

Analytical Medicinal Chemistry

**16:663:511 (3 credits)
Spring 2005**

**Time: M, W 4:30-7:30 pm
(Lectures end before spring break)**

Place: Pharmacy 323A

Course Description: The *Analytical Medicinal Chemistry* course focuses on the fundamental analytical chemistry concepts in drug discovery and development, and presents examples of modern applications of analytical methods in pharmaceutical research. Topics such as chromatographic separations (*e.g.*, GC, LC, CE), tandem mass spectrometry (qualitative and quantitative analysis), NMR, LC-MS, CE-MS, LC-FT-IR, MALDI, and ICP-MS will be discussed. Modern applications in the analysis of small and large molecules in the pharmaceutical and biotech industry (*e.g.*, PK, metabolism, lead optimization, Combi-Chem, metabonomics, proteomics, and genomics) will be discussed.

Course Instructors:

Longqin Hu, Ph.D. (Coordinator)
Associate Professor of Medicinal Chemistry

Ray Bakhtiar, Ph.D.
Senior Research Fellow, Merck Research Laboratory

Course Material:

Handouts and Class Lectures

Examinations:

Two exams (a mid-term and a comprehensive final) and
One term paper

Grading:

Mid-Term	40%
Term Paper	10%
Term Paper presentation	10%
Final Examination (cumulative)	40%
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Total	100%

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Tentative Course Outline:

Lectures 1-5	Introduction to Separation Science Gas Chromatography Liquid Chromatography: RP- and NP-HPLC Capillary Electrophoresis Affinity Chromatography Size Exclusion Chromatography Chiral Chromatography (GC, CE, and LC) Chromatographic Separation and Purification of Bio-molecules
Lectures 6-8	LC Detectors Spectrophotometric Detection Mass Spectrometry Electrochemical Detection IR and FT-IR Lasers NMR Specialized Detection Systems
Lectures 9-20	Bio-Mass Spectrometry Proteomics Genomics Biomarkers Metabonomics Combi-Chem Pharmacokinetics and Biotransformation
Lectures 21-26	Selected Topics LC-MS and LC-MS/MS Method Development Method Validation, FDA Guidelines, GLP, GMP, GCP Tandem MS Structure Assignment and Interpretation Data Mining and Visualization In Vitro Screening (<i>e.g.</i> , PGPs, Caco-2)

Week	Day	Date	Lecture Topic	Week	Day	Date	Lecture Topic	Week	Day	Date	Lecture Topic
1	T	18-Jan		6	Th	24-Feb			Sa	2-Apr	
1	W	19-Jan	L1 - Introduction to Anal Separations	6	F	25-Feb			Su	3-Apr	
1	Th	20-Jan	(Hu)		Sa	26-Feb		12	M	4-Apr	
1	F	21-Jan			Su	27-Feb		12	T	5-Apr	
	Sa	22-Jan		7	M	28-Feb	L20-21 - Bio-Mas Spectrometry (Bakhtiar)	12	W	6-Apr	
	Su	23-Jan		7	T	1-Mar		12	Th	7-Apr	
2	M	24-Jan	L2-3 - Introduction to Anal Separations	7	W	2-Mar	L22-23 - Method development & validation	12	F	8-Apr	
2	T	25-Jan	(Hu)	7	Th	3-Mar	(Bakhtiar)		Sa	9-Apr	
2	W	26-Jan	L4-5 - GC (Bakhtiar)	7	F	4-Mar			Su	10-Apr	
2	Th	27-Jan			Sa	5-Mar		13	M	11-Apr	
2	F	28-Jan			Su	6-Mar		13	T	12-Apr	
	Sa	29-Jan		8	M	7-Mar	L24-25 - Interpretation & data mining	13	W	13-Apr	
	Su	30-Jan		8	T	8-Mar	(Bakhtiar)	13	Th	14-Apr	
3	M	31-Jan	L6-7 - HPLC (Bakhtiar)	8	W	9-Mar	L26-27 - In vitro screening (Bakhtiar)	13	F	15-Apr	
3	T	1-Feb		8	Th	10-Mar			Sa	16-Apr	
3	W	2-Feb	L8-9 - Other chromatography (Bakhtiar)	8	F	11-Mar			Su	17-Apr	
3	Th	3-Feb			Sa	12-Mar		14	M	18-Apr	
3	F	4-Feb			Su	13-Mar		14	T	19-Apr	
	Sa	5-Feb		9	M	14-Mar	Spring Break	14	W	20-Apr	Term paper due on April 20th
	Su	6-Feb		9	T	15-Mar	Spring Break	14	Th	21-Apr	
4	M	7-Feb	L10-11 - Bio-Mas Spectrometry (Bakhtiar)	9	W	16-Mar	Spring Break	14	F	22-Apr	
4	T	8-Feb		9	Th	17-Mar	Spring Break		Sa	23-Apr	
4	W	9-Feb	L12-13 - Bio-Mas Spectrometry (Bakhtiar)	9	F	18-Mar	Spring Break		Su	24-Apr	
4	Th	10-Feb			Sa	19-Mar		15	M	25-Apr	Term paper presentation
4	F	11-Feb			Su	20-Mar		15	T	26-Apr	
	Sa	12-Feb		10	M	21-Mar	Final Examination	15	W	27-Apr	Term paper presentation
	Su	13-Feb		10	T	22-Mar		15	Th	28-Apr	
5	M	14-Feb	Mid-Term Exam	10	W	23-Mar		15	F	29-Apr	
5	T	15-Feb		10	Th	24-Mar			Sa	30-Apr	
5	W	16-Feb	L14-15 - Bio-Mas Spectrometry (Bakhtiar)	10	F	25-Mar			Su	1-May	
5	Th	17-Feb			Sa	26-Mar		16	M	2-May	
5	F	18-Feb			Su	27-Mar		16	T	3-May	Reading Day
	Sa	19-Feb		11	M	28-Mar		16	W	4-May	Reading Day
	Su	20-Feb		11	T	29-Mar					FINAL
6	M	21-Feb	L16-17 - Bio-Mas Spectrometry (Bakhtiar)	11	W	30-Mar					
6	T	22-Feb		11	Th	31-Mar					
6	W	23-Feb	L18-19 - Bio-Mas Spectrometry (Bakhtiar)	11	F	1-Apr					