## **CHEM 344**

# **Introductory Organic Chemistry Laboratory**

2-credits

**Laboratory Manual** 

**Spring 2019** 

**University of Wisconsin-Madison** 

#### **Course Instructors**

	Dr. Nicholas J. Hill	Dr. Aubrey Ellison	Dr. Brian J. Esselman
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#### **Teaching Assistants**

Names, contact information, and office hours of course teaching assistants are not available prior to the printing deadline for this laboratory manual. Your section TA will provide this information during the first meeting of the course.

#### **Course Website**

https://canvas.wisc.edu/courses/125443

#### **Course Description and Mission Statement**

Chemistry 344: Introductory Organic Chemistry Laboratory introduces the basic synthesis, purification, and characterization techniques of organic chemistry, along with critical interpretation of experimental and theoretical data. The course is primarily face-to-face in the classroom and laboratory, with some online components. The laboratory includes material from both Chemistry 343 and 345.

(Intermediate level; physical science breadth; counts as L&S credit)

Chemistry 344 will provide students with opportunities to learn organic chemistry theory and practice via effective pedagogical and assessment techniques. Students will perform organic chemical reactions in a safe manner, collect authentic data using state of the art instrumentation, analyze those data using modern physical organic chemistry concepts, and explain their reasoning in written and visual format.

#### **Course Requisites**

Completion of or concurrent enrollment in CHEM 345. Students may not repeat CHEM 344 if previously earned credit for CHEM 344. There is no requisite of a C or better in CHEM 345, since we permit concurrent enrollment.

#### **Course Meeting times**

Monday & Wednesday: 7:45 – 11:50 AM, 1:20 – 5:25 PM, 5:40 –9:45 PM Tuesday & Thursday: 7:45 – 11:50 AM, 1:20 – 5:25 PM, 5:40 –9:45 PM

The course meets in various classrooms and laboratories in the chemistry department. Consult your individual schedule for details on the location of your course section.

## **CHEM 344 Laboratory Manual Table of Contents**

- 1. Safety
- 2. Keys to Success in the Lab
- 3. Separation of a Mixture by Extraction
- 4. Computational Molecular Modeling
- 5. Nucleophilic Substitution Reactions  $(S_N 1/S_N 2)$
- 6. Elimination Reactions (E1/E2)
- 7. Oxidation of 4-*tert*-Butylcyclohexanol
- 8. Reactions of Nitrogen Functional Groups
- 9. Wittig Synthesis of Ethyl Cinnamate
- 11. EAS Nitration of Bromobenzene
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- 14. Formation of a Biaryl by Suzuki-Miyaura Coupling
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## **Appendices**

- A. Spectroscopy Sample Submission and Data Analysis Information
- F. Obtaining Your NMR and GC-MS Data
- I. Recommended MestReNova Setup; Work-up of <sup>1</sup>H- and <sup>13</sup>C-NMR Data
- S. <sup>1</sup>H-, <sup>13</sup>C-, and <sup>19</sup>F-NMR Chemical Shift Correlation Tables
- V. <sup>1</sup>H-NMR Chemical Shift Parameters for Aliphatic, Vinyl, and Aryl Protons
- Y. <sup>1</sup>H- and <sup>13</sup>C-NMR Chemical Shifts for Common Solvents in CDCl<sub>3</sub>
- Z. Physical Properties of Common Solvents
- AA. Typical  $J_{H-H}$ ,  $J_{H-F}$ , and  $J_{C-F}$  Coupling Values
- CC. Infrared Absorption Correlation Table
- DD.  $pK_a$  Table
- EE. Cyclohexane A-values; Isotope Data for Common Nuclei
- FF. Table of Common EI-MS Fragmentations
- GG. Periodic Table of Pauling Electronegativity Values
- HH. General Procedure for Recrystallization
- II. Thin-Layer Chromatography Background

