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20.320 Practice Problem Catalog

2009 PSET 1 Problem 1
- General problem statement: Influenza hemagglutinan pH dependent conformational change that helps escape lysosomal degradation
- Program used: Python
- Utility: coding practice to understand protein conformation
- Broad topic: Protein structure

2009 PSET 1 Problem 2
- General problem statement: Residues responsible for pH dependent conformational change in Influenza hemagglutinan.
- Program used: CLUSTALW and Biopython
- Utility: Practice problem with concepts and different biologically relevant programs
- Broad topic: Protein structure, function

2009 PSET 1 Problem 3
- General problem statement: Cystic Fibrosis is a genetic disease leading to alterations in folding of the CTFR protein, which is a traffic ATPase.
- Program used: None
- Utility: Great conceptual problem for recitation
- Broad topic: Protein folding, energetics, Gibbs Free Energy

2009 PSET 2 Problem 1
- General problem statement: A key histidine plays a role in the pH-dependent conformational change of influenza hemagglutinans, analyzing the electrostatics of different conformations
- Program used: Biopython
- Utility: Good mix of coding to achieve conceptual results
- Broad topic: Protein folding, electrostatics

2009 PSET 2 Problem 2
- General problem statement: Understanding the Chou- Fasman algorithm to predict the propensity for alpha-helices vs beta sheets in the influenza hemagglutinans HA_2 chain based on its sequence
- Program used: Python, PyMOL
- Utility: Not for recitation
- Broad topic: Predicting protein structure

2009 PSET 2 Problem 3
- General problem statement: Predicting protein-protein interaction in the *lacI* binding lac operon system, followed by a 'novel' binding event
- Program used: None

- Utility: Good for recitation
- Broad topic: Predicting structure, Predicting interactions

2009 PSET 3 Problem 1
- General problem statement: Interactions between GCSF and GCSR-receptor found in bone marrow precursors and neutrophils are dependent on the energetics of different protein variants.
- Program used: None
- Utility: Great for recitation
- Broad topic: Thermodynamic cycles, protein-protein interactions

2009 PSET 3 Problem 2
- General problem statement: Using a toy protein-protein interaction (PPI) network to analyze probabilities of pathways and interactions
- Program used: Python
- Utility: Not too coding intensive, basic concepts with extension to medical application
- Broad topic: Protein-Protein interaction (graphs/networks)

2009 PSET 3 Problem 3
- General problem statement: General Metropolis algorithm to find energy minimum based on the Boltzmann distribution
- Program used: Python
- Utility: Good practice for data analysis, not much biological relevance
- Broad topic: Energetics, data minimization

2009 PSET 5 Problem 1
- General problem statement: Screening for drugs based on binding affinity and performing Isothermal Titration Calorimetry to understand the thermodynamics of binding
- Program used: None
- Utility: Great for recitation
- Broad topic: ITC

2009 PSET 5 Problem 2
- General problem statement: Dasatinib is a small molecule tyrosine kinase inhibitor specific for the Src and Abl kinase families, but it is thought that it has some specificity for binding EphB4. Utilize SPR to learn about specificity and binding kinetics
- Program used: None
- Utility: Great for recitation
- Broad topic: SPR, binding kinetics

2009 PSET 5 Problem 3
- General problem statement: Analyze SUB1 signaling through many potential interacting partners by setting up a protein microarray experiment and analyzing data to determine parameters such as K_d to inform likely signaling partners.
- Program used: MATLAB
- Utility: Good intro to transforming data and plotting in MATLAB
- Broad topic: Protein microarray experiments, binding parameters

2009 PSET 6 Problem 1
- General problem statement: The effects of uncompetitive enzyme inhibitors are analyzed by deriving a new form of the Michaelis-Menton equation and looking at the effects of uncompetitive inhibitors on enzyme parameters.
- Program used: None
- Utility: Great for recitation
- Broad topic: Enzyme kinetics, Enzyme inhibitors

