

# ALL LECTURES IN SB228

1. Introduction
2. Molecular Architecture I
3. Molecular Architecture II
4. Molecular Simulation I
5. Molecular Simulation II
6. Bioinformatics I
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## 1. Introduction

### 1.1. Principles of Biology

1. SB228 Lecture 1 Lecture1
2. Principles of Biology. Concept 1.1
3. Principles of Biology
4. The Cycle of Life
5. Structural Overview of Biology
6. Informatics Overview of Biology
7. Spontaneous Self-Organization
8. Energy Landscapes
9. What Drives Folding

### 1.2. Structure is Central

10. Structure is Central. Concept 1.2
11. Structure is Central
12. Cellular Cities
13. Membrane Dynamics
14. Enzymes Catalyze Reactions
15. The Core Machinery of Life
16. Drug Binding to Receptor
17. Fibrous Proteins in Disease

### 1.3. Protein Images

18. Protein Images. Concept 1.3
19. What Does a Protein Look Like
20. Protein in Water
21. See the Protein alone
22. See the Bonded atoms
23. Try to See the Main Chain 1
24. Try to See the Main Chain 2
25. Try to See the Main Chain 3
26. Try to See the Chain Path
27. For Function Show Surface

### 1.4. Fundamental interactions

28. Fundamental interactions. Concept 1.4
29. Fundamental interactions
30. What is an atom
31. What is a Molecule
32. Forces Between atoms
33. Total Potential Energy
34. Bond Stretching
35. Bond angle Bending
36. Bond Twisting
37. Van Der Waals interaction
38. Electrostatics interaction
39. Hydrogen Bonds 1
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41. Water Energy and Dipole
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### 1.5. Complex interactions

43. Complex interactions. Concept 1.5
44. Complex interactions
45. Moving Over Energy Surface
46. Simulating Crystals
47. Simulating Liquids
48. Liquids argon and Water
49. Solutions Urea
50. Solutions Methane
51. Hydrophobic Effect
52. Explaining Hydrophobicity
53. Explaining the Dielectric Effect
54. Energy and Springs 1
55. Energy and Springs 2
56. Strength of interactions

### 1.6. Useful tools

57. Useful tools. Concept 1.6
58. Useful tools
59. Web Searching Google
60. Web Searching Pubmed
61. Molecular Graphics 1
62. Basic Molecular Graphics
63. Molecular Graphics Rasmol
64. Molecular Graphics Pymol
65. Movie of Pymol Demonstration
66. Molecular Graphics Others
67. Capturing Pictures

<b>2. Molecular Architecture I</b>	
<b>2.1. Polypeptide Chain</b>	<b>2.2. Amino acids</b>
1. SB228 Lecture 2 Lecture2 2. Lecture 2 Contents 3. Polypeptide Chain. Concept 2.1 4. The Polypeptide Chain 5. Chemical Structure 6. The Peptide Group	7. Amino acids. Concept 2.2 8. Amino acids 9. Amino acid Side Chains 10. Amino acid Names 11. Amino acid Classification 1 12. Amino acids Gly and Pro 13. Amino acids Cys 14. Amino acids Leu and Phe 15. Amino acids Glu and arg 16. Amino acids Val and Ile 17. Amino acid Classification 2
<b>2.3. Degrees of Freedom</b>	<b>2.4. Reverse Turns</b>
18. Degrees of Freedom. Concept 2.3 19. Degrees of Freedom 20. Backbone Degrees of Freedom 21. Steric Clashes Limit Phi, Psi 22. Ramachandran Diagram 23. Different Backbone Conformations 24. Contour Plots 25. Phi, Psi Distributions a, G, P, N 26. Phi, Psi Distributions a, M, F, V 27. Side Chain Conformations	28. Reverse Turns. Concept 2.4 29. Reverse Turns 30. Beta Turns 31. Virtual Bonds 32. Beta Turn Types
<b>2.5. The alpha Helix</b>	<b>2.6. The Beta Sheet</b>
33. The alpha Helix. Concept 2.5 34. The alpha-Helix 35. Proteins Have Helices 36. The alpha Heli 37. The Helix Surface 38. Helix Surface Ridges 39. Helix Ridge Lines 40. Different Possible Helices 41. 310 Explained 42. Alpha-Helix Dipole 1 43. Alpha-Helix Dipole 2	44. The Beta Sheet. Concept 2.6 45. Beta Sheets 46. Proteins Have Strands 47. The Beta Strand 48. Beta Sheet 49. Beta Sheets are Solid 50. Beta-Sheet Sidedness 51. Real Sheets are Twisted 1 52. Real Sheets are Twisted 2 53. The Beta Hairpin

