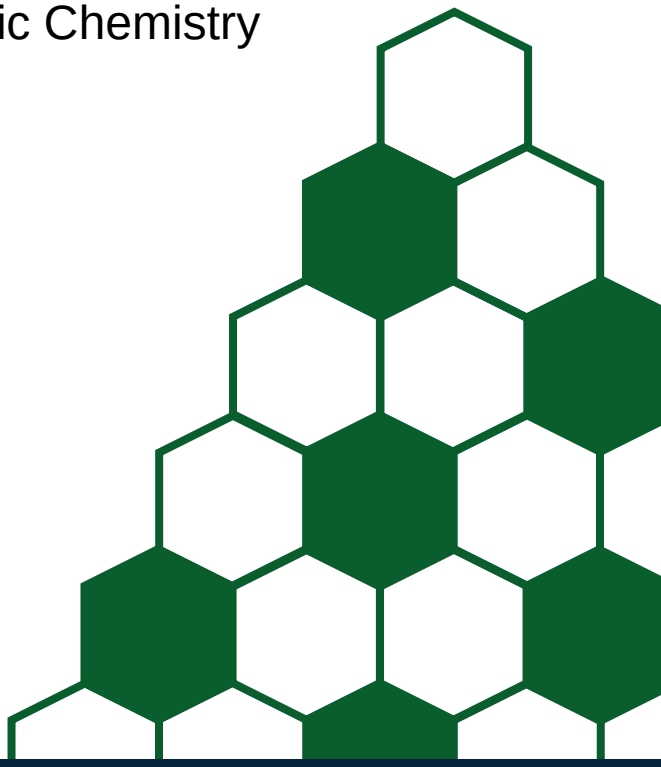
Using Nuclear Magnetic Resonance (NMR) Spectroscopy

Documentation Project Plan

Project Manager: Rachelle Gervacio

Client: CHEM-3206: Advanced Organic Chemistry Lab Instructor



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Project Overview

This project overview describes general information about my planned training manual: **A Guide to Using Nuclear Magnetic (NMR) Spectroscopy.**

Document description

I am creating a 22-page (8.5″ × 11″, spiral-bound) training manual for undergraduate university students completing organic chemistry experiments in an NMR facility. The training manual will contain conceptual information about key NMR spectroscopy principles and applications. Its contents describe detailed procedures specifically for using a 400 MHz Bruker NMR spectrometer and TopSpin 3.2 NMR software to analyze and identify a sample of unknown organic compounds.

Purpose and objective

The training manual's primary purpose is to train CHEM-3206: Advanced Organic Chemistry Lab students to use an NMR spectrometer at the University of Winnipeg's NMR facility. The client, a university chemistry instructor, also wants the training manual to prepare students for their fourth-year honours course, which requires using NMR spectroscopy for their final capstone research project.

The training manual's secondary purpose is to replace existing documentation that requires major content, formatting, and design revisions. The current NMR procedures are included in a 76-page supporting information (SI) document primarily intended for university chemistry instructors. I will revise and repurpose the SI document's content for a different audience: a cohort of undergraduate university students.

Scope

Because the SI document contains 76 pages about chromatography, mass spectrometry, and NMR spectroscopy, the client has asked me to only include relevant procedures for two types of NMR spectroscopy methods: proton (^{1}H) NMR and carbon (^{13}C) NMR.

The project's scope will focus on training students to use an NMR spectrometer safely and properly. Therefore, the training manual will contain topics about NMR safety guidelines and NMR spectroscopy procedures. The procedures will describe NMR sample preparation, NMR data acquisition, and NMR spectra production.

Audience analysis

My intended audience is a cohort of undergraduate university students taking a third-year advanced organic chemistry course. The students do not have experience using NMR hardware or software, and they will use the training manual in an NMR facility with strict safety protocols and expensive laboratory equipment.

The following list describes general information about a typical advanced organic chemistry student:

- They range in age from 20 to 25.
- They are enrolled as third- or fourth-year science majors.
- They are considering applying for graduate or professional studies.
- They are highly extrinsically motivated by grades and course completion.

Attitudes

The students are highly motivated to get good grades on their laboratory exercises because organic chemistry is a demanding course required for their degree program. As a result, they want to understand and complete their experiments as quickly as possible to move on to the next laboratory exercise. They do not want to read lengthy and redundant information they already know. Additionally, some students do not fully recognize the practical applications of NMR spectroscopy and instead regard it as another mandatory laboratory exercise.

Abilities

The students have proficient reading and problem-solving skills, which are necessary to conduct chemistry experiments at the third-year level. Furthermore, the students have intermediate computer literacy skills and know how to browse the internet, use a word processor, and create spreadsheets. They can also perform chemistry laboratory techniques, such as chemical synthesis and distillation, and they have general laboratory safety skills.

