[A-3]COURSE SYLLABUS

1. Course Description (Approximately 100 words)

This course deals with quantum mechanical calculations for molecular structures. . Ab initio methods are introduced at the Hartree Fock level and extensions at higher levels of are outlined through explicit examples. The further extensions of these calculations in explicit solvent models is considered next. Calculations of molecular frequencies, thermodynamic functions and NMR frequencies is also outlined. Methods employed in geometry optimization and computations of transition states is also described.

2. Course Goals and Objectives (Approximately 100 words)

By the end of the course the students should be able to:

Invent computer methods to predict the three-dimensional folded structure of a protein—and the pathway by which folding occurs—from its amino acid sequence, so information from the human genome can be translated into the encoded protein structures.

Devise experimental tests to establish the reliability of new theoretical treatments.

Invent new computer tools and logistics methods to reduce significantly the time needed for commercializing new drugs.

3. Textbook (Title, Author, Publisher, Year of Publication, etc.)

Introductory books on quantum chemistry, statistical mechanics and computer programming fundamentals.

4. Reference

Introductory books on quantum chemistry, statistical mechanics and computer programming fundamentals.

5. Course Requirements and Grades

CAT 30%
EXAM 70%

6. Course Calendar

Week	Main Content
1	Ab initio methods –I (Hartree Fock), Ab initio methods - II (Post Hartree Fock
2	Density functional methods, Softwares for quantum mechanical calculations
3	Different forms of inputs for Ab initio calculations, Computation of single poir
4	Geometry optimization
5	Electron densities and electrostatic potentials
6	Analysis of output for Gausian programmes – I
7	Analysis of output for Gausian programmes – II
8	Molecular frequencies
9	Modeling in solutions - I
10	Modeling in solutions - II
11	Thermodynamic functions
12	NMR frequencies
13	QSAR, Transition states
14	FINAL EXAMINATION