## 3. Molecular Architecture II

<b>3.1. Helix-Helix Packing</b>		<b>3.2. Helix-Sheet Packing</b>	
<ol style="list-style-type: none"> <li>1. SB228 Lecture 3 Lecture3</li> <li>2. Lecture 3 Contents</li> <li>3. Helix-Helix Packing. Concept 3.1</li> <li>4. Helix-Helix-Packing</li> <li>5. Pairs of alpha-Helices</li> <li>6. Helix Ridge Lines</li> <li>7. Common Helix Packings</li> <li>8. Helix Packing Omega 140 -40</li> <li>9. Helix Packing Omega 20 -160</li> <li>10. Common Helix Packings Revisited</li> </ol>		<ol style="list-style-type: none"> <li>11. Helix-Sheet Packing. Concept 3.2</li> <li>12. Helix-Sheet-Packing</li> <li>13. Alpha-Helix and Beta-Sheet</li> <li>14. Common Helix-Strand Packings</li> <li>15. Pair of Beta-Sheets</li> <li>16. Common Strand Strand Packings</li> </ol>	
<b>3.3. Architectural Principles</b>		<b>3.4. Folding Unit Classification</b>	
<ol style="list-style-type: none"> <li>17. Architectural Principles. Concept 3.3</li> <li>18. Architectural Principles</li> <li>19. Close Packing in Proteins</li> <li>20. Hydrogen Bonding in Proteins</li> <li>21. Buried Waters in Proteins</li> <li>22. Cavities in Proteins</li> <li>23. Domains in Proteins 1</li> <li>24. Domains in Proteins 2</li> <li>25. Contact Order</li> </ol>		<ol style="list-style-type: none"> <li>26. Folding Unit Classification. Concept 3.4</li> <li>27. Folding Unit Classification</li> <li>28. Folding Units</li> <li>29. All-Alpha Proteins 1</li> <li>30. All-Alpha Proteins 2</li> <li>31. All-Beta Proteins 1</li> <li>32. All-Beta Proteins 2</li> <li>33. Alpha Beta Proteins 1</li> <li>34. Alpha Beta Proteins 2</li> <li>35. Alpha Beta Proteins 3</li> <li>36. Explain Beta-Barrel</li> <li>37. Bab Chirality</li> <li>38. Bab Chirality Why</li> <li>39. Alpha Plus Beta Proteins</li> </ol>	
<b>3.5. Sample Folds</b>		<b>3.6. Classification Databases</b>	
<ol style="list-style-type: none"> <li>40. Sample Folds. Concept 3.5</li> <li>41. Some Examples</li> <li>42. Small Proteins</li> <li>43. Coiled-Coil Proteins</li> <li>44. Membrane Proteins</li> <li>45. Simple all-Alpha Fold</li> <li>46. All-Beta with Long Beta-Hairpins</li> <li>47. Antiparallel all-Beta Fold</li> <li>48. Parallel all-Beta Fold</li> <li>49. Simple alpha Beta Fold</li> </ol>		<ol style="list-style-type: none"> <li>50. Classification Databases. Concept 3.6</li> <li>51. Classification Databases</li> <li>52. Cath</li> <li>53. Cath Mainly alpha</li> <li>54. Cath Mainly Beta</li> <li>55. Cath Mixed alpha-Beta</li> <li>56. Cath Few Secondary Structures</li> <li>57. Cath Drill Down to a Level</li> <li>58. Cath Drill Down to H Level</li> <li>59. Cath Hierarchy</li> <li>60. Cath the Numbers</li> <li>61. Other Databases Scop</li> <li>62. Other Databases Dali 1</li> <li>63. Other Databases Dali 2</li> <li>64. Comparing Cath Scop Dali</li> </ol>	

