Syllabus – Fall 2009
CHEM 5181 – Mass Spectrometry and Chromatography

University of Colorado at Boulder – Department of Chemistry and Biochemistry

Tuesdays 11:00-12:15 & & Thursdays 10:50-12:05
Ekeley W166

Taught by:

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Office Hours: Tue & Thu immediately after class till 1 pm in Ekeley E150 or M329.

Labs and Final Project at Mass. Spec. Facility Directed by:

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Course Objectives

After taking this course you should have developed a basic understanding of the main types of techniques and instruments used in mass spectrometry and chromatography, as well as a basic familiarity with interpreting their data. We will focus on the fundamentals, applicability, extractable information, advantages and limitations of each technique.

You are likely to encounter in your graduate and professional careers many problems for which techniques that we do not cover in the course (or that don't even exist today) are very appropriate. Another way to state our objective is that after taking this course you should be able to ask intelligent questions, look for the information you need, and 1) decide whether the information provided by the technique is useful for your problem; and 2) quickly learn to use the technique and interpret the data it produces.

Course prerequisites

The course prerequisites are undergraduate physics (electric and magnetic fields and forces, heat transfer, fluid mechanics), calculus, probability and statistics, and basic physical chemistry. You are responsible for supplemental work that you may need to catch up in any of the prerequisite areas.

Textbooks: (should be available at the UMC bookstore): Hoffmann & Stroobant. *Mass Spectrometry*, 2nd Ed., Wiley, 2002. $60 *(QD96.M3 H6413 2001)* and McLafferty & Turecek. *Interpretation of Mass Spectra*, 4th Ed., 1993. $39 *(QC454 .M22 1993)*

There is no textbook for the chromatography part, as we have not found a good one. Past students may have the Braithwaite book that is a good reference. We will provide reading materials for some of the chapters. See below for others reference books.

Web page for the course

http://www.colorado.edu/chemistry/chem5181/

We will bring printed notes before every class and post the lecture notes on the web AFTER each lecture. Do not print the notes on the web before class, as those are from previous course offerings and will be changing. The page contains reading materials classified as "required", "suggested", and "advanced."

Email list for the course

The email list for the course is: chem-5181@lists.colorado.edu

It is *essential* that you be subscribed to the email list as some announcements will only be sent by email. I have subscribed all the students that are on the class roster. You can also subscribe on your own by sending a message to listproc@lists.colorado.edu with the following message body (the subject line doesn't matter):

Subscribe chem-5181 Your Name

If you drop the course you can unsubscribe from the list by sending a message to listproc@lists.colorado.edu with the following message body (the subject line doesn't matter):

Unsubscribe chem-5181

Homework and Exam Legibility

It is often a significant problem to "decode" homeworks and exam if the writing is too small or messy, or if they are poorly organized. We may take points out for poor legibility. For homeworks, we prefer if you type them in a computer, although this is not required. A neat handwritten homework is just as good. The current homework will be posted on the course page in Word to save you the typing, should you decide to type your homework.

Please list the units of all results (SI units if possible).

Policy about Homework Collaboration

It is OK to discuss the problems in small groups, and in fact this will help you learn (teach each other, bounce ideas, etc.). However everyone is still responsible for working out and writing their own solution separately. If you don't go through the effort of understanding and solving every problem yourself (after discussing it with others if you want) you will find yourself at a large disadvantage in the exams where you have to solve new problems very quickly. To reiterate, it is OK to discuss the problems but not to write solutions together or to compare them or the results. If you do any of the later, it often becomes obvious when grading because multiple people have the same wrong solutions to several problems.

Course Grading Policy

The grade will be determined as the weighed average of the following parts (subject to change):

- 20% homework, journal skims, and in-class quizzes
- 15% labs (at MS facility)
- 20% 2 midterms

- 15% final project (with MS facility)
- 15% final exam
- 5% presentation of a paper to the class
- 10% class participation

Late homeworks will not be graded unless we have agreed to an extension ahead of time. If they are graded, the grade will be multiplied by 0.7 to discourage lateness. No exceptions except in cases of personal (not academic) hardship. If you cannot come to class a day in which a homework or lab is due, you can (a) turn it in ahead of time; (b) type it or scan it and email it to Jose. If you scan it, make sure that the scan is legible and that the file is not so large that it may cause email problems (so < 5 MB).

Prize for Best Grade in the Course

The student with the highest grade at the end of the course will receive a free copy of the book "Measuring Mass: From Positive Rays to Proteins", M. Grayson, Ed., 2002. This is a very nice review of the history of mass spectrometry that was recently produced to commemorate the 50 years of the American Society for Mass Spectrometry (ASMS).

