducing IR as a qualitative technique
Good laboratory practice

At the end of the module the student is expected to be able to:

Perform qualitative IR spectroscopy of pure compounds selecting appropriate measurement techniques
Describe why molecules absorb infrared radiation
Explain different types of infrared spectrometers
Interpret spectra and use search libraries

General learning outcomes (to which this module is contributing)

3. understand, select and apply a set of instrumental analytical techniques appropriate for a given problem;

Summary of Course Content:

IR spectroscopy is a work horse in the analytical laboratory. This module will give knowledge of the theory and practice of how to obtain and recognise high quality spectra for compound identification, explorative analysis and multivariate classification.

The module includes lectures in

- Theory (vibrations, frequencies, selection rules, molecular interactions.)
- instrumentation (instrumental components, spectrometers, sampling accessories)
- sampling techniques
- information enhancement (noise reduction, spectral subtraction, differentiation, library search)
- spectrum interpretation of organic compounds

Assessment Methods:

Oral or written exam

Relevant literature:

Günzler, Helmut and Gremlich, Hans-Ulrich: IR spectroscopy : an introduction
Translated by Mary-Joan Blümich
Wiley-VCH Verlag GmbH, 69469 Weinheim, Germany 2002
ISBN 3-527-28896-1

Module Title:

Atomic Spectroscopy

Module Code: AM09

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Notional Learning Hours

- (a) Contact time: 10 h
- (b) Private study: 40 h

Format of Teaching:

Lectures and seminars: 10 h
Laboratory practices: 0 h
Others (specify): 0 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Due to Covid-19 all classes will be on-line. Therefore, there will be 6 h of formal lectures, arranged in slots of 120 minutes, and practical works will be exemplified on-line by the lecturer.

Convener:

The name of the member of permanent staff responsible for the module

Maria Clara Costa

University:

The name of the University and Department responsible for the module

Universidade do Algarve /Departamento de Química e Farmácia

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

- To introduce fundamental concepts of Atomic Spectroscopy (AS)
- To introduce the instrumentation used in the most common AS techniques: Flame and Electrothermal Atomic Absorption Spectroscopy; Plasma Emission Atomic Spectroscopy, Atomic Fluorescence.
- To introduce the sources of error and methods for validating results in AS.

General learning outcomes (to which this module is contributing)

3. Understand, select and apply a set of instrumental analytical techniques appropriate for a given problem

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

This module introduces concepts of fundamental AS. It then explores the most widely used AS techniques: Flame and Electrothermal Atomic Absorption Spectroscopy; Plasma Emission Atomic Spectroscopy and Atomic Fluorescence. For each technique, the principles, instrumentation, limitations and typical applications are presented.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Laboratory report and/or a questionnaire test.

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Lecture notes will be available for students.

Recommended reading:

"Quantitative Chemical Analysis", Daniel C. Harris, Freeman, 6th ed., 2003.

"Analytical Chemistry", R. Kellner, J.M. Mermet, M. Otto, H.M. Widmer, Wiley-VCH Verlag, Weinheim, Germany, 1998.

"Principles of Instrumental Analysis", D.A. Skoog, F.J. Holler, T.A. Nieman, 5th ed., Saunders College, Florida, 1998

"Chemical Analysis – Modern Instrumentation Methods and Techniques", F. Rousseac, A. Rousseac, Wiley, 2000

"Analytical Instrumentation – Performance, Characteristics and Quality", G. Currell, Wiley, 2000.

Module Title:

Mass spectrometry and hyphenated techniques

Module Code: AM10

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Notional Learning Hours

(c) Contact time: 10 h

(d) Private study: 40 h

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Formal lectures in 60/90 min timetable

Convener:

The name of the member of permanent staff responsible for the module

Encarnación Moyano

University:

The name of the University and Department responsible for the module

University of Barcelona. Department of Chemical Engineering and Analytical Chemistry.

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

- To introduce the fundamentals aspects of mass spectrometry
- To recognize and understand the main components of a mass spectrometer
- To fully understand the fundamentals and the main characteristics of the most common ionization sources and mass analyzers
- To understand the fundamentals of tandem mass spectrometry
- To explore the fundamentals of mass spectrometry data interpretation
- To understand basic concepts and practical aspects of coupling mass spectrometry to separation techniques: GC-MS, LC-MS
- To explore the principles of qualitative and quantitative analysis in separation techniques-mass spectrometry
- To acquire basic knowledge to use the technology in different application fields (environmental, food analysis, pharmaceutical industry, etc.)

