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Technology Report

The Shrewd Guess: Can a Software System Assist Students in Hypothesis-Driven Learning for Organic Chemistry?

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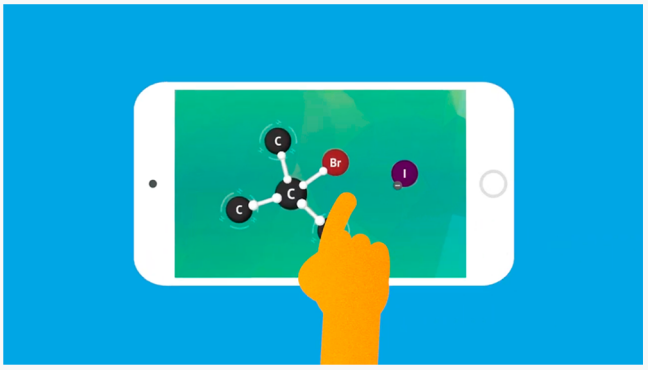
ABSTRACT: The mechanism maps that guide student instruction in organic chemistry curricula are structural representations of bond-breaking and bond-making events that transform a reactant into a product. For students, these pathways represented by electron pushing formalism (EPF) can be challenging to navigate. For instructors, providing formative feedback to students to support their learning of the EPF arrow system is difficult to provide in a timely manner. The Mechanisms App ("the App") was developed as a method for students to explore the electron movement of organic chemistry through a touch screen interface of a smart phone or tablet with real-time feedback of these moves. In this paper, the pedagogical content of the App and its backend system is described. This system produces a graphical record of a user's move within the App and is called a decision tree. A study of students' use of the App in two different modes was devised to understand whether the in-app experience can facilitate a hypothesis-driven approach to learning EPF. Examples of classroom implementation for the App in a variety of institutions and future research are also described.



KEYWORDS: *Upper-Division Undergraduate, Second-Year Undergraduate, Organic Chemistry, Constructivism, Mechanisms of Reactions, Computer-Based Learning, Assessment*

INTRODUCTION

Mechanisms, or electron-pushing formalism (EPF), depict the bond-making and -breaking within organic chemical reactions and are the maps that guide student instruction in curricula. Experts use chemical knowledge to reason how electrons will move in a mechanism to explain and predict reaction pathways.[1] Too often for students, including graduate students, the mechanistic routes through organic reactions seem to be filled with dead ends and roadblocks.[2−4] Even when students are given the destination—the product of the reaction—they can be more likely to adopt incorrect reasoning to describe the mechanistic steps of the reaction path.[5−7]

The question becomes how best to help students understand the EPF reasoning of organic chemistry and move beyond memorizing a procedure to explaining a process.[8−14] Research has shown that novice learners in organic chemistry focus on surface features when presented with an organic reaction, while experts "see" deeper concepts during each step of a mechanistic pathway.[15,16] Recent studies have shown that the use of animations help students to move to a more dynamic, and expert, view of reactions.[17] The Mechanisms app by Alchemie ("the App") was developed as a touch-screen software interface to enable students to make sense of the EPF of organic chemistry through experimentation.[18] In the App, students investigate reactions by moving electrons to make and break bonds, to which the App responds immediately using graphical and audio feedback.

The guiding principles which grounded the original development of the App came from Jerome Bruner's landmark book published in 1960, *The Process of Education*.[19] Bruner was one of 35 scientists, mathematicians, psychologists, and other scholars invited to a 10-day conference in 1959 with a goal of improving science and mathematics instruction for a new workforce as the nation faced rapidly changing technology. From the conference proceedings, discussions thereafter, and Bruner's reflection after the conference came this work which delineates Bruner's early ideas on cognitive constructivism. Three of the tenets of *The Process of Education* are

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Table 1. Pedagogical Content in the Sections of Mechanisms

