Total Synthesis and Activation Methods

- 1. Course number and name: 020STMCS2 Total Synthesis and Activation Methods
- 2. Credits and contact hours: 4 ECTS credits, 2x1:15 contact hours
- 3. Names of instructors: Joseph Bejjani

4. Instructional materials:

- Course handouts
- Lab manual
- References
 - Carey et Sundberg. *Chimie organique avancée*. De Boeck (available at the campus library)
 - Brückner, R., 1999. *Mécanismes réactionnels en chimie organique*. De Boeck (available at the campus library)
 - Clayden, Greeves, Warren, and Wothers, *Chimie organique*. De Boeck (available at the campus library)
 - BERTRAND, GRÉE, LALLEMAND et NIEF. Synthèse organique Principes et outils. Ecole Polytechnique (available at the campus library)
 - Hammerich, O. and Speiser, B., 2015. Organic electrochemistry: revised and expanded. CRC Press.
 - Mason, T.J. and Peters, D., 2002. *Practical sonochemistry: Power ultrasound uses and applications*. Woodhead Publishing.
 - Novak, F.M. ed., 2011. Sonochemistry: Theory, Reactions, Synthesis, and Applications. Nova Science Publishers, New York.
 - Kappe, C.O., Stadler, A. and Dallinger, D., 2012. *Microwaves in organic and medicinal chemistry*. John Wiley & Sons.
 - Jacques Drouin. *Manipulations commentées de chimie organique*. De Boeck (available at the campus library).
 - Jacques Mesplède et Christine Saluzzo. 100 manipulations de chimie organique et inorganique. Bréal (available at the campus library)

5. Specific course information

a. Catalog description:

Total synthesis, Industrial alternatives, Synthesis planning, Retrosynthesis techniques, Solutions to chemoselectivity problems, Protection of functional groups and applications, Enantiomer resolution techniques, Asymmetric induction, Prediction of the stereochemistry of products resulting from diastereoselective reactions, Strategies of asymmetric syntheses, Enzymatic engineering and industrial asymmetric synthesis, Fields of synthetic chemistry, Profile of synthetic chemistry companies, Accessibility of starting substrates, Sources of organic compounds, SynGas, Production of basic compounds, REACH regulations and procedures to follow, Green chemistry and engineering, Parameters to assess the "green" nature of a chemical process, Bioprocesses and biotechnologies, Green alternatives to conventional solvents,

Principle of electrosynthesis, Advantages and disadvantages of electrosynthesis, The different types of electrosyntheses, Electrocatalytic reactions, Principle of sonochemistry, Constraints and limitations of sonochemistry, Transducers and sonochemistry on an industrial scale, Principle of microwave activation, Microwave activation and dielectric properties of materials, Microwave heating and conventional thermal heating, Microwave effects, Multi-step synthesis in lab.

b. Prerequisites: 020CORNI3 Organic Chemistry

c. Required/Selected Elective/Open Elective: Required

6. Specific goals for the course

a. Specific outcomes of instruction:

- Use retrosynthesis techniques to design an efficient synthesis of a given target molecule from simple and available molecules
- Choose reagents and adequate methods of protection and deprotection to synthesize highly functionalized compounds while taking into account the problems of regio-, chemo- and stereoselectivity that may arise
- Predict the results of diastereoselectivity and asymmetric induction in chemical reactions
- Use electrochemistry, ultrasonic and microwave techniques to perform more efficient industrial syntheses
- Plan the development of an industrial synthesis process while taking into account safety measures, environmental, economic and legislative aspects
- Perform multistep syntheses of organic compounds that possess biological activities or interesting characteristics.
- Communicate the results of experimental work in the form of a scientific article

b. PIs addressed by the course:

PI	1.3	2.2	4.2
Covered	Х	Х	Х
Assessed	Х	Х	Х

7. Brief list of topics to be covered

- Total synthesis: definition, general overview, examples of important total syntheses, uses and advantages, industrial alternatives with instructive illustrations
- Retrosynthesis techniques
- The different types of chirality
- Enantiomer resolution methods
- Prochirality
- Asymmetric induction
- Transition state models to explain and predict asymmetric induction
- Diastereoselectivity with supporting transition state models
- Asymmetric synthesis methodologies

- Protections and deprotections of functional groups
- Laboratory work: multi-step synthesis of a compound with interesting biological activity
- The fields of synthetic chemistry
- Available starting substrates
- Sources of raw materials
- Heavy chemicals and basic chemicals
- The REACH regulation: overview, usefulness, approach and procedures
- Green chemistry and green engineering
- Parameters for assessing the "green" nature of a chemical process
- Bioprocesses and biotechnologies
- Electrosynthesis as a green alternative
- Green solvents
- Electrosynthesis: principle, advantages and disadvantages, and the different types
- Sonochemistry
- Microwave activation