Research Article

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An exploration of the proton NMR problem-solving approaches of undergraduate students

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Abstract: Problem-solving is an important component of chemistry teaching and learning. It often requires both conceptual knowledge and problem-solving skills. This study aims to examine how students solve tasks related to proton ^{1}H NMR spectroscopy. This study included 24 voluntary participants enrolled in second-semester organic chemistry labs in two different instructional settings (online or in person). The data were collected through interviews conducted via Webex video conferencing software and used a think-aloud protocol. The data were analyzed using an inductive coding approach to identify students' problem-solving approaches and resources they used when solving a given ^{1}H NMR task that involved matching protons in a compound to specific peaks in the spectrum. The resources framework was used to capture students' conceptual resources and problem-solving approaches. Results revealed that participants used more productive approaches than unproductive approaches while solving the problem; however, most students relied on one basic NMR concept to draw conclusions about the identity of a given peak. Also, when we observed the problem-solving resources that students utilized based on how they received NMR instruction (online or in-person), we did not observe major differences between the problem-solving resources that students used.

Keywords: nuclear magnetic resonance (NMR); organic chemistry; undergraduate; problem-solving

1 Introduction

Problem-solving is a fundamental skill in chemistry, it is essential in our day-to-day life, and is a process we follow to obtain a solution. However, we may be unaware of the pathway that leads to this solution (Greenbowe, 1983). The process of solving a problem is often challenging for students because when they encounter a new problem they have not seen before, they fail to recognize the steps needed to obtain the solution.

Problem-solving is also an area of great interest in chemistry education research and researchers have studied various facets of it in the field of chemistry. One such study conducted by Surif et al. (2014) investigated students' achievement levels when solving algorithmic, conceptual, and open-ended problems. According to their findings, an overwhelming 96 % of the students were able to solve algorithmic problems effectively. However, only 54 % and 15 % of students could successfully answer conceptual and open-ended questions, respectively. This study highlights a significant challenge that students encounter when solving conceptual and open-ended problems, likely due to a lack of a deep understanding of the underlying concepts. This underscores the importance of prioritizing the development of students' conceptual understanding, which is vital to solving problems in chemistry effectively.

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Researchers have also explored the influence of different factors on students' ability to solve problems effectively (Lopez et al., 2014). In this study, the researchers used multivariate regression analysis to explore the relationship between prior science achievement, knowledge structures, spatial ability, gender, and ethnicity in relation to problem-solving performance in organic chemistry. The findings indicated that knowledge structures (the organization of knowledge around core ideas) emerged as a significant predictor of problem-solving performance. In particular, the organization of knowledge played a significant role in explaining the variability in students' scores related to their performance.

Although there have been numerous studies investigating the challenges that students encounter when solving problems in organic chemistry and different methods for helping students with these challenges (Lieber & Graulich, 2020), limited research has been conducted on how undergraduate students approach spectroscopic problem-solving, particularly proton NMR. Thus, this study aims to investigate the NMR problem-solving processes and compare their problem-solving strategies in two distinct instructional settings: online versus in-person instruction. By examining the similarities and differences in problem-solving approaches between different instructional environments, this study seeks to provide valuable insights into effective approaches for teaching and supporting students in spectroscopic problem-solving related to proton NMR.

2 Literature review

2.1 NMR spectroscopy

Nuclear magnetic resonance spectroscopy (NMR) is one of the most widely used analytical tools throughout academia and industry. NMR spectroscopy can be used to get information about the structure of a compound (Giuliano & Carey, 2020; Karty & Melzer, 2018; Parker, 1988; Pavia et al., 2014; Schummer, 2002). Due to its importance, NMR spectral data interpretation is covered in most undergraduate organic chemistry curriculums. Also, some undergraduate students receive hands-on experience in using NMRs. A survey involving four-year undergraduate institutions in organic chemistry laboratories conducted in 2011 has indicated that more than 70 % of the institutions give students hands-on experience in using NMRs (Martin et al., 2011). However, problem-solving related to NMR spectroscopy can still be challenging for students (Angawi, 2014). It often requires sound conceptual knowledge of NMR concepts and high-level problem-solving skills (Angawi, 2014). Although conceptual understanding is sometimes inferred as problem-solving, problem-solving, and conceptual understanding are different. With sound conceptual knowledge one can attempt to solve problems, but solving problems requires conceptual knowledge along with critical thinking and reasoning skills (Holme et al., 2015).

Learning how to approach spectroscopic problem-solving is also a complicated task. There is no straightforward way to solve NMR problems (Angawi, 2014). Students can receive assistance from textbooks. Textbooks are highly regarded as trustworthy resources that provide valuable support to students. Authored by subject matter experts, these educational materials offer detailed explanations of NMR concepts, accompanied by numerous worked examples, practice questions, and answers to self-assessment questions. Furthermore, textbooks feature a diverse range of questions, addressing both individual spectral features and combinations of such features (Anderson et al., 2020). In addition to questions solely focused on proton NMR, some textbooks feature combinations of questions that require students to extract information from various other spectra such as IR, ^{13}C NMR, 2D-NMR and Mass Spectrometry. However, authors have observed that the problems in the textbooks may not provide an equal emphasis on all the necessary concepts that require solving ^{1}H NMR questions (Anderson et al., 2020). Frequently, the questions in the textbooks test students' knowledge of one concept, and the questions that require the integration of all the conceptual knowledge, like the number of signals, splitting patterns, chemical shift, and integration, are limited (Anderson et al., 2020).

In addition to the aforementioned traditional methods, students can now enhance their understanding of NMR spectroscopy through computer-based and web-based tools. Mnova and Mestrelab Research are examples of computer-based NMR prediction tools that enable students to visualize spectra without the need for costly instrument time, reagents, or solvents (Kolonko & Kolonko, 2019). Moreover, incorporating web-based teaching methods has been explored in the literature as an effective approach to teaching NMR. One challenging concept in NMR education is understanding spin-spin splitting patterns. Azman and Esteb (2016) introduced a novel approach using a coin-flipping analogy and a freely accessible web app to teach the fundamentals of spin splitting. The results of their study demonstrated that incorporating the web app in teaching splitting patterns yielded significant benefits compared to traditional methods. Students showed improved comprehension of the origins of splitting, the peak's shape, and the associated ratio when using the web app. These advancements in computer and web-based tools contribute to a more comprehensive and accessible education in NMR spectroscopy.

Furthermore, in 2022, a novel educational website (www.nmr-challenge.com) was launched, providing a comprehensive collection of over 160 NMR spectral assignments obtained from actual samples (Socha et al., 2023). Each assignment includes NMR spectra of an unidentified compound, presenting students with the challenge of determining its chemical structure. The assignments range from basic to advanced levels, with basic assignments offering one-dimensional ^{1}H and ^{13}C NMR spectra, while advanced assignments include two-dimensional correlation spectra. To enhance the learning experience, the website incorporates an interactive chemical structure drawing tool, providing instant feedback on proposed structures. The assignments are categorized based on their level of difficulty to ensure the engagement of both beginner and advanced students. Additionally, the website will regularly introduce new spectral problems, ensuring a continuous learning resource for students.

Another web-based platform that helped students practice proton NMR questions is nmr.cheminfo.org, introduced by Patiny et al. (2018). This online platform offers students an online alternative to desktop software packages that exist for NMR spectral interpretation. It provides a set of exercises and tools to help students to solve NMR problems. It is clear that recent advances in technology are revolutionizing the NMR spectroscopy learning experiences of students.

2.2 Evidence-based research studies on students' problem-solving approaches in spectroscopy

Only a handful of research studies can be found in the literature about students' approaches to spectroscopic problem-solving. In one such study, the authors investigated how students solve spectroscopic problems (Cartrette & Bodner, 2010). The researchers tried to understand how the study participants determined the structure of a molecule using the molecular formula, IR, and proton NMR. The results suggested that more successful participants used a consistent approach and drew molecular fragments at intermediate stages in solving the question.

Other studies used eye-tracking techniques to determine how students solve NMR spectra. A study by Topczewski et al. (2017) compared how novice students (students taking the course currently) and experts (graduate and advanced undergraduate students) solve NMR spectroscopic questions. Gaze frequency and gaze order data were used to identify the problem-solving approaches of the study participants (Topczewski et al., 2017). They found significant differences in gaze patterns among the expert and novice groups, as well as between two categories of novice students (advanced and early). These findings suggest that different spectral data interpretation approaches exist between these groups. Experts mainly gazed between the ^{1}H NMR data and the correct structure. Advanced novice students, on the other hand, scanned possible structures more than connecting ^{1}H NMR resonances to a given structure. Early novice students showed a more expert-like strategy than the advanced group, but they were unable to understand the connection between ^{1}H NMR data and the correct structure.

Connor et al. also used eye-tracking to investigate how undergraduate and doctoral students solve ^{1}H NMR and IR spectra (Connor et al., 2020). The study involved 18 undergraduate students and seven doctoral students. Their eye movements were tracked to determine their cognitive processes associated with NMR problem-solving. One of the significant findings of this study was that undergraduate students used an uninformed bidirectional approach, whereas doctoral students used an informed unidirectional approach. In other words, undergraduate students had to frequently move back and forth between reference tables and frequency axis since they had difficulty processing the data and needed to refresh their working memories more often. In contrast, the doctoral students seemed more familiar with processing NMR data and could process the data uni-directionally moving only toward one direction. For instance, they only moved from the molecule to the chemical shift axis in the first synthesis example (Connor et al., 2020).

Hence, there are only a limited number of research studies on how students approach spectroscopic problem-solving. More studies are needed to fully understand students' approaches to solving different types of spectroscopic problems. By understanding students' productive and unproductive approaches, we can develop improved methods for teaching NMR problem-solving to students at the undergraduate level. Notably, previous research studies use NMR tasks that provide students with a molecular formula and then ask them to solve the structure using the given NMR and other spectral data. However, it is also important to explore how students solve NMR tasks that are commonly used by organic chemists. For instance, most organic chemists already have some idea of what the structure of their target synthesized compound should be and then use the NMR spectrum to verify if the compound has been synthesized. We used this approach in our study and designed a task where students needed to match the peaks of the proton NMR to the given molecular structure.