## Spring 2019 CHEM 344 Lab Schedule

Date		Monday	Tuesday	Wednesday	Thursday
Jan	21	No Class	No Class	Spectroscopy I	Spectroscopy I
	28	check-in/Spectroscopy II	check-in/Spectroscopy II	Spectroscopy III	Spectroscopy III
Feb	4	WebMO I	WebMO I	Review 1/WebMO II	Review 1/WebMO II
	11	Spec/WebMO Exam	Spec/WebMO Exam	Extraction I	Extraction I
	18	Extraction II	Extraction II	Oxidation	Oxidation
	25	Review 2	Review 2	$S_N 1$	$S_N 1$
Mar	4	$S_N 2$	$S_N 2$	E1	E1
	11	E2	E2	Midterm exam	Midterm exam
	18	Spring break	Spring break	Spring break	Spring break
	25	EAS nitration	EAS nitration	EAS acylation	EAS acylation
Apr	1	Review 4	Review 4	Imine	Imine
	8	Aldol	Aldol	Review 5	Review 5
	15	Wittig	Wittig	Suzuki	Suzuki
	22	Review 6	Review 6	No Class	No Class
	29	Review 7	Review 7	No Class	No Class

**Review** – no laboratory work scheduled. In-class active-learning activities led by TA. Additionally, your TA will be available to answer questions and assist with laboratory reports. Lab reports may be due on review days (see lab report hand-in schedule below).

Friday March 29 last day to drop class Friday May 3 last day of classes

Final Exam: 05-05-2019, 7:45 AM, Locations TBD

## Spring 2019 CHEM 344 Lab Report Submission Schedule

Date		Monday	Tuesday	Wednesday	Thursday
Jan	21	No Class	No Class		
	28				
Feb	4				
	11			WebMO	WebMO
	18				
	25	Extraction	Extraction	Oxidation	Oxidation
Mar	4				
	11	$S_N 1/S_N 2$	$S_N 1/S_N 2$		
	18	Spring break	Spring break	Spring break	Spring break
	25	E1/E2	E1/E2		
Apr	1	EAS nitration	EAS nitration	EAS acylation	EAS acylation
·	8			Imine	Imine
	15	Aldol	Aldol		
	22	Wittig	Wittig	Suzuki	Suzuki
	29		_	_	

Lab reports must be handed to your TA at the start of the discussion session. Work submitted after the submission deadline will be considered late and graded according to the late work policy (see page xiv).

## Spring 2019 CHEM 344 Lab Report Return Schedule

Date		Monday	Tuesday	Wednesday	Thursday
Jan	21	No Class	No Class		
	28				
Feb	4				
	11				
	18	WebMO	WebMO		
	25				
Mar	4	Extraction	Extraction	Oxidation	Oxidation
	11				
	18	Spring break	Spring break	Spring break	Spring break
	25	$S_N 1/S_N 2$	$S_N 1/S_N 2$		
Apr	1	E1/E2	E1/E2		
	8	EAS nitration	EAS nitration	EAS acylation	EAS acylation
	15			Imine	Imine
	22	Aldol	Aldol	Wittig	Wittig
	29	Suzuki	Suzuki		

#### **Chemistry 344 Learning Outcomes**

Students will:

- understand the role of spectroscopy and spectrometry in organic structure elucidation and be able to use spectral data to analyze pure samples and product mixtures;
- understand and be proficient in the safe use of basic apparatus, glassware, and techniques for the synthesis, isolation, and purification of organic molecules;
- will be able to use computational chemistry to support their data analysis, and to predict and rationalize experimental outcomes;
- will be able to use the electronic and molecular structure of organic molecules to predict and rationalize chemical reactivity;
- will be able to use molecular orbitals, potential energy surfaces, and electron-pushing reaction mechanisms to describe chemical reactivity with an emphasis on the reactions of alcohols, alkyl halides, aromatic compounds, and carbonyl-containing compounds.

#### **Chemistry 344 (2 credits) Credit Hour Accounting**

The University defines one credit as the learning that takes place in *at least* 45 hours of learning activities, which include time in lectures or class meetings, in person or online, labs, exams, presentations, tutorials, reading, writing, studying, preparation for any of these activities, and any other learning activities. Learning in Chemistry 344 is spread across multiple platforms and the numbers provided below are a good-faith estimate of the time required, exact hours will vary.

