GEORGE MASON UNIVERSITY

SCHOOL OF SYSTEMS BIOLOGY

BINF 731: Protein Structure Analysis. **Fall 2020**

Instructor: Iosif Vaisman
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Office Hours: By appointment
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Textbook: see course reading materials at http://binf.gmu.edu/vaisman/binf731/papers.html

Credit hours: 3.0 Credits
Meeting days and times: Thursday, 4:30 pm - 7:10 pm
Building and room: Online (using Blackboard Collaborate Ultra)

Course description: Review of computational methods for the analysis, classification and prediction of three-dimensional protein structures. The course covers theoretical approaches, techniques and computational tools for protein structure analysis. The topics also include protein geometry and topology, 3D structure databases, protein modeling and engineering.

Course Requirements: The course will include reading assignments and project assignments. The results of project assignments will be presented in the online format. The date of the final exam can be found in the GMU academic calendar.

Grading: grades will be based on project assignments (66%) and exam (34%).

Course Outline

1. Complexity of protein structure and protein folding
2. Methods for experimental determination of three-dimensional structure
   a. X-ray crystallography
   b. Neutron diffraction
   c. NMR
3. Protein structure verification and validation
4. Protein structural hierarchy
   a. Structural building blocks
   b. Secondary and supersecondary structures
   c. Ramachandran diagram
   d. Secondary structure assignment and prediction
5. Protein structure classification
6. Protein structure databases
7. Protein models
   a. All-atom models
   b. Residue-based models
   c. Simplified residue alphabets
   d. Lattice models
8. Protein visualization
9. Protein modeling

    a. *Ab initio* methods (QM, DFT)
    b. Energy based methods (energy minimization, molecular dynamics, simulated annealing)
    c. Stochastic searches (Monte Carlo, genetic algorithms)
10. Knowledge based protein modeling
    a. Comparative modeling
    b. Fold recognition
11. Protein structure prediction and structural genomics
12. Computational analysis of protein-protein, protein-DNA, and protein-ligand interactions.
13. Structure-function relationship in proteins, computational mutagenesis.
14. Protein engineering

Course website: http://binf.gmu.edu/vaisman/binf731/

Policies

- It is expected that students adhere to the George Mason University Honor Code as it relates to integrity regarding coursework and grades. The Honor Code reads as follows: "To promote a stronger sense of mutual responsibility, respect, trust, and fairness among all members of the George Mason University community and with the desire for greater academic and personal achievement, we, the student members of the University Community have set forth this: Student members of the George Mason University community pledge not to cheat, plagiarize, steal and/or lie in matters related to academic work." More information about the Honor Code, including definitions of cheating, lying, and plagiarism, can be found at the Office of Academic Integrity website at http://oai.gmu.edu

- Students are encouraged to discuss course content, labs, and similar activities with other students; however, all assignment submissions must contain only original, individually completed work, unless a different arrangement approved by the instructor.

- Posting or sharing course content (e.g., recordings, exams, or anything not created by the student), using any non-electronic or electronic medium (e.g., web site) where it is accessible to someone other than the individual student is strictly prohibited without prior instructor's approval.

- Students must follow the university policy for Responsible Use of Computing (see http://universitypolicy.gmu.edu/policies/responsible-use-of-computing/).

- Students are responsible for the content of university communications sent to their Mason email account and are required to activate their account and check it regularly. All communication from the university, college, school, and program will be sent to students solely through their Mason email account.

- Students with disabilities who seek accommodations in a course must be registered with George Mason University Disability Services. Approved accommodations will begin at the time the written letter from Disability Services is received by the instructor (see https://ds.gmu.edu/).