Chemistry
Education Research
and Practice

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| Journal: | *Chemistry Education Research and Practice* |
| Manuscript ID | RP-ART-07-2022-000208.R1 |
| Article Type: | Paper |
| Date Submitted by the Author: | 08-Feb-2023 |
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# Metacognitive Regulation in Organic Chemistry Students: How and Why Students Use Metacognitive Strategies When Predicting Reactivity

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## Abstract

Problem solving is a key component of authentic scientific research and practice in organic chemistry. One factor that has been shown to have a major role in successful problem solving in a variety of disciplines is metacognitive regulation, defined as the control of one's thought processes through the use of planning, monitoring, and evaluation strategies. Despite the growing interest in assessing and promoting metacognition in the field of chemical education, few studies have investigated this topic in the context of organic chemistry students. To gain a deeper understanding of how and why students make use of strategies related to metacognitive regulation in their approaches to solving problems, we conducted interviews with Organic Chemistry I, Organic Chemistry II, and graduate organic chemistry students and used multiple measures to examine students' metacognition. As a part of these interviews, students verbalized their thoughts as they worked on complex predict-the-product problems and completed a self-report instrument indicating which planning, monitoring, and evaluation strategies they had used while completing each problem. Think-aloud protocols were analyzed for the presence of each of the behaviors included on the self-report instrument, and students' use of metacognitive strategies was compared to identify differences between students with different levels of experience and between students who generated more and less successful solutions to the problems. Students who generated more successful solutions to the problems tended to report using a greater number of metacognitive strategies. When asked why they did or did not use certain metacognitive strategies, students indicated a number of factors, such as not feeling able to use these strategies effectively or believing that using these strategies was unnecessary. The results of this study support the importance of teaching metacognitive problem-solving strategies in organic chemistry courses and suggest several methods for the assessment and instruction of metacognition.

## Introduction

In teaching chemistry, our major goal is to help students develop their ability to engage in chemical thinking and to ask and answer questions related to authentic chemical practices (Talanquer and Pollard, 2010; Sevian and Talanquer, 2014). Efforts to reform chemistry curricula have emphasized the importance of guiding students toward understanding and applying fundamental chemical concepts across a variety of situations and toward engaging in practices that are both central to the discipline and broadly useful for non-chemistry and chemistry majors alike (Cooper and Stowe, 2018; National Research Council, 2012). An essential component of authentic scientific research and practice in organic chemistry is problem solving, defined by Schoenfeld (2016) as “learning to grapple with new and unfamiliar tasks when the relevant solution methods (even if only partly mastered) are not known” and by Wheatley (1984) as “what you do, when you do not know what to do.” Much of the research in organic chemistry education has therefore focused on how students solve different types of problems and how problem-solving strategies can be taught (Graulich, 2015). The types of problems that are most commonly used to assess student knowledge in organic chemistry courses can be classified into three major categories (Austin et al., 2015; Helix et al., 2022). These include predict-the-product problems that ask students to predict the outcome of a given chemical reaction, mechanism problems that require students to explain how a reaction occurred, and synthesis problems that ask students to design a series of reactions to generate a given molecule. Each of these problem types corresponds to an authentic question routinely encountered by practicing organic chemists.

Among the types problems commonly used to assess student knowledge, predict-the-product problems are distinctive in that students are not provided with an endpoint to work towards. Studies have shown that when students attempt to solve mechanistic problems in which the final product is given, they typically focus on proposing steps that “get me [closer] to the product” by reducing the number of structural differences between the reactants and products (Bhattacharyya and Bodner, 2005; Caspari et al., 2018; Ferguson and Bodner, 2008). Work by DeCocq and Bhattacharyya (2019) demonstrated that knowing the overall product of a transformation led to a dramatic change in the reasoning strategies organic chemistry students used when asked to provide the intermediate product and curved arrows for a single elementary step of a multi-step mechanism. In the absence of information about the final product of the transformation, students primarily proposed intermediate products based on their knowledge of the chemical properties of the reactants. After students were provided with the final product, many changed their answers to structures that more closely resembled this product. It is clear from these studies that student reasoning is highly affected by the information given in the problem statement, and that students’ approaches to problems in which the ultimate product is not known, such as predict-the-product problems, may more accurately reflect their ability to engage in chemical reasoning. For this reason, along with the relatively small number of studies investigating student reasoning on problems of this type and level of difficulty, recent work in our research group has centered on investigating student approaches to open-ended predict-the-product problems that are relatively complex and potentially ambiguous (Helix et al., 2022).

Our previous research on student approaches to open-ended predict-the-product problems involved analyzing think-aloud interviews in order to categorize student approaches in terms of common problem-solving actions (Helix et al., 2022). The results of this analysis were used to develop a general workflow model that describes the ways in which students with different levels of expertise in organic chemistry solve problems that rely on predicting reactivity. While completing this work, we became interested in examining additional strategies that students engage in while solving these types of problems, especially those that may differentiate between successful and unsuccessful problem solvers. One of the factors that has been shown to have a significant impact on problem-solving across disciplines is a student's ability to engage in metacognition, defined as the knowledge and control of one's own thought processes (Flavell, 1979; Rickey and Stacy, 2000; Schoenfeld, 2016). There has been growing interest among chemical education researchers in assessing and promoting metacognition, yet few studies have focused on organic chemistry courses (Arslantas et al., 2018). In a review of research conducted in the field of organic chemistry education, Graulich (2015) suggested that one of the main areas of future progress in this domain should be fostering metacognitive and learning strategies. Developing ways to teach metacognition and scaffold the development of specific metacognitive problem-solving skills in this context is made easier by having an understanding of both how and why students use these strategies in their approach to solving organic chemistry problems. This study therefore builds upon our previous research on student approaches to complex predict-the-product problems by providing a more comprehensive, multi-method examination of students' use of metacognitive regulation strategies when solving problems of this type. In addition to determining which metacognitive behaviors are exhibited by students with different levels of experience in organic chemistry and exploring the connection between students' metacognitive regulation and their success in solving problems, we also discuss students' reasons for using these strategies.

*Theoretical Framework*

<u>Metacognition and Its Importance in Problem Solving</u>

Metacognition, commonly defined as "thinking about thinking," refers to the awareness and control of one's own cognitive processes (Flavell, 1979; Livingston, 2003). This complex construct can be divided into two major components: metacognitive knowledge and metacognitive regulation (Schraw and Moshman, 1995; Livingston, 2003). Metacognitive knowledge refers to what a person knows about their own thinking processes, and includes declarative, procedural, and conditional knowledge (Jacobs and Paris, 1987). Declarative knowledge involves knowing about one's thought processes and the factors that influence one's learning, procedural knowledge relates to knowing how to use strategies and skills to accomplish tasks, and conditional knowledge involves knowing when and in what context it is appropriate to use different strategies (Jacobs and Paris, 1987). Metacognitive regulation refers to the strategies used to control one's thinking and learning and includes the skills of planning, monitoring, and evaluation (Schraw and Moshman, 1995). Planning typically takes place before beginning a task and can involve activating relevant background knowledge, setting goals, making predictions, selecting strategies to use, and allocating time and resources (Schraw and Moshman, 1995). Monitoring would occur during the process of completing the task; this would include checking one's understanding and determining whether one's chosen strategies are working (Schraw and Moshman, 1995). Evaluation would then involve reflecting upon and assessing the outcomes of a task as well as the processes used while completing that task (Schraw and Moshman, 1995). In our study, we focused on the regulatory component of metacognition, which is particularly vital for successful problem solving (Davidson et al., 1994).

