^{1}H NMR Spectrum: A Team-Based Tabletop Game for Molecular Structure Elucidation

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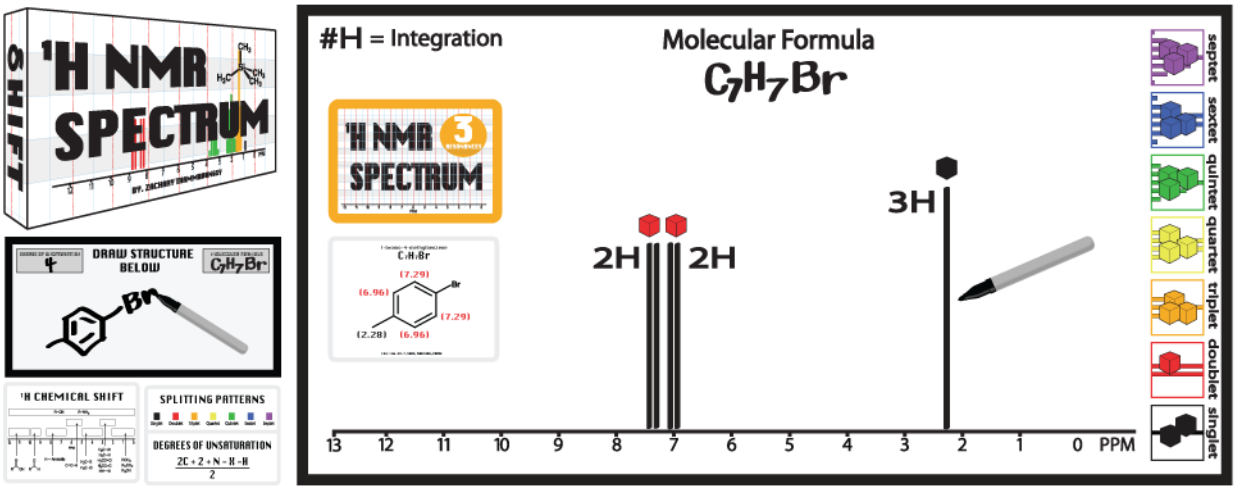
ABSTRACT

The ^{1}H NMR Spectrum game, the first example of a team-based tabletop game focused on elucidating the structures of organic small molecules using ^{1}H NMR spectra, was developed and deployed in a college level organic chemistry lecture course and laboratory course. The tabletop game was designed as a collaborative and competitive group activity to encourage multiple rounds of play to help students reinforce their ^{1}H NMR spectra interpretation skills. While playing in either team-based or free-for-all mode, students analyzed the provided chemical shifts, splitting patterns, integrations, and molecular formula within a designated time limit to correctly deduce the structure associated with the ^{1}H NMR spectrum. After playing the game, students in a lecture course and a laboratory course self-reported that they felt more comfortable solving ^{1}H NMR spectroscopy questions, found the game to be an appealing study aid, and were able to complete multiple rounds of play to strengthen their skills in interpreting ^{1}H NMR spectra. The ^{1}H NMR Spectrum tabletop game may serve as an engaging and competitive group learning tool to supplement teaching on ^{1}H NMR spectroscopy.

GRAPHICAL ABSTRACT



KEYWORDS

Second-Year Undergraduate, Organic Chemistry, Collaborative / Cooperative Learning, Hands-On Learning / Manipulatives, Puzzles/ Games, Problem Solving, NMR Spectroscopy, Student-Centered Learning

INTRODUCTION

Solving the structures of organic small molecules based on their ^{1}H nuclear magnetic resonance (NMR) spectra is a key skill emphasized in undergraduate organic chemistry courses.[1,2] Successful structure determination requires students to complete multiple complex tasks: interpreting chemical shifts, splitting patterns, and integrations to solve molecular structures.[3–6] The combination of active learning techniques and repeated practice in an enjoyable format may promote students' abilities to elucidate molecular structure from ^{1}H NMR spectra.[7,8]