There is also no study about how students in different instructional settings (online and in-person labs) solve ^{1}H NMR spectroscopic problems. Therefore, it is worth understanding how the instructional format (in-person or online) may affect students' NMR problem-solving skills. To this end, our study investigated the ^{1}H NMR problem-solving approaches of students enrolled in online and in-person settings.

3 Theoretical perspectives

3.1 Resources framework

The theoretical underpinning for this research study is the resources framework by Hammer and Elby (2003). According to Elby and Hammer, resources are fine-grained cognitive units activated based on the context or task (2010). The cognitive resources can be procedural, epistemological, or conceptual (Becker et al., 2017). In this study, among these three types of resources, we will be focused on the conceptual and procedural resources that students use to solve problems related to NMR. Procedural resources are resources that are readily observable when carrying out a procedure (Wittmann & Black, 2015).

The fundamental conceptual resources that students can utilize when solving proton NMR problems typically involve the resources activated in counting the number of signals, identifying the chemical shift based on the environment, determining the splitting pattern, and determining the integration. However, the resources that students activate during the problem-solving process are not explicit. We can only see them if they utilize these resources as a problem-solving approach. Therefore, our focus is not to characterize the activation of fine-grained resources based on the prompt but to focus on how students use these activated resources in problem-solving as a problem-solving approach. To capture students' problem-solving approaches, we used a grain size different from Hammer and Elby, called mesoscopic grain size. This grain size is bigger than the fine-grained resource level and smaller than the concept level (Figure 1). This mesoscopic grain size is based on the idea of Wittmann (2006) and Wittmann and Black (2015). This mesoscopic grain size has been previously used by Rodriquez et al. in examining problem-solving approaches of students solving chemical kinetics problems (2019).

Context-based resource activation differs from the transfer of stable knowledge units, where you can identify misconceptions and replace them with correct ideas (Hammer et al., 2005). Moreover, this framework suggests that resources are not inherently right or wrong, but they may be productive or unproductive for the task under consideration. When students encounter an unfamiliar problem, they search their resource pool and try to activate something useful for the context. As educators, we can improve our instructional methods by helping students consistently activate productive resources.

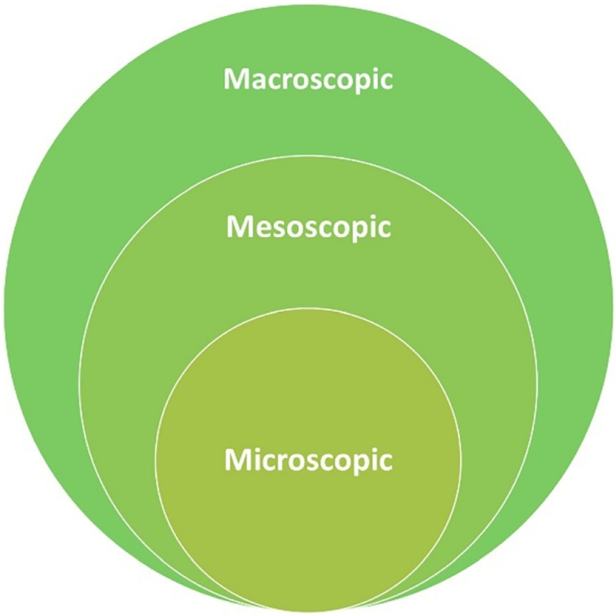

Figure 1: The grain size of cognitive resources.

4 Research questions

The research questions that guide our research are:
(1) What conceptual and procedural problem-solving resources do students apply to the given proton NMR task?
(2) What are the frequently used problem-solving resources when students approach this task?
(3) What are the productive and unproductive problem-solving resources that students utilize for the given task?
(4) Is there a difference in the problem-solving resources that students use based on whether they received instruction online or in-person?

5 Methodology

5.1 Participants and setting

The data was collected from students enrolled in second-semester organic chemistry labs at a public research-intensive university in the southeastern United States. This study was conducted from Fall 2020 to Spring 2022. Participants were recruited via online announcements using the institution's course management system. The method of instruction for Fall 2020, Spring 2021, and Summer 2021 was online (due to the COVID-19 pandemic). Students in Fall 2021 and Spring 2022 received in-person laboratory instruction. Three different instructors taught the sections from which the data was collected.

Twenty-four undergraduates volunteered to participate in the qualitative interviews; 22 of them were STEM majors (Biology, Chemistry, Biomedical Science, or Neuroscience), and two were post-baccalaureate students. Thirteen study participants were senior students, seven juniors, and two sophomore students. Details of the demographics of the study participants can be found in Table 1. All individuals gave consent to participate in the study, and IRB approval was obtained. We offered a $10 Amazon gift card to those who participated in the interviews.

5.2 NMR course content – online course

Proton NMR spectroscopy was taught in the second-semester organic chemistry laboratory course at the institution where the study took place. In Fall 2020, Spring 2021, and Summer 2021, the laboratory instruction was online and held as synchronous lectures via WebEx. The synchronous lecture was about 50 min once per week. During that time, the instructor discussed how to identify the number of signals based on nonequivalent protons, how to determine chemical shift values based on shielding and de-shielding effects, how to use the chemical shift table, and how to determine the splitting patterns (first and second order splitting). The integration

Table 1: Demographics of interview participants.

	Online	In-person
Major		
Bio-Medical Science	1	0
Biology	3	4
Chemistry	5	4
Neuroscience	3	2
Post Baccalaureate	2	0
Academic classification		
Sophomore	2	0
Junior	1	6
Senior	9	4
Post Baccalaureate	2	0

concept was briefly covered in those lectures. This information was revealed during the discussions we had with the instructors who taught the course, in student interviews, and when we reviewed the course material. Students used an online platform called Lab Flow (https://www.catalystedu.com/labflow) (CatalystEdu, 2018) to do lab quizzes and assignments (Figure 2). There was also a video on interpreting proton NMR spectrums on that platform. This video was around 12 min long and gave a brief overview of the NMR technique, its uses, what is proton NMR, how the data is collected in the NMR machine, how protons will get shielded or deshielded based on the environment, the integration concept, splitting patterns and at the end, there was one question on how to use all these information of chemical shift, splitting and integration to solve the spectrum of ethyl acetate. The students could watch the video as often as they like and participate in NMR-related quizzes online. These quizzes assessed their knowledge of matching a set of given compounds to their corresponding NMR spectrums based on integrating all the NMR concepts they learned. Also, there were questions about drawing representative NMR spectrums when a compound name was given. A chemical shift table was also available for students to use.

5.3 Course content and description – in person

The students enrolled in in-person labs had the opportunity to learn the same concepts covered in online labs related to proton NMR. In addition to that, the students had in-person labs to get hands-on experience. The lab is project-based, and students work independently to synthesize a series of six compounds related to chalcone and isoxazole derivatives (Henary et al., 2015; Tomaszewski, 2011). The students determine the successfulness of their synthesis based on IR, ^{1}H NMR, ^{13}C NMR spectroscopy, and melting point analysis. Students did not perform the NMR analyses themselves but had the opportunity to use ^{1}H NMR data collected for their synthesized compounds to interpret the success of their syntheses. Table 2 provides a summary of various aspects of the online and in-person courses.

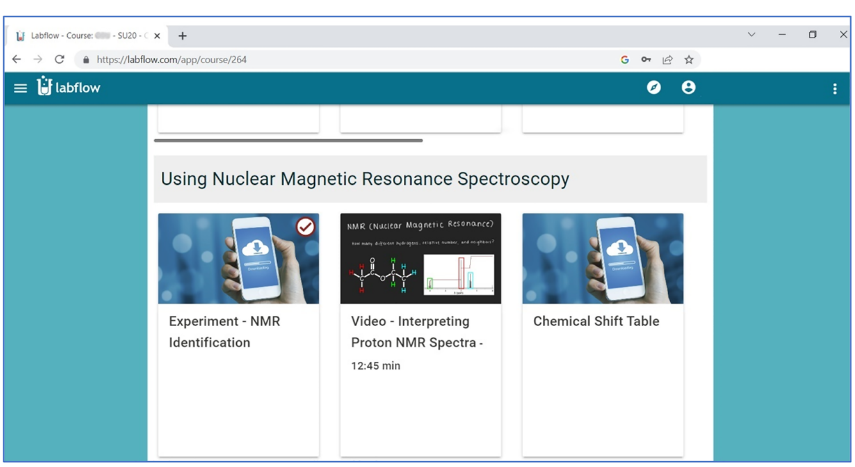

Figure 2: Lab flow interphase.

Table 2: Summary of online and in person course content and description.

	Online	In-person
Course content and material	Instructor provided PowerPoint uploaded to online course management system	
Lecture time	One 50 min lecture (synchronous via Webex)	One 50 min in-person pre-lab lecture
Recommended textbook	Experimental organic chemistry – A small scale approach, 2nd edition (Wilcox and Wilcox, 1995)	
Homework assignments	Post lab report – containing matching compound peaks to spectrum (among the set of spectrums provided, the students need to select which spectrum matches to Ex: methyl butanoate) The spectrums were zoomed in to help recognize the multiplicities, spectrums were free from solvent and impurity peaks, integration values were given)	Worksheet questions included questions like matching molecular structure to spectrum, questions on chemical shift, and splitting pattern
Evaluation methods	Pre-lab quiz with basic questions about NMR concepts – the solvents used in NMR, the radiation type involved, defining of terms such as upfield and downfield. Post-lab quiz is given as a homework assignment for the students to work on their own and submit on a deadline. Proton NMR in the final exam	After the NMR instruction was covered quizzes include questions about proton NMR. The final exam also assessed NMR concepts
Review session	Whole semester review session which also reemphasize the concepts learned about proton NMR	
Office hours	Via WebEx During this time the student can meet the instructor and discuss any questions they have	In-person
Other resources	Lab flow – instructional video on proton NMR (12 min) Recording of the online synchronous lecture Chemical shift table	Not available
Hands on experience	Not available	Had the opportunity to analyze proton NMR spectra of their synthesized compounds and determine the successfulness of their synthesis

5.4 Pilot study and refinement of the interview protocol

We piloted our interview protocol with five students: two junior students, two senior students, and one graduate student. Adjustments were made to the interview protocol by removing some of the tasks we had in the initial interview draft to fit the interview time limit of around 1 h, and minor modifications were made to the tasks that were confirmed to be included in the final interview protocol. Additionally, to check the content validity of the tasks, we interviewed one chemistry instructor with more than six years of experience teaching NMR at the undergraduate level at the time of data collection and adjusted some of the questions based on her comments.