2009 PSET 6 Problem 2
- General problem statement: Analyze enzyme-substrate kinetics by calculations simplified by the quasi-steady state assumption and compare the results of a system of equations with and without applying the Michaelis Menton approximation
- Program used: MATLAB
- Utility: Mix of concepts and coding, solving ODEs
- Broad topic: QSSA, Michaelis Menton, ODEs

2009 PSET 6 Problem 3
- General problem statement: Enzymes often produce many products by interacting with different substrates with different specificities and efficiencies. This problem analyzes how competitive inhibition can affect product formation under different conditions
- Program used: MATLAB
- Utility: Conceptual results, coding heavy
- Broad topic: Enzyme competition

2010 PSET 1 Problem 1
- General problem statement: Characterize binding kinetics of candidate drugs by using SPR.
- Program used: None
- Utility: Great conceptual questions on SPR, good for recitation or exam review
- Broad topic: SPR, binding kinetics

2010 PSET 1 Problem 2
- General Problem Statement: Simulate Isothermal Titration Calorimetry (ITC) to control for immobilization artifacts of the SPR experiment from PSET 1-1
- Program used: Parts in MATLAB
- Utility: Conceptual parts good for recitation or exam review, applications in MATLAB can be included or not
- Broad topic: ITC, binding kinetics

2010 PSET 1 Problem 3
- General Problem Statement: Quantify the relation between a ligand and receptor using radioactive labeling and compare to SPR results
- Program used: Parts in MATLAB
- Utility: Good combination of concepts and using simple coding to understand the concepts
- Broad topic: Binding kinetics, SPR

2010 PSET 2 Problem 1
- General Problem Statement: Understand enzyme kinetics from the perspective of an engineer optimizing production or a headache drug
- Program used: MATLAB
- Utility: Using MATLAB to expand understanding
- Broad topic: Enzyme kinetics, QSSA

2010 PSET 2 Problem 2
- General Problem Statement: Analyze protein microarray data from the Jones et al paper with respect to EGFR family receptors
- Program used: MATLAB
- Utility: Teaches how to use coding to analyze data
- Broad topic: Protein microarrays

2010 PSET 2 Problem 3
- General Problem Statement: Yeast surface display is a new experiment (not discussed in class) that can be used to quantify protein-ligand interactions.
- Program used: Parts in MATLAB
- Utility: Great extension problem, recitation or exam question to extend on previous experiments to determining binding kinetics
- Broad topic: Binding kinetics, determining parameters

2010 PSET 3 Problem 1
- General Problem Statement: Understand enzyme inhibitors and differences between competitive, non-competitive, and uncompetitive inhibitors.
- Program used: Parts in MATLAB
- Utility: Great for recitation, exam review
- Broad topic: Enzyme inhibitors

2010 PSET 3 Problem 2
- General Problem Statement: Analyze the Huang-Ferrell model for the MAP kinase cascade both conceptually and by modulating their model.
- Program used: MATLAB (skeleton code provided)
- Utility: Implementing signaling cascades in MATLAB
- Broad topic: Kinase cascades

2010 PSET 3 Problem 3
- General Problem Statement: Understand the properties of a phosphorylation and dephosphorylation of cognate and non-cognate substrates of a particular kinase.
- Program used: MATLAB
- Utility: Some parts useful conceptually in recitation
- Broad topic: Modeling phosphorylation/dephosphorylation

2010 PSET 4 Problem 1
- General Problem Statement: Explore a system of EGFR receptor internalization in response to antibody treatment and the effects of antibody binding to surface receptor levels
- Program used: Parts in MATLAB
- Utility: Parts good for recitation or exam review (real-life application of concepts)
- Broad topic: Receptor endocytic trafficking

2010 PSET 4 Problem 2
- General Problem Statement: Analyze the Haugh paper discussed in class to understand the model
- Program used: None
- Utility: Deeper analysis of papers discussed in class
- Broad topic: Ligand effects, Haugh model

