JOURNAL OF CHEMICAL EDUCATION

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Introducing Molecular Structural Analysis Using a Guided Systematic Approach Combined with an Interactive Multiplatform Web Application

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Cite This: *J. Chem. Educ.* 2020, 97, 4330−4338 Read Online

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ABSTRACT: Performing the identification of organic chemical compounds from a set of spectroscopic data gives the opportunity to students to develop critical thinking and problem-solving skills. In this context, we developed a student-centered methodology for teaching molecular structural analysis to first-year undergraduate students. This systematic approach was implemented during classroom-training sessions and complemented by a home-based training program. Home-based activities involved a multiplatform Web-based application (ULg Spectra) combined with guided inquiries. ULg Spectra offers fully interactive tutorial/drill materials relying on mass, infrared, and nuclear magnetic resonance spectra (i.e., one-dimensional ^{1}H NMR and ^{13}C NMR spectra and two-dimensional ^{1}H−^{13}C HSQC spectra). A survey indicates that the vast majority of students valued the ULg Spectra application combined with guided inquiries, especially in terms of usability and usefulness. This approach prompted them to actively engage in problem solving, and student autonomy was improved. Statistical data demonstrated that low-, medium-, and high-training students' groups showed increasing performance in the final exam. Interestingly, a statistically significant increase in final grades and success rate was also observed compared to previous years.

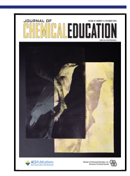
KEYWORDS: *First-Year Undergraduate/General, Analytical Chemistry, Organic Chemistry, Computer-Based Learning, Inquiry-Based/Discovery Learning, Problem Solving/Decision Making, IR Spectroscopy, Mass Spectrometry, NMR Spectroscopy, Student-Centered Learning*

■ INTRODUCTION

The interpretation of spectroscopic data to solve chemical structures is a key topic included in undergraduate organic chemistry courses. In addition to building practical skills in chemistry, students get the opportunity to develop critical thinking and authentic problem-solving skills.[1] Students' representations constructed during this kind of problem solving provide a clearer understanding of their conceptual development.[2] Indeed, the analysis of spectroscopic data is a complex process in which students have to learn how to extract relevant information obtained from various analytical methods and organize it to find out an evidence-based chemical structure. This challenging task is somewhat comparable to (i) receiving the pieces of a jigsaw puzzle, (ii) organizing them, and (iii) fitting them together to achieve a conclusive outcome. Students have to deal with different aspects of mass (MS), infrared (IR), and nuclear magnetic resonance (NMR) spectra. At the beginning, students perceive this task as an uphill struggle, but when a systematic and illustrated method is followed, we have noticed that they can work in play-learning mode.

Molecular structural analysis (MSA) is frequently taught by a traditional lecture-oriented method followed by worked examples. However, education and cognitive research showed that greater student participation in the learning process, leading in increased engagement, yields improved results.[3] This can be reached by shifting from a faculty-centered teaching to a student-centered learning.[4] Challenge problems,[5] guided-inquiry methods,[6−8] and computer tools[9] can easily be integrated into the traditional class structure and allow a smooth entry into student-centered pedagogy. This blended learning is a challenging approach consisting of a thoughtful

Received: April 7, 2020
Revised: October 9, 2020
Published: November 11, 2020



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J. Chem. Educ. 2020, 97, 4330−4338