5.5 Data collection

The data were collected through a think-aloud protocol. Participants were asked to verbalize their thoughts and annotate on the WebEx screen (Figure 3) while solving the NMR question.

All interviews were conducted one week before or after their final exam or within the final exam week. Before each session, participants were given an overview of the task, what was expected from them, and how to annotate on the screen using WebEx tools. During the interview, students were told they could access the chemical shift table at any point. On average, the interview was about 1 h. All sessions were video recorded.

The interview protocol was composed of six tasks. Each of the first four tasks was based on a foundational NMR concept or skill, which included identifying the number of signals, splitting patterns, and chemical shifts. Here, we focus on students' NMR problem-solving approaches in detail, and we will include only the data we collected from one task. (Please refer to Section 1.1 in Supplementary Document for all NMR tasks). In this task, students were asked to match the structure of a compound to its signals on the ^{1}H NMR spectrum in the selected question. The spectrum that was used in the task was clear and did not have any impurity or solvent peaks (Figure 4). Integration values and multiplicities were not provided. The students can determine the individual peaks based without

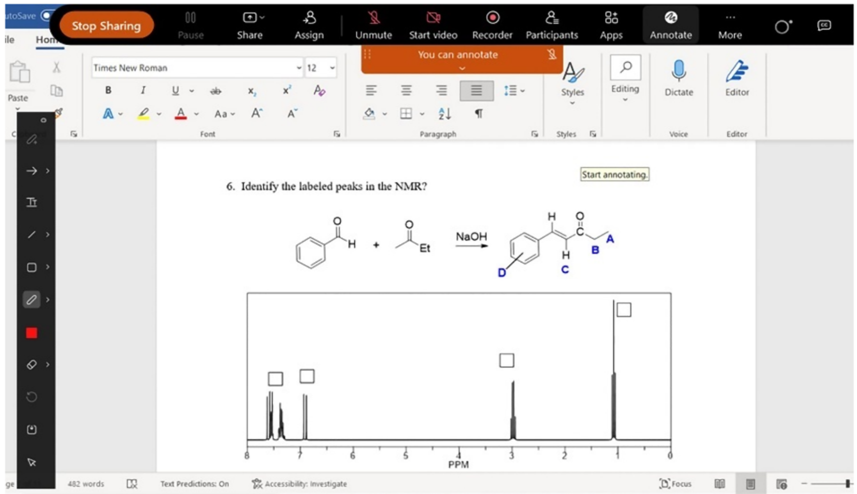

Figure 3: An example of the WebEx screen visible to the student when conducting the interview.

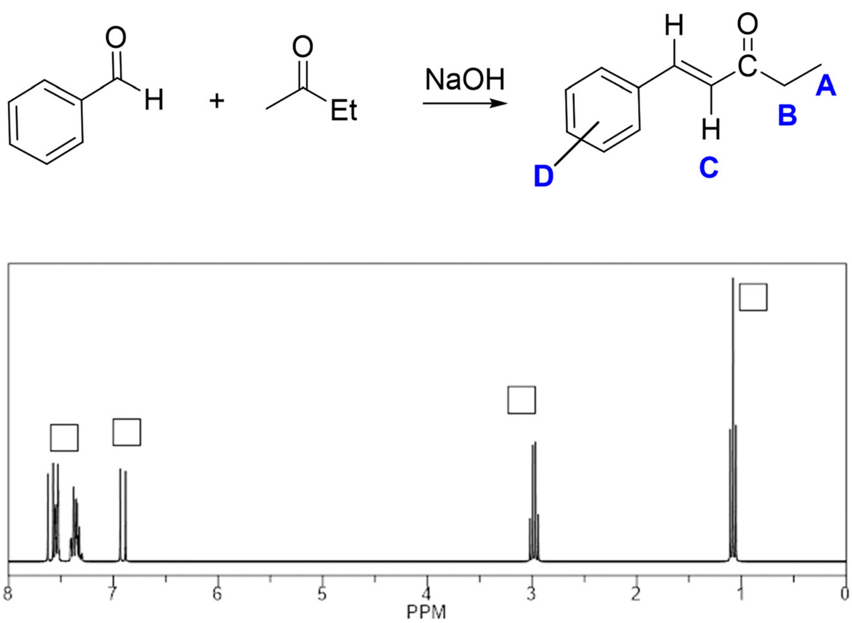

Figure 4: Spectral interpretation task.

providing this information and using other information like chemical shift, and multiplicities information. We utilized ChemDraw software to derive the spectra for the study. Recognizing that NMR analysis can be intellectually challenging (Connor et al., 2019; Topczewski et al., 2017), we aimed to simplify the task to focus on the main principles of NMR spectroscopy. Also, considering the demographics of our students which mainly consist of non-chemistry majors, we decided to adopt a simplified approach. Consequently, we chose not to incorporate a real-life NMR spectrum, omitting any solvent or impurity peaks as it would have added complexity. Our primary objective was to assess the students' fundamental comprehension of NMR principles.

5.6 Identify the labeled peaks in the NMR

We acknowledge that in our NMR spectra, the peaks in the benzene region are grouped together and not individually resolved. As a result, we decided to group these peaks together and label them as a single signal, designated as signal D, for the purpose of interpretation in the given question. This approach was taken to simplify the analysis and facilitate a clearer understanding of the spectra.

5.7 Data analysis

The interviews were transcribed verbatim. The images of the students' work were also embedded in the transcripts to improve the clarity of the student's interview data. We conducted the first round of open coding to identify the problem-solving approaches of students during their problem-solving process. To do so, we arranged the transcript data into a table consisting of two columns. The first column contained verbatim transcript data, and the second column was used to write down the problem-solving approach identified during coding. The data arranged in this format helped us track their problem-solving process chronologically. Then, we uploaded these transcripts in table form to NVivo 12 software to code their problem-solving approaches.

After identifying the problem-solving approaches each student used, we categorized students' problem-solving approaches as productive or unproductive based on the resources framework. If the problem-solving approach helped them towards a correct solution, we categorized it as productive. If the problem-solving approach did not help them get to the correct solution, we categorized it as an unproductive problem-solving approach. We also developed problem-solving maps for each student, to create a visual representation of their problem-solving process.

The first author (SKG) developed the initial coding scheme to identify the problem-solving approaches that students used using the transcripts. All transcripts were used to develop the initial coding scheme. Then, one transcript was randomly selected for collaborative coding with members of the research team. This team was composed of an expert in the field, one Ph.D. student, and two undergraduate students. The collaborative coding session helped to fine-tune the initial coding scheme for problem-solving approaches.

After establishing the initial codes, we coded each transcript using the constant comparative analysis method (Strauss & Corbin, 1990). If we identified a new code, we went back and checked whether that code was present in our earlier coded transcripts.

5.8 Inter-rater reliability

To establish interrater reliability, first, we selected one interview transcript and coders SKG and trained undergraduate (RNS) coded it independently to identify the problem-solving approaches. The reliability calculated was around 55 %, which was low. Then, a thorough discussion about the definition of the codes and the clarity of the codes and unitization issues were resolved between the two coders (SKG and RNS). Then in the second round, we selected another transcript from the online group, and the coders coded it independently and checked for the agreement. This time the agreement was around 80 % for the problem-solving approaches, indicating a strong agreement. To further establish the interrater reliability, we checked another transcript, but this time we selected one in-person transcript. The agreement was around 85 % which was a strong agreement. Then, the first and second coders (RNS) coded the rest of the transcripts to identify the problem-solving approaches.

6 Results and discussion

RQ 1 – Students in our sample utilized a range of problem-solving approaches in response to the given task. The codebook, which contains the full list of problem-solving approaches, including sample quotes, can be found in the Supplementary Information. A summary of the codes is shown in Table 3.

Next, we will look closely at the cognitive and procedural resources students used when considering the four major components of NMR problem solving – counting the number of signals, determining the chemical shift, determining the splitting pattern and integration, and how students used them as a problem-solving approach in dealing with this task. We selected these four features because they are the foundational proton NMR features in the organic chemistry content map published by the ACS Exams Institute (Raker et al., 2013) and are covered universally in the undergraduate organic chemistry curriculum. Moreover, they are the basic NMR concepts covered in standard organic chemistry textbooks (Anderson et al., 2020). Spectral features other than these four, for instance, spin coupling, and determination of diastereotropic protons are taught in some universities but not in all institutions in the undergraduate organic chemistry curriculum. Hence, not considered the basic features related to proton NMR spectroscopy (Anderson et al., 2020).

6.1 Counting the number of signals

The number of equivalent protons in the structure will determine the number of signals that will appear in the spectrum. This problem-solving approach was less frequently used (2.4 %). Mia is one student who started the task

Table 3: Code book (code name, and description).

