UAB
Universitat Autònoma de Barcelona

# Supramolecular Chemistry and Molecular Recognition

Code: 106819
ECTS Credits: 6

2025/2026

| Degree | Type | Year |
|---|---|---|
| Nanoscience and Nanotechnology | OB | 3 |

## Contact

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## Teachers

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## Teaching groups languages

You can view this information at the end of this document.

## Prerequisites

It is recommended having studied and passed the 2nd year subjects "Chemistry of the Elements", "Organic Chemistry", and "Thermodynamics, Kinetics and Phase Transformations"

Although the classes are in Catalan, much of the material that the student will have to work, as well as the main bibliographic sources, are written in English. Therefore, good knowledge of this language is recommended.

## Objectives and Contextualisation

In this subject, the students will learn the basis of in Supramolecular Chemistry, which will allows them to recognize molecular recognition phenomena from a chemical point of view and to understand the processes involved in the formation of self-assembled supramolecular structures.

The specific objectives of this subject are:

· To introduce the concept of Supramolecular Chemistry, to study the chemical interactions on which it is based and know the main methods of characterization and manipulation of the supramolecular complexes.
· To apply the basics of Supramolecular Chemistry to the understanding of the processes of molecular

recognition both at a chemical and biological level.
· To use the basics of Supramolecular Chemistry to interpret the formation of self-assembled supramolecular structures.

## Learning Outcomes

1. CM19 (Competence) Work independently to solve problems and practical cases related to nanoscale phenomena.
2. KM31 (Knowledge) Describe the fundamental interactions involved in supramolecular chemistry that lead to the formation and manipulation of supramolecular complexes.
3. SM31 (Skill) Design nanomaterials and nano-systems that suit different technological specifications and uses.

## Content

1. Introduction to Supramolecular Chemistry.

Supramolecular systems. Supra molecular forces (van der Waals, hydrogen, ion-ion, ion-dipole, dipole-dipole, ion-π, π-π, hydrophobic). Relationship between strength and directionality. Coordination chemistry: metallic centers and ligands. Basic concepts in supramolecular chemistry: host-guest systems and self-assembling; association constants and selectivity; complementarity, preorganization and cooperativity.

2. Characterization and manipulation of supramolecular systems.

X-ray diffraction. Mass spectrometry. Spectroscopic techniques (UV-vis, IR, NMR). Electrochemical techniques. Electrochemical and photochemical manipulation of supramolecular systems.

3. Complexation and molecular recognition.

Recognition of cations, anions and neutral molecules. Association constants. Stoichiometry. Applications.

4. Self-assembly and self-organization.

Concept of self-assembly and self-organization. Self-assembling based on intermolecular interactions (amphiphilic molecules). Self-assembling based on coordination in metal centers (helicates, racks, ladders, grids). Mechanical self-assembling (rotaxanes, catenanes, knots).

5. Supramolecular interactions and molecular recognition in biological systems. Biological structures and processes based on supramolecular interactions: nucleotides and DNA; peptides and proteins; lipids and membranes; virus.

LAB EXPERIMENTS

Experiment 1. Determination of critical micelle concentration by means of conductivity measurements

Experiment 2. Characterization of the inclusion complex between cyclodextrin and phenolphthalein by means of UV-vis spectroscopy

Experiment 3. Synthesis and characterization of an anion-binding host

## Activities and Methodology

| Title | Hours | ECTS | Learning Outcomes |
|---|---|---|---|
| Type: Directed | | | |
| Laboratory teaching | 14 | 0.56 | |
| Problems and Exercices | 8 | 0.32 | |
| Theoretical classes | 22 | 0.88 | |
| Type: Supervised | | | |
| Tutorial classes | 1 | 0.04 | |
| Type: Autonomous | | | |
| Exercices | 20 | 0.8 | |
| Laboratory | 30 | 1.2 | |
| Preparation of laboratory experiments | 5.75 | 0.23 | |
| Self study | 44 | 1.76 | |

Students will have to develop different types of activities throughout this course:

a) Guided activities: Theoretical classes and exercises will be held in the classroom. On the other hand, students will also carry out laboratory experiments consisting of the synthesis and / or characterization of supramolecular systems.
All the materials needed for these activities will be found in the space of the course on the Virtual Campus.

b) Supervised activities: Tutorial classes would be done in order to monitor one of the assessment activities that students must work on, which consists in reading, understanding and writing a scientific article related to the subject.

c) Autonomous activities: Students will have to study the contents of the course, solve problems, prepare laboratory experiments, summarize and present a scientific article.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

## Assessment

## Continous Assessment Activities

| Title | Weighting | Hours | ECTS | Learning Outcomes |
|---|---|---|---|---|
| Laboratory | 15% | 0.25 | 0.01 | KM31 |
| Presentation of a scientific paper | 15% | 2 | 0.08 | CM19, KM31 |

| | | | | |
|---|---|---|---|---|
| Writting Exams | 70% | 3 | 0.12 | KM31, SM31 |

The assessment will have two options: continuous assessment, and single assessment.