Knowledge

The students understand organic chemistry concepts and reactions. They are familiar with NMR spectroscopy and most NMR terminology, and they know how to analyze NMR spectra. Also, they have experience following laboratory instructions and writing formal laboratory reports.

To accommodate the client's requests and the audience's needs and experience, I will use a concise, formal writing style and include NMR terminology. I will write at a higher language level, use plain language wherever possible, and include pictures that depict specific steps to make the NMR procedures both clear and precise. I will also format the training manual as a physical document so that students can refer to procedures while using the NMR spectrometer.

For more information about my information design decisions, refer to the content plan on page 3.

Content Plan

This content plan describes the documentation project's information design goals and strategies for the planned training manual. It also contains the document outline, which summarizes the training manual's core topics and the estimated number of pages and photos.

Information design

This subsection describes my design decisions for the training manual's content and format.

Structure

Front matter will include a title page, table of contents, and statement of purpose to help students familiarize themselves with the document's subject and contents. Content will use a chronological and task-based organizational pattern to organize and categorize topics. In other words, students will initially read the manual from beginning to end as they learn and perform sequential tasks required to use an NMR spectrometer safely and properly. After the first reading, students will be able to use the manual as a reference when needed. The back matter will contain an appendix with a glossary, relevant NMR webpage links, and NMR facility contact information for students who need supplementary information not already in the body section.

Contents

The two prerequisite topics (Introduction and Getting Started) will be located at the beginning of the training manual to familiarize students with NMR concepts, hardware and software, and facility safety guidelines before they start using the NMR spectrometer. These will be followed by three procedural topics (Preparing an NMR Sample, Acquiring NMR Data, and Processing an NMR Spectrum) to describe the tasks required to process and analyze an NMR sample.

For a detailed document outline of the training manual's contents and descriptions of each topic, refer to Table 1 on page 4.

Format, style, and language

Because the NMR facility prohibits electronics and magnetic objects near the NMR spectrometer, I will format the training manual as a physical document. I will export the training manual as a .pdf file and use spiral binding. Spiral binding will allow students to open the training manual a complete 360 degrees, and the document can lie completely flat and take up less amount of space when students fold its pages back.

I will use a concise, formal writing style to maintain stylistic consistency with the chemistry department's existing training and laboratory documents. To address the students' education level and laboratory experience, I will write at a higher language level and use NMR terminology to ensure that students learn specific definitions that are a part of their course curriculum. When describing procedural information, I will use plain language wherever possible to make the steps clear and straightforward.

Graphics

I plan to include large photographs (.jpg files) of the NMR hardware setup and correctly prepared NMR samples for students to compare with their samples. I will also include cropped screenshots with callouts (.png files) for key procedural steps that involve using the TopSpin 3.2 software. Small icons (.png files) inside text boxes will emphasize important warnings and notes, as well as large flow charts (.png files) to summarize the NMR spectroscopy procedures.

Document outline

Table 1 shows the document outline and estimated numbers of photos and pages for the training manual's topics. The training manual will contain approximately **18 photos** and **22 pages**.

Table 1. The training manual's document outline and estimated numbers of photos and pages.

Topic	Description	No. of Photos	No. of Pages
1. **Introduction** a) About nuclear magnetic resonance (NMR) spectroscopy b) NMR facility overview	▪ Overview of general NMR spectroscopy concepts. ▪ Overview of the University of Winnipeg's NMR hardware setup.	2	2
2. **Getting Started** a) NMR safety guidelines b) TopSpin 3.2 general overview	▪ List of safety guidelines and procedures for emergency situations. ▪ Overview of TopSpin 3.2's graphical user interface.	4	5
3. **Preparing an NMR Sample** a) Common NMR preparation mistakes	▪ Procedures for preparing an NMR sample for analysis.	2	3
4. **Acquiring NMR Data** a) Proton (^{1}H) NMR b) Carbon (^{13}C) NMR	▪ Procedures for using the NMR spectrometer and TopSpin 3.2 to analyze an NMR sample and acquire data. This topic will describe procedures for two types of NMR methods: proton (^{1}H) and carbon (^{13}C) NMR spectroscopy.	5	5
5. **Processing an NMR Spectrum** a) Proton (^{1}H) NMR b) Carbon (^{13}C) NMR	▪ Procedures for using TopSpin 3.2 to process and produce an NMR spectrum. This topic will describe procedures for two types of NMR methods: proton (^{1}H) and carbon (^{13}C) NMR spectroscopy.	5	5
6. **Appendix** a) Glossary b) Interesting NMR links c) NMR facility contact Information	▪ List of NMR-related key terms. ▪ List of links to NMR-related webpages. ▪ Contact information for the University of Winnipeg's NMR facility and security office.	0	2
Total		**18 photos**	**22 pages**

Resource Plan

This resource plan describes the five phases involved in the training manual's documentation process. It also outlines each resource's responsibilities during each development phase.

