Unit I:

Dr. Zahra Alghoul – Analytical Techniques in Drug Design

Course Objective:

The drug design process goes through several steps that include synthesis, characterization, and packaging. In this series of activities, students will use analytical chemistry techniques for characterization of pharmaceutical solutions, tablets, and ointments. The selected experiments introduce students to measurement techniques, general laboratory skills for preparation of standard solutions and samples for analysis, and identification and quantification of compounds through instrumental analysis.

Course Outline:

- Improving accuracy and precision in experimental analysis
- Analysis of analgesic drugs using high-performance liquid chromatography
- Characterization of sulfathiazole (solubility, melting point, pKa, polymorphism)
- Kinetics of drug decomposition, aspirin as an example (effect of storage conditions such as temperature and humidity on shelf life)
- Determination of the diffusion parameters of a drug (aspirin) through a membrane
- Characterization of tonicity of pharmaceutical solutions
- Characterization of pharmaceutical powders and granules

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\text{Acetylsalicylic Acid (ASA)} + \text{H}_2\text{O} \rightarrow \text{Salicylic Acid (SA)} + \text{Acetic Acid}
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Unit II:

Dr. Jennifer Caroll- Natural Products and Drug Discovery

Course Objective:

The isolation and characterization of natural products is the cornerstone of pharmaceutical development. Up to 80% of currently available pharmaceuticals are originally sourced from nature, or are derivatives of naturally occurring compounds (1). Our “Natural Products and Drug Discovery” project will introduce students to the fundamentals of isolation, biological testing and structure elucidation of small molecules. Students will become familiar with organic structure analysis including current literature database searches, steam distillation, chemically active extraction and spectroscopic characterization. Analysis of small molecules will include techniques such as gas chromatography, mass spectroscopy and nuclear magnetic resonance.

Course Outline:

- Introduction to Natural Products and Literature Searching
- Separation and Purification of Small Molecules
- Introduction to Spectroscopy
- Structure Elucidation and De-replication

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Unit III:

Dr. Emily Fogle – Protein Chemistry

Course Objective:

Students will learn about protein chemistry and performing assays:

- Become familiar with the use of pipets and other volumetric equipment in a biochemistry lab
- Use a standard curve to determine the concentration of an unknown protein
- Manipulate and analyze protein structure using the viewer Jmole/Firstglance
- Understand the importance of non-covalent interactions in protein-protein and protein-ligand interactions using Jmol/Firstglance to visualize and compare non-covalent interactions in protein structure
- Learn to perform an enzyme-linked immunosorbent assay (ELISA)
- Understand the antibody-antigen interactions and how the ELISA technique uses antibodies to detect and quantitate an analyte
- Determine IC50 values for inhibitors of an enzyme and correlate the values to the non-covalent interactions observed in protein structure

Course Outline:

- Determining concentration of an unknown protein
- ELISA immunoassay
- Protein structure viewing exercise to investigate inhibitor binding
- Activity assays for acetylcholinesterase
- Determination of IC50 values for inhibitors of acetylcholinesterase
Unit IV:

Dr. Erik Sapper - Data-Driven Discovery of New Drugs and Active Molecules

Course Objective:

Molecular modeling, informatics, and quantitative structure-activity relationships (QSAR) are powerful tools used to infer complex relationships within extremely large and complex data sets. An example of one such application is in the discovery of new pharmaceutical drugs and active compounds. Large sets of known molecules and their properties may be used in a computational process for discovering new molecules based on performance trends, analysis of molecular descriptors, and leveraging of machine learning models such as artificial neural networks and evolutionary algorithms. Students will leave the workshop with a better understanding of how data science and informatics may be used to accelerate the discovery of new drugs and active molecules.

Course Outline:

This hands-on session will introduce and guide students through three stages of a data-driven discovery project:

- Analysis of a training set of molecules having known properties
- Discovery of molecular descriptors suitable for data analysis
- Development, cross-validation, and use of equations that predict the performance of novel and newly proposed pharmaceutical drugs.