OPTION A: Continuous assessment (this is the option by default)

The assessment will be carried out by means of several evidences:

Written exams: There will be two midterm exams throughout the course, one in the middle and the other at the end of the semester.
Each of these exams will have a weight of 35% on the final grade. If the average mark of these two exams is less than 5, a final exam will be required at the end of the semester (as long as more than 2/3 of assessment tasks have been passed), which will include the contents of the whole course, and the mark will be the 70% of the total (it will replace the partial exams).
In order to do the final exam the student will have to appear in both partial sessions. Students wanting to improve their mark may also be present at the final exam; If the mark of this exam is greater than the average of the two partial exams, the final exam will be the 70% of the final. Otherwise, the exam grades will correspond to the final exam mark.

Laboratory: Laboratory experiments will be evaluated by carrying out a small written test at the end of the last practice session, which will be equal to 15% of the final mark of the subject.

Written work on a scientific article: The students will be distributed in groups of 3-5 students, and each of these groups will be assigned a subject related to the contents of the subject. Students will have to look for a scientific article focused on this topic, read it, analyze it, and prepare a presentation in the English language that will be evaluated. This activity will have a weight of 15% on the final grade of the subject.

In order to pass the subject, students must have:

1) An average grade of exams exceeding 5.

2) An average grade over 5.

3) Have attended the three practice sessions in the laboratory. In the event of having completed less than one third of the evaluable evidence of the course and / or having failed in an unjustified manner in any of the practice sessions in the laboratory, the students will be evaluated as "not presented".

OPTION B: Single assessment (to select this option, the student must communicate it to the Academic Office (Gestión Académica) of the Faculty of Sciences and to the professor or professors of the subject in the periods of time established for the purpose)

The single assessment is exclusively applied to the written exams, and it will consist in a single exam where all the contents of the subject will be evaluated with exercises of different typology (multiple choice, problem solving, concepts development, etc.).

The mark of this assessment will count the 70% of the final mark for the subject. The other percentage will be obtained by making the laboratoy exercises (15%) and by making the work/report on the scientific paper (15%). To pass this subject the student must get a mark greater than 5,0 over 10 in this test, to attend the laboratory exercises and to have obtained an overall mark greater then 5,0 over 10.

The single assessment of the written exams will be at the same day, time and place than the last written test of the continuous assessment. Those students getting marks lower than 5,0, will have a second opportunity to retake the assessment which will be at the same day, time and place that the retake exam for the continuous assessment, providing the student had follow the laboratory exercises and performed the report/work on the scientific paper.

## Bibliography


- P.D. Beer, T.A. Gale, Barendt, J.Y.C. Lim, *Supramolecular Chemistry*, Oxford University Press (Oxford Chemistry Primers), Oxford, UK, 2022.
- J.W. Steed, D.R. Turner, K. Wallace, *Core Concepts in Supramolecular Chemistry and Nanochemistry* , Wiley, Chichester, 2007.
- P.D. Beer, P.A. Gale, D.K. Smith, *Supramolecular Chemistry*, Oxford University Press (Oxford Chemistry Primers), New York, 1999.
- J.W. Steed, P.A. Gale, *Supramolecular Chemistry: from Molecules to Nanomaterials*, Wiley, Chichester, 2012.


## Software

Teams, Microsolft Office, OBS Studio

## Groups and Languages

Please note that this information is provisional until 30 November 2025. You can check it through this link. To consult the language you will need to enter the CODE of the subject.

| Name | Group | Language | Semester | Turn |
|---|---|---|---|---|
| (PAUL) Classroom practices | 1 | Catalan | first semester | afternoon |
| (PLAB) Practical laboratories | 1 | Catalan | first semester | morning-mixed |
| (PLAB) Practical laboratories | 2 | Catalan | first semester | morning-mixed |
| (TE) Theory | 1 | Catalan | first semester | afternoon |