General learning outcomes (to which this module is contributing)

3. Understand, select and apply a set of instrumental analytical techniques appropriate for a given problem
6. Critically analyse and evaluate data using statistical tools and software

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

This module explores the fundamental aspects of mass spectrometry and topics that will be discussed include: (a) mass spectrometry basics, (b) theoretical and practical aspects of the most popular ionization techniques, (c) the basics of the main mass analyzers, (d) fundamentals of tandem mass spectrometry and an introduction to popular MS/MS instrument types (e.g., QqTOF, QqQ, QIT, LIT, FTICR), and (e) an overview of mass spectral interpretation, (f) basic aspects of coupling mass spectrometry to separation techniques (GC-MS, LC-MS), (g) mass spectrometry of small and large molecules, (h) an overview of mass spectral interpretation for qualitative analysis and (i) the principles of quantitative analysis using mass spectrometry

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

- Written Examination (80%)
- Resolution of practical exercises (20%)

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

- J.H. Gross. Mass Spectrometry: a textbook. Springer, 2nd edition, 2011.
- F.W. McLafferty and F. Turecek. Interpretation of mass spectra. University Science Books, 4th edition, 1993.
- E. de Hoffmann and V. Stroobant. Mass Spectrometry. Principles and Applications. J. Wiley and Sons, 3rd edition, 2007.
- J. Barker, D.J. Ando, R. Davis, M.J. Frearson. Mass Spectrometry. ACOL, 1999.
- B. Ardrey. Liquid Chromatography-Mass Spectrometry: An introduction. J. Wiley and Sons, 2004.
- www.spectroscopynow.com

Module Title:

Electroanalytical Techniques

Module Code:

AM11

Pre-requisites (if any)

No pre-requisites are required

Notional Learning Hours

(a) Contact time: 10 h

(b) Private study: 40 h

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Formal lectures in 60 - 120 min. timetable

Convener:

Bartłomiej Cieślak

University:

Gdańsk University of Technology / Faculty of Chemistry / Department of Analytical Chemistry

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

1. To familiarize the students with the basics of electrochemistry
2. To introduce students the main electrochemical techniques used in analytical chemistry
3. To present some novel approaches of electrochemical analysis

General learning outcomes (to which this module is contributing)

At the end of the module the student is expected to:

1. Understand the basics of electrochemistry
2. Know the most important equations used in electrochemical analysis
3. Recognize the differences between chosen electroanalytical methods
4. Understand and recognize the advantages and disadvantages of chosen electroanalytical methods

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

The module will start with familiarizing students with the most crucial definitions and equations connected with electrochemistry. The basics will be discussed before introducing students the use of electrochemical analysis. The most frequently used electroanalytical methods, such as potentiometry or amperometry, will be described. Some novel approach, which is used in the analytical laboratories and industry, such as stripping voltammetry will also be discussed and described.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Homework and participation in the class discussions (30 %)

Test of exam (70 %)

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

F. Scholz, „Electroanalytical Methods – Guide to Experiments and Applications”, ISBN 978-3-642-02915-8, by Springer in 2010

J. Wang, “Analytical Electrochemistry, 3rd Edition”, ISBN: 978-0-471-67879-3, by WILEY in 2006

P. T. Kissinger, W. R. Heineman „Laboratory Techniques in Electroanalytical Chemistry”, ISBN 9780824794453, by CRC Press in 1996

Module Title:

Gas Chromatography

Module Code:

AM12

Pre-requisites (if any)

Notional Learning Hours

(e) Contact time: 10 h

(f) Private study: 10 h

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Formal lectures in 60/90 min timetable

Convener:

Enrique Durán Guerrero

University:

University of Cadiz, Analytical Chemistry Department

Module Description - The Purpose or Aims:

3. To introduce fundamental concepts on chromatography
4. To describe the Gas Chromatography instrumental system
5. To apply fundamental concepts on Gas chromatography

General learning outcomes (to which this module is contributing)

At the end of the module the learner is expected to be able to:

3. Correctly understand the basic principles of chromatography
4. Critically analyze and evaluate the efficiency of a chromatographic system
5. Correctly identify and describe the principles and instrumentation in the gas chromatographic techniques
6. Correctly describe different applications of gas chromatography

Summary of Course Content:

This module introduces concepts of fundamental chromatography. It then explores the most widely used gas chromatographic instrumental techniques. It shows how to choose the best analytical conditions for a gas-chromatographic analysis. The principles, instrumentation, limitations and typical applications of GC are presented.