Section	Categories	Details
Tutorial (How to Play)	Movement, Electrons & Bonds, Formal Charge, Decision Point, Interface	Interactive tutorials introducing the interface of the app
Essentials (100 puzzles)	Intro Reactions, Structure, Acid Base Reactions, Addition Reactions, Carbonyl Reactions	Five sections from both semesters of organic chemistry, with content starting with basic terminology and structural concepts, such as stability and resonance
Substitution and Elimination Reactions (60 puzzles)	Substitution Reactions, Elimination Reactions, and a combined section with both types of reactions	Three sections of content: S_N1/S_N2 then E1/E2, in the combined section students must decide which of the four pathways is favored
Oxygen-containing Functional Groups (65 puzzles)	Alcohol Reactions, Aldehyde and Ketone Reactions, Carboxylic Acid Reactions	Three sections which survey the mechanisms of oxygen containing functional groups
Pi Systems (40 puzzles)	Triple Bond Reactions, Electrophilic Aromatic Substitution (EAS) Reactions	Two sections of content which further investigate the formation and reactions of pi bonds

1. Understanding the structure of a subject, that is, the fundamental principles of a discipline rather than a mastery of facts, will allow learners to make connections between ideas and solve new problems.
2. To develop an intuition for problem-solving, which for Bruner meant being able to arrive at a plausible conclusion without going through all the analytical steps, learners must construct their ideas by testing hypotheses and learning from these experiments.
3. To encourage connections between prior knowledge and build new ideas, a spiral curriculum should be used where basic ideas are first introduced and used, then applied to more complex concepts, and then revisited throughout the learning of a discipline.

As the App was developed, these three principles were employed in designing the user experience (UX), the user interface (UI), and the pedagogy within the App.[20] The overarching technical development objectives were to provide the scaffolding (through repetition and spiraling of content) and immediate feedback for EPF moves from the software (to foster experimentation with concepts) to assist students in a better grasp of the structure of organic chemistry.

Though the mode of instruction in the App employs game-based learning methods,[21] the content and pedagogy of the App is less aligned with games and more with interactive simulations,[22] which allow for manipulation and control of the variables within an interface to modify and explore submicroscopic interactions dynamically. Visualizations and applications similar to the App include The Connected Chemistry Curriculum,[23] PhET simulations for chemistry,[24] and the Molecular Workbench by the Concord Consortium.[25] However, a differentiating feature of the App is the addition of a playful UX/UI design to lower the barrier to use for students who have come to expect an engaging experience in a mobile application.[26]

This paper highlights the features of the App that were inspired by the Bruner principles and their usefulness through a study of organic chemistry students. After two years of use in college classrooms, the anchoring question this technology report begins to answer is, what scaffolding pieces facilitate hypothesis-driven learning with an interactive learning tool? In *The Process of Education*,[19] Jerome Bruner stated "The shrewd guess, the fertile hypothesis, the courageous leap to a tentative conclusion—these are the most valuable coin of the thinker at work." It is anticipated that by evaluating processes to encourage hypothesis-driven learning, this research can assist in further research and development and the implementation of other dynamic visualizations and formative assessment collection systems.

MECHANISMS (THE APP): CONTENT, IN-APP RESOURCES, AND DATA SYSTEM

The App was first released in spring 2018 after 5 years of design and development and with funding from the National Science Foundation[20] with a tutorial system and 60 interactive exercises ("puzzles"), 20 each in the reaction categories Acid/Base, Addition, and Carbonyls. Currently, the software system has 265 puzzles divided into the following categories: Tutorial, Essentials, Substitution and Elimination Reactions, Oxygen-Containing Functional Groups, and Pi Systems (Table 1).

Each of the puzzles has its own short video (30−90 s) that can be accessed from within the App. A web-based instructor dashboard allows faculty to assign sets of puzzles for either in-class or out-of-class work. These assignments are delivered as a separate category in the App on the students' device. The App is free to download from the AppStore and Google Play.[18] To accommodate students without access to smartphones or tablets, the App is available as a web-based product.[27] The Tutorial and 50 puzzles of the Essentials section are free to use, the remaining content of 215 puzzles is available for a fee.

The depiction of the EPF within the App is dynamic movement of electrons guided by the user's finger and does not include any curved arrows. This was a decision made during early development as on a touchscreen even if there were an arrow when electrons are moved from source to sink, the head of an arrow would not be visible underneath a finger on the screen. Additionally, arrows are symbols to represent movement, but through the dynamic interface, the movement can be directly shown, thus eliminating the need for the curved arrow symbol. As an example, a user can reveal hidden electrons from the nucleophile with a tap and then drag them to make a bond with the electrophile, but there is no way to move the electrons in the opposite direction.

