SHIV NADAR UNIVERSITY

UNDERGRADUATE COURSE PROPOSAL

I. **COURSE TITLE: Informatics & Medicinal Chemistry**

II. **COURSE CODE (PLEASE CROSS-LIST IF APPLICABLE): CHY 332**

III. **COURSE CREDITS (L:T:P): 4** (3L: 0T: 1P)

IV. **TOTAL CONTACT HOURS/ BATCH/WEEK (L:T:P): 3L:0T:2P**

V. **NO. OF BATCHES: 1**

VI. **COURSE TYPE (MAJOR/UWE/CCC/REAL/VELS/IC), PLEASE MENTION ALL THAT APPLIES & WRITE CREDITS FOR EACH ONE: MAJOR/UWE**

VII. **PREREQUISITE/S (IF ANY): CHY221, CHY112**

VIII. **COURSE COORDINATOR/INSTRUCTOR(S):** *N. Sukumar* **(course coordinator);** *Bani Kant Sarma*

IX. **SCHOOL/ DEPARTMENT: Chemistry**

X. **DISCIPLINES TO WHICH THE COURSE MAY BE OF INTEREST: Chemistry, DLS**

XI. **COURSE CONTENT:**

1. **Introduction** (*5 classes*)

- Drug Discovery in the Information-rich age (*1 lecture*)
- Introduction to Pattern recognition and Machine Learning (*1 lecture*)
- Supervised and unsupervised learning paradigms and examples (*1 lecture*)
- Applications potential of Machine learning in Chem- & Bioinformatics (*1 lecture*)
- Introduction to Classification and Regression methods (*1 lecture*)

2. **Representation of Chemical Structure and Similarity** (*10-12 classes*)

- Sequence Descriptors
- Text mining
- Representations of 2D Molecular Structures: SMILES
- Chemical File Formats, 3D Structure
- Descriptors and Molecular Fingerprints
- Topological Indices
- Substructural Descriptors
- Physicochemical Descriptors
- Descriptors from Biological Assays
- Representation and characterization of 3D Molecular Structures

- Pharmacophores
- Molecular Interaction Field Based Models
- Local Molecular Surface Property Descriptors
- Quantum Chemical Descriptors
- Shape Descriptors
- Protein Shape Comparisons, Motif Models
- Molecular Similarity Measures
- Cluster and Diversity analysis
- Network graphs
- Self-Organized Maps
- Semantic technologies and Linked Data

3. **Mapping Structure to Response: Predictive Modeling** (*8 classes*)

- Linear Free Energy Relationships
- Quantitative Structure-Activity/Property Relationships (QSAR/QSPR) Modeling
- Ligand-Based and Structure-Based Virtual High Throughput Screening
- 3D Methods - Pharmacophore Modeling and alignment
- ADMET Models
- Activity Cliffs
- Structure Based Methods, docking and scoring
- Model Domain of Applicability

4. **Data Mining and Statistical Methods** (*8 classes*)

- Linear and Non-Linear Models
- Feature selection
- Principal Component analysis (*1 lecture*)
- Partial Least-Squares Regression
- kNN, Classification trees and Random forests
- Introduction to Neural Nets
- Support vector machines classification and regression (*3 classes*)
- Data preprocessing and performance measures in Classification & Regression (*1 lecture*)
- Introduction to evolutionary computing (*1 lecture*)
- Data Fusion
- Model Validation
- Best Practices in Predictive Cheminformatics

5. **Medicinal Chemistry** (*6-8 classes*)

- Sources of Bioactive compounds and their sources
- High-throughput screens of compound collections
- Combinatorial chemistry in drug discovery
- Peptidometics in drug design
- Macrocycles and their advantages
- mAB vs small molecules in drug discovery

XII. RECOMMENDED BOOK(S):

1. Johann Gasteiger, Thomas Engel, Chemoinformatics: A Textbook (Wiley-VCH, 2003)
2. Jürgen Bajorath (Editor), Chemoinformatics and Computational Chemical Biology (Methods in Molecular Biology) (Humana Press, 2004)
3. Leach & Gillet, An Introduction to Chemoinformatics
4. D.Sriram and P. Yogeswari, Medicinal Chemistry (2nd edition, Pearson)
5. Graham L. Patrick, An Introduction to Medicinal Chemistry (4th edition, Oxford University Press)

XIII. ASSESSMENT SCHEME:

Lab assignments (40%), 2 exams (40%), presentations (20%)

Passing grade: 40%

Assured **A** grade: 80%

Required attendance: 75%