Assessment Methods:

3. Group Work Discussion (30%)
4. Oral Exposition (40%)
5. Written Report (30%)

Threshold

Learning Outcome 1 – to be able to describe the factors affecting the separation of a chromatographic system.

Learning Outcome 2 – to correctly calculate efficiency parameters for a chromatographic column.

Learning Outcome 3 – to correctly identify the components of a given gas chromatographic system.

Learning Outcome 4 – to correctly identify whether a sample could be analyzed by gas chromatography.

Good

Learning Outcome 1 – to be able to explain the separation of different compounds by a chromatographic system.

Learning Outcome 2 – to correctly analyze the efficiency of a chromatographic system and design solutions to increase its performance.

Learning Outcome 3 – to correctly describe the components of a given gas chromatographic system.

Learning Outcome 4 – to correctly describe the analysis of a sample by gas chromatography.

Excellent

Learning Outcome 1 – to be able to predict the separation of different compounds by a chromatographic system, considering the factors involved.

Learning Outcome 2 – to develop a laboratory quality control plan for chromatographic equipment, based on the efficiency of each equipment.

Learning Outcome 3 – to correctly describe the influence of the components of a gas chromatographic system on the results obtained.

Learning Outcome 4 – to correctly define what type of analysis could be performed by each gas chromatographic system.

Relevant literature:

Lecture notes will be available for students.

Recommended reading:

"Quantitative Chemical Analysis", Daniel C. Harris, Freeman, 6th ed., 2003.

"Analytical Chemistry", R. Kellner, J.M. Mermet, M. Otto, H.M. Widmer, Wiley-VCH Verlag, Weinheim, Germany, 1998.

"Principles of Instrumental Analysis", D.A. Skoog, F.J. Holler, T.A. Nieman, 5th ed., Saunders College, Florida, 1998

"Chemical Analysis – Modern Instrumentation Methods and Techniques", F. Rousseac, A. Rousseac, Wiley, 2000

"Analytical Instrumentation – Performance, Characteristics and Quality", G. Currell, Wiley, 2000.

Module Title:

Liquid Chromatography

Module Code:

AM13

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Notional Learning Hours

(g) Contact time: 10 h

(h) Private study: 25 h

Format of Teaching:

Lectures and seminars: 9 h

Laboratory practices: 0 h

Others (specify): 1 h (on line connection to a liquid chromatographic system)

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Formal lectures in 100/120 min timetable, with some practical exercises and discussion.

Convener:

The name of the member of permanent staff responsible for the module

Marta Ferreiro González

University:

The name of the University and Department responsible for the module

University of Cadiz (Spain)

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

- To introduce the fundamentals of liquid chromatography
- To study the effect of mobile phase composition on the separation performance
- To discuss about the main instrumental components of a liquid chromatographic system

General learning outcomes (to which this module is contributing)

At the end of the module the learner is expected to be able to:

5. To correctly identify and describe the fundamentals of liquid chromatography
6. To correctly select the most adequate conditions (column, mobile phase, pH, elution mode) to separate a set of compounds of different chemical characteristics
7. To correctly select the best detection system for a given analytical problem
8. To establish the adequate working conditions for the analysis of a sample with compounds of different polarity

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

This module introduces the fundamental aspects of liquid chromatography. Topics to be discussed include: basic concepts on LC, retention parameters, band broadening, column efficiency in LC, column packing materials, bonded phases, effect of pH on selectivity, column evaluation, elution modes, LC instrumentation (pumping system, injectors, detectors).

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

LO1-LO4 – Assignment and critical exposition about the state-of-the-art of an analytical problem solved using liquid chromatography (50%)

LO1-LO4 – Work assignment (30%)

LO1 and LO3 – Written examination (20%)

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Lecture notes will be available for students.

