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Article

A Digital and Interactive Tool to Learn ^{1}H NMR Spectroscopy: The SpinDrops Learning Environment

Dominik Diermann,* Dennis Huber, Steffen J. Glaser, and Jenna Koenen

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ABSTRACT: Nuclear magnetic resonance (NMR) spectroscopy is one of the most important spectroscopy methods in modern chemistry, yet students need help learning and understanding its complex nature. Empirical investigations show that simulation and (interactive) visualizations can support students by offering new possibilities for investigating connections and direct effects of parameter changes. Therefore, this article introduces a digital and interactive learning environment that addresses students' learning difficulties to facilitate the understanding of crucial ^{1}H NMR background knowledge. The *SpinDrops Learning Environment* (SDLE) covers practically useful, basic concepts for interpreting a ^{1}H NMR spectrum from a theoretical point of view. It includes new interactive visualizations and a dynamic and realistically simulated ppm-spectrum. To evaluate the role and influence of interactivity by parameter control regarding students' learning processes and conceptual understanding, we designed two SDLE versions differing in the degree of interactivity and dynamics. We then asked $N = 50$ students to work with the learning environment in a pre-post study with questionnaires on affective constructs and a ^{1}H NMR knowledge test on conceptual understanding. $N = 12$ students additionally took part in a think-aloud study. The results showed that students benefit from learning with the SDLE as their conceptual understanding and NMR-related interest, self-efficacy, and estimated knowledge increase significantly. Although the SDLE showed significantly positive effects on students' learning results and processes, the difference in the degree of interactivity and dynamics inside the software only had a small impact, as revealed in the quantitative and qualitative data.

KEYWORDS: *digital learning environment, NMR spectroscopy, interactivity, simulation*

■ INTRODUCTION

Many science students and researchers face understanding difficulties regarding ^{1}H nuclear magnetic resonance (NMR) spectroscopy and spectra interpretation. Here, we introduce the interactive and digital *SpinDrops Learning Environment* (SDLE). This article presents its development and empirically collected effects on students' conceptual understanding and motivational beliefs, namely, self-estimation of knowledge, interest, and self-efficacy regarding principles for the interpretation of ^{1}H NMR spectra.

■ THEORETICAL BACKGROUND

Nuclear magnetic resonance (NMR) spectroscopy of ^{1}H nuclear spins, or ^{1}H NMR spectroscopy, is arguably the most important and most used spectroscopic method for chemistry research and daily lab work. Therefore, probably every student who deals with chemistry learns about NMR in their study life.[1,2] ^{1}H NMR spectroscopy is a powerful method to analyze the molecular structure of unknown reactants or to control a recently done synthesis path. However, most students need help understanding the background of NMR spectroscopy and the corresponding interpretation of NMR spectra: Studies in this field revealed some difficulties regarding explaining the number (and position) of signals (more precisely, their multiplet components), their distinction, the "N+1"-rule, shielding effects on nuclear spins/ppm values,[3,4] the interpretation of the coupling constant,[5] the abstract nature of certain concepts,[2] or the use of adequate terms and language.[2,6] Unfortunately, we still only know little about learning processes and understanding regarding NMR, as only a few empirical investigations or bigger educational projects on the topic can be found.[1,5,7]

Recent work investigated how NMR spectra are interpreted: Connor et al.[3] classified corresponding invalid chemical assumptions (into five categories) and were able to observe some common misleading heuristics for spectra analysis (like overgeneralization or neglecting certain spectral features).

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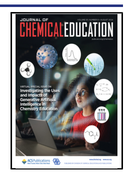

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Literature suggests that interpreting spectra correctly demands experience and application opportunities so students learn to recognize and focus on important aspects.[1,3−5,7,8] This seems to be an important skill for successful NMR spectroscopy educators as well.[2,9]

Experts seem to have a well-founded knowledge basis (also about theoretical backgrounds)[7] to better identify, make sense of, and connect spectral information to certain molecular structures.[1,3−5] It seems to be a big challenge to consider and process the many different spectral features and information[1−3,8] (not only the number and position of signal or the splitting of peaks[5]). Especially novices and less successful students seem to struggle with this, as they often act in inefficient and unsystematic ways.[3−5] Interpreting spectra could also be seen as a problem-solving approach,[5] so that efficient strategies and broad background knowledge are important. Another study by Connor et al.[4] compared novices' and experts' information processing during the interpretation of ^{1}H NMR spectra and derived necessary areas of understanding containing the fundamental knowledge of basic principles. They also derived recommendations for teaching, for example, to let students predict the influence of certain variables for a spectrum and to provide guidance. Other ideas to support learning might be to explicitly address wrong assumptions,[3] to let students check on their reasoning,[3,5] or to promote a systematic and consistent step-by-step approach.[2,5] Fantone et al.[2] reinforce the claim for scaffolding and gradual teaching of individual features by Anderson et al.[10] Both express the need for new additional learning opportunities. It becomes clear that students need support to understand ^{1}H NMR spectroscopy.[7,8]

However, the question of how NMR and its complex nature can be best understood and taught is not yet fully answered. Current approaches are mostly limited to textbooks,[10] simple explanation videos, spectra collections as exercises, or some online software tools,[11−13] but some offer innovative ways, for example, game-like digital spectra analysis or prediction tools,[14] a cooperative learning course,[15] guided inquiry tutorials with digital media,[16] benchtop spectrometers,[17] or visualization and simulation tools of spin states, the NMR experiment, pulses, and NMR spectra for self-study.[18]

Effective (digital) tools to learn (^{1}H) NMR spectroscopy need to address these suggestions and to realize such mentioned support based on empirical evidence.

Several studies show that, for example, tools like interactive simulations and dynamic visualizations can foster students' understanding—especially in a science-related context.[19,20] Computer-based simulations and visualizations can benefit the learning of science,[21−24] as they can facilitate the comprehension of connections, relations, and direct effects of some parameter changes, which can be ideally executed by the learner interactively.[19] Moreover, they can help learners reveal knowledge deficits and directly assess their learning,[25] as they can include texts or questions to stimulate thinking and control learning. Interaction between the software and the user seems particularly favorable regarding learning success.[26−29]

However, well-known learning theories like the cognitive load theory[30,31] or the theory of multimedia learning,[32] as well as further empirical results, suggest that visualizations and simulation tools must be carefully designed in terms of content structure (intrinsic load), design, features, and possibilities to interact (extrinsic load or if contributing to learning germane load)—especially for complex contents or ideas (like ^{1}H NMR). Here, the intrinsic load is already high by its nature, so some kind of guidance and instruction might be needed.[33] There are promising hints that simulation tools (for example, embedded into a digital learning environment) might support students learning and understanding. However, results could differ for learning ^{1}H NMR as they also depend on the level of interactivity, complexity, and the risk of mental exhaustion.[19,34]

There are several approaches to developing digital learning environments (that could be defined as self-controlled programs/software) about chemistry, physics, or further scientific topics[19,35−38] in which students can engage with scientific concepts in more or less open tasks. Digital learning environments are possibly adaptive to different levels of preknowledge, cognitive skills, learning paces, and individual demands for guidance, help, feedback, and support.[39] Therefore, they potentially foster students' understanding and are promising tools for learning.