Many approaches to aid students in learning to solve NMR spectra problems have been published, including laboratory activities, repositories of practice problems, and collaborative learning activities.[5,9–12] These learning aids are useful to supplement teaching on NMR spectroscopy, a topic that many students find challenging; however, many of these aids lack mechanisms to allow students to review and study NMR concepts multiple times. Engaging in multiple rounds of practice can help students become proficient at determining structures from spectra once they have grasped the fundamental concepts of NMR spectroscopy. A game that combines a repository of problems with

collaborative aspects of other activities could provide students with an engaging way to practice their NMR spectra interpretation skills.

Tabletop games have been used in the chemical education realm as active learning tools and have been shown to foster a more cohesive student-centered learning environment, where students are able to engage in the material.[13-14] A variety of tabletop games have been published for organic chemistry learners that span devising synthetic strategies to learning functional groups.[15–23] Although web-based and app-based games for ^{1}H NMR spectroscopy exist, to our knowledge no tabletop game that focuses on solving a molecular structure based solely on the ^{1}H NMR spectra has been reported.[11,24] A tabletop ^{1}H NMR game would allow students to reinforce ^{1}H NMR spectra interpretation while encouraging students to engage in repeated practice elucidating unknown structures.

To provide students with enjoyable, repeated rounds of interpreting ^{1}H NMR spectra, we gamified the practice process. We took components from traditional methods used to reinforce ^{1}H NMR solving skills, such as homework sets and low-stakes quizzes, and added teams as a cooperative component to create a tabletop game. We also included a point system to incentivize students to play multiple rounds and to create a competitive gameplay element.

General gameplay in the ^{1}H NMR Spectrum tabletop game (Figure 1) comprises two steps. One player (the structure giver) selects a card that depicts the structure of an organic small molecule and draws the corresponding ^{1}H NMR spectrum on a whiteboard. The remaining players attempt to deduce the structure from the depicted spectrum. To accommodate learners at different stages, structure cards can range from level one (simple structures with a single resonance signal) to level seven (more complex structures with seven resonance signals). In this study, we conducted the gameplay with only the materials for levels two and three, and these materials are included in the Supporting Information. The game can be played in teams (team-based mode) or with a group of students competing against each other (free-for-all mode), and the length of play can be varied by the number of structures attempted.