Development process

The documentation project will involve five phases of development. Figure 1 summarizes the five phases involved in the training manual's documentation development process.

Figure 1. The documentation development process involving five phases.

Table 2 shows the resources and tasks for each phase in the documentation development process.

Table 2. The tasks and resources required to complete each documentation development phase.

Phase	Resource(s)	Task(s)
1) Plan	Project manager	▪ Discuss the project requirements with the client. ▪ Define the project's scope and goals. ▪ Estimate the project's schedule, budget, and resources. ▪ Create a document outline and content plan.
2) Design	Project manager	▪ Define usability and accessibility goals. ▪ Conduct audience and task analysis. ▪ Identify appropriate writing style and style guide.
3) Develop	Project manager	**Writing:** ▪ Research project topic and gather sources. ▪ Review and modify content from existing documentation. ▪ Write a draft for conceptual, procedural, and reference topics. **Editing:** ▪ Revise draft for its accordance with its rhetorical situation and SME feedback. ▪ Revise draft for organization, consistency, and content gaps and accuracy. ▪ Revise draft for its accordance with the specified style guide. **Proofreading:** ▪ Review, revise, and finalize the draft for mechanical and formatting errors. **Illustrating:** ▪ Create and edit photos, screenshots, and icons. **Testing:** ▪ Test and revise documentation for errors and inconsistencies.
	Subject-matter expert	▪ Discuss training manual concepts, procedures, and references with the project manager. ▪ Test documentation with the project manager.
4) Produce	Project manager	▪ Identify production requirements and format. ▪ Gain approval from the client to finalize and publish the document. ▪ Distribute the finalized document to the client.
	Subject-matter expert	▪ Review and approve the finished document.
5) Evaluate	Project manager	▪ Evaluate the project's final budget and schedule development. ▪ Meet with the client to discuss the final document, areas for improvement, and overall project effectiveness. ▪ Create a report that summarizes documentation results.

Project Schedule

This project schedule includes the time estimates for creating the training manual. For a detailed schedule, refer to the Excel file titled **NMR Spectrometer Training Manual - Project Schedule.xlsx** to see the time durations and tasks involved in all five phases of documentation development.

Project topic estimates

Table 3 shows the estimated time requirements for developing the training manual's planned topics. Table 4 on page 8 shows the estimated time requirements with a 20% fudge factor to account for errors in assumptions and unanticipated circumstances.

Table 3. Development time estimates for each training manual topic.

Topic	Quantity	Estimated no. of days*	Total days**
1. **Introduction** a) About nuclear magnetic resonance (NMR) spectroscopy b) NMR facility overview	2 pgs. 2 illus.	**Writing:** 2 × 5 hrs. = 10 / 8 hrs. = 1.5 days **Editing & proofreading:** 2 × 1 hr. = 2 / 8 hrs. = 0.5 day **Illustrating:** 2 × 0.75 hr. = 1.5 / 8 hrs. = 0.5 day	**3 days**
2. **Getting Started** a) NMR safety guidelines b) TopSpin 3.2 general overview	5 pgs. 4 illus.	**Writing:** 5 × 5 hrs. = 25 / 8 hrs. = 3.5 days **Editing & proofreading:** 5 × 1 hr. = 5 / 8 hrs. = 1 day **Illustrating:** 4 × 0.75 hr. = 3 / 8 hrs. = 0.5 day	**5 days**
3. **Preparing an NMR Sample** a) Common NMR preparation mistakes	3 pgs. 2 illus.	**Writing:** 3 × 5 hrs. = 15 / 8 hrs. = 2 days **Editing & proofreading:** 3 × 1 hr. = 3 / 8 hrs. = 0.5 day **Illustrating:** 2 × 0.75 hr. = 1.5 / 8 hrs. = 0.5 day **Testing:** 3 × 0.5 hrs. = 1.5 / 8 hrs. = 0.5 day	**4 days**
4. **Acquiring NMR Data** a) Proton (^{1}H) NMR b) Carbon (^{13}C) NMR	5 pgs. 5 illus.	**Writing:** 5 × 5 hrs. = 25 / 8 hrs. = 3.5 days **Editing & proofreading:** 5 × 1 hr. = 5 / 8 hrs. = 1 day **Illustrating:** 3 × 0.75 hr. = 2.25 / 8 hrs. = 0.5 day **Testing:** 5 × 0.5 hrs. = 2.5 / 8 hrs. = 0.5 day	**6 days**
5. **Processing an NMR Spectrum** a) Proton (^{1}H) NMR b) Carbon (^{13}C) NMR	5 pgs. 5 illus.	**Writing:** 5 × 5 hrs. = 25 / 8 hrs. = 3.5 days **Editing & proofreading:** 5 × 1 hr. = 5 / 8 hrs. = 1 day **Illustrating:** 3 × 0.75 hr. = 2.25 / 8 hrs. = 0.5 day **Testing:** 5 × 0.5 hrs. = 2.5 / 8 hrs. = 0.5 day	**6 days**
6. **Appendix** a) Glossary b) Interesting NMR links c) NMR facility contact information	2 pg. 0 illus.	**Writing:** 2 × 2 hrs. = 4 / 8 hrs. = 0.5 day **Editing & proofreading:** 2 × 0.5 hr. = 1 / 8 hrs. = 0.5 day **Illustrating:** N/A	**1 day**

