CHEM 6572
Macromolecular Structure
Fall 2011
Revised 8/20/2011

Description: This course covers the principles of protein and nucleic acid structure, stability and dynamics. Topics will include interactions, conformations, forces and thermodynamics that govern 3D structures of biological polymers, and detailed descriptions of their structures. This course will also introduce students to methods used to visualize and analyze large molecules in 3D, and methods used to determine 3D structures.

Instructor: Prof. Loren Williams
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E-mail can only be accepted from Georgia Tech accounts. When sending an e-mail message, please put the following information in the subject line:
CHEM 6572, firstname lastname, subject.
Example: CHEM 6572, Marie Curie, request for meeting on May 13

Place and time: 10:05 am - 10:55 am MWF Molecular Sciences & Engr 1201A.

Office hours: Mon and Fri 11 AM, or by appointment. To make an appointment, please contact my administrator, Sue Winters (sue.winters@chemistry.gatech.edu). It is best to check with her before you plan to visit my office.

Textbooks:
Required: Branden and Tooze, Introduction to Protein Structure, Second Edition, Garland Publishing, 1999.
Supplementary: Some material will be presented from:
R.D. Blake, Informational Biopolymers of Genes and Gene Expression, University Science Books, 2005
Voet and Voet, Biochemistry, Fourth Edition, John Wiley & Sons, Inc. 2010.
These supplementary texts are not required.

Additional Reading/Study Materials:
A number of papers from the primary literature will be posted. Approximately half of these papers will be required reading and the remainder will be optional supplementary reading. Slides will be posted.

Computer Software and Hardware:
You will need access to a computer with an internet connection, and the ability to run certain free software that is downloaded from the internet. We will be using PYMOL in class, so that might be easiest for you to use if you are not already committed to another molecular visualization software package. You will not need a laptop in class!!

Grades: will be based on four exams (60% total), homework assignments and quizzes (25%), and class participation (15%). Exams and quizzes will cover assigned reading and class discussions. Quizzes will be announced at least one class in advance.

Historically, students with class averages of 80-100 received an “A”; those with averages 60-79 received a “B”, those with averages 40-59 received a “C”.

Exam dates: September 14, October 12, November 16, and December 16 (11:30 am).

Syllabus

Brief Review of Kinetics, Thermodynamics, Driving Force and Equilibrium
Brief Review of Molecular Structure
The Liquid of Life: Water
Forces that stabilize macromolecular structure
- short range repulsion
- charge-charge
- dipole interactions (dipole-charge, dipole-dipole, etc)
- induced dipole
- hydrogen bonds
- screening and dielectric effects

The Covalent Structure of Biopolymers
- Amino Acids
- The Peptide Bond
- Protein Rotamers: Ramachandran plots
- The Nucleic Acid Bases
- The Nucleic Acid Backbone
- Nucleic Acid Rotamers

Introduction to PYMOL: visualization software
Introduction to Databases
- Protein Data Bank
- Sequence Databases, Blast Searches and Alignments

Protein Folding
- The alpha-helix
- The beta-sheet
- Fibrous Proteins
- Turns
- Alpha-Domain Structures
- Alpha/Beta Structures
- Beta Structures
- Protein Folding

Nucleic Acids Structure
- Base pairs and base triples
- Helical Structures: A, B and Z-helices
- Cation Binding
- Triplexes and Quadruplexes
- RNA Structures
- DNA-small molecule interactions
- Supercoiling and Condensation

Protein-Nucleic Acid Interactions and Complexes
- Transcription Factors
- The Nucleosome
- The Ribosome
- Viruses

Introduction to Structure Determination
- X-ray diffraction

NMR spectroscopy
Structure, Prediction and Design
Proteins
RNA