Activity	Time in class (hr)	Time out of class (hr)	
Spectroscopy 1 - 3	9	1	_
WebMO 1 & 2	8	2	
Extraction 1 & 2	5.5	3	
Bleach Oxidation	3.5	3	
$S_N 1/S_N 2$	3.0	5	
E1/E2	5	5	
EAS - nitration	2.5	3	
EAS - acylation	2.5	2	
Imine	1.5	2	
Wittig	2.5	2	
Aldol	2.5	2	
Suzuki	2	3	
Review Days (6)	6		
Exam 1	2	3	
Exam 2	2	3	
Final Exam	2	3	
Total	59.5	42	101.5

#### **Course Communication**

Email, office hours, and Piazza are the primary modes of non-classroom communication in CHEM 344. This is a demanding course and you will require assistance from your instructors to have success and gain the most from the experience.

For all logistical, enrollment, and excused absence-related issues it is acceptable to contact your instructors via email. Please send a single email to all course instructors (page ii) and your TA. Use "CHEM 344" in the subject line. For all other course content-related communications, students must use Piazza (see the course Canvas page for details).

Piazza Communication or Office Hours	Email Communication
Help with pre- or post-lab questions	Registration, scheduling, or enrollment
General organic chemistry background questions	Excused absence
Course schedule	Individual course-related issues
Quiz or exam content	McBurney Faculty Notifications
Issues involving retrieving/solving spectra	Health-related accommodations
Issues accessing/using course software	
Questions regarding Academic Integrity issues	

#### **McBurney Accommodations**

If you have McBurney accommodations, please request a Faculty Notification Letter through McBurney Connect. You are encouraged to email the course instructors and your TA if you would like to arrange an individual meeting. Please do this as close to the start of the semester as possible to allow us to better accommodate your needs. Accommodations for exams and quizzes will be coordinated with the chemistry undergraduate office.

#### McBurney Disability Resource Center syllabus statement

The University of Wisconsin-Madison supports the right of all enrolled students to a full and equal educational opportunity. The Americans with Disabilities Act (ADA), Wisconsin State Statute (36.12), and UW-Madison policy (Faculty Document 1071) require that students with disabilities be reasonably accommodated in instruction and campus life. Reasonable accommodations for students with disabilities is a shared faculty and student responsibility.

Students are expected to inform the course instructors and their TA of their need for instructional accommodations by the end of the third week of the semester, or as soon as possible after a disability has been incurred or recognized. Instructors and TAs will work either directly with you or in coordination with the McBurney Center to identify and provide reasonable instructional accommodations. Disability information, including instructional accommodations as part of a student's educational record, is confidential and protected under FERPA.

http://mcburney.wisc.edu/facstaffother/faculty/syllabus.php

#### **Health-related Accommodations**

If you have health-related issues (such as severe allergies, chemical sensitivity, respiratory illnesses, etc.) that may impact your participation in the lab course, please contact all course instructors (page ii) to arrange a meeting. Students who are pregnant or are trying to become pregnant should contact a laboratory director as soon as possible prior to the start of lab work.

#### **Institutional statement on diversity**

Diversity is a source of strength, creativity, and innovation for UW-Madison. We value the contributions of each person and respect the profound ways their identity, culture, background, experience, status, abilities, and opinion enrich the university community. We commit ourselves to the pursuit of excellence in teaching, research, outreach, and diversity as inextricably linked goals.

The University of Wisconsin-Madison fulfills its public mission by creating a welcoming and inclusive community for people from every background – people who as students, faculty, and staff serve Wisconsin and the world.

https://diversity.wisc.edu/

## **Grades and Grading Philosophy**

## **Laboratory Reports**

Experiment	<b>Total Points</b>
Chapter 3 Extraction	55
Chapter 4 WebMO	45
Chapter 5 S <sub>N</sub> 1 & S <sub>N</sub> 2	65
Chapter 6 E1 & E2	60
Chapter 7 Oxidation & TLC	40
Chapter 8 Imine	45
Chapter 9 Wittig	45
Chapter 11 EAS Nitration	55
Chapter 12 EAS Acylation	50
Chapter 14 Suzuki	45
Chapter 17 Aldol	45
<b>Total points</b>	550

#### **Exams**

The first exam of the semester covers the spectroscopy and WebMO material and is worth 75 pts.

