**Analytical Spectroscopy (26:160:547): NMR & Mass Spectrometry**

**Spring Semester 2023**

**Graduate course offering in Structure Characterization by Nuclear Magnetic Resonance (NMR) and Mass Spectrometry (MS).**

**NMR Facility Director:** NMR, Raman, and IR spectroscopies Pavel Kucheryavy, LSC-I 001A  
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E-mail: pavel.kucheryavy@rutgers.edu

**MS Facility Manager:** Mass Spectroscopy Roman Brukh  
Phone: 973-353-5254  
E-mail: rbrukh@rutgers.edu

**Time/Days:** 6:00-9:00 PM/ Mondays  
**Location:** Life Science Center I, Room 103  
**Starting/Ending Dates:** 01-23-2023/04-30-2023

**Course description:**

**The NMR part** of the course will cover mostly NMR spectroscopy. One class off in this course will be dedicated to other analytical methods such as IR and Raman spectroscopy methods. In NMR part of the course basic principles of NMR spectroscopy, common type of experiments, optimization of the parameters for experiment and analysis of the results. It will be focused mostly on the liquids NMR, including common 1D, 2D, dynamic methods, such as T1/T2 and DOSY, as well as solid state NMR. One class of the NMR section will be dedicated to the practical session where student will set up their experiments in person and analyze the obtained data.

The NMR part covers the physical basis of NMR, chemical shifts and couplings, FT NMR, NMR relaxation, NMR hardware, NMR data acquisition and processing, the NOE, multi pulse and two-dimensional NMR, and dynamic NMR.

**The MS part** covers the physical and chemical principles of mass spectrometry. The main types of techniques and instruments will be discussed, including ion sources (EI, ESI, MADLI, etc.), mass analyzers (including quadrupole, FTMS, TOF, Orbitrap), tandem MS, and MS-chromatography coupling. The instrument calibration and basics of MS data interpretation will be covered. Specific examples of the application of MS to the determination of the molecular structure will be presented. Students (groups) will submit a small final project, which includes the design of an MS experiment, running the experiment, and data interpretation. After taking this course students should have developed an understanding and ability to use the instruments in the MS facility.

**Prerequisites:** There are no prerequisites for this course

**Learning Goals:** Upon successful completion of this course, the student should be able to:

1) Recognize the importance in the application of NMR spectroscopy and mass spectrometry and its application in organic chemistry and material science;
2) Understand the nuclear magnetic properties of certain nuclei that lead to signals in NMR spectra;
3) Understand basic methodological parameters employed in NMR experiments (pulse sequences) that will yield specific chemical or structural information;
4) Critically evaluate and interpret NMR spectra from both 1D and 2D experiments to elucidate and confirm structures;
5) Effectively communicate the “language” (jargon) used in NMR, both in oral and written contexts.
6) Effectively use modern NMR processing software.
7) Understand principles of IR and Raman spectroscopies as well effectively analyze and interpret the spectra.

Grading and Evaluation Process:

<table>
<thead>
<tr>
<th>Component</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Problem Sets (14), take home (1.75% each)</td>
<td>25%</td>
</tr>
<tr>
<td>Exam 1, in class (100 Pts)</td>
<td>20%</td>
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<tr>
<td>Exam 2, in class (100 Pts)</td>
<td>20%</td>
</tr>
<tr>
<td>Final Exam, take home (100 Pts)</td>
<td>25%</td>
</tr>
<tr>
<td>Total</td>
<td>100%</td>
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</tbody>
</table>

Problem Sets:

Exams: The three exams will cover materials of the lectures, assigned readings, and problem sets respectively from the first, middle and last segments of the course.

Letter Grades of A, B, C, D and F will be assigned based on the following scale:
A = 90-100; B = 80-89; C = 70-79; D = 60-69; F = below 60


Recommended software: Topspin 4.14 for simulations and data processing. It is currently free for academic users.

