STUDENT GRANTS FOR MASTERS

DEGREE IN

FINE CHEMISTRY EXPERIMENTATION

PROFESSIONAL INTRODUCTION COURSE IN THE AREA OF FINE CHEMICALS COMPANIES

TENTH YEAR OFFERED

STARTING: 2017/2018

A JOINT INITIATIVE OF

UNIVERSITAT AUTÒNOMA DE BARCELONA AND ESTEVE QUÍMICA S.A.

INTRODUCTION TO THE MASTERS DEGREE

Entry into the employment market for university graduates is a priority concerns for the Universitat Autònoma de Barcelona and for the chemicals company Esteve Química, S. A. (EQ Esteve). Together they have designed the **Master in Fine Chemistry Experimentation,** a two-year course for professional orientation in the area of fine chemicals companies, with the aim of helping young graduates to find an occupation that matches their education and skills.
This is a training Masters degree that aims to provide employment opportunities for new university graduates with no professional experience who want to train in a major company in the fine chemicals sector following a period at the university.

What are the objectives of the Master in Fine Chemistry Experimentation?

The objectives are basically:

1) to offer new graduates from all Spanish universities the opportunity to see the operations of a major fine chemical company and
2) help new graduates to enter the employment market and occupy position s of responsibility related to their university education.

What benefits does the Master in Fine Chemistry Experimentation offer students? And what does it offer the company?

This Masters degree brings many benefits to university graduates. It opens the door and offers the possibility of overcoming that great initial obstacle of having no professional experience; it offers the chance to see a large company in operation, to receive complementary training to broaden that received at the university and to put theoretical knowledge into practice. And finally, the enormous opportunities for entry into the labour market that are presented to grant holders by EQ Esteve itself, or other companies in the sector, cannot be underestimated.
Clearly, our Masters degree also offers benefits to EQ Esteve, among which we can highlight the valuable human capital that they have to opportunity to train to carry out activities in one of their departments.
Moreover, they will work at all times with university graduates able to offer the EQ Esteve crucial values for the growth and prosperity of the company, such as enthusiasm and the daily energy of young people who see themselves at the starting point of a new stage in their lives.

What kind of professional is EQ Esteve looking for?

EQ Esteve is looking for professionals without professional experience who they can train. Professional experience is a requirement which, in this Masters course, is overtaken by other requirements such as enthusiasm, creativity, willingness to learn and undertake a new professional

path. The UAB, as a public university, wants to play a part in facilitating this possibility for young graduates.

Who is this programme aimed at?

Candidates eligible to apply for these grants should satisfy the following requirements:

- Possess a Degree in Chemistry, Biochemistry or Chemical Engineering obtained within the last 4 years.
- Have been successful in the selection process for the award of an EQ Esteve grant to undertake this Masters degree.
- Not have received a grant to study this Master in the past.

Holding a grant for the study of this Masters degree is not compatible with any remunerated employment, the receipt of unemployment benefit, or any other grant.

What documentation is necessary?

The period for presenting applications will be approximately from July, 1st to September, 23rd, yearly.

Candidates should present the following documentation:

- Passport size photograph (in electronic format)
- Photocopy of national identity document or other document that accredits identity
- Curriculum vitae
- Photocopy of academic record in which details of the grant competitions appear
- Photocopy of documents and certifications that endorse the merits and circumstances outlined in the application or CV.

All documentation should be handed into the Secretary's Office of the Department of Chemistry at the Universitat Autònoma de Barcelona.

ORGANISATIONAL STRUCTURE OF THE MASTERS DEGREE

Coordination and management
Carles Jaime Cardiel. Professor of Organic Chemistry at the Department of Chemistry of the UAB.
Ramon Alibés Arqués. Associate professor of Organic Chemistry at the Department of Chemistry of the UAB.