■ RESEARCH PROJECT AND AIM OF RESEARCH

To support the learning of ^{1}H NMR, a digital and interactive learning environment that allowed learners to dive into the basics of ^{1}H NMR spectroscopy was developed, implemented, and evaluated. Coherently, we present the newly developed *SpinDrops Learning Environment* (SDLE), containing interactive and dynamic simulations and visualizations of submicroscopic processes and/or corresponding ^{1}H NMR spectra. Our learning environment was empirically validated regarding its content structure,[40] designed based on theoretical considerations and ideas, and implemented inside the existing SpinDrops software [SpinDrops is a free software developed by the Glaser research group at the Technical University of Munich to provide rich visualization of spin system dynamics, pulse sequences, and quantum mechanical backgrounds (product operators) during NMR experiments (www.spindrops.org); the *SpinDrops Learning Environment* is available as a module inside the SpinDrops software (see Supporting Information).][41]

Of course, we wanted to empirically investigate how effective the SDLE is as a learning tool and if it positively affects students' motivation and interest. Our primary research questions for the study presented in this article are therefore

- RQ 1: Are there improvements regarding conceptual understanding, motivation, interest, and ^{1}H NMR self-estimated knowledge while learning with the *SpinDrops Learning Environment*?
- RQ 2: How does interactivity by parameter control inside the *SpinDrops Learning Environment* affect students' conceptual understanding and learning process?
- RQ 3: How do affective variables, cognitive load, or preknowledge affect students' performance and conceptual understanding while learning with the *SpinDrops Learning Environment*?
- RQ 4: Are there common patterns in students' learning strategies while they learn with the *SpinDrops Learning Environment*?

■ MATERIALS AND METHODS

The content structure of the SDLE consists of those theoretical backgrounds that are principally important for practical spectra analysis (Figure 1). They were identified in an online survey with lectures.[40] They are namely the precession movement and

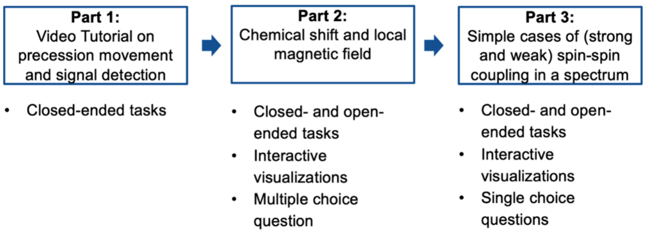

Figure 1. Content structure and design features of the *SpinDrops Learning Environment* (SDLE).

signal detection (provided as a video tutorial in which the user also gets familiar with the most common SDLE features; Part 1), the chemical shift and local magnetic field (responsible for the signal's position; Part 2), as well as simple cases of (strong and weak) spin−spin coupling in a spectrum (responsible for the signal's structure; Part 3). A first exploratory, qualitative pilot study with $N = 8$ students and $N = 2$ NMR experts (study A) had a great influence on the current design and content selection. The results also led to an adaption of some usability aspects and a rework of technical difficulties. After this first pilot study A, a revised learning environment version without technical issues that students can work on for around 60−75 min on their PC or Mac was obtained. (Download links are available in the Supporting Information.)

The learning environment is based on educational science design principles: Guided discovery/guided activity,[33,42−44] explanation texts, gradually more open-ended tasks, multiple-choice tasks for learning control, hints and feedback given by a pedagogical agent if necessary,[45−47] and possibilities to interact with the software and its simulations/visualizations. Learners, for example, can change spin system parameters (like ppm values or coupling constants) and directly see how this affects a realistic simulated ^{1}H NMR spectrum. Learners can also change these parameters in newly developed interactive visualization schemes on the local magnetic field or coupling trees (Figure 2) and directly see how this affects the visualization and the ^{1}H NMR spectrum. Further screenshots of the SDLE and its design elements are added to the Supporting Information.

To investigate the effects of the SDLE and especially the effects of the interactive visualizations and features have on learning and understanding NMR spectroscopy and how learners work with the software, a main study (study B) with two different versions of the learning environment was conducted in a pre-post-design—one with a higher amount of dynamics and interactions (version V1) and one with a lower interaction level (version V2). Version V2 featured static pictures instead of interactive visualizations, and it was impossible to jump back and check what has been done in previous tasks.

In summary, $N = 50$ chemistry students ($N = 38$ bachelor students currently attending a ^{1}H NMR lecture and $N = 12$ master students) were randomly assigned to one of the two versions ($N = 26$ to V1 and $N = 24$ to V2). Both groups had to answer the same questionnaire before and after studying with the SDLE. The questionnaire included empirically validated scales on motivation/self-efficacy (five items[48] on a scale from 1 to 5), interest (nine items[49] on a scale from 1 to 5), and knowledge self-estimation (six items on a scale from 1 to 5, based on the different content/parts of the SDLE and orientated on existing item formulations[48,50]), as well as a self-constructed, in advance piloted and validated, subject knowledge test on conceptual understanding of the covered ^{1}H NMR content: Based on our online survey and the corresponding choice of the content structure of the learning environment, we previously designed 44 items and validated them with $N = 36$ students from Germany (with an anonymous online test). Due to the limited lecture time to conduct study B, we only kept 14 single-choice items with the best selectivity and difficulty values. A few items were also included due to the importance of the underlying concept. The test covered chemical shift, spin−spin coupling, and overall ^{1}H NMR spectra analysis and interpretation. Each item gave one or two points if answered correctly. An exploratory factor analysis (maximum likelihood with varimax rotation) showed the best-fitting model with only one common factor (Bartlett

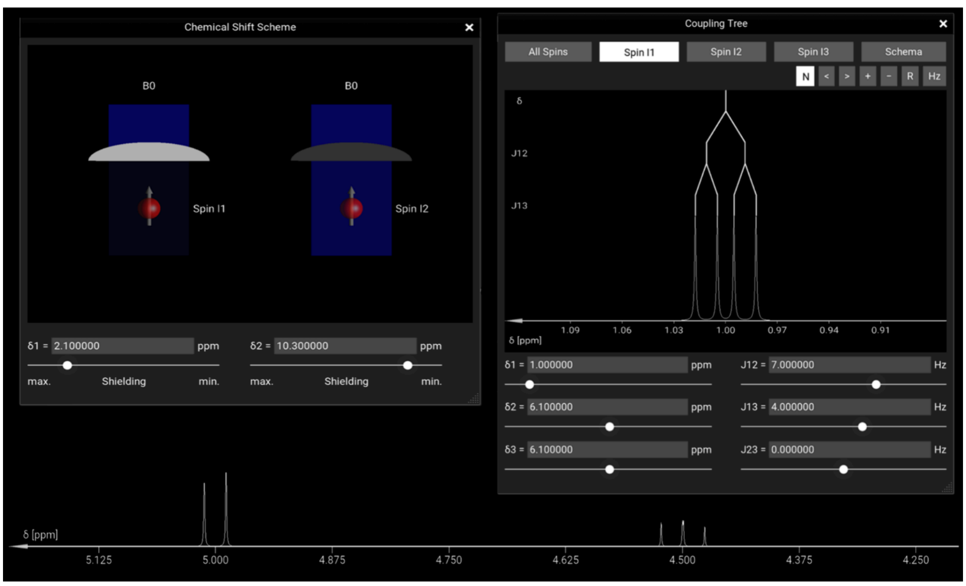

Figure 2. Interactive visualization schemes on the local magnetic field (left) and coupling tree (right) and the realistically simulated ^{1}H NMR ppm spectrum (bottom) inside the SDLE.

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J. Chem. Educ. 2024, 101, 3202−3215

test $p < 0.001$; KMO values of 0.57 pre and 0.59 post), leading us to interpret all questions' overall test results as a valid indicator for students' knowledge.

A copy of the questionnaires and the ^{1}H NMR knowledge test can be found in the Supporting Information. Figure 3 shows an overview of the study design aiming to answer the research questions from above.

