**CHEM777 Principles of Medicinal Chemistry. Fall 2017.**

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

**Instructor**: Dr. Ashok Maliakal ashok.maliakal@gmail.com
Phone: 908-591-3529.
Office hour: by appointment.

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

**Prerequisites:** Undergraduate organic chemistry. Undergraduate biochemistry.

**Schedule**

Sep 11 Drug target. Reading assignment: chapter 1, 2, 6.

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

Sep 18 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 25 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

Oct 2 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 9 Pharmacokinetics. Reading assignment: chapter 11.
- Drug absorption and distribution
- Drug metabolism
- Prodrug

Oct 16 First exam.

Oct 23 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 30 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 6 Antibacterial agents. Reading assignment: chapter 19.
- Drugs targeting bacterial cell wall synthesis
- Drugs targeting plasma membrane
- Drugs targeting protein synthesis
- Antibacterial resistance

Nov 13 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 20 Biogenic amine-related drugs. Reading assignment: chapter 22, 23, 25.

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

Nov 27. Discussion of projects

Dec 4. Exam II.

Dec 11 Presentations.

Dec 18 Final project report due.

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