Metacognition has been shown to have a significant impact on problem-solving success in specific disciplines such as chemistry (Rickey and Stacy, 2000; Gulacar et al., 2020) and mathematics (Jacobse and Harskamp, 2012; Schoenfeld, 1987; Artz and Armour-Thomas, 1992) as well as in general critical thinking tasks (Swanson, 1990; Ku and Ho, 2010). Schoenfeld (1987), for example, found that in the absence of metacognitive regulation, college students enrolled in his mathematical problem-solving course often continued down unproductive paths, despite having the requisite mathematical knowledge to solve the problem, because they did not pause to consider whether they were making progress in the right direction. This indicates that simply being familiar with the relevant concepts is not sufficient for solving genuine problems. Work by Swanson (1990) suggests that a high level of metacognition could in fact compensate for lower aptitudes; using think-aloud interview techniques, he observed that children with higher levels of metacognition performed better on problem-solving tasks than those with lower metacognitive activity regardless of differences in general academic aptitude. This association between metacognitive ability and problem-solving skills underscores the importance of studying metacognition in disciplines where problem solving is a central practice.

### Measuring Metacognition

Methods of assessing metacognition can be divided into two major categories: on-line measures and off-line measures (Van Hout-Wolters, 2009). On-line measures, also known as concurrent measures, are taken at the same time as a study participant is completing a task. Examples include think-aloud interviews, observations, eye-tracking, and logging of participants' actions while performing a task on a computer (Van Hout-Wolters, 2009). Off-line measures, which commonly take the form of self-report questionnaires or retrospective interviews, are administered asynchronously with task performance. Learners are asked to report on their likelihood of engaging in certain metacognitive behaviors or using particular metacognitive strategies, either in a specific context or in general. The decision regarding which type of measure to use depends on several factors, one of which is a researcher's belief about the theoretical nature of metacognition. One of the major assumptions underlying the use of different measures of metacognition is whether metacognition is conceptualized as a general aptitude or a specific event (Winne and Perry, 2000). When metacognitive ability is seen as an aptitude or trait, it can be assumed that students' use of metacognitive strategies is stable across different situations and contexts. If metacognition is instead viewed as an event, it would be expected that students' metacognitive behavior would vary depending on the contextual features and demands of a task. Concurrent measures are bound to a specific task and would therefore correspond with the assumption that metacognition is an event (Winne and Perry, 2000). Self-report measures, on the other hand, are more typically used when measuring metacognition as an aptitude. In general, self-report measures only weakly correlate with concurrent measures, which indicates that the choice of measurement may have a significant impact on the results of a study (Craig et al., 2020; Van Hout-Wolters, 2009). According to Desoete (2008), when it comes to measuring metacognition, there is evidence that "how you test is what you get" (Desoete, 2008, p. 204). For this reason, one's choice of assessment should be carefully considered when measuring metacognition.

There are benefits and drawbacks to the various measures of metacognition. Concurrent assessments are generally considered to better align with actual behavior than off-line measures, likely because these measures require the learner to make judgments based on reconstructing their previous cognitive processes from memory (Van Hout-Wolters, 2009; Veenman et al., 2006). The issue of distortion due to memory failure can be partially mitigated by administering self-report measures immediately after completing a task and asking students to consider their behavior in a specific situation (Ericsson and Simon, 1993; Veenman, 2011). While this does not resolve all of the issues with self-report questionnaires, including the inclination to give socially desirable responses, being asked to consider one's behavior in a specific situation can make it easier for participants to recall their actual behavior (Van Hout-Wolters, 2009). Task-specific questionnaires typically correlate more strongly with concurrent methods than general questionnaires; for example, Schellings et al. (2013) observed a correlation of $r$=0.63 between think-aloud protocols and a task-specific questionnaire that was directly based on a taxonomy for coding those think-aloud protocols (Schellings et al., 2013). The major drawback of concurrent assessments is that they tend to be much more time-consuming to administer and analyze, so it is not typically feasible to use them with large groups. Also, though thinking aloud is not considered to alter student behavior apart from increasing the time taken to complete a task, assessing metacognition in this way may lead to underestimations of metacognitive behavior (Ericsson and Simon, 1993; Veenman, 2011). This is because students may not be consciously aware of their self-regulatory processes, as these processes are often highly automated in adults (Schraw et al., 2006; Veenman et al., 2006). To overcome the drawbacks associated with these individual measures of metacognition, many researchers have emphasized the advantage of using multiple methods to assess metacognition (Cooper et al., 2008; Desoete, 2008; Schellings et al., 2013; Veenman, 2005).

### Metacognition in Chemical Education

Metacognition has been studied extensively as a psychological construct since the 1970s, but it is primarily in the past two decades that interest has grown in studying metacognition in the context of chemical education (Avargil et al., 2018; Arslantas et al., 2018; Lavi et al., 2019). Much of this work has centered on evaluating interventions designed to promote metacognitive behaviors in chemistry students. Interventions that involve explicitly teaching metacognitive learning strategies to students in introductory or general chemistry courses were found to result in improved course grades (Cook et al., 2013; Mutambuki et al., 2020) and increases in student self-efficacy (Graham et al., 2019). Other interventions made use of pre- or post-class activities such as online homework-based metacognitive training in a general chemistry course (Casselman and Atwood, 2017) or the use of question-embedded videos as a replacement for pre-class textbook readings involving organic chemistry concepts (Pulukuri and Abrams, 2021). These interventions both led to improvements in learning outcomes and metacognitive skillfulness as measured by calibration accuracy. Several interventions focused more closely on the connection between metacognition and successful problem solving. Parker-Siburt and coworkers (2011) developed and evaluated a general chemistry recitation section that was designed to help students develop metacognitive and problem-solving skills through the process of analyzing, solving, and manipulating problems (Parker Siburt et al., 2011). Heidbrink and Weinrich (2021) conducted think-aloud problem-solving interviews with biochemistry students and determined that implicitly targeting metacognition via reflective prompts resulted led to increases in the number of students who exhibited metacognitive behaviors related to declarative knowledge, conditional knowledge, monitoring, and evaluating (Heidbrink and Weinrich, 2021). Sandi-Urena, Cooper, and Stevens (2011) found that a collaborative intervention involving problem-solving and reflective prompting led to an increase in metacognitive awareness and in the ability to solve difficult non-algorithmic chemistry problems in the treatment group as compared to the control group in a general chemistry laboratory course (Sandi-Urena et al., 2011).