Recommended reading:

7. Liquid Chromatography : Fundamentals and Instrumentation. Salvatore Fanali, Paul R. Haddad, Colin Poole, Marja-Liisa Riekkola, and Marja-Liisa Riekkola. Elsevier 2017
8. Selection of the HPLC Method in Chemical Analysis. Serban Moldoveanu , and Victor David. Elsevier 2016
9. Liquid chromatography.: Applications. Colin Poole. Elsevier 2017

Module Title:

Extraction methods in Analytical Chemistry

Module Code:

AM14

Pre-requisites (if any)

Recommended (although not mandatory) to have been taken "Liquid Chromatography" and "Gas Chromatography" modules

Notional Learning Hours

(i) Contact time: 10 h

(j) Private study: 10 h

Format of Teaching:

Lectures and seminars: 10 h

Laboratory practices: 0 h

Others (specify): 0 h

Teaching Strategy:

Formal lectures in 60/90 min timetable

Convener:

Enrique Durán Guerrero

University:

University of Cadiz, Analytical Chemistry Department

Module Description - The Purpose or Aims:

6. To introduce fundamentals of the different extraction methods employed in analytical chemistry: ultrasound assisted extraction (UAE), microwave assisted extraction (MAE), pressurized fluid extraction (PFE), supercritical fluid extraction (SFE), solid-phase extraction (SPE), solid-phase microextraction (SPME), stir bar sorptive extraction (SBSE), headspace sorptive extraction (HSSE), solid-phase dynamic extraction (SPDE).
7. To introduce fundamentals about influential variables of each extraction method.
8. To show the problems related with the stability of samples under different extraction conditions.

General learning outcomes (to which this module is contributing)

At the end of the module the learner is expected to be able to:

7. Correctly describe the different extraction methods.
8. Correctly develop and optimize an extraction method, taking into account the different implied variables.
9. Select the most adequate extraction technique on the basis on the kind of compounds they are trying to extract

Summary of Course Content:

Extraction methods are widely used in Analytical Chemistry and they are essential in chromatography to concentrate and/or isolate compounds from complex matrixes. The fundamentals and limitations of ultrasound assisted extraction, microwave assisted extraction, pressurized fluid extraction, supercritical fluid extraction solid-phase extraction, solid-phase microextraction, stir bar sorptive extraction, headspace sorptive extraction and solid-phase dynamic extraction are going to be introduced. Moreover, possible influential variables of each extraction method will be discussed in order to achieve the best overall analytical conditions. Several applications are going to be presented in order to make the students able to choose the best extraction technique on the basis of the composition of the sample.

Assessment Methods:

6. Group Work Discussion (30%)
7. Oral Exposition (40%)
8. Written Report (30%)

Threshold

Learning Outcome 1 – to correctly describe the fundamentals of a given extraction method.

Learning Outcome 2 – to be able to identify the main variables implied in each extraction method.

Learning Outcome 3 – to be able to identify if what extraction technique(s) can be applied for some compounds

Good

Learning Outcome 1 – to identify what kind of samples can be extracted with each extraction method.

Learning Outcome 2 – to be able to identify the possible influence of the variables on the method.

Learning Outcome 3 – to be able to determine what compound cannot be extracted by some extraction techniques.

Excellent

Learning Outcome 1 – to be able to determine the operational conditions for each extraction technique and to know the advantages and disadvantages of each one.

Learning Outcome 2 – to be able to correctly develop an extraction method.

Learning Outcome 3 – to be able to choose the most adequate extraction technique depending on the compound to be extracted

Relevant literature:

Lecture notes will be available for students.

Recommended reading:

"Analytical Chemistry", R. Kellner, J.M. Mermet, M. Otto, H.M. Widmer, Wiley-VCH Verlag, Weinheim, Germany, 1998.

"Principles of Instrumental Analysis", D.A. Skoog, F.J. Holler, T.A. Nieman, 5th ed., Saunders College, Florida, 1998

"Handbook on Analytical Separations" R.M. Smith Ed. Vol. 3.

"Environmental Analysis" W. Kleibohmer. Elsevier, 2004.

"Supercritical Fluid Extraction" L. Taylor. Wiley, New York, 1996

"Solid-Phase Extraction: Principles and Practice" E.M Turman, M.S. Mills, Wiley, New York, 1998.

Module Title:

Quality Parameters and Optimization in Chromatography

Module Code:

AM15

Pre-requisites (if any)

AM12, AM13, DA04

Notional Learning Hours

(a) Contact time: 12 h

(b) Private study: 368 h

Format of Teaching:

Lectures and seminars: 8 h

Exercises: 4 h

Teaching Strategy:

Formal lectures in 60 min timetable.