*Code name	Description
Problem identification	Tries to identify what the question is asking and what they need to do.
Number of signals	
Number of signals – chemical environment	Try to identify different types of signals based on different chemical environments.
Number of signals – symmetry	Use of symmetry principle in identifying signals.
Reasoning about splitting pattern	
Splitting pattern using $n + 1$ rule	Application of the $n + 1$ rule to determine the splitting pattern of signals based on neighboring hydrogens.
Splitting patterns from the spectrum	Using splitting patterns from the spectrum to identify signals.
Reasoning about chemical shift	
Inductive effect-based reasoning for chemical shifts	Use of inductive effect when reasoning about the chemical shift.
Chemical shift – structure-property relationship	Try to correlate structure to its properties to chemical shift.
The reasoning for chemical shift based on stability	Use stability to differentiate relative positions of signals in the NMR spectrum.
Use of chemical shift table	Use of chemical shift table to identify peaks.
Acknowledge the ambiguity of chemical shift values.	Have the idea that chemical shift values aren't discrete values but can be within a range.
Chemical shift table as evidence	Use the chemical shift table as evidence to differentiate signals.
Chemical shift table to identify chemical shift ranges	Chemical shift table to identify chemical shift ranges.
The reasoning of chemical shift based on resonance	Use resonance to different relative positions of signals in the NMR spectrum.
Determination of integration values of signals	Use of integration concept to identify signals.
Compare and contrast	
Compare and contrast the chemical shift	Compare and contrast the chemical shift values of signals.
Compare and contrast the splitting pattern	Compare and contrast the splitting patterns of signals.
Reflection	
Change answer	Change the answer as new information becomes apparent.
Confirm	The student uses NMR concepts to identify the signals during the first or second round of analysis. During this time, they confirm, validate, or verify initial data or answers.
Process of elimination	After identifying all the other signals, use the process of elimination to find the last signal.
Make a plan	Make a plan on the order to follow when identifying the signals.
Random guess	Did not provide any reasoning or backing about selecting the choices
Implement peak labeling	Label the identified peaks in the spectrum

[a]Primary codes are bolded, and secondary codes are unbolded.

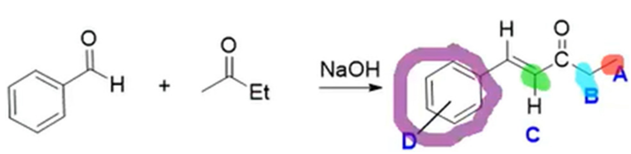

Figure 5: Drawing of Mia.

by counting the number of signals. Mia counted the number of signals by attending to the environments that the protons were in (Figure 5).

Interviewer: So, how do you start this kind of question?

Mia: Um, so I would look at the environments and what they are attached to

Interviewer: Okay,

Mia: so, um, A is one environment [highlighted A in red], B is one environment [highlighted B in blue]. C is also an environment [highlighted C in green] because it's attached to carboxyl, it's attached to double bond and it's also attached to a, um carbonyl group.

Interviewer: yeah.

Mia: And then Um, D it is also a whole environment.

The provided excerpt describes Mia's approach to solving this spectroscopic problem by counting the number of signals based on the environments in which the protons are located. Mia demonstrates an understanding that the number of non-equivalent protons in a structure corresponds to the number of signals observed in the spectrum. By analyzing the molecule's structure and identifying the different environments to which the protons are attached, Mia accurately determines the number of signals for regions labeled A, B, and C.

However, it is notable that Mia did not discuss the number of different environments in region D, even though there are three distinct sets of protons present. The study acknowledges that this oversight may be attributed to how the problem was presented, specifically grouping the aromatic protons in the spectra. This deliberate grouping was done to avoid the challenge of distinguishing individual signals for aromatic protons, which can be difficult due to their overlapping nature.

This observation highlights an important aspect of spectroscopic problem-solving, namely the need for careful consideration of how task is presented and the potential impact it may have on students' interpretations. In this case, grouping the aromatic protons obscured the ability to differentiate their signals individually, possibly leading to Mia's interpretation.

Overall, this highlights the importance of providing clear and representative spectroscopic data to students, allowing them to accurately analyze and interpret the spectra. It also underscores the need for educators to be aware of potential challenges and limitations associated with presenting spectroscopic data, particularly when dealing with overlapping signals or complex molecular structures. By addressing these considerations, instructors can enhance students' problem-solving abilities and promote a more comprehensive understanding of spectroscopy.

Another problem-solving approach that students used when counting the number of signals is symmetry. Mary is one such student who used this approach. This student mentioned that not every hydrogen in the benzene ring shows up as a separate signal due to the symmetry in the benzene ring. Using symmetry in this way was a productive approach that helped students to identify the number of signals. The following is an example from Mary who used symmetry to determine signals C and D.

Mary: But I want to say that this one is D [indicating the most deshielded aromatic protons] and this one [see student notation in Figure 6]is C ***because, um, there is*** *…* ***there is symmetry in the ring, yeah, there's symmetry in the ring,*** *but C, C is a doublet.*

Mary's utilization of symmetry to determine the number of signals in a benzene ring exemplifies the effectiveness of this method in spectroscopy analysis. By recognizing the inherent symmetry within the benzene structure, Mary was able to discern that not every hydrogen atom would generate a distinct signal. This crucial insight prevented her from overestimating the number of expected signals and facilitated a more precise interpretation of the NMR spectrum. By incorporating symmetry considerations, Mary demonstrated her ability to navigate the complexity of molecular structures and harness symmetry as a powerful tool in NMR analysis.

Determining symmetry in counting the number of signals in NMR holds significant importance due to its profound impact on the analysis process. The integration of symmetry considerations enables students and researchers to streamline their interpretation of NMR spectra, simplifying the identification and characterization of different proton environments. When combined with other fundamental NMR techniques, such as chemical shift values and splitting patterns, symmetry analysis provides valuable insights into the molecular system under

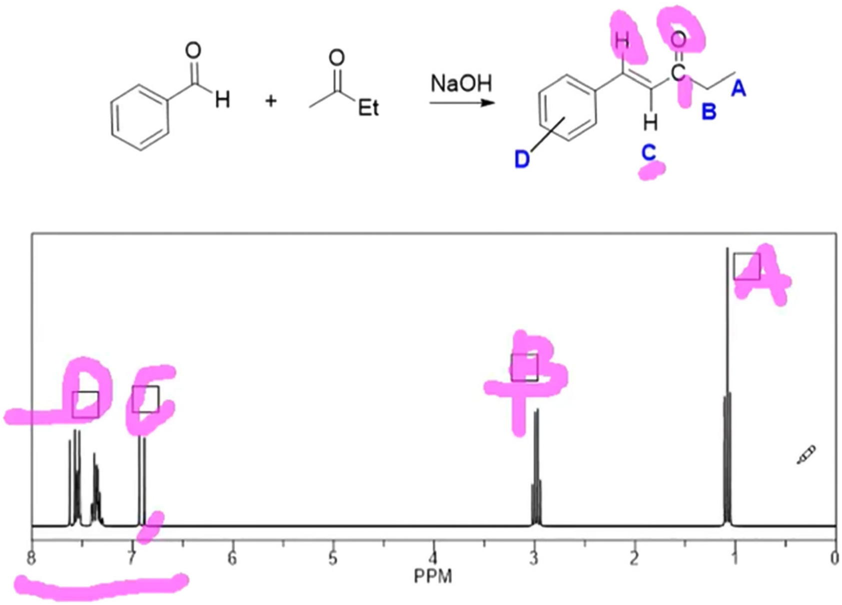

Figure 6: Mary's annotation on the NMR task.

investigation. By applying this holistic approach, students can gain a comprehensive understanding of the structural characteristics embedded within the molecule, enhancing their ability to elucidate intricate details and derive meaningful conclusions from the spectroscopic data.

6.2 Determination of chemical shift

Problem-solving approaches related to chemical shifts were one of the most used problem-solving approaches by students (see Table 3). Students used various relationships or principles to determine the chemical shift such as inductive effect-based reasoning, structure-property relationship, and stability. Also, some students used the provided chemical shift table in determining the chemical shift.

6.2.1 Inductive effect-based reasoning on chemical shift

Although most students had productive ideas about inductive effect-based chemical shift determination, Lia used the idea of inductive effect in an unproductive manner (Figure 7). When attempting to identify the signals, she recalled that when a proton is closer to oxygen (she meant the oxygen of the carbonyl group), it will be more deshielded.

> *Lia: We'll automatically … here, um, this, the D is the most downfield so I would say that the D is going to be … the no … downfield I'm sorry this …* ***the D is the most like, it's the farthest away from that oxygen. So, I would say that the D is the most upfield*** *[see Figure 7 for Lia's annotations].*

And she continued using the same principle in determining the rest of the signals.

> *Lia: and then the, um the B and the A are close … The B itself is closest to the umm carbon double bond oxygen, so I would say that The B is right here (Figure 7) and then I would say that this is C (Figure 7). Because it's also the next closest one, and then the, A is a little bit farther from that. So, it would be upfield.*

Lia had some productive ideas about the inductive effect and about how it relates to shielding and deshielding principles and in determining the chemical shift values. However, she had some challenges connecting these two concepts. That is, she did not incorporate other ideas that affect chemical shifts beyond inductive effects such as

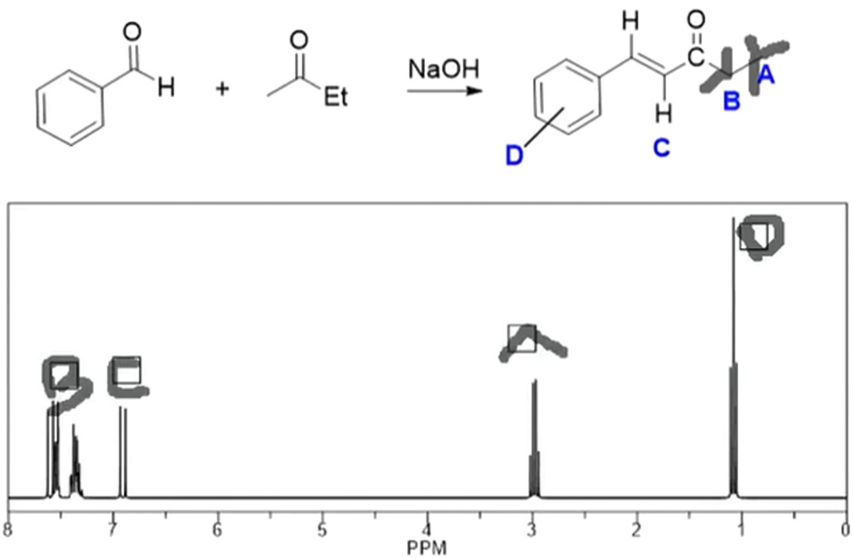

Figure 7: Drawing of Lia.

the anisotropy of the aromatic ring. The presence of an aromatic ring introduces a unique electronic environment, characterized by ring currents and π-electron delocalization, leading to distinctive shielding and deshielding effects. Neglecting these additional factors can limit the accuracy and completeness of the chemical shift determination.

