Fau	COURSE CHANGE REQUEST Undergraduate Programs			UUPC Approval <u>4/24/23</u> UFS Approval SCNS Submittal			
FLORIDA Depart	Department Chemistry and Biochemistry			Confirmed			
ATLANTIC UNIVERSITY College	College : Science			Banner Posted Catalog			
Current Course CHM 4350 Current Course Prefix and Number CHM 4350 Structural Bio			ourse Title				
Syllabus must be attached for ANY changes to current course details. See <u>Checklist</u> , Please consult and list departments							
that may be affected by the ch Change title to:	anges; attach aoc	cumentation.	Change description to	:			
RI Structural Biochemistr	у		Course emphasizes a computer-based approach to teaching structural biochemistry. It uses hands-on experience to develop essential skills for				
Change prefix			understanding relationships betwee biomolecules. State-of-the-art soft	een structure and function of ware for visualization, manipulation and			
From: To:			simulation of various biomolecules is used throughout. This course contains an assignment or multiple assignments designed to help students				
Change course number			conduct research and inquiry at a				
From:	From: To:			Change prerequisites/minimum grades to: BCH 3033 with minimum grade of "C"			
Change credits*							
From:	Т о:						
Change grading			Change corequisites to:				
From:	To:						
Change WAC/Gordon Ru Add	le status** Remove		Change registration co	antrols to:			
Change General Education Requirements*** Add Remove **** *Review Provost Memorandum **WAC/Gordon Rule criteria must be indicated in syllabus and							
approval attached to this form. See <u>WAC Guidelines</u> . ***General Education criteria must be indicated in syllabus and approval attached to this form. See <u>GE Guidelines</u> .			Please list existing and new pre/corequisites, specify AND or OR and include minimum passing grade (default is D-).				
Effective Term/Year Spring 2024 for Changes:			Terminate course? Effective Term/Year for Termination:				
Faculty Contact/Email/Phone Maciej Stawikowski, mstawikowski@fau.edu, 561-297-4871							
Approved by Andrew Lebuh's.				Date 3/30/23			
Department Chair				4-5-23			
College Curriculum Chair			4/9/22				
College Dean UUPC ChairChlyn Williams				4/24/23			
Undergraduate Studies Dean Dan Meeroff				4/24/23			
UFS President		\mathcal{W}					
Provost							

Email this form and syllabus to mjenning@fau.edu seven business days before the UUPC meeting.

RI: Structural Biochemistry (CHM 4350) CRN # 0000

Syllabus Spring 20XX semester

NUMBER OF CREDIT HOURS: 3

TIME: Tuesday/Thursday, 2:00 PM – 3:20

LOCATION: PS-334

INSTRUCTOR: Dr. Maciej Stawikowski Department of Chemistry and Biochemistry PS-310 Office Phone 561-297-4871 E-mail: mstawikowski@fau.edu

OFFICE HOURS Tuesdays, 2PM-3PM, PS 310

TEXTS

No textbook is required. The following materials are recommended:

- 1. Introduction to protein structure; 2th edition, C. Branden & J. Tooze. ISBN-10: 0815323050.
 - 2. Introduction to Proteins: Structure, Function, and Motion; A. Kessel & N. Ben-Tal. ISBN-10: 1439810710.
- 3. Lehninger Principles of Biochemistry; 4th edition, D. L. Nelson & M.M. Cox. ISBN-10: 0716743396.
- 4. UCSF Chimera User's Guide. <u>https://www.cgl.ucsf.edu/chimera/docs/UsersGuide/</u> Recommended.
- 5. All online e-books freely available to FAU students and recommended by the instructor.

PREREQUISITE: BCH 3033 with minimum grade of "C"

CATALOG DESCRIPTION

Course emphasizes a computer-based approach to teaching structural biochemistry. It uses hands-on experience to develop essential skills for understanding relationships between structure and function of biomolecules. State-of-the-art software for visualization, manipulation and simulation of various biomolecules is used throughout. This course contains an assignment or multiple assignments designed to help students conduct research and inquiry at an intensive level.

COURSE DESCRIPTION

This course is an introduction to structural biochemistry with an emphasis on computer-based approach, hands-on experience to develop essential skills for understanding of relationships

between structure and function of biomolecules. A workshop format (introductory lecture followed by hands-on practice) will be carried out throughout all sessions. Classes will be held in computer labs. Each session will be composed of approximately 45 min. of lecture and 45 min. of hands-on training.

RESEARCH-INTENSIVE (RI) DESIGNATED COURSE

This course contains an assignment or multiple assignments designed to help students conduct research and inquiry at an intensive level. If this class is selected to participate in the university-wide assessment program, students will be asked to complete a consent form and submit electronically some of their research assignments for review. Visit the Office of Undergraduate Research and Inquiry (OURI) for additional opportunities and information at http://www.fau.edu/ouri.