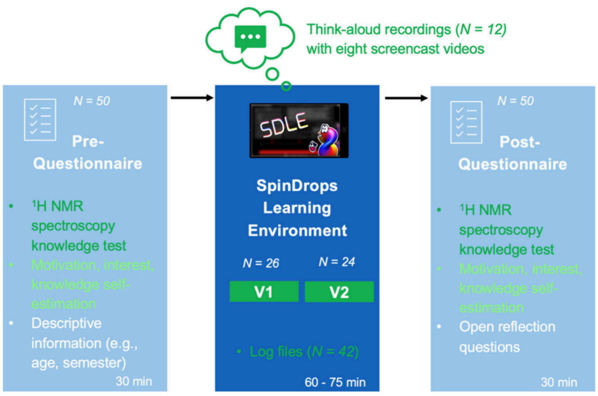

Figure 3. Study design of the leading investigation (study B) on the SDLE. Elements intended to answer research question 1 are colored in light green, and elements regarding research questions 2 to 4 are colored in dark green.

A subgroup of $N = 12$ students additionally worked on the SDLE using the think-aloud method. Together with eight screencast videos, we were able to have a closer, qualitative look at learning processes and the strategies students used. Inside the SDLE, there are two multiple-choice questions for learning control (after parts two and three) and single-choice questions on cognitive load.[51] These answers, among other usage information, e.g., the order in which students clicked on buttons or changed parameters, were collected by automatically generated log files [of which we could collect $N = 42$ (All studies mentioned in this article were performed in compliance with the relevant (German) laws and ethical and institutional (Technical University of Munich) guidelines; all participants were informed about the voluntary data collection and the anonymous data processing in advance; informed consent was obtained in the form of a signed declaration of data security (think-aloud studies) or ticking a mandatory cross in questionnaires; all participants were free to take part in each study; not taking part had no negative consequences).]

The data was checked for normal distribution, which was true for most scales (including the pre-time subject knowledge test on conceptual understanding, motivation and self-efficacy, knowledge self-estimation, and interest at post-time; Shapiro–Wilk and Kolmogorov–Smirnov tests). In a few cases (post-time subject knowledge test and interest pretest), the data at least fulfilled the preconditions for a *t*-test (Levene tests for variance homogeneity). Therefore, means for the related items on each scale were calculated and compared using *t*-tests. We also calculated reliability values (Cronbach's alpha) for each scale (Figure 4). The statistic software *R-studio*[52] was used for analyzing the data from the questionnaires and subject knowledge tests. *MAXQDA Analytics Pro 2022*[53] served for transcript coding and qualitative content analysis.[54] The Supporting Information contains a copy of the (shortened) codebook and its category descriptions.

RESULTS

Study A: Evaluation of Usability

The first SDLE version was evaluated within study A. Here, $N = 8$ students and $N = 2$ NMR experts worked with this version

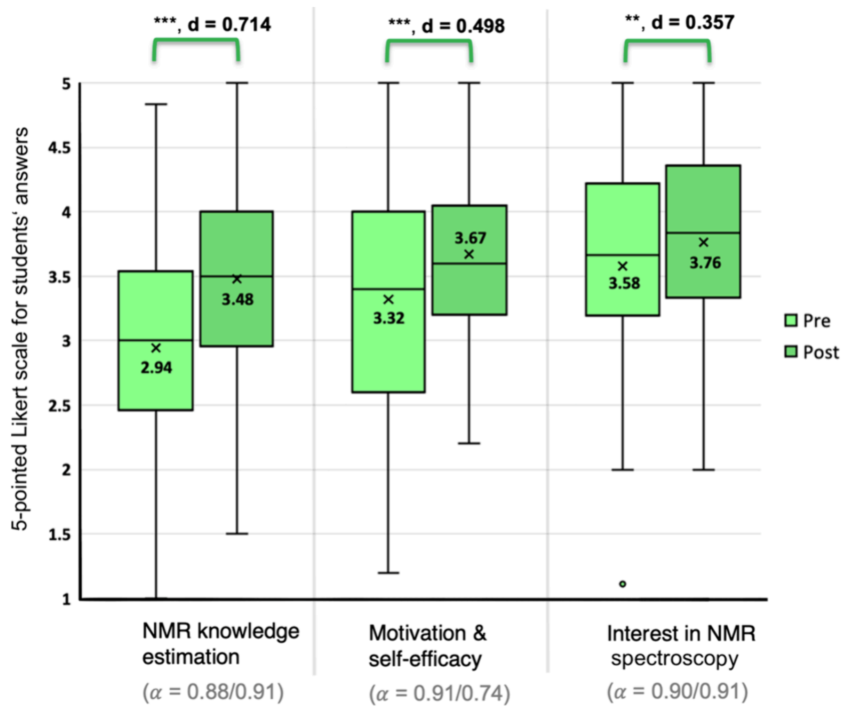

Figure 4. Boxplots of the responses of all $N = 50$ participants (versions V1 and V2 combined) for the scales (from left to right) "NMR knowledge estimation", "Motivation and self-efficacy", and "Interest in NMR spectroscopy" in a pre (light green)-post (dark green) comparison. Means are visualized by crosses and written in black. Significant differences are indicated by * for $p < 0.05$, ** for $p < 0.01$, and *** for $p < 0.001$.

and thought aloud. Qualitative content analysis[54] clarified that students assessed the SDLE as helpful. However, the cognitive load and the number of details within the environment had to be reduced. Results indicated a need for preknowledge, as this first SDLE version started on a slightly too high level and included too many details. We also identified and addressed major understanding problems based on this first data.

Consequently, some tasks were shortened, some explanations and hints were rewritten, the content structure was rearranged, a manual and an introduction/explaining video tutorial about the software environment and its features were added, not necessary information was "hidden" behind a special button, and minor technical changes were made. In addition, we could fix technical problems that occurred during the pilot study. Some changes were also applied to the additional visualization schemes (Figure 2). The experts' perspectives helped correct possibly misleading statements and coherently structure the final version of the SDLE.

Nevertheless, promising indicators of students' beneficial learning could be identified, e.g., students felt "better about interpreting spectra" after working through the SDLE. Statements that describe conceptual understanding and learning success were often found together with using SDLE features like hints, feedback, or interactive visualizations.

We finalized the SDLE based on the obtained qualitative data, assuming it would be a helpful tool for learning and revising the basics of ^{1}H NMR spectroscopy.

Study B: Questionnaires and ^{1}H NMR Knowledge Test on Conceptual Understanding

In December 2022 and January 2023, the final version of the SDLE was used in study B to investigate our assumption and answer the given research questions. Finally, N = 50 mainly Bachelor of Science (undergraduate; 58%), Master of Science (graduate; 34%), and further chemistry students (8%) participated in the study. Students, on average, were 21.1 years old and in their fourth semester. Thirty-one participants identified as male, 19 as female, and most had never used the SpinDrops software before (88%).

The questionnaires (quantitative data) showed little (and no significant) differences between the two versions, so the following results are based on the data from both versions, in other words, the SDLE in general and all 50 students.

Affective Constructs

Figure 4 shows the pre- and post-results for the relevant scales of affective variables. Participants estimated their NMR-related knowledge as significantly higher after they studied with the SDLE (see Table 1 for detailed values). The NMR knowledge estimation in the prequestionnaire can be seen as an indicator of students' preknowledge. Therefore, the investigated group of students was at quite a high level on average (M_{pre}= 2.94 on a scale from 1 to 5). They showed the biggest pre-post increase regarding the single items on the concept of spin−spin coupling, followed by the chemical shift. Working with the SDLE also significantly raised students' NMR-related motivation and self-efficacy and NMR-related interest (see Table 1). All answer means (for all students and all items corresponding to each scale) are written inside the boxes in Figure 4.

