Course Syllabus

Jump to Today ✎ Edit

POINT 1902 LOMA
NAZARENE UNIVERSITY

Department of Chemistry

CHEMISTRY 3051

Organic Structure Elucidation

2 Units (plus 0 unit CHE1003L corequisite laboratory)

Fall 2026 - Quad 2

	Instructor title and name: Dr. Katherine Maloney, Professor of Chemistry
Meeting times: MWF 12:15 - 1:20 pm	**Phone:** 619-849-3425
Meeting location: RLC 102	**Email:** kmaloney@pointloma.edu (mailto:kmaloney@pointloma.edu)
Final Exam: 10:30 am -1:00 pm on Monday, December 14th	**Office hours:** • Tuesday 9-10 am, 12-1 pm • Wednesday 3:30-4:30 pm (sometimes) • Friday 3:30-4:30 pm • and by appointment in Rohr Science 316 (if 1-3 students) or 350 (if >3 students)

PLNU Mission

To Teach ~ To Shape ~ To Send

Point Loma Nazarene University exists to provide higher education in a vital Christian community where minds are engaged and challenged, character is modeled and formed, and service is an expression of faith. Being of Wesleyan heritage, we strive to be a learning community where grace is foundational, truth is pursued, and holiness is a way of life.

COURSE DESCRIPTION

From the PLNU Catalog: Introduction to modern spectrometric techniques for elucidating the structure of organic compounds, including one- and two-dimensional nuclear magnetic resonance spectroscopy, infrared spectroscopy and mass spectrometry. Course includes a weekly laboratory. Offered on a Quad basis.

COURSE LEARNING OUTCOMES

At the end of the course you will be able to:

1. Describe principles underlying modern organic spectroscopic methods.
2. Acquire spectroscopic data using the PLNU Fourier transform infrared (FTIR) spectrometer and nuclear magnetic resonance (NMR) spectrometer on unknown organic molecules.
3. Process and interpret electron impact mass spectrometric (EIMS), IR, and 1D and 2D NMR data to elucidate the structures of unknown organic molecules.
4. Write reports in the style of a *Journal of Natural Products* manuscript describing the structure elucidation of two unknown compounds.

REQUIRED TEXTS AND RECOMMENDED STUDY RESOURCES

Introduction to Spectroscopy (https://www.cengage.com/c/introduction-to-spectroscopy-5e-pavia/9781285460123PF/?filterBy=Student) , by Pavia, Lampman, Kriz and Vyvyan, Cengage Learning, 5th Edition, **2017**. *Required*

Pocket Guide to Biomolecular NMR (https://link.springer.com/book/10.1007/978-3-642-16251-0) , by Doucleff, Hatcher-Skeers, and Crane, Springer, **2011**. *Recommended.* Necessary readings from this excellent text will be provided.

INTRODUCTION PROBLEMS

A few short Introduction Problems will be assigned daily and will often be used to begin class dis[illegible]n. The questions will be based on that day's reading assignment and will cover new material. You w[illegible]k

on these problems outside of class. Answers to Intro Problems will be uploaded to Canvas to verify *participation* and *effort*.

ASSIGNMENTS

Problems requiring greater thought and reflection will be completed outside of class and will be due periodically throughout the course. (See the course schedule for due dates.) In the interest of providing rapid feedback despite the large class size, only one or two of the assigned problems will be graded for correctness, with the rest graded only for completion. *(Note that you won't be told which problem will be graded, so you would be wise to do your best on each!)* You are strongly encouraged to compare *all* your answers to the answer key, which will be posted on Canvas after the due date.

SPECIAL TOPICS PRESENTATIONS

Elucidating the complete structures of organic molecules can often require more niche techniques that are beyond the scope of this quad class; often these are highly dependent on the type of molecule being studied. Some of these techniques have come into common use only recently. In small groups, you will do a deep dive into one special method of your choice and present that method to the rest of the class.

EXAMS

There will be one midterm exam (one hour, in class) and one cumulative final exam (two and a half hours) during finals week. See the course schedule for the dates of the exams.