## 4. Molecular Simulation I

4.1. Underlying Principles		4.2. Simulation Methods	
<ol style="list-style-type: none"> <li>1. SB228 Lecture 4 Lecture4</li> <li>2. Lecture 4 Contents</li> <li>3. Underlying Principles. Concept 4.1</li> <li>4. Underlying Principles</li> <li>5. Boltzmanns Distribution</li> <li>6. Entropy and Free Energy1</li> <li>7. Absolute Probabilities</li> <li>8. Dynamic Properties</li> <li>9. Types of Motion</li> <li>10. Crossing Energy Barriers</li> <li>11. Rates of Motion</li> </ol>		<ol style="list-style-type: none"> <li>12. Simulation Methods. Concept 4.2</li> <li>13. Simulation Methods</li> <li>14. Moving Over Energy Surface</li> <li>15. Reaction Coordinates</li> <li>16. Protein Folding Landscape</li> <li>17. Levinthals Paradox</li> <li>18. Resolve Paradox</li> <li>19. Simple Energy Minimization</li> <li>20. Convergent Energy Minimization</li> <li>21. Monte Carlo Methods</li> <li>22. Simulated annealing</li> </ol>	
4.3. Molecular Dynamics		4.4. Simulating Solutions	
<ol style="list-style-type: none"> <li>23. Molecular Dynamics. Concept 4.3</li> <li>24. Molecular Dynamics</li> <li>25. Molecular Potential Energy</li> <li>26. Molecular Dynamics theory</li> <li>27. Molecular Dynamics Procedure</li> <li>28. Molecular Dynamics Procedure 1</li> <li>29. Molecular Dynamics Procedure 2</li> <li>30. Molecular Dynamics Procedure 3</li> <li>31. Units in Force Fields</li> </ol>		<ol style="list-style-type: none"> <li>32. Simulating Solutions. Concept 4.4</li> <li>33. Simulating Liquids.</li> <li>34. Water is a Very Simple Molecule</li> <li>35. Simulating Liquids</li> <li>36. Liquids argon and Water</li> <li>37. Pure Water Dynamics</li> <li>38. Properties of Liquid Water</li> <li>39. Hydrophobic Effect</li> <li>40. Simulating Hydrophobic Effect</li> <li>41. Voronoi Decomposition</li> <li>42. Voronoi analysis of Contacts</li> <li>43. Hydrophobic Clusters Cross Box</li> <li>44. Methane Solution Dynamics</li> <li>45. Butane Solution Dynamics</li> <li>46. Benzene Solution Dynamics</li> <li>47. Hydrophobic Energy and Contact Surface</li> <li>48. Hydrophobic Solutes Perturb Water Density</li> <li>49. Large Density Changes</li> </ol>	
4.5. Simulating alpha-Helix		4.6. Simulating Folded Protein	
<ol style="list-style-type: none"> <li>50. Simulating alpha-Helix. Concept 4.5</li> <li>51. Dynamics of the alpha-Helix</li> <li>52. Alpha-Helix Dynamics</li> <li>53. Water allows Hydrogen Bonds to Break</li> </ol>		<ol style="list-style-type: none"> <li>54. Simulating Folded Protein. Concept 4.6</li> <li>55. Dynamics of Folded Protein</li> <li>56. Protein in Water1</li> <li>57. Protein Dynamics</li> <li>58. RMS Deviation from X-Ray</li> <li>59. Hydrogen Bond Stability</li> <li>60. Four Classes of Water Molecules</li> <li>61. Density of Surface Water</li> <li>62. Orientation of Surface Water</li> <li>63. Properties of Water Molecules</li> </ol>	
4.7. History of Simulation			
<ol style="list-style-type: none"> <li>64. History of Simulation. Concept 4.7</li> <li>65. Los alamos 1943-45</li> <li>66. Levinthal 1966</li> <li>67. Levinthal Movies</li> <li>68. 50 Years of Simulation</li> </ol>			

