CHEMISTRY 599  SPECIAL TOPICS  
MASS SPECTROMETRY IN MECHANISM AND STRUCTURE INVESTIGATION  
FALL SEMESTER 2022

| INSTRUCTOR | Prof. Valery V. Fokin  
|            | MCB-359  
|            | (213) 740-5964  
|            | fokin@usc.edu  
|            | Office Hours:  
|            | by appointment  
|            | Co-instructor: Dr. Dmitry Eremin, MCB-396,  
|            | eremin@usc.edu |

| HELPFUL BACKGROUND | CHEM 526 AND (CHEM 515 or CHEM 516), can be taken concurrently |

| LECTURE | Tentatively Wed and Fri, 1:30-2:50 (pending TA schedules)  
| Location will be announced. |

| COURSE CONTENT AND LEARNING OBJECTIVES | The goals of this course are two-fold. First, it will introduce the students to the important physical aspects of catalytic organic and organometallic reactions. Using examples from recent literature, we will learn about modern methods of obtaining mechanistic parameters, the importance of obtaining robust data, and methods for its processing. We will also examine applications of catalytic processes in industrial and research setting. Next, we will examine modern mass spectrometry techniques. With the recent literature examples, we will learn about modern applications of mass spectrometry in organic and organometallic chemistry, biochemistry and medical research. We will have several hands-on sessions on high-end MS instruments at the Chemistry Department and Agilent Center of Excellence in Biomolecular Characterization. |

| ACADEMIC INTEGRITY | All USC students are responsible for reading and following the Student Conduct Code, which appears in the SCampus and at https://policy.usc.edu/student/scampus/  
| | The USC Student Conduct Code prohibits plagiarism. Some examples of what is not allowed by the conduct code: copying all or part of someone else’s work (by hand or by looking at others’ files, either secretly or if shown), and submitting it as your own; giving another student in the class a copy of your assignment solution; consulting with another student during an exam; modifying a graded assignment before asking for re-grading, letting your lab partner prepare the report and expect |
a grade for their work. If you have questions about what is allowed, please discuss it with the instructor.

Students who violate University standards of academic integrity are subject to disciplinary sanctions, including failure in the course and suspension from the University. Since dishonesty in any form harms the individual, other students, and the University, policies on academic integrity will be strictly enforced. We expect you to familiarize yourself with the Academic Integrity guidelines found in the current Scampus. Violations of the Student Conduct Code will be filed with the Office of Student Conduct, and appropriate sanctions will be given.

This policy does not apply to discussion, exchange of information, working together, etc. On the contrary, we encourage that you consult with classmates regarding learning material and homework assignments. Team projects require that you work with your team and assist your partner as much as he or she assists you. However, for individual marks, it is required that you prepare the final product by yourself.

**TEXTS**

Primary literature and/or links to it will be provided before starting a new topic.

**GRADING**

The course will be graded on the basis of 2 homework projects (50 points each) and a final assignment (100 points), due on December 11 (Friday).

**Total 200 points**

---

**Tentative schedule**

<table>
<thead>
<tr>
<th>DATE</th>
<th>TOPIC</th>
<th>ITEMS DUE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weeks 1-2</td>
<td>Introduction to multistep reactions, catalysis, mechanism and kinetics.</td>
<td></td>
</tr>
<tr>
<td>Weeks 3-4</td>
<td>Thermodynamics and kinetics. Rate laws and their meaning.</td>
<td></td>
</tr>
<tr>
<td>Weeks 5-6</td>
<td>Mechanistic investigation of multistep processes.</td>
<td>Homework 1</td>
</tr>
<tr>
<td>Weeks 7-8</td>
<td>Linear free energy relationships. Hammett plots and Hammond postulate.</td>
<td></td>
</tr>
<tr>
<td>Week 9</td>
<td>Examples of studies of homogeneous catalytic processes.</td>
<td></td>
</tr>
<tr>
<td>Week 10</td>
<td>Mass spectrometry: theoretical aspects and general principles.</td>
<td></td>
</tr>
<tr>
<td>Week 11</td>
<td>Ionization technics: from small molecules to tissue analysis.</td>
<td></td>
</tr>
<tr>
<td>Week 12</td>
<td>Practical class: Familiarization with modern instruments.</td>
<td></td>
</tr>
<tr>
<td>Week 13</td>
<td>Mass spectra interpretation. Fragmentation principles. Structure elucidation.</td>
<td>Homework 2</td>
</tr>
<tr>
<td>Week 14</td>
<td>Mass spectrometry of biomolecules. Peptide sequencing.</td>
<td></td>
</tr>
<tr>
<td>Week 15</td>
<td>Presentations and discussion of final projects.</td>
<td>Final project</td>
</tr>
</tbody>
</table>
Grading breakdown

