BIO4010W: Macromolecular Structure and Bioinformatics

Lectures TBA

Lecturer TBA

Office hours: By appointment (Zoom) – email me for an appointment

Topics covered:

Introduction to Biological macromolecules and genetic material
1)   Types of macromolecules and their function(s)
2)   The evolving view of the nature of genetic material, the central dogma of molecular biology, gene structure and information content
3) Bioinformatics, genomics, proteomics – an overview of the emerging field

Biological databases and database searches
1) The various biological databases – an overview
2) NCBI, Uniprot in depth
3) Efficient strategies for database searches
4) Understanding and scrutinizing database annotation

The primary structure of proteins
1) Introduction to the hierarchical structure of proteins
2) The building blocks – detailed study of amino acids
3) Linear arrangement of the amino acids in the polypeptide chain, the peptide bond and spatial arrangements of the side-chains. 4) Chemistry and geometry of the peptide bond

The secondary structure of proteins
1) Introduction to secondary structure elements
2) Detailed study of the alpha-helix
3) Detailed study of beta-sheets
4) Properties and functions of loop regions
5) Topology diagrams as representations of secondary structure elements 6) Super-secondary structures or motifs

The tertiary and quaternary structure of proteins 1)
Introduction to the three-dimensional structure of proteins
2) What holds a protein into its tertiary structure?
3) Domain and domain folds
4) Quaternary structure of proteins
5) Structural classification of proteins – Protein structure databases

Protein databank and three-dimensional representations of proteins
1) What is the PDB?

2) Nature of three-dimensional structural data
3) Understanding the format of a PDB file; other file formats.

Computer graphics-based visualization and modeling of the three dimensional structures of macromolecules
1) Visualizing and animating structures of macromolecules 2)
Overview of a popular program: Pymol

Introduction to computational tools for studying proteins-Part 1.
1) Protein sequence analysis
2) Protein characterization tools
3) Overview of proteomics

Introduction to computational tools for studying proteins-Part 2.
1) Secondary structure prediction tools
2) Modeling the three-dimensional structure of proteins
3) Structure-function relationships in proteins

Course Schedule: Available on blackboard

Class format:
In addition to traditional lectures, small take-home writing and analyses projects will be assigned on a regular basis to stimulate exploration of the field of bioinformatics. A more involved take-home project will aim to tackle a given biological problem using computational methods. Students will do assignments which will be evaluated periodically throughout the length of the course. Mini-quiz type exercises, in-class writing, and group exercises/ teamwork will be incorporated in the classes as required. "Blackboard" will be used for disseminating information, handouts etc.

Reading Material:
This course is designated as a OER (Open Educational Resources) /ZTC (Zero textbook cost) course and there is no formal textbook requirement for this course. "Blackboard" will be used for disseminating all reading material including peer reviewed open access articles, links to open educational resources, and all instructor designed reading material for the course.

Reading and Video List: Available on blackboard within the 'Resources' and 'Reading material' folders.

Online Course Access and technology requirements:
The course is hybrid and will require a computer (desktop/laptop with any operating system installed) and internet access for the online lectures/homework etc. Information for all software installations and licenses needed to operate the software will be provided in class

and if needed, step by step instructions or video recordings will be made accessible to all students. The lectures of the course will be held at a fixed time in person and using "Zoom"; mandatory participation is required **with cameras turned on**. Asynchronous activities such as discussion forums, assignments, etc. will be flexible in time but must be completed by the assigned deadlines. There will be links to help documents/videos for technology troubleshooting in addition to office hours where individual one on one help can be provided as needed.

Note: For all online tests, **your cameras must be turned on**.

Class Policy:
- Plagiarism is unacceptable and any attempt to do so will be graded with a zero.
- Lateness and absence will be noted and will result in penalties in your final grade.
- Late assignments will be penalized.
- Group activities require equal participation and any member who does not adequately participate will be penalized.

Academic Integrity Policy
Academic dishonesty is prohibited in The City University of New York and is punishable by penalties, including failing grades, suspension, and expulsion. Examples of academic dishonesty include cheating, plagiarism, internet plagiarism, obtaining unfair advantage, and falsification of records. A full definition of each form of academic dishonesty, as well as procedures for imposition of sanctions for violations of the CUNY. Policy on Academic Integrity, may be accessed at:
*www.brooklyn.cuny.edu/pub/documents/**academicintegritypolicy**.pdf*

Grading*:

Standard testing methods: 50%
Quizzes 10%
Regular reinforcement and assessment of concepts learnt in class. Multiple choice and/or short written answers/explanations
Midterm 20%
Multiple choice and/or short written answers/explanations
Approximately halfway through the course
Final 20%
Multiple choice and/or short written answers/explanations.

Written and other methods to assess learning: 50%
Take-home term project 20%
Individual or group project involving use and analysis of the learnt computational tools 20%
Class/Team participation and attendance 10%

Grade Basis

98.00	A+
93.00	A
89.00	A-
83.00	B+
79.00	B
73.00	B-
69.00	C+
63.00	C
59.00	C-
53.00	D+
49.00	D

*All assignments/tests will be graded, and feedback provided within a maximum of 2-3 days of submission for most assignments except lengthy written assignments that take longer to grade.

Learning Outcomes

Students successfully completing the course should be able to:

- Navigate biological databases and extract required biological data efficiently.
- Analyze protein sequences to predict functional motifs, domain architecture, secondary and tertiary structure, and other indicators of function.
- Model and refine the three-dimensional structure of proteins, visualize the structure, and map the biophysical properties of the protein sequence onto the modeled structure.
- Perform sequence and structure comparisons of two or more sequences.
- Predict protein-ligand interaction.
- Critically and comprehensively review the scientific literature pertaining to their research topic.
- Frame a robust hypothesis for their study.
- Communicate results in the format of a scientific manuscript/presentation.

Department Goals and Objectives to be covered in this course:

CORE BIOLOGICAL KNOWLEDGE
Cell Biology:
Demonstrate a working understanding of the Central Dogma.
Describe the bio-molecular structure and function of proteins.

PRACTICAL COMPETENCIES

- Independently investigate biological phenomena using the scientific method and proven research tools and methods.
- Develop familiarity with laboratory and research procedures by
  - formulating hypothesis.
  - reading scientific literature.
  - designing and carrying out experiments.
  - preparing results in tabular and graphical form.
- Communicate scientific results in class.

PROFESSIONAL ATTITUDES AND ETHICAL RESPONSIBILITIES OF BIOLOGICAL RESEARCH

- Adhere to the highest professional standards of the scientific community.
- Evaluate important technological advances and discoveries with respect to
  - impact on the environment
  - impact on society