Inductive effect-based reasoning is a commonly employed problem-solving approach used by students to determine the chemical shift in spectroscopic analysis. This approach relies on understanding the influence of electron-withdrawing or electron-donating groups on the chemical environment of a proton, which in turn affects its chemical shift value. In this study, 19 students used this approach and they mostly had productive ideas about inductive effect-based chemical shift determination.

To effectively apply inductive effect-based reasoning in determining chemical shifts, students should consider the overall electronic environment of a proton and evaluate the relative strengths of electron-withdrawing and electron-donating groups present in the molecule. It is also beneficial to refer to established trends and patterns in chemical shift values, such as those found in chemical shift tables or databases, to guide the analysis.

In summary, Lia's experience highlights the importance of integrating various concepts and factors that influence chemical shift values in spectroscopy analysis. While the inductive effect is a critical consideration, other ideas, such as the anisotropy of aromatic systems are needed to obtain a more comprehensive understanding. By considering a broader range of factors and their interplay, students can enhance their ability to accurately interpret spectroscopic data and arrive at reliable conclusions about chemical shift values. A holistic approach that encompasses multiple principles and concepts ensures a more thorough and precise analysis in the field of spectroscopy.

6.2.2 Structure-property relationship-based method in determining the chemical shift

Structure-property relationship-based chemical shift determination was another student -derived problem-solving approach that students used. This problem-solving approach was productive to identify A and B signals but did not help to identify C and D signals. This approach was used by six students. Here is an example quote from Bill:

> *Bill: And B is a secondary alkane. Okay. I just know that the shifts [of] the primary alkane is more closer upfield. It's more closer upfield. Secondary alkane is more … are in between … is less upfield than the primary alkanes and tertiary alkanes are even less upfield compared to A.*

Bill's problem-solving resource utilized a type of structure-property relationship. He used the idea of primary, secondary, and tertiary alkanes to determine chemical shift values, which was a productive approach given the context of the question to identify signals A and B but was not productive when identifying C and D. He switched to a different approach of splitting pattern to identify signal C and D.

> *Bill: this guy (C) is doublet and this guy (trying on identifying neighboring protons for signal D) here, this neighboring, well sometimes, I got confused on how to name. I'm just I'm just going to treat this (signal D) as a multiplet for now.*

Above example shows that Bill's understanding of why certain peaks would appear in specific chemical shift ranges of the NMR spectrum was limited by a surface-level recollection of where certain peaks would appear, rather than a deep understanding of the underlying principles of chemical shift. Additionally, although this use of structure-property relationship is not explicitly taught in the context of the reasoning behind the chemical shift values of signals in proton NMR, students use it as a resource while solving NMR tasks.

6.2.3 The stability-based method in determining the chemical shift

Below is an example in which John utilized a stability-based resource to determine the chemical shift: this is also student-derived problem-solving approach to determine chemical shift and it is important to note that this approach has not been specifically taught in the classroom. But stability and reactivity are heavily discussed in organic chemistry courses and as such some students have developed unproductive student-derived resources based on those and utilize them to explain NMR chemical shifts.

> *John: So, first, if I'm recalling the chemical shift table correctly yeah, definitely. I could be calling it wrong. I believe I saw a* ***CH_3 group that was one of the more rightmost*** *[upfield]and at around one [ppm] and* ***it's going to be more stable of course.*** *So. Immediately I thought, okay, the CH_3 because it has* ***the most number of hydrogens bonded to it that will be my rightmost or the lowest ppm shift****, so that's why I put A at the 1 peak. B having two [hydrogens] greater than one so I put this up at that at that 3 [ppm] peak. C following the trend.*

John's strategy was used successfully to identify signals A, B, and C. However, he encountered difficulty when using this resource to determine the chemical shift for signal D. Although stability is a resource that students may use, it is not directly applicable to proton NMR problem-solving and appears to be a student-generated resource.

The idea of stability is an unproductive resource that was incompatible with the context of this task especially when determining the location of the signals for the benzene ring. Therefore, John had to alter his approach by recalling the chemical shift of aromatic hydrogens and thus, was able to correctly predict the signal for D.

> *John: Yes, because if I recall correctly, aromatics such as benzene worth, had a higher ppm than like the CH_3 group.*

This example emphasizes the possibility that students can arrive at the correct answer using an inappropriate resource. Thus, it highlights the importance of employing assessment questions that ask students to provide reasoning and not merely an answer to a problem. This approach can help students to enhance their understanding and allows instructors to identify and provide feedback when inappropriate resources are utilized by students.

6.2.4 The use of the chemical shift table when reasoning about the chemical shift

A few students (N = 6) consulted the provided chemical shift table to either search for a specific chemical shift value or to substantiate their reasoning. Additionally, some students acknowledged that chemical shift values are not discrete but can have a range by utilizing the chemical shift table. Although the problem-solving approach of using the chemical shift table when reasoning about chemical shift was not frequently, it was typically used productively.

6.3 Conceptual reasoning on the splitting pattern

Conceptual reasoning on the splitting pattern was the most frequently used code and students used it productively and unproductively. Some students applied the $n + 1$ rule unproductively. For example, sometimes students would count the number of hydrogens on the same carbon to determine the splitting pattern instead of counting the neighboring protons for the n in the $n + 1$ rule. It indicates that some students improperly use the $n + 1$ rule and did not know the underlying concepts and reasonings for why signals split. This observation was previously mentioned in literature (Connor et al., 2019). For example, when attempting to identify signals, Lia noted that signals A and B appeared to resemble an ethyl group. She then looked at the structures and identified that signal A has three hydrogen atoms, while signal B has two hydrogen atoms. However, when attempting to apply the $n + 1$ rule to predict the number of peaks in each signal, Lia made an error. Instead of counting the adjacent hydrogen atoms as "n" in the $n + 1$ rule, she incorrectly counted the total number of hydrogen atoms in each signal, not the neighboring hydrogens:

> *Lia: The C is more upfield than B Um, just because normally the, um, well, also doing it based off of the like peak, so this right here (Figure 8, she refers to Hydrogens drawn on the structure for signal A and B)* ***would technically be like an ethyl****. So, you would count this technically is. hold on, let me see if I can. Yeah, so this would technically count,* ***this was like 2 hydrogens and then this like, this A, would count as 3 hydrogens.***

> *Lia: So, based off of that, the B has more and it makes kind of sense more sense just looking at the spectrum, and then you can see, like the hydrogen here (Shows the hydrogen on the structure labeled as C). So, if you do the n + 1 and there's only one hydrogen there, it makes sense that there's gonna be 2 [doublet] Like, right here (showing 6.9 ppm doublet in the spectrum of Figure 8) for the C. And then it also makes sense for the, A, because the A has 3 H. So, n + 1, which is why it looks like there's 4 on that A. (Figure 8).*

Lia had a productive idea here and observes that sometimes the splitting patterns in NMR spectra may not exactly match the pattern that is expected. However, despite this productive idea, her unproductive application of the $n + 1$ rule and unproductive ideas about chemical shift led her to an incorrect solution. This highlights that students need to triangulate data and use multiple pieces of information to solve NMR questions.

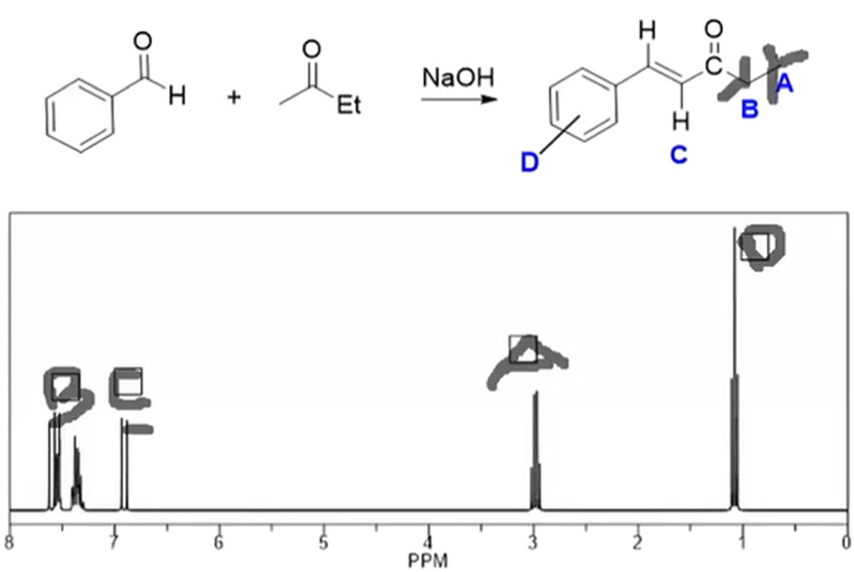

Figure 8: Drawing of Lia. (The $n + 1$ rule is a productive heuristic resource that can help students quickly determine the splitting pattern. However, Lia is using that resource in an unproductive way in solving this task and she gets stuck when reasoning about signal B).

> *Interviewer: Okay. What is the splitting pattern of B?*

> *Lia: The B is the same thing? It just for me B this is where I always say, like, it looks like sometimes there's moments where it's like, the chart,* ***and it's necessarily doesn't match up with the n + 1 because for B if there's 2 hydrogens right here,*** *obviously the 2 doesn't match up with how many looks like there's in there, because it looks like there might be 4. hmm.*

If Lia had a productive understanding of chemical shift, she may have been able to catch the error in her application of the $n + 1$ rule. This is because chemical shift can provide important information about the chemical environment of a molecule and having a solid understanding of both chemical shift and the $n + 1$ rule can help ensure accurate interpretation of NMR spectra.