To evaluate interventions designed to promote metacognition and to investigate the nature of metacognition in chemistry problem solving, chemical education researchers need to assess students' metacognitive ability. Researchers have most commonly used self-report instruments, either alone or in combination with other methods, for this purpose. Examples of general metacognitive self-report instruments that have been applied to chemical education research include the Inventory of Metacognitive Self-Regulation (development: Howard et al., 2000; use with students who had completed a general chemistry course: Wang, 2015) and the Metacognitive Awareness Inventory (development: Schraw and Dennison, 1994; use with students enrolled in a general chemistry course: Gulacar et al., 2020). The Metacognitive Activities Inventory (MCAI), developed by Cooper and Sandi-Urena (2009), is an example of a domain-specific self-report instrument that was designed to measure metacognitive skillfulness in chemistry problem solving. Cooper and Sandi-Urena validated the use of this instrument among students enrolled in general chemistry I and graduate students (Cooper and Sandi-Urena, 2009). Concurrent methods such as think-aloud interviews (Heidbrink and Weinrich, 2021; Kadioglu-Akbulut and Uzuntiryaki-Kondakci, 2020; Wang, 2015) and an automated online instrument known as Interactive MultiMedia Exercises or IMMEX (Cooper et al., 2008) are among the other measures researchers have used to assess metacognition in chemistry students. Several of these studies made use of multiple measures (Cooper et al., 2008; Kadioglu-Akbulut and Uzuntiryaki-Kondakci, 2020; Wang, 2015). In their investigation of metacognition use in general chemistry problem-solving, Cooper, Sandi-Urena, and Stevens (2008) observed convergence between the scores students received on the MCAI (a self-report instrument) and the IMMEX (a concurrent measure). Wang (2015) examined characteristics of students' metacognition in different general chemistry topics using data from self-report measures, think-aloud interviews, and students' judgments of their performance. Kadioglu-Akbulut and Uzuntiryaki-Kondakci (2020) investigated the effectiveness of self-regulatory instruction in a high school chemistry classroom using the Cognitive and Metacognitive Strategies Scale (a self-report instrument), think-aloud protocols, and journal entries.

Despite the growing interest in the role of metacognition in chemistry education, few studies have focused on organic chemistry students. In a recent review of metacognition in higher education chemistry, 27 out of the 31 articles that met the inclusion criteria examined metacognition in students that were enrolled in introductory, general, or preparatory chemistry courses (Arslantas et al., 2018). Problems students encounter in organic chemistry courses differ from those encountered in general chemistry courses in that they are primarily non-mathematical and require a different set of fundamental skills (Cartrette and Bodner, 2010). According to Dye and Stanton (2017), many of the students they interviewed as part of their study on metacognition in upper-division biology students stated that organic chemistry was the first course in which they had to be metacognitive to succeed, likely due to their lack of experience with the type of problem solving required in organic chemistry courses (Dye and Stanton, 2017). This suggests that investigating metacognition in organic chemistry students would be particularly valuable.

To our knowledge, only four reports on metacognition in organic chemistry students have been published (Graulich et al., 2021; Lopez et al., 2013; Mathabathe and Potgieter, 2017; Pulukuri and Abrams, 2021). Lopez et al. (2013) investigated the study strategies used by ethnically diverse organic chemistry students and found that students typically used strategies that involved reviewing course materials rather than more metacognitive study strategies and that there were no significant correlations between study strategies used and course performance. Mathabathe and Potgieter (2017) examined organic chemistry students' use of metacognitive regulation during the collaborative planning of a laboratory group project. Based on previous coding schemes described in the literature as well as inductive analysis of transcripts of these collaborative planning sessions, the authors devised a coding scheme and decision tree for the classification of verbalizations related to planning, monitoring, control, and evaluation. Their coding scheme also classified verbalizations according to the type of regulation (self or other), area of regulation (cognition, task performance, or behavior), and depth of the regulatory behavior (high or low). Graulich et al. (2021) described the use of a scaffold that was designed to guide students through solving an organic chemistry case-comparison problem using a combination of instructional prompts and metacognitive suggestions. After writing down their initial solution and explanation for the given case-comparison problem, students watched videos of peers solving the same problem, completed a scaffolded analysis of these peer-solutions with a partner, developed a general procedure for handling contrasting cases tasks, and then revised their initial explanations. The authors found that this scaffolded activity led students to improve the quality of their mechanistic explanations. Pulukuri and Abrams (2021) compared metacognitive monitoring proficiency and learning gains between students who used different learning resources and found that students who learned organic chemistry concepts from question-embedded videos did better on both outcomes than those who learned from a textbook. Each of these studies suggests ways that metacognition can be observed in or encouraged in organic chemistry students.

## Problem Statement and Research Questions

The present study provides a link between two areas of study in chemical education: problem solving in organic chemistry and metacognition. While many studies have explored student approaches to solving organic chemistry problems, including predict-the-product problems (Cruz-Ramírez de Arellano and Towns, 2014; Finkenstaedt-Quinn et al., 2020; Grove et al., 2012a; Grove et al., 2012b; Helix et al., 2022; Webber and Flynn, 2018), none have focused specifically on investigating students' self-reported or concurrent use of metacognitive strategies during the process of solving organic chemistry problems. The major aim of this work is to characterize the behaviors related to metacognitive regulation that students exhibit when approaching relatively complex predict-the-product problems. We also sought to determine the reasons why students use certain metacognitive strategies because, while there are some reports on why students use metacognitive strategies in the context of reading comprehension (Andriani and Mbato, 2021; Thuy, 2020), there are none related to problem solving. Without an understanding of why students choose to use or not use metacognitive strategies, one cannot design effective instruction that will persuade students to adopt these strategies. Understanding which metacognitive strategies students with different levels of expertise use when working on organic chemistry problems, how the use of these strategies connects to successful problem solving, and why students choose to engage in these behaviors would provide a useful starting point for instructors to design interventions that teach these strategies to students. In this investigation, we were therefore guided by the following research questions:

1. What metacognitive strategies do undergraduate and graduate students use when solving organic chemistry problems?
2. How do students who are more and less successful at solving organic chemistry problems differ in their use of metacognitive regulatory strategies?
3. What reasons do students have for using or not using metacognitive strategies while solving organic chemistry problems?

## Methods

### *Participants and Context*

All work was conducted at the University of California, Berkeley, a large, research-intensive public institution located in the Western United States, during the 2020-2021 academic year. This study was approved by the university's Institutional Review Board (IRB), Protocol #2015-08-7858, and informed consent was obtained from all participants. Interviews were conducted with undergraduate and graduate students who were enrolled in organic chemistry courses or were conducting research related to organic chemistry. Undergraduate interview participants were recruited from two courses, Chem 3A (Organic Chemistry I) and Chem 3B (Organic Chemistry II), both of which are intended for students who are not majoring in chemistry, chemical biology, or chemical engineering. Recruitment announcements were posted on the learning management systems for these courses at the end of the Fall 2020 semester. Graduate students were recruited at the end of the Spring 2021 semester via an email sent to all students enrolled in the synthetic or chemical biology divisions of UC Berkeley's chemistry Ph.D. program. Students were entered into a gift card drawing as a reward for their participation. In total, 10 Organic Chemistry I students, 16 Organic Chemistry II students, and 12 graduate students participated in interviews. A summary of information about the interview participants' educational and demographic background is included in Table 1. All participants were asked questions about their year in their program and their undergraduate major or graduate research topic during the interview, and most of the undergraduate and all of the graduate student participants also completed a survey that contained questions about demographic information prior to the interview.

