Applied Spectroscopy

Title	Applied Spectroscopy
Semester	E2023
Master programme in	Chemical Biology
Type of activity	Course
Teaching language	English
Study regulation	Read about the Master Programme and find the Study Regulations at ruc.dk Læs mere om uddannelsen og find din studieordning på ruc.dk

REGISTRATION AND STUDY ADMINISTRATIVE

Registration	Sign up for study activities at stads selvbetjeningwithin the announced registration period, as you can see on the Studyadministration homepage. When signing up for study activities, please be aware of potential conflicts between study activities or exam dates. The planning of activities at Roskilde University is based on the recommended study programs which do not overlap. However, if you choose optional courses and/or study plans that goes beyond the recommended study programs, an overlap of lectures or exam dates may occur depending on which courses you choose.
Number of participants	
ECTS	5
Responsible for the activity	William Goldring (goldring@ruc.dk) Anders Malmendal (amalm@ruc.dk) Torben Lund (tlund@ruc.dk)
Head of study	Anders Malmendal (amalm@ruc.dk)
Teachers	
Study administration	INM Registration & Exams (inm-exams@ruc.dk)
Exam code(s)	U60043

ACADEMIC CONTENT

Overall objective	Spectroscopic methods play an important role in the analysis and identification of molecules and their structures. Nuclear Magnetic Resonance (NMR), Infra-red spectroscopy (IR) and mass spectrometry (MS) are used to characterize a diverse range of molecules, many of which are derived from a wide variety of sources or used in numerous applications. Some examples include molecules isolated from Nature (plants, animals and other biological sources) that possess important biological activity, or molecules involved in the discovery and development of medicines, such as the products of organic chemistry reactions. The central theme of the course is the application of spectroscopic techniques for the structural analysis and identification of organic and bioorganic molecules including macromolecules. During lectures, the students will be acquainted with the theory behind each method, including one- and two-dimensional proton and carbon Nuclear Magnetic Resonance (NMR) spectroscopy and electron and electrospray ionization mass spectrometry (EI- and ESI-MS). Throughout the course, problem solving exercises and worked examples discussed in class will demonstrate and illustrate approaches employed for the analysis and interpretation of different types of spectral data, which are used to reveal detailed structural information, and ultimately facilitate the identification or characterization of known and unknown molecules of varying degrees of complexity. Applied Spectroscopy students will therefore analyze and discuss spectra recorded for a number of organic molecules, with an emphasis on the interpretation of the data. This will enhance an understanding of the theory and concepts described, and reveal the power of the spectroscopic methods when used in combination.
Detailed description of content	The central theme of this course is the application of spectroscopic techniques for the structural analysis and identification of organic molecules. During lectures, the applications of one- and two-dimensional proton and carbon Nuclear Magnetic Resonance (NMR) spectroscopy and electron impact mass spectrometry (EI-MS) are described and illustrated. The underlying theory and worked examples discussed in class will facilitate the interpretation of spectra for the identification or characterization of known and unknown molecules of varying degrees of complexity. Furthermore, advanced applications of these techniques will be introduced and discussed in the context of difficult to solve molecular structure assignment and determination problems. Throughout the course, students will therefore analyze and discuss different types of spectra recorded for a number of organic molecules, and learn how to interpret the data to reveal detailed structural information. This will enhance an understanding of the theory and concepts described, and reveal the power of the spectroscopic methods when used in combination. **Detailed Teaching Objectives and Learning Outcomes** After successful completion of the course the student will be able to demonstrate and apply: **Knowledge of** • Fundamental NMR and MS theory, together with the concepts of wavenumber, chemical shift and coupling, and fragmentation, respectively.

- The typical position and pattern of NMR absorptions, and MS fragmentation, in relation to compound structure and the influence of functional groups.
- Advanced methods and applications for the determination of molecular structure.

Skills in

- Interpretation and analysis of NMR and mass spectra for the identification of functional groups, fragments, stereochemistry, bonding arrangement and overall structures in organic molecules.
- Solving moderate to complex structure identification problems.
- Problem-solving, independent learning and the application of methods to solve unfamiliar problems.

