

**Post Graduate Diploma in Chemoinformatics**  
**Annual Examinations – 2006**

**Paper: PGDC – 106**  
**Computational Chemistry**

Time allowed: Three hours

Maximum Marks: 80

**SECTION – I**

Marks

Q1. Answer all the objective type questions given below:

1X20=20

- i) Molecular dynamics is based on \_\_\_\_\_ algorithm.
- ii) The equation for Lennard –Jones Potential is \_\_\_\_\_.
- iii) Proteins are made up from \_\_\_\_\_.
- iv) STO and GTO stands for \_\_\_\_\_.
- v) The force field (Potential) describes the \_\_\_\_\_ ~~between the atoms.~~
- vi) In Ultra Violet ~~photo electron spectroscopy~~ the source of radiation is \_\_\_\_\_.
- vii) Counter ions like  $Mg^{2+}$  interact with macro ions by \_\_\_\_\_ interaction.
- viii) Insight II is a program used for \_\_\_\_\_.
- ix) The non bonded energy of a molecule represents \_\_\_\_\_.
- x) Conformational searching involves \_\_\_\_\_ parts.
- xi) SHAKE is a method to realize \_\_\_\_\_.
- xii) G N Ramachandran plot is used to describe \_\_\_\_\_.
- xiii)  $\Delta G_{solv} = \Delta G_{ele} + \underline{\hspace{1cm}} + \underline{\hspace{1cm}} + \underline{\hspace{1cm}} + \underline{\hspace{1cm}} + \Delta G_{others}$
- xiv) In  $\alpha$ -helix of proteins the structure repeats itself every \_\_\_\_\_  $\text{\AA}^0$  along the helix axis.
- xv) In Homology modeling, loop building of proteins only adds \_\_\_\_\_ atoms.
- xvi) SCRF model describes solvent as a continuum of \_\_\_\_\_.
- xvii) 3D structure of biomolecules can be viewed by using \_\_\_\_\_.
- xviii) In potential energy surface concept the total molecular wave function is \_\_\_\_\_.
- xix) The stretching energy of a molecule is based on \_\_\_\_\_.
- xx) Two software packages used for energy minimization are \_\_\_\_\_ and \_\_\_\_\_.

**SECTION – II**

Answer any six questions. All questions carry equal marks.

5X6=30

1. Explain with examples Inter and Intra molecular interactions.
2. Conformational searching can be done manually. Describe the procedure giving examples.

3. Discuss the basis of Quantum theory and its boundary conditions.
4. What are the basic sets, how were they developed, how do you select basic set for energy minimization of a molecule.
5. Give in detail the two models of Continuum solvation.
6. Compare Monte Carlo Simulation with Brownian Dynamic Simulation.
7. What type of information is required to build a molecule manually? Explain with examples.
8. How will you perform comparative protein structure modeling by MODELLAR?

### SECTION – III

Answer any three questions. All questions carry equal marks.

10X3=30

1. Force field parameters are important aspects of Molecular Mechanics. Explain in detail with examples.
2. Give a detailed account of energy minimization process. Discuss in brief software used for it.
3. Various techniques have been used to simulate the structure and dynamics of bio molecules. Support the statement by describing various explicit simulation methods.
4. Homology modeling is the best alternative when the structure of protein cannot be solved by X- ray diffraction or NMR techniques. Explain all the steps involved in support of the above statement.