**Table 1. Summary of Information Related to Interview Participants' Demographic and Educational Background**

| Type of Information | Undergraduate Participants (N=26) | Graduate Participants (N=12) |
|---|---|---|
| Gender | Women (65%)<br>Men (19%)<br>Non-Binary or Unsure (4%)<br>Did Not Answer (15%) | Men (66%)<br>Women (25%)<br>Non-Binary or Unsure (8%) |
| Race/Ethnicity | East Asian (50%)<br>South Asian (15%)<br>African American/Black (8%)<br>Mexican American/Chicano (8%)<br>White/Caucasian (8%)<br>Did Not Answer (20%) | White/Caucasian (75%)<br>American Indian/Alaska Native (8%)<br>East Asian (8%)<br>Mexican American/Chicano (8%)<br>Middle Eastern/North African (8%)<br>South Asian (8%) |
| Year in Undergraduate or Graduate Program | First Year (12%)<br>Second Year (85%)<br>Third Year (4%) | First Year (25%)<br>Second Year (17%)<br>Third Year (8%)<br>Fourth Year (42%)<br>Fifth Year (8%) |
| Undergraduate Major or Graduate Research Focus | Life Science (77%)<br>Engineering (15%)<br>Public Health (8%)<br>Social Science (4%) | Organic Chemistry (100%)<br>Biological Chemistry (58%)<br>Analytical Chemistry (16%)<br>Inorganic Chemistry (16%)<br>Materials Chemistry (8%) |

It is important to note that the undergraduate students who volunteered to participate in interviews are not a fully representative sample of those enrolled in Organic Chemistry I or II. Overall, the undergraduate interview participants received final percentage grades in the course that were 0.5 standard deviations above the class average, and less than 20% received a grade lower than the class mean. However, as shown in Figure 1, the undergraduate interviewees did differ widely in their performance in the course, ranging from over one standard deviation below the class average to over one standard deviation above the class average. Grade data was not collected for the graduate student participants.

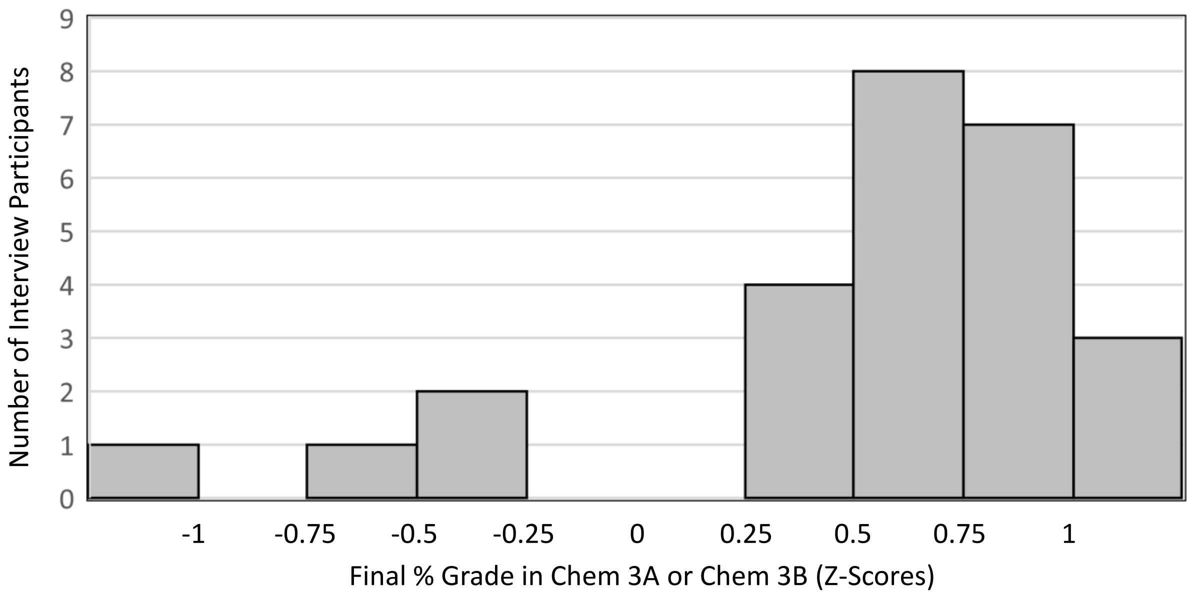


**Figure 1.** Distribution of final percentage grades among undergraduate interview participants in the organic course they were enrolled in at the time of the interview. Raw percentage scores were converted to z-scores in order to present data combined from the different courses.

*Development of List of Metacognitive Strategies Used in Interview Coding Scheme and Self-Report Instrument*

An initial list of 37 metacognitive skills that we believed would help students succeed in solving organic chemistry problems was developed in consultation with chemistry and education faculty members and graduate students. This list consisted of items drawn from the Cooper and Sandi-Urena's (2009) Metacognitive Activities Inventory (MCAI) and Schraw and Dennison's (1994) Metacognitive Awareness Inventory (MAI), some of which were modified to better suit the context of problem-solving in organic chemistry, as well as additional metacognitive behaviors that we had observed students engaging in during think-aloud interviews as part of our previous study into student approaches toward open-ended predict-the-product problems (Helix et al., 2022). When deciding what to include in this initial list, we prioritized behaviors that we believed would be useful for students when solving organic chemistry problems and that were related to the planning, monitoring, and evaluation skills that comprise the construct of metacognitive regulation.

This initial list of metacognitive activities was introduced to seven students who had previously taken one or more organic chemistry courses and had volunteered to participate in focus groups. During these focus groups, students completed a survey that asked how often they engaged in each activity while working on organic chemistry problems. They were then asked to provide feedback on the clarity of the questions and instructions. The wording of some items was changed in response to this round of feedback, while other items were removed from the list entirely. The final list (see Table 2) was narrowed down to nine strategies that students might use during the planning phase before attempting a solution, five monitoring strategies that students might use during the problem-solving process, and six strategies that students could use to evaluate the products and process of their approach after reaching a solution. We believed that this list could function as a measure of students' use of metacognitive regulation strategies in the context of both a self-report instrument and a coding scheme for use with interview transcripts. To ensure this dual functionality, we also conducted pilot interviews with five Organic Chemistry I or Organic Chemistry II students during the semester before the main data collection took place. These pilot interviews followed the same protocol described in the "interview protocol" section of this work. Transcripts of the think-aloud problem-solving portion of these pilot interviews, as well as similar interviews that one of the authors had conducted with students enrolled in different organic chemistry courses, were analyzed to determine whether student usage of each skill was evident or not evident in order to confirm that these behaviors could be detected in students' verbalizations of their thinking processes.