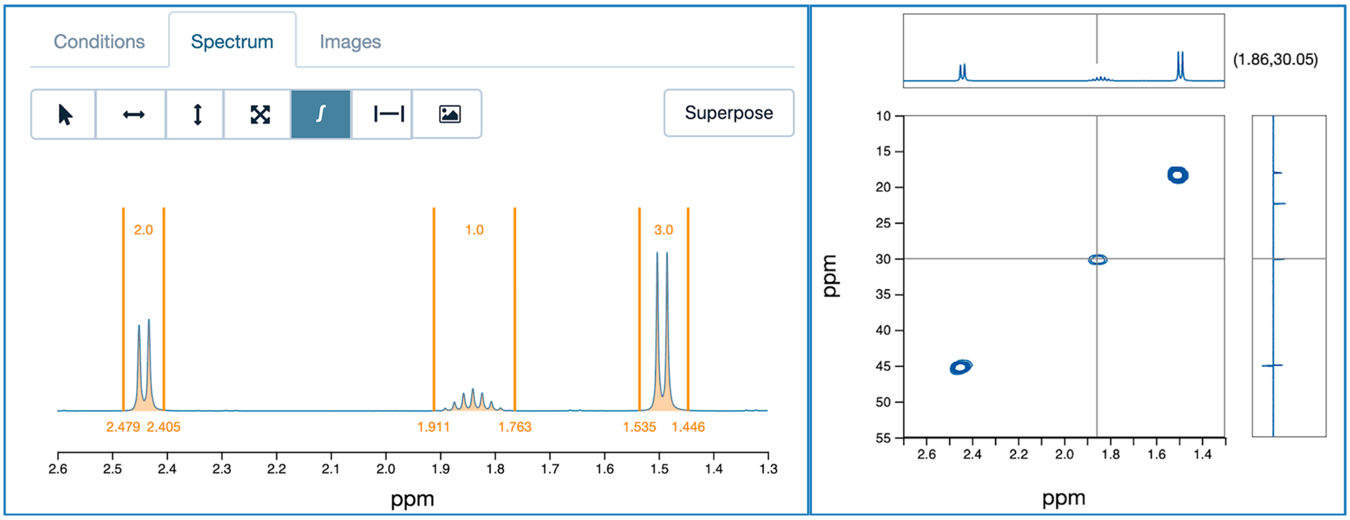

Figure 1. Display of two typical spectra: (Left) ^{1}H NMR spectrum illustrating the zoom, peak integration, and calibration functions of the application and (Right) ^{1}H−^{13}C HSQC spectrum with the corresponding 1-D ^{1}H NMR (top) and 1-D ^{13}C NMR (right) projections (with the cursor position coordinates in ppm in the top right corner).

integration of classroom face-to-face and digital methods of teaching and learning.[10,11]

Here we report the systematic approach used to teach MSA to first-year undergraduate students. This method is based on four main aspects:

- Traditional lectures
- Tutorial sessions of problem solving in which a systematic method is taught, relying on an interactive multiplatform Web-based application, developed at the University of Liège
- Students' home-based training using a guided inquiry
- Conditional access to a working session based on two previous exam tests, after getting a digital badge

After developing a theoretical understanding of spectroscopic methods based on textbooks,[12−16] a new interactive tool was introduced and used by the students in combination with tutorial sessions of problem solving. This tool, named ULg Spectra (ULg is an abbreviation for University of Liège), is a second-generation multiplatform Web-based application. The first-generation software tool was previously described,[17] and statistical data on first-year undergraduate student exam results provided evidence that its use effectively contributes to improving their performance. The second version was developed taking into account students' comments obtained from a previous survey.[17] It is a multiplatform Web-based application (https://www.ulgspectra.ulg.ac.be)[18] and therefore does not require any software installation. It is more user-friendly, more interactive, and faster. ULg Spectra contains a spectral database including many sets of exercises labeled with their difficulty levels. These difficulty grades follow the experience gained by the students and are adapted to lecturer's requisites. This new version of ULg Spectra is fully interactive and covers mass spectrometry and IR spectroscopy as well as one-dimensional (1-D) and two-dimensional (2-D) ^{1}H and ^{13}C NMR spectroscopy. 2-D NMR includes ^{1}H−^{1}H COSY (correlation spectroscopy), ^{1}H−^{13}C HSQC (heteronuclear single quantum correlation) and ^{1}H−^{13}C HMBC (heteronuclear multiple bond correlation) spectroscopy.[17,18]

ULg Spectra was integrated to tutorial sessions of problem solving teaching a systematic analysis approach based on data tabulation and partial structure analysis.[19] It was also used during students' home-based training, either individually or in informal collaborative groups. In that case, it was complemented with a guided inquiry on our institutional online educational platform (eCampus), built on Blackboard. Because educational badges were found to improve engagement and learning,[20−22] a digital badge system was also implemented as an additional incentive to train. Peer-to-peer interactions were encouraged through an online discussion forum as it is a widely accepted tool to enhance learner understanding and engagement.[23] Written interactions about science concepts help students clarify and share knowledge among peers.[24,25]

■ METHODOLOGY

The MSA teaching method described here was used in the Organic Chemistry course of first-year undergraduate veterinary students and involved a total of 226 students. These students are not chemistry students and often do not perceive the direct interest of this subject in their curriculum. The vast majority of them had no experience with MSA prior to the course. In this context, critical thinking, scientific rigor, and student engagement were thought to be very important and emphasized.

Theoretical concepts of MS, IR, and NMR spectroscopy were taught during 4 h of formal lecture (i.e., two class periods) and illustrated by textbook spectra.[12−16] At the end of the lecture, the ULg Spectra application was introduced as part of the lecture component.

ULg Spectra application

ULg Spectra is a spectral database containing exercises with different difficulty levels. Spectra are derived from real compounds and can display solvent and/or impurity peaks. Therefore, they are a valuable resource for students to develop critical-thinking skills through relevant problem-solving strategies.[26]