COURSE OBJECTIVES / LEARNING OUTCOMES

We will use state-of-the-art software that will allow for visualization, manipulation and simulation of various biomolecules including proteins, nucleic acids, lipid membranes and their interactions. Students will learn how to identify and describe molecular interactions at different levels. We will work with different biological databases to obtain different data: from sequence to 3-dimensional structures. Participants will learn how use various computer programs to manipulate 3D structures, create publication-quality molecular images to be incorporated in scientific presentations and literature reports. State-of-the-art 3D printing technique will be incorporated into the teaching giving student better perspective on three-dimensional aspect of biomolecular architecture. During this course students will be involved in 3D printing of molecular models.

STUDENT LEARNING OUTCOMES (SLOs)

SLO 1: Knowledge.

Students will demonstrate ability to complete an independent research project, including writing a summary report and oral presentation at the end of the course.

SLO 2: Formulate Questions.

Students will formulate or identify research questions and evaluate the literature to integrate basic principles and knowledge of biomolecular interactions and their application do design and virtually screen protease inhibitors.

SLO 3: Plan of Action.

Students will develop and implement an experimental approach to address research and inquiry questions or scholarly problems. Students' plan of action will be evaluated in the written assignment.

SLO 4: Critical Thinking.

Students will apply critical thinking skills to evaluate available information through literature search regarding the practical application of protein modeling, drug design and computer simulations. *SLO 5: Ethical Conduct.*

Students will identify and follow significant ethic issues while conducting research and inquiry. *SLO 6: Communication.*

Students will convey their research and inquiry in both oral and written formats.

RESEARCH ASSIGNMENTS

- 1. Explore the biochemistry of various proteolytic enzymes and related information in various databases, to determine enzyme mode of action, structure, and existing inhibitors.
- 2. Prepare 3D model structure of the enzyme in question. Determine binding site and protein properties.
- 3. Identify 3D structures of existing enzyme inhibitor. Identify relevant publication. Determine drug-likeness properties of that compound and keep it as a reference.
- 4. Perform virtual docking of 10 selected compounds from ZINC database to selected enzyme. Determine binding strength. Select top 3 results and determine drug-likeness of identified inhibitors and compare it with existing inhibitor.
- 5. Prepare the presentation on the same topic and present it in class.

INTEGRATION OF SLO'S AND ASSIGNMENTS

SLOs

Assignment requirements and assessments

- 1. Knowledge Students will master research methodologies related to drug design and simulations. Students will demonstrate knowledge of biomolecular interactions, the relationships between structure and function of various enzymes. Students will learn practical skills of computer-based molecular model visualization, manipulation and analysis. They will learn principles of bioinformatics skills such as homology model building, mutational analysis, molecular docking and molecular dynamics simulations. The knowledge and skills will enable them for the design of novel enzyme inhibitors. The acquired knowledge, critical thinking and thoughtful analysis of protein-ligand interactions will help students in their future research endeavors.
- 2. Formulate Questions Students will conduct background research to determine what has been done to address research question and confirm that the research is unique. The ability to identify the key critical question applicable to the selected field of study will be assessed.

Students will be divided into groups – each working on different molecular target (enzyme).

Ultimately, all groups will try to answer the following questions:

1. What is the best inhibitor scaffold that can achieve the best binding/inhibition?

2. Can we modify existing scaffolds to obtain better/more selective enzyme inhibitors?

3. Which enzyme residues are responsible for inhibitor binding/interaction?

4. How key interacting atoms/groups could be further modified to achieve better binding/selectivity?

5. How to increase the cell uptake of the inhibitor?

3. Plan of Action Students will recognize new inhibitor scaffold candidates by analyzing 3-dimensional structures of known enzyme inhibitors found in macromolecular structure databases. They will also analyze literature data to confirm the validity of their findings.

Structural Biochemistry (CHM 4350)

Students will develop practical skills for advanced molecular model visualization, manipulation and computer-based simulation.

Student will search ZINC, a free database of commercially-available compounds for virtual screening. ZINC contains over 230 million purchasable compounds in ready-to-dock, 3D formats.

After identifying mode of action, active site and already known enzyme inhibitors students will perform virtual screening of compounds selected from ZINC database. Docked models will be scored according to docking software (Autodock Vina) scoring function. Identified inhibitors will als be evaluated for drug likeness, using bioinformatics tools. The aforementioned actions will be performed in a recurring manner until satisfactory criteria are met (e.g. strong inhibitor binding).

