

3. DTA of a multicomponent inorganic salt. Identify endothermic and exothermic transitions.
4. Interpretation of recorded TGA/DSC thermograms from literature or instruments.
5. SEM image analysis using provided micrographs. Measure particle size, surface texture, and morphology.
6. TEM micrograph interpretation. Determine lattice fringes, particle shape, and crystallite boundaries.
7. Visit/demo of SEM/TEM facility (if available). Instrument components, vacuum system, sample mounting.
8. Software simulation of electron beam interactions. Use open-source or institutional software for understanding signal generation.

ESSENTIAL/RECOMMENDED TEXTBOOKS

Theory:

1. **Skoog, Holler, and Crouch**, *Principles of Instrumental Analysis* (7th Ed.) – Cengage
2. **Willard, Merritt, Dean, and Settle**, *Instrumental Methods of Analysis* – CBS Publishers
3. **Tiwari, Ashutosh**, *Nanomaterials: A Guide to Fabrication and Applications* – Wiley
4. **Ertl, G., Knözinger, H., & Weitkamp, J.**, *Handbook of Heterogeneous Catalysis (vol. 1: Characterization Techniques)* – Wiley-VCH
5. **Brown, M.E.**, *Introduction to Thermal Analysis: Techniques and Applications* – Springer
6. **N.K. Kaushik and Shulka**, *Thermal Analysis Techniques and Applications*, IK International.

Practicals and Data Interpretation:

1. Practical Manual of Instrumental Techniques for Chemistry Students – University-level lab manuals
2. Lab Guide for Materials Characterization – Any departmental handout or material characterization facility guide
3. SEM/TEM Micrograph Interpretation Manual – Available from JEOL/FEI training resources
4. Online Spectral/Imaging Databases – NIMS, SpringerMaterials, NIST, etc.

Note: Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.

DISCIPLINE SPECIFIC ELECTIVE 9

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		

CHEMINFORMATICS	4	2	0	2	12 th Class: Physics, Chemistry, Mathematics	-
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Course Objectives:

- The aim of the course is to introduce the students to computational drug design through structure-activity relationship, QSAR and combinatorial chemistry. The students will learn about the target analysis, virtual screening for lead discovery, structure based and ligand-based design method and the use of computational techniques, library preparation and data handling.

Learning Outcomes:

By the end of the course, the students will be able to:

- Have a comprehensive understanding of drug discovery process and techniques including structure-activity relationship, quantitative structure activity relationship and the use of cheminformatics in this, including molecular modelling and docking studies.
- Appreciate role of modern computation techniques in the drug discovery process and perform their own modelling studies.

THEORY:

UNIT 1:

(4 hours)

Introduction to Cheminformatics: History and evolution of cheminformatics, Use of cheminformatics, Prospects of cheminformatics, Molecular modelling and structure elucidation.

Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

UNIT 2:

(12 hours)

Searching chemical structures: Full structure search, sub-structure search, basic ideas, similarity search, three-dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

Applications: Prediction of Properties of Compounds; Linear Free Energy Relations; Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modeling Toxicity.

UNIT 3:

(6 hours)

Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra; Computer Assisted Structure elucidations; Computer Assisted Synthesis Design

UNIT 4:

(8 hours)

Introduction to drug design; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and Structure Based Drug design; Application of Cheminformatics in Drug Design.

Practical:

(60 hours)

- Overview of Rational Drug Design, Ligands and Targets
- In silico representation of chemical information

- i. CIF IUCr Crystallographic Information Framework
 - ii. CML Chemical Markup Language
 - iii. SMILES -- Simplified Molecular Input Line Entry Specification
 - iv. InChi -- IUPAC International Chemical Identifier
3. Chemical Databases and Data Mining
 - i. Cambridge Structural Database CCDC CSD
 - ii. Crystallographic Open Database COD
 - iii. Protein Data Bank PDB Ligand Explorer
 - iv. ChempSpider
 4. Molecular Drawing and Interactive Visualization
 - i. ChemDraw
 - ii. MarvinSketch
 - iii. ORTEP
 - iv. Chimera, RasMol, PyMol
 5. Computer-Aided Drug Design Tools
 - i. Molecular Modeling Tools
 - ii. Structural Homology Modeling Tools
 - iii. Docking Tools and Screening Tools
 6. Building a Ligand
 - i. Building ab initio
 - ii. Building from similar ligands
 - iii. Building with a known macromolecular target
 - iv. Building without a known macromolecular target
 - v. Computational assessment of activity and toxicity and drugability.

References:

1. **Leach, A. R.; Gillet, V. J. (2007)**, An introduction to Chemoinformatics, **Springer**.
2. **Gasteiger, J.; Engel, T. (2003)**, Chemoinformatics: A text-book. **Wiley-VCH**.
3. **Gupta, S. P. (2011)**, QSAR & Molecular Modeling. **Anamaya Pub.**
4. **Gasteiger, J.** Handbook of cheminformatics: from data to knowledge in 4 volumes, **Wiley**.

Note: Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.

DISCIPLINE SPECIFIC ELECTIVE 10

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		