The formative feedback of the App is delivered to students through visuals, text, and sounds (Figure 1). Every puzzle starts with a Task Card (Figure 1a). Most of these cards include images of curved arrows for one of the mechanistic steps the student will encounter during the reactions. Students can access a list of goals (examples are, "Form the more stable carbocation", "Show the resonance delocalization", "Perform a nucleophilic attack") at any time during game play (Figure 1b). Immediate move assessment happens when a move is not allowed mechanistically; the bond snaps back into position and delivers a "cat hiss" correction sound. Sometimes this correcting feedback is accompanied by a hint button, which gives specific instructions on why a move is incorrect (Figures 1c and d). When the puzzle is complete, a "Goals Achieved" sign is displayed, and stars appear on the goal card (Figures 1e and f).

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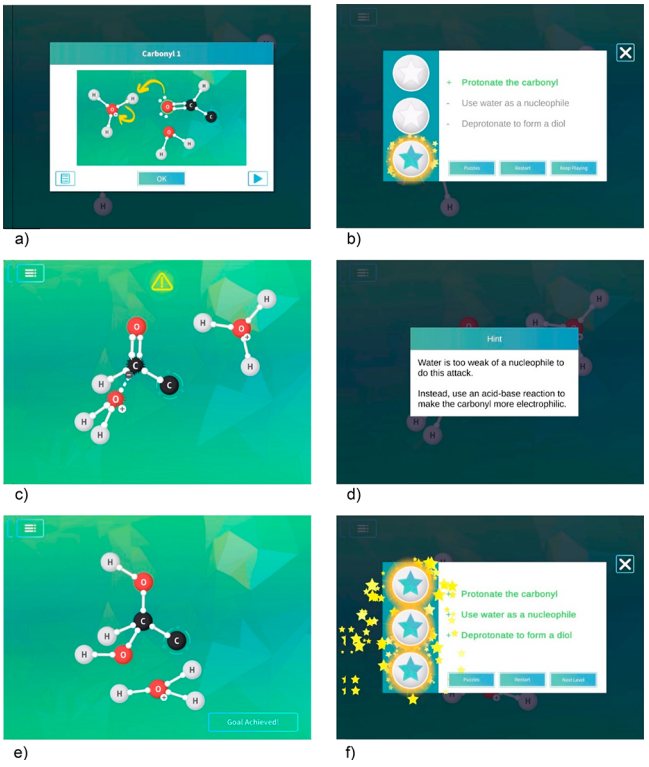

Figure 1. Scaffolding resources of the App from top left: (a) Task Card, (b) goals of puzzle, (c) immediate move assessment, (d) hint after incorrect move, (e) final product with goal achieved feedback, (f) stars appearing when goals are achieved.

The backend data system of the App has been designed to capture all student moves and interactions within the user interface. Some of this data is delivered to instructors through the dashboard. At this time instructors can access each student's progress (number of stars earned) on required puzzles, if attempts were made within a designated time frame, and also how many moves and how much time the student used to solve each assigned puzzle. The state of the puzzle during the session, that is, the connectivity of atoms as the result of a move, are represented in the database as SMILES (Simplified Molecular Input Line Entry System) strings, which is a method of representing molecular structure with a line of text.[28] These representations can be used to understand user interactions within the App. The graphical replay of each puzzle session, as a sequence of allowed and error moves, is called a decision tree. (Examples of decision trees are included in the Supporting Information.) The development team has used deidentified decision trees to analyze common errors to build the in-app hint system. Instructors and students do not currently have access to these decision trees.

The challenge to the pedagogy and development team has been to build enough scaffolding for novice learners while allowing the spirit of experimentation and hypothesis-testing to be part of the experience. An "Expert Mode" feature, which removed access to the Goal Card and in-app hints, was added to allow students to assess their understanding without the extra help. By testing the usability of the App with students in either the Regular or Expert modes, the development team wanted to discover which scaffolding resources were more effective in creating an interface which would promote hypothesis-driven mechanistic reasoning skills.