Some Information about Grades

Grading is absolute, we don't grade on a curve. Not everyone has gotten an A in past offerings of this course (although we would be very happy if that was the case), and from experience a good grade requires hard work. FYI in the previous four years we gave in total 3 A, 11 A-, 20 B+, 7 B, 4 B-, and 2 C+. You need to get at least a B- for the course to count towards graduate credit and a B (average of all courses) to avoid being placed on probation (for CHEM graduate students).

The correspondence between numeric and letter grades is as follows:

	From	To		From	To
A	100	95	C	61	56
A-	94	88	C-	55	49
B+	87	82	D+	48	43
B	81	75	D	42	36
B-	74	69	D-	35	30
C+	68	62	F	29	0

Please don't obsess about grades! They are much less important in grad school than they were in undergrad. They should not become an end in themselves (the "professional student syndrome"), rather they should be a feedback tool to help you identify your strengths and weaknesses and to learn.

Note that we determine the grading policy, and always make an effort to grade all students with the same criteria. For this reason we cannot change your grades unless we made a mistake. So please don't tell us something like "yes, it is true I made that mistake in that question, but I think you should only discount 2 points instead of the 4 you took for it."

Reading Assignments

Many lectures will have a required reading assignment, either as indicated in the course schedule, or announced in class. You are responsible for the material in the readings, and we may have questions about it in class quizzes or homeworks.

Labs & Final Project with the MS Facility

Two labs and one final project will be carried out in groups of 3 students, using the resources of the MS facility. Each group will turn in a single lab report.

Structure of final project

The purpose of the final project is to allow you to perform additional experiments with the instruments at the mass spec facility with more time and focus that is possible for the labs. The project will be carried out in groups of 3 students.

You have to turn in a 1-2 page project proposal. We will get back to you quickly about whether we think the project is viable for the class. Then you have to schedule time to use the instruments at the mass spec facility as needed. The project will be graded based on (1) creativity; (2) quality and readability of the project report; (3) A brief presentation in class; and (4) your good organization and coordination with Dr. Kato in the use of the MS facility (e.g. start the project early rather than leave it for the last week, clean up after yourselves, etc.).

Structure of Student Presentations

Students will be required to present a review of a recent journal paper on either mass spectrometry or chromatography to the instructors and students during a class period. The purpose is to gain familiarity with current topics in the field as well as to understand and practice scientific presentation skills. Students should begin considering articles for presentation as soon as possible, preferably selecting one related to proposed research, and check with the instructors for their suitability no later than 2 weeks prior to presentation (so that there is time to find a new one, should the chosen one not work). A portion of one class lecture will be dedicated to discussing presentation concepts and skills.

Attendance Policy

You are required to attend all the lectures and labs. If you need to miss a lecture, let us know ahead of time and prepare a 2-page (double spaced) summary of the notes and reading for that day. This summary may be graded. If you need to miss a lab, please join another group.

Changes to the Course During the Semester

As with life, this syllabus is subject to change. We may make some changes to the course during the semester if we think is appropriate, including to lectures, assignments, presentations, and exams.

Policy on Course Auditing

We prefer that you take the course for credit as you will get more out of it this way and it also makes it easier for us to teach it. However we may allow interested people who do not have enough time to take the course for credit to audit the course, on a case-by-case basis.

Feedback on the Course

We are always experimenting with some new ideas as we try to improve the course, some of which were suggested from previous years' students. The only purpose of having a course is that it will be useful to you, the students. Thus don't hesitate to give us feedback early on about what's working or not working – chances are that we can fine-tune the course as we go along, as we have done in previous years.

Midway and at the end of the course we will send a Zoomerang questionnaire with specific questions about the course, so that we can use your experience to improve the next offering. We ask that you take this seriously as it really helps us improve. You will get some class credit for doing this as part of the class participation grade (proportional to the total number of respondents since the responses are anonymous). Responses from previous students are posted on the class web page.

Recommended Reference Books

All of these books are in Norlin Library. Library call numbers are below the title. The "new" price on Amazon.com as of Aug. 2003 is given as a reference. Note that may of these books can be purchased "used" at much lower prices on Amazon.com and other online sellers.

Also note that lots of information on these topics is available on the course web page and other web sites. Check the course page for some major links in the subject, or of course use Google to search around.

