

# MEDICINAL CHEMISTRY AND DRUG DESIGN

Spring, 2021 (ver. 2.4 updated 11/11/2020)

## CHEM 577a

Units: 2

Introduction to fundamentals of medicinal chemistry with special attention to the drug discovery process

Prerequisites: None

Instruction mode: Lecture, January 18 – March 10

MW 11:00-12:20pm

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 15 – April 28

MW 11:00-12:20pm

Grading Option: Letter (can audit for grade "V")

## Instructor: Charles McKenna

Office: LJS 268

Office Hours: 5:00-6:00pm Mondays and Wednesdays or by appointment.

Contact Info: mckenna@usc.edu. Office: (213) 740-7007

## Website:

Blackboard

## Dornsife IT Help

Hours of Service: Mon-Fri, 9am – 5pm

Contact Info:

- Phone support: 213-740-2775
- Email support: ts@dornsife.usc.edu

## 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

Textbook: "An Introduction to Medicinal Chemistry" Graham L. Patrick. Oxford University Press, New York, 2017.

Required weekly readings posted in the syllabus. Additional materials for the class will be presented on Blackboard.

## Grading Breakdown

### CHEM 577a

Homework	280 points	70%
Final/Presentation	120 points	30%
<b>TOTAL</b>	<b>400 points</b>	<b>100%</b>

### CHEM 577b

Homework	200 points	50%
Final/Presentation	200 points	50%
<b>TOTAL</b>	<b>400 points</b>	<b>100%</b>

## Grading Scale

Course final grades will be determined using the following scale

A	95-100	B	83-86	C	73-76	D	63-66
A-	90-94	B-	80-82	C-	70-72	D-	60-62
B+	87-89	C+	77-79	D+	67-69	F	59 and below

## 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](mailto: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.

Course Schedule	Monday	Wednesday
<b>CHEM 577a</b> Week 1 (1/18)	<b>University Holiday</b> (Martin Luther King's Birthday) – No Class	<b>Chalk/talk:</b> Class organization
Week 2 (1/25)	<b>Chalk/talk:</b> History of drug discovery <b>Chapter 1:</b> Drugs and drug targets	<b>Chalk/talk:</b> Amino Acids/Peptides/Proteins/Enzyme kinetics 1 <b>Chapter 2:</b> Protein structure and function
Week 3 (2/1)	<b>Chalk/talk:</b> Enzyme kinetics II <b>Chapter 3:</b> Enzymes: structure and function	<b>Chalk/talk:</b> Medicinal chemistry of imaging probes
Week 4 (2/8)	<b>Chalk/talk:</b> Curies/radiation therapy; Elion/drugs <b>Chapter 7:</b> Enzymes as drug targets	<b>Chalk/talk:</b> Homework 1 solutions <b>Chapter 4:</b> Receptors: structure and function <b>Homework 1 DUE</b>
Week 5 (2/15)	<b>University Holiday</b> (President's Day) – No class	<b>Chalk/talk:</b> Acids/bases I <b>Chapter 5:</b> Receptors and signal transduction
Week 6 (2/22)	<b>Chalk/talk:</b> Drug patents/ Acids/bases II <b>Chapter 8:</b> Receptors as drug targets	<b>Chalk/talk:</b> Homework 2 solutions <b>Chapter 10:</b> Miscellaneous drug targets <b>Homework 2 DUE</b>
Week 7 (3/1)	<b>Chalk/talk:</b> Cocaine/Abzymes; <b>Chapter 11:</b> Pharmacokinetics and related topics	<b>Chalk/talk:</b> FINAL/Presentation hints <b>Chapter 12:</b> Drug discovery: finding a lead
Week 8 (3/8)	<b>Chalk/talk:</b> Homework 3 solutions <b>Chapter 15:</b> Getting the drug to market <b>Upload Presentation slides DUE</b> <b>Homework 3 DUE</b>	FINAL/Presentations (5x5+1) (PechaKucha) Coronavirus Mini-Colloquium
<b>CHEM 577b</b> Week 9 (3/15)	<b>Chalk/talk:</b> Class organization <b>Chapter 13:</b> Drug design: optimizing target interactions	<b>Chalk/talk:</b> Antifungal agents <b>Chapter 14:</b> Drug design: optimizing access to the target
Week 10 (3/22)	Special guest presentation (NIH-NCI/Ellison Institute): Dr Jerry Lee	<b>Chapter 17:</b> Computers in medicinal chemistry; <b>Chapter 18:</b> Quantitative structure-activity relationships (QSAR)
Week 11 (3/29)	<b>Chalk/talk:</b> Homework 4 solutions + 'Bayes...? What was that about?' <b>Chapter 19:</b> Antibacterial agents <b>Homework 4 Due</b>	<b>Chalk/talk:</b> High throughput drug screening – virtual/real chimiothèques <b>Chapter 6:</b> Nucleic acids
Week 12 (4/5)	<b>Chalk/talk:</b> Case study: cisplatin <b>Chapter 9:</b> Nucleic acid as drug targets	<b>Wellness Day!</b> <b>Chapter 23:</b> Drugs acting on the adrenergic nervous system (self-read)
Week 13 (4/12)	<b>Chalk/talk:</b> Homework 5 solutions <b>Chapter 20:</b> Antiviral agents <b>Homework 5 DUE</b>	<b>Chalk/talk:</b> Case Studies: antivirals <b>Chapter 21:</b> Anticancer agents
Week 14 (4/19)	<b>Chalk/talk:</b> Psychoactive drugs <b>Chapter 24:</b> Opioid analgesics (read Special guest presentation: Dr Carolina Garri (NIH-NCI/Ellison Institute)	<b>Chalk/talk:</b> Homework 6 solutions; Final/presentation hints <b>Chapter 26:</b> Cardiovascular drugs <b>Upload Presentation slides DUE</b> <b>Homework 6 DUE</b>
Week 15 (4/26)	FINAL/Presentations (10x10+5)	FINAL/Presentations (10x10+5)

## 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, <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](http://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](http://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](http://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](http://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](http://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](http://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](http://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](http://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](http://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](http://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](http://dps.usc.edu)