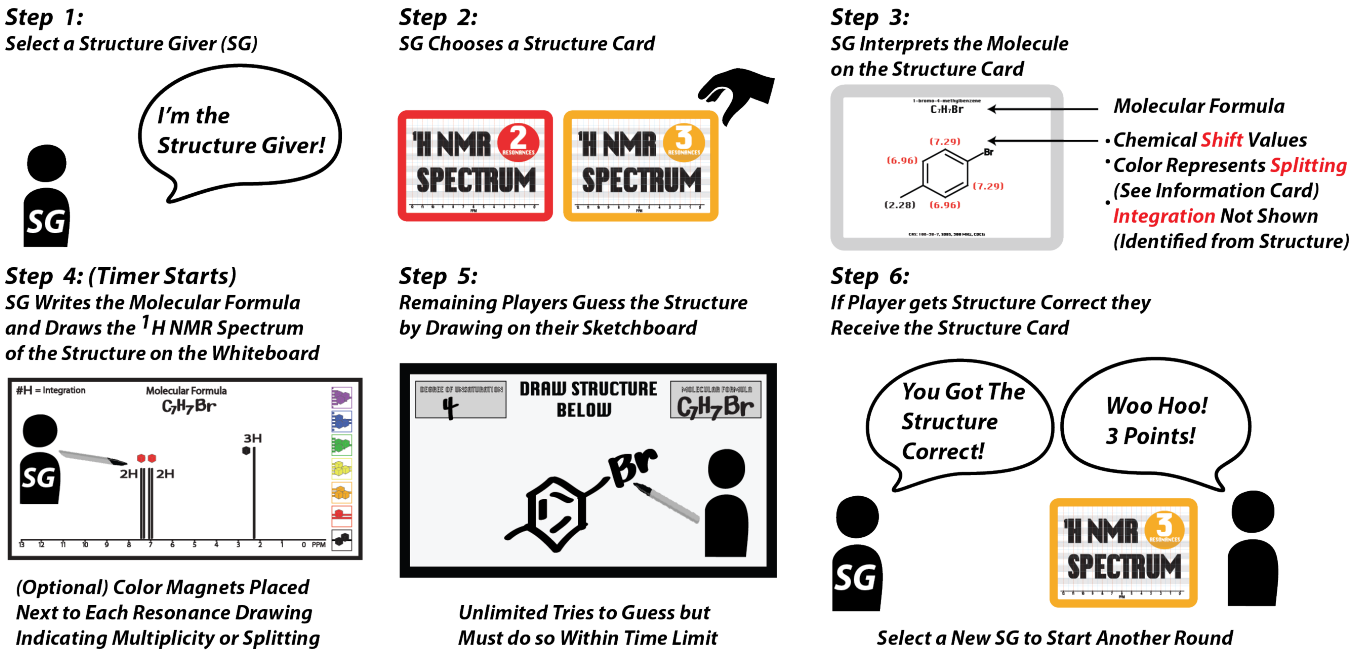


Figure 1. General gameplay of the 1H NMR Spectrum game.

MATERIALS

Materials needed for the ^{1}H NMR Spectrum game include materials available in the Supporting Information and common commercial items. The Structure Cards and Sketchboards, which are printed and laminated for game play, can be downloaded from the Supporting Information. The game also requires one or more whiteboards and dry erase markers. Optional materials include small cloths or erasers for cleaning dry erase ink, small cubic magnets, and colored tape. After the materials have been assembled, the ^{1}H NMR Spectrum game can be played in a variety of settings, including classrooms, laboratories, discussions and recitations, office hours, tutoring sessions, and at home.

GAMEPLAY

The ^{1}H NMR Spectrum game can be played in either team-based or free-for-all modes depending on the availability of space for collaboration. The two modes of gameplay are described in more detail in the following section, and rules of play for each setting can be found in the Supporting Information. In both modes, the game is played in rounds, where only one player, designated as the structure giver, is allowed to select and look at one structure card at a time. The structure giver may choose a card from the level that they feel best suits their skills and comfort. This card displays the molecular formula, chemical structure, chemical shifts, and splitting patterns of a small molecule. The proton integration is omitted but can be deduced by the structure giver based on the provided structure. The

structure giver provides clues to other players by drawing the ^{1}H NMR spectrum and molecular formula on a whiteboard. If needed, the structure giver may use colored magnets on the whiteboard to represent splitting patterns in the event spectrum resonance signals overlap and are challenging to distinguish.

The remaining players have unlimited attempts within five minutes, beginning when the structure giver starts drawing, to determine the molecular structure based on the ^{1}H NMR spectrum drawn on the whiteboard by drawing the structure on their Sketchboard. Because the purpose of the ^{1}H NMR is to incentivize students to practice interpreting spectra, there is no penalty for guessing. Including such a penalty could discourage students from providing a wrong answer in front of their peers. The first person to correctly draw the molecular structure wins the round and keeps the structure card. A new round begins at the end of the time period, and a different player becomes the structure giver. At the end of the game, points are tallied based on the number displayed on the front of each structure card. The player or team with the most points is declared as the winner. Game length can be adjusted as needed by altering the number of rounds or time allotted per round in both modes.