<table>
<thead>
<tr>
<th>Assignment</th>
<th>Points</th>
<th>% of grade</th>
</tr>
</thead>
<tbody>
<tr>
<td>Homework 1</td>
<td>50</td>
<td>25</td>
</tr>
<tr>
<td>Homework 2</td>
<td>50</td>
<td>25</td>
</tr>
<tr>
<td>Final project</td>
<td>100</td>
<td>50</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>200</strong></td>
<td><strong>100</strong></td>
</tr>
</tbody>
</table>

Statement on Academic Conduct and Support Systems

Academic Conduct:

Plagiarism – presenting someone else's ideas as your own, either verbatim or recast in your own words – is a serious academic offense with serious consequences. Please familiarize yourself with the discussion of plagiarism in SCampus in Part B, Section 11, “Behavior Violating University Standards” [policy.usc.edu/scampus-part-b](http://policy.usc.edu/scampus-part-b). Other forms of academic dishonesty are equally unacceptable. See additional information in SCampus and university policies on scientific misconduct, [policy.usc.edu/scientific-misconduct](http://policy.usc.edu/scientific-misconduct).

Support Systems:

*Counseling and Mental Health* - (213) 740-9355 – 24/7 on call
[studenthealth.usc.edu/counseling](http://studenthealth.usc.edu/counseling)
Free and confidential mental health treatment for students, including short-term psychotherapy, group counseling, stress fitness workshops, and crisis intervention.

*National Suicide Prevention Lifeline* - 1 (800) 273-8255 – 24/7 on call
[suicidepreventionlifeline.org](http://suicidepreventionlifeline.org)
Free and confidential emotional support to people in suicidal crisis or emotional distress 24 hours a day, 7 days a week.

*Relationship and Sexual Violence Prevention Services (RSVP)* - (213) 740-9355(WELL), press “0” after hours – 24/7 on call
[studenthealth.usc.edu/sexual-assault](http://studenthealth.usc.edu/sexual-assault)
Free and confidential therapy services, workshops, and training for situations related to gender-based harm.

*Office of Equity and Diversity (OED)* - (213) 740-5086 | Title IX – (213) 821-8298
[equity.usc.edu, titleix.usc.edu](http://equity.usc.edu, titleix.usc.edu)
Information about how to get help or help someone affected by harassment or discrimination, rights of protected classes, reporting options, and additional resources for students, faculty, staff, visitors, and applicants.

*Reporting Incidents of Bias or Harassment* - (213) 740-5086 or (213) 821-8298
[usc-advocate-simplicity.com/care_report](http://usc-advocate-simplicity.com/care_report)
Avenue to report incidents of bias, hate crimes, and microaggressions to the Office of Equity and Diversity |Title IX for appropriate investigation, supportive measures, and response.

*The Office of Disability Services and Programs* - (213) 740-0776
[dsp.usc.edu](http://dsp.usc.edu)
Support and accommodations for students with disabilities. Services include assistance in providing readers/notetakers/interpreters, special accommodations for test taking needs, assistance with architectural barriers, assistive technology, and support for individual needs.
USC Campus Support and Intervention - (213) 821-4710
campussupport.usc.edu
Assists students and families in resolving complex personal, financial, and academic issues adversely affecting their success as a student.

Diversity at USC - (213) 740-2101
diversity.usc.edu
Information on events, programs and training, the Provost’s Diversity and Inclusion Council, Diversity Liaisons for each academic school, chronology, participation, and various resources for students.

USC Emergency - UPC: (213) 740-4321, HSC: (323) 442-1000 – 24/7 on call
dps.usc.edu, emergency.usc.edu
Emergency assistance and avenue to report a crime. Latest updates regarding safety, including ways in which instruction will be continued if an officially declared emergency makes travel to campus infeasible.

USC Department of Public Safety - UPC: (213) 740-6000, HSC: (323) 442-120 – 24/7 on call
dps.usc.edu
Non-emergency assistance or information.