2010 PSET 4 Problem 3
- General Problem Statement: Analyze the effects of negative feedback in the MAPK model
- Program used: MATLAB (skeleton code provided)
- Utility: Pseudo-implementation
- Broad topic: MAPK pathway, negative feedback

2010 PSET 5 Problem 1
- General Problem Statement: Understand and generate feed forward loops (FFLs) in the context of glycolysis and gene circuit design
- Program used: None
- Utility: Understanding cell logic networks
- Broad topic: FFLs

2010 PSET 5 Problem 2
- General Problem Statement: Understand transcriptional regulation in the form of differential equations, be able to understand term contributions, and extend to different applications (siRNA)
- Program used: Parts in MATLAB (for plotting)
- Utility: good for recitation or exam review
- Broad topic: Transcriptional regulation

2010 PSET 5 Problem 3
- General Problem Statement: Understand properties of interlinked positive feedback loops with biological implications
- Program used: Parts in MATLAB
- Utility: understanding how to model feedback loops
- Broad topic: Transcriptional regulation, positive feedback

2010 PSET 6 Problem 1
- General Problem Statement: Analyze the properties of protein engineering scaffolds such as Ankyrin repeat protein, Affibody, and 10th Fibronectin domain 3.
- Program used: PyRosetta
- Utility: Intro to using PyRosetta for understanding protein structure
- Broad topic: Protein structure

2010 PSET 6 Problem 2
- General Problem Statement: Explore the conformational energy of two tri-peptides
- Program used: PyRosetta
- Utility: coding intro to conformation/energetics
- Broad topic: Protein structure/conformation

2010 PSET 6 Problem 3
- General Problem Statement: Use alanine scanning to understand the role of residues on hGH binding to its receptor
- Program used: None
- Utility: Great for recitation, exam review
- Broad topic: Protein structure

2010 PSET 6 Problem 4
- General Problem Statement: Understand protein folding and energetics in the context of p53 mutations in cancer that alter protein folding
- Program used: None
- Utility: Great for recitation, exam review
- Broad topic: Protein folding

2010 PSET 6 Problem 5
- General Problem Statement: Analyze a nonlinear biochemical circuit of a system with two transcription factors that mutually repress eachother.
- Program used: Parts in MATLAB
- Utility: Parts good for writing a model and learning mathematical representations
- Broad topic: ??

2010 PSET 7 Problem 1
- General Problem Statement: Use the Chou-Fasman algorithm to analyze secondary structure and mutations that can alter structure
- Program used: Python
- Utility: Good coding exercise to analyze mutation effects
- Broad topic: Predicting Structure

2010 PSET 7 Problem 2
- General Problem Statement: Analyze multiple sequence alignment in the EGFR family ligands
- Program used:
- Utility: good review problem
- Broad topic: Predicting structure, Specificity

2010 PSET 7 Problem 3
- General Problem Statement: Understand the sequence of Bone Morphogenic Protein-2.
- Program used: MATLAB or Python, PyMol may be helpful
- Utility: good practice problem
- Broad topic: Protein sequence, interactions

2011 PSET 1 Problem 1
- General Problem Statement: PyRosetta Tutorial
- Program used: PyRosetta
- Utility: Learning the new interface
- Broad topic: PyRosetta Tutorial

2011 PSET 1 Problem 2
- General Problem Statement: Understand the structure of P-Glycoprotein, a multidrug resistance transporter.
- Program used: PyRosetta
- Utility: Using the program to understand structure functio
- Broad topic: Protein structure

2011 PSET 1 Problem 3
- General Problem Statement: Calculate the folding energetics of Chymotrypsin Inhibitor 2 and multiple mutants
- Program used: None
- Utility: Great recitation problem, very basic
- Broad topic: Protein folding, energetics

2011 PSET 2 Problem 1
- General Problem Statement: Analyze experimental results of alanine scanning performed to evaluate the importance of resides involved in IL4 binding its receptor, IL4-BP.
- Program used: part in PyMol (visualization tool)
- Utility: Great for recitation and exam review
- Broad topic: Interaction energetics