Exercises (30/60 min)

Convener:

Svein A. Mjøs

University:

University of Bergen

Module Description - The Purpose or Aims:

At the end of the module the learner is expected to be able to:

1. Understand the basic concepts of separation (peak resolution, selectivity, efficiency) and which factors that will have influence on separation in liquid and gas chromatography.
2. Evaluate efficiency and selectivity of a chromatographic system using common parameters such as separation number, theoretical plates and peak capacity.
3. Choose a suitable optimization strategy and apply the technique to optimize a system (e.g. experimental designs, simplex optimization).
4. Use retention indices, relative retention, and other methods for standardization of chromatographic retention.

General learning outcomes (to which this module is contributing)

3. understand, select and apply a set of instrumental analytical techniques appropriate for a given problem;
6. critically analyse and evaluate data using statistical tools and software

Summary of Course Content:

To make participants able to identify the most critical parameters for separation and to be able to evaluate quality of separation in chromatographic methods. To introduce basic method optimization strategies and to make participants able to optimize chromatographic methods. To introduce methodologies for standardization of retention and to introduce the principles of multi-dimensional separation.

Assessment Methods:

Written exam or assignment

Relevant literature:

Lecture notes will be available for students.

Recommended reading: "Quantitative Chemical Analysis", Daniel C. Harris, Freeman (Chapters on chromatography).

"Principles of Instrumental Analysis", Skoog, Holler, Nieman/Crouch, (Chapters on chromatography).

Selected papers, to be defined

Data Analysis

Module Title: <i>Statistics</i>
Module Code: DA01
Pre-requisites (if any) None
Notional Learning Hours (a) Contact time: 10 h (b) Private study: 40 h Format of Teaching: Lectures and seminars: 10 h Teaching Strategy: Regular lectures. Daily exercises, which are followed up the next day.
Convener: Bjørn Grung
University: University of Bergen
Module Description - The Purpose or Aims: This module trains students to work with random and systematic deviation. It introduces the basic concepts in statistics: data variability, the concept of probability and probability distributions. It describes how to estimate the mean and standard deviation of a population from small sets of data, and how to propagate these deviations when experimental results are used in calculations. The module serves as an introduction to later, more advanced modules. At the end of the module, the learner is expected to be able to: <ol style="list-style-type: none">1. Choose the best parameters to describe a given set of data2. Understand how to use statistical tables (Z, T, chi-square)3. Estimate the confidence interval of a result from a limited set of repeated experiments4. Estimate the confidence interval of a value calculated from several experimental variables.5. Calculate how errors propagate through a calculation6. Perform linear regression by hand
General learning outcomes (to which this module is contributing) 6: To critically analyse and evaluate data using statistical tools and software

Summary of Course Content:

Deviations in experimental results: random, systematic and gross. How to measure and how to minimize random and systematic deviations. Parameters for measuring data dispersion. Parameters for measuring data location. The concept of probability and the role of statistics in Quality Control. Random distributions. Gaussian distribution. The Central Limit Theorem. Confidence intervals. Propagation of random and of systematic errors. Linear regression.

Assessment Methods:

School exam. 2 hours.

Relevant literature:

Lecture notes will be available to students

Recommended reading:

• Peter C. Meyer, Richard E. Zund, "Statistical Methods in Analytical Chemistry", 2nd. Ed., John Wiley & Sons, 2000.

• James N. Miller, Jane C. Miller, "Statistics and Chemometrics for Analytical Chemistry", 4th ed., Prentice Hall, 2000.

Module Title:

Statistical decision and analysis of variance

Module Code:

DA02

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Notional Learning Hours

(k) Contact time: 10 h
(l) Private study: 40 h

Format of Teaching:

Lectures and seminars: 10 h
Laboratory practices: 0 h
Others (specify): 0 h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

10 h of formal lectures in 60-120 min timetable including computer seminars (with Excel spreadsheet). Teaching will be interactive, combining lectures with computer exercises. Therefore, each student will need a computer (personal or university provided) with the Microsoft Excel application installed to attend the classes. Due to present health restrictions, teaching will be online and thus, the computer must be provided with webcam, microphone and headphones for good student-professor interaction.