All of the exercises are numbered and sorted into three categories, namely, Easy, Medium, and Hard. An exercise can be searched by its number, difficulty level, or student section (e.g., veterinary students, chemistry students, ...). Full spectral data are stored, making the application fully interactive. This

https://dx.doi.org/10.1021/acs.jchemed.0c00329
J. Chem. Educ. 2020, 97, 4330−4338

includes MS, IR, ^{1}H NMR, ^{13}C NMR, ^{1}H−^{13}C HSQC, ^{1}H−^{1}H COSY, and ^{1}H−^{13}C HMBC spectra. Hands-on experience and interactive data handling were emphasized as they increase students' motivation and performance compared to theoretical lessons and traditional paper-based exercises.[17,27] All of the spectra can be zoomed. Peak integration and calibration can be performed on ^{1}H NMR spectra (Figure 1). NMR spectra can be overlaid where appropriate. The concepts required for 2-D NMR are quite sophisticated, especially in the context of first-year undergraduate students. From our experience in the field, ^{1}H−^{13}C HSQC spectra are simpler and less intimidating. It is an appropriate way to enter the 2-D NMR world. So, although ULg Spectra also includes ^{1}H−^{1}H COSY and ^{1}H−^{13}C HMBC spectra, only ^{1}H−^{13}C HSQC spectra were used in the present study (Figure 1). Getting started with the ULg Spectra application is fast and easy through a video tutorial.[28] The access is available to students at the University of Liège through a simple login procedure. A demo version is accessible without login.[18]

Technical Considerations

ULg Spectra is a three-tier Web-based application composed of (i) a client application running in the browser, (ii) a back-end server exposing web services, and (iii) a relational database where the data are stored. The client-side application leverages the latest Web technologies to efficiently render interactive charts in the browser. It consists of a single-page Web application (SPA) developed with the VueJS framework[29] and using D3.js[30] for the rendering of SVG graphics. It can run in modern web browsers, on any platform, and does not require the installation of third-party software. The back-end server is a NodeJS application implementing a REST API. The server makes the exercises present in the PostgreSQL database available to the clients through this API. The event-driven and asynchronous NodeJS runtime allows the server to handle many concurrent connections. CPU-intensive operations, such as the computation of contour lines for 2-D spectra (Conrec algorithm), are delegated to native C++ add-ons in order to optimize the performances. The overall application is based on state-of-the-art technologies and has been designed to be scalable. For example, multiple instances of the stateless back-end server can be deployed behind a load balancer.

First Tutorial Session of Problem Solving

After the theoretical explanation of MS, IR, and NMR spectroscopy, students have to learn how to apply these fundamental concepts in order to solve molecular structural analysis problems through tutorial sessions and home training. The first tutorial session of problem solving summed up the data to collect from the different spectra and to organize in order to get an evidence-based chemical structure (Table 1). The index of hydrogen deficiency was also defined. Afterward, 10 questions were asked to test students' comprehension. Six were multiple-choice questions, and four were open questions. Students had 5 min to think about each question, which was based on a particular item in Table 1. An example is shown in Figure 2.

This first session was completed by the demonstration of a full MSA problem from the ULg Spectra database, including EI-MS, IR, ^{1}H NMR, ^{13}C NMR, and ^{1}H−^{13}C HSQC spectra. This exercise was chosen in the "Easy" category. It was solved by the teaching assistant interacting with the students, following the items summarized in Table 1 and based on data tabulation. Colors were used to highlight partial structure correlations.

Table 1. Summary of Data to Collect from EI-MS, IR, and NMR Spectra and Information to Infer

Spectra Source	Data to Analyze	Information to Infer
EI−MS	Molecular ion peak	Molecular weight determination
	Even- or odd-numbered molecular ion?	Nitrogen rule
	Molecular ion pattern	Isotope assessment (^{13}C, ^{37}Cl, ^{81}Br)
	Main fragment peaks	Main fragmentation pathways (without rearrangement)
IR	Main vibrational bands in the 4000−1300 cm^{-1} region	Functional groups determination
^{1}H NMR	Number of signals	Number of nonequivalent proton types
	Chemical shift	Chemical proton environment
	Signal integration	Number of equivalent protons
	Multiplicity	Number of equivalent proton neighbors
^{13}C NMR (APT[a])	Number of signals	Number of nonequivalent carbon types
	Positive or negative signal?	Differentiation of quaternary carbon/methylene and methyl/methine
^{1}H−^{13}C HSQC	Correlation peak observed	Proton(s) directly linked to carbon
	No correlation peak	Quaternary carbon or proton(s) directly linked to heteroatom

[a]APT mode: Attached proton test mode allowing the observation of all carbons as positive or negative signals depending on the number of protons attached.

First Home Training of Problem Solving

Afterward, students were asked to use ULg Spectra at home in order to solve another "Easy-type" full exercise. An extensive inquiry, on the eCampus platform, guided the students through this first home training. Students had to analyze each spectrum using ULg Spectra and answer guiding questions on eCampus in parallel. Various types of questions were used: i.e., students were asked to locate the molecular ion peak in the image of the EI-MS spectrum using coordinate settings, complete a sentence using a drop-down menu, and answer dichotomous (true/false) and multiple-choice questions. Feedback for correct and incorrect answers was automatically displayed at the end of the test. Multiple attempts were allowed. When the test was successfully completed, students got access to a final question to check the structure they obtained.

Other On-Campus Tutorial Sessions and Home Training

Three additional tutorial sessions were scheduled, focusing on full MSA problems of increasing difficulty from the ULg Spectra database. The same systematic approach was used. An example of an exercise solved during one of these sessions is available in the Supporting Information. On-campus tutorial sessions allowed face-to-face and eye-to-eye interactions. The teaching assistant could pay particular attention to students' needs and difficulties. She regularly asked the students whether they had clearly understood. Reciprocal exchanges were fostered.