2011 PSET 2 Problem 2
- General Problem Statement: Understand secondary structures by analyzing contact maps
- Program used: None
- Utility: Great for recitation and exam review
- Broad topic: Protein structure

2011 PSET 2 Problem 3
- General Problem Statement: Computationally simulate alanine scanning in a leucine zipper protein which is a dimer
- Program used: Python
- Utility: computational problem
- Broad topic: Interaction energetics

2011 PSET 2 Problem 4
- General Problem Statement: Use the Chou-Fasman algorithm to analyze secondary structure of sequences
- Program used: Python
- Utility: practice understanding the algorithm, computationally heavy
- Broad topic: Predicting structure

2011 PSET 2 Problem 5
- General Problem Statement: DNA sequence motif prediction of a transcription factor
- Program used: none
- Utility: good recitation or exam review (hand calculations)
- Broad topic: Protein specificity

2011 PSET 3 Problem 1
- General Problem Statement: Expand on material from a guest lecture on optimizing binding for bZIP using protein binding arrays
- Program used: none
- Utility: good review if topic is covered, basic
- Broad topic: Specificity

2011 PSET 3 Problem 2
- General Problem Statement: Use thermodynamic cycles and alanine scanning to understand GCSF interactions to inform drug design changes
- Program used: none
- Utility: Great for recitation or exam review
- Broad topic: Drug design

2011 PSET 3 Problem 3
- General Problem Statement: Use a minimization algorithm to identify low energy states for re-packing the side chains of the GCSF/GCSF complexes to form a rotor
- Program used: PyRosetta, PyMol
- Utility: coding heavy
- Broad topic: Protein design

2011 PSET 3 Problem 4
- General Problem Statement: Analyze multiple sequence alignment in the EGFR family ligands
- Program used:
- Utility: good review problem
- Broad topic: Predicting structure, Specificity

2011 PSET 4 Problem 1
- General Problem Statement: learn how to repeat a problem from homework 1 (generating a Ramachandran plot in PyRosetta) in MATLAB.
- Program used: MATLAB
- Utility: Learning to plot in MATLAB
- Broad topic: Practice in MATLAB

2011 PSET 4 Problem 2
- General Problem Statement: Analyze protein-ligand complex formation
- Program used: MATLAB
- Utility: learning to plot and curve fitting in MATLAB
- Broad topic: Practice in MATLAB

2011 PSET 4 Problem 3
- General Problem Statement: Plan Isothermal Titration Calorimetry (ITC) experiments to identify thermodynamic properties of a drug-substrate interaction
- Program used: none
- Utility: Great for recitation or exam review
- Broad topic: ITC

2011 PSET 5 Problem 1
- General Problem Statement: Derive and understand the concept of the Pseudo-first order approximation for protein-ligand binding
- Program used: none
- Utility: Great recitation or exam review problem
- Broad topic: Binding kinetics

2011 PSET 5 Problem 2
- General Problem Statement: Use ITC to understand binding kinetics and thermodynamic properties
- Program used: none
- Utility: Good recitation and exam review problem
- Broad topic: ITC

2011 PSET 5 Problem 3
- General Problem Statement: Understand dynamics of ODE systems of protein-ligand interactions prior to reaching equilibrium
- Program used: MATLAB
- Utility: Learning MATLAB ODE solvers
- Broad topic: ODE dynamics

2011 PSET 6 Problem 1
- General Problem Statement: Understand the dynamics of the TGFβ ligand and receptor system
- Program used: none
- Utility: Great exam review question
- Broad topic: Receptor ligand oligomer formation

2011 PSET 6 Problem 2
- General Problem Statement: Michaelis-Menton Kinetics and competitive inhibitors
- Program used: none
- Utility: Great recitation or exam review problem
- Broad topic: Enzyme kinetics, inhibitors

2011 PSET 6 Problem 3
- General Problem Statement: Analyze protein binding array data to extract kinetic parameters
- Program used: MATLAB
- Utility: Practice using MATLAB to analyze data
- Broad topic: Protein binding array, kinetic parameters

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