In addition, 2 cumulative exams covering all techniques, reactions, and concepts in CHEM 344 are given (*i.e.* one mid-term exam and one final exam). Each cumulative exam is worth 100 points.

Assessment	Points
Spectroscopy/WebMO Exam	75
Midterm Exam (materials through E1/E2)	100
Final Exam (all materials)	100
Total exam points	275

In total, there are 550 + 275 = 825 points available in the course.

#### Grades must reflect achievement.

The instructors of this course do their utmost to ensure that your grade accurately reflects your achievement as measured by a variety of assessments. Your achievement will be assessed via quizzes, exams, pre-laboratory assignments, and post-laboratory data analysis.

All TAs use the same grading rubrics for lab reports in order to ensure grading consistency within the course. **The final letter grade is not based upon total course points.** Instead, the grade is based upon a normalized score (*z-score*) which can be compared to all students in the course. Note that adjustments will be made to this method for particularly high achieving sections.

To determine your normalized score on any particular work, apply the following formula:

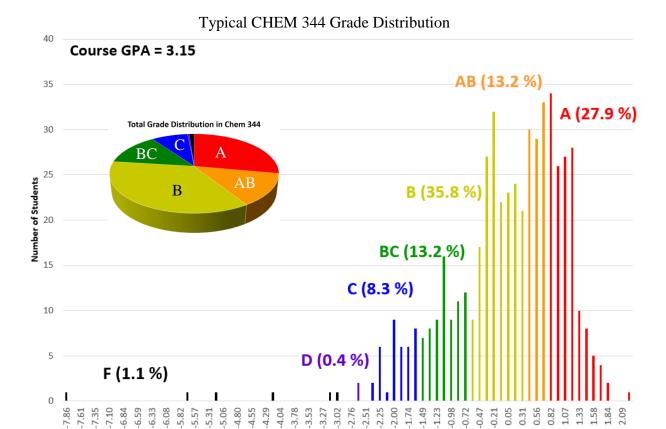
$$Normalized \ Score = \frac{Your \ Score - Your \ Section \ Average \ Score}{Your \ Section \ Standard \ Deviation}$$

We will provide regular grade reports via email to help you track your progress.

The overall GPA of the course will be approx. 3.15, though it will be slightly higher in some sections and slightly lower in others. The final grade distribution will resemble the pie chart on page xii.

## **Common Chemistry 344 Grading Questions/Clarifications**

Common Question/Myth	Clarification
There are only three A grades assigned	There is no predetermined number of letter grades. In the
per section.	recent past, there have been as many as 7 As and as few
	as 2 As in a section of 18 students.
I got 82% of the course points, what is	CHEM 344 does not use arbitrary grade cut-offs of 90%
my letter grade?	= A, 80% = B, etc. An entirely standardized grading
	scheme is not viable in a large laboratory course which
	has many units of assessment and up to 36 different TAs.
	Instead of arbitrary cut-offs, grades are determined by the
	normalized score for each student within the section.
Grading is solely based upon TA	All TAs follow detailed guidelines for grading lab reports
opinion/preference. My TA is a	and standard keys for exams (all of which are written by
"hard grader" and so my grade will	the course instructors), but there is always some variation
be lower than if I had another TA.	in grading. This is why a normalized score is used for
	grade calculations.
Grades cannot be estimated until the	The normalized score for any report, quiz, or exam is
end of the course.	calculated via the formula shown below.
	$Normalized\ Score = rac{Your\ Score - Your\ Section\ Average\ Score}{Your\ Section\ Standard\ Deviation}$
	Individual grade reports will be sent to you periodically
	during the semester.
My friend in another section got a	The raw point scores themselves do not matter.
higher score on the exam than I and	Only the normalized score in your section matters for all
my classmates do, does that mean we	exams and lab reports.
all failed?	



