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Using Jigsaw-Style Spectroscopy Problem-Solving To Elucidate Molecular Structure through Online Cooperative Learning

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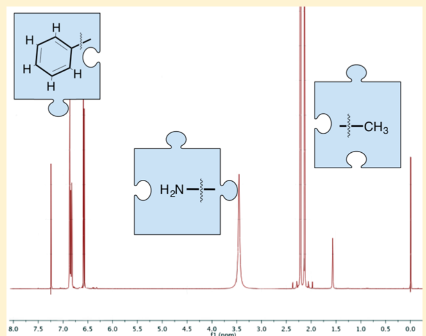
Supporting Information

ABSTRACT: Cooperative learning was employed as an instructional approach to facilitate student development of spectroscopy problem solving skills. An interactive online environment was used as a framework to structure weekly discussions around spectroscopy problems outside of class. Weekly discussions consisted of modified jigsaw-style problem solving activities in which students cooperatively interpreted infrared and nuclear magnetic resonance spectra. Students' use of the discussion site was monitored and revealed that they accessed discussions in the days prior to examinations. Together with attitudinal surveys, which were used to gauge student perceptions of the activities, these results indicate that students found the discussions to be a useful resource for learning spectroscopy.



KEYWORDS: *Second-Year Undergraduate, Organic Chemistry, Collaborative/Cooperative Learning, Problem-Solving/Decision-Making, Internet/Web-Based Learning, Multimedia-Based Learning, IR Spectroscopy, NMR Spectroscopy*

Teaching problem solving is a primary goal of chemistry education.[1,2] Unfortunately, students frequently leave chemistry courses without developing problem solving abilities.[3,4] As instructors, we often mistake student engagement with routine textbook exercises as problem solving. However, true problem solving, described by Wheately as "what you do when you don't know what to do," occurs when students are faced with a novel problem that places them in unfamiliar territory.[5] Numerous studies have investigated problem solving in chemistry in order to identify strategies employed by students in this context.[6−11]

One challenging area of organic chemistry instruction is spectroscopic identification. Solving organic structures through spectroscopic interpretation begins with learning to read, analyze, and fully interpret spectra, which requires practice, access to authentic spectra and, most importantly, a social context which functions as a source of diverse views to challenge the students and stimulate the learning process.[12,13] Spectroscopy problems which ask students to predict molecular structures based on spectral data are particularly challenging for students because they require multiple steps during which students must repeatedly draw on their knowledge of different chemistry concepts such as electronegativity and bond order in addition to NMR-specific topics like shielding and splitting.[14−16] These sorts of problems demand a high level of information processing[17] and a solid understanding of fundamental NMR spectroscopy concepts. Thus, students who rely on algorithmic strategies to solve these types of problems are often unsuccessful.[16] Bodner identified successful spectroscopy problem solvers as those students who adopted more consistent approaches, which involved drawing molecular fragments as they worked, more efficiently mining spectral data, and checking their final answer against the spectra provided.[16] Providing students with activities and learning strategies that promote alternatives to rote memorization and algorithmic heuristics[11] is expected to help them develop more meaningful problem solving skills.

Numerous studies have praised student-centered, cooperative learning in which the course instructor plays the part of a discussion facilitator.[18−22] In this format, students tend to engage in higher-order thinking, which promotes active learning in the discussion space and results in higher student satisfaction.[23−26] Slavin defined cooperative learning as (ref 23, p 160):

> *A set of educational strategies in which students work together in small groups to help each other learn academic content.*

Cooperative learning is an instructional strategy that is shown to improve students' problem solving ability. Towns reported that students who participate in cooperative learning

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activities "move away from rote learning strategies and more toward meaningful strategies."[18] Likewise, in her assessment of the effect of collaborative groups on students' problem solving strategies, Cooper found that students who participated in collaborative work developed improved problem solving strategies that they continued to employ when they worked individually.[19] Cooperative learning was previously applied to NMR spectroscopy and was reported to improve student achievement on exams.[14] In some cases, cooperative online learning offers a more feasible alternative to in-class implementation, and several investigations of utilizing online environments to promote collaborative learning in the context of chemistry have been reported.[20−22,27,28]

■ ONLINE ENVIRONMENT

Students and instructors can access a wealth of organic spectroscopy learning resources online that range significantly in difficulty and focus. Such Web sites are useful as supplementary teaching tools[29−35] because they offer practice beyond what is available in a typical organic chemistry textbook and a few allow students to interact with spectra by providing magnification and integration tools. However, these sites typically provide single answers rather than elaborated solutions for each problem and do not situate the problems within a context of other laboratory tasks,[36,37] such as how to determine if a reaction has occurred by comparing spectra of starting material and product. Thus, students are not able to examine how a peer or an expert gleans important information from different parts of a spectrum. Furthermore, online resources are not always a good fit because tools hosted by other educational institutions usually contain information or topics that are not covered, or that are presented in a different order, than at a student's home institution.