## 5. Molecular Simulation II

<b>5.1. Normal Mode theory</b>		<b>5.2. Protein Normal Modes</b>	
<ol style="list-style-type: none"> <li>1. SB228 Lecture 5 Lecture5</li> <li>2. Molecular Simulation II</li> <li>3. Normal Mode theory. Concept 5.1</li> <li>4. Normal Mode Dynamics</li> <li>5. Basic theory</li> <li>6. Normal Modes in High Dimensions1</li> <li>7. Normal Modes in High Dimensions2</li> <li>8. Normal Modes in High Dimensions3</li> <li>9. Molecular Potential Energy</li> <li>10. Potential Energy in torsion Space</li> <li>11. Theory of Normal Modes I</li> <li>12. Theory of Normal Modes II</li> </ol>		<ol style="list-style-type: none"> <li>13. Protein Normal Modes. Concept 5.2</li> <li>14. Rates of Vibration</li> <li>15. Amplitudes of Vibration</li> <li>16. Trypsin inhibitor Modes</li> <li>17. BPTI Normal Modes Movie</li> <li>18. Lysozyme Modes</li> <li>19. Lysozyme Normal Modes Movie</li> <li>20. Ribonuclease Modes</li> <li>21. Ribonuclease Normal Modes Movie</li> </ol>	
<b>5.3. Unfolding alpha Helix</b>		<b>5.4. Unfolding Proteins</b>	
<ol style="list-style-type: none"> <li>22. Unfolding alpha Helix. Concept 5.3</li> <li>23. Alpha-Helix Unfolding</li> <li>24. Why Simulate Unfolding</li> <li>25. Unfold alpha-Helix</li> <li>26. Effect of Temperature</li> <li>27. Helix Less Stable in Water</li> <li>28. Water allows Hydrogen Bonds to Break</li> <li>29. Helix Unfolding Movie</li> <li>30. Distributions in Solution</li> </ol>		<ol style="list-style-type: none"> <li>31. Unfolding Proteins. Concept 5.4</li> <li>32. Protein Unfolding</li> <li>33. What Happens to Secondary Structure</li> <li>34. Protein Unfolding1 Movie</li> <li>35. What Happens to aromatic Sidechains</li> <li>36. Protein Unfolding2 Movie</li> <li>37. Unfolding Pathway</li> <li>38. Connection to Experiment1</li> <li>39. Connection to Experiment2</li> <li>40. Connection to Experiment3</li> </ol>	
<b>5.5. Folding Simplified Chains</b>		<b>5.6. Folding Simulations</b>	
<ol style="list-style-type: none"> <li>41. Folding Simplified Chains. Concept 5.5</li> <li>42. Fold Simplified Proteins</li> <li>43. Why is Folding So Difficult</li> <li>44. Simplified Models for Folding1</li> <li>45. Virtual Bonds</li> <li>46. Simplified Models for Folding2</li> <li>47. Cartoon Folding Movie</li> <li>48. 3x3x3 Cube Protein Folding</li> <li>49. Lattice Model of Folding</li> </ol>		<ol style="list-style-type: none"> <li>50. Folding Simulations. Concept 5.6</li> <li>51. Folding Simulations</li> <li>52. Need Massive Computational Resources</li> <li>53. Villin Folding</li> <li>54. IBM Blue Gene Project</li> <li>55. IBM Blue Gene Design</li> <li>56. Folding at Home</li> <li>57. Folding at Home Helix Folding</li> <li>58. Pande Helix Folding Movie</li> <li>59. Pande Villin Folding Movie</li> <li>60. Folding at Home Rates</li> </ol>	