Learning outcomes:

- Understand the factors that influence wavenumber, chemical shift and coupling patterns, and fragmentation.
- Be able to examine an organic molecule and predict the chemical shift and splitting pattern of a given proton or carbon atom.
- Interpret a spectrum, or combine information from a set of spectra, to confirm or identify moderately complex known and unknown organic structures.
- Choose optimal spectroscopic techniques for molecular structure identification.

Course material and Reading list

Textbook:

D. L. Pavia, G. M. Lampman, et al., Introduction to Spectroscopy, 5th Ed., Cengage Learning, 2015.

Other materials:

Powerpoint slides and problems will be posted on Moodle during the course.

Overall plan and expected work effort

5 ECTS corresponds to 135 hours of work

The work load for the student:

Preparation time Contact time

- Lectures, workshops and preparation: 55 hours

Study and preparation time:

- Reading and self-revision problems: 20 hours
- Theoretical problem preparation: 20 hours
- Reading time: 20 hours
- Revision and exam preparation: 20 hours

- Total 135 hours

Format

Evaluation and feedback

The course includes formative evaluation based on dialogue between the students and the teacher(s).

Students are expected to provide constructive critique, feedback and viewpoints during the course if it is needed for the course to have better

quality. Every other year at the end of the course, there will also be an evaluation through a questionnaire in SurveyXact. The Study Board will handle all evaluations along with any comments from the course responsible teacher.

Furthermore, students can, in accordance with RUCs 'feel free to state your views' strategy through their representatives at the study board, send evaluations, comments or insights form the course to the study board during or after the course.

Programme

The course is organized around a combination of lectures (powerpoint, boardwork, and discussion) and problem solving workshops. See study.ruc.dk for a detailed coure schedule, and the course page on Moodle for a schedule, course description and other documents, together with lecture notes and problem solving questions.

Each lecture section is followed by a problem solving workshop, organized according to the course schedule on Moodle. Students will find questions associated with a particular lecture section either at the end of the set of lecture notes, or as separate files uploaded to the course Moodle page.

Students are expected to complete or attempt the problem solving questions associated with a particular workshop, before it takes place, and be prepared to present their solutions, in whole or in part, during the workshop.

ASSESSMENT

Overall learning outcomes

After successful completion of the course the student will be able to:

- describe and apply fundamental NMR and MS theory, together with the concepts of chemical shift and coupling, and fragmentation, respectively
- identify and interpret the typical position and pattern of NMR absorptions, and MS fragmentation, in relation to compound structure and the influence of functional groups
- employ advanced methods and applications for the determination of molecular structure
- interpret and analyze NMR and mass spectra for the identification of functional groups, fragments, stereochemistry, bonding arrangement and overall structure in organic molecules, together with biological molecules in pure form and as a part of mixtures
- solve moderate to complex structure identification problems
- solve unfamiliar problems through the application of skills and strategies in problem-solving and independent learning
- describe the factors that influence wavenumber, chemical shift and coupling patterns, and fragmentation
- examine an organic molecule and predict the chemical shift and splitting pattern of a given proton or carbon atom
- interpret a spectrum, or combine information from a set of spectra, to confirm or identify moderately complex known and unknown organic structures
- choose optimal spectroscopic techniques for molecular structure identification
- translate between molecular structure and spectroscopic output