- 4. Critical Students will 1) analyze obtained structural information about the putative inhibitor, 2) analyze literature data supporting their ideas, 3) will discuss their thinking, predictions and possible pitfalls to be encountered during data analysis/molecular simulations.
- 5. Ethical Conduct Students will apply the codes of academic integrity making sure that their work adheres to ethical guidelines. It is strongly recommended that students complete the Responsible conduct of research (RCR) certificate through the CITI training of academic research on-line at http://www.fau.edu/graduate/events/citi-training.php.
- 6. Communication Students will prepare 15 minutes-long oral presentation to the class that covers:
 - background literature data review for selected enzyme,
 - inhibitor design approach,
 - results of their simulation
 - -comparison/discussion of the results with published data,

Students are encouraged to submit their research projects to the Undergraduate Research Symposium held at Florida Atlantic University (Boca Raton campus) each Spring Semester. Use the following link for more information:

http://www.fau.edu/ouri/undergrad_symposium.php

COURSE EVALUATION METHOD

Students will be required to practice the use of various programs and study given problems at home before class meets.

There will be three major exams during the semester: two progress exams (non-cumulative) and a comprehensive final exam. The comprehensive final exam is cumulative and may relate to any topic covered during the semester. The comprehensive final exam will be given during exam week at the end of the semester in accordance with the published FAU exam schedule.

The exam will consist of short answer questions (essay and word problems) and results of analysis of computer molecular models and biochemical problems. Software-relates skills will also be tested.

Each progress exam will be 60 minutes long while the final exam will be 90 minutes long. The exams will test the material covered in classes as well as material from assigned readings/practice problems.

Students are also expected to prepare a final presentation on selected biochemistry/medicine related subject that encompasses biomolecular structure – activity relationships (as per research assignment). It is expected that students demonstrate acquired in class skills to effectively communicate the topic. The presentation is based research assignment as assigned by the instructor. Students will be evaluated based on provided presentation rubric.

Tentative exam dates:

Exam 1: TBD Exam 2: TBD Research Presentations: TBD Final exam: TBD

Each exam will be held in PS 334, during regular class hours.

Any dispute concerning exam grades during the semester must be brought to instructor's attention within one week after grades are posted. No appeal will be considered at a later date.

ASSESMENT AND GRADING SCALE

Final grade in this course will be calculated as a sum of points earned during exams and research presentation:

Exam 1: 20 points Exam 2: 20 points Final exam: 20 points Research project and presentation: 40 points

TOTAL: 100 points

There will be no rounding.

Extra credit assignments may be offered throughout the semester. No extra credit assignments will be given to <u>an individual student</u> as a means of improving the grade. Giving such credit is unfair to the rest of the class. Furthermore, a student who was not able to master the class material cannot be expected to successfully complete additional, higher-level assignments.

All grades will be posted on Canvas.

COURSE GRADING SCALE

А	A-	B+	В	B-	C+	С	C-	D+	D	F
93.0-	89.0-	85.0-	82.0-	78.0-	74.0-	70.0-	67.0-	63.0-	60.0-	0-
100%	92.9%	88.9%	84.9%	81.9%	77.9%	73.9%	69.9%	66.9%	62.9%	59.9%

INCOMPLETE GRADE

Incompletes will not be given unless a) a student is passing the course and b) a student encounters severe and unexpected problems and was not able to complete some portion of the work assigned to all students as a regular part of the course. Incompletes are given only by arrangement with the instructor. Students are expected to make up incompletes as soon as reasonably possible. Incompletes are <u>not</u> given because a student is doing poorly in the course.

MAKEUP TESTS POLICY

A student who misses any exam during the semester (or the final exam) will receive a grade of 0 unless a) student notifies the instructor <u>prior</u> to the exam that he or she will be absent and b) the student presents a legitimate, documented reason that meets FAU criteria for missing the exam. If these conditions are met, a make-up exam will be considered.

Make up exam will not be given unless a written and verifiable reason is approved either prior to the exam or within 24 hours of the exam date. Unexcused absence from an exam will result in a zero score being recorded. If a student is unable to complete the required coursework for health or personal/family reasons, an incomplete <u>may</u> be issued, according to University policy on Incompletes.

ATTENDANCE POLICY

Students are expected to attend all of their scheduled University classes and to satisfy all academic objectives as outlined by the instructor. The effect of absences upon grades is determined by the instructor, and the University reserves the right to deal at any time with individual cases of non-attendance. Students are responsible for arranging to make up work missed because of legitimate class absence, such as illness, family emergencies, military obligation, court-imposed legal obligations or participation in University-approved activities. Examples of University-approved reasons for absences include participating on an athletic or scholastic team, musical and theatrical performances and debate activities. It is the student's responsibility to give the instructor notice prior to any anticipated absences and within a reasonable amount of time after an unanticipated absence, ordinarily by the next scheduled class meeting. Instructors must allow each student who is absent for a University-approved reason the opportunity to make up work missed without any reduction in the student's final course grade as a direct result of such absence.