After each on-campus session, students could train at home solving extra drill exercises. Home training allowed students to proceed in their own environment. A set of relevant exercises

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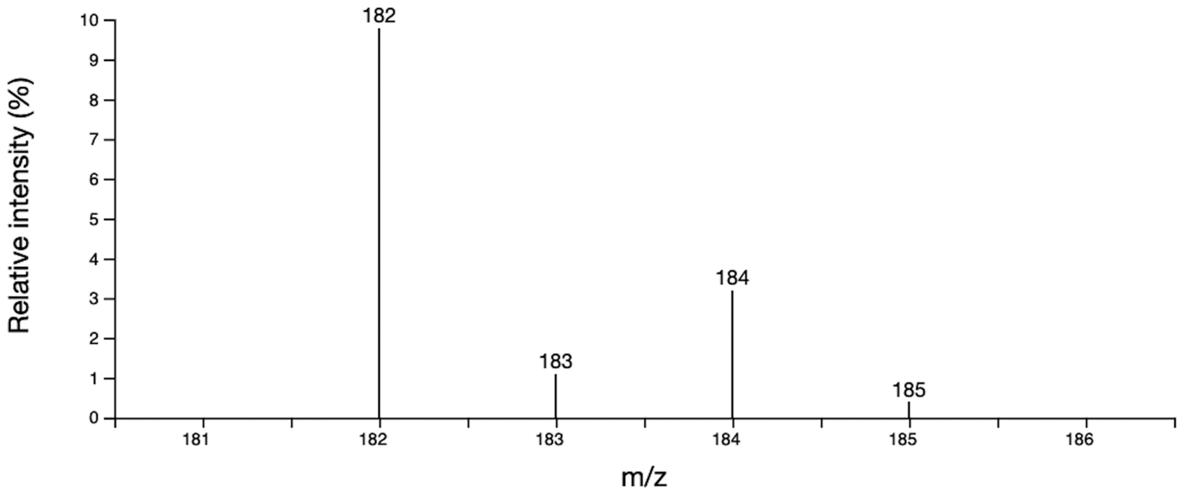
J. Chem. Educ. 2020, 97, 4330−4338

This is the isotopic pattern of a molecular ion:



Which of the following is NOT true?

The molecule includes:

1) an even number of nitrogen atom(s).

2) approximately 10 carbon atoms.

3) 1 chlorine atom.

4) 1 bromide atom.

[Answer: 4]

Figure 2. Example of a multiple-choice question used during the first tutorial session of problem solving, with the answer provided in brackets.

Table 2. Synopsis of the Two Types of Guided Inquiry Used during Home Training

Inquiry Type	Test	Aim	Tasks for Students	Topics Covered
Extensive	Preliminary test with feedback for correct and incorrect answers	Step-by-step assistance	Answering ~12 questions	Molecular ion mass Nitrogen rule Molecular ion pattern and isotope assessment (^{13}C, ^{37}Cl, ^{81}Br) Main fragmentation pathways Functional group(s) Number of equivalent protons and their chemical environment Number of nonequivalent carbon types Features of $^{1}H-^{13}C$ HSQC spectrum Molecular formula Index of hydrogen deficiency
	Final test[a]	Check the molecular structure	Naming the obtained structure or selecting the correct structure in a multiple-choice question	
Short	Preliminary test	Verify basic hints	Answer 4 questions	Molecular ion mass Molecular formula Index of hydrogen deficiency Functional group(s)
	Final test[a]	Check the molecular structure	Naming the obtained structure or selecting the correct structure in a multiple-choice question	

[a]The preliminary test has to be successfully completed to get access to the final test.

from the ULg Spectra database were coupled to a guided inquiry on the eCampus course dedicated to these first-year undergraduate students. Two types of guided inquiry were available (Table 2): either an extensive inquiry, as described before, or a short inquiry. The extensive inquiry was a kind of step-by-step assistance with automatic feedback. A full example of an extended guided inquiry is available in the Supporting Information, along with detailed feedback for incorrect and

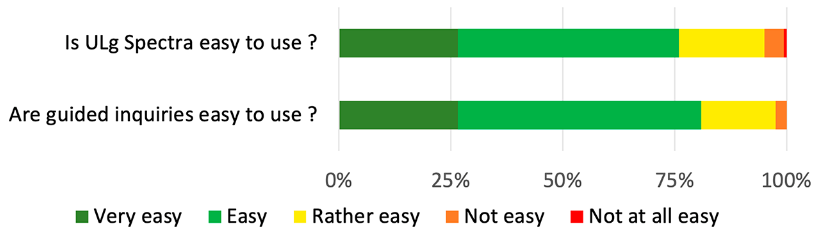


Figure 3. ULg Spectra combined with guided inquiries was overall perceived by students as usable (n = 162).