## 6. Bioinformatics I

<b>6.1. Data in Biology</b>		<b>6.2. Statistics of Comparison</b>	
<ol style="list-style-type: none"> <li>1. SB228 Lecture 6 Lecture6</li> <li>2. Bioinformatics I</li> <li>3. Data in Biology. Concept 6.1</li> <li>4. Data in Biology</li> <li>5. Strings</li> <li>6. Human Genome</li> <li>7. Relationships</li> <li>8. Multiple Sequence alignments</li> <li>9. 3-D Data</li> <li>10. Sequence Objects</li> <li>11. Structure Objects</li> </ol>		<ol style="list-style-type: none"> <li>12. Statistics of Comparison. Concept 6.2</li> <li>13. Statistics is Important in Bioinformatics</li> <li>14. Mean</li> <li>15. Standard Deviation</li> <li>16. Uniform Distribution</li> <li>17. Binomial Distribution</li> <li>18. Normal Distribution</li> <li>19. Extreme Value Distributions</li> <li>20. Expectation Values1</li> <li>21. Expectation Values2</li> </ol>	
<b>6.3. Data Visualization</b>		<b>6.4. Databases</b>	
<ol style="list-style-type: none"> <li>22. Data Visualization. Concept 6.3</li> <li>23. Data Visualization</li> <li>24. Intuitive Clustering</li> <li>25. Hierarchical Clustering</li> <li>26. K-Means Clustering</li> <li>27. Roc analysis</li> <li>28. True or False</li> <li>29. Roc Curve Examples</li> <li>30. Views of Structure Space1</li> <li>31. Views of Structure Space2</li> </ol>		<ol style="list-style-type: none"> <li>32. Databases. Concept 6.4</li> <li>33. Databases</li> <li>34. Protein Database RCSB</li> <li>35. Protein Database PDBLITE</li> <li>36. RNA Structure Database</li> <li>37. Membrane Protein Data Base</li> <li>38. Organic Molecule Structures</li> <li>39. Small Molecule Database</li> <li>40. Pathway Databases1</li> <li>41. Pathway Databases2</li> </ol>	
<b>6.5. Web Resources</b>		<b>6.6. Sequence Comparison</b>	
<ol style="list-style-type: none"> <li>42. Web Resources. Concept 6.5</li> <li>43. Web Resources</li> <li>44. Ensembl EBI Sanger Genome Viewer1</li> <li>45. Ensembl EBI Sanger Genome Viewer2</li> <li>46. NCBI Genome Viewer1</li> <li>47. NCBI Genome Viewer2</li> <li>48. NCBI is the Place for Sequence</li> <li>49. EBI is the Place for tools</li> </ol>		<ol style="list-style-type: none"> <li>50. Sequence Comparison. Concept 6.6</li> <li>51. Sequence Comparison</li> <li>52. Identical Comparison</li> <li>53. Identical Trace</li> <li>54. Mismatch Comparison</li> <li>55. Mismatch Trace2</li> <li>56. Deletion Comparison</li> <li>57. Deletion Trace</li> <li>58. Deletion-Insertion Comparison</li> <li>59. Deletion-Insertion Trace</li> <li>60. Scoring Matrix</li> <li>61. Gap Penalties</li> <li>62. Dynamic Programming</li> <li>63. Dynamic Programming1</li> <li>64. Dynamic Programming2</li> <li>65. Advanced Methods</li> <li>66. FASTA</li> <li>67. Blast and Psi-Blast</li> <li>68. Blast Compare Sequences</li> </ol>	

## 7. Bioinformatics II

7.1. Structure Comparison		7.2. Structure and Sequence	
<ol style="list-style-type: none"> <li>1. SB228 Lecture 7 Lecture7</li> <li>2. Bioinformatics II</li> <li>3. Structure Comparison. Concept 7.1</li> <li>4. Structure Comparison</li> <li>5. Structure Superposition</li> <li>6. Simple Structural alignment</li> <li>7. Distance and Similarity</li> <li>8. Structural in action</li> <li>9. Structural alignment</li> <li>10. Protein Structure Similarity Measures</li> </ol>		<ol style="list-style-type: none"> <li>11. Structure and Sequence. Concept 7.2</li> <li>12. Comparing Sequence-Structure Comparison</li> <li>13. Sequence Score Distribution1</li> <li>14. Sequence Score Distribution2</li> <li>15. Sequence Score Distribution3</li> <li>16. Sequence Score is Extreme Value Distribution</li> <li>17. Structure Score Distribution1</li> <li>18. Structure Score Distribution2</li> <li>19. Structure Score Distribution3</li> <li>20. Structure Score Follows Extreme Value</li> <li>21. Statistical Significance</li> <li>22. Similarity Measures</li> </ol>	
7.3. Structural Genomics		7.4. Expression Patterns	
<ol style="list-style-type: none"> <li>23. Structural Genomics. Concept 7.3</li> <li>24. Structural Genomics Project</li> <li>25. What Can One Do With Structural Genomics</li> <li>26. Structural Genomics and Modeling</li> <li>27. Expectations From Structural Genomics</li> <li>28. JCSG Center</li> <li>29. BSGC Center</li> <li>30. MCSG Center</li> <li>31. NYSG Center</li> <li>32. TBSG Center</li> <li>33. Structural Genomics Output</li> </ol>		<ol style="list-style-type: none"> <li>34. Expression Patterns. Concept 7.4</li> <li>35. Microarray Basics1</li> <li>36. Oligo DNA Microarrays</li> <li>37. cDNA Expression arrays</li> <li>38. More Expression array Cartoons</li> <li>39. Scientific american Explains1</li> <li>40. Scientific american Explains2</li> <li>41. Cleaning Up Oligo Chips1</li> <li>42. Noisy Background</li> </ol>	
7.5. Discovering Drugs		7.6. Diagnosing Disease	
<ol style="list-style-type: none"> <li>43. Discovering Drugs. Concept 7.5</li> <li>44. Drug Binding</li> <li>45. Structure Based Drug Design</li> <li>46. Drug Docking</li> <li>47. Autodock</li> <li>48. Autodock Movies1</li> <li>49. Benzamidine Trypsin.mov</li> <li>50. Autodock Movies2</li> <li>51. Biotin Streptavidin.mov</li> <li>52. Drugs from Sequence</li> </ol>		<ol style="list-style-type: none"> <li>53. Diagnosing Disease. Concept 7.6</li> <li>54. Pharmacogenomics</li> <li>55. Protein 2-D Gels</li> <li>56. Expression array Diagnosis1</li> <li>57. Expression array Diagnosis2</li> </ol>	

