MEDICINAL CHEMISTRY AND DRUG DESIGN (updated 3/17/19)

CHEM 577a
Units: 2
Introduction to fundamentals of medicinal chemistry with special attention to the drug discovery process
Prerequisites: None
Instruction mode: Lecture, January 7 – February 27
Grading Option: Letter (can audit for grade “V”)

CHEM 577b
Units: 2
Concepts, methods and examples of current approaches to drug design including computer-based molecular modeling techniques.
Prerequisites: CHEM 577a
Instruction mode: Lecture, March 4 – April 24
Grading Option: Letter (can audit for grade “V”)

Instructor: Charles McKenna
Office: LJS 268/MCB 260/261 MCH
Office Hours: 12:30 – 1:30PM Wednesdays
Contact Info: mckenna@usc.edu. Office: (213) 740-7007 / (213) 740 999

Website:
Dr. Bruno Herreros
Office: SGM 426
Phone: (213)740-7039
Email: herreros@usc.edu
Office hours: By appointment

Contact for lab computer support:
Jaime Avila
Office: SGM 418
Phone: (213) 740-7039
Email: avila@usc.edu

Dornsife IT Help
Hours of Service: Mon-Fri, 9am – 5pm
Contact Info:
• Phone support: 213-740-2775
• Email support: ts@dornsife.usc.edu
• Walk-In support: ACB 530

Learning Objectives
Students will gain in depth knowledge of the goals, methods, and salient examples of modern drug design from a medicinal chemistry perspective.

Course Notes
Class information will be posted on the class website during the course as needed.

Required Readings and Supplementary Materials
Required weekly readings posted in the syllabus. Additional materials from the literature will be presented during the course.

Grading Breakdown
CHEM 577a
Homework 280 points 70%
Final/Presentation 120 points 30%
TOTAL 400 points 100%

CHEM 577b
Homework 200 points 50%
Final/Presentation 200 points 50%
TOTAL 400 points 100%
Grading Scale
Course final grades will be determined using the following scale

<table>
<thead>
<tr>
<th>Grade</th>
<th>Range</th>
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<tbody>
<tr>
<td>A</td>
<td>95-100</td>
</tr>
<tr>
<td>A-</td>
<td>90-94</td>
</tr>
<tr>
<td>B+</td>
<td>87-89</td>
</tr>
<tr>
<td>B</td>
<td>83-86</td>
</tr>
<tr>
<td>B-</td>
<td>80-82</td>
</tr>
<tr>
<td>C+</td>
<td>77-79</td>
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<tr>
<td>C</td>
<td>73-76</td>
</tr>
<tr>
<td>C-</td>
<td>70-72</td>
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<tr>
<td>D+</td>
<td>67-69</td>
</tr>
<tr>
<td>D</td>
<td>63-66</td>
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<tr>
<td>D-</td>
<td>60-62</td>
</tr>
<tr>
<td>F</td>
<td>59 and below</td>
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Grading Timeline
Within one class interval (exams) or one week for papers and homework.

Additional Policies
Late assignments will be penalized. Missed classes may be excused with email explanation. Attendance is expected for all course sessions. Lectures will use PowerPoint slides and online materials.

Academic Integrity
USC seeks to maintain an optimal learning environment. General principles of academic honesty include the concept of respect for the intellectual property of others, the expectation that individual work will be submitted unless otherwise allowed by an instructor, and the obligations both to protect one’s own academic work from misuse by others as well as to avoid using another’s work as one’s own. All students are expected to understand and abide by these principles. SCampus, the Student Guidebook, contains the University Student Conduct Code (see University Governance, Section 11.00), while the recommended sanctions are located in Appendix A.

Students with Disabilities
Any student requesting academic accommodations based on a disability is required to register with Disability Services and Programs (DSP) each semester. A letter of verification for approved accommodations can be obtained from DSP. Please be sure the letter is delivered to me (or to TA) as early in the semester as possible. DSP is located in STU 301 and is open 8:30 a.m.–5:00 p.m., Monday through Friday. Website for DSP and contact information: (213) 740-0776 (Phone), (213) 740-6948 (TDD only), (213) 740-8216 (FAX) ability@usc.edu.