**Table 2. Final List of 20 Strategies Included in the Interview Coding Scheme and Self-Report Instrument.**

| Type of Strategy | Individual Item on Self-Report Instrument/Coding Scheme | Abbreviation |
|---|---|---|
| Planning | I set goals (ex. "I need to make this bond," or "I want to make this functional group") before attempting a solution. | Set Goals |
| | Before I started working, I sorted through the information in the problem to determine what is relevant.[a] | Sort Relevant Info |
| | Before I started working, I looked for any reactions I recognized. | Look for Reactions Recognized |
| | I reflected upon things I know that are relevant to the problem before I started working.[a] | Reflect Relevant Knowledge |
| | I tried to relate unfamiliar problems with previous problems I've encountered.[a] | Relate to Previous Problems |
| | I jotted down my ideas or things I know that are related to the problem before attempting a solution.[a] | Jot Down Ideas |
| | I made predictions about what would happen before I started working on the problem. | Make Predictions |
| | I brainstormed multiple ways to solve a problem before I actually started solving it.[b] | Brainstorm Multiple Ways |
| | I considered whether my proposed steps were reasonable before I actually started solving the problem.[a] | Consider If Plan Reasonable |
| Monitoring | When I was in the middle of working on the problem, I paused to consider whether there was another way to solve it.[b] | Consider Another Way |
| | While I was working on the problem, I paused to consider whether I was making progress toward my goals.[b] | Monitor Progress Toward Goals |
| | I paused to consider whether what I was doing was correct while I was working on the problem.[b] | Monitor Correctness |
| | I took note of what I was uncertain about as I worked on the problem. | Note Uncertainty |
| | As I worked on the problem, I periodically checked back over what I had done so far to make sure my overall approach was reasonable. | Periodically Check If Reasonable |

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|---|---|---|
| Evaluation | I thought about whether my answer was reasonable after I finished the problem.[a] | Consider If Answer Reasonable |
| | I made sure that my solution actually answered the question.[a] | Check If Answered Question |
| | I checked back over my work after I finished the problem to make sure I didn't make any mistakes.[a] | Check For Mistakes |
| | Once I reached an answer, I checked to see that it agreed with what I predicted.[a] | Check If Agreed With Prediction |
| | Once I finished the problem, I summarized the main take-away lesson I learned.[b] | Summarize Main Takeaways |
| | After I finished the problem, I considered how I might change my approach for future problems. | Consider Changes For Future |

[a] Duplicated or modified from an existing item on the MCAI (Cooper and Sandi-Urena, 2009).
[b] Duplicated or modified from an existing item on the MAI (Schraw and Dennison, 1994).

*Interview Protocol*

Each undergraduate or graduate student volunteer participated in an individual interview, which typically lasted about an hour. Because this study was conducted during the COVID-19 pandemic, all interviews took place over the Zoom video conferencing platform. Interviews were audio and video recorded for later viewing and transcription.

The components of the interview protocol and timeline are provided in Figure 2. Copies of the interview protocol and the surveys students completed during the interview are provided in Appendices S1 and S2 of the Electronic Supplementary Information. At the beginning of the interview, a PDF file containing the problems used in the interview was emailed to each participant. Participants were then asked to state their undergraduate major or graduate research focus, their year of study, and each organic chemistry course they had taken or taught. . After they answered these introductory questions, students were given guidelines for how they should use the think-aloud technique to verbalize their thoughts while solving a problem. They were then asked to solve an organic chemistry problem while vocalizing their thought processes. A list of the problems completed by the study participants and their accepted answers is included in Figure 3. The same instructions were given for all problems: "Predict the major organic product(s) of the following reactions. Please indicate stereochemistry where appropriate." Participants were asked to either use the screenshare feature while annotating the PDF file or, if they preferred to write on paper, angle their camera toward that sheet of paper. Students worked on the problem without interruptions, except for occasional prompts to speak up or brief feedback on their think-aloud technique, until they indicated that they had reached their final answer. Students were then provided with a link to a survey hosted on Qualtrics, where they were asked to indicate whether they had used in each of the 20 metacognitive strategies introduced in Table 2 while solving the first interview problem. For each item, students were able to select "yes" or "no." As a part of this survey, students were also asked how frequently they used each strategy when working on homework and exam problems in their organic chemistry course; however, this component of the data collection was completed as a part of a broader study involving additional chemistry courses and is beyond the scope of this work. Students were then asked several questions about their problem-solving approach, including questions about their reasons for carrying out certain metacognitive activities either on the problem they had just worked on during the interview or in their organic chemistry course in general. Following this discussion, students were asked to complete a second problem, which had identical instructions, while thinking aloud. They were then prompted to fill out a second survey to indicate whether they had used each strategy while working on that problem. Students were permitted to review their written work (i.e. any notes, annotations, chemical structures, or mechanistic drawings they wrote down while working on each problem) while completing each self-report survey.

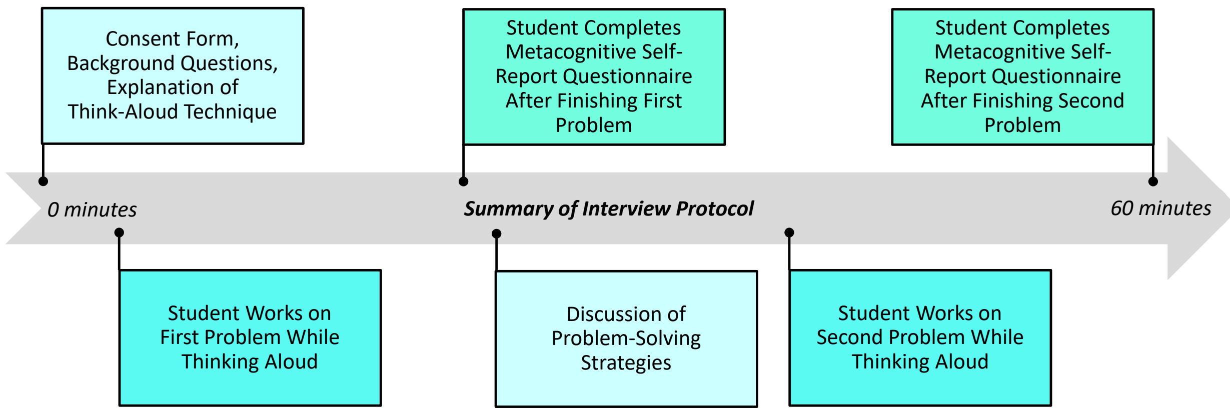

**Figure 2.** Summary of interview protocol, including typical one-hour timeline.

We chose to use both concurrent and self-report measures in order to get a more complete understanding of students' usage of strategies related to metacognitive regulation when solving organic chemistry problems. The think-aloud interview method was chosen because it allows for an in-depth analysis of students' problem-solving processes, and concurrent measures of metacognition are considered to better align with actual behavior as compared to off-line methods (Veenman et al., 2006). However, data collected using think-aloud protocols may not be complete if interview participants do not or can not verbalize all of their thoughts (Veenman, 2011). For this reason, we chose to additionally ask students about their behavior using a retrospective, task-specific self-report questionnaire. Because memory distortions are likely to increase with the interval between task performance and retrospective reports, we chose to administer this questionnaire immediately after students finished solving each problem (Ericsson and Simon, 1993; Veenman, 2011). Considering the minimal interval between completion of the problem-solving task and self-report questionnaire, we expected that reviewing their written work would provide sufficient cues to minimize memory distortions without the additional time required to allow participants to fully review their recorded think-aloud protocol. There is considerable precedent for similar study designs in which students think aloud while completing a task and then complete a retrospective questionnaire about their strategy usage directly after task completion without reviewing their process (Bannert and Mengelkamp, 2008; Desoete, 2008; Merchie and Van Keer, 2014; Rogiers et al., 2020; Schellings, 2011; Schellings et al., 2013; Veenman and van Cleef, 2019).