*Estimated number of days for each development task was rounded up to the nearest half or whole day.
**Total days were rounded up to the nearest whole day.

Total	25 days

Table 4. Development time estimates for each training manual topic with a 20% fudge factor.

Topic	Total days	Total days with 20% fudge factor*
1. **Introduction** a) About nuclear magnetic resonance (NMR) spectroscopy b) NMR facility overview	**3 days**	3 + (0.2 × 3) = **4 days**
2. **Getting Started** a) NMR safety guidelines b) TopSpin 3.2 general overview	**5 days**	5 + (0.2 × 5) = **6 days**
3. **Preparing an NMR Sample** a) Common NMR preparation mistakes	**4 days**	4 + (0.2 × 4) = **5 days**
4. **Acquiring NMR Data** a) Proton (^{1}H) NMR b) Carbon (^{13}C) NMR	**6 days**	6 + (0.2 × 6) = **8 days**
5. **Processing an NMR Spectrum** a) Proton (^{1}H) NMR b) Carbon (^{13}C) NMR	**6 days**	6 + (0.2 × 6) = **8 days**
6. **Appendix** a) Glossary b) Interesting NMR links c) NMR facility contact information	**1 day**	1 + (0.2 × 1) = **2 days**
Total	**25 days**	**33 days**

*Total days with 20% fudge factor were rounded up to the nearest whole day.

Table 5 shows the estimated total number of days required for each documentation development phase. The training manual will require approximately **50 days** to create and produce.

Table 5. Time estimates for each documentation development phase.

Phase	Total days
1. **Plan**	6 days
2. **Design**	4 days
3. **Develop**	33 days
4. **Produce**	3 days
5. **Evaluate**	4 days
Total	**50 days**

Project Budget

This project budget summarizes the required expenses for the training manual's documentation project. Table 6 shows the estimated costs for developing and producing the training manual. US dollar costs were converted to Canadian dollars (conversion rate: 1USD = 1.32CAD).

The estimated total cost for creating and producing the training manual is **$41.58**.

Table 6. The estimated expenses for the training manual's documentation project.

Category	Item	Quantity	Duration	Cost	Subtotal
Resource	Project manager ▪ Rachelle Gervacio	1	3 months	N/A	N/A
	Subject-matter expert ▪ Advanced Organic Chemistry lab instructor	1	3 months	N/A	N/A
Information Sources	Supporting information for published Journal of Chemical Education article	1	N/A	N/A	N/A
	Organic chemistry student laboratory manual	1	N/A	N/A	N/A
	University of Winnipeg's NMR facility website	1	N/A	N/A	N/A
Tools	Microsoft Word	1	3 months	N/A	N/A
	Adobe Photoshop (subscription)	1	1 month	$41.58	$41.58
Printing services*	Training manual ▪ 22 pages ▪ Plastic spiral binding	20	N/A	N/A	N/A

*The University of Winnipeg will cover all printing expenses.

Total	$41.58

Project Risk Mitigation

This project has two critical success factors necessary for development: regular contact with the SME and authorized access to the university's NMR facility. Without these critical success factors, I cannot verify the training manual's accuracy, document the TopSpin 3.2 software, or test the NMR procedures. I would not be able to write any core topics involving hands-on interaction with the NMR hardware and software.

To ensure the project's success, I made an alternative plan in case I encounter any problems during documentation development. If I cannot contact my SME, I can contact two people who have proficient knowledge and experience using an NMR spectrometer: the university's NMR facility technician and a fourth-year chemistry honours student. Both individuals have agreed to answer my questions and give me access to the NMR facility if I need additional time documenting and testing procedures.

Before I can use the NMR spectrometer, I will need to participate in a mandatory 1-hour safety training session. The NMR facility technician has already given me his availability for NMR training, so I can start documenting the NMR procedures as soon as possible.