CHEM777 Principles of Medicinal Chemistry. Fall 2014.

Text Book: *An Introduction to Medicinal Chemistry*, 5th Edition, Graham L. Patrick, Oxford.

Instructor: Dr. Ashok Maliakal ashok.maliakal@gmail.com
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Office hour: by appointment.

Grading: Quizzes 20%
Midterm I 25%
Midterm II 25%
Final project 30%

Prerequisites: Undergraduate organic chemistry. Undergraduate biochemistry.

Schedule

Sep 7 Drug target. Reading assignment: chapter 1, 2, 6.

- Medicine and chemistry
- Drug targets
- Binding and molecular interactions
- Biomolecular structures

Sep 14 Proteins as drug targets: enzymes. Reading assignment: chapter 3, 7.

- How do enzymes catalyze reactions?
- Reversible inhibitors and inhibition kinetics
- Suicide inhibitors
- Transition state analogues
- Case study: Parkinson's disease
- Isozymes: cyclooxygenases

Sep 21 Proteins as drug targets: receptors and signal transduction. Reading assignment: chapter 4, 5, 8.

- Neurotransmitter and hormones
- Ion channels
- G-protein-coupled receptors
- Receptor tyrosine kinases
- Agonists and antagonists

Sep 28 Nucleic acids as drug targets. Reading assignment: chapter 6, 9.

- Review of genetics
- Automated synthesis of biomolecules.
- mRNA targeting: antisense DNA
- mRNA targeting: ribozymes and RNA interferences
- DNA targeting: artificial transcription factors, triplex-formation oligonucleotides, and polyamides.
- DNA targeting: DNA damaging reagents.
- Gene therapy

- Delivery of nucleic acids

Oct 5 Pharmacokinetics. Reading assignment: chapter 11.
- Drug absorption and distribution
- Drug metabolism
- Prodrug

Oct 12 First exam.

Oct 19 Drug development. Reading assignment: chapter 12, 13, 14.
- Drug target
- Finding a lead
- Evaluating drug activities.
- Optimizing interactions
- Optimizing access to the target
- Case study: ACE inhibitors

Oct 26 Molecular docking and 3D-QSAR. Reading assignment: chapter 17, 18.
- Computational chemistry
- Molecular docking
- QSAR
- 3D-QSAR

Final Project Starts!
- Find your group members
- Select a drug
- Search literature
- Develop your own strategy
- Write a report

Nov 2 Antibacterial agents. Reading assignment: chapter 19.
- Drugs targeting bacterial cell wall synthesis
- Drugs targeting plasma membrane
- Drugs targeting protein synthesis
- Antibacterial resistance

Nov 9 Antiviral and anti-cancer agents. Reading assignment: chapter 20, 21.
- Life cycle of viruses
- Anti-HIV drugs
- Anti-influenza drugs
- Cancer biology
- Anti-cancer drugs targeting DNA
- Anti-cancer drugs targeting biosynthetic pathways
- Anti-cancer drugs targeting tubulin assembly and disassembly

- Anti-cancer drugs targeting kinases (special topic: aptamers)
- Antibody-drug conjugates

Nov 16 Biogenic amine-related drugs. Reading assignment: chapter 22, 23, 25.

- Muscle contraction and relaxation
- Cholinergic receptor
- Adrenergic receptors
- Histamine receptors
- Neurotransmitter reuptate inhibitors

Nov 23 Exam II.

Nov 30 Discussion of projects.

Dec 7 Presentations.

Dec 14 Final project report due.

NJIT Honor code will be upheld. Any violations will be brought to the immediate attention to the Dean of Students.