Convener:

The name of the member of permanent staff responsible for the module

Martí Rosés

University:

The name of the University and Department responsible for the module

Universitat de Barcelona / Analytical Chemistry

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

1. To introduce the fundamentals and importance of statistical decision
2. To evaluate the different sources that contribute to data variability
3. To differentiate between random and controlled factors that contribute to data variability
4. To apply statistical tests and analysis of variance to design and validate analytical methods

General learning outcomes (to which this module is contributing)

6. Critically analyse and evaluate data using statistical tools and software

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

This module will discuss the fundamentals and applicability of statistical decision tests: comparison of a mean to a reference value or comparison of two means (z-tests and t-tests, including paired t-test), comparison of variances (F-test). It will also discuss the fundamentals, applications and limitations of the analysis of variance. This will include the use of one-way and two-ways ANOVA in the analysis of data variability caused by different sources, experimental design and interlaboratory tests.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

1. Written examination (80%)
2. Computer and written assignment (20%)

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

- J.N. Miller and J.C. Miller: 'Significance tests', chapter 5 in "Statistics and Chemometrics for Analytical Chemistry". 4th ed. Prentice and Hall, 2000.
- D.C. Harris: 'Statistics', chapter 4 in "Quantitative Chemical Analysis". 6th ed. W.H. Freeman & Co., 2003.

Module Title:

Uncertainty Measurement

Module Code: DA03

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module. Students are required to have a basic knowledge of analytical chemistry and statistics.

Notional Learning Hours

- (a) Contact time: 10 h
- (b) Private study: 40 h

Format of Teaching:

Lectures and seminars: 10 h (6 h theory and 4 h exercises)

Laboratory practices: - h

Others (specify): - h

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

The relevance and principles of the evaluation of the measurement uncertainty are presented in an interactive way and exercises to solve specific problems are solved in the classroom.

Convener:

The name of the member of permanent staff responsible for the module

Ricardo Bettencourt da Silva (<http://mechem.rd.ciencias.ulisboa.pt/>)

University:

The name of the University and Department responsible for the module

University of Lisbon – Faculty of Sciences - Chemistry and Biochemistry Department

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

1. To raise awareness of the importance of measurement uncertainty evaluation
2. To introduce the concepts of measurement traceability and uncertainty
3. To introduce the principles of the ISO guide to the expression of uncertainty in measurement (GUM)
4. To present the principles of alternative approaches for measurement uncertainty evaluation (“bottom-up” approach, “top-down” approach based on intralaboratory data and “top-down” approach based on interlaboratory data).

General learning outcomes (to which this module is contributing)

At the end of the module the learner is expected to be able to:

1. Define the traceability of measurements in chemistry
2. Evaluate the uncertainty associated with volumetric, gravimetric and instrumental quantification steps
3. Evaluate the uncertainty associated with simple chemical measurements using the “bottom-up” approach
4. Evaluate the uncertainty associated with complex chemical measurements using the “top-down” approach based on interlaboratory data.
5. Evaluate the uncertainty associated with complex chemical measurements using the “top-down” approach based on intralaboratory data.
6. Evaluate the conformity of a sample with a legal or specification limit considering the measurement uncertainty.
7. Select the most adequate approach for measurement uncertainty evaluation taking the target measurement uncertainty and the needed resources for the evaluation into account.

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

This module aims at raising the awareness for the need to report measurements traceable to an adequate reference and with an objective quantification of their quality (i.e. measurement uncertainty).

The basics of measurement traceability and uncertainty are introduced. The principles of the GUM are presented and applied to the evaluation of the uncertainty of simple measurements.

The principles of the most popular alternatives to the “bottom-up” approach are presented, namely the “top-down” approach based on intralaboratory data and the “top-down” approach based on interlaboratory data.

The application of the more pragmatic approaches to complex measurements is presented.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

Assessment method: Final exam to be solved in one working day.

Threshold

LO1 – State the relevance of reporting measurements with uncertainty.

LO2 – Clarify the role of measurements traceability on their comparability.

LO3 – Explain the general principles of the studied approaches for the evaluation of the measurement uncertainty.

LO4 – Describe how measurement uncertainty should be considered in the evaluation of sample compliance with a legal or specification limit.

LO5 – Evaluate the uncertainty associated with an operationally defined measurement using data from a collaborative trial (i.e. “top-down” approach based on interlaboratory data).

Good

LO1 – Distinguish different measurands associated with the analysis of the same analyte in the same item.

LO2 – Describe the traceability of measurements in chemistry.

LO3 – Evaluate the uncertainty associated with single analytical steps

LO4 – Describe the most relevant advantages and disadvantages of the studied approaches for the evaluation of the measurement uncertainty.

LO5 – Evaluate the uncertainty associated with a complex measurement using the “top-down” approach based on intralaboratory data.

Excellent

LO1 – Evaluate the uncertainty associated with simple measurements using the bottom-up approach.

