

SEMESTER -V
CHEMINFORMATICS
PRACTICAL

Program: B.Sc.
Course Code: U20/CHE/SEC/502/P
Course Type: SEC 2
No. of Credits: 3

Max. Hours: 45
Hours per week: 3
Max. Marks: 50

COURSE OBJECTIVE:

To provide a basic learning in the emerging area of chemical sciences and usage of cheminformatics in the industry.

COURSE OUTCOMES:

- CO 1:** introduce students to different methods of cheminformatics, provide examples on the use of cheminformatics in modern drug research.
- CO 2:** Gain practical experience through exercises with representative methods used in cheminformatics.

PRACTICAL SESSIONS

1. Construction of small molecules.
2. Energy minimization and generation of SMILES Notation.
3. Property calculation.
4. QSAR Equation generation (linear regression method/multiple linear regression).
5. Searching RCSB for protein information, download protein and Literature search.
6. Protein preparation.
7. Active site identification and grid Generation.
8. Docking of ligand.
9. Protein ligand interaction studies.
10. Design of new molecules

SEMESTER - V
CHEMINFORMATICS
PRACTICAL MODEL PAPER

Course Code: U20/CHE/SEC/502/P

Credits: 3

Max Marks: 50

Max. Time: 2 Hrs

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| 1. Construction of molecules using Chems sketch | 10 M(CO1) |
| 2. Calculation of properties using pkcsm and excel sheet preparation | 10M (CO1) |
| 3. QSAR equation generation and validation | 15 M (CO2) |
| 4. VIVA | 10 M |
| 5. Attendance | 5M |