Table 1. Detailed Values and Statistics for the Pre-Post Differences of Affective Constructs (N = 50)

Construct	M_{pre}	SD_{pre}	M_{post}	SD_{post}	t-test statistics
NMR knowledge self-estimation	2.94	1.16	3.48	1.04	$t(49) = 5.049$, $p < 0.001$, $d = 0.714$
motivation and self-efficacy	3.32	1.12	3.67	0.99	$t(49) = 3.524$, $p < 0.001$, $d = 0.498$
interest in NMR	3.58	1.16	3.76	1.05	$t(49) = 2.527$, $p = 0.007$, $d = 0.357$

^{1}H NMR Knowledge and Conceptual Understanding

Figure 5 displays students' pre- and post-test results. Overall, all students achieved a significantly higher test score after working with the SDLE than they did before (see Table 2 for detailed values). The subgroup of students working with version V1 (higher interactivity and dynamics) on their own also achieved significantly higher test results in the pre-post comparison. The same is true for version V2 with lower interactivity.

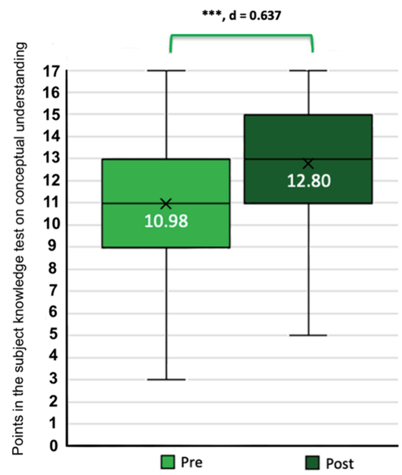

Figure 5. Boxplots of the ^{1}H NMR spectroscopy subject knowledge test results of all N = 50 students in a pre (green; left)-post (dark green; right) comparison. Means are visualized by crosses and written in white. Significant differences are indicated by * for $p < 0.05$, ** for $p < 0.01$, and *** for $p < 0.001$.

The groups of V1 and V2 are comparable to each other as no significant difference was found between their individual pretest results (t-test). We could find significant differences neither between the two groups' individual post-test scores nor between their respective pre-post differences (t-tests, Welch-tests, and ANCOVA with preknowledge). However, there were descriptive tendencies toward a higher test-score increase for those learning with the higher dynamic version V1 (average mean difference of 2.12 points compared to 1.50 points for V2). The positive but parallel development of the test results suggests that the SDLE as a whole supports learning, yet interactivity plays a minor role in learning outcomes.

We were interested in whether a higher expression of the affective constructs affects the test results and calculated linear and multiple regression models to see if the post-test results (and, therefore, students' final knowledge level) were moderated by any other variable. This means that the post-test results are not significantly influenced by any other variable than the knowledge self-estimation after learning with the learning environment. Students with one more points on this scale, on average, achieved 1.27 points more in the postknowledge test (R^2 = 0.129; $F(1,48)$ = 7.12, p = 0.010; y =

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J. Chem. Educ. 2024, 101, 3202−3215

Table 2. Detailed Values and Statistics for the Pre-Post Differences of the Results of the Subject Knowledge Test for Conceptual Understanding

	M_{pre}	SD_{pre}	M_{post}	SD_{post}	*t*-test statistics
Version V1 (higher interactivity, $N = 26$)	10.58	3.35	12.69	3.36	$t(25) = 3.614$, $p < 0.001$, $d = 0.709$
Version V2 (lower interactivity, $N = 24$)	11.42	3.41	12.92	2.47	$t(23) = 2.687$, $p = 0.007$, $d = 0.549$
Overall ($N = 50$)	10.98	3.37	12.80	2.93	$t(49) = 4.508$, $p < 0.001$, $d = 0.637$

Table 3. Detailed Values and Statistics for the Pre-Post Differences of Affective Constructs for the Two Groups K0 (Lower Pre-knowledge, $N = 21$) and K1 (Higher Pre-knowledge, $N = 29$) for All $N = 50$ students (Both Versions Combined)

construct	group	M_{pre}	SD_{pre}	M_{post}	SD_{post}	*t*-test statistics
Subject knowledge test on conceptual understanding	K0	7.81	2.34	10.86	3.12	$t(20) = 3.896$, $p < 0.001$, $d = 1.742$
	K1	13.28	1.73	14.21	1.80	$t(28) = 2.830$, $p = 0.004$, $d = 1.070$
NMR knowledge self-estimation	K0	2.69	0.62	3.15	0.73	$t(20) = 2.882$, $p = 0.005$, $d = 1.289$
	K1	3.13	0.99	3.72	0.83	$t(28) = 4.121$, $p < 0.001$, $d = 1.558$
Motivation and self-efficacy	K0	3.16	1.05	3.65	0.66	$t(20) = 2.813$, $p = 0.005$, $d = 1.258$
	K1	3.43	0.87	3.69	0.70	$t(28) = 2.166$, $p = 0.019$, $d = 0.819$
Interest in NMR	K0	3.32	0.93	3.59	0.85	$t(20) = 1.945$, $p = 0.033$, $d = 0.870$
	K1	3.77	0.69	3.89	0.70	n.s.

$8.385 + 1.268x$; $f = 0.37$, medium effect). Pearson's correlation test (for all participants) coherently showed a significant correlation with a correlation coefficient of $r = 0.36$ ($t(48) = 2.668$, $p = 0.010$). This means that higher values for self-estimation also had higher values in the postknowledge test, which showed that students estimate their learning success realistically and personally realize that they learned something. Also, the significant relation between students' pre- and post-test results (linear regression; $R^2 = 0.357$; $F(1,48) = 26.69$, $p < 0.001$, $y = 7.087 + 0.520x$) was not significantly moderated by any other measured affective variable, meaning that no variable was found, that predicts changes between pre- and post-test results. One possible interpretation for the missing link between post-test results (cognitive learning results) and the affective constructs of self-efficacy and interest, as well as students' preknowledge estimation, is that students with higher or lower primary self-efficacy or interest could benefit from the SDLE—in different ways. Learners, for example, are free in their pace and the amount of support provided by the software's hints and help, so the SDLE might be suitable for heterogeneous groups of students.

Cognitive Load

There were two items on cognitive load (labeled invested mental effort and perceived task difficulty[51]) at two places inside the SDLE: after the part on the chemical shift and after the part of spin−spin coupling. Students' answers to these could be collected in anonymous and automated log files. The means of all sets of answers showed that students rate the tasks on spin−spin coupling as significantly more mentally demanding (invested mental effort) than the first ones on the concept of chemical shift ($t(32) = 3.464$, $p = 0.001$, $d = 0.603$). They also estimated task difficulty higher for the tasks on coupling ($t(32) = 2.410$, $p = 0.022$, $d = 0.420$).

A linear regression analysis on the influence of the measured cognitive load on students' subject knowledge (test result in the post-test) revealed significant results only for perceived task difficulty. Thus, 20.4% of the variation in post-test scores can be explained by the perceived task difficulty ($R^2 = 0.204$; $F(1,31) = 7.953$, $p = 0.008$). For each higher unit on the difficulty estimation scale (regarding all SDLE tasks in summary and independent from the version), students' test results decreased by 1.22 points ($y = 17.648-1.223x$). This could be rated as a strong effect ($f = 0.51$) and indicates that a higher (estimated) cognitive load, in fact, undermined learning results.

