Universidad Zaragoza

Year : 2020/21

63024 - Food metabolites analysis at trace levels

Syllabus Information

Academic Year: 2020/21
Subject: 63024 - Food metabolites analysis at trace levels
Faculty / School: 105 - Facultad de Veterinaria
Degree: 566 - Master's in Food Quality, Safety and Technology
ECTS: 3.0
Year: 1
Semester: Second semester
Subject Type: Optional
Module: ---

1.General information

1.1.Aims of the course

1.2.Context and importance of this course in the degree

1.3.Recommendations to take this course

2.Learning goals

2.1.Competences

2.2.Learning goals

2.3.Importance of learning goals

3.Assessment (1st and 2nd call)

3.1.Assessment tasks (description of tasks, marking system and assessment criteria)

4.Methodology, learning tasks, syllabus and resources

4.1.Methodological overview

The learning process begins with participative group lectures, combined with practical sessions in the computer room to provide skills to manage various tools and resources related to essential aspects of the subject and other individual activities (resolution of questionnaires and exercises, the study of practical cases derived from the theoretical classes, analysis, and synthesis of bibliographic material, preparation of presentations).

Laboratory practical sessions will be intercalated between the theory blocks so that students can apply in a practical way the knowledge acquired during theory classes.

4.2.Learning tasks

The course includes the following activities:

1. Six lectures in group (10.5 h)
2. Two seminars of 1.5 and 2 h of presentation and discussion of papers
3. Two practical sessions at the laboratory (6 h)
4. Four practical sessions with software at the computer room (8 h)
5. One session in an external laboratory (2 h)
6. Preparation of papers and reports (15 h student only)
7. Questionnaires solving (30 h student only)

4.3.Syllabus

Lecture 1 (2.0 h): Key knowledge for trace analysis in food. Why trace analysis and what traces must be analyzed in food. Specific problems. Techniques available to address these analysis. Molecular keys to detectability and ease of isolation. Introduction to mass spectrometry. Basic concepts of MS.

Practical session 1 (1.5 h computer room): Databases of chemical interest to obtain properties related to extractability and detectability. Effects of pH. Basic online tools for obtaining spectrometric data.

Lecture 2 (2.0 h): Mass analyzers. Basic properties, types and features. Ion sources and ionization mechanisms in mass spectrometry. General description of the coupling to gas and liquid chromatography systems, characteristics and limitations.

Lecture 3 (2.0 h): General introduction to chromatography, with detail in gas chromatography (GC). Key concepts. Optimization of chromatographic separation. GC columns. Selection of stationary phases.

Lecture 4 (2.0 h): Carrier gas dynamics. Gas Chromatography injection techniques.

Practical session 2 (1.5 h computer room): Excel tools for modeling the chromatographic process (separation), pressure and flow conditions, and injection. Other online tools of interest.

Lecture 5 (2.0 h): Overview of Liquid Chromatography. Instrumentation in HPLC systems: degassers, mixers, pumps, injectors. LC columns. Particle size and efficiency. Types and supports of stationary phases. Operation modes: normal phase, reverse phase and HILIC. Mobile phase selection and selectivity.

Lecture 6 (2.0 h): Sample preparation and method development in GC-MS. Working with volatile molecules (isolation, preconcentration and injection): vapor phase approaches (static headspace, SPME, dynamic headspace); liquid-liquid, SPE, and SBSE methods.

Lecture 7 (2.0 h): Key knowledge for the development of non-volatile trace analysis methods. Working with non-volatile molecules (preconcentration and isolation): QUECHERS methods, restricted access media, MIPs and others. Instrumental techniques: LC-fluorescence and LC-MS. Criteria for choosing LC-MS systems. Acquisition modes: quantitative MRM or data independent acquisition. Keys to developing quantitative methods: crossover point, retrospective analysis, ionic suppression, normative considerations for the identification of food analytes.

Lecture 8 (2.0 h): Key knowledge for the identification of metabolites. How to identify a molecule. The metabolomic approach to identify markers and pathways: workflow and tools. Work schemes to isolate and identify bioactive molecules (semi-preparative chromatography).

Practical session 3 (4.0 h laboratory): Isolation and determination of volatile compounds. A simplified food sample containing volatile compounds of different volatility will be provided. Students will apply different procedures for the isolation and preconcentration of the analytes (HS, SPME, L-L, SPE, P&T) and will collaborate in the preparation of the GC system for its analysis and in the integration of the chromatograms. The chromatograms obtained using different isolation techniques will be compared. Students will process the data obtained to estimate detection limits, percentage of transferred mass, repeatability, concentrations and uncertainties in the determination.

Practical session 4 (2.0 h laboratory): Analysis of biogenic amines by selective SPE isolation, derivatization and quantification by HPLC with fluorescence detector. Students will apply a procedure of isolation, preconcentration, derivatization, and HPLC analysis of biogenic amines in simplified foods. Students will have to carry out the complete procedure, perform its calibration, partial validation and analyze a standard sample.

Practical session 5 (3.0 h computer room): Practical problems with gas chromatography software and real data in which students will carry out practical exercises to work on the concepts of searching for compounds by name in the spectrum library, TIC (Total Ion Current) chromatogram and acquired m/z interval, extraction of ion chromatograms, localization of a compound from its mass spectrum, identification with spectrum libraries, selection of m/z fragments for quantitative analysis, detection of interferences.

Practical session 5 (2.0 h computer room): software practice in which students will work with data from a metabolomic experiment. Students will act on each of the steps of the metabolomic strategy: sample selection, signal processing, statistical analysis, metabolite identification, integration into metabolic pathways, and markers search.

4.4.Course planning and calendar

Further information concerning the timetable and lectures and work presentations concerning to dates and important events related to the subject are in details described in the Faculty of Veterinary Science website: (http://veterinaria.unizar.es/). This website is updated at the beginning of the academic course.

Course will be start with lectures while practical sessions will be introduced after the corresponding theoretical contents.

4.5.Bibliography and recommended resources

Recommended bibliography at: https://biblioteca.unizar.es/ Additional resources related to databases, software, and other material will be delivered to students as they need them.