*Problem Design*

The problems students completed during the think-aloud portion of the interview, along with the accepted answers for each problem, are shown in Figure 3. Mechanistic drawings showing the formation of these products are provided in Appendix S5. Each of these problems was previously used when conducting think-aloud interviews with a different population of undergraduate and graduate organic chemistry students at this institution as a part of our ongoing research into student approaches to open-ended predict-the-product problems (Helix, 2021; Helix et al., 2022). In the present study, Problems A and B were completed by undergraduates enrolled in Organic Chemistry I, while Problems C and D were completed by undergraduates enrolled in Organic Chemistry II as well as graduate students.

The order in which each participant completed the problems was randomized. Several possible reactions could occur in Problem A, including an acid-catalyzed hydration of the alkene or epoxide or an intramolecular cyclization involving both functional groups. Problem B is an E2 reaction followed by an addition of methanol to the resulting alkene under acidic conditions. This addition of methanol includes a carbocation rearrangement. The reactants in Problem C could undergo either a Mannich reaction or an amine-catalyzed intramolecular aldol reaction. The first step of Problem D involves hydrolysis of the acetal to generate an aldehyde, which then reacts with a Horner-Wadsworth-Emmons (HWE) reagent in the second step. The product of the HWE reaction could then potentially cyclize to form a six-membered ring via an intramolecular oxa-Michael addition.

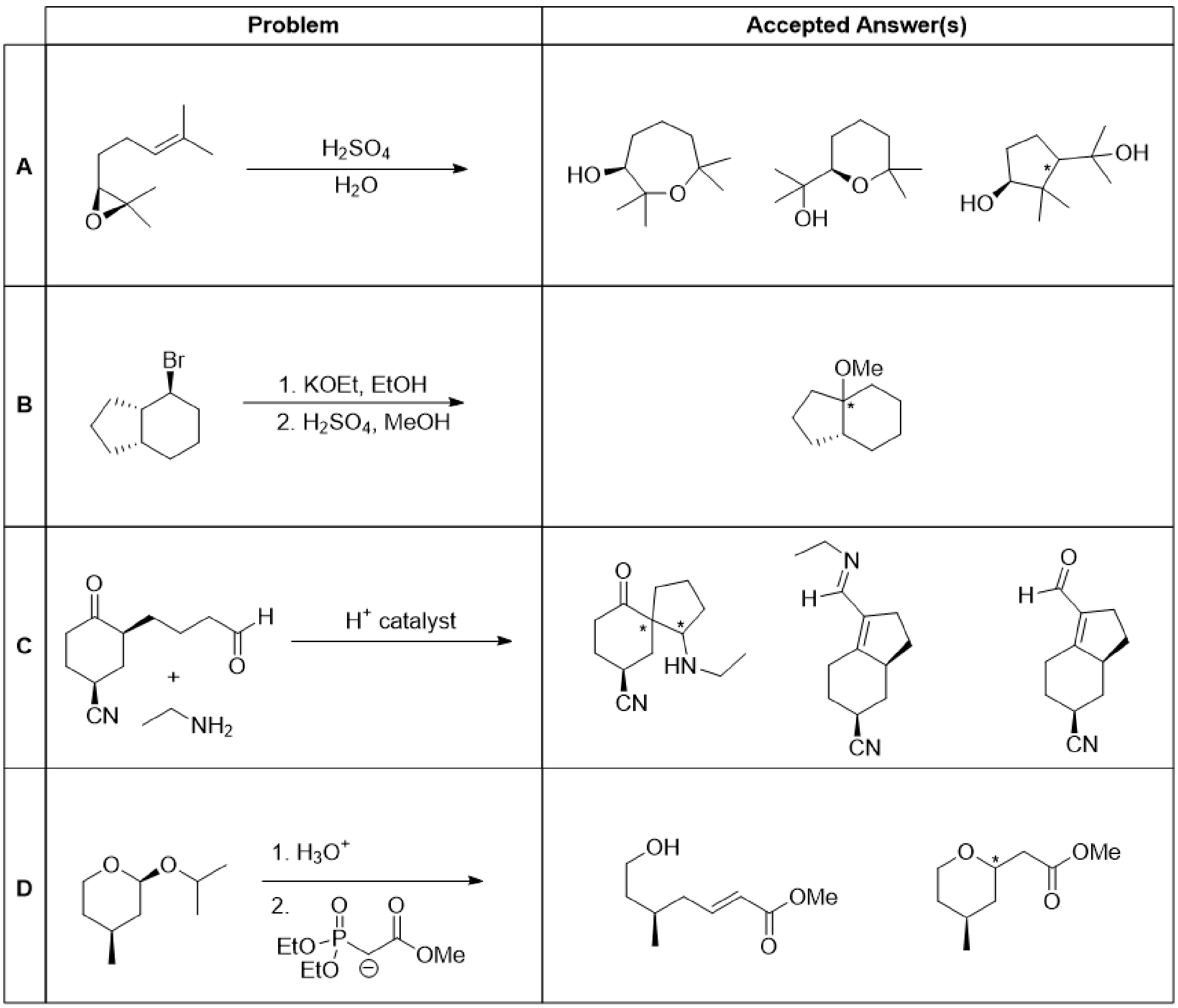


**Figure 3.** Organic chemistry problems that students completed during think-aloud interviews. Problems A and B were completed by Organic Chemistry I students, while problems C and D were completed by Organic Chemistry II students and graduate students.

We believed that, for the majority of interview participants, these problems would function as novel problems as opposed to routine exercises (Bodner, 2003). Whether any given chemistry question functions as a problem or an exercise depends on how familiar the person solving the task is with the material rather than on the innate difficulty of the task. For example, a stoichiometry problem that would serve as a routine exercise for a practicing chemist would be a novel problem for a student enrolled in their first chemistry course. The practicing chemist would likely complete the task in a logical, linear fashion based on recalled algorithms, while the student may take a more circuitous approach involving false starts and dead ends. The ambiguity and open-endedness of the chosen problems presented an opportunity for us to investigate how students approach less familiar problems where simple recall of information is not enough, and made it more likely that students would display the use of metacognitive behaviors during the process of solving these problems (Carr and Taasoobshirazi, 2008). Prior studies suggest that concurrent assessment of metacognitive regulation should be conducted using tasks that are of a level of complexity that would require the interview participants to intentionally control their thinking processes (Shin et al., 2003). Multiple sources of ambiguity were included in the design of these problems, including polyfunctional starting materials, an absence of detailed reaction conditions (e.g. temperature, equivalents), and the possibility of multiple potential products or completing solution pathways. Pilot interviews conducted with Organic Chemistry I and Organic Chemistry II students during the semester prior to the main study confirmed that students were generally interpreting the problems as expected and were able to at least generate some reasonable ideas about each problem despite their potential difficulty.