Interestingly, students who worked with the SDLE version V2 (lower interactivity) estimated the overall cognitive load (mean over all four items on a 7-point Likert scale) as slightly lower than those who worked with version V1 ($M_{V1} = 4.02$, $SD_{V1} = 1.07$; $M_{V2} = 3.63$, $SD_{V2} = 0.84$). However, no significant difference was found here. This seems surprising as it leads to the assumption that the mentioned differences in interactivity did not influence the cognitive load. The reasons might be a too low number of students or the fact that the SDLE (and its content and other features) is already so demanding that the differences in the interactivity only play a subordinated role.

Multiple Choice (MC) and Single Choice (SC) Items Inside the SDLE

We briefly mention the findings of the multiple choice and single choice items inside the SDLE after each of the two parts on chemical shift and spin−spin coupling, which also appeared in the log files. Further details on these results can be found in the Supporting Information. Regarding the part on chemical shift, there was one multiple choice question with four possible answers (two correct, two incorrect). Students could reach up to four points here and add three more points from three single-choice questions after the part on spin−spin coupling. Most students answered both questions correctly (a Wilcoxon-Test with $V = 863$, $p < 0.001$ and $V = 338.5$, $p < 0.001$ compared and showed significantly higher scores than the scales mid in both tasks), again independent from the SDLE version. This reinforces the finding that the SDLE can foster students' conceptual understanding, even though those questions are relatively easy as they are supposed to function as a basic learning control. Those two questions (after each part) did not correlate with each other (as they cover different concepts), and only the questions on spin−spin coupling correlated significantly with the post-test results ($r = 0.82$; $t(25) = 7.277$, $p < 0.001$). This might be due to the focus of the multiple choice question on theoretical backgrounds which were closely related to the directly taught topics (the subject knowledge test instrument focused a bit more on practical application in new contexts).

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J. Chem. Educ. 2024, 101, 3202−3215

Table 4. Categorized and Clustered Responses on the Open Question (a) About Students' Precepted Learning Process and Success with the SDLE with the Number of Occurrences on the Right[a]

Category	Number of students, who mentioned the category*
Learning success and deeper understanding (of connections)	13
Supportive visualizations/schemes and figures	6
SDLE as introduction into NMR (+ revision possibility)	6
Helpful hints and feedback	4
Helpful explanations/texts and tasks/structure of the SDLE	4
Non-transparent or complex tasks/challenges	4
Helpful interactivity and dynamics	3
Time problems (could not finish in time)	3
Positive emotion and motivation	2
(Positive) Usability	2
Confusing additional interactive schemes (e.g., coupling trees)	1
Difficulties in usage (e.g., continue button)	1
Possibility for self-regulated learning	1

[a]The colored highlights resemble similar categories received from question (b) in Table 5. Single responses could be counted in more than one category if they mentioned several aspects (*).

Table 5. Categorized and Clustered Responses on the Open Question (b) about Additional Notes and General Feedback about the SDLE with the Number of Occurrences on the Right[a]

Category	Number of students, who mentioned the category*
Negative usability aspects: controls/windows (optic and design)	4
Positive emotion and motivation	3
Learning success and deeper understanding (of connections)	3
SDLE as introduction into NMR (+ revision possibility)	3
Supportive visualizations/schemes and figures	3
(Positive) Usability	2
Wish for additional information (e.g., 2D NMR) or additional exercises	2
Wish for additional explanation on coupling trees	1
Non-transparent tasks/challenges	1
Good addition to the lecture	1
Criticism on the introductive tutorial video	1
Helpful explanations/texts and tasks/structure of the SDLE	1

[a]The colored highlights resemble similar categories received from question (a) in Table 4. Single responses could be counted in more than one category if they mentioned several aspects (*).

Cluster Analysis: Influence of Preknowledge

We also analyzed if we could identify specific groups/clusters of students with unique traits and characteristics who particularly benefit from the SDLE. As the SDLE covers difficult and cognitively demanding topics, it made sense to cluster depending on the level of preknowledge indicated by the ^{1}H NMR subject knowledge pretest results. With a cutoff point of 10.5 points (from 17 at best), we identified two groups with lower (K0, $N = 21$) and higher (K1, $N = 29$) preknowledge, assuming advantages for group K1 since they already know more and might be able to focus on new important information. For both groups, we could not find significant differences between versions V1 and V2 (using t-test), so both are combined to present these further results (descriptively, the knowledge test result improvements in group K1 were higher for version V1 and in group K0 higher for version V2). All values and t-test statistics for this section are presented in Table 3. Both groups showed significant increases in the pre-post knowledge test results, yet group K0 (lower preknowledge) benefits more than group K1 (higher preknowledge) comparing the pre-post-means with t-tests. Not surprisingly, students in group K1 showed significantly better post-test results ($t(48) = 4.795$, $p < 0.001$). However, the increases in terms of the pre-post score differences were significantly higher for group K0. Therefore, especially students with lower preknowledge (but not exclusively) showed better learning success regarding understanding ^{1}H NMR and interpreting spectra after using the SDLE. This shows that the learning environment is also suitable for beginners.

While the NMR-related self-efficacy and knowledge self-estimation increased significantly in both groups, students interest only increased significantly in the group K0 with lower preknowledge. At the single postmeasurement time, the scale means of interest and self-efficacy were not significantly different between the groups K1 (higher preknowledge) and K0 (lower preknowledge). These findings also suggest that students with lower preknowledge achieve the same level of self-efficacy and interest as students with higher preknowledge after learning with the SDLE.

Feedback on Acceptance and Usability

The post-test questionnaire included two open, reflective questions on acceptance and usability, asking for (a) students' precepted learning process and success with the SDLE and (b)

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J. Chem. Educ. 2024, 101, 3202−3215

additional notes and general feedback about the SDLE. We clustered the received responses based on the answers, which are presented in Tables 4 and 5.

It became clear that students assessed their learning as successful and the SDLE as a supportive and helpful tool for learning and revising ^{1}H NMR spectroscopy (self-regulated or in addition to a lecture), even in terms of a deeper understanding of connections and backgrounds. These statements fit the previously presented quantitative results. Most students also rated the features and design elements as helpful, although some described the tasks as too complex or nontransparent.

Most categories in Table 5 resembled those from Table 4. Students additionally mentioned minor negative aspects regarding the controlling elements and the design of the SDLE, which can easily be fixed in the next SDLE version (e.g., color design or size of windows or figures on the screen).

Learning Time with Interactive Visualizations

The log files included time stamps. Thus, it was possible to calculate how much time participants spent on the tasks in which they either used the interactive visualizations (see Figure 2) in version V1 or static, nonanimated pictures of the schemes in version V2. Working times on the two open tasks on the chemical shift and the local magnetic field (M_{V1_cs} = 574 s, SD_{V1_cs} = 321 s; M_{V2_cs} = 667 s, SD_{V2_cs} = 353 s) were slightly but not significantly different between the versions (using t-test as we found homogeneity of variances). In the next SDLE part, students took significantly more working time with the coupling trees (version V1) in the two open tasks on spin−spin coupling (M_{V1_ssc} = 995 s, SD_{V1_ssc} = 547 s; M_{V2_ssc} = 369 s, SD_{V2_ssc} = 227 s) than they needed in version V2. We used a Wilcoxon rank sum test here (W = 244, p < 0.001), as the data showed inhomogeneous variances. This could mean they had more difficulties with these tasks or the interactive visualizations. Another interpretation would be that they interacted more with the software, leading to a potentially higher processing depth through the additional investigation time and possibilities.

Study B: Qualitative Think-Aloud Data

So far, we have looked at the (quantitative) results from the ^{1}H NMR spectroscopy knowledge test instrument and the questionnaires, and we have compared the two different interactive SDLE versions, V1 and V2 (with statistical methods). As there were only minor differences regarding learning or affective outcomes (self-efficacy, interest), we will use the qualitative data from the subgroup of students who worked with the SDLE with the think-aloud method to dive deeper into learning processes and strategies.

