### IV Year M.Tech (Int) Biotechnology Sem-VI

**Subject:** Introduction to Molecular modelling and Chemoinformatics  
**Course Code:** BI-605  
**Faculty:** Dr.K.V.Swamy

<table>
<thead>
<tr>
<th>Unit</th>
<th>Topics</th>
<th>No Of Lectures</th>
<th>Lecture Serial No</th>
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</table>
| **Unit-1**  
Introduction to molecular graphics  
- Different coordinate systems  
- Basic principle of molecular graphics and structure visualization.  
- Different molecular graphics packages  
- Protein Data Bank.  
| -2 | 2 |
| **Unit-2**  
Building of small molecules  
- Methods used in building small molecules using crystal, cartesian, polar and chemical internal coordinates  
- Building of Biopolymers DNA oligopeptides in different secondary structure  
| -2 | -10 |
| **Unit-3**  
Optimization of geometries of small molecules  
- Energy minimization by systematic search Method  
- Plotting conformation energy contours (Ramachandran plot), and finding out minimum energy conformation  
- Gradient based Energy minimization  
- Molecular mechanics approach  
- Molecular Dynamics method  
- Monte Carlo method  
- Genetic algorithm  
| -2 | -24 |
| **Unit-4**  
Use of Quantum chemical methods for geometry optimization  
- Schrödinger equation  
- Basic Formalism in quantum mechanics  
- Schrödinger equation for a multi- electron atom  
- Schrödinger equation for a molecule  
- Hartree- Fock Method  
- Different MO methods  
- Molecular electrostatic potential  
- Optimization of geometries of small molecules  
- Quantum chemical indices  
| -3 | -33 |

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**L T P Hr C:** 3 0 4 7 5

Mail : info.biotech@dpu.edu.in, Website: biotech.dpu.edu.in.
Books recommended:

1) Molecular modeling: Principles and applications by Andrew Leach, publisher- Prentice Hall 2001
2) Molecular Modeling, Holtje and Folkers G Weinheim New York

Evaluation scheme

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<thead>
<tr>
<th>S. No</th>
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<tr>
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