Emergency Preparedness/Course Continuity in a Crisis
In case of a declared emergency if travel to campus is not feasible, USC executive leadership will announce an electronic way for instructors to teach students in their residence halls or homes using a combination of Blackboard, teleconferencing, and other technologies. See the university’s site on Campus Safety and Emergency Preparedness.
<table>
<thead>
<tr>
<th>Course Schedule</th>
<th>Monday</th>
<th>Wednesday</th>
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<tbody>
<tr>
<td><strong>CHEM 577a</strong></td>
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<tr>
<td>Week 1 (1/7)</td>
<td>Chalk/talk: Class organization; History of drug discovery</td>
<td>Chalk/talk: Introductory Chapter 1: Drugs and drug targets: an overview</td>
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<tr>
<td>Week 2 (1/14)</td>
<td>Chalk/talk: Enzyme kinetics Chapter 2: Protein structure and function</td>
<td>Chalk/talk: Enzyme kinetics Chapter 3: Enzymes: structure and function</td>
</tr>
<tr>
<td>Week 3 (1/21)</td>
<td>University Holiday (Martin Luther King's Birthday) – No class</td>
<td>Chalk/talk: Medicinal chemistry of imaging probes</td>
</tr>
<tr>
<td>Week 4 (1/28)</td>
<td>Chalk/talk: Curies/radiation therapy Chapter 7: Enzymes as drug targets <strong>Homework 1 DUE</strong></td>
<td>Chalk/talk: Elion/drug discovery Chapter 4: Receptors: structure and function</td>
</tr>
<tr>
<td>Week 5 (2/4)</td>
<td>Chalk/talk: Acids/bases Chapter 5: Receptors and signal transduction</td>
<td>Chalk/talk: Aredia patent Chapter 8: Receptors as drug targets <strong>Homework 2 DUE</strong></td>
</tr>
<tr>
<td>Week 6 (2/11)</td>
<td>Chalk/talk: Cocaine/Abzymes Chapter 10: Miscellaneous drug targets</td>
<td>Chalk/talk: Homework 2 solutions Chapter 11: Pharmacokinetics and related topics</td>
</tr>
<tr>
<td>Week 7 (2/18)</td>
<td>University Holiday (President's Day) – No class</td>
<td>Chalk/talk: FINAL/Presentation hints Chapter 12: Drug discovery: finding a lead <strong>Homework 3 DUE</strong></td>
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<tr>
<td>Week 8 (2/25)</td>
<td>Chalk/talk: Homework 3 solutions Chapter 15: Getting the drug to market <strong>Upload Presentation slides DUE</strong></td>
<td>FINAL/Presentations (5x5+1) (PechaKucha) <strong>Homework 4 DUE</strong></td>
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<tr>
<td><strong>CHEM 577b</strong></td>
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<tr>
<td>Week 9 (3/4)</td>
<td>Chalk/talk: Class organization Chapter 13: Drug design: optimizing target interactions</td>
<td>Chalk/talk: Homework 4 solutions Chapter 14: Drug design: optimizing access to the target</td>
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<tr>
<td>Break (3/11)</td>
<td>Spring Break – No class</td>
<td>Spring Break – No class</td>
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<tr>
<td>Week 10 (3/18)</td>
<td>Chalk/talk: Special guest presentation: Dr J Lee (NIH/Ellison Institute) Chapter 17: Computers in medicinal chemistry</td>
<td>Chalk/talk: High throughput drug screening – virtual/real chimiothèques Chapter 18: Quantitative structure-activity relationships (QSAR) <strong>Homework 5 DUE</strong></td>
</tr>
<tr>
<td>Week 12 (4/1)</td>
<td>Chalk/talk: Antifungal agents Chapter 9: Nucleic acids as drug targets</td>
<td>Chalk/talk: Case studies: antivirals Chapter 20: Antiviral agents <strong>Homework 6 DUE</strong></td>
</tr>
<tr>
<td>Week 13 (4/8)</td>
<td>Chalk/talk: Homework 6 solutions Chapter 21: Anticancer agents</td>
<td>Chalk/talk: Case study: cisplatin Chapter 23: Drugs acting on the adrenergic nervous system</td>
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<tr>
<td>Week 14 (4/15)</td>
<td>Chalk/talk: Final/presentation hints Chapter 24: The opioid analgesics</td>
<td>Chalk/talk: Homework 7 solutions Chapter 26: Cardiovascular drugs <strong>Upload Presentation slides DUE</strong> <strong>Homework 7 DUE</strong></td>
</tr>
<tr>
<td>Week 15 (4/22)</td>
<td>FINAL/Presentations (10x10+5)</td>
<td>FINAL/Presentations (10x10+5)</td>
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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. Other forms of academic dishonesty are equally unacceptable. See additional information in SCampus and university policies on scientific misconduct, http://policy.usc.edu/scientific-misconduct.

Support Systems:
Student Counseling Services (SCS) – (213) 740-7711 – 24/7 on call
Free and confidential mental health treatment for students, including short-term psychotherapy, group counseling, stress fitness workshops, and crisis intervention. engemannshc.usc.edu/counseling

National Suicide Prevention Lifeline – 1 (800) 273-8255
Provides free and confidential emotional support to people in suicidal crisis or emotional distress 24 hours a day, 7 days a week. www.suicidepreventionlifeline.org

Relationship and Sexual Violence Prevention Services (RSVP) – (213) 740-4900 – 24/7 on call
Free and confidential therapy services, workshops, and training for situations related to gender-based harm. engemannshc.usc.edu/rsvp

Sexual Assault Resource Center
For more information about how to get help or help a survivor, rights, reporting options, and additional resources, visit the website: sarc.usc.edu

Office of Equity and Diversity (OED)/Title IX Compliance – (213) 740-5086
Works with faculty, staff, visitors, applicants, and students around issues of protected class. equity.usc.edu

Bias Assessment Response and Support
Incidents of bias, hate crimes and microaggressions need to be reported allowing for appropriate investigation and response. studentaffairs.usc.edu/bias-assessment-response-support

The Office of Disability Services and Programs
Provides certification for students with disabilities and helps arrange relevant accommodations. dsp.usc.edu

Student Support and Advocacy – (213) 821-4710
Assists students and families in resolving complex issues adversely affecting their success as a student EX: personal, financial, and academic. studentaffairs.usc.edu/ssa

Diversity at USC
Information on events, programs and training, the Diversity Task Force (including representatives for each school), chronology, participation, and various resources for students. diversity.usc.edu

USC Emergency Information
Provides safety and other updates, including ways in which instruction will be continued if an officially declared emergency makes travel to campus infeasible. emergency.usc.edu

USC Department of Public Safety – UPC: (213) 740-4321 – HSC: (323) 442-1000 – 24-hour emergency or to report a crime.
Provides overall safety to USC community. dps.usc.edu