Makeup examinations will be given only for excused absences. In such cases, appropriate documentation must be provided within two days of the end of the excused absence.

LABORATORY

In the laboratory component of this course, you will apply what you are learning in class to the structure elucidation of two organic unknowns. Since you will be acquiring your own data on each instrument (of which there is typically only one), you may need to sign-up online for times during the week to perform the lab. For lab each week, you and a partner will *(1)* acquire data using PLNU instrumentation, *(2)* perform an in-depth analysis of the data, and *(3)* answer analysis questions regarding your results. Two formal reports (one for each unknown) will also be due during the semester. Additional details regarding each aspect of the laboratory can be found in the lab manual, which will be distributed in the second week of class.

COURSE SCHEDULE AND ASSIGNMENTS

Note: This schedule is subject to change. Any substantial changes (i.e. changes to anything other than *Details* or *Readings*) will be announced on the *Announcements* page in Canvas, and modified here in the *Syllabus*.

CHE3051 Schedule : Full Calendar

	Date	Topic/Assignment	Reading	In Lab
0	Mon 10/19	Quad 1		
	Wed 10/21	Intro to organic structure analysis	How to solve the NYT Crossword Puzzle	
	Fri 10/23	*Fall Break - no class*		
1	Mon 10/26	Mass spectrometry, part I: the molecular ion	-*Skim* Chapter 3 -*Read* Sections 3.6, 3.7, 1.4, 1.5	
	Wed 10/28	Mass spectrometry, part II: fragmentation	-*Read* Sections 4.1 & 4.2 -*Skim* the rest of Chapter 4	Unknown 1: GCMS data; Reading & writing about structure elucidation
	Fri 10/30	Infrared spectroscopy	-*Read* Sections 2.4, 2.8, 2.9, 2.23 -*Skim* the rest of Chapter 2	
2	Mon 11/2	Interpreting IR spectra	-Pavia Chapter 2	**GCMS Questions Due Monday**
	Wed 11/4	Intro to 1H NMR spectroscopy **Assignment 1 Due** (*MS & IR)*	-Doucleff, Chapter 1	Unknown 1: IR
	Fri 11/6	Chemical shift and equivalence	-*Read* Sections 5.8, 5.9, 5.13 -*Skim* the rest of Chapter 5	
3	Mon 11/9	Intro to spin-spin coupling	-Doucleff, Sections 2.1, 2.2 -Pavia, Sections 5.1, 7.5, 7.6	**IR Questions Due Monday**
	Wed 11/11	Coupling constants and exchange	-Pavia, Sections 7.1, 7.2	Unknown 1: 1D NMR
	Fri 11/13	Intro to 13C NMR spectroscopy	-Pavia*, skim* Sections 6.2-6.9 -*Read* Sections 6-6.1, 6.11-6.13, 6.17	
4	Mon 11/16	13C Chemical shifts and DEPT **Assignment 2 Due** *(1H NMR)*	-Pavia, Sections 6.10, 9.4	**1D NMR Questions Due Monday**
	Wed 11/18	Intro to 2D NMR	-Doucleff, Chapter 2 -Pavia, *read* Section 9.6 -*flip through* Sections 9.7-9.10	Unknown 2: GCMS & IR
	Fri 11/20	**Midterm exam (MS, IR, 1D NMR)**		
5	Mon 11/23	1H-1H COrrelation SpectroscopY (COSY)	-Pavia, Section 9.7	**Unknown 1 Report Due Monday**
	Wed 11/25	*Thanksgiving Break*		
	Fri 11/27	*Thanksgiving Break*		
6	Mon 11/30	One-bond heteronuclear experiments: HETCOR, HSQC/HMQC **Assignment 3 Due** *(13C NMR)*	-Pavia, Section 9.7B, 9.8	
		Heteronuclear multiple bond		Unknown 2:

	Wed 12/2	correlation (HMBC) and Heteronuclear 2-Bond Correlation (H2BC)	TBD	1D & 2D NMR
	Thu 12/3	***Field trip to the DEA Lab in Vista***		
	Fri 12/4	NOESY	-Doucleff, Section 3-3.2 -Pavia, Sections 6.5, 9.10	
7	Mon 12/7	Special Topics presentations	TBD	**Unknown 2 Report Due Monday**
	Wed 12/9	Special Topics presentations	TBD	Dereplication: SMART NMR & GNPS
	Fri 12/11	Solving structure elucidation problems **Assignment 4 Due** *(2D NMR)*	-Pavia, Section 9.11, Chapter 11	
8	Mon 12/14	**Comprehensive Final Exam**	10:30 am - 1:00 pm	Dereplication Questions Due

Full Calendar

ASSESSMENT AND GRADING

The activities described above will contribute to your total course grade according to the following distribution:

Assignments	10%
Intro Problems, EdPuzzles & Participation	10%
Laboratory	30%
Stereochemistry Presentation	10%
Midterm exam	15%
Final exam	25%

Student grades will be posted in the Canvas grade book throughout the course. Letter grades will be assigned at the end of the course based on your percentage of total possible points, according to the following scale:

A	B	C	D	F
A 93-100	B+ 87-89	C+ 77-79	D+ 67-69	F Less than 59
A- 90-92	B 83-86	C 73-76	D 63-66	
	B- 80-82	C- 70-72	D- 60-62	

FINAL EXAMINATION POLICY

Successful completion of this class requires taking the final examination on its scheduled day. The final examination schedule is posted on the **Traditional Undergraduate Records: Final Exam Schedules (http://www.pointloma.edu/experience/academics/class-schedules)** site. If you find yourself scheduled for three (3) or more final examinations on the same day, you are authorized to contact each professor to arrange a different time for one of those exams. However, unless you have three (3) or more exams on the same day, no requests for alternative final examinations will be granted.

STATE AUTHORIZATION

State authorization is a formal determination by a state that Point Loma Nazarene University is approved to conduct activities regulated by that state. In certain states outside California, Point Loma Nazarene University is not authorized to enroll online (distance education) students. If a student moves to another state after admission to the program and/or enrollment in an online course, continuation within the program and/or course will depend on whether Point Loma Nazarene University is authorized to offer distance education courses in that state. It is the student's responsibility to notify the institution of any change in his or her physical location. Refer to the map on **State Authorization (https://www.pointloma.edu/offices/office-institutional-effectiveness-research/disclosures)** to view which states allow online (distance education) outside of California.

PLNU COPYRIGHT POLICY

Point Loma Nazarene University, as a non-profit educational institution, is entitled by law to use materials protected by the US Copyright Act for classroom education. Any use of those materials outside the class may violate the law.

PLNU RECORDING NOTIFICATION

In order to enhance the learning experience, please be advised that this course may be recorded by the professor for educational purposes, and access to these recordings will be limited to enrolled students and authorized personnel.
Note that all recordings are subject to copyright protection. Any unauthorized distribution or publication of these recordings without written approval from the University (refer to the Dean) is strictly prohibited.

PLNU ACADEMIC HONESTY POLICY

Students should demonstrate academic honesty by doing original work and by giving appropriate credit to the ideas of others. Academic dishonesty is the act of presenting information, ideas, and/or concepts as one's own when in reality they are the results of another person's creativity and effort. A faculty member who believes a situation involving academic dishonesty has been detected may assign a failing grade for that assignment or examination, or, depending on the seriousness of the offense, for the course. For all student appeals, faculty and students should follow the procedures outlined in the University Catalog. See **Academic Policies (https://pointloma-public.courseleaf.com/tug-catalog/academic-general-policies/)** for definitions of kinds of academic dishonesty and for further policy information.

ARTIFICIAL INTELLIGENCE (AI) POLICY

You are allowed to use Artificial Intelligence (AI) tools (e.g., ChatGPT, Gemini Pro 1.5, GrammarlyGo, Perplexity, etc.) in this course. Any work that utilizes AI-based tools must be clearly identified as such, including the specific tool(s) used. Please use **this Purdue resource (https://guides.lib.purdue.edu/c.php?g=1371380&p=10135074)** to guide your citations when using AI.

