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COURSE SYLLABUS

1. Identification

Code and title: QUP 130 – Special Topics in Multidimensional Chromatography
Professors: Claudia Alcaraz Zini and Rosângela Assis Jacques
Level: Master and Doctorate
Credit hours: 2
Revised: August_2021

2. Summary

Introduction to multidimensional chromatographic techniques, history, fundamentals, instrumentation, modulators, nomenclature, abbreviations, analysis of complex mixtures by GCxGC (petroleum and derivatives, fixed oils, essential oils, aromas and fragrances, environmental samples, biological samples, forensic samples, etc), future perspectives.

3. Objective

Basic concepts related to comprehensive multidimensional chromatography and partial fractions, both with regard to gas chromatography and with regard to liquid chromatography. In addition, the student should know how to apply this knowledge in practical cases related to the analysis of complex samples, such as oil and derivatives, environmental samples, forensics, aromas, food and beverages, etc.

4. Contents

- Introduction to multidimensional chromatographic techniques: Comprehensive Two-Dimensional Liquid and Exclusion Chromatography (LC×SEC), Comprehensive Two-Dimensional Liquid and Gas Chromatography (LC×GC), Comprehensive Two-Dimensional Liquid Chromatography (LC×LC), Nano LC: principles, evolution, columns , state of the art detection systems; applications; Comprehensive Two-Dimensional Supercritical Gas Chromatography (SFC×GC), Comprehensive Three-Dimensional Gas Chromatography (GC×GC×GC), Size Exclusion Chromatography, Liquid and Comprehensive Three-Dimensional Capillary Electrophoresis (SEC×LC×CZE), Liquid Chromatography Coupled with Gas Chromatography In-line Comprehensive Two-Dimensional (LC-GC×GC), Comprehensive Two-Dimensional Gas Chromatography with Two Parallel Columns in the Second Dimension (GG×2GC), gas chromatography coupled with a mass spectrometry detector (GC/MS), etc.
- History of two-dimensional chromatography, with emphasis on heart-cut GC×GC and comprehensive GC×GC.
- Fundamentals (orthogonality, diagram types, roof effect, choice of columns as a function of phases and dimensions, chirality, in-phase and out-of-phase modulation, primary peak, modulation cycle, out-of-cycle peak, etc.).
- Nomenclature and abbreviations.
- Instrumentation (modulators, detectors).
- Data processing (retention rates, interpretation, chemometrics)
- Applications: petrochemicals (diesel, gasoline, biodiesel and diesel blends, heavy fractions), aromas and fragrances and essential oils, pharmaceutical industry (solvent residues, drugs),

essential and fixed oils, environmental samples (pesticides in fruits and vegetables, air and aerosols, cigarette smoke, pyrolysis products), forensic samples (fires, oil spills), biological samples (drugs, steroids, steroids, metabolomics).
- Future perspectives (data processing, data interpretation, field analysis, new modulators)

5. Assessment

The student will be assessed through: (i) Monograph: each student will write a monograph, which will be presented both in written form and in an illustrated oral presentation (poster, transparencies, slides) of about 30 minutes on topics of interest to the discipline. A summary of the work will be given to colleagues on the day of the presentation or (ii) Occasional works: Each student must read, prepare and present a scientific article in the area of Multidimensional Chromatography, presenting it orally with visual resources (poster, transparencies, slides) , delivering a text related to the work to the teacher and a summary to the colleagues on the day of the presentation. A knowledge check exercise, with or without consultation, can also be used, depending on the knowledge profile of the class. The student, who obtains a final grade of A, B or C, awarded as per the list below, will be considered approved:
A: grade equal to or above 9.0
B: grade equal to or above 7.5 and below 9.0
C: grade equal to or above 5.0 and below 7.5
D: grade below 5
FF: lack of frequency

6. Methodology

Lectures, exercises lists, seminars and examinations.

7. Bibliography

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