We anticipated that one way to more readily integrate cooperative problem solving would be to use a locally designed online resource where students from the same course can approach spectroscopy problems as a group and learn problem analysis together outside of regular class time.[38] Online cooperative learning approaches were shown to be successful in other chemistry problem solving contexts.[20−22] The approach described here is in contrast to other approaches, which dedicate class time to allow for group-based spectroscopy solving in-person.[39,40]

The impact of classroom environment on cooperative learning has previously been investigated.[41−46] Some aspects of face-to-face social interaction are not possible when cooperative work is done online, particularly when it is text-based. For instance, gesturing, which conveys information beyond that of verbal communication, is not always captured in online environments, and therefore, students may be hindered in communicating with each other.[44] However, technology rich environments free students and instructors up for activities that may not be feasible within the time constraints of the traditional classroom. They provide a platform for instructors to collect data about the learning process and to assess their students. Further, they enable students to explore complex material, such as spectroscopy, on their own time.[45]

In constructing the discussion prompts, we further recognized that in a research lab setting, chemists interpret spectra as experimental data that is obtained directly from an NMR spectrometer. Spectra derived from authentic sources are rarely, if ever, taken on samples that are free from solvents, trace impurities, or reaction byproducts, and they often exhibit splitting patterns and overlapping signals that add challenges to their interpretation far beyond the standard, first-order textbook examples. By providing students with authentic spectra, we aimed to push students to develop meaningful problem-solving strategies by presenting them with unfamiliar and authentic spectroscopy problems.

Small group discussions around structure elucidation from NMR and IR data were hosted online using VoiceThread,[38,47] an interactive site that facilitates communication around visual prompts. The site can host images, presentations, and videos with which students can interact by commenting through text, voice, or video. Students can also utilize a doodle tool, which converts any slide into a virtual whiteboard on which they can draw or label images, such as an ^{1}H NMR spectrum. The doodle tool is one way to support communication that might otherwise be difficult using an online system. For instance, verbal explanations often use words that have a deictic function, such as "this" or "that", which are not easily understood in text-based supports.[44] Such communication is facilitated by the doodle tool because students can use it to reference the specific objects that they are discussing.

VoiceThread is inexpensive for individual instructors, easy to use, and is therefore accessible to individuals at all institution types.[47] However, one potential limitation to the software is that it is asynchronous. In some respects this is useful, because students can participate outside of class on a flexible time schedule. However, this aspect of the framework means that students do not always respond to each other's comments in real time or near real time as might be desirable for some types of cooperative learning.

■ PEDAGOGICAL DESIGN

The cooperative learning activities were designed based on a modification of the jigsaw approach, in which small groups of students work individually on components of a larger topic or problem and then later synthesize their collective knowledge.[48] This approach requires individual responsibility while also promoting group understanding of a larger topic. In a typical activity, each student was tasked with analyzing a small feature of a spectrum (Table 1), such as a peak in a ^{1}H NMR spectrum, using their interpretation to contribute to an overall group assessment of the posted spectrum leading to elucidation of the molecular structure (Figure 1). The approach allows for accessible tasks, while still providing a complex learning environment without overwhelming the students.[49]

The jigsaw activities were implemented in three sections (N = 48 students) of a second-semester organic chemistry lab course. Nonparticipating students (N= 303) were assigned comparable work to do individually. The participating sections were selected based on the graduate student teaching assistants who were assigned to teach them and IRB approval was obtained for the comparative study. Within each section, small self-organized groups of 4−6 students worked together to solve a new spectroscopy problem each week. The problems were constructed to parallel the course syllabus and increased in difficulty as the term progressed; the problems ranged from simple IR and NMR spectra to complex problems involving multiple sources of information in addition to a spectrum, such as partial IR and ^{13}C NMR data or reaction information. Students were also prompted to read each others' posts and offered critiques, alternate viewpoints, problem solving advice, or additional reasoning in support of a previously posted