Form of examination	Individual oral exam based on a portfolio. The character limit of the portfolio is 2,400-24,000 characters, including spaces. Examples of written products are exercise responses, talking points for presentations, written feedback, reflections, written assignments. The preparation of the products may be subject to time limits. The character limits include the cover, table of contents, bibliography, figures and other illustrations, but exclude any appendices. Time allowed for exam including time used for assessment: 30 minutes. The assessment is an overall assessment of the written product(s) and the subsequent oral examination. Permitted support and preparation materials for the oral exam: Personal notes, own reports and assignments. Assessment: 7-point grading scale. Moderation: Internal co-assessor
Form of Re-examination	Samme som ordinær eksamen / same form as ordinary exam
Type of examination in special cases	
Examination and assessment criteria	The portfolio consists of a set of recorded spectra of an unknown compound and a written report of the data for each organised into tables, and including a detailed analysis and assignment of the signals. The portfolio concludes with a solution to the identity of the unknown compound, including its structure and a discussion of functional groups and sub-structures derived from the analysis of the data. Oral examination: the student will start with a summary of the findings of the portfolio followed by questions by the examiners. Assesment criteria: It will be assessed to which degree the student ● Is able to interpret and analyse IR, NMR and mass spectra for the identification of functional groups, fragments and structures in organic molecules. ● Demonstrate the ability to solve structure identification problems. ● Understands the factors that influence wavenumber, chemical shift and coupling patterns, and fragmentation. ● Is able to examine an organic molecule and predict the chemical shift and splitting pattern of a given proton or carbon atom. ● Interprets a spectrum, or combines information from a set of spectra, to confirm or identify moderate to complex unknown organic structures. ● Chooses optimal spectroscopic techniques for molecular structure identification. Oral examination: all the above and: ● Presents and defends analysis and interpretation of the data Whether the performance meets all formal requirements in regards to both written and oral exam

Exam code(s)	Exam code(s) : U60043

Course days:

Hold: 1

Applied Spectroscopy (CB)

time	23-10-2023 08:15 til 23-10-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	25-10-2023 14:15 til 25-10-2023 16:00
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	26-10-2023 08:15 til 26-10-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	30-10-2023 08:15 til 30-10-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	01-11-2023 14:15 til 01-11-2023 16:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	28b.0-01 - store teorirum (30)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	02-11-2023 08:15 til 02-11-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	06-11-2023 08:15 til 06-11-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	08-11-2023 14:15 til 08-11-2023 16:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	09-11-2023 08:15 til 09-11-2023 10:00
location	28b.0-05 - lille teorirum (20)

Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	13-11-2023 08:15 til 13-11-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	15-11-2023 14:15 til 15-11-2023 16:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	16-11-2023 08:15 til 16-11-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	20-11-2023 08:15 til 20-11-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	22-11-2023 14:15 til 22-11-2023 16:00
forberedelsesnorm	ikke valgt

forberedelsesnorm D-VIP	ikke valgt
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	23-11-2023 08:15 til 23-11-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	27-11-2023 08:15 til 27-11-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	Anders Malmendal (amalm@ruc.dk) William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	29-11-2023 14:15 til 29-11-2023 16:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	30-11-2023 08:15 til 30-11-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	Anders Malmendal (amalm@ruc.dk) William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	04-12-2023 08:15 til 04-12-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk) Anders Malmendal (amalm@ruc.dk)

Applied Spectroscopy (CB)

time	06-12-2023 14:15 til 06-12-2023 16:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt
location	28b.0-01 - store teorirum (30)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	07-12-2023 08:15 til 07-12-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk) Anders Malmendal (amalm@ruc.dk)

Applied Spectroscopy (CB)

time	11-12-2023 08:15 til 11-12-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	Anders Malmendal (amalm@ruc.dk) William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	13-12-2023 14:15 til 13-12-2023 16:00
forberedelsesnorm	ikke valgt

forberedelsesnorm D-VIP	ikke valgt
location	28b.0-05 - lille teorirum (20)
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy (CB)

time	14-12-2023 08:15 til 14-12-2023 10:00
location	28b.0-05 - lille teorirum (20)
Teacher	Anders Malmendal (amalm@ruc.dk) William Goldring (goldring@ruc.dk)

Applied Spectroscopy - Hand-in of portfolio (CB)

time	19-12-2023 10:00 til 19-12-2023 10:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt

Applied Spectroscopy - Exam (CB)

time	12-01-2024 08:15 til 12-01-2024 16:00
Teacher	William Goldring (goldring@ruc.dk)

Applied Spectroscopy - Hand-in of portfolio (reexam) (CB)

time	31-01-2024 10:00 til 31-01-2024 10:00
forberedelsesnorm	ikke valgt
forberedelsesnorm D-VIP	ikke valgt

Applied Spectroscopy - Reexam (CB)

time	27-02-2024 08:15 til 27-02-2024 12:00
forberedelsesnorm	ikke valgt

forberedelsesnorm D-VIP	ikke valgt
Teacher	William Goldring (goldring@ruc.dk)