*Data Analysis*

Students' answers to the interview problems were evaluated for correctness, with partial credit given for partially correct answers or pathways. Approximately 30% of students' answers to each of the interview problems were scored by two researchers (KAB and AMB). The interrater reliability between the two researchers as measured by percent agreement was 88%, and the Spearman's rho correlation between the two raters' scores was 0.985 ($p < 0.001$). The remaining students' answers were scored by a single researcher (KAB). Rubrics used to score each question are provided in Appendix S5. Average scores received on each problem were calculated for the Organic Chemistry I, Organic Chemistry II, and graduate students, and are reported as percentages, e.g. a score of 3 points on an individual problem scored out of 4 points would correspond to a percent score of 75%.

Interviews were fully transcribed, and the transcripts were annotated to indicate what students were writing as they spoke aloud. These transcripts were then coded by several members of the research team using MaxQDA qualitative data analysis software. Two different coding schemes were developed, one for analysis of the think-aloud portion of the interview and the other for analysis of the discussion portion. Definitions and examples of all codes are provided in Appendices S3 and S4. The first scheme includes codes that correspond to each of the 20 metacognitive strategies included in Table 2. These codes were assigned to each think-aloud problem transcript according to whether a student's usage of each skill was evident or not evident in the transcript. Definitions and criteria for the inclusion or exclusion of certain statements under each code were developed following extensive discussion between members of the research team, which included undergraduates who were currently enrolled in organic chemistry courses. The second scheme was developed to categorize the most common reasons that students gave for using or not using the metacognitive strategies described in Table 2. Codes and their definitions were developed inductively using a constant comparative method that consisted of reading the transcripts, noting down emerging themes and potential codes, and meeting to discuss agreements and disagreements between members of the research team. Saturation was reached with a set of 16 codes: nine corresponding to reasons students reported using the metacognitive skills, and seven corresponding to reasons for not using these skills. Similar codes were categorized into a total of seven major themes by two members of the research team. A list of these themes, codes, and their descriptions is included in Table 3.

After coding approximately 10% of the transcripts as a group, each remaining think-aloud or discussion transcript was coded independently by at least two members of the research team. The average interrater agreements between pairs of researchers for metacognitive skills observed during the think-aloud interview and for reasons for using or not using metacognitive strategies mentioned during the discussion portion of the interview were κ=0.83 and κ=0.80, respectively. All members of the research team met periodically to compare notes on the coding process and resolve any discrepancies in coding.

**Table 3. List of Codes Developed to Classify Reasons Students Gave for Using or Not Using Metacognitive Strategies.**

| Themes | Codes | Descriptions |
|---|---|---|
| **Reasons for Using Strategies: The student uses this strategy because...** | | |
| Using strategy helps them solve the problem efficiently | Avoid wasting time/effort | It helps them avoid wasting time or effort during the problem-solving process. |
| | Get started/narrow focus | It helps them get started on the problem or narrow their focus to certain pathways. |
| | Builds confidence | It helps them feel more confident in their answer or thought process. |
| | Many reactions to consider | They recognize that a wide variety of reactions or types of reactivity exist and could possibly be relevant to the problem. |
| | Keeps them from forgetting | It helps prevent them from forgetting an idea or piece of information. |
| Using the strategy helps them solve the problem correctly | Keeps them on right track | It helps them stay on the right path and continue making progress toward an answer. |
| | Helps avoid mistakes | It helps them avoid making mistakes. |
| Someone encouraged use | Someone encouraged use | Another person, such as an instructor or tutor, encouraged them to use this skill. |
| Helps them learn/improve | Helps them learn/ improve | It helps them learn or improve their knowledge or problem-solving skills. |
| **Reasons for Not Using Strategies: The student does not use this strategy because...** | | |
| Using the strategy is detrimental to their success | Prevents success: distracting | It distracts them and they therefore consider it to be detrimental to their success in solving the problem. |
| | Prevents success: other | They consider it to be detrimental to their success in solving the problem for another reason, or they state that it is detrimental without stating a specific reason. |
| They are not able to use the strategy | Issues with timing | There is not typically enough time for them to use it. |

| | | |
|---|---|---|
| | Unable to use effectively | They believe they are unable to use the skill effectively, often because they do not feel experienced enough to do so. |
| Using the strategy is unnecessary | Unnecessary: have answer | They consider it to be unnecessary when they have already found an answer to the problem. |
| | Unnecessary: redundant | They consider it to be unnecessary because they either use a different strategy for the same purpose or use a similar strategy at a different time in the problem. |
| | Unnecessary: other | They consider it to be unnecessary for another reason, or they state that it is unnecessary without stating a specific reason. |

After coding was complete, the average number of strategies students were observed using and the number of strategies that they self-reported using on at least one of the interview problems was calculated for Organic Chemistry I students, Organic Chemistry II students, and graduate students. The number of strategies students were observed using was determined using the coding scheme, while the number of strategies they self-reported using was determined using the surveys students took after completing each problem. The average percent agreement between observed and self-reported use of metacognitive skills was then calculated for each of these groups. A percent agreement of zero would indicate that there was no overlap between the strategies that a student self-reported using and the strategies that they were observed using on a specific problem. Percentages of students who self-reported or were observed using a strategy on at least one of the interview problems were also calculated for each of these groups. The average number of strategies students self-reported or were observed using was also calculated for students who received a performance score of less than or equal to 60% on the interview problems and those who scored greater than 60% on the interview problems. T-tests were used to compare self-reported and observed strategy usage between these groups of higher and lower-performing students. IBM SPSS 27.0 was used for all statistical analysis. The number of times that students gave a certain reason for using or not using one of the 20 metacognitive strategies during the discussion portion of the interview was also determined.

## Results and Discussion

This study seeks to examine the behaviors related to metacognitive regulation that students exhibit when approaching complex, open-ended organic chemistry problems. We first discuss which metacognitive strategies were used by students with different levels of organic chemistry experience, based upon data from self-report instruments as well as observations of students' problem-solving processes during think-aloud interviews. As part of this analysis, we also consider the discrepancies between these two different measures of metacognitive skillfulness. We then describe how these students' use of metacognitive strategies relates to their success in problem solving by presenting both aggregate quantitative data and summaries of a selection of individual interview transcripts. After presenting the "what" and "how" of the metacognitive behaviors that students demonstrate when working on organic chemistry problems, we conclude with a discussion of students' reasoning behind using or not using these strategies.

*Research Question 1: What metacognitive strategies do undergraduate and graduate students use when solving organic chemistry problems?*

In our analysis, we were interested in determining which out of the list of twenty metacognitive strategies were used most and least frequently by students, and whether this varied between students with different levels of experience. Percentages of students who self-reported using or were observed using each of the listed metacognitive strategies are displayed in Table 4. Before commenting on discrepancies between these two measures of metacognition, we will discuss instances where these two measures were generally in agreement.