CODE OF ACADEMIC INTEGRITY

Students at Florida Atlantic University are expected to maintain the highest ethical standards. Academic dishonesty is considered a serious breach of these ethical standards, because it interferes with the university mission to provide a high quality education in which no student enjoys an unfair advantage over any other. Academic dishonesty is also destructive of the university community, which is grounded in a system of mutual trust and places high value on personal integrity and individual responsibility. Harsh penalties are associated with academic dishonesty. For more information, see <u>University Regulation 4.001</u>.

Withdrawal:

Please check the official FAU website regularly for the most up to date information on last day to withdraw without a "W" & last day to withdraw without an "F" dates for this semester.

DISABILITY POLICY STATEMENT

In compliance with the Americans with Disabilities Act Amendments Act (ADAAA), students who require reasonable accommodations due to a disability to properly execute coursework must register with Student Accessibility Services (SAS) and follow all SAS procedures. SAS has offices across three of FAU's campuses – Boca Raton, Davie and Jupiter – however disability services are available for students on all campuses. For more information, please visit the SAS website at <u>www.fau.edu/sas/</u>.

COUNSELING AND PSYCHOLOGICAL SERVICES (CAPS) CENTER

Life as a university student can be challenging physically, mentally and emotionally. Students who find stress negatively affecting their ability to achieve academic or personal goals may wish to consider utilizing FAU's Counseling and Psychological Services (CAPS) Center. CAPS provides FAU students a range of services – individual counseling, support meetings, and psychiatric services, to name a few – offered to help improve and maintain emotional well-being. For more information, go to http://www.fau.edu/counseling/

<u>Anti-Discrimination and Anti-Harassment Policy:</u> Students, faculty and staff at Florida Atlantic University are expected to abide by the published anti-discrimination and anti-harassment policy: http://www.fau.edu/regulations/chapter5/Reg%205.010%206-2015.pdf

CLASS ETIQUETTE POLICY

University policy on the use of electronic devices states: "In order to enhance and maintain a productive atmosphere for education, personal communication devices, such as cellular telephones and pagers, are to be disabled in class sessions."

- The use of cell phones or other communication devices for talking or texting is disruptive, and is therefore prohibited during class. A ringing or vibrating phone is just as bad, turn it off before class begins.
- Students are permitted to use personal computers during class for note-taking and other class-related work only.
- No food, drinks, chewing gums, snacks or similar items are permitted in class.
- Bringing-in visitors to the computer lab is not acceptable.

Policy on the Recording of Lectures

Students enrolled in this course may record video or audio of class lectures for their own personal educational use. A class lecture is defined as a formal or methodical oral presentation as part of a university course intended to present information or teach students about a particular subject. Recording class activities other than class lectures, including but not limited to student presentations (whether individually or as part of a group), class discussion (except when incidental to and incorporated within a class lecture), labs, clinical presentations such as patient history, academic exercises involving student participation, test or examination administrations, field trips, and private conversations between students in the class or between a student and the lecturer, is prohibited. Recordings may not be used as a substitute for class participation or class attendance and may not be published or shared without the written consent of the faculty member.

Failure to adhere to these requirements may constitute a violation of the University's Student Code of Conduct and/or the Code of Academic Integrity.

CLASS SCHEDULE

Below is the tentative schedule, which is subject to change due to environmental, pedagogical, or other factors deemed appropriate by the instructor.

Week	In Class	Exams/presentations
1	Amino acids and protein primary structure. Introduction to UCSF Chimera software.	
2	Non-covalent interactions in biomolecules.	
3	Protein secondary structures.	
4	Protein tertiary and quaternary structure. Protein Domains and Motifs.	
5	Nucleotides and nucleic acids.	
TBD		Exam 1
6	Carbohydrates and glycoproteins.	
	Introduction to 3D printing of biomolecules	
7	Structure and organization of biological	
ľ	membranes. Membrane proteins.	
8	Biomolecular structure determination methods.	
9	Protein-protein interactions. Case studies.	
10	Protein-ligand interactions. Case studies.	
TBD		Exam 2
11	Computational methods for structure prediction.	
12	Protein stability and dynamics.	
13	Biomolecular software – showcase and demonstration. Biological databases and data mining.	
14	Molecular structure description: analysis of literature examples; from writing to making molecular movies; creating stunning presentations; Practice examples.	
TBD		Research Presentations
TBD		Final exam

Required course materials:

USB flash drive – 16GB or more.