Teaching staff

Teaching staff of the UAB

Ángel Álvarez Larena. Director of the X-Ray Diffraction Service at the UAB.
Mercè Granados Juan. Professor of the Dept. of Analytical Chemistry, Univ. Barcelona.
Jordi Coello Bonilla. Professor of Analytical Chemistry, Department of Chemistry.
Pere de March Centelles. Professor of Organic Chemistry a, Department of Chemistry.
Josep Font Cierco. Professor of Organic Chemistry, Department of Chemistry.
Carles Jaime Cardiel. Professor of Organic Chemistry, Department of Chemistry.
Félix Busqué Sánchez. Associate professor of Organic Chemistry, Department of Chemistry.
Ramon Alibés Arqués. Associate professor of Organic Chemistry, Department of Chemistry.
Teodor Parella Coll. Director of the Nuclear Magnetic Resonance Service of the UAB.
Albert Virgili Moya. Professor of Organic Chemistry, Department of Chemistry.

Experts not attached to the UAB

Josep Montefusco Monferrer. Graduate in Law (UAB), specialist in intellectual property rights.
Rafael Pi Subirana. Doctor in Chemical Sciences (UAB), expert in experiment design and patents agent.

Experts from EQ Esteve

Martí Bartra Sanmartí. Director of the scientific area of the R+D Department.
Ramon Berenguer Maimo. Head of the pilot plant section of the R + D Department.
Montserrat Closa Calvo. Head of the analytical development section of the R + D Department.
Montserrat Monsalvatje Llagostera. Head of the synthesis laboratories section of the R + D Department..
Jordi Redondo Moreno. Head of the spectroscopic techniques section of the R + D Department.

ACADEMIC INFORMATION

1. Grant holder selection process

The selection of grant award winners and the allocations of places will be carried out by the directors of the Masters programme together with representatives form EQ Esteve.
During the selection process account will be taken of:
· The appropriateness of the candidate according to the profile required by the company.
· Academic record.
· other studies and complementary activities. (Other knowledge, languages, computer skills etc.)
· Personal interview.
The results of the selection process will be made known to the candidates.

2. Registration

Accepted students should register at the School for Postgraduate Studies during the month of December 2008.
Students will be cover by an accident and health insurance policy.
Once registered, grant holders should sign the cooperation agreement with the UAB, and will receive a receipt and a copy of the agreement by registered mail at the address indicated on the registration form.

3. Obligations and withdrawals

Grant holders must respect all the regulations of EQ Esteve, fulfil their working hours and carry out the tasks allocated to them, follow the theory classes and respect professional secrets both during their period at the company and once the grant period has expired.
Grants will be cancelled in the following cases:
- where there is any irregularity in the application information
- if registration is not carried out
- if grant holders do not present themselves at the company on the appointed date and time
- if grant holders fail to fulfil any of their obligations

In the case of voluntary withdrawal from the place by the grant holder, this should be communicated in writing to the directors of the Masters programme and to the company with at least 15 days notice.

4. Starting date

Grant holders will start work in the company (EQ Esteve, C/ Caracas, 17-19, 08030 Barcelona) on each January, 1st.
Registration will take place on the administration office of the Department of Chemistry at UAB.
Telephone 93 5811997

5. **Evaluation**

Evaluation of theory classes will be continuous and may include projects and exams.
In order to obtain the Masters qualification attendance is required at least 90% of the theory sessions (not counting justified absences) and have achieved a positive evaluation in all of them. it is also necessary to satisfy at least 90% of the practical hours (not counting justified absences) and the presentation of the research project.

6. Award of the degree and request for academic certificates

A pass in all the theory and practical credits at EQ Esteve and in the research project leads to an overall pass and the award of the Masters degree. Students will be informed of their eligibility to receive the masters degree and any modifications to the registration documents that are required should be made at that time (address, contact telephone number, etc.) and the cost of processing the qualification should be paid.
The Academic Management Office at the School for Postgraduate Studies is responsible for the administration and sending of the Masters degrees to the addresses supplied by students. Certificated are issued in approximately one year.

Students may request a "substitute certificate", free of charge. This certificate may only be issued once. If students require information about the classes taken, a different certificate is required and this costs approximately €25. In both cases these certificates should be requested expressly in writing by the interested party from:
Continuing Education Academic Management at ep.formcont@uab.es

PRGRAMMES FOR ATTENDED CLASSES

Subject: Structural Determination and RMN (4 ECTS credits)

Lecturers: Dr. Albert Virgili Moya
Dr. Teodor Parella Coll

1. Introduction:

Review of the rudiments of different spectroscopes: mass spectrometry, nuclear magnetic resonance (NMR) spectrometry.