Team-Based Play

In team-based play, two teams of up to three students each compete against each other. The teams share one whiteboard and one optional set of colored magnets. Each player has an information card, a Sketchboard, and a dry erase marker. Teams take turns solving as many structures as possible in five minutes. The team structure giver for the round must choose one structure card at a time and draw the ^{1}H NMR spectrum on the whiteboard. Structure givers may employ strategy when deciding which level of card to select. Choosing lower level cards may allow their teammates to solve more structures. However, choosing higher level cards provides more points for each structure solved. The remaining team members collaborate to interpret the ^{1}H NMR spectrum and draw the corresponding structure of the molecule on a Sketchboard. Concurrently, the opposing team should also collaborate to determine their own answer. If more time is available, the team structure giver can choose another structure card to solve. If the team cannot correctly determine any of the structure cards chosen, the opposing team may steal the structure cards by providing the correct structure in a single attempt per structure card. Structure card points are tallied to determine the winning team after a designated number of

rounds. At the end of a game, each team rotates to compete against a different team so that the same teams do not compete against each other for every game.

Free-for-All Play

In free-for-all mode, groups of up to five students share one whiteboard and one optional set of colored magnets. Each player has an information card, a Sketchboard, and a dry erase marker. Each player takes a turn as the structure giver while other players attempt to interpret the ^{1}H NMR spectrum and draw the structure of the molecule on their Sketchboard individually. Depending on the scoreboard, the structure giver may employ a strategy to maximize their chance of winning by deciding which level card to select. Choosing a lower-level card may allow their opponents to score less while also receiving a point. However, choosing a higher-level card could increase the level of difficulty and prevent their opponent from scoring. In this mode, the round ends when the first player to correctly guess the structure. Structure card points are tallied to determine the winning team after a designated number of rounds.

GAME EVALUATION AND DISCUSSION

Students in a sophomore-level organic chemistry lecture course (n = 53) and a laboratory course (n = 115) played the game, and their self-reported comfort levels for solving ^{1}H NMR structures and preferences for study aids were assessed using pre- and post-game surveys. Students in the lecture course played the game in team-based mode during class time. The game was introduced after students learned fundamental NMR spectroscopy concepts in two prior class meetings. Students in the laboratory course played the game during the last class meeting as a final exam review exercise. The laboratory students learned NMR spectroscopy in a prerequisite lecture course and reviewed NMR spectroscopy concepts at the beginning of the laboratory course. Student responses to surveys were used with approval by the University of California, Irvine, Institutional Review Board (IRB 2018-4211).

Surveys were administered before and after students played the ^{1}H NMR Spectrum game to determine if students' self-reported ability to solve ^{1}H NMR structure problems and preferred methods for studying NMR spectroscopy changed (Table 1). When students were asked to self-report their ability to solve ^{1}H NMR problems before they played the game, 26% of students in the lecture course and 33% of students in the laboratory course chose good or very good, indicating that most students

did not have high confidence in their ability to solve ^{1}H NMR spectroscopy problems (Figure 2).[25–27] After the students played the game, more students responded either good or very good when asked the same question — 50% of students in the lecture course and 54% of students in the laboratory course. This increase suggests that students became more confident in their ability to solve ^{1}H NMR spectroscopy problems.

To determine if the game is amenable to multiple rounds of play, we asked students in the post-game survey how many rounds they were able to complete during class. When playing in team-based mode, 76% of students in the lecture class reported solving four or more problems (Figure 2). In the laboratory course where students played in free-for-all mode, only 46% of students reported solving four or more problems while playing. Thus, both groups of students successfully played multiple rounds and solved multiple structures. Students who played in a team-based mode, were able to solve more structures during gameplay as compared to students who played in the free-for-all mode. Two differences between team-based and free-for-all gameplay could explain this variability in the amount of structures solved. In team-based play, the structure giver prompted their teammates to solve as many structure problems as possible in the five-minute round. By contrast, the structure giver in free-for-all play only presented one spectrum to be solved during their turn. Additionally, each team in the team-based mode rotated after each round to play against multiple other teams in the course. This competitive aspect might have prompted students to keep playing.

