

Chem/Biochem 597A: Drug Design

Spring 07

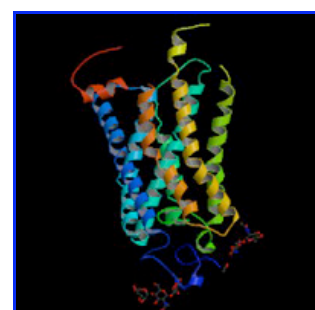
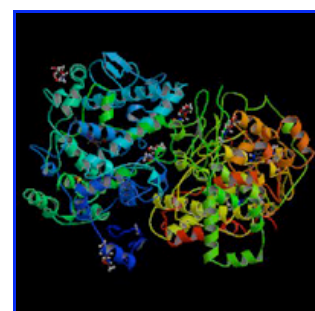
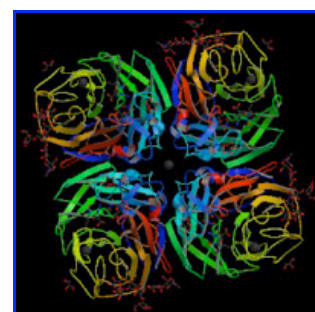
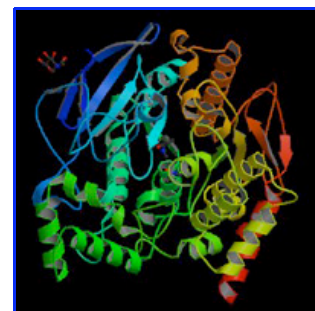
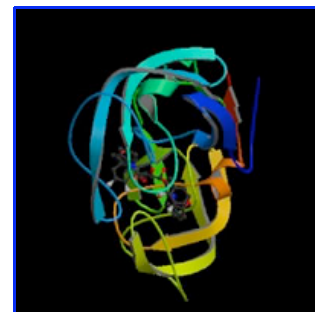
T&Th 1:00-2:15pm
LGRT 1033

Instructors: Lila M. Gierasch (gierasch@biochem.umass.edu, 814 Lederle Tower, 5-6094)
Scott C. Garman (garman@biochem.umass.edu, 1021K Lederle Tower, 7-4488)

Today is July 5, 2007

[Glossary](#)