2. Obtaining one-dimensional NMR spectra:

The experimental act: available variables.

The most common nuclei in organic chemistry, measures of: chemical displacement, coupling constants, relaxation time, spin systems, Nuclear Overhauser Effect (NOE), diffusion constants.

Manipulation of a free induction decay (FID) and obtaining a spectrum. Spectra edition.

Example of obtaining different spectra from the nucleus of a molecule: 1H, 13C, 19F...DEPT, SELNOE, HETNOE. Data production and structure elucidation.

NMR at variable temperature.

3. Obtaining two-dimensional NMR spectra:

The experimental act: available variables.

The most important homo- and heteronuclear experiments, direct and long distance connectivity, nuclear Overhauser effect (NOESY and ROESY), diffusion velocity measurements.

Manipulation of a free induction decay (FID) series and obtaining a bi-dimensional spectrum. Phase-sensitive spectra.

Examples of two-dimensional spectra: COSY, TOCSY, HSQC, HMBC, NOESY, ROESY, data production and structure elucidation.

4. Resolution of structures with the help of combined IR, MS, RMN spectra.

Subject: Advanced Aspects of Organic Synthesis (4 ECTS credits)

Lecturer: Dr. Josep Font Cierco

1. **Objectives of organic synthesis**. Molecular complexity. Synthesis and retrosynthesis, Production of the synthetic tree. Search for advanced synthetic intermediaries.
2. **Functional groups**. Transformations between functional groups. Logical disconnections according to functional groups. Protection of functional groups: characteristics of a protector group, orthogonal and sequential protection.
3. **Review of formation methodologies for C-C and C=C links.** New methodologies for the formation of C-C and C=C links: use of transition metals especially as catalysers; radicalary reactions.
4. **Ring formations**. Reactions to the formation of 6, 5, 4 and 3 valve cycloalkanes. Macrocycles.
5. **Selectivity**: Chemical selectivity. Regioselectivity. Steroselectivity. Examples selected from each category.
6. **Asymmetrical synthesis**. Methods employed in enentioselective synthesis: resolution, chiral precursors, chiral auxiliaries, chiral catalysers, enzymes.
7. **Aspects of sustainability applied to organic synthesis. Economy** Atom economy. non-polluting solvents. Reactions in aqueous environments. Catalytic reactions vs. equimolar or quasiequimolar reactions. Supported catalysers.

Subject: Organic Heterocyclic Chemistry (2.5 ECTS credits)

Lecturer: Dr. Pere de March Centelles

1. **Introduction.** Nomenclature. Electronic structure. Aromatic character. Monocyclic and polycyclic systems. Reactivity and regioselectivity.
2. **Five-member rings with a heteroatom.** Synthesis and reactivity of furans, pyrroles, tiophens, indoles and benzofurans.
3. **Six- member rings with a heteroatom.** Synthesis and reactivity of pyridines, quinolines and isoquinolines.
4. **Five-member rings with two or more heteroatoms.** Synthesis and reactivity of imidazoles, pyrazoles, oxazoles and isoxazoles.
5. **Pericyclic thermal reactions.** Frontier molecular orbitals. Regioselectivity, periselectivity and stereoselectivity. 1.3 dipole concept.
6. **[2+2] and Hetero-Diels-Alder reactions.** Use of ketenes, imines, isocyanates, olefins, carbonyl compounds, nitrils, nitrous and azabutadien derivatives.
7. **Propargylic dipoles.** Nitryl ylides. Nitryl oxides. 1.3 heterodisubstituted systems. Diazoalkynes. Azides.
8. **Allylic dipoles.** Azomethine ylides Nitrones. Ozone and ozonolysis.

Subject: Extension of Technical Instruments (2.5 ECTS credits)

Lecturers: Dr. Santiago Maspoch Andrés
Dr. Marcel Blanco Romia
Dr. Jordi Coello Bonilla

1. Spectroscopic techniques (IR, NIR)
Fundamentals. Spectral registration methods. Applications in the chemical and pharmaceutical industries. Examples of application to process control. Introduction of the PAT concept.

2. Chromatography of gases
Injection. Detection: FID, ECD, MS. Example of development of HRGC methods. Head-space. Quantification by external standard or by standard additions.