We transcribed and coded the think-aloud data from N = 12 students (N = 5 worked with the SDLE version V1, N = 7 with version V2). The codebook (see Supporting Information) was developed deductively based on theoretical models,[55,56] reworked, and complemented inductively. It was also used for the mentioned study A and slightly adapted for study B. For coding and analyzing the transcripts, we used the *MAXQDA Analytics Pro 2022* software.[53] Three of the 12 transcripts (25%) were coded twice, achieving excellent intercoder reliability of an overall Cohens κ = 0.90,[57] which showed that two independent persons interpreted these transcripts mostly similarly.

Reviving the previous and anticipating the following results, again, only a few differences (regarding strategies, learning outcomes, or processes) between the SDLE versions V1 (high interactivity) and V2 (lower interactivity) arose from the qualitative data. Sometimes, there were hints toward a higher processing depth if students worked with version V1. Independent from the version, the think-aloud data also showed that the SDLE supports students' learning and conceptual understanding.

Cognitive Processes and Conceptual Understanding

Segments expressing cognitive processes or conceptual understanding were coded into four categories of rising processing depth (reproduction, selection, organization, and integration) and whether the statement is correct or if it expresses a conceptual misunderstanding. We did not see significant differences between versions V1 and V2 in any of the categories (Table 6).

Table 6. Subcategories for the Main Category "Cognitive Processes and Conceptual Understanding/Learning"[a]

	V1 (higher interactivity, N = 5)	V2 (lower interactivity, N = 7)	overall (N = 12)
Reproduction	30% (4%)	31% (6%)	31% (5%)
Selection	38% (5%)	40% (4%)	39% (4%)
Organization	17% (5%)	11% (7%)	13% (7%)
Integration	3% (3%)	2% (2%)	2% (2%)
Misunderstanding/ Misconception	12% (2%)	16% (7%)	14% (5%)

[a]Pictured are the relative parts of the subcategories to the main category (in %; in the format mean (standard deviation) in comparison between SDLE version V1 and V2).

Based on all 12 cases, there are significant differences between the individual extent of the subcategories "reproduction" − "integration", "selection" − "integration", and "selection" − "organization" (Friedmann-test: $\chi^2(3)$ = 35.10; all p < 0.001). We used nonparametric tests here, which are more suitable for the smaller number (N = 12) of participants' transcripts, as they are also called assumption-free and do not build on normal distribution.[58,59] This means that students mainly expressed cognitive processes on the level of reproduction and selection, meaning that they mostly make sense of one or two connections at a time. Analogously, limited to version V1 there only is a significant difference between "selection" and "integration" ($\chi^2(3)$ = 14.76; p = 0.002) and limited to V2 ($\chi^2(3)$ = 20.471) between "reproduction" − "integration" (p = 0.037), "selection" − "integration" (p < 0.001), and "selection" − "organization" (p = 0.037). By comparing the number of codes expressing understanding and the subcategory of "misunderstanding/misconception" (paired Wilcoxon tests), V1 students (p = 0.029) and V2 students (p = 0.011−0.018) both revealed significantly more understanding than misunderstanding codes on the levels of reproduction and selection up to organization.

Strategies and Heuristics

Whenever a statement could not be classified as a cognitive process, it was coded with other categories on typical strategies (e.g., working with the interactive schemes or the simulated ppm spectrum or using the hints or feedback) and heuristics (or problems during the task solution process with the software). For most subcategories, we also noted whether the respective approach contributed to the overall task solution or if it did not. We counted the relative appearances of each code

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J. Chem. Educ. 2024, 101, 3202−3215

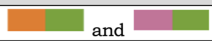
Code pattern and number of occurrences …		in version V1 (n = 5).	in version V2 (n = 7).	in total (N = 12).
1		28	44	72
2		32	30	62
3		61	64	125
4	e.g. 	4	6	10

Figure 6. Common code patterns and the number of occurrences in the transcripts are divided into versions V1 and V2. The length of the transcripts was 222,6 codes for V1 and 262 for V2 on average. Color code: "*cognitive processes and conceptual understanding/learning*" is green, "*misunderstanding/misconception*" is red, "*change/use parameters interactively (SpinDrops)*", "*usage of hints (SpinDrops)*", and "*usage of feedback (SpinDrops)*" are yellow, "*usage of common heuristics*" is pink, "*metacognitive strategies*" are orange, and "*reading the tasks/texts*" is light green.

in each transcript and calculated (assumption-free) Wilcoxon rank sum tests to compare two codes or versions. They showed major differences regarding the categories as follows:

- The feedback was more often useless to students with version V2 than to those with version V1 ($W = 7.5$, $p = 0.049$). Without the control opportunity with interactive tools, the feedback might be less beneficial for understanding.
- Regarding different and typical heuristics, students compared things with each other, jumped back, or looked into the handbook to recheck some ideas. This last heuristic was found more often in version V2 ($W = 7$, $p = 0.046$), maybe because students compensated for the lack of their own possibilities to change parameters and check ideas.
- The newly developed interactive schemes on the local magnetic field/electronic shielding and the coupling trees (Figure 2) were only available in V1. Both led more often to correct understanding/were more often correctly used than not ($V = 0$, $p = 0.090$ for the first and $V = 1$, $p = 0.052$ for the second one). As neither difference was significant, we cannot make final statements on the effects of these additional interactive elements/simulation tools.
- Only in version V1, we found significantly more codes resembling that the optional hints led to a correct result than codes showing that they still led to a wrong procedure ($V = 0$, $p = 0.048$). At the same time, we could not see a significant difference in version V2 ($V = 1$, $p = 0.053$). One possible interpretation is that the hints are especially handy if the cognitive load by various interaction possibilities is higher. They then make it easier to structure the working process and focus on the essential parts.

Correlations and Common Patterns

In the following, we will look at code relations and common patterns. This will provide insights into how the appearing categories/codes relate to each other or appear together (high correlations) or in which order they typically appear. Especially, relations between the main categories of "cognitive processes and conceptual understanding/learning" and "strategies and heuristics" seemed to be of greater importance as they show which strategies and features lead to learning success.

The codes "reading the tasks/texts" and "metacognitive strategies" correlate with cognitive learning processes in both SDLE versions V1 and V2 (according to *MAXQDA*). Therefore, students can already make sense of the provided explanation texts and learn with them. The integration of knowledge especially seemed to require metacognitive activity. This makes sense, as experts in any subject tend to monitor and regulate their learning activity.[60,61] Students who read the optional hints and the final feedback often showed cognitive learning processes on levels of selection and organization up to integration (integration only in version V1) in the immediate surroundings. Also, the hints were primarily coded as helpful. Based on the distance and correlations between codes, useful heuristics for positive learning outcomes inside the SDLE were "comparison and revision" and "paraphrasing the task". The first heuristic describes students who check their ideas and compare the changes they made/the spectra they designed with previous spectra or figures. They also jumped back (only possible in version V1) and looked something up in the SDLE manual/handbook. Students also benefited from reformulating the task in their own words or breaking it down into little subtasks (mainly on the levels of reproduction and selection).

The interactive schemes like the coupling trees, which were only present in version V1 (higher interactivity), could foster learning mainly on the levels of reproduction and selection but sometimes up to organization. However, their usage also appeared together with learning difficulties.