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Table 1. Student Tasks in Jigsaw Molecular Structure Elucidation Activity

Spectrum Type	Activity Tasks	Example
^{1}H NMR	Analyze spectral feature and propose substructure	"I think there is an ethyl group present in this molecule, because there is a triplet peak at about 0.8 ppm and there is a quartet peak at about 1.4 ppm. This is consistent with where protons on sp^3 hybridized carbons are found."
^{1}H NMR or IR	Interpret molecular formula and propose viable functional groups	"There are 5 carbons, 12 hyrdrogens, and two oxygens and so there are no units of usaturation. Because there are no units of unsaturation and two oxygen atoms there could be an ether group."
^{1}H NMR or IR	Link two spectral features together based on analysis previously performed by peers	"Since we've already figured out that this is an aromatic ring, I figure that it has to be substituted in more than one spot. In particular, I wouldn't be surprised if this was substituted on both the first and third carbon, because otherwise there would be fewer peaks."
Combined ^{1}H NMR with supplementary IR or ^{13}C NMR	Analyze supplementary information (^{13}C NMR or IR) provided in a combination problem	"There is an IR peak at around 1750, which is probably some type of carbonyl. Maybe an ester since there are two oxygen atoms."
Synthesis	Propose a way to modify the molecule and indicate how the product would impact spectrum	"With electrophilic aromatic substitution, we can add groups onto the aromatic ring. By adding HNO_3, a nitro group can be attached. The nitro group has no H's of it's own, but would influence other peaks on the aromatic ring. NO_2 is electron withdrawing, which will result in a downshift of existing peaks in a ^{1}H-NMR."

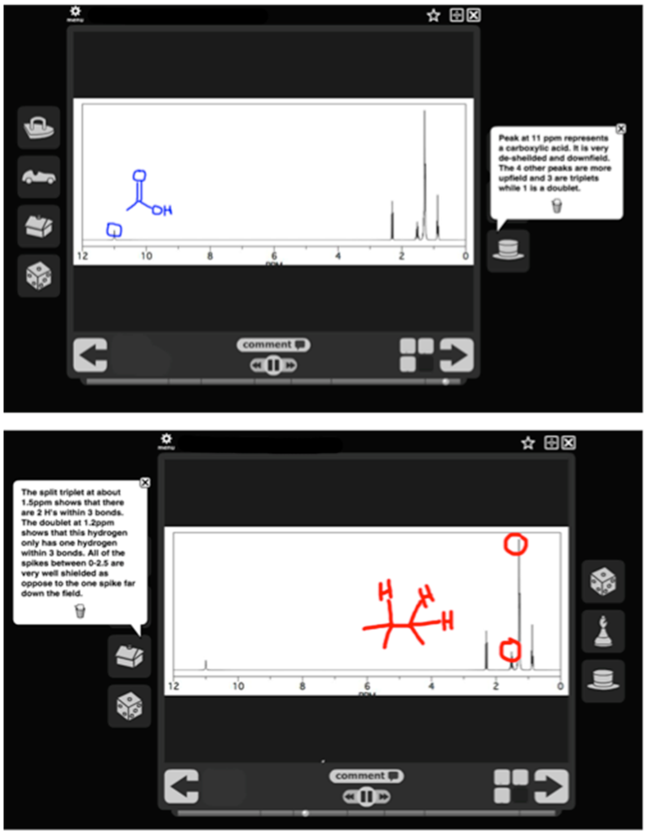

Figure 1. Screenshots of the online interface illustrating individual student contributions to the elucidation of a molecular structure based on a ^{1}H NMR spectrum. In each case, the student explains their analysis by using a text response tool and indicates the spectral feature of interest and it is corresponding structure using the doodle tool.

comment. They reported spending 15−60 min per week on the activity.

To promote a multifaceted learning experience in later assignments, students were prompted to not only analyze a spectrum but also propose reactions to alter the functionalities present in the molecule. Students were further asked to consider how their proposed synthetic steps would affect the spectra of the molecule. By supplying the scaffold for the integration of chemical synthesis into the spectroscopy discussions but not specifying specific synthetic routes to follow, students were free to take ownership of the problems by proposing their own organic transformations.[50]

The jigsaw modules were paired with individual homework sets that employed "documented problem solution" writing[51] during which students reflected on their own problem solving process. The purpose of this activity was to reinforce cooperative learning with individual reflection. Each week students wrote about how to solve one or more problem from the set as if they were explaining it step-by-step to a peer.