LOMA WRITING CENTER

The Loma Writing Center exists to help all members of the PLNU community cultivate transferable writing skills to engage their academic, professional, personal, and spiritual communities. We work toward this goal by conducting one-on-one consultation sessions, supporting writing education across the PLNU community, and participating in ongoing writing center research.

Getting feedback from the Loma Writing Center while you're in the process of working on an assignment is a great way to improve the quality of your writing and develop as a writer. You are encouraged to talk with a trained writing consultant about getting started on an assignment, organizing your ideas, finding and citing sources, revising, editing for grammar and polishing final drafts, and more. For information about how to make in-person or online appointments, see **Loma Writing Center webpage (https://www.pointloma.edu/centers-institutes/loma-writing-center)** or visit the Loma Writer Center on the first floor of the Ryan Library, room 221.

- Appointment Calendar: **https://plnu.mywconline.com/ (https://plnu.mywconline.com/)**
- Website: **https://www.pointloma.edu/centers-institutes/loma-writing-center (https://www.pointloma.edu/centers-institutes/loma-writing-center)**
- Email: **writingcenter@pointloma.edu (mailto:writingcenter@pointloma.edu)**

PLNU ACCOMMODATIONS POLICY

PLNU is committed to providing equal opportunity for participation in all its programs, services, and activities in accordance with the Americans with Disabilities Act (ADA). Students with disabilities may request course-related accommodations by contacting the Educational Access Center (EAC), located in the Bond Academic Center (EAC@pointloma.edu or 619-849-2533). Once a student's eligibility for an accommodation has been determined, the EAC will work with the student to create an Accommodation Plan (AP) that outlines approved accommodations. Professors are able to view a student's approved accommodations through Accommodate.

PLNU highly recommends that students speak with their professors during the first two weeks of each semester/term about the implementation of their approved accommodations in that particular course. Accommodations are not retroactive; as such, clarifying with the professor at the outset is one of the best ways to promote positive academic outcomes.

Students who need accommodations for a disability-related need should contact the EAC as early as possible (i.e., ideally before the beginning of the semester) to assure appropriate accommodations can be provided. In accordance with ADA, accommodations cannot constitute a fundamental alteration to course outcomes; therefore, planning ahead is vital in establishing appropriate accommodations for equal access to the course. It is the student's responsibility to make the first contact with the EAC. Students cannot assume that because they had accommodations in the past, their eligibility at PLNU is automatic. All determinations at PLNU must go through the EAC process. This is to protect the privacy of students with disabilities who may not want to disclose this information and are not asking for any accommodations.

PLNU ATTENDANCE AND PARTICIPATION POLICY

Regular and punctual attendance at all class sessions is considered essential to optimum academic achievement. If the student is absent for more than 10 percent of class sessions, the faculty member will issue a written warning of de-enrollment. If the absences exceed 20 percent, the student may be de-enrolled without notice until the university withdrawal date or, after that date, receive an "F" grade.

ASSIGNMENTS AT-A-GLANCE

The table below lists our assignments and their due dates. Click on any assignment to review it.

Course Summary:

Date	Details	Due

Date	Details	Due
Mon Nov 4, 2024	Intro Problems 5 (https://canvas.pointloma.edu/courses/87514/assignments/1366668)	due by 12:15pm
	GCMS Questions (https://canvas.pointloma.edu/courses/87514/assignments/1366653)	due by 5pm
Wed Nov 6, 2024	Intro Problems 6 (https://canvas.pointloma.edu/courses/87514/assignments/1366669)	due by 12:15pm
Fri Nov 8, 2024	Intro Problems 7 (https://canvas.pointloma.edu/courses/87514/assignments/1366670)	due by 12:15pm
Mon Nov 11, 2024	Intro Problems 8 (https://canvas.pointloma.edu/courses/87514/assignments/1366671)	due by 12:15pm
	FTIR Questions (https://canvas.pointloma.edu/courses/87514/assignments/1366650)	due by 5pm
Wed Nov 13, 2024	Intro Problems 9 (https://canvas.pointloma.edu/courses/87514/assignments/1366672)	due by 12:15pm
Fri Nov 15, 2024	Intro Problems 10 (https://canvas.pointloma.edu/courses/87514/assignments/1366655)	due by 12:15pm
Mon Nov 18, 2024	Intro Problems 11 (https://canvas.pointloma.edu/courses/87514/assignments/1366656)	due by 12:15pm
	1D NMR Questions (https://canvas.pointloma.edu/courses/87514/assignments/1366644)	due by 5pm

