## **BIOSC 1540 - Computational Biology**

Spring, 2019

## **Course Schedule**

Date	Topic	Instructor	Exercises
Jan. 8 <sup>th</sup>	Review Syllabus Comp Bio: General Overview UNIX Command Line (Intro)	Jacob Durrant	
Jan. 10 <sup>th</sup>	UNIX Command Line	Jacob Durrant	UNIX homework
Jan. 15 <sup>th</sup>	Basic Python	Jacob Durrant	Python Homework
Jan. 17 <sup>th</sup>	Computational Genomics	Miler Lee	Homework: TBA
Jan. 22 <sup>nd</sup>	High-Performance Computing	Kim Wong	Homework: TBA
Jan. 24 <sup>th</sup>	Machine Learning	Jacob Durrant	Homework: TBA
	Discuss Group Projects		
Jan. 29 <sup>th</sup>	EXAM 1	(No Class)	
Jan. 31st	Intro to Proteins & Ligands	Jacob Durrant	Video: What is a Protein?
Feb. 5 <sup>th</sup>	Ligand/Protein Binding	Jacob Durrant	Homework: PoseView
Feb. 7 <sup>th</sup>	Cheminformatics 1	Jacob Durrant	Due: Background-Research Rough Draft (Group Project)
Feb. 14 <sup>th</sup>	Small-Molecule Drugs	Jacob Durrant	Homework: Predict Chemical Properties
Feb. 19 <sup>th</sup>	Small-Molecule Models	Jacob Durrant	Due: Materials-and- Methods/Results-and- Discussion Rough Draft #1 (Group Project)
Feb. 21st	Ligand-Based CADD	Jacob Durrant	Homework: TBA
Feb. 26 <sup>th</sup>	Catch-up Day (Python Packages, Command-line Programs)	Jacob Durrant	Homework: TBA
Feb. 28st	EXAM 2	(No Class)	
Mar. 5 <sup>th</sup>	Determining Protein Structures	Jacob Durrant	Due: Edited/Revised Group Projects (Everything So Far, Compiled into One Document)
			Swap Projects (Peer Review)
Mar. 7 <sup>th</sup>	Search & Visualize Proteins	Jacob Durrant	Homework: UniProt and PDB Searching and Visualization
Mar. 12 <sup>th</sup>	No Class (Spring Break)		

Mar. 14 <sup>th</sup>	No Class (Spring Break)		
Mar. 19 <sup>th</sup>	Alignment and Homology Models	Jacob Durrant	Homework: SWISS-MODEL  Due: Peer-Reviewed Group  Projects
Mar. 21 <sup>st</sup>	Druggable Proteins	Jacob Durrant	Homework: FTMAP
Mar. 26 <sup>th</sup>	Protein Simulations 1	Jacob Durrant	Homework: TBA
Mar. 28 <sup>th</sup>	Protein Simulations 2	Jacob Durrant	Homework: NAMD and VMD
Apr. 2 <sup>nd</sup>	CADD and Protein Flexibility	Jacob Durrant	Reading: Molecular Dynamics Simulations and Drug Discovery
Apr. 4 <sup>th</sup>	Computational Alchemy	Jacob Durrant	Homework: TBA
Apr. 9 <sup>th</sup>	Structure-Based CADD	ТВА	Homework: TBA
			Due: Final Written Project Reports
Apr. 11 <sup>th</sup>	Project Presentations		Group Oral Presentations (10 Minutes per Group)
Apr. 16 <sup>th</sup>	Project Presentations		Group Oral Presentations (10 Minutes per Group)
Apr. 18 <sup>th</sup>	EXAM 3	(No Class)	

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CADD and Protein Flexibility	Jacob Durrant	Reading: Molecular Dynamics Simulations and Drug Discovery
Computational Alchemy	Jacob Durrant	Homework: TBA
Structure-Based CADD	TBA	Homework: TBA
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Project Presentations		Group Oral Presentations (10 Minutes per Group)
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