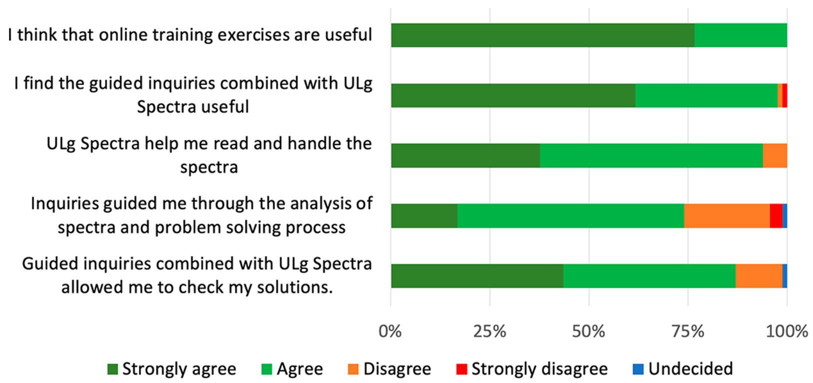


Figure 4. Majority of students have positive perceptions of ULg Spectra combined with guided inquiries (n = 162). The label "undecided" was attributed to the students who ticked both "agree" and "disagree" boxes in the form.

correct answers. The short inquiry was aimed at letting the students check the structure they obtained for a given exercise. In each case, the difficulty level was clearly refined in the context of first-year undergraduate veterinary course requirements and labeled with a bronze/silver/gold medal. Bronze medal exercises were for beginners. Silver medal exercises correspond to the difficulty level required to pass the final exam, and gold medals were for students seeking to go further with more challenging exercises. All of the inquiries allowed multiple attempts, as they were designed as training formative tools.

To promote students' engagement and training, a digital badge system was also implemented. Students obtained this badge after solving at least three problems of the ULg Spectra database and filling out the associated extensive or short inquiry questionnaire. These students gained access to a working session based on two previous exam tests. Besides, an intranet discussion forum was created to foster peer-to-peer interactions. In the past, students sent their questions and misunderstandings to the teaching assistant by email. This was not efficient because the teaching assistant often had to answer several times the same questions from different students, and this caused inequity between students as most of them were not aware of these further explanations. An online discussion forum has several advantages falling within active−constructive−interactive processes.[24] Writing down a question is an active and even constructive process as the students have to highlight the subject of misunderstanding and elaborate what a text sentence or a solution step means to them or what is the stumbling block to understanding. Moreover, mutual support and peer-to-peer interactivities are encouraged, and finally, knowledge is clarified and shared among peers.[23] This intranet discussion board was moderated by the teaching assistant.

■ EVALUATION OF THE METHODOLOGY

Evaluation of ULg Spectra Combined with Guided Inquiries

The determination of a chemical structure is included in the second-semester organic chemistry course of first-year undergraduate veterinary students. Of 226 students registered for the June exam, 162 students took an active part in ULg Spectra combined with guided inquiries, i.e., 72%. These students obtained a badge by solving at least three problems of the ULg Spectra database and filling out the associated extensive or short inquiry questionnaire. Consequently, they gained access to one additional on-campus session simulating two exam tests. For each test, students had approximately 45 min to solve a problem before getting a model resolution. The teaching assistant moved among students while they were solving the test and answered their questions. It was noticed that students tended to be more actively engaged in solving the test compared to previous years. Indeed, the students asked more questions, and more students tried to solve the problems and suggested a chemical structure. In the past, this simulation test was also scheduled 1 or 2 weeks after the last tutorial session, but its access was free (i.e., no conditional access requiring a digital badge), and a lot of students appeared passive, to lack motivation and to just wait for the given solution. Our new systematic learning method including online training and conditional access to this additional working session appeared to improve student engagement.

At the end of this working session, students were asked to fill out an anonymous survey about online training using ULg Spectra combined with guided inquiries. A total of 162 students answered questions about usability (Figure 3) and usefulness (Figure 4). The survey included the opportunity to write comments about the strengths and weaknesses of ULg Spectra combined with guided inquiries.

https://dx.doi.org/10.1021/acs.jchemed.0c00329
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Usability. For the majority of the students (95%), the use of ULg Spectra was very easy (27%), easy (49%), or rather easy (19%). Students became rapidly familiar with the main functionalities of this application as 74% of the students needed only 1 h or less and 19% needed 2 h to get sufficient mastery of the application. Guided inquiries on our eCampus educational platform were perceived as usable by 98% of the students with the following distribution: very easy (27%), easy (54%), and rather easy (17%).

Usefulness. All of the students provided very positive assessments of the usefulness of online exercises to gain practical skills in MSA. Guided inquiries were also very positively perceived as 98% strongly agree or agree that they were useful. Ninety-four percent of the respondents found ULg Spectra to be helpful to read and handle spectra. Seventy-four percent considered that the inquiries on our eCampus platform guided them through the analysis of spectra and the problem-solving process. This percentage is somewhat lower probably because of the number of extensive inquiries, i.e., a step-by-step assistance with automatic feedback, that was limited to one per difficulty level, whereas the number of short inquiries was larger. That is probably why two students ticked both "agree" and "disagree" boxes in the form. In their comments, 12% of the students explicitly asked for more extensive guided inquiries. Eighty-seven percent of the respondents considered that the guided inquiries combined with ULg Spectra allowed them to check the chemical structure they obtained for a given exercise. This is consistent with the larger number of short checking inquiries.