LO2 – Develop strategies for the optimization of measurement cost and quality based on the uncertainty budget.

LO3 – Develop models for “worst-case” measurement uncertainty evaluations.

LO4 – Describe the limitations of data from a collaborative trial to estimate the uncertainty associated with a rational measurement.

LO5 – Describe how the intralaboratory data needed for the evaluation of the measurement uncertainty should be collected.

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

1. JCGM, International Vocabulary of Metrology – Basic and General Concepts and Associated Terms (VIM 3rd edition), JCGM 200, BIPM, 2012 (https://www.bipm.org/utis/common/documents/jcgm/JCGM_200_2012.pdf).
2. JCGM, Evaluation of measurement data - Guide to the expression of uncertainty in measurement, JCGM 100, BIPM, 2008 (https://www.bipm.org/utis/common/documents/jcgm/JCGM_100_2008_E.pdf).
3. S.L.R. Ellison, A. Williams (eds), Eurachem/CITAC guide: Quantifying Uncertainty in Analytical Measurement, Third edition, Eurachem, 2012 (https://www.eurachem.org/images/stories/Guides/pdf/QUAM2012_P1.pdf).
4. V.J. Barwick, S.L.R. Ellison, Part (d): Protocol for uncertainty evaluation from validation data, VAM Project 3.2.1 Development and Harmonisation of Measurement Uncertainty Principles, LGC/VAM/1998/088, 2000 (http://blpd.dss.go.th/training/dwdocuments/enews/VAM_uncertainty-0452.pdf).
5. R. Cordeiro, C. Rosa, R.J.N.B. Silva, Measurements recovery evaluation from the analysis of independent reference materials: Analysis of different samples with native quantity spiked at different levels, *Accred. Qual. Assur.* 23 (2018) 57-71 (<https://link.springer.com/article/10.1007/s00769-017-1296-2>).
6. R.J.N.B. Silva, A. Williams (Eds.), Eurachem/CITAC Guide: Setting and Using Target Uncertainty in Chemical Measurement, Eurachem, 2015 (https://www.eurachem.org/images/stories/Guides/pdf/STMU_2015_EN.pdf).

Module Title:

Experimental Design and Optimization

Module Code:

DA04

Pre-requisites (if any)

DA01

Notional Learning Hours

- (a) Contact time: 10 h
- (b) Private study: 40 h

Format of Teaching:

Lectures and computer exercises

Teaching Strategy:

Classroom lectures and computer exercises. Students carry out the exercises first, and then they are repeated in a plenary session.

Convener:

Bjørn Grung

University:

University of Bergen

Module Description - The Purpose or Aims:

- To introduce fundamentals of experimental design and optimization for analytical methods
- To introduce several ways to run an experimental design
- To show how to apply experimental design and optimization reducing the number of experiences

General learning outcomes (to which this module is contributing)

3. understand, select and apply a set of instrumental analytical techniques appropriate for a given problem;
6. critically analyse and evaluate data using statistical tools and software

Summary of Course Content:

Experimental design and optimization is a set of tools for reducing the number of experiments needed to arrive at an analytical result. Several considerations, regarding the most adequate design is going to be presented as a way to help the students to know how to decide the best option depending on the specific problem. The software package Sirius will be used.

Students should be able to pick an appropriate design, set up the design matrix, perform calculations and interpret the results.

Assessment Methods:

A report demonstrating how a multi-factor optimization task was carried out.

Relevant literature:

Lecture notes and scientific papers will be made available.

Recommended reading: R.G. Brereton (2003): Chemometrics – Data analysis for the Laboratory and Chemical Plant, Wiley

Module Title:

Pattern Recognition and Classification

Module Code:

DA05

Pre-requisites (if any)

Any module(s) which must have been taken prior to the current module, or any specific background required to take this module.

Previous background/knowledge about general statistics (from a previous module, for example) would be desirable.

Notional Learning Hours

(m) Contact time: 10 h

(n) Private study: 25 h

Format of Teaching:

Lectures and seminars: 8 h

Laboratory practices: 0 h

Others (specify): 2 h (examples with computer)

Teaching Strategy:

Please show how the contact hours are to be allocated in terms of the type of class involved.

Formal lectures in 100/120 min timetable, with some practical exercises and discussion.

Convener:

The name of the member of permanent staff responsible for the module

José María Palacios-Santander

University:

The name of the University and Department responsible for the module

University of Cadiz (Spain)

Module Description - The Purpose or Aims:

This should specify the purpose of the module where it fits into the programme specification and what it aims to provide. Please list the Aims in numerical order.