Overall, it is important that students acknowledge that when solving NMR problems, it is important to consider multiple pieces of information, including chemical shift, peak splitting, and peak intensities to avoid errors and ensure accurate interpretation.

6.3.1 Determination of splitting pattern using spectrum

The effective use of representations is crucial for one's problem-solving success (De Leone & Gire, 2006). It applies to solving proton NMR problems also in which students must deduce information from the NMR spectrum. This includes looking along the X-axis in the NMR spectrum to determine chemical shift values and the use of peak shape to determine splitting patterns and integration. That is, starting at the spectrum and then making determinations about the structure rather than from structure to spectrum.

Students oftentimes used this spectrum-based approach in determining the splitting pattern. Eli is one of the students who used this approach, and she used this approach productively.

Eli: Okay. Here can't quite read this. I'm thinking 1,2,3,4 [she is counting the number of peaks in the signal at 3 ppm on the spectrum] and this 1, I think is 1, 2 3 [she is counting the number of peaks in the signal at 1 ppm on the spectrum] (Figure 9). So then for 7 and 8 [ppm]. We know that's usually what, um the benzene ring. It was a benzene signal, I wanna say this one is D [label D signal]

Interviewer: So, among the two signals at 7 ppm and 8 ppm how do you know that the last signal is D?

Eli: Because it has like, multiple peaks and that's like commonly what the benzene peaks look like.

Interviewer: Oh, okay.

Understanding splitting patterns is an important aspect of interpreting NMR spectra, and it can be approached using different methods. One commonly used approach is the application of the $n + 1$ rule, which predicts the number of peaks in a splitting pattern based on the number of neighboring protons. However, another effective method is to analyze the spectrum itself to gain insights into the splitting patterns.

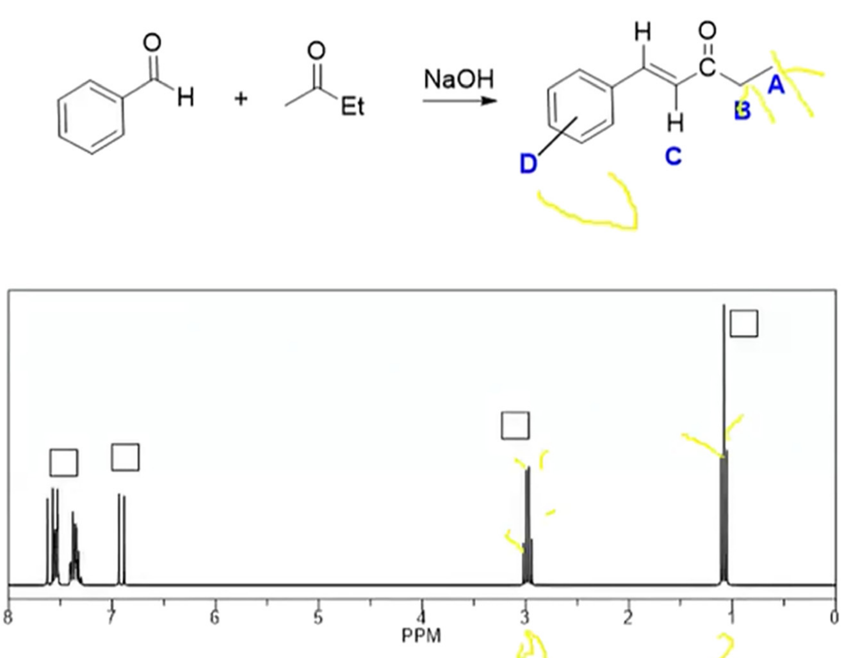

Figure 9: Drawing of Eli.

Eli, as a student who adopts a spectrum-based approach to determine splitting patterns, exemplifies how we can use representations productively and highlights their significance in solving proton NMR problems. By closely examining the peaks in the spectrum, Eli can observe the multiplet patterns and deduce information about the neighboring protons and their arrangement within the molecule. This approach not only demonstrates Eli's ability to effectively utilize representations but also emphasizes the benefits of this method in problem-solving.

6.4 Integration

Integration is one of the basic NMR concepts, that oftentimes, do not get an equal emphasis in undergraduate instructional settings (Anderson et al., 2020). However, it has been mentioned as a required component in proton NMR problem-solving in ACCM (Anchoring Concepts Content Map) for ACS exams (Raker et al., 2013). Also, it is one of the proton NMR concepts that do not receive equal emphasis in most textbooks (Anderson et al., 2020).

During our interview sessions with students and instructors, it was brought to our attention that the integration concept was briefly covered during instruction. So, students had mixed ideas about the integration concept, and some students were able to use the integration concept productively and some did not have any clue about what is meant by integration. Out of the group, only eight students were able to utilize the integration approach in either a productive or unproductive manner. It should be noted that the integration values were not explicitly stated in the question, which may have contributed to the infrequency of its use among the students.

Interviewer: Okay, like, can you tell me what is the integration of B?

Aria: Oh, are you asking for a number? Integration would be.

Interviewer: It's okay if you don't know.

Aria: Yeah, I don't think I have a number. I just know it's like, when they kind of like, combine, but I don't have a number.

Other students seemed confident in using the integration concept in their problem-solving process. The following is an example from Ben's interview.

Ben: For A, I want to say. It's this. (Label A on the spectrum)

Interviewer: What makes you think that is signal A?

Ben: um. A few things, first of all it's the highest peak. Which means that there's quite a few protons there, which would make sense for A

The findings from the interview sessions strongly emphasize the critical need for adequate instruction and equal emphasis on the concept of integration in undergraduate proton NMR instruction. It is crucial to incorporate integration into the instructional curriculum in a manner that effectively conveys its relevance and enables students to utilize it proficiently in problem-solving. By incorporating integration into instructional materials, textbooks, and examination questions, instructors can ensure that students develop a comprehensive understanding of this concept and its practical application in NMR spectroscopy. The observed mixed understanding and utilization of integration among students further emphasize the imperative for enhanced instruction and curriculum development in this specific area. By providing explicit coverage of integration and integrating it comprehensively into instructional materials, educators can facilitate students in developing a stronger grasp of this concept and its significance in the context of NMR spectroscopy.

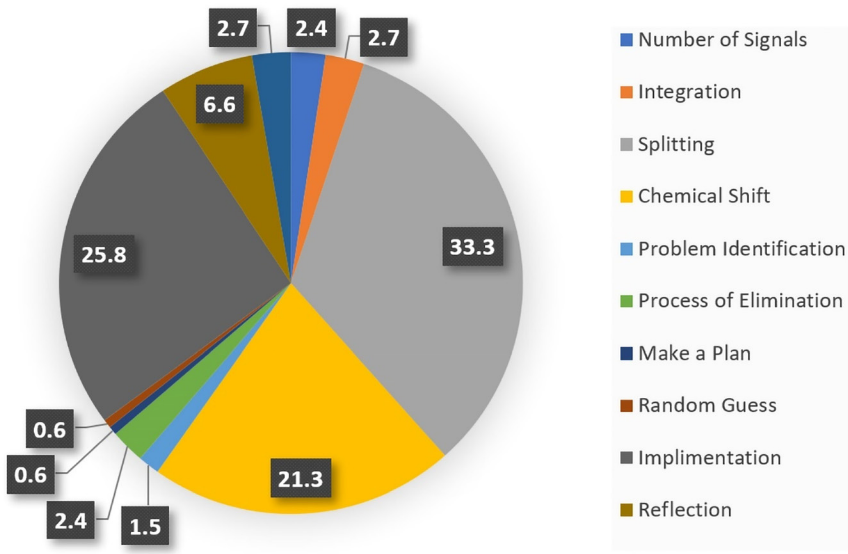

Figure 10: Frequency percentage of the problem-solving approaches for the task.

6.5 RQ 2. Frequency of problem-solving approaches that students used for the task

Beyond the resources directly related to the number of signals, chemical shift, and splitting patterns, students also employed other problem-solving approaches and resources such as random guessing, problem identification, process of elimination, reflection, and compare and contrast. Details of these approaches are described in the Supplementary Document.

Figure 10 illustrates the distribution of problem-solving approaches employed by students for the task, expressed as a percentage frequency. The most frequently used problem-solving approaches are determining the splitting pattern, chemical shift determination, and implementation. Problem-solving approaches outside of these three were less frequently used (<10 %). Again, the problem-solving approaches students used may be a consequence of the task itself.

The analysis of problem-solving approaches employed by students reveals that approaches outside of the three major categories (splitting pattern determination, chemical shift determination, and implementation) were utilized less frequently, with a frequency of less than 10 %. This observation suggests that these approaches may have been perceived as less effective or relevant by the students, or they may not have been explicitly emphasized in the instructional context. However, it is essential to consider that the infrequent usage does not necessarily imply a lack of value, but rather indicates their relatively lower prominence in the problem-solving process for the specific tasks at hand.

Furthermore, the diverse range of problem-solving approaches exhibited by students underscores their resourcefulness and adaptability in tackling proton NMR problems. These approaches showcase the students' capacity for critical thinking, problem identification, and the application of various cognitive strategies to arrive at solutions. The variability in problem-solving approaches also highlights the significance of cultivating a comprehensive problem-solving toolkit to help students to tackle problems.

6.6 RQ 3. The productive and unproductive problem-solving approaches that students use

Figure 11 illustrates the productive and unproductive problem-solving approaches that students used. Random guessing was the least productive approach, while the integration approach was used unproductively 44 % of the time. Conceptual reasoning for splitting pattern and chemical shift determination were used unproductively approximately 14 % and 10 % respectively. All other problem-solving approaches were used successfully 100 % of the time.