Version V1 showed slightly higher percentages of codes resembling learning success (in comparison to misunderstandings) than V2. Moreover, students using version V2 (lower interactivity) showed only partially correct statements on the integration level. However, these differences were not significant. *MAXQDA* can display the order in which codes appear in each transcript with process diagrams (see Supporting Information).

For both SDLE versions combined, we can derive some common patterns of codes (see Figure 6):

1. "Metacognitive strategies" (orange) and "heuristics" (pink) were often directly followed by "cognitive processes or conceptual understanding" (green)
2. "Reading the task/text" (light green) already led directly to "cognitive processes or conceptual understanding" (green)
3. Generally, the usage of SpinDrops (yellow) was often followed by "cognitive processes or conceptual understanding" (green)
4. We often found the sequence: "misunderstandings/misconception" (red) > "strategies/usage of SpinDrops" (yellow) > "cognitive processes or conceptual understanding" (green) (Figure 6). Thus, the SDLE could help to overcome understanding problems/difficulties and finally led to a correct understanding.

Learning Difficulties and Understanding Problems

Finally, using the results from the think-aloud part, some difficulties could be identified (in both versions) and can be

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J. Chem. Educ. 2024, 101, 3202−3215

addressed in a future SDLE version. Only minor technical issues (e.g., view and window size) were found.

Table 7 shows the categorized understanding difficulties students showed during their work with the SDLE (they understandably struggled the most with the open-ended tasks). Interestingly, the problem of comparing different functional groups and their effects on the chemical shift moderated by the electronic shielding appeared most frequently. Related to this, some students also had difficulties correctly connecting the shielding strength to the final ppm value. Here, the interactive visualizations could sometimes help students understand these relations. The coupling concept was also challenging: Students could not always predict or explain the necessary circumstances for a doublet or a triplet to appear in the ^{1}H NMR spectrum or explain overlapping signals correctly. Finally, the precession movement (mostly the relation between Larmor frequency and the ppm-value) caused some misunderstandings. Due to the findings of the lecturers' online survey[40] and time reasons, the SDLE covered the concepts of precession and spin properties only briefly at the beginning.

Table 7. Categorized and Clustered Understanding Difficulties from the Think-Aloud Transcripts with Numbers of Occurrences on the Right[a]

understanding/learning difficulty	number of occurrences
Compare/distinguish shielding and deshielding effects by functional groups (strength and resulting ppm values), e.g., CN-group vs Cl/Br-atoms	15
Understand relation between electronic shielding and chemical shift (ppm value): stronger/weaker shielding → lower/higher local magnetic field → lower/higher Larmor frequency → lower/higher ppm value	8
Multiplet structure: Understand and identify conditions for doublets, doublets of doublets, and triplets	6
Distinguish between different frequencies (Larmor, offset, ...) and relate them to ppm-values and spectrum-frequency (TMS)	6
Relation of Larmor/offset frequency and precession movement (speed; direction in rotating frame)	5
Remember typical numbers for coupling constants *J* between given spins	2
Distinguish between weak and strong coupling	2
Recognize and understand the overlap of two (or more) signals (structure)	1
Identify/characterize chemically equivalent spins	1
Relating proton-spin from molecules to corresponding signal in the spectrum	1

[a]If a problem appeared more than once in one transcript, it was counted each time. Similar statements were aggregated.

In summary, the results from the qualitative think-aloud data revealed little to no differences between students who learn with version V1 or V2. Therefore, the level of interactivity had a minor impact on students' learning processes and outcomes. However, some tendencies point toward a higher processing depth with the higher interactive version V1. Independently from the SDLE version, the qualitative data underlined our previous findings: The SDLE, with its features and visualization tools, is a valuable instrument to learn and recap the basics of ^{1}H NMR spectroscopy.

DISCUSSION

Study A

Of course, the findings from study A were limited in scope. It aimed to first-time evaluate the SDLE in terms of usability, comprehensibility, extent, and technical functionality in a qualitative investigation. Regarding its goal, the study collected first positive results with respect to students' learning, students' learning difficulties, and hints for a rework in which the learning environment was improved. Some of the most significant changes were the addition of an introductory SDLE tutorial video, which also briefly covers the concept of nuclear spin and precession movement, the adaption of the additional interactive visualizations, and the rework of the chapter on spin−spin coupling. Despite the relatively small number of students, we could finalize the SDLE toward a more comprehensible structure.

Based on experts' estimations, mistakes and poorly structured or formulated texts inside the SDLE were corrected. Therefore, the SDLE offers a validated, correct, and broad approach to learning or revising the basics of ^{1}H NMR spectroscopy.

Interestingly, we already saw some similar findings to those from study B, e.g., the helpful hints or the most common strategies and heuristics.

General Discussion

Our extensive, interactive, and innovative software for learning ^{1}H NMR spectroscopy meets the wish for learning opportunities expressed by previous research.[2,10] The SDLE was developed considering different empirical results about specific design elements and features (e.g., scaffolding elements like hints and feedback, guided discovery, ...). Its content structure was also selected based on empirical evidence: We conducted an online survey[40] about lecturers' estimation of the essential concepts for understanding ^{1}H NMR and interpreting ^{1}H NMR spectra. The results confirmed that chemical shift (local magnetic field and ppm-values) and spin−spin coupling (multiplet fine structure of signals) should be central. We then designed a new approach to teach these concepts interactively with the SpinDrops software.[40] Unlike most other ideas,[11−13] the SDLE is not only about practical and step-by-step spectra interpretation, which is sometimes possible without a correct understanding of the underlying concepts. The software starts one step earlier by covering the theoretical basics of spectra interpretation, which is necessary for developing expertise.[4] To become an expert, it is important to acquire a wide knowledge basis over a long time and through reflection processes, actively engaging with explicit content, and connecting theoretical backgrounds and practical skills.[62,63]

Quite in line with the known students' difficulties and recommendations for teaching, the SDLE stepwise explains[1,2] problematic topics,[3−5] like the signal position due to shielding effects (chemical shift), different multiplet signals (coupling), the coupling constant, or the "N+1"-rule. It includes tasks with concrete examples that build on each other to master individual spectral features: The first tasks cover the concept of chemical shift without coupling effects which then appear in later tasks (and not directly altogether). Thereby, it relies on scaffolding,[2,10] feedback, and optional hints and offers students the possibility to interactively change parameters and to predict and check the individual effects on a ^{1}H NMR spectrum.[3−5]

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J. Chem. Educ. 2024, 101, 3202−3215

The test instrument on ^{1}H NMR subject knowledge is new and self-designed. The first task selection was orientated on typical (German and English) textbooks and the first concepts from the SDLE. Then, experts stated their opinions on the tasks. After revision, we implemented a more extended version of the test using an online survey tool (Unipark). Students with different knowledge levels from all around Germany answered the tasks. Therefore, we could evaluate the tasks and questions qualitatively and choose the ones with the most suitable difficulty and selectivity. Some tasks were included due to the importance of their covered concepts, and some finally needed to be excluded because of the available time frame for study B. Of course, these development processes must be considered when interpreting our findings. As other empirically validated scales and the think-aloud data fit the implications from the test results, the subject knowledge test can be considered as a validated indicator for students' knowledge level and learning success.

Study B

We have chosen a study design that allows us to make statements on the influence of interactivity and dynamic presentation inside the SDLE on learning processes and learning outcomes regarding the basics of ^{1}H NMR spectroscopy, as the only difference for participants was the degree of interactivity between the two versions V1 and V2.

The tools and features the SDLE was built on (mainly simulations/visualization tools and scaffolding) have already been proven to enhance science-related learning and support learning processes in various empirical investigations.[19,21−23,33,42,43]

Naturally, the presented results of study B are limited to the moderately high number of 50 German students, who were randomly assigned to one of the two SDLE versions. Students participated voluntarily and without reward in the study. Therefore, they either might be a motivated group of students or might see a high demand for additional exercise.