This modified jigsaw method should be easily adaptable in other classrooms, because it is not necessary to develop unique spectral problems for the discussions. Although we used authentic spectra, many of the structure elucidation problems used in the discussions were adapted from organic texts or materials available online. An example problem, which was modified for jigsaw, is provided in the Supporting Information section.

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Table 2. Grading Rubric for Online Cooperative NMR Spectroscopy Problems

Score	Criteria
Outstanding	1. Provided a thorough explanation of one feature of the spectrum[a,b] and described how each connects to a proposed molecular structure/substructure such as a functional group or group of atoms.
	2. Used the drawing tool to clearly indicate the spectral feature of interest and the proposed molecular substructure they attribute to it.
	3. Provided a reasonable interpretation of the spectral feature based on the information provided.[c]
	4. Connected their analysis to another students' comment regarding a different feature of the spectrum or responded to another students comment in some way.
Satisfactory	1. Provided an explanation of a single spectral feature, but the explanation is not thorough or does not include analysis of one aspect or neglected to fully connect to a proposed structure.
	2. Did not use the drawing tool to indicate the spectral feature of interest of the molecular substructure proposed.
	3. Interpreted the data, but some element was incorrect based on the available information.
	4. Did not connect their analysis to another's comment regarding a different feature of the spectrum or respond to another students' comment in some way.
Unsatisfactory	1. Posted a comment, but it was very brief and did not include discussion of two or more aspects of the spectral feature and did not connect to a proposed molecular structure.
	2. Did not use the drawing tool to indicate the spectral feature they discussed of the molecular structure they proposed.
	3. Did not propose a molecular structure for the single spectral feature or multiple aspects of their interpretation were incorrect based on the information provided.
	4. Did not connect their analysis to another students' comment regarding a different feature of the spectrum of respond to another students' comment in some way.

[a]Analysis of ^{1}H NMR should include peak position, peak splitting, and integration. [b]Analysis of IR should include peak position, shape, and magnitude. [c]Note: there may be more than one "correct" interpretation of a spectral feature.

■ FEEDBACK AND GRADING

Providing students with timely feedback is an important component of the assignment because it maximizes learning gains and helps students to adapt to the style of the activity, which may be unlike the work they typically encounter in science classes. Feedback can be provided in two ways: (1) through comments provided directly in the online discussion or (2) by discussion of common misconceptions or incorrect interpretations during class. One advantage of providing individual feedback directly in the online discussion is that it allows the instructor to connect directly with individual students when it might not otherwise be feasible during class. Furthermore, the online discussion provides a rich source of information to the instructor about the common misinterpretations and incorrect or partial understandings around particular elements of spectroscopy so that they can be addressed in class.

Successful cooperative learning requires individual accountability to promote positive interdependence among group members and can be achieved through the use of individual scoring and task specialization.[23] Therefore, students were graded on their individual contributions to the problem (Table 2) for three of the five assigned tasks. Criteria 1−3 focus on ensuring that individual students made a solid contribution to the problem. It is also important to help students learn the material from different perspectives, and so criterion 4 was included to emphasize cooperative discussion. Students may be reluctant to comment on or respond to other students' posts, and the instructor should model how to make a positive and constructive comment when providing feedback to each group. Cooperative learning activities should also include a group goal,[23] which could be further reinforced by offering bonus points to each student in a group who successfully solves the structure.

■ STUDENT RESPONSE

User activity logs were analyzed to assess the frequency and timing of students' use of VoiceThread. Although the assignments only required students to visit VoiceThread once per assignment, students accessed the online tool repeatedly throughout the term. For example, during the week prior to the final exam, a discussion section with only 16 students generated 119 total views. Among all participating sections, the average number of views per student per day ranged from 0 to 4, spiking on the due date for each assignment (Figure 2) and in

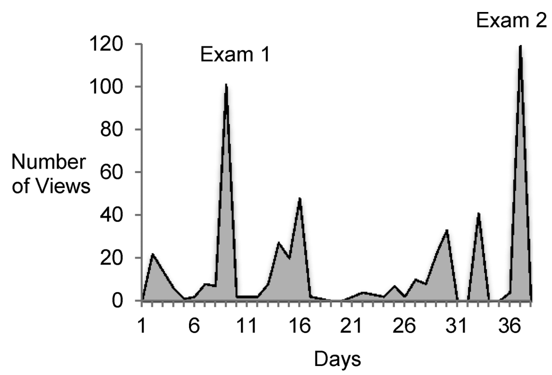

Figure 2. Graph of the raw number of discussion views throughout the second half of the term and in advance of both course mid-term examinations.

the days prior to each exam. The raw number of views for individual students ranged from 0 to 22 on a single day. One possible explanation for repeated viewing of the discussions is that students found them to be a useful resource for study.