## 8. Prediction I

<b>8.1. Why Predict Structure</b>		<b>8.2. Knowledge-Based Physics</b>	
<ol style="list-style-type: none"> <li>1. SB228 Lecture 8 Lecture8</li> <li>2. Structure Prediction I</li> <li>3. Why Predict Structure. Concept 8.1</li> <li>4. Human Genome</li> <li>5. Half of Proteins Are Novel</li> <li>6. Is There a Finite Number of Folds</li> <li>7. Chothias 1,000 Fold Hypothesis1</li> <li>8. Chothias 1,000 Fold Hypothesis2</li> </ol>	<ol style="list-style-type: none"> <li>9. Knowledge-Based Physics. Concept 8.2</li> <li>10. Knowledge-Based Physics</li> <li>11. Knowledge-Based Energies1</li> <li>12. Environmental Energies</li> <li>13. Pair-Wise Energies</li> <li>14. Knowledge-Based Geometry</li> <li>15. Fragment Libraries</li> <li>16. Fit and Complexity</li> <li>17. Knowledge-Based Simulation</li> </ol>		
<b>8.3. CASP</b>		<b>8.4. Predict Secondary Structure</b>	
<ol style="list-style-type: none"> <li>18. CASP. Concept 8.3</li> <li>19. What is CASP</li> <li>20. CASP Targets</li> <li>21. The CASP Process</li> <li>22. CASP Statistics</li> <li>23. Hubbard Plots</li> <li>24. GDT-TT Score</li> <li>25. Assessment</li> <li>26. CASP2 Experiences</li> <li>27. Simple Z-Score Sum</li> <li>28. Which Targets are Which</li> </ol>	<ol style="list-style-type: none"> <li>29. Predict Secondary Structure. Concept 8.4</li> <li>30. Predict Secondary Structure</li> <li>31. Predicting Secondary Structure</li> <li>32. Secondary Structure States</li> <li>33. Early History2</li> <li>34. Chou-Fasman Secondary Structure</li> <li>35. Early Blind Experiment</li> <li>36. Statistical Preferences</li> <li>37. Amino Acid Classification</li> <li>38. Elementary Neural Network</li> <li>39. Training a Neural Network</li> <li>40. Sequence Profile</li> <li>41. Rost 1993 Neural Network</li> <li>42. Jones 1999 Neural Network</li> <li>43. Secondary Structure Prediction Quality</li> <li>44. Historical Record of Best Predictions At CASP</li> </ol>		
<b>8.5. Sidechain Prediction</b>		<b>8.6. Homology Modeling</b>	
<ol style="list-style-type: none"> <li>45. Sidechain Prediction. Concept 8.5</li> <li>46. Side Chain Modeling</li> <li>47. Basic Idea1</li> <li>48. Basic Idea2</li> <li>49. Basic Idea3</li> <li>50. Simulated Annealing</li> <li>51. Segment Match Modeling</li> <li>52. Mean Field1</li> <li>53. Mean Field2</li> <li>54. Generalized Self-Consistent Mean-Field1</li> <li>55. Generalized Self-Consistent Mean-Field2</li> <li>56. Some Other Methods</li> </ol>	<ol style="list-style-type: none"> <li>57. Homology Modeling. Concept 8.6</li> <li>58. What is Homology Modeling</li> <li>59. Loop Methods Are Varied</li> <li>60. A Multiple Sequence Alignment</li> <li>61. Fssp Structural Alignments2</li> <li>62. Servers and Meta Servers</li> <li>63. Comparative Modeling Servers and Creators</li> <li>64. Meta Servers Are Winners</li> </ol>		