Date	Topic	Notes	Links
	Introductory material	<ul style="list-style-type: none"> • Syllabus pdf; • Term_Paper_info 	<ul style="list-style-type: none"> • Drug design glossary; • Petsko and Ringe (from UMass sites only);
T Jan 30	LMG: Intro to course; Drug discovery timeline part 1	<ul style="list-style-type: none"> • Lecture 1 ppt 	<ul style="list-style-type: none"> • Drug discovery tutorial; • DrugResearcher.com
Th Feb 1	LMG: Intro to proteins	<ul style="list-style-type: none"> • L2 preview ppt; • Lecture 2 pdf 	
T Feb 6	LMG: Physical methods in drug discovery	<ul style="list-style-type: none"> • L3_outline ppt; • Lecture 3 pdf 	<ul style="list-style-type: none"> • Fluorescence html; • Freire ITC pdf; • Blundell X-ray pdf; • Giralt NMR pdf; • Pellecchia NMR pdf (or .doc version)
Th Feb 8	SCG: Drug discovery timeline part 2: Lead optimization to clinical trials	<ul style="list-style-type: none"> • L4_outline pdf; • Lecture 4 pdf 	<ul style="list-style-type: none"> • Phase 1 mishap html; • Phase 3 withdrawal html; • ClinicalTrials.gov
T Feb 13	SCG: Pharmacokinetics and pharmacodynamics	<ul style="list-style-type: none"> • Lecture 5 pdf 	<ul style="list-style-type: none"> • Goodman chapt1 pdf;
Th Feb 15	SCG: Intro to transmembrane receptors	<ul style="list-style-type: none"> • L6_outline pdf; • Lecture 6 pdf 	<ul style="list-style-type: none"> • Fillmore GPCR 2004.pdf; • Kroeze GPCR pdf
T Feb 20	Quiz	<ul style="list-style-type: none"> • Quiz key pdf 	<ul style="list-style-type: none"> • Quiz histogram
Th Feb 22 (optional)	Special lecture: 10:00AM, LGRT 1634 <i>Jonathan Greer, Abbott: Careers in the Pharmaceutical Industry</i>		
Th Feb 22	<i>Jonathan Greer, Abbott: Structure-Based Drug Design</i>	(see handout)	<ul style="list-style-type: none"> • Frag based design pdf; • Business Week story
T Feb 27	Discussion: Structure-based drug design, Target selection		
Th Mar 1	<i>Sherin Abdel-Meguid, ProXyChem: Target Selection</i>	<ul style="list-style-type: none"> • AbdelMeguid ppt 	<ul style="list-style-type: none"> • Targets for medicine pdf
T Mar 6	Discussion: Target selection, High throughput screening		From Seena: <ul style="list-style-type: none"> • Drug discovery tools pdf; • Drug discovery products
Th Mar 8	<i>Angela Cacace, Pfizer: High Throughput Screening</i>	<ul style="list-style-type: none"> • Cacace pdf 	<ul style="list-style-type: none"> • HTS design pdf; • HTS considerations pdf; • HTS fluorescence pdf; • HTS robotics pdf; • Allosteric screening pdf; • Cell & target assays pdf; • SSprang G prof primer pdf
T Mar 13	Discussion: High throughput screening, Combinatorial libraries		
Th Mar 15	<i>Pat Walters, Vertex: Combinatorial Libraries</i>	<ul style="list-style-type: none"> • Walters pdf 	<ul style="list-style-type: none"> • Virtual screening pdf; • Chemical libraries pdf
	Spring Break		
T Mar 27	Discussion: Combinatorial libraries, Reducing lead time		
Th Mar 29	Discussion: SAR in tuberculosis		
T Apr 3	<i>Chris Lipinski, Melior Discovery: Reducing Lead Time</i>	<ul style="list-style-type: none"> • Lipinski ppt 	<ul style="list-style-type: none"> • Chemical space pdf



Th Apr 5	<i>Cindy Dowd, NIAID: SAR in Tuberculosis</i>	• Dowd pdf	• Progress in TB pdf ; • Thiolactomycin SAR pdf ; • Nitroimidazopyran pdf ; • PA-824 resistance pdf
T Apr 10	Discussion: SAR in tuberculosis, GPCRs		
Th Apr 12	Field Trip to Vertex Pharmaceuticals		• Vertex trip pdf ; • Directions to Vertex
T Apr 17	No class; Monday class schedule		
Th Apr 19	<i>Jean Lachowicz, Schering Plough Research Institute: GPCRs as Drug Targets</i>	• Lachowicz ppt	• Schizophrenia animal models pdf
T Apr 24	Discussion: GPCRs, COX-2 inhibitors		
Th Apr 26	<i>John Talley, Microbia: Discovery and Development of COX-2 Inhibitors</i>	• Talley pdf	• Ulcer study pdf ; • Celebrex clinical trial pdf ; • Binding studies pdf ; • Myocardial infarct pdf ; • Cardio risk pdf ; • Breast cancer pdf ; • Cox2 safety pdf ; • Forbes profile ; • Whitehead story
T May 1	No Class: Protein folding diseases meeting		
T&W May 1-2	Protein folding diseases meeting at UMass	• Registration ; • Meeting flyer pdf	• Misfolding intro pdf ; • Folding diseases pdf ; • Dobson folding pdf ; • Sitia QC pdf ; • Goldberg degradation pdf ; • Selkoe folding pdf
Th May 3	No Class		
T May 8	Discussion: COX-2 inhibitors, Protein folding diseases		
Th May 10	<i>Stewart Fisher, Astra Zeneca: Identifying New Antibacterial Agents</i>	• Fisher ppt	• Antibacterial discovery pdf
T May 15	Wrap up; Papers due		

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