Problem Solving Media. Students were also asked to select their most preferred exercise media, either traditional paper exercises or online versions, and to explain their choice. Students could give multiple arguments. Sixty-five percent preferred online exercises against 23% who chose traditional paper exercises. 8% ticked both boxes, and 3% did not answer.

Among the 106 students who preferred online exercises, 89% emphasized the improved readability of the online spectra (zoom and cursor tools). Moreover, 10% mentioned that analysis of spectra was easier and faster, especially $^{1}H-^{13}C$ HSQC spectra. In this context, it was noticed that even though the concepts required for 2-D NMR are quite sophisticated, $^{1}H-^{13}C$ HSQC spectroscopy was overall positively perceived by the students. Very interestingly, 25% valued the gain of autonomy through interactivity, and they highlighted that thorough data handling allowed a better understanding of MSA. Some students (9%) also mentioned that interactivity fostered their ability to perform the entire reasoning by themselves: i.e., select relevant pieces of information from each spectrum and organize them to find out an evidence-based chemical structure. On the contrary, fixed-image spectra of paper exercises are less readable and required highlighting some appropriate details. Seven percent of the students who preferred the online exercise valued the centralized exercise database linked with the possibility to check the solution. Practical aspects were also appreciated (9%): i.e., students were free to train wherever they wanted and use their favorite device, such as a tablet computer. Four percent of the students who preferred the online exercise pointed out the ecological gain as there is no need to print any document. Finally, 2 students explicitly mentioned that the online exercise became a play activity.

Among the 38 students who preferred traditional paper exercises, 50% found paper handling easier and faster, probably relying on habitual behavior as noted by some students. Thirty-two percent appreciated the details already highlighted in the paper exercises because these hints simplified the problem-solving process. As expected, some of these students (26%) also chose traditional paper exercises because the final exam is still paper-based.

Strengths. Additionally, students were asked to comment on the strengths and weaknesses of ULg Spectra combined with guided inquiries. Among the 162 students filling out the survey, 44% emphasized the opportunity to check the chemical structure obtained after problem solving. Interestingly, 33% gave positive in-depth comments on the learning process and problem-solving approach. These students highlighted that guided inquiries allowed them to identify, understand, and correct their mistakes. This approach encouraged them to actively engage in problem resolution before getting the answer. It allowed them to verify their understanding and led them to self-assessment. Besides, 31% of the students appreciated the large number of exercises available for training. Twenty-eight percent liked the usability, readability, and interactivity of this approach. Twelve percent underlined the improved autonomy as they can proceed at their own pace, wherever and whenever they want. One student also noticed that the digital badge control had a positive effect as it fostered him/her to work. Moreover, 3% of the students valued the framework of the overall systematic approach including on-campus tutorial sessions even though this aspect was not the direct subject of the survey.

Weakness. In their comments, students also suggested some improvements. Among the 162 students filling out the survey, 32% would like to get some hints after multiple attempts or more feedback for incorrect answers in short guided inquiries. Twelve percent even asked to obtain a complete resolution after multiple attempts. Fourteen percent of respondents would like a larger number of exercises combined with short guided inquiries whereas 12% asked for more exercises combined with extensive guided inquiries. Clearly, weaknesses include two aspects: (i) an overall increase of the number of exercises with guided inquiries, which corroborates that they are perceived as useful, and (ii) a need for more step-by-step assistance (probably from students with learning disabilities).

Evaluation of the Overall Systematic Approach

Exams were organized in June and focused on the interpretation of MS, IR, and NMR spectra to get the chemical structure. These exams were paper-based, and a detailed answer with relevant points was graded. Students were required to determine the molecular weight of the unknown compound, explain the main fragmentation pathways from the MS spectrum, identify the possible functional groups from the IR spectrum, interpret ^{1}H NMR, ^{13}C NMR, and $^{1}H-^{13}C$ HSQC spectra (chemical shift and multiplicity), calculate the index of hydrogen deficiency, and finally come up with an evidence-based chemical structure. Student's exams were also examined to evaluate the adoption by the students of the systematic approach developed during the on-campus tutorial session, outlining key steps to take into account during problem solving. This approach followed the items listed in Table 1 and was based on systematic data tabulation using significant colors to highlight connections between pertinent complementary information. Our findings are in line with those of Domin and Bodner (ref 2, p 837):

There is a relationship between symbolic systems we present to students when teaching and the representation they construct when solving chemistry problems.