AUGSBURG UNIVERSITY USABILITY SURVEY

In the spring of 2019, six students were recruited for think-aloud interviews; all subjects were in second semester organic chemistry at Augsburg University (a private, liberal arts institution located in Minneapolis, MN), and the study was conducted the week before the final exam. All student testing and data analysis was approved as ethical by Augsburg University's IRB #2019-24-03. Arbitrarily, three participants used the App in Regular mode (Patrick, Rochelle, and Sam) and three used Expert Mode (Emma, James, and Kim) to work through the Aldehyde and Ketone 13 puzzle, an aldol reaction of acetone with benzaldehyde. All students had used the App for class activities prior to the interviews. All names are pseudonyms.

This puzzle has five states in moving from the starting material to the final product (Figure 2). Because each of these moves requires both making and breaking of bonds, the minimum number of moves needed to solve the puzzle is ten. The decision trees of the six participants were used to analyze total number of moves in the puzzle session, according to whether the moves were mechanistically allowed or were error moves, and when these moves occurred with respect to the five intermediate states of the aldol reaction (Tables 2 and 3). From the transcripts and videos of the subjects using the App, the number of times in-app resources were used by the participant was counted during the puzzle solution activity (Table 2). The decision trees of the six participants are available in the Supporting Information.

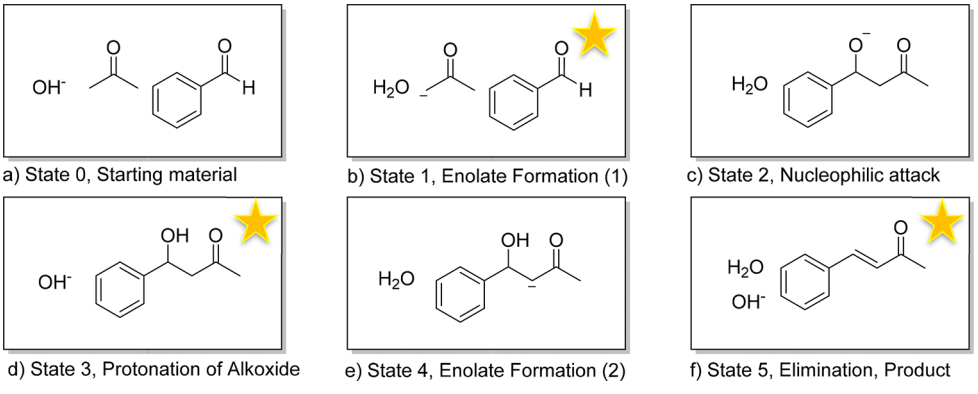

Figure 2. States of the puzzle Aldehyde and Ketone 13 from the Mechanisms App, the stars indicate where the three goals of the puzzle are earned.

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Table 2. Usability Testing of the App with Three Users in Regular Mode and Three Users in Expert Mode (No Access to the List of Goals or in-App Hints)

User	Mode	Puzzle Complete?	Total Number of Moves	Number of Error Moves	Frequency of Use: Task Card	Frequency of Use: Goals	Frequency of Use: Hint
Patrick	Regular	Yes	29	11	2	2	2
Rochelle	Regular	Yes	13	3	4	1	1
Sam	Regular	Yes	46	20	4	5	1
Emma	Expert	No	24	16	1		
James	Expert	Yes	57	25	1		
Kim	Expert	Yes	20	4	2		

Table 3. Error Moves by Users by Type for Each Step of Mechanism

User	Mode	Number of Error Moves	Enolate Formation (1)	Nucleophilic Attack	Protonation of Alkoxide	Enolate Formation (2)	Elimination
Patrick	Regular	11	8	0	1	1	1
Rochelle	Regular	3	0	0	0	3	0
Sam	Regular	20	1	1	1	11	6
Emma	Expert	16	9	0	7		
James	Expert	25	0	10	6	5	4
Kim	Expert	4	0	0	0	0	4