Table 1. Pre-activity and post-activity survey questions.

Survey questions	Response Options
How would you rate your ability to solve 1H NMR spectroscopy problems?	Five item Likert scale: very weak to very good
Which of the following sounds appealing for studying 1H NMR spectroscopy? Select all that apply.	Flash cards Videos 1H NMR card game Textbook readings Practice quizzes 1H NMR phone app
While playing the 1H NMR card game, approximately how many 1H NMR spectra did your team solve?	1 2 3 4 more than 4

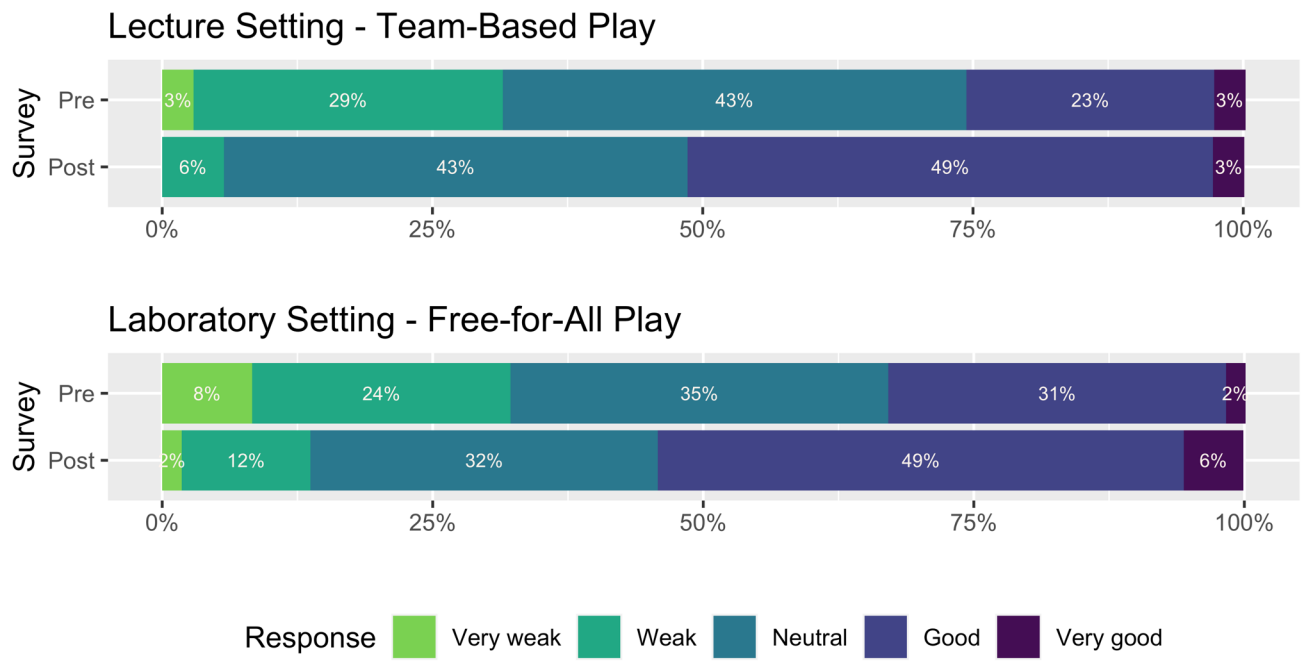


Figure 2. Student self-reported ability to solve ^{1}H NMR spectroscopy problems pre- and post-gameplay. Responses ranged from very weak to very good.