Indeed, when scoring the final test, we noticed that for 93% of the nonblank copies, students used our systematic approach at least to some extent. Three representative students' exams with fully good structuration level are available in the Supporting Information, along with examples of copies corresponding to the first, second, and third quartile scores. (These examples are provided with the students' consent.) The structuration level was evaluated and divided into six categories as shown in Figure 5. For grades greater than or equal to 13/20, the level of structuration was fully good or very good. For grades lower than or equal to 6/20, problem resolutions showed poor, very poor, or even not at all structuration. Clearly, data confirm the link between the final scores and the structuration level, but it is not the sole parameter to consider. The in-depth understanding of theoretical concepts is obviously important. Usually, students with fully good and very good structuration levels also understand underlying fundamental concepts. But, some students with poor structuration level can have more misunderstandings than other students characterized by a very poor structure. In other words, in some cases, a systematic approach is attempted but the connections between the data collected and the information inferred are not made properly.

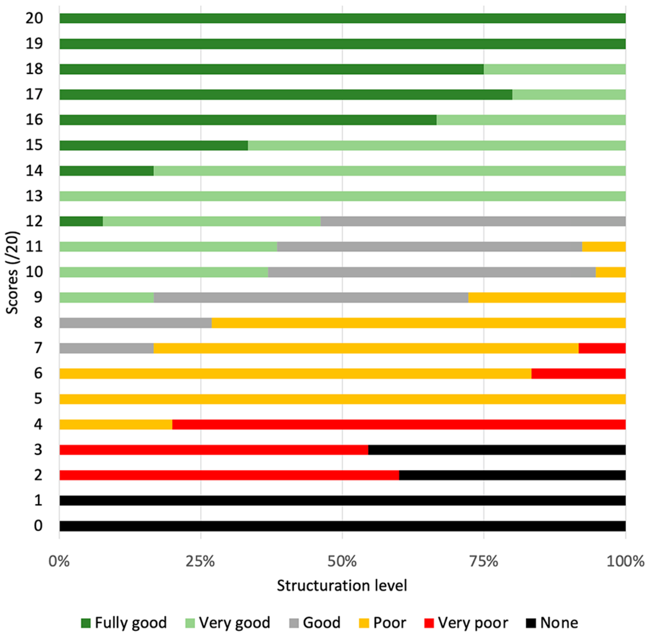

Figure 5. Exam scores were clearly linked to the structuration level ($n = 226$). The score of 0 was obtained by students who just handed in a blank copy.

Link between Participation in ULg Spectra and Performance at Summative Assessment

In order to evaluate the link between students' engagement in ULg Spectra and their subsequent performance in the final exam, students were classified into four groups, according to the number of exercises they solved using ULg Spectra combined with eCampus guided inquiries: no or low training (less than 3 solved exercises), medium training (3 to 5 solved exercises), high training (6 to 10 solved exercises), or very high training (more than 10 solved exercises). Data were analyzed using a Kruskal–Wallis nonparametric test, followed, if significant, by a Steel–Dwass–Critchlow–Fligner test for posthoc pairwise analysis (XLSTAT). The results of the 4 groups are illustrated in Figure 6. Low-, medium-, and high-training groups showed significantly increasing performance ($p < 0.0001$). The difference in performance between the high- and very-high training groups was not statistically significant ($p = 0.056$).

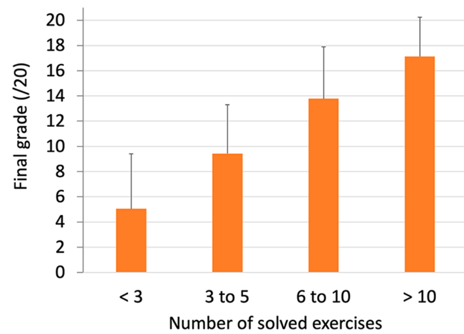

Figure 6. Summative assessment grade based on the number of solved exercises (mean ± SD). Low-, medium-, and high-training groups showed significantly increasing performance ($p < 0.0001$). The difference in performance between the high and very high training groups was not statistically significant ($p = 0.056$).

The performances of the students who benefited from this new pedagogical engineering ($n = 226$) was subsequently compared with those of the students who took the exam in the previous two years ($n = 372$). The distribution of final grades (first exam sessions) is illustrated in Figure 7. The mean grade increased (9.3 ± 5.3 for the 2019 cohort, against 8.6 ± 5.4 for the 2017 and 2018 cohorts) (Figure 7), which was a statistically significant result (Mann–Whitney U test, $p = 0.033$). Despite no change in the median (9.0/20), Box plots (Figure 7) suggest that the new pedagogical engineering mainly benefited the "average" students, as the first quartile increased from 5.0 to 6.0/20 and the third quartile increased from 11.0 to 12.0/20. The most interesting consequence is that the success rate, corresponding to a grade greater than or equal to 10/20, was significantly higher with the new pedagogical engineering: 49.1% in 2019 against 39.8% in 2017–2018 (Chi-square test with 1 DoF, $p = 0.026$).

■ CONCLUSION

The determination of the chemical structure from spectroscopic data provides opportunities for emphasizing fundamental chemical concepts and their application, making connections between various analytical topics. This kind of problem solving requires practical skills and drill. A systematic methodology for teaching molecular structural analysis to veterinary school first-year undergraduate students taking an organic chemistry course was developed and implemented. Such a specific student population was selected as a challenging cohort as many of them barely perceive the (added) value or concrete usefulness of this matter in their curriculum.

