

**Syllabus**  
**CHEM 579/BINF 739**  
**Modern Methods of Drug Discovery**  
**Mondays, Aug 27-Dec 18, 2007**  
**4:30-7:10 pm, Bull Run Hall, room 248**

**Instructors:** Dr. Robin Couch ([rcouch@gmu.edu](mailto:rcouch@gmu.edu)), Dr. Saleet Jafri ([sjafri@gmu.edu](mailto:sjafri@gmu.edu)),  
Dr. Vijayasarathy Srinivasan ([vsriniva@gmu.edu](mailto:vsriniva@gmu.edu)).

**Course description:**

This course provides an introduction to the process of drug discovery. In this course we will cover modern methods and strategies of drug target identification, lead molecule identification, and lead optimization.

**Student learning goals:**

After taking this course you should have an understanding of the methods and strategies involved in the drug discovery process including (1) methods used to identify potential drug targets, (2) approaches to screening for lead molecules, (3) sources of lead molecules, including natural products, synthetic libraries, and *in silico* structure-based molecules, (4) lead optimization, and (5) the future directions of drug development, including the promise of personalized medicine.

**Required course materials:**

Abbreviated lecture notes are available for download at <http://www.binf.gmu.edu/jafri/chem579-binf739/>. You will be expected to supplement these lecture notes during class discussions. Additional handouts will also be provided during class. *Modern Methods of Drug Discovery*, edited by Alexander Hillisch and Rolf Hilgenfeld, *Enzymes* (second edition) by Robert A. Copeland, *Chemoinformatics in Drug Discovery*, edited by Tudor I. Oprea, and *Bioinformatics and Drug Discovery*, edited by Richard S. Larson are the textbooks upon which this course is primarily based. However, since the lecture notes will be provided, **the purchase of these textbooks is optional**. These books can be obtained from the Mercer Library Reserves Desk on a two hour loan.

**Requirements and methods of evaluation:**

Your grade will be based on one **Midterm Exam (35%)**, one **Research Project (25%)** and a **Final Exam (40%)**. The Final Exam is cumulative.

Your **Research Project** will consist of a **written report** describing a protein that you believe would make an excellent drug target. You must contact me ASAP with the name of your selected protein since no two students may write about the same protein simultaneously. Selection preference is based upon the order in which I'm contacted. You are expected to obtain all relevant information by performing a literature search (eg. PubMed). In your paper you should thoroughly describe why the protein is a good target for drug development, including any experimental data that validates your protein selection. Be sure to include in your paper a thorough description of your protein (eg its biology, mechanism of action (including catalytic mechanism, if appropriate), structural information, etc). Indicate if there are lead molecules available for your protein. If so, what is the mechanism of action? Indicate in detail how you would identify additional lead molecules for your protein (include a descriptive experimental protocol for doing this). The paper should be written in a format to convince the reader that your target deserves exploration and justifies funding.

## ***Presentation/Lecture List***

- Week 1***      ***Aug 27, 2007*** Course Overview, Policies and Procedures.  
Lecture 1: Modern Methods of Drug Discovery: An Introduction. (RC)
- Week 2***      ***Sept 3, 2007*** No class this week.
- Week 3***      ***Sept 10, 2007*** Lecture 2: Methods to Identify Potential Drug Targets: a) Proteomics. (RC)
- Week 4***      ***Sept 17, 2007*** Lecture 3: Methods to Identify Potential Drug Targets: b) Genomics. (SJ)
- Week 5***      ***Sept 24, 2007*** Lecture 4: Methods to Identify Potential Drug Targets: c) Bioinformatics.  
(SJ)
- Week 6***      ***Oct 1, 2007*** Midterm exam (RC)
- Week 7***      ***Oct 9, 2007*** \*\*\* Tuesday Lecture \*\*\* Lecture 5: Target Validation. (RC)
- Week 8***      ***Oct 15, 2007*** Lecture 6: Drug Lead Identification: Rational Design, High Throughput  
Screening, Natural Products, and Synthetic Libraries. (RC)
- Week 9***      ***Oct 22, 2007*** Lecture 7: Lead Optimization: Physicochemical Concepts in Drug Design.  
(RC)
- Week 10***     ***Oct 29, 2007*** Lecture 8: 3D-QSAR. (SJ)
- Week 11***     ***Nov 5, 2007*** Lecture 9: Malaria and Drug Design. (VS)
- Week 12***     ***Nov 12, 2007*** Lecture 10: Tuberculosis and Drug Design. (VS)
- Week 13***     ***Nov 19, 2007*** Lecture 11: Drug Lead Identification: *In silico* Structure-Based Molecules.  
(RC)
- Week 14***     ***Nov 26, 2007*** Lecture 12: The Future of Drug Design; Review; Research Project Due (RC)
- Week 15***     ***Dec 11-18, 2007*** Final Exam (RC)