To reiterate the first premise of the Chemistry 344 grading philosophy, **grades will be based solely upon achievement**. The following will not be taken into consideration when determining your final grade:

- Effort/hard work
- Time spent on coursework
- Number of posts/replies/etc. on Piazza
- Attitude toward organic chemistry
- Attendance and/or participation in discussion or office hours
- How much you perceive your instructor(s) like/dislike you
- Needing a specific letter grade for graduate or professional school admissions
- Wanting a specific letter grade to maintain or improve your GPA
- Wanting to take a course for which Chem 344 is a prerequisite

#### **CHEM 344 Laboratory Safety Policy Summary**

You are required to follow the rules and guidelines discussed in the lab safety video presentation and Chapter 1 of this manual. In summary:

Place book bags, coats etc. on the hangers and shelves at the front of the lab. Do not block the pathway, exit, or fire extinguisher with your belongings. Do not store bags, coats, etc. in the corridor.

A lab coat must be worn at all times in the laboratory.

Your entire foot must be covered by shoes or a combination of shoes and socks. No sandals, flip-flops, open-toed/heeled shoes.

Regardless of weather conditions, trousers covering the entire leg must be worn in the lab. Shorts are not acceptable.

Gloves and goggles must be worn at all times in the lab. Gloves must be removed and discarded before leaving the lab.

Do not eat/drink/chew in the lab. Do not inhale or ingest chemicals.

No smoking or open flames.

Cell phones, laptops, music devices, and earphones/earbuds are not allowed in the lab.

#### Follow all safety instructions given by your TA!

#### Access to the lab

The only times that you are allowed access to the organic teaching labs are during the scheduled meeting times for the lab session in which you enrolled. You may not work in the lab at any other time. Unless you are enrolled in the scheduled lab session you are not allowed in the lab. There are no visitors allowed.

#### Lab equipment

You have been assigned a lab bench space and a drawer containing lab equipment. During checkin, make sure that every item that is listed on the yellow check-in sheet is present in the drawer and is in good condition. Replace any piece of glassware that is chipped or cracked! Wash any glassware you consider to dirty. You are responsible for keeping all equipment clean and in good condition, and accounting for it at the end of the semester.

#### **CHEM 344 Exam Conflict Policy**

Instructors of daytime courses often schedule exams that conflict with a scheduled CHEM 344 class meeting time. If you miss a CHEM 344 lab session due to an exam given in another course, you will be required to use your excused absence (see page xv) to cover the missed lab session. You will not be allotted any extra excused absences.

According to the timetable and Faculty Document 1585a:

"Instructors who schedule evening exams should make every possible effort to accommodate students with unavoidable conflicts. It is the instructor's responsibility to assure that all students with conflicts between daytime courses with evening exams and evening courses are treated fairly and without penalty.

If a scheduling conflict exists between the evening exam of a daytime course and a regularly scheduled evening course, then the evening course takes precedence over the exam."

It is the responsibility of the instructor who schedules the conflicting exam to offer you an alternate exam time that does not conflict with your CHEM 344 or other class time. Thus, it is your responsibility to check for any exams that conflict with your CHEM 344 class time and contact the instructor of the conflicting course as soon as possible so an accommodation can be made. No make-up lab sessions are available to students who miss a CHEM 344 lab session due to a conflicting exam.

#### **CHEM 344 Late Work Policy**

The schedule for submission of all graded material is available on page v of this manual. Partial or complete lab reports submitted up to 24 hours after the printed submission deadline will receive a maximum of 50% of the total points available (*i.e.* your lab report will be graded and the points you obtain multiplied by 0.5). Partial or complete reports submitted >24 hours after the printed submission deadline will not be graded for credit (*i.e.* you will receive 0 pts for the work).

Pre-lab work submitted after the start of the discussion session will not be graded for credit.

It is your responsibility to be aware of all deadlines for submission of work to your TA.