This blended learning approach relies on student-centered pedagogy and associates on-campus tutorial sessions with a complementary home-based training program. On-campus sessions emphasized eye-to-eye interactions and gaze stimuli as they can effectively modulate visual attention and action

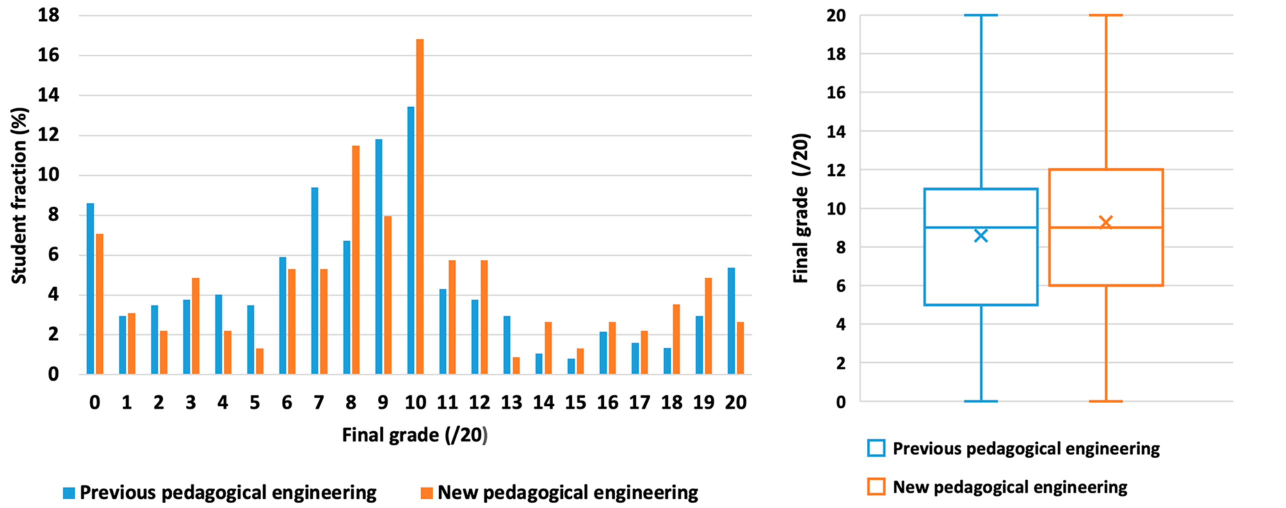

Figure 7. (Left) Summative assessment grades' distribution corresponds to a statistically significant increase in students' performance after the implementation of the new pedagogical engineering ($p = 0.033$). (Right) Box Plots illustrate higher mean final grades (X) and increasing first and third quartiles.

control in human observers and engage in reciprocal exchanges.[31] The home-based training strategy was designed using the active−constructive−interactive framework proposed by Chi.[24] This framework consists of a taxonomy that ranks activities from passive to active to constructive to interactive, in terms of learning benefits.[32] Our methodology involves high-ranking activities based on an interactive multiplatform Web application, some guided-inquiry tools which are both active and interactive, and a constructive/interactive intranet discussion forum. Besides, a digital rewarding badge system is used as an additional incentive to train and slightly gamify the learning process.

A survey indicates that the majority of students have positive perceptions of the ULg Spectra application combined with guided inquiries, especially in terms of usability, usefulness, readability, and interactivity. Interesting positive in-depth comments on learning and problem solving were also collected. In addition to being a valuable resource for students to check their answers, guided inquiries prompted them to engage further in challenging problems because these tools allowed them to identify, understand, and correct their mistakes. The improved autonomy was also appreciated.

We believe that teaching molecular structural analysis with such an approach not only makes the course to better be perceived by the a priori not convinced students but also contributes to settle the required scientific approach foundations of these future veterinarians. Indeed, the interactivity enhances their ability to critically observe and collect scientific information, combine them, and finally think by themselves to propose an evidence-based chemical structure, which is a basic scientific version of the observation of symptoms intended for diagnostic purposes.

Statistical data on exam question scores provide evidence that students' home training using ULg spectra combined with guided inquiry effectively contributes to improving their final exam performance: higher final grades and a higher success rate are indeed observed compared to previous years.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.0c00329.

Typical worked example problem resolution taught during an on-campus session, showing the systematic data tabulation using significant colors to highlight connections between pertinent complementary information (PDF)

Full example of an extended guided inquiry, with detailed feedback for correct and incorrect answers (PDF)

Three representative student's exams with fully good structuration level and other examples of copies corresponding to the first, second, and third quartile scores (These examples are provided with the students' consent.) (PDF)

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https://dx.doi.org/10.1021/acs.jchemed.0c00329
J. Chem. Educ. 2020, 97, 4330−4338

https://pubs.acs.org/10.1021/acs.jchemed.0c00329

Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

We thank Michelle Dupont for her useful IT support.

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