# Biomolecular Modeling (G25.2601–001)

## SYLLABUS

<table>
<thead>
<tr>
<th>Week/s</th>
<th>Topics</th>
<th>Reading</th>
<th>Homework</th>
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<tr>
<td>1–2</td>
<td><strong>Panoramic view into 21st century biology:</strong> The genomics revolution and the rise of computational biology</td>
<td>Chaps. 1, 2, articles 1–4; [1: Molecular modeling and visualization with VMD]</td>
<td>[Modeling assignment]</td>
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<td>3</td>
<td><strong>Introduction to molecular modeling and simulation:</strong> problems, challenges, and approaches</td>
<td>Chaps. 3, 4, articles 8, 20, 21; [2: Sequence and structure databases, intro. to modeling (book asst. 1)]</td>
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<td>4</td>
<td><strong>Continued Introduction to molecular modeling and simulation:</strong> challenges and approaches as exemplified by four types of problems: protein folding, nucleic-acid/protein interactions, chromatin folding, and RNA folding</td>
<td>Chaps. 5, 6, articles 9, 18, 24; [3: Intro. to PDB and structure manipulation (book asst. 2)]</td>
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<td>5</td>
<td><strong>Basic protein structure</strong></td>
<td>Chap. 7, article 26; [4: Pentapeptide (met-enkephalin) structure analysis (book asst. 3)]</td>
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<td>6</td>
<td><strong>Nucleic acid structure, basic and advanced topics:</strong> DNA structure variability, sequence effects, and higher-order structures; RNA structure and function</td>
<td>Chap. 8, 9; [5: Creating Ramachandran plots (book asst. 4) and 6: Protein/DNA complexes (book asst. 5)]</td>
<td>[4: Term Project: Successes and failures of molecular modeling (book asst. 9, due end of term)]</td>
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<td><strong>Spring Break</strong></td>
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<td>7</td>
<td><strong>Introduction to quantum and molecular mechanics</strong></td>
<td>Chap. 10; [7: Homology contest (book asst. 6)]</td>
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<td>8–9</td>
<td><strong>Biomolecular force fields</strong>&lt;br&gt;Nonbonded computations</td>
<td>Chap. 11; [8: Nonbonded computations (book asst. 8)]</td>
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<td>10</td>
<td><strong>Field perspective:</strong> molecular modeling and simulation, a field coming of age</td>
<td>Chap. 12, article 29; [9, first half: Article discussion assignment on Schlick et al. (2010)]</td>
<td>[9: second half: Article discussion assignment on Shaw et al. (2010)] [12: Monte Carlo simulations (book asst. 12)]</td>
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<td>11</td>
<td><strong>Class discussion on Schlick et al. (2010); Begin Minimization Methods</strong></td>
<td>Chap. 13; [10: Molecular geometry (biphenyl) optimization (book asst. 10)]</td>
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<td>12</td>
<td><strong>Complete Minimization methods; Monte Carlo methods</strong></td>
<td>article 33; [11: Global optimization contest (book asst. 11)]</td>
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<td>13–14</td>
<td><strong>Molecular dynamics methods</strong></td>
<td>articles 5, 7, 10, 16, 19, 22; [9, second half: Article discussion assignment on Shaw et al. (2010)] [12: Monte Carlo simulations (book asst. 12)]</td>
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<td>15</td>
<td><strong>Class discussion/debate on Shaw et al. (2010)</strong></td>
<td>[13: Protein dynamics with NAMD]</td>
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**Textbook**


**Other Reference Books**


**Article Reading list**

**General Perspective Articles on the Biology and Modeling**


**General Review Articles on Modeling**


**Specific / Advanced Topics**

**Homology Modeling**


**Membranes Simulations**


**Computational Aided Drug Design**


**Implicit Solvent Modeling**


**Monte Carlo Simulations**


**Multiscale modeling**