#### **CHEM 344 Lab Absence Policy**

You are expected to attend every lab session during the course (and to arrive on time). You may, however, need to miss a lab session due to circumstances beyond your control. The course policies and procedures that you need to follow are detailed below. It is your responsibility to understand and follow these policies.

#### What if I need to miss a lab session?

All CHEM 344 students are granted one (1) Excused Absence (EA). The EA can be used if you need to miss a laboratory session. *The EA cannot be used on the day of an exam. Students who miss an exam will receive a score of zero*.

#### Who should I inform, and when?

By email, you should inform your laboratory TA, Dr. Hill, Dr. Ellison, and Dr. Esselman as soon as you know that you will use the EA. (Write one email, copy everyone listed above). You must submit the EA form to your TA **no later** than the returning lab session. The EA form is printed on page xvii of this lab manual.

#### Will using the EA affect my grade?

You will neither gain an advantage nor be penalized by using the EA. You are required to complete the lab report for the day you missed and submit it at the regularly scheduled time using stock data downloaded from the course Canvas page. Any lab reports due on the day you are absent must be submitted to your TA at the start of the next discussion session. The points associated with the observations during the laboratory session will be prorated from the score of your pre-lab assignment (whether it is a one day or multiple day lab). The EA cannot be used retroactively to negate a lower-than-desired lab report score.

#### What happens if I am late to the pre-laboratory discussion?

Each meeting of the course begins at 7:45 AM, 1:20 PM, or 5:40 PM. You are expected to attend each session on time. You will not be allowed into the laboratory for the day's experimental work without permission from one of the laboratory directors if you are more than 15 minutes late to the session. This is critical for your success in the laboratory as well as for the safety of all students and TAs. You may be required to use your excused absence if you are late for the session.

## What happens if I have not completed or submitted the pre-lab material?

You will not be allowed into the laboratory for the day's experimental work without permission from one of the laboratory directors. Appropriate preparation is critical for your success in the laboratory as well as for the safety of all. You may be required to use your excused absence if you do not submit the pre-lab material.

Excused Absence Form for CHEM 344 Spring 2019		
Student name:		
TA name:		
Experiment and date missed:		
Student signature:		
TA signature:		
Date:		
Hand this form to your TA no later than the day you return from your absence.		

#### Maximizing your learning in an ethical manner

The instructors of CHEM 344 continually aim to improve student learning and update the curriculum. Integral to this mission is the development of new experiments and assessments. For existing experiments, this goal is partly achieved by the introduction of new pre- and post-lab questions each semester. We also regularly introduce new experiments into the CHEM 344 repertoire. The majority of you will not take another organic chemistry course, but the thought processes, ability to learn and communicate new concepts, and data analysis skills you acquire from CHEM 344 will be invaluable in your future studies and careers. With this in mind, we strongly encourage you to approach the data analysis and pre-/post-lab assessments in this course using of all of the resources provided and endorsed by the teaching staff. These include instructor office hours/drop-ins, TA office hours, Piazza, talking to your TA and classmates in lab, and organized study groups.

It is an unfortunate fact that students often attempt to take shortcuts in the course by submitting work copied from their classmates or previous students of the course. We are aware that CHEM 344 computational/spectral data and answers to lab report questions from previous semesters are available to many of you, and that there is a temptation to use these resources. Not only does this behavior hinder your learning of the material and the growth you should experience in the course, it is unethical, fraudulent, and constitutes academic misconduct.

In this course, as in all scientific endeavors, claiming credit for the work of another is academic misconduct. Despite unambiguous communication of our expectations, multiple students have ignored the academic misconduct policies of this course in recent semesters. All of them were assessed a significant point penalty for the plagiarized work, and several were awarded a grade of F in the course and had a letter detailing their misconduct placed on file with the Dean of Students office. Clearly, we treat academic misconduct with the seriousness it deserves, and are obliged to deal with all cases that are brought to our attention (see pages xx and xxi in lab manual and <a href="https://www.students.wisc.edu/doso/academic-integrity/">https://www.students.wisc.edu/doso/academic-integrity/</a>). At this point in your academic career, you are expected to be fully aware of the requirements for academic integrity, and the definitions, scope, and consequences of academic misconduct at UW-Madison. We urge you to make sure that all experimental, computational, and spectral data submitted for grading in CHEM 344 have been obtained and generated by you from your material, or have been obtained in accordance with our stock data policy.

