Universitat Autònoma de Barcelona

Industry and Research in Chemistry: Specialized Topics in Theory and Practice 2016/2017

Code: 42424
ECTS Credits: 9

Degree	Type	Year	Semester
4313385 Industrial Chemistry and Introduction to Chemical Research	OB	0	1

Contact

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Use of languages

Principal working language: english (eng)

Prerequisites

none

Objectives and Contextualisation

Industrial Chemistry and Introduction to Chemical Research is a mandatory module of the Masters Program in Industrial Chemistry and Introduction to Chemical Research. The objective of this course is to acquiere new knowledge and abilities in fields related to Industrial Chemistry and Chemical Research: Regulations, Patents, Experimental design, Job searching, Introduction to computational chemistry, NMR , Introduction to photochemistry, Resource optimization and environmental assessment of chemical processes, Risk and safety in chemical facilities, and Laboratory instrumental techniques and chemical analysis (including mass spectrometry, chromatography, microscopy, XRD, ICP and laboratory advanced techniques).

Skills

- Correctly apply new information capture and organisation technologies to solve problems in professional activity.
- Correctly evaluate the risks and environmental and socio-economic impact associated to special chemical substances.
- Define specialised concepts, principles, theories and facts in the different areas of Chemistry.
- Design processes that imply the treatment or elimination of dangerous chemical products.
- Evaluate the human, economic, legal and ethical dimension of professional practice, as well as the environmental implications of one's work.
- Identify information in the scientific literature using the appropriate channels and integrating said information to approach and contextualise a research issue.
- Operate with advanced instrumentation for chemical evaluation and structural determination.
- Students should be able to integrate knowledge and face the complexity of making judgements from information which, being incomplete or limited, include reflections on the social and ethical responsibilities linked to the application of their knowledge and judgements
- Students should know how to communicate their conclusions, knowledge and final reasoning that they hold in front of specialist and non-specialist audiences clearly and unambiguously
- Use scientific terminology in the English language to defend experimental results in the context of the chemistry profession.

Learning outcomes

1. Apply advanced analytical and instrumental techniques in a chemistry laboratory.

2. Characterise materials and biomolecules.
3. Compare microscopy and spectroscopy techniques for applications of differing natures.
4. Correctly apply new information capture and organisation technologies to solve problems in professional activity.
5. Describe quality and patent regulations.
6. Design chemical experiments.
7. Design chemical processes that respect the environment.
8. Evaluate risks and security in chemical facilities and laboratories.
9. Evaluate the human, economic, legal and ethical dimension of professional practice, as well as the environmental implications of one's work.
10. Identify information in the scientific literature using the appropriate channels and integrating said information to approach and contextualise a research issue.
11. Know the environmental risks associated to special substances and chemical processes.
12. Students should be able to integrate knowledge and face the complexity of making judgements from information which, being incomplete or limited, include reflections on the social and ethical responsibilities linked to the application of their knowledge and judgements
13. Students should know how to communicate their conclusions, knowledge and final reasoning that they hold in front of specialist and non-specialist audiences clearly and unambiguously
14. Use scientific terminology in the English language to defend experimental results in the context of the chemistry profession.

Content

M1: Industry and Research in Chemistry: Specialized Topics in Theory and Practice

- Regulations.

- Patents.

- Experimental design.

- Job searching.

- Introduction to computational chemistry.

- NMR (theory + problem resolution + introductory practical course)

- Introduction to photochemistry.

- Resource optimization and environmental assessment of chemical processes.

- Risk and safety in chemical facilities.

- Laboratory instrumental techniques and chemical analysis.

Mass spectrometry, chromatography
Microscopy
XRD
ICP
Laboratory advanced techniques

Methodology

Lectures / Individual work:
The student acquires the knowledge of the course by attending the lectures and complementing them with the individual work. The lectures may include problem solving (theoretically based or practical exercises) and seminars.

Laboratory work
Laboratory practices will be held to achieve specific and relevant competencies.

Activities

Title	Hours	ECTS	Learning outcomes
Type: Directed			
Individual work	141	5.64	2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14
Laboratory Practice	21	0.84	1, 3, 4, 6, 7, 8, 9, 10, 11, 12, 13, 14
Lectures	47	1.88	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14

Evaluation

Continual assessment

Evaluation activities

Title	Weighting	Hours	ECTS	Learning outcomes
Presentations	20%	8	0.32	4, 6, 7, 8, 9, 10, 11, 12, 13, 14
Reports	40%	0	0	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14
Theoretical - practical tests	40%	8	0.32	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14

Bibliography

Patents

http://www.ub.edu/centredepatents/es/
http://www.oepm.es/es/propiedad_industrial/index.html
http://www.epo.org/law-practice.html
http://e-courses.epo.org/wbts/htgaep_en/index.html

Experimental design

Richard G. Brereton, "Applied Chemometrics for Scientists", 2007, chapter 2, Wiley Chichester.
Rolf Carlson & Johan E. Carlson, "Design and optimization in organic synthesis", 2005, Series Data Handling in Science and Technology Vol. 24, Elsevier Amsterdam.
Gareth A. Lewis; Didier Mathieu & Roger Phan-Tan-Luu, "Pharmaceutical experimental design", 1999, Marcel Dekker NY.

Introduction to computational chemistry

C. J. Cramer, "Essentials of Computational Chemistry: Theories and Models", 2004, Wiley, 2nd edition.
F. Jensen, "Introduction to Computational Chemistry", 2007, Wiley, 2nd edition.
E. G. Lewars, "Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics", 2011, Springer, 2nd edition.
D. C. Young, "Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems", 2001, Wiley.

Introduction to Photochemistry

Angelo Albini, "Photochemistry: Past, Present and Future", 2016, Springer-Verlag, Berlin Heidelberg.

Resource optimization and environmental assessment of chemical processes

Xavier Domènech, "Química Verde", 2005, Editorial Rubes, ISBN 9788449701818.
Risk Assessment and Sustainable Chemistry: http://www.epa.gov/nrmrl/std/index.html
Life Cycle Assessment: http://www.epa.gov/nrmrl/std/lca/resources.html
Donald Mackay, "Multimedia Environmental Models", 2001, Lewis Publishers, ISBN 1-56670-542-8.

Risk and safety in chemical facilities

D.J. Knight, "EU Regulation of Chemicals: REACH", 2005, Rapra Review ReportN. 181, RapraTechnology Limited, Shawbury UK.

Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency.

Laboratory instrumental techniques and chemical analysis

Thomas T. Tidwel, "Wilhelm Schlenk: The Man Behind the Flask", Angew. Chem. Int. ed. 2001, 40, 331-337.

Duward F. Shriver, M. A. Drezdzon, "The Manipulation of Air-Sensitive Compounds", 1986, J. Wiley and Sons: New York.