[A-3]COURSE SYLLABUS

1. Course Description (Approximately 100 words)

This course introduces the students to molecular modelling and drug designing. Students will have an understanding of Molecular Geometry which deals with Molecular Geometry and Coordinate Space for Optimization of Algorithm of Molecular Geometry. They will also deal with Molecular Dynamics, historical Perspective and Viewpoint of Pharmacophore, Molecular Docking, and the library and Database of the same. They will be introduced to Software Resources such as Molecular Mechanics (MM3 and MM4), Huckel-MO-Calculator, Semiempirical (MOPAC), SciQSAR, a linear-regression- based QSAR, Chem3D, HyperChem, among others.

2. Course Goals and Objectives (Approximately 100 words)

By the end of this course, the students should be acquainted with theoretical and practical knowledge of molecular modeling tools and techniques for drug design and discovery, the knowledge of molecular modeling software will be useful for for commercial projects related to drug discovery and developments which has also been clearly discussed. The detailed knowledge and skill is given in the course and the students get acquired the same after studying the course.

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

a. Molecular Modeling in Methods and Principles in Medicinal Chemistry by HansDieter Holtje and GerdFolkers, Third edition, Volume 5, 1996, VCH Publishers,
New York, NY (USA).

b. Structure-Based Ligand Designin Methods and Principles in Medicinal Chemistry
by Klaus Gubernator, Hans-Joachim Bohm, Volume 6, 1997, VCH Publishers,
New York, NY (USA).

4. Reference

a. Advanced Computer- Assisted Techniques in Drug Discovery in Methods and Principles in Medicinal Chemistry by Han van de Waterbeemd (ed.) Volume 3, 1994, VCH Publishers, New York, NY (USA).

b. Virtual Screening for Bioactive Molecules by in Methods and Principles in Medicinal Chemistry, Edited by Hans-Joachim Bohm and Gisbert Schneider, Volume 10, 2000.

5. Course Requirements and Grades

EXAMINATION = 70%
C.A.T. = 20%
ASSIGNMENT = 10%

TOTAL = 100%

6. Course Calendar

Week	Main Content
1	INTRODUCTION TO MOLECULAR MODELING
2	QUANTUM MECHANICS
3	Molecular Mechanics Force Field
4	ENERGY MINIMISATION
5	Pro-drugs
6	ION CHANNEL AS DRUG TARGET
7	C.A.T.
8	PHARMACOKINETICS
9	The drug discovery process
10	PHARMACOPHORE
11	Chemical database
12	PubChem
13	PDBsum
14	EXAMINATION