We approach every semester with optimism that we have designed a challenging course that is rich with opportunities for deep learning. All of the teaching staff strive to make CHEM 344 a rewarding experience for each student. The main determinant of your experience and learning outcome in this course, however, is you. We encourage you to engage with the course material and all available resources in a manner that is both ethical and which maximizes your learning.

The course and university academic misconduct policies are outlined on the subsequent pages.

You are required to sign and submit an academic integrity declaration form (page 1-7) prior to beginning laboratory work.

#### **CHEM 344 Academic Integrity Policies**

All work submitted by a student for grading in CHEM 344 is required to be the product of that student alone. This will be assumed to be the case unless the work is clearly labeled otherwise.

All laboratory reports are submitted individually; there are no partner or group laboratory reports.

All laboratory work is performed by the student and the data obtained are recorded directly into the lab notebook during the lab session. All data recorded must pertain to actual measurements and observations made by the student on their own experiment (even when working in pairs).

Calculations, interpretation, and assignment of NMR, GC-MS, IR, WebMO, or any other form of data, answers to pre- and post-lab questions, and all other items submitted for grading must be the original work of each individual student (even when working in groups).

Submission of work copied directly from any another student (including a lab partner), the lab report of a previous student, a textbook, web-site, journal article, etc., without citation or reference, or possession of another student's lab report (graded or ungraded) are all considered to be plagiarism and will be dealt with according to University guidelines for academic misconduct. Enabling any of the above actions is also considered to be academic misconduct and will be dealt with according to University guidelines. At a minimum, such behavior will result in a significant point deduction for each lab report in question.

Information on academic misconduct is available from the website of the Office of the Dean of Students (http://students.wisc.edu/doso/acadintegrity.html).

It is your responsibility to understand the definition, scope, and consequences of academic misconduct.

#### Generation and use of WebMO data

You are required to understand and adhere to the following policies pertaining to the generation and use of WebMO data:

- As with all material submitted for grading in CHEM 344, all WebMO data and images submitted for grading by you must be entirely your own work. Specifically, this means that all WebMO-related images, job numbers, and data that appear in your lab report must have been generated by you in your own WebMO account.
- Each WebMO calculation you run will have a unique 6-digit job number. The unique job number for each relevant calculation must be written on the lab report cover sheet, and must correspond to the data presented in your lab report.
- Sharing of a WebMO account between 2 or more students is not permitted under any circumstances. Should evidence suggest that a single account has been used by multiple students, all students involved will be under suspicion of academic misconduct. Information on academic misconduct is available from the website of the Office of the Dean of Students (https://www.students.wisc.edu/doso/academic-integrity/).
- The WebMO activity of all students enrolled in CHEM 344 is checked regularly during the semester. Should evidence suggest that data have been plagiarized, all students involved will be under suspicion of academic misconduct.
- Keep your web browser up to date "I couldn't see the molecule/my computer would not start/etc." is not a valid reason for sharing data or not doing the calculations. Links to browsers such as Firefox and Chrome are provided on the course Canvas page.

**Summary**: you are required to perform every WebMO calculation yourself in your own WebMO account. Sharing of WebMO data between you and your lab partner or anyone else will be considered as academic misconduct. All data you present must be traceable to specific 6-digit job numbers. **Do not delete any data from your account. You must keep these jobs as a record of your work.** 

It is your responsibility to understand the definition, scope, and consequences of academic misconduct.

#### CHEM 344 NMR/GC-MS/IR Stock Data Policy

All of the experiments in CHEM 344 involve the post-lab analysis of spectroscopic data obtained from the compound(s) that you synthesized in the lab. The data will be posted on the appropriate experiment page of the CHEM 344 course Canvas page.

IR and GC-MS data are provided as a pdf file.