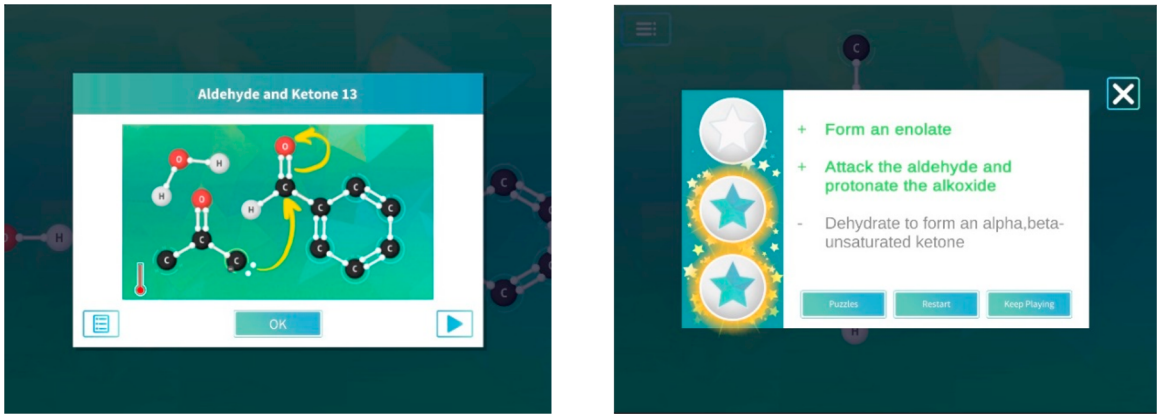

Figure 3. On the left (a) is the Task Card and on the right (b) is the card showing the goals for puzzle Aldehyde and Ketone 13.

Regardless of the mode, the first scaffolding resource, the Task Card, is encountered as the puzzle is opened. For Aldehyde and Ketone 13, the card depicts the second step of the mechanism (Figure 3a). Only those participants in Regular Mode could access the Goal Card (Figure 3b) of the puzzle at any time during the session. The participants in Expert Mode would see when they had achieved a specific goal, but the remaining goals descriptions were not visible to them.

Though the participants in the Regular mode all completed the puzzle, the efficiency of moving through the states of the session varied. The excess number of moves, beyond error moves, were from users moving back and forth with allowable mechanistic moves, such as breaking a bond that was just formed or changing the resonance state of the molecule. Though the Task Card was available to Patrick and provided a structure of State 1, he did not use the card as he tried various moves to form the first enolate. He did encounter a hint while moving from State 0 to State 1, but it was not helpful in discovering the correct acid−base reaction, and most of his moves involved using the hydroxide as either a nucleophile or a base with the benzaldehyde instead of with acetone. Once he used hydroxide to form the enolate of acetone to move to State 1, he progressed efficiently to State 3. Sam, however, reached State 3 in a total of nine moves (as opposed to Patrick's 19), but then used 22 moves to form the second enolate and reach State 4. During these moves, Sam was intent on deprotonating the methyl group. Though a hint was delivered during these moves, he did not click on it at the time. Of the three participants in Regular mode, Rochelle was the most efficient puzzle solver, and her error moves occurred as she attempted to use an intramolecular deprotonation method to form the second enolate, State 4.

All three of the participants in the Regular mode used the Task Card and the Goal Card in helping to develop a method for solving the puzzle, and all encountered at least one in-app hint during the session. Only for Sam was that hint used to move his problem-solving forward. It helped him test eliminating the hydroxyl group and form a conjugated system in the final elimination step. "So, I'm trying to form a conjugated system. Hmm. Then, it would make sense to go there [moves lone pair on carbon to form a C═C bond]. OH is a bad leaving group, but I guess I can try it [achieves State 5, the puzzle solution]." All three of these participants remarked about the unlikeliness of hydroxy as a leaving group.

For the participants in the Expert Mode group, the only in-app resource available was the Task Card. Emma did not finish the puzzle and was the only participant to restart the puzzle. In her first attempt, she used nine moves and could not move

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forward after she had used hydroxide as a nucleophile with carbonyl of benzaldehyde. (If she had been in Regular mode, she would have been prompted with a hint at this step.) In her second puzzle attempt, she did successfully reach State 2 in five moves but hit a stopping point after converting the alkoxide to a carbon−oxygen double bond, because "I know like oxygen would rather make a double bond and not have any charge, but I do not know what to do with the hydrogen." James spent nearly 25 min on the puzzle, and though he moved to State 1 in only 2 moves, he used 29 moves to reach State 2, 9 moves for State 3, 7 moves for State 4, and 10 moves for State 5. At one point (after reaching State 3 and protonating the alkoxide), the interviewer did prompt James to look for sites of reactivity, and he was able to recognize that there was an α carbon with two hydrogens. His multiple moves did not appear to be random, as he described chemical principles during the process. In the final step of the puzzle, he was asked about why he formed a double bond, "Well, one, I haven't tried it yet, and two, well the OH could leave if this is under basic conditions. That would make sense. I've never thought of it as a good leaving group. This ring could leave too, but if the ring leaves, it's losing its aromaticity. I'll try the OH." Kim moved efficiently to State 4 and then used a total of 12 moves with 4 error moves to perform the elimination reaction to reach State 5. From the Task Card, she noticed the thermometer: "Oh, there is heat. Heat means elimination. Which do I eliminate? Maybe? Okay, I'm gonna try eliminating the hydroxide, I don't think it's something that's gonna happen, but let's see. Oh, there we go. I'm done. Okay."