We also wanted to determine if students' choice of study aid for learning ^{1}H NMR spectroscopy changed after playing the game. Before playing the game, practice quizzes (66%) were the most popular study aid for lecture students; whereas flash cards (43%) were the most popular study aid for the laboratory students (Figure 3). The students in both courses showed modest interest in the game pre-activity, where 31% of lecture students and 35% of lab students reported the game to be an appealing study aid. The low level of interest in the game pre-activity could be explained by the fact that the students were not introduced to the game before the survey and did not have any context of what the game would be like. Post-activity, the game became almost as appealing as practice quizzes for the lecture students, where 51% of students voted in favor of the game. Practice quizzes were still the most popular study aid for these students. The lecture students' focus on practice quizzes likely stems from the lecture course structure, in which frequent low-stakes quizzes were used as a significant component of assessments. The majority of the laboratory students (58%) reported the game as the most appealing study aid, where the game gained popularity by 23% post-activity. Thus,

the survey responses suggest that the students in both settings found the game to be an appealing study aid for learning ^{1}H NMR spectroscopy.

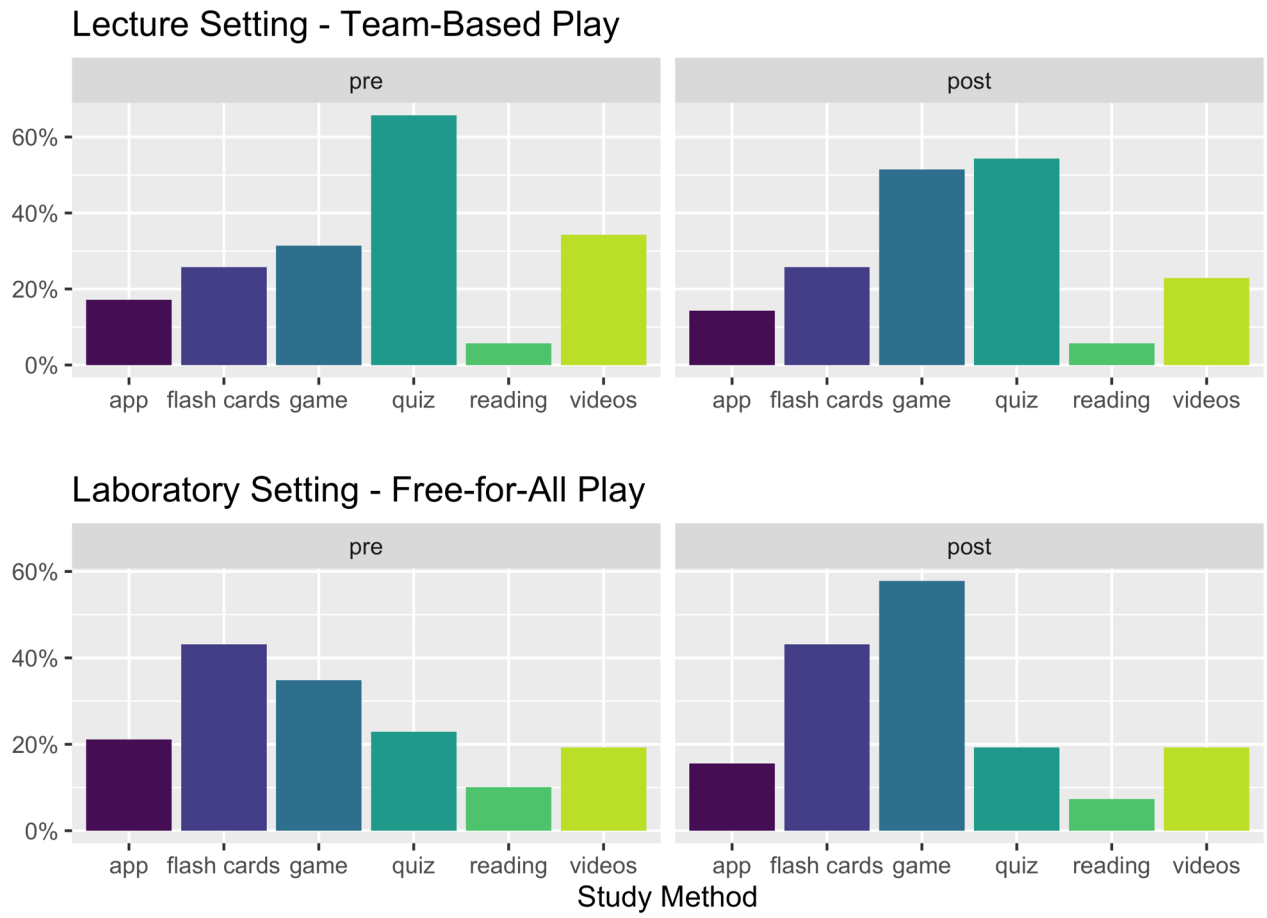


Figure 3. Student responses to pre- and post-activity survey questions, "Which study aid is appealing for learning 1H NMR spectroscopy (select all that apply)?"

In the post-activity survey, we also solicited free response comments from both groups of students who played the 1H NMR Spectrum game to determine their perceptions of the game. In general, students from both courses stated that they enjoyed the game and that the game helped reinforce concepts in 1H NMR spectroscopy. Some students noted that they enjoyed the competitive nature of the game, making it amenable to multiple rounds of play. Representative feedback from students included these comments:

- *"Very fun and clever game. I enjoyed playing and my teammates and I learned more about NMR in a fun way."* (lecture course)
- *"I had a lot of fun playing the card game. I was really struggling with splitting patterns but after some practice, the card game helped to reinforce the things I had studied."* (lecture course)

- *"It was really fun. It fed my competitive spirit. I think I did well because it did not feel like a pressured exam."* (laboratory course)
- *"I think the game is very well set up and I would definitely want to buy it once it comes up. My biggest trouble is to remember important chemical shifts, and no other studying method has helped me as much as this method."* (laboratory course)