You are required to use MestReNova to process and analyze your own experimental NMR data. MestReNova is available for download from the University of Wisconsin chemistry department website.

In cases where your experimental NMR data are unusable, you are required to use MestReNova to process and analyze the stock FID data file for the specific experiment. The stock data file contains authentic student data (i.e. usable, but not necessarily perfect data) and will be posted on the course Canvas page next to the experimental data.

#### Points to note:

- A spectrum generated from stock FID data **must** be accompanied by an explanation of why the stock data were necessary, along with a hardcopy of your own experimental NMR spectrum.
- You will not receive credit for the NMR portion of the lab report if you submit only the prepared stock spectrum (watermarked "Stock Spectrum").
- You are required to process and work-up the spectrum yourself in MestReNova.
- Do not use another student's NMR data or spectrum (see preceding pages for background).

Valid reasons for using stock data	Invalid reasons for using stock data
fid file missing (sample not run)	Impurities are present in my experimental data
NaN error (no data in fid file)	I can't be bothered to find my data.
GC-MS only shows baseline	My GC-MS has an extra signal.
Only baseline noise/no signals present	I don't know how to find my data/install MNova

Post on Piazza or bring your data to office hours if you have any questions on these policies.

#### **CHEM 344 Suggested Reading**

There is no required textbook for CHEM 344, but it is assumed that you have access to a copy of "Organic Chemistry" by Loudon, 6<sup>th</sup> Ed. and CHEM 343/345 lecture notes.

The content of a discussion section will be based upon the material found in the corresponding chapter of the textbook and the current CHEM 344 lab manual. However, your TA may introduce concepts that are not covered in the textbook or the lab manual. It is your responsibility to be familiar with <u>all</u> concepts covered in the discussion. It is strongly recommended that you read the textbook content prior to attending the pre-lab discussion.

	Experiment	Location in Loudon 6 <sup>th</sup> Ed.
3	Mass spec/IR and NMR Separation of a Mixture by Extraction	Chapters: 12, 13, 14.3B, 14.3C, 15.2, 16.3, 19.3, 20.3, 21.4, 23.4, AII, AIII, & AIV Chapters: 3, 8.6, 18.7 20.4, & 23.5
4	Computational Molecular Modeling	Chapters: 1, 12, 13, 15.1, 16.1-16.3, 19.7, 26.2
5/20	Nucleophilic Substitution Reactions ( $S_N1/S_N2$ )	Chapters: 9, 10.3, 18.7, & 23.6
6	Elimination Reactions (E1/E2)	Chapters: 9 & 10.2
7	Oxidation of 4-tert-Butylcyclohexanol	Chapters: 6.6, 10.5, & 10.6
8	Reactions of Nitrogen Functional Groups	Chapters: 19.11, 21.8, & 23.7
9	Wittig Synthesis of Ethyl Cinnamate	Chapters: 19.13
10	Stereochemistry of a Carbonyl Reduction	Chapters: 10.9, 13.3, & 19.8
11	Electrophilic Aromatic Substitution – Nitration	Chapters: 16, 18.9, 23.9, 23.10, 26.3, & 26.4
12	Electrophilic Aromatic Substitution – Acylation	Chapters: 16, 18.9, 23.9, 23.10, 26.3, & 26.4
13/21	Grignard Reaction	Chapters: 9.8, 19.9, & 21.10
14	Formation of a Biaryl by Suzuki-Miyaura Coupling	Chapters: 18.5 & 18.6
15	Cu/TEMPO Catalyzed Aerobic Oxidation of a Primary Alcohol	Chapters: 10.5, 10.6, & 17.5
16	Biginelli Multicomponent Reaction	Chapters: 19.7 & 19.11
17	Aldol Condensation	Chapters: 22.4
19	Radical Bromination of Bibenzyl	Chapters: 5.6 & 17.2
22	Nucleophilic Aromatic Substitution (S <sub>N</sub> Ar)	Chapters: 18.1 - 18.4
23	Wittig Synthesis – Diels-Alder Reaction	Chapters: 15.3, 19.13, 28.1, 28.3