3. Chromatography of liquids
Normal phase. Reverse phase. Development of HPLC methods. Chromatography of chiral composites.

4. Extension of chromatographic techniques. HPLC-masses coupling
Evolution of HPLC columns. Chromatography – mass detector coupling. Thermal and electrospray interphases. API and APCI techniques. Examples of application.

5. Capillary electrophoresis
Fundamentals. Examples of application.

Subject: Industrial Application of Experiment Design: Products, Processes and Formulations (2 ECTS credits)

Lecturer: Dr. Rafael Pi Subirana

Introduction:
The philosophy of Experiment Design as an alternative to the traditional focus.

Tools:
Factorial designs.
Central compound designs.
Latin squares
Designs of mixtures.
Combined designs.

Question to resolve:
What influences the system?
What is the influence like?
What model does the system describe?
What is the best composition?
What is the optimal composition?

Areas of application:
Screening of process factors and raw materials
Optimisation
New products and formulas
New processes
Modification of existing products and formulas
Modification of existing processes
Continued improvement of processes, products and formulas
Technical help service
Analytical methods

Subject: Organic Molecular Modelling (1.5 ECTS credits)

Lecturer: Dr. Carles Jaime Cardiel

Theme 1. **Molecular modelling.** Generalities. Molecular models. Systems of molecular modelling: theoretical bases. A force field in detail.

Theme 2. **Applications of MM to confirmational analysis.** Generalities: the problem of the global minimum. How many confomers does a compound contain? Configurational assignment with thee MM/^{1}H-RMN compound.

Theme 3. **Molecular dynamics I.** Qualitative introduction. Simulation convergence, Differences to Monte-Carlo methods. Molecular interactions. Docking. An example – cyclodextrines: complexing geometry, inclusion simulation, dimers.

Theme 4. **Molecular dynamics II. Free energy perturbation.** Basic concepts. Enantio-differentiation. Rotaxanes: identifying the problem, transactional isomery, effects of solvents.

Subject: Crystalline Polymorphism focussed on Pharmaceutical Solids (1.5 ECTS credits)

Lecturer: Dr. Ángel Álvarez Larena

1- Polymorphs, solvates and amorphs: structural and thermodynamic considerations.
2- Analytical techniques: thermal analysis, spectroscopy, microscopy, diffraction techniques, complementary analysis.
3- Structure-properties relation, Crystallisation.
4- Obtaining and predicting polymorphs and solvates. Obtaining amorphous solids.

Subject: ISO Regulations and Analytical validation Procedures (1 ECTS credit)

Lecturers: Dr. Santiago Maspoch Andrés
Dr. Marcel Blanco Romia
Dr. Jordi Coello Bonilla

1. Introduction and ISO regulations
Introduction to quality. Quality certification systems. ISO9000:2000. Pharmaceutical industry: good laboratory practice. ISO17025.

2. Guides
FDA and EMEA guides. ICH guide. Introduction to Q2-Q8 guides. Pharmacopoeias.

3. Validation of an analytical method
Selectivity, exactitude, precision, linearity, limits to detection and quantification. Interlaboratory precision.

Subject: Patents in the Pharmaceutical Industry (1 ECTS credit)

Lecturer: Montserrat López Bellosta

Theme 1. R+D for a new pharmaceutical. Patentability requirements. Industrial application. Novelty. Inventive activity. Descriptive Sufficiency. Expert in the subject. Duration and effects of the patent. Exception to exclusive rights. Patent modes.

Theme 2. Procedures for concession of patents. Writing the patent. lab books. Patent novelty .

Theme 3. Protection of data in the Pharmaceutical Dossier register in the area of industrial property. new indications. line extensions. Data protection versus protection by patent. Processing of line extensions under EU and Spanish legislation. R+D and line extensions. Data protection on the pharmaceutical sector and line extensions.

Theme 4. Patent infractions. literal infraction. Infraction by equivalence. Claims and description of the patent. Proof of infraction. Procedural mechanisms for obtaining proof of infraction. Procedures for verifying the facts. Precautionary measures. Judicial procedures for patents. Actions conferred by the patent. Oral judgement. Damages. Patent litigation: proof. Reversal of the burden of proof. Declaration of non-infraction of the patent. Nullity of the patent.