Date	Details	Due
Wed Nov 20, 2024	Intro Problems 12 (https://canvas.pointloma.edu/courses/87514/assignments/1366657)	due by 12:15pm
	Assignment 2 (https://canvas.pointloma.edu/courses/87514/assignments/1366646)	due by 5pm
Fri Nov 22, 2024	Midterm Exam (https://canvas.pointloma.edu/courses/87514/assignments/1366673)	due by 1:20pm
Mon Nov 25, 2024	Intro Problems 13 (https://canvas.pointloma.edu/courses/87514/assignments/1366658)	due by 12:15pm
	Unknown 1 Report (https://canvas.pointloma.edu/courses/87514/assignments/1366676)	due by 5pm
Mon Dec 2, 2024	Intro Problems 14 - HETCOR (https://canvas.pointloma.edu/courses/87514/assignments/1366659)	due by 12:15pm
Wed Dec 4, 2024	Intro Problems 15 - HMBC (https://canvas.pointloma.edu/courses/87514/assignments/1366660)	due by 12:15pm
	Assignment 3 (https://canvas.pointloma.edu/courses/87514/assignments/1366647)	due by 5pm
Fri Dec 6, 2024	Intro Problems 16 - NOESY (https://canvas.pointloma.edu/courses/87514/assignments/1366661)	due by 12:15pm
Mon Dec 9, 2024	Intro Problems 17 (https://canvas.pointloma.edu/courses/87514/assignments/1366662)	due by 12:15pm

Date	Details	Due
Wed Dec 11, 2024	Intro Problems 18 (https://canvas.pointloma.edu/courses/87514/assignments/1366663)	due by 12:15pm
Fri Dec 13, 2024	Intro Problems 19 (https://canvas.pointloma.edu/courses/87514/assignments/1366664)	due by 12:15pm
	Assignment 4 (https://canvas.pointloma.edu/courses/87514/assignments/1366648)	due by 5pm
Tue Dec 17, 2024	Unknown 2 Report (https://canvas.pointloma.edu/courses/87514/assignments/1366677)	due by 5pm
Wed Dec 18, 2024	Final Exam (https://canvas.pointloma.edu/courses/87514/assignments/1366651)	due by 1pm
Wed Oct 21, 2026	Intro Problems 1 (https://canvas.pointloma.edu/courses/87514/assignments/1366654)	due by 12:15pm
Mon Oct 26, 2026	Intro Problems 2 (https://canvas.pointloma.edu/courses/87514/assignments/1366655)	due by 12:15pm
Wed Oct 28, 2026	Intro Problems 3 (https://canvas.pointloma.edu/courses/87514/assignments/1366656)	due by 12:15pm
Fri Oct 30, 2026	Intro Problems 4 (https://canvas.pointloma.edu/courses/87514/assignments/1366657)	due by 12:15pm
Wed Nov 4, 2026	Assignment 1 (https://canvas.pointloma.edu/courses/87514/assignments/1366645)	due by 5pm

Date	Details	Due
	Dereplication Questions (https://canvas.pointloma.edu/courses/87514/assignments/1366649)	
	GCMS Instrument Training (https://canvas.pointloma.edu/courses/87514/assignments/1366652)	
	Optional Structure Elucidation Practice Problems (https://canvas.pointloma.edu/courses/87514/assignments/1366674)	
	Special Topic Presentation (https://canvas.pointloma.edu/courses/87514/assignments/1366675)	