1. Course: CHEM 599-659 Selected Topics in Chemistry: Medicinal Chemistry

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<td>9:30-10:45</td>
<td>ST 127</td>
<td>Dr. D. Derksen</td>
<td>SB 231</td>
<td><a href="mailto:dderksen@ucalgary.ca">dderksen@ucalgary.ca</a></td>
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To avoid IT problems, it is recommended that the students use their U of C account for all course correspondence. Please use “CHEM 599/659 inquiry” as the Subject of your e-mail.

Desire 2 Learn (D2L): CHEM 599 L01 - (Winter 2019) - Selected Topics in Chemistry: Medicinal Chemistry
https://d2l.ucalgary.ca/d2l/home/171384

Departmental Office: Room SA 229, Tel: (403) 220-5341, e-mail: chem.undergrad@ucalgary.ca

2. Course Description: An introduction to concepts in medicinal chemistry including synthesis, lead discovery, rational drug design, receptors and basics of metabolism.

3. Reference Textbooks (Suggested, not required):

4. Topics Covered and Suggested Readings:

   Course Contents

   1) Historical Overview of Drug Discovery and Introduction
      - Drugs discovered without rational design
      - Overview of modern rational drug design
      - Stages of drug discovery
      - ADME

   2) Lead Discovery and Lead Modification
      - Lead discovery
        - Endogenous ligands and natural products
        - Fragment-based lead discovery
      - Lead modification
        - Solid phase peptide and organic synthesis
        - Structure-activity-relationship (SAR) studies
        - Isosteres
        - Conformational analysis and constraints
        - Peptidomimetics/Amino acids
        - Heterocycle synthesis
      Common reactions in medicinal chemistry
        - Cross coupling
        - Amide bond forming methods
        - pKa
        - Synthetic design
        - SciFinder and Reaxys

   3) Physiochemical properties
      - Rules for rapid profiling from structures
      - Lipophilicity
      - pKa
- Solubility
- Permeability

4) Receptors/Enzymes
   - Drug-receptor interactions
   - How interactions are determined
   - Drug and receptor chirality
   - Overview of enzymes as catalysts
   - Inhibition and inactivation
   - Irreversible enzyme inhibitors

5) Barriers to effective drugs/ metabolism
   - BBB, plasma stability
   - Pathways for drug deactivation and elimination
   - Phase I transformations and mechanisms
   - Phase II transformations and mechanisms
   - P450 inhibition, hERG blocking, toxicity
   - Intro to pharmacokinetics

6) Graduate student proposals/presentations

CUMULATIVE FINAL

Department Approval Electronically Approved Date January 6, 2020