Part I: General Books Covering Many Analytical Techniques, with good sections on MS and/or Chromatography

Author	Publisher	Title	$ New Amazon	Comments
Schwedt	Wiley	The Essential Guide to Analytical Chemistry *(QD75.2.S3913 1997)*	$65	Small book with great illustrations, Great reference, highly recommended!
Settle (Ed.)	Prentice-Hall	Handbook of Instrumental Techniques for Analytical Chemistry *(QD79.I5 H36 1997)*	$115	Good general reference about analytical techniques
Skoog, Holler, & Nieman	Brooks-Cole	Principles of Instrumental Analysis, 5th Ed. *(QD73 .S56 1998)*	$141	General reference, similar to above
Rubinson & Rubinson	Prentice-Hall	Contemporary Instrumental Analysis *(QD79.J5 R83 2000)*	$127	General reference, similar to above

Part II: Books on Mass Spectrometry

Author	Publisher	Title	$ New Amazon	Comments
Lambert et al.	Prentice-Hall	Organic Structural Spectroscopy *(QD272.S6 O74 1998)*	$94	Very good set of chapters on MS by Graham Cooks
Watson	Lippincott-Raven	Introduction to Mass Spectrometry *(QP519.9.M3 W37 1997)*	$110	Good general reference, similar to Hoffman & Stroobant (we used this book as CHEM-5181 text in 2002)
Barker	Wiley	Mass Spectrometry, 2nd Ed. *(QD96.M3D38 1999)*	$80	Introductory reference

Dawson (Ed.)	Elsevier	Quadrupole Mass Spectrometry *(QD96.M3.Q3 1976)*	$99	Standard reference on quadrupoles
Smith & Busch	Wiley	Understanding Mass Spectra *(QD96.M3S65 1999)*	$70	Alternative to McLafferty for MS interpretation
Cotter	ACS Books	Time of Flight Mass Spectrometry: Instrumentation and Applications in Biological Research *(QP519.9.M3 C68 1997)*	$125	Good reference on TOF, especially for Bio-MS
March & Todd (Ed.)	CRC	Practical Aspects of Ion Trap Mass Spectrometry (Volumes 1-3) *(QD96.M3 P715 1995)*	$189, $189, & $115	Edited book (one author per chapter); comprehensive reference on Ion traps
Lee	Wiley	A Beginner's Guide to Mass Spectral Interpretation *(QD96.M3 L44 1998)*	$55	Introductory reference on interpretation

Part III: Books on Chromatography and Capillary Electrophoresis

Author	Publisher	Title	$ New Amazon	Comments
Miller	Wiley	Chromatography: Concepts and Contrasts, *(QD79.C4 M55 2005)*	$83	Good general reference
Braithwaite & Smith	Kluwer	Chromatographic Methods *(QD79.C4 B73 1996)*	$96	Good general reference, used as textbook in Fall'02 and Fall'03
McNair & Miller	Wiley	Basic Gas Chromatography *(QD79.C45M425 1998)*	$37	Good *short* reference book, read it if you use GC a lot
Grant	Wiley	Capillary Gas Chromatography, 1995 *(QD79.C45G73)*	$185	Detailed reference
Weston & Brown	Academic	HPLC & CE *(QD79.C454 H63 1997)*	$82	Good reference with lots of pointers to the research literature
Snyder, Kirkland, & Glajch	Wiley	Practical HPLC Method Development, 2nd Ed. *(QP519.9.H53S69 1997)*	$100	Bible of HPLC
Cunico, Gooding, & Wehr	Bay Bioanalytical Labs	Basic HPLC and CE of Biomolecules, *(QP519.9.H53 C86 1998)*	$40	Good, practical reference, read it if you use these techniques a lot for biomolecules
Fritz & Gjerde	Wiley-VCH	Ion Chromatography *(QD79.C453 G52 2000)*	$120	General reference on IC (with a chapter on CE)
Weinberger	Academic Press	Practical Capillary Electrophoresis, 2nd Ed. *(QP519.9.C36 W45 2000)*	$105	General reference on CE

Your comments about all of these books (whether you found them useful or not, and if so for which questions/chapters, etc.) as well as on any other books in these subjects are highly appreciated.

Students with Disabilities

If you qualify for accommodations because of a disability, please submit to me a letter from Disability Services in a timely manner so that your needs may be addressed. Disability Services determines accommodations based on documented disabilities. Contact: 303-492-8671, Willard 322, and http://www.Colorado.EDU/disabilityservices

Policy on Sexual Harassment

The University of Colorado at Boulder policy on Discrimination and Harassment (http://www.colorado.edu/policies/discrimination.html, the University of Colorado policy on Sexual Harassment and the University of Colorado policy on Amorous Relationships applies to all students, staff and faculty. Any student, staff or faculty member who believes s/he has been the subject of discrimination or harassment based upon race, color, national origin, sex, age, disability, religion, sexual orientation, or veteran status should contact the Office of Discrimination and Harassment (ODH) at 303-492-2127 or the Office of Judicial Affairs at 303-492-5550. Information about the ODH and the campus resources available to assist individuals regarding discrimination or harassment can be obtained at http://www.colorado.edu/odh