In an end-of-term survey, all students were asked to rank their course resources on a 5-point Likert scale (Figure 3) from extremely useless (1) to extremely useful (5). On average, participating students ranked their online discussions as *useful* (3.2, SD = 1.2), which was ranked higher in learning value than the course textbook (participating students 2.9, SD = 1.1; nonparticipating students 2.6, SD = 1.0). External Internet resources were rated the most highly by both groups (participating students 3.7 SD = 1.2; nonparticipating students 4.1, SD = 1.2).

Students also responded to an open-ended question that asked them to comment on their general perception of the

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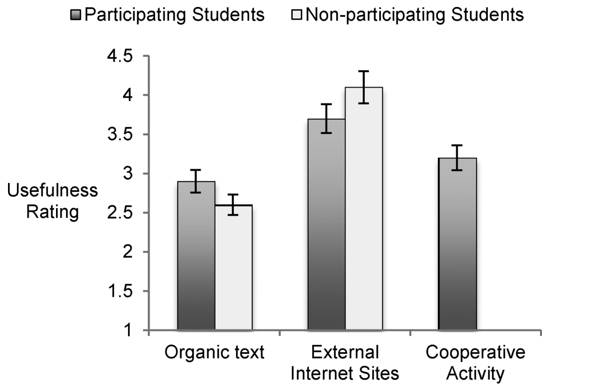

Figure 3. On an end-of-term survey, students ranked the usefulness of course resources for studying spectroscopy on a Likert-scale where 1 = extremely useless and 5 = extremely useful.

online discussions. The response rate was 88% of survey respondents and the majority of student comments were positive (71%). The following are example comments:

Student 1: It forced me to practice IR and NMR when I would have otherwise neglected to do so, which was helpful. Comments should be required to be video because it forces you to explain it out loud, which takes more understanding than simply writing it.

Student 2: I thought the discussions were incredibly useful and helped me prepare for the exam. The feedback from them was also helpful and helped me know what to study.

The comment by Student 1 above, which suggests that submissions to the discussion should be video in order to more effectively promote discussion, is notable for several reasons. The student certainly has a point that speaking the answers aloud may require a better understanding of the spectrum at hand. However, the video responses provided another unanticipated benefit: students found them amusing. We observed that video responses generated more traffic and more interest than the text responses. For example, one student group posted a 5 min long skit that included a "fire-side chat" about predicting ^{1}H NMR peaks of various aromatic compounds accompanied by John Coltrane.

Many students' comments, such as that made by Student 2, reflect that the students found the discussions to be useful in preparing for course exams. Although students also seemed to rewatch them for entertainment or social purposes, the student comments also corroborate the usage data. Together with the survey data, which indicate students found them to be a useful resource, these results suggest that some students also re-examined the discussions for the purposes of studying.

CONCLUSIONS

Cooperative learning is an evidence-based instructional practice that supports student development of problem solving skills. We describe a practical application of cooperative learning based on a modified jigsaw approach, which is designed to support students' as they learn to use spectral data to elucidate the structure of a molecule. These rather complex and daunting problems are broken down into accessible pieces so that students can work in small groups to arrive at a solution. This model is transportable to other classrooms because most standard spectroscopy problems can be adapted for use. Online cooperative activities are a useful resource for instructors because it enables them to monitor student learning. Additionally, the students, who reported the resource's usefulness in a survey, frequently accessed the discussions prior to exams.

Identifying a suitable discussion space for students at all levels is an important part of constructing an effective course. Online discussion spaces are useful tools for facilitating evidence-based pedagogical methods, such as cooperative problem solving, when it might not otherwise be practical. Explanation of data and lab results is a critical skill in science, and cooperative online discussion activities, such as those presented here, are appropriate for other science disciplines, in lab and lecture and in K−12 settings.

ASSOCIATED CONTENT

Supporting Information

Example assignments. This material is available via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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