As far as students' difficulties regarding chemical shift and coupling are concerned, our results confirm previous findings: As Table 7 shows, students have problems with the relation of shielding effects and ppm values/signal positions and with the distinction (and explanation) of multiplet signals. The effective use of metacognitive strategies we found in the think-aloud data indicates that self-regulation and a systematic and organized strategy are beneficial for understanding ^{1}H NMR spectroscopy and spectra interpretation.[3−5] The most useful heuristics found in this study also support the recommendations of breaking spectra interpretation down into the investigation of individual features[2,5] and providing the opportunity to check ideas.[3,5] The strategy of defining the current problem in one's own words also seems to be beneficial for some students, confirming previous insights.[15]

Although most previous works focus on spectra interpretation,[11−14] there are some approaches that mainly teach theoretical backgrounds[15] or make use of comparable design elements[16] like the SDLE. Kolonko and Kolonko,[16] for example, used guided inquiry tutorials on similar content combined with computer-based tools (for spectra visualization and prediction) and also achieved significant increases in content knowledge and better self-estimation by students. Angawi[15] counted on a cooperative learning course structure on spectra analysis (without using digital media). Here, students collaboratively worked on gradually more difficult problems, receiving some help. They showed significantly better learning results compared to the classical course structure and gave overall positive feedback.

Together, all findings complement the picture that guidance, support (e.g., by digital tools like the SDLE), and a successive increase of complexity are needed to master (^{1}H) NMR spectroscopy and all the different spectral data.

Study B's main result, according to which the two SLDE versions, with their different level of interactivity and dynamics, led to nearly the same outcomes of the used instruments like the ^{1}H NMR knowledge test, needs to be further discussed. There may be too small differences between the two versions regarding interactivity. However, we could only include more differences by changing the covered contents or neglecting moral or technical considerations. Another explanation could be that other features (e.g., scaffolding) are more impactful than interactivity: Then, we could not see significant effects, as these other features do not differ and play a more prominent role, overshadowing possible interactivity influences.

Generally, interactivity, dynamics, and parameter control might play a minor role in complex content like NMR and, therefore, only show minimal effect in our study.[34] By its nature, subjects like NMR already place a high intrinsic cognitive load on learners.[30,31] The additional complexity of interactivity might then overload learners' information processing capacity.[64,65] Therefore, effects on learning indeed depend on the unique content and its complexity.

With the complexity and intrinsic load of ^{1}H NMR spectroscopy, a high degree of interactivity or a more dynamic presentation might undermine positive learning results. This might be why we only found so few differences between students who worked with the different versions regarding cognitive and affective variables. However, the visualization and its added cognitive load can also lead to the possibility of engaging more with the learning subject by triggering cognitive processes.[66,67] From this point of view, interactivity would benefit deeper processing and understanding. Thus, we identified hints that this interactivity could also benefit understanding this subject field as learners' engagement can be increased. It could also be asked how far students really used the interactive features and visualizations during their learning process or if they did not engage with them, which, of course, then would lead to minor differences in the results.

Positive and negative effects of high freedom of interaction could also "cancel" each other: Self-regulated learning and useful visualization might benefit learning, while the higher (intrinsic and germane) cognitive load might undermine students' learning.[64] We can see some tendencies for this assumption in the qualitative think-aloud data.

The subject knowledge test on conceptual understanding needed to be relatively short (lack of lecture time for the study) and, therefore, may be not detailed enough to picture all the differences in students' knowledge.

We were interested in whether the additional interactive elements (e.g., the visualization of the local magnetic field or the coupling trees; see Figure 2) support learning, as could be deducted from the theory. Nevertheless, we could only partially confirm this assumption statistically. This could be due to the high cognitive demand for students to understand and interact with these elements. Students might need further help understanding and using them correctly, as the descriptions might be too long or complicated. Another reason for the little insights from the qualitative data can be the

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J. Chem. Educ. 2024, 101, 3202−3215

coding strategy, as we primarily were interested in cognitive processes. Statements/coding units that were coded in this category then were coherently not identified or counted as strategies or interactions with SpinDrops or the interactive elements a second time. We want to investigate these new additional interactive schemes on their own in greater detail in the future.

CONCLUSION AND IMPLICATIONS FOR TEACHING

The *SpinDrops Learning Environment* stands out as a promising approach to improving students learning and understanding of ^{1}H NMR in a self-regulated way, as the overall test results significantly increased and students' knowledge self-estimation, interest, self-efficacy, and motivation were influenced positively. Therefore, students (at any point while studying ^{1}H NMR spectroscopy in their study course) can learn or revise the most important basics of ^{1}H NMR at their own pace with a theory-based, developed, and empirically validated tool. Interestingly, high interactivity and a higher level of dynamics do not influence learning in a way that was measurable with our instruments. Future research needs to confirm this finding and, moreover, should investigate further possibilities to support and scaffold students' learning of ^{1}H NMR spectroscopy. Our findings supplement the empirical foundations for this.

The common patterns and strategies inside the SDLE may be transferable to working with ^{1}H NMR spectra in general. This suggests providing students with comparable spectra or example signals in many possibilities to exercise and revise. Students can learn or revise the basics of ^{1}H NMR spectroscopy, which are fundamental for spectra analysis at their own pace. They have the opportunity to take hints, jump back, and look up specific topics in a self-regulated way. Lecturers might also want to apply the SDLE in their lectures or recommend the software to their (chemistry) students who have problems understanding NMR spectroscopy and interpreting spectra and/or low motivation and interest.

The log files have yet to be fully analyzed and might provide further insights into learning processes with the SDLE (e.g., if all students actually worked with the interactive elements). Like a design-based research approach, we can continuously adapt the SDLE based on new insights or ideas to further support students' learning. Additionally, the design principles and the general concept of an interactive learning environment inside SpinDrops can be transferred to other topics (e.g., quantum mechanical questions). The presented development process and study results can also yield important insight for other digital learning environments.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.4c00151.

Download links for the German *SpinDrops-Lernumgebung* and the English *SpinDrops Learning Environment* for PC and Mac; a shortened codebook for transcripts (translated into English); the complete pre- and postquestionnaires (translated), including the ^{1}H NMR subject knowledge test on conceptual understanding (with correct answers); additional figures and tables (on further results of study B) as well as screenshots from the *SpinDrops Learning Environment* (Figures S1−S4 and Tables S1−S3) (PDF)

AUTHOR INFORMATION

Corresponding Author

Dominik Diermann − *Technical University of Munich, TUM School of Social Sciences and Technology, Department of Educational Sciences, Munich, Bavaria 80333, Germany;* orcid.org/0000-0002-2633-3888; Email: dominik.diermann@tum.de

Authors

Dennis Huber − *Technical University of Munich, TUM School of Natural Sciences, Department of Chemistry, Garching, Bavaria 85748, Germany; Munich Center for Quantum Science and Technology (MCQST), Munich, Bavaria 80799, Germany;* orcid.org/0000-0002-5182-6078

Steffen J. Glaser − *Technical University of Munich, TUM School of Natural Sciences, Department of Chemistry, Garching, Bavaria 85748, Germany; Munich Center for Quantum Science and Technology (MCQST), Munich, Bavaria 80799, Germany*

Jenna Koenen − *Technical University of Munich, TUM School of Social Sciences and Technology, Department of Educational Sciences, Munich, Bavaria 80333, Germany;* orcid.org/0000-0002-3591-617X

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jchemed.4c00151

Notes

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