1. To introduce fundamentals of pattern recognition and classification methods and its applications
2. To discuss and analyze several scientific publications regarding the state-of-the-art of this module
3. To practice with real data from analytical problems.

General learning outcomes (to which this module is contributing)

At the end of the module the learner is expected to be able to:

1. Understand the principles of pattern recognition and classification
2. Correctly select and apply these chemometric tools to analytical problems
3. Interpret the results obtained after using these tools

Summary of Course Content:

This should be a summary paragraph of list of the topics to be covered by the module

Pattern recognition and classification methods provide an approach to the interpretation of the multivariate data often encountered in analytical chemistry. Widely used methods include mapping and display, discriminant development, clustering, and modeling. These methods can be applied to a great variety of chemical problems with the aim of classification. This classification developed from spectral, chromatographic, or compositional data may be desirable for any number of purposes within quality control, including source identification, detection of odorants, presence or absence of a disease in a patient or animal from which a sample has been taken, and food quality testing, to name a few. After studying the fundamentals of these chemometric tools, some analytical problems based on real data as well as their possible interpretations will be discussed.

Assessment Methods:

Details of assessment methods should include forms of assessment and the contribution of each to the summative assessment of the module. The relationship to the learning outcomes of the module should be explicit and the numbers of the various learning outcomes should be attached to the assessment methods listed. Please list in numerical order

LO1 & LO2 – Assignment and critical exposition about the state-of-the-art of pattern recognition and classification (60%)
LO3 – Work assignment (40%)

Relevant literature:

Details on any resources required and should be included (e.g core texts; recommended reading material, etc)

Lecture notes will be available for students.

Recommended reading:

10. "Handbook of Chemometrics and Qualimetrics", D. L. Massart, B. G. M. Vandeginste, L. M. C. Buydens, S. De Jong, P. J. Lewi, J. Smeyers-Verbeke, Elsevier, The Netherlands, 1997.
11. "Applied Chemometrics for Scientists", R. G. Brereton, John Wiley & Sons, Ltd., England, 2007.
12. "A Practical Guide to Scientific Data Analysis", David Livingstone, John Wiley & Sons, Ltd., England, 2009.

<p>Module Title:</p> <p><i>Multivariate Data Analysis</i></p>
<p>Module Code:</p> <p>DA06</p>
<p>Pre-requisites (if any)</p> <p>DA01, DA04</p>
<p>Notional Learning Hours</p> <p>(a) Contact time: 10 h</p> <p>(b) Private study: 40 h</p> <p>Format of Teaching:</p> <p>Lectures and supervised computer exercises.</p>
<p>Convener:</p> <p>Bjørn Grung</p>
<p>University:</p> <p>University of Bergen</p>
<p>Module Description - The Purpose or Aims:</p> <p>To introduce the concept of latent variables</p> <p>Using latent variables to detect and describe the main variation patterns in a data set</p> <p>Using Principal Component Analysis for exploratory data analysis and classification</p> <p>Introducing Partial Least Squares Regression as an alternative to Multiple Linear Regression</p> <p>At the end of the module the student is expected to be able to:</p> <p>Understand the mathematics behind latent variable methods</p> <p>Perform an adequate pretreatment of a data set prior to multivariate analysis</p> <p>Use commercial software to perform PCA on a data set</p> <p>Perform calibration and prediction using Partial Least Squares</p>
<p>General learning outcomes (to which this module is contributing)</p> <p>6. critically analyse and evaluate data using statistical tools and software</p>
<p>Summary of Course Content:</p> <p>Data sets from the modern analytical laboratory are usually highly collinear in nature. Modern analytical instruments produce huge amounts of data. To find the information present in such data sets require the use of multivariate modeling techniques. Principal Component Analysis (PCA) is demonstrated to be an extremely powerful tool for detection of sample and variable correlations. Various useful plots that aid the analyst in his quest for information are presented. Various common types of data pretreatment are presented. Multivariate calibration with PLS is introduced.</p>
<p>Assessment Methods:</p> <p>Computer exercise with a written report.</p>
<p>Relevant literature:</p> <p>Lecture notes and scientific papers will be available for students.</p> <p>Recommended reading: R.G. Brereton (2003): Chemometrics – Data analysis for the Laboratory and Chemical Plant, Wiley</p>