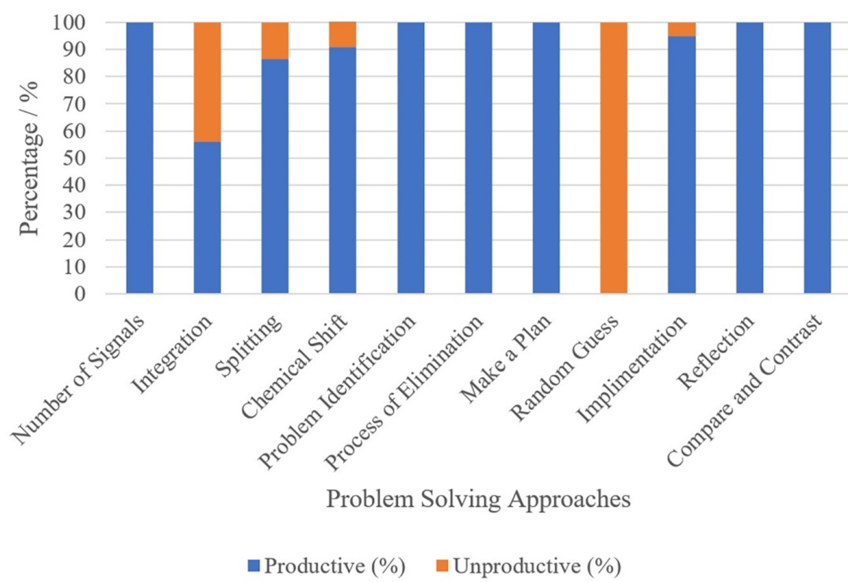

Figure 11: Productive and unproductive use of problem-solving approaches that students used for the task.

Among the various problem-solving approaches, random guessing emerged as the least productive, indicating its limited effectiveness in solving proton NMR problems. This finding underscores the significance of employing systematic and informed strategies, rather than relying on chance alone, when approaching spectroscopic problem-solving tasks.

Moreover, the integration approach was utilized unproductively in 44 %, suggesting that students encountered difficulties in effectively applying the concept of integration in their problem-solving process. Integration plays a critical role in determining the structure of a given molecule. The high percentage of unproductive use suggests that students may have struggled with the interpretation and application of integration values.

Additionally, conceptual reasoning for splitting pattern determination and chemical shift determination was employed unproductively in approximately 14 % and 10 % of instances, respectively. This finding implies that some students faced challenges in understanding and applying the fundamental concepts underlying splitting patterns and chemical shifts. These concepts are essential in proton NMR analysis, significantly contributing to the determination of molecular structure and connectivity. The unproductive utilization of these approaches highlights the need for enhanced instruction and conceptual understanding in these specific areas.

Conversely, all other problem-solving approaches were successfully employed 100 % of the time. These approaches likely encompassed strategies such as problem identification, process of elimination, reflection, compare and contrast, making a plan, and counting the number of signals. The consistent success with these approaches suggests that students effectively utilized these resources to navigate through the problem-solving process.

The findings depicted in Figure 11 emphasize the importance of providing targeted instruction and support in areas where students encounter difficulties. The unproductive use of certain problem-solving approaches, particularly integration and conceptual reasoning for splitting pattern and chemical shift determination, underscores the need for additional emphasis on these concepts during instruction. By addressing these challenges and fostering a deeper conceptual understanding, educators can enhance students' problem-solving abilities in the context of proton NMR analysis.

6.7 RQ 4. The comparison of the problem-solving approaches that students used based on how they received instruction (online vs. in-person instruction)

We did not observe a notable difference in the use of problem-solving approaches in online and in-person groups. Figure 12 show the online and in-person comparison of problem-solving approaches that students used.

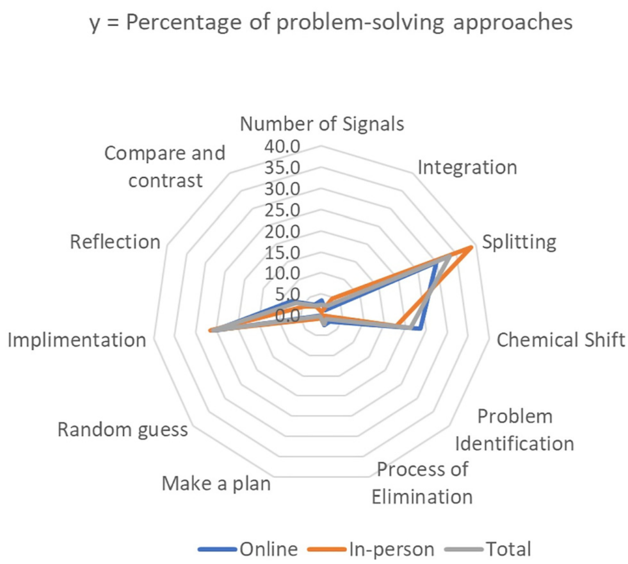

Figure 12: The comparison of problem-solving approaches that students used (online, in-person, total).

Figure 12 is a radar chart, which is a type of two-dimensional chart commonly used to represent two or more quantitative variables represented on axes starting at the same starting point. In this instance, the chart portrays the frequency percentage of problem-solving approaches, with each problem-solving approach plotted along its own axis, and all the axes converge at the center of the chart. The chart compares the frequency percentage of problem-solving approaches employed by two groups: the online group, indicated by a blue line, and the in-person group, indicated by an orange line. The gray line denotes the total. Based on the chart, it can be observed that the frequency percentage of problem-solving approaches used by the in-person and online groups largely overlap, suggesting that there is no major difference in the use of problem-solving approaches between the two groups.

The absence of a substantial difference in the use of problem-solving approaches between online and in-person groups suggests that students in both settings were able to employ similar resources to solve NMR problems. This implies that online instruction can effectively facilitate the development of problem-solving skills in this domain, comparable to traditional in-person instruction.

However, it is important to acknowledge that the absence of a significant difference in problem-solving approaches between online and in-person instruction does not imply overall equivalence between the two modes. Various factors, such as the quality of instruction, availability of resources, and individual student characteristics, can still impact learning outcomes. However, in the specific context of employing problem-solving approaches for proton NMR analysis, the findings suggest that online instruction can be equally productive as in-person instruction.

It is crucial to consider the potential benefits and challenges associated with online instruction. While online learning offers flexibility and accessibility, it may require additional measures to ensure effective instruction, student engagement, and access to necessary resources. Conversely, in-person instruction provides face-to-face interaction and immediate support but may have limitations in terms of scheduling and human or instrumental resources.

The findings from the comparison of problem-solving approaches in the online and in-person groups shed light on the adaptability and effectiveness of online instruction for developing problem-solving skills in proton NMR analysis. These results can guide educators in designing online instructional strategies that effectively promote critical thinking, conceptual understanding, and application of problem-solving approaches in the domain of spectroscopy.

7 Conclusions

In this qualitative study, we investigated how undergraduate students solve a proton NMR question which requires the incorporation of all basic concepts related to proton NMR, counting the number of signals, determining the splitting pattern, determining chemical shift and integration. Additionally, we have identified the problem-solving resources employed by the participants when approaching the task at hand. Furthermore, we have also determined the frequency of problem-solving approaches used by research participants.

In the given task, students were given the structure and the spectrum, and they had to identify the matching peaks in the spectrum. Our results revealed that participants used more productive approaches than unproductive approaches while solving the problem. When we looked at the online and in-person groups separately, we did not observe any difference between the problem-solving approaches that students used.

One of the primary rationales for selecting this particular task was to evaluate the student's capacity to apply triangulation techniques when processing data derived from various fundamental NMR concepts. Most students relied solely on one basic NMR concept to draw conclusions about a given peak. This approach often resulted in a protracted and unproductive process of trial and error when attempting to arrive at the correct answers. John serves as a prime example of this phenomenon, where he switched answers several times.

8 Implications

8.1 For teaching

Our study suggests that educators should provide students with a broad range of questions rather than limiting them to a narrow set of examples. We observed that some students developed their own resources, such as structure-property relationships, to determine chemical shifts. However, if instructors design tasks that address the limitations of certain problem-solving approaches, it can help students gradually develop a deeper understanding of the appropriate resources required to activate in diverse contexts of problems.

Our findings also indicate that students occasionally arrive at the correct answer through flawed reasoning. This highlights the importance of using two-tier questions in assessment whenever appropriate, as previously noted in Mutambuki and Fynewever's study (2012). Two-tier questions, comprising a first-tier question followed by a reasoning tier, play a crucial role in monitoring and assessing students' reasoning abilities. These types of questions provide instructors with valuable insights into whether students are arriving at the correct answers for the appropriate reasons. By incorporating the reasoning tier, educators can gain a deeper understanding of students' cognitive processes and identify any misconceptions or gaps in their understanding.

Moreover, both conceptual knowledge and well-developed problem-solving skills are required to become a competent problem solver. Instructors should give equal emphasis to all the requisite concepts related to proton NMR. It was noted that students paid more attention to certain problem-solving approaches pertaining to concepts like splitting patterns and chemical shifts, and comparatively less attention to those related to integration. A strong grasp of concepts like integration can assist students in developing their problem-solving skills. Hence, it is imperative for instructors to give equal importance to all four fundamental concepts of proton NMR instead of focusing solely on one or two concepts while neglecting the others.

When helping students to develop problem-solving skills, chemistry teachers and instructors should explicitly model their NMR problem-solving process (Wood, 2006). Also, guided inquiry activities that incorporate predefined templates for signal analysis can serve as effective tools to guide students through the problem-solving process. After tabulating their data using the provided template, students can utilize the results to construct partial structures. Subsequently, this information can be combined with additional data, such as IR, mass, and ^{13}C NMR, to construct the complete structure.

Furthermore, group activities can be an excellent way to supplement individual practice and enhance learning outcomes. Collaborative learning environments provide opportunities for students to share their knowledge and perspectives, co-construct knowledge, and learn from one another (Mooring et al., 2022). During our study, it came to our attention that Lia, when attempting to identify the signals, utilized an unproductive approach for inductive effect-based reasoning. She incorrectly recalled that a proton becomes more deshielded when it is closer to oxygen (the oxygen of the carbonyl group). However, we observed that if Lia had been part of a collaborative group, there would have been a higher likelihood of someone in the group recognizing the inadequacy of this approach. Through collaborative efforts, they could have collectively constructed knowledge and increased the chances of arriving at the correct answer.