- *"I think the game is very well set up and I would definitely want to buy it once it comes up. My biggest trouble is to remember important chemical shifts, and no other studying method has helped me as much as this method."* (laboratory course)

Overall, the students had a positive impression of the game, enjoyed the competitive nature of the game, and were able to review concepts in 1H NMR spectroscopy multiple times, all of which were goals when we designed the game.

INSTRUCTOR CONSIDERATIONS

When introducing the ^{1}H NMR Spectrum game, instructors should consider appropriate timing with their course content, what mode of play is best suited to their teaching space, and what duration of play fits their time constraints. The ^{1}H NMR Spectrum game is designed to incentivize students to practice deducing structures from spectra. Accordingly, students should play the game after learning fundamental NMR spectroscopy analysis skills. When choosing team-based or free-for-all play modes, instructors should consider the physical space available. Team-mode play requires multiple physical spaces that each contain whiteboards and can accommodate up to six students. Free-for-all play can be arranged in a single area that allows students to gather close enough to see the whiteboard. Instructors can adjust game duration to suit their class time constraints. Game play duration in our examples was set for thirty minutes (lecture) and twenty-five minutes (laboratory). Time allotted for each round can be increased or shortened as needed.

CONCLUSION

The ^{1}H NMR Spectrum tabletop game allows students to practice solving ^{1}H NMR spectra in an engaging, low stakes environment and encourages many rounds of gameplay to reinforce concepts important for solving ^{1}H NMR spectra problems. The game is amenable to use as an active learning tool in small and large lectures, discussions and recitations, laboratories, office hours, tutoring sessions, and at home. Students self-reported an increased level of ability in solving ^{1}H NMR spectra

after playing the game and reported the game as an appealing study aid for learning ^{1}H NMR spectroscopy. In a future study we intend to investigate the effect of playing the game on students' performance on NMR-related course assessments. We envision that the ^{1}H NMR Spectrum game will allow students to practice their spectroscopy skills in a way that builds confidence, enjoyment, and collaboration.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available:

Rulebook: Team-based Mode (PDF)

Rulebook: Free-for-All Mode (PDF)

Instructional Video (mp4)

Printable Materials (PDF)

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