## 9. Prediction II

9.1. Fold Recognition		9.2. Fold Recognition at CASP	
<ol style="list-style-type: none"> <li>1. SB228 Lecture 9 Lecture9</li> <li>2. Structure Prediction II</li> <li>3. Fold Recognition. Concept 9.1</li> <li>4. Fold Recognition</li> <li>5. Comparative Modeling vs Threading</li> <li>6. Threading Covers More of Protein Space</li> <li>7. What is Fold Recognition</li> <li>8. What is Threading</li> <li>9. Simple Example</li> <li>10. A Different Threading</li> <li>11. Gaps in Threading</li> <li>12. Frozen approximation</li> <li>13. Use a Sequence Profile</li> <li>14. Profile Matching1</li> <li>15. Profile Matching2</li> <li>16. Deletions Using Structure</li> <li>17. Insertions Using Structure</li> <li>18. Getting Good alignments Summary</li> </ol>		<ol style="list-style-type: none"> <li>19. Fold Recognition at CASP. Concept 9.2</li> <li>20. Fold Recognition at CASP</li> <li>21. CASP4 Threading Servers and Creators</li> <li>22. Fold Recognition Meta Servers are Winners</li> </ol>	
9.3. Progress at CASP		9.4. Early ab initio Prediction	
<ol style="list-style-type: none"> <li>23. Progress at CASP. Concept 9.3</li> <li>24. Progress at CASP</li> <li>25. Explanation of Scoring index</li> <li>26. Best Results at CASP1 to CASP4</li> <li>27. Measuring Target Difficulty</li> <li>28. CASP Progress</li> </ol>		<ol style="list-style-type: none"> <li>29. Early ab initio Prediction. Concept 9.4</li> <li>30. Ab initio Early History</li> <li>31. Early History</li> <li>32. Coordinate and Distance Deviation</li> <li>33. Folding as a Random Walk</li> <li>34. Wide Distribution of Folds</li> <li>35. Very Simple Lattice Model</li> <li>36. Potential Energy in torsion Space0</li> <li>37. Folding With Restraints1</li> <li>38. Folding With Restraints2</li> <li>39. Diversity of Folds</li> </ol>	
9.5. Modern New Fold Prediction		9.6. Winning NF Methods at CASP	
<ol style="list-style-type: none"> <li>40. Modern New Fold Prediction. Concept 9.5</li> <li>41. Modern New Fold Prediction</li> <li>42. A Paradigm for Predicting Structure</li> <li>43. Energy Vs Rms Cartoons</li> <li>44. Energy Vs Rms Reality</li> <li>45. Energy Vs Rms</li> <li>46. Hierarchical Structure Prediction</li> <li>47. Getting an average Model</li> <li>48. Hierarchical Prediction Does Well</li> <li>49. Folding Energy Functions</li> <li>50. Potential Energy in torsion Space</li> <li>51. Energy Minimization Folds the Chain</li> <li>52. Cooperative Hydrophobic Packing</li> <li>53. Cooperative Hydrogen Bonds1</li> <li>54. Cooperative Hydrogen Bonds2</li> <li>55. Minimization Gives Good Folds</li> </ol>		<ol style="list-style-type: none"> <li>56. Winning NF Methods at CASP. Concept 9.6</li> <li>57. CASP4 New Fold Winners</li> <li>58. Winning NF Methods at CASP4</li> <li>59. Segment Exchange Monte Carlo</li> <li>60. Fragment insertion Monte Carlo</li> <li>61. New Potential Improves Recognition</li> <li>62. Lattice Monte Carlo</li> <li>63. Complicated Lattice</li> <li>64. Structure Prediction by Minimization</li> <li>65. All-Beta Prediction Success</li> <li>66. Segment Folding Monte Carlo</li> <li>67. Segment Folding Prediction</li> <li>68. CASP5 New Fold Winners</li> <li>69. Winning NF Methods at CASP5</li> <li>70. Baker at CASP51</li> <li>71. Baker at CASP52</li> <li>72. Shortle at CASP5</li> <li>73. CASP5 Lessons</li> <li>74. CASP Summary</li> </ol>	