

Indústria i Recerca Química: Aspectes Especialitzats Teòrico-Pràctics

2014/2015

Codi: 42424

Crèdits: 9

| Titulació | Tipus | Curs | Semestre |
|--|-------|------|----------|
| 4313385 Química Industrial i Introducció a la Recerca Química/Industrial Chemistry and Introduction to Chemical Research | OB | 0 | 1 |

Professor de contacte

Nom: Jordi Garcia-Anton Aviño

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Utilització de llengües

Llengua vehicular majoritària: anglès (eng)

Grup íntegre en anglès: No

Grup íntegre en català: Sí

Grup íntegre en espanyol: No

Equip docent

Teodor Parella Coll

José María Paulis Fernández

Maria Dolors Baró Mariné

José Luis Bourdelande Fernández

Jordi Coello Bonilla

Agustí Lledós Falcó

Cristina Palet Ballús

Juan Francisco Piniella Febrer

Josefina Pons Picart

Manel del Valle Zafra

Angel Álvarez Larena

José Peral Pérez

Equip docent extern a la UAB

Mireia Condom Ejarque

Rafael Pi

Prerequisits

none

Objectius

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 acquire 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).

Competències

- 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 ones 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.

Resultats d'aprenentatge

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 ones 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.

Continguts

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

Metodologia

Classes de Teoria / Treball Individual:

L'alumne adquireix els coneixements propis de la assignatura assistint a les classes magistrals i complementant-les amb l'estudi personal dels temes explicats. Les classes de teoria poden incloure classes magistrals, resolució de problemes (cassos pràctics o supòsits teòrics) i seminaris.

Pràctiques de Laboratori:

Es programen pràctiques de laboratori per assolir les competències específiques corresponents.

Activitats formatives

| Títol | Hores | ECTS | Resultats d'aprenentatge |
|------------------------|-------|------|--|
| Tipus: Dirigides | | | |
| Classes de Teoria | 47 | 1,88 | 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14 |
| Sessions de laboratori | 21 | 0,84 | 1, 3, 4, 6, 7, 8, 9, 10, 11, 12, 13, 14 |
| Treball Individual | 141 | 5,64 | 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14 |

Avaluació

L'avaluació de l'assignatura inclou:

- Defensa oral de treballs
- Proves teòriques i/o pràctiques
- Lliurament de treballs i informes

Activitats d'avaluació

| Títol | Pes | Hores | ECTS | Resultats d'aprenentatge |
|-----------------------------|-----|-------|------|---|
| Defensa oral de treballs | 20% | 8 | 0,32 | 4, 6, 7, 8, 9, 10, 11, 12, 13, 14 |
| Proves teòriques pràctiques | 40% | 8 | 0,32 | 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14 |
| Treballs / informes | 40% | 0 | 0 | 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14 |

Bibliografia

Experimental design

Richard G. Brereton, "Applied Chemometrics for Scientists". Wiley Chichester, 2007, chapter 2.

Rolf Carlson & Johan E. Carlson, "Design and optimization in organic synthesis". Series Data Handling in Science and Technology Vol. 24. Elsevier Amsternam (2005).

Gareth A. Lewis; Didier Mathieu & Roger Phan-Tan-Luu. "Pharmaceutical experimental design". Marcel Dekker NY(1999).

Patents

<http://www.ub.edu/centrepatents/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

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.

Resource optimization and environmental assessment of chemical processes

Xavier Domènech, "Química Verde", Editorial Rubes, 2005, 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" Lewis Publishers, 2001, ISBN 1-56670-542-8

Risk and safety in chemical facilities

D.J. Knight, "EU Regulation of Chemicals: REACH", Rapra Review Report N. 181, Rapra Technology Limited, Shawbury UK, 2005

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. Drezdson "The Manipulation of Air-Sensitive Compounds" 1986, J. Wiley and Sons: New York

