Computational Drug Design CSE 873 (3-0)

1. **Rationale:**

Drug discovery is expensive, slow, and risky and traditionally takes 12 years and over $2.5B for a single success out of 100,000 compounds. But the game is changing. AI, machine learning, and *in silico* modeling are slashing timelines, cutting costs, and boosting success rates. Virtual screening, predictive algorithms, and multi-omics are turning trial-and-error into smart, targeted innovation. The future of drug discovery is digital, data-driven, and dramatically faster. Most of the contents of the course are already up to date; however, there is a need to revise some topics as per recent paradigm shift.

2. **Educational Objectives**

a. Understand challenges related to computational predictions, data privacy, and regulatory acceptance of *in silico* drug design.
b. Application and development of automated workflows for high-throughput virtual screening and hit-to-lead optimization.
c. To understand the development and application of modern *in silico* tools in different phases of drug discovery.
d. To understand optimization and selection of feature for the design of new drug candidates for better optimal efficacy and safety profiles.

3. **Course Outcomes**

a) After completing this course student will be able to understand the application and algorithms of different computational tools in drug discovery. Additionally, students will get awareness regarding current challenges in global pharmaceutical industry.
b) Students will be able to develop virtual screening pipelines integrating ligands- -structures and machine learning based methodologies.
c) Students will be able to construct, optimize and validate the hit identification and lead optimization using high-throughput screening methods.

4. **Recommended Reading:**

a. Computational Drug Discovery: Methods and Applications by Vasanthanathan Poongavanam, Vijayan Ramaswamy, DOI:10.1002/9783527840748, 2024

b. Protein-Protein Docking, Methods and Protocols by Agnieszka A. Kaczor, 2024,
c. Virtual Screening for Bioactive Molecules by in Methods and Principles in Medicinal Chemistry, Edited by Hans-Joachim Bohm and Gisbert Schneider, Volume 10, 2000.
d. Pharmacophore and Pharmacophore Search in Methods and Principles in Medicinal Chemistry, Edited by Thierry Langer and Rémy D. Hoffmann, Volume 32, 2006.