Group activities should include predicting and sketching out NMR peaks based on organic compound structures before consulting the spectrum, which would be an effective strategy for enhancing NMR problem-solving abilities. This approach encourages students to actively engage with the material and develop a deeper understanding of NMR concepts, as well as the relationship between structure and spectral peaks. Additionally, verifying their predictions against the actual spectrum, and discussing it with peers, will be an excellent way for the students to develop their critical thinking and problem-solving skills.

8.2 For research

The findings in this research demonstrate that research should not only focus on students' conceptual understanding but also need to develop some new strategies to help students to aid with problem-solving. Also, looking deeply into how NMR material is presented to students and how it will help to develop students' conceptual knowledge and problem-solving abilities could be another area of focus. Also, how students solve proton NMR problems in various difficulty levels and students' representational competence in solving spectroscopic questions could be another area to explore. As in this study, it will also be important to further explore how students solve tasks that are related to spectroscopic problems faced by everyday organic chemists in the laboratory.

Furthermore, it is worth noting that currently, there is a lack of established concept inventory within the field of NMR, with the exception of the NMR lexical representational competence inventory (Connor et al., 2021). Therefore, the development of a comprehensive concept inventory for NMR represents a promising avenue for future research in this domain.

Another area that is worth exploring is the comparison between in-person and online instruction in various other aspects of conceptual gains and the development of problem-solving skills related to proton NMR. Additionally, it would be worthwhile to investigate how hands-on experiences aid in the development of skills and proficiency in NMR problem-solving, as compared to online instruction.

9 Limitations

This study was carried out with 24 participants and at one institution; therefore, the generalizability of the results may be limited. Additionally, our analysis focused on only one task, which may not provide a comprehensive understanding of participants' problem-solving approaches and success in proton NMR. For example, the limitations of certain problem-solving approaches like structure-property relationship and stability-based methods in determining chemical shift if we used more than one task.

Moreover, it is worth noting that the use of a think-aloud protocol may cause some stress on participants, and solving questions virtually on a screen may create fatigue in some participants. Additionally, the spectrum we utilized was devoid of solvent peaks, which may not accurately reflect the NMR spectra encountered by chemists in real-world scenarios. However, we were able to gain knowledge of the resources students elicit around basic NMR concepts.

Supplementary Information

1.1 NMR interview questions
1.2 Complete code book

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References

Anderson, S. Y. C., Ong, W. S. Y., & Momsen, J. L. (2020). Support for instructional scaffolding with ^{1}H NMR spectral features in organic chemistry textbook problems. *Chemistry Education: Research and Practice*, *21*(3), 749–764.

Angawi, R. F. (2014). Using a problem solving-cooperative learning approach to improve students' skills for interpreting ^{1}H NMR spectra of unknown compounds in an organic spectroscopy course. *Journal of Chemical Education*, *91*(6), 823–829.

Azman, A. M., & Esteb, J. J. (2016). A coin-flipping analogy and web app for teaching spin–spin splitting in 1H NMR spectroscopy. *Journal of Chemical Education*, *93*(8), 1478–1482.

Becker, N. M., Rupp, C. A., & Brandriet, A. (2017). Engaging students in analyzing and interpreting data to construct mathematical models: An analysis of students' reasoning in a method of initial rates task. *Chemistry Education: Research and Practice*, *18*(4), 798–810.

Cartrette, D. P., & Bodner, G. M. (2010). Non-mathematical problem solving in organic chemistry. *Journal of Research in Science Teaching*, *47*(6), 643–660.

CatalystEdu. (2018). Lab Flow. https://www.catalystedu.com/labflow

Connor, M. C., Finkenstaedt-Quinn, S. A., & Shultz, G. V. (2019). Constraints on organic chemistry students' reasoning during IR and ^{1}H NMR spectral interpretation. *Chemistry Education: Research and Practice*, *20*(3), 522–541.

Connor, M. C., Glass, B. H., Finkenstaedt-Quinn, S. A., & Shultz, G. V. (2020). Developing expertise in ^{1}H NMR spectral interpretation. *The Journal of Organic Chemistry*, *86*(2), 1385–1395.

Connor, M. C., Glass, B. H., & Shultz, G. V. (2021). Development of the NMR lexical representational competence (NMR-LRC) instrument as a formative assessment of lexical ability in ^{1}H NMR spectroscopy. *Journal of Chemical Education*, *98*(9), 2786–2798.

De Leone, C. J., & Gire, E. (2006). Is instructional emphasis on the use of non-mathematical representations worth the effort? *AIP Conference Proceedings*, *818*(1), 45–48.

Elby, A., & Hammer, D. (2010). Epistemological resources and framing: A cognitive framework for helping teachers interpret and respond to their students' epistemologies. *Personal Epistemology in the Classroom: Theory, Research, and Implications for Practice*, *4*(1), 409–434.

Giuliano, R., & Carey, F. (2020). *Organic chemistry 11th Edition*. McGraw-Hill Higher Education.

Greenbowe, T. J. (1983). *An investigation of variables involved in chemistry problem solving*. Purdue University.

Hammer, D., & Elby, A. (2003). Tapping epistemological resources for learning physics. *Journal of the Learning Sciences*, *12*(1), 53–90.

Hammer, D., Elby, A., Scherr, R. E., & Redish, E. F. (2005). Resources, framing, and transfer. In *Transfer of learning from a modern multidisciplinary perspective* (pp. 89–119). Greenwich, Connecticut: Information Age Publishing.

Henary, M., Owens, E. A., & Tawney, J. G. (2015). Creative report writing in undergraduate organic chemistry laboratory inspires nonmajors. *Journal of Chemical Education*, *92*(1), 90–95.

Holme, T. A., Luxford, C. J., & Brandriet, A. (2015). Defining conceptual understanding in general chemistry. *Journal of Chemical Education*, *92*(9), 1477–1483.

Karty, J., & Melzer, M. (2018). *Organic chemistry: Principles and mechanisms*. W. W. Norton.

Kolonko, E. M., & Kolonko, K. J. (2019). Introducing NMR spectroscopy using guided inquiry and partial structure templating. *Journal of Chemical Education*, *96*(5), 912–919.

Lieber, L., & Graulich, N. (2020). Thinking in alternatives—a task design for challenging students' problem-solving approaches in organic chemistry. *Journal of Chemical Education*, *97*(10), 3731–3738.

Lopez, E. J., Shavelson, R. J., Nandagopal, K., Szu, E., & Penn, J. (2014). Factors contributing to problem-solving performance in first-semester organic chemistry. *Journal of Chemical Education*, *91*(7), 976–981.

Martin, C. B., Schmidt, M., & Soniat, M. (2011). A survey of the practices, procedures, and techniques in undergraduate organic chemistry teaching laboratories. *Journal of Chemical Education*, *88*(12), 1630–1638.

Mooring, S. R., Burrows, N. L., & Gamage, S. (2022). Flipped classrooms in organic chemistry—a closer look at student reasoning through discourse analysis of a group activity. In *Student reasoning in organic chemistry* (pp. 159–178). Royal Society of Chemistry.

Mutambuki, J., & Fynewever, H. (2012). Comparing chemistry faculty beliefs about grading with grading practices. *Journal of Chemical Education*, *89*(3), 326–334.
Parker, S. P. (1988). *Spectroscopy source book*. McGraw-Hill (Tx).
Patiny, L., Bolaños, A., Castillo, A. M., Bernal, A., & Wist, J. (2018). Teaching NMR spectra analysis with nmr.cheminfo.org. *Magnetic Resonance in Chemistry*, *56*(6), 529–534.
Pavia, D. L., Lampman, G. M., Kriz, G. S., & Vyvyan, J. A. (2014). *Introduction to spectroscopy*. Cengage Learning.
Raker, J., Holme, T., & Murphy, K. (2013). The ACS exams institute undergraduate chemistry anchoring concepts content map II: Organic chemistry. *Journal of Chemical Education*, *90*(11), 1443–1445.
Rodriguez, J.-M. G., Bain, K., Hux, N. P., & Towns, M. H. (2019). Productive features of problem solving in chemical kinetics: More than just algorithmic manipulation of variables. *Chemistry Education: Research and Practice*, *20*(1), 175–186.
Schummer, J. (2002). In P. Morris (Ed.), *The impact of instrumentation on chemical species identity: From chemical substances to molecular species*. The Royal Society of Chemistry.
Socha, O., Osifová, Z., & Dračínský, M. (2023). NMR-Challenge.com: An interactive website with exercises in solving structures from NMR spectra. *Journal of Chemical Education*, *100*(2), 962–968.
Strauss, A., & Corbin, J. (1990). *Basics of qualitative research*. Sage Publications.
Surif, J., Ibrahim, N. H., & Dalim, S. F. (2014). Problem solving: Algorithms and conceptual and open-ended problems in chemistry. *Procedia – Social and Behavioral Sciences*, *116*, 4955–4963.
Tomaszewski, R. (2011). A science librarian in the laboratory: A case study. *Journal of Chemical Education*, *88*(6), 755–760.
Topczewski, J. J., Topczewski, A. M., Tang, H., Kendhammer, L. K., & Pienta, N. J. (2017). NMR spectra through the eyes of a student: Eye tracking applied to NMR items. *Journal of Chemical Education*, *94*(1), 29–37.
Wilcox, C. F., & Wilcox, M. F. (1995). *Experimental organic chemistry: A small-scale approach* (2nd ed.). Prentice-Hall.
Wittmann, M. C. (2006). Using resource graphs to represent conceptual change. *Physical Review Special Topics – Physics Education Research*, *2*(2), 020105.
Wittmann, M. C., & Black, K. E. (2015). Mathematical actions as procedural resources: An example from the separation of variables. *Physical Review Special Topics – Physics Education Research*, *11*(2), 020114.
Wood, C. (2006). The development of creative problem solving in chemistry. *Chemistry Education: Research and Practice*, *7*(2), 96–113.

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