From this limited study of six students, we have found the most important in-app feature for fostering testing and experimentation in solving mechanism problems within the App is the immediate move assessment interaction, which allows students to use their conceptions (or in some cases, misconceptions) to try out possibilities. Though this immediate feedback was useful at a granular level, the Goal Card helped students to break down the reaction into key steps and frame their hypotheses within a chemical concept framework. If accessed, the Task Card could be helpful for a few of the moves. Though there were embedded hints to be uncovered by the users on certain error moves, either the notification was not prominent enough for the student to notice the hint, or the hint did not convey the information needed for the user.

CLASSROOM IMPLEMENTATION AND FUTURE RESEARCH

A key resource external to the App is the classroom support that frames the use of a learning tool.[29] The fifth author, Michael Wentzel, remarked that the students at Augsburg University were encouraged to write out the mechanisms on paper as they manipulated bonds and electrons within the App during in-class and out-of-class assignments. Two studies which compared students using the App to students solving similar mechanisms problems with traditional paper-and-pencil methods, found that both groups tackled the respective problems in a similar manner regardless of modality.[30,31] The research team asked instructors (authors Yee, Kabrhel, and Evans) at a variety of institutions to share their implementation strategies for the App. In all three cases, the App was used during class activities (as opposed to strictly outside of class) and was a complement to traditional methods of lecture, discussion, or structure drawing (Table 4).

Table 4. Case Studies

Institution	Hartnell College	University of Wisconsin-Green Bay	Georgia Tech
Description or institution	2-year college in Salinas, CA	4-year primarily undergraduate public university, satellite campus	Large, urban R1 public research institution
Course	Organic II, Spring 2019Organic I, Fall 2019	Organic I, Fall 2018Organic II, Spring 2019Organic II, Fall 2019	Organic II, Fall 2019 (with biochemistry focus)
Reasons for using the App	To facilitate EPF learning. From observations that students had difficulty knowing how to start a mechanism, and when they would draw arrows, they would begin in the wrong place. The App does not allow these moves.	To incorporate new technology on the classroom iPads which were used to enhance traditional teaching methods.	To add variety to mostly pencil-and-paper activities, the App was used as a problem-solving tool during in-class activities while teaching using a flipped-classroom practice.
Class implementation	During the first semester, the App was used mostly as an out-of-class activity. Students were encouraged to draw out mechanisms as the used the App, but this process was not explicitly modeled. During the second semester of use, the App was used during class to show mechanisms and students were prompted to verbalize what was happening during in the App during the discussion.	The App was used as part of weekly homework assignments. Mechanisms were demonstrated in class using the App to show example problems. The App was also incorporated into a section of the take-home final exam.	The App was used in class and was part of the class discussion after a "mini-lecture." Students were encouraged to verbalize mechanistic reasoning as they used the App and to draw out the reaction steps as they proceeded with problem solving using the App.

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Further research is ongoing in a first semester organic chemistry course at a large public university to compare how students answer questions within the App during a quiz sections, through collection of their move-by-move data, to their traditional EPF answers on an exam a few days later. What is yet to be studied is whether combining the software system's real-time move assessment with traditional methods of structure drawing can help students more successfully navigate the route from reactant to product using EPF in an organic chemistry mechanism. In terms of development, the translation of data from the backend system to actionable skill assessment of EPF conceptual understanding and delivery of those assessments to both students and instructors is yet to be accomplished.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.0c00246.

Graphical outputs from the App (the decision trees) of the participants in the Augsburg usability study (PDF)

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Notes

The authors declare the following competing financial interest(s): Authors J.E.W., J.E., S.E.W., and G.J.M. have received compensation for work performed as employees or contractors of Alchemie, the producer of Mechanisms.

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