EXPECTATIONS

- Professional demeanor required, respecting each other and instructor.
- No food or open beverage containers in the classroom - University and School policy.
- If necessary, the syllabus may be modified at any point during the semester.
- Class attendance taken and required. **EXCUSED ABSENCES MUST BE GRANTED BY INSTRUCTOR IN ADVANCE** *

* Unexcused absences that are not the result from illness (confirmed by a Doctor's note) or extreme extenuating circumstances will be taken in the grading. One unexcused absence will result in the loss of the student’s attendance grade (10% of the total grading points).

Academic Calendar: https://myrun.newark.rutgers.edu/s23
Final Exam Schedule: https://scheduling.newark.rutgers.edu/ru-n-final-exam-schedule-spring-2023-tentative/

Academic Integrity
As an academic community dedicated to the creation, dissemination, and application of knowledge, Rutgers University is committed to fostering an intellectual and ethical environment based on the principles of academic integrity. Academic integrity is essential to the success of the University's educational and
research missions, and violations of academic integrity constitute serious offenses against the entire academic community. The entire Academic Integrity Policy can be found here: http://academicintegrity.rutgers.edu/academic-integrity-policy/

Your health and well-being matter, and Rutgers has put in place a number of resources that are intended to help students through the challenges that might emerge during these times. Information on many of these resources appears below. Please let us know immediately if you are experiencing circumstances that are negatively impacting your academic performance. We also strongly encourage you to contact your academic advisor.

Accommodation and Support
Rutgers University Newark (RU-N) is committed to the creation of an inclusive and safe learning environment for all students. RU-N has identified the following resources to further the mission of access and support:

• Absences: All students are responsible for timely notification of their instructor regarding any expected absences. The Division of Student Affairs can provide assistant for absences related to religious observance, emergency or unavoidable conflict (illness, personal or family emergency, etc.) Students should refer to the University’s Course Attendance policy (10.2.7), for complete expectations and responsibilities. The office can be contacted at: (973) 353-5063 or deanofstudents@newark.rutgers.edu.

• Disabilities: The Office of Disability Services (ODS) is responsible for the determination of appropriate accommodations for students who encounter barriers due to disability. Once a student has completed the ODS process (registration, initial appointment, and submitted documentation) and reasonable accommodations are determined to be necessary and appropriate, a Letter of Accommodation (LOA) will be provided. The LOA must be given to each course instructor by the student and follow up with a discussion. This should be completed as early in the semester as possible as accommodations are not retroactive. More information can be found at ods.rutgers.edu. Contact ODS: (973) 353-5375 or ods@newark.rutgers.edu.

• Temporary Conditions/Injuries: The Division of Student Affairs can assist students who are experiencing a temporary condition of injury (broken or sprained limbs, concussions, or recovery from surgery). Students experiencing a temporary condition or injury should submit a request for assistance at: https://temporaryconditions.rutgers.edu.

• Pregnancy: The Office of Title IX and ADA Compliance is available to assist students with any concerns or potential accommodations related to pregnancy. Students may contact the office at (973) 353-1906 or TitleIX@newark.rutgers.edu.

• Gender or Sex-Based Discrimination or Harassment: The Office of Title IX and ADA Compliance can assist students experiencing any form of gender or sex-based discrimination or harassment, including sexual assault, sexual harassment, relationship violence, or stalking. Students can report an incident to the office at: (973) 353-1906 or TitleIX@newark.rutgers.edu. Incidents may also be reported by using the following link: tinyurl.com/RUNReportingForm. For more information, students should refer to the University’s Student Policy Prohibiting Sexual Harassment, Sexual Violence, Relationship Violence, Stalking and Related Misconduct located at: http://compliance.rutgers.edu/title-ix/about-title-ix/title-ix-policies/.
• Interpersonal Violence: The Office for Violence Prevention and Victim Assistance can provide any student with confidential support. The office is a confidential resource and does not have a reporting obligation to report information to the University's Title IX Coordinator. Students can contact the office at: (973) 353-1918 or run.vpva@rutgers.edu. There is also a confidential, text-based line students can text for support: (973) 339-0734.

• Crisis and Concerns: The Campus Awareness Response and Education (CARE) Team works with students in crisis to develop a support plan to address personal situations that might impact academic performance. Students may contact the CARE Team at: http://tinyurl.com/RUNCARE or careteam@rutgers.edu.

• Stress, Worry, or Concerns about Well-Being: The Counseling Center has confidential therapists available to support students. To schedule an appointment: counseling@newark.rutgers.edu or (973) 353-5805. If a student is not quite ready to make an appointment with a therapist but is interested in self-help, check out TAO at Rutgers-Newark for an easy, web-based approach to self-care and support: https://tinyurl.com/RUN-TAO.

• Emergencies: Call 911 or contact Rutgers University Police Department (RUPD) at (973) 353-5111.

Learning Resources:
• Rutgers Learning Center (tutoring services)
  (973) 353-5608
  https://sasn.rutgers.edu/student-support/tutoring-academic-support/learning-center

• Writing Center (tutoring and writing workshops)
  (973) 353-5847
  nwc@rutgers.edu
  https://sasn.rutgers.edu/student-support/tutoring-academic-support/writing-center

Please note that, if necessary, the syllabus may be modified at any point during the semester.
Course calendar:

<table>
<thead>
<tr>
<th>Week</th>
<th>Date</th>
<th>Topic</th>
<th>Instructor</th>
<th>Assignment</th>
<th>Due date</th>
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<tbody>
<tr>
<td>1</td>
<td>Jan 23</td>
<td>Introduction to the course, History of NMR, Principles of NMR and</td>
<td>PK</td>
<td>NMR 1</td>
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<tr>
<td></td>
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<td>instrumental aspects</td>
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<td>2</td>
<td>Jan 30</td>
<td>Chemical Shifts, Coupling Constants, Decoupling, Common 1D NMR</td>
<td>PK</td>
<td>NMR 1</td>
<td>Feb 06</td>
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<td>3</td>
<td>Feb 06</td>
<td>Quadrupolar NMR, 2D NMR</td>
<td>PK</td>
<td>NMR 2</td>
<td>Feb 13</td>
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<td>4</td>
<td>Feb 13</td>
<td>Structural information from 2D NMR</td>
<td>PK</td>
<td>NMR 3</td>
<td>Feb 20</td>
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<tr>
<td>5</td>
<td>Feb 20</td>
<td>Other methods: DOSY, T1/T2, Screening, Solid State NMR</td>
<td>PK</td>
<td>NMR 4</td>
<td>Feb 27</td>
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<td>6</td>
<td>Feb 27</td>
<td>Practical Session</td>
<td>PK</td>
<td>NMR 5</td>
<td>Mar 6</td>
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<td>7</td>
<td>Mar 06</td>
<td>Raman and IR spectroscopy NMR Exam</td>
<td>PK</td>
<td>NMR 6</td>
<td>Mar 20</td>
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<td>8</td>
<td>Mar 20</td>
<td>Introduction to MS, Principles of MS</td>
<td>RB</td>
<td>MS 1</td>
<td>Mar 27</td>
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<td>9</td>
<td>Mar 27</td>
<td>Isotopic composition and accurate mass</td>
<td>RB</td>
<td>MS 2</td>
<td>Apr 3</td>
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<td>10</td>
<td>Apr 03</td>
<td>Ionization sources</td>
<td>RB</td>
<td>MS 3</td>
<td>Apr 10</td>
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<td>11</td>
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<td>Mass analyzers</td>
<td>RB</td>
<td>MS 4</td>
<td>Apr 17</td>
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<td>12</td>
<td>Apr 17</td>
<td>Tandem mass spectrometry</td>
<td>RB</td>
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<td>13</td>
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<td>Practical session</td>
<td>RB</td>
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<tr>
<td>14</td>
<td>May 01</td>
<td>Interpretation of MS spectrum</td>
<td>RB</td>
<td>MS 7</td>
<td>May 8</td>
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<td>May 08</td>
<td>Final Exam</td>
<td>PK, RB</td>
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