Some strategies were used by nearly every student, others were rarely used by any student, and others were used more often by more or less experienced students. Among undergraduates in either organic chemistry course and graduate students, more than 90% reported and were observed sorting through the problem statement to determine what was relevant, reflecting upon prior knowledge they had that was relevant to the problem at hand, and monitoring whether what they were doing was correct as they worked on the problem. On the other hand, fewer than 50% of students reported or were observed jotting down their ideas prior to starting the problem, summarizing the main takeaway lessons learned after finishing the problem, or considering ways they might change their approach for future problems. It may be that students view the initial planning strategies such as sorting through the problem statement or reflecting upon their prior knowledge as necessary for determining how to solve the problem at hand, while evaluation strategies related to learning from the experience of doing problems, such as summarizing main takeaway lessons or considering how they might change their approach for the future, are primarily useful for improving one's performance on future problems.

Strategies with differences in usage between groups of students included making predictions and setting goals before beginning the problem, which were both performed more often by graduate students according to both measures. Both of these strategies require a student to think multiple steps ahead before beginning to work on the problem, which is likely more difficult for the undergraduate students, who had less experience with solving organic chemistry problems. Organic Chemistry I students, who had the least experience with organic chemistry, were more likely than other students to take note of what they were uncertain about when solving the problem; 100% of these participants exhibited this behavior according to both self-report surveys and observations.

Comparing the individual metacognitive problem-solving strategies that participants in this study self-reported using to other studies that make use of metacognitive self-report instruments is difficult because most report only composite survey scores. However, several of the strategies interview participants were observed using have been reported in other studies of chemistry students' approaches to solving problems. For example, based on analyzing students' responses to organic chemistry synthesis problems on exams (Bodé and Flynn, 2016) and during think-aloud interviews (Webber and Flynn, 2018), Flynn and coworkers found that students wrote down functional groups and identified other relevant explicit and implicit features of the problem, attempted multiple solutions, and rejected certain proposed reaction pathways. These strategies correspond most closely to several planning and monitoring strategies commonly used by participants in the present study, namely the "Sort Relevant Info," "Reflect Relevant Knowledge," "Jot Down Ideas," "Brainstorm Multiple Ways" or "Consider Another Way," and "Consider If Plan Reasonable" or "Monitor Correctness" strategies. Students have been observed using similar strategies during think-aloud interviews involving organic chemistry mechanism and predict-the-product problems (DeCocq and Bhattacharyya, 2019) and molecular polarity or thermodynamics problems (Wang, 2015). A few other studies have also reported how often students used certain metacognitive strategies. In their study of students' approaches to open-ended chemistry problems, Overton et al. (2013) found that only 10 of 27 interview participants evaluated their answers; evaluation strategies were also used relatively infrequently among our sample.

Heidbrink and Weinrich (2021) found that 23 out of 25 interview participants exhibited monitoring strategies such as appraising one's work or one's thought process when solving buffer problems, while fewer (19 out of 25) used planning strategies like goal setting or allocating resources or evaluation strategies like reflecting on their answer or identifying areas where they struggled in solving the problem. The monitoring strategies exhibited by the students in Heidbrink and Weinrich's study mostly closely correspond with the "Monitor Correctness" strategy described in this work, which we also observed in nearly all of the think-aloud protocols (36 out of 38). In sum, while few prior studies have provided quantitative information on the proportion of students who use some of the individual metacognitive problem-solving strategies described in this work, our findings are generally consistent with the literature on problem solving in chemistry.

**Table 4. Percent of Interview Participants Who Used Listed Strategies While Solving At Least One Interview Problem, Grouped by Course. Increased Color Saturation Indicates a Larger Percentage.**

| Strategy | Percent Self-Reporting Use of Strategy | | | Percent Observed Using Strategy | | |
|---|---|---|---|---|---|---|
| | Organic I (*N*=10) | Organic II (*N*=16) | Graduates (*N*=12) | Organic I (*N*=10) | Organic II (*N*=16) | Graduates (*N*=12) |
| Set Goals | 80 | 69 | 92 | 10 | 13 | 33 |
| Sort Relevant Info | 90 | 94 | 100 | 100 | 100 | 100 |
| Look for Reactions Recognized | 100 | 94 | 100 | 60 | 31 | 75 |
| Reflect Relevant Knowledge | 100 | 100 | 100 | 100 | 94 | 100 |
| Relate to Previous Problems | 80 | 100 | 92 | 10 | 6 | 0 |
| Jot Down Ideas | 50 | 38 | 33 | 40 | 31 | 25 |
| Make Predictions | 70 | 63 | 100 | 60 | 50 | 83 |
| Brainstorm Multiple Ways | 60 | 38 | 50 | 60 | 69 | 75 |
| Consider If Plan Reasonable | 90 | 94 | 67 | 40 | 19 | 42 |
| Consider Another Way | 100 | 88 | 92 | 80 | 69 | 83 |
| Monitor Progress Toward Goals | 100 | 75 | 75 | 10 | 13 | 8 |
| Monitor Correctness | 100 | 94 | 100 | 90 | 94 | 100 |
| Note Uncertainty | 100 | 75 | 83 | 100 | 81 | 67 |
| Periodically Check If Reasonable | 90 | 69 | 75 | 40 | 50 | 33 |
| Consider If Answer Reasonable | 90 | 100 | 100 | 50 | 88 | 100 |
| Check If Answered Question | 100 | 88 | 100 | 10 | 31 | 17 |
| Check For Mistakes | 60 | 69 | 67 | 10 | 63 | 33 |
| Check If Agreed With Prediction | 80 | 44 | 75 | 0 | 6 | 0 |
| Summarize Main Takeaways | 40 | 19 | 25 | 0 | 0 | 8 |
| Consider Changes For Future | 50 | 31 | 33 | 0 | 0 | 0 |

Though some strategies were used approximately equally often according to both self-report and concurrent measures, there was in general a large discrepancy between the two measures. Table 5 summarizes the average number of strategies that Organic Chemistry I, Organic Chemistry II, and graduate students used during the interview according to both measures. On average, the number of strategies students reported using while solving either one of the interview problems was 66% greater than the number of strategies that they were observed using according to coding of their think-aloud interview transcripts. The average percent agreement between self-reported and observed usage of metacognitive regulatory strategies, which takes into account agreement between the two measures for each individual strategy, was 57%. Correlations between the two measures were weak and non-significant (first problem: $r = 0.15$, $p = 0.38$; second problem: $r = 0.19$, $p = 0.25$). This is consistent with the finding that self-reports tend to only weakly correlate with concurrent measurements of metacognitive behavior (Craig et al., 2020; Van Hout-Wolters, 2009). In a meta-analysis of studies assessing metacognitive skills, for example, Craig et al. (2020) found that analyzing 21 studies that correlated off-line and on-line measures of metacognition resulted in a pooled effect size estimate of 0.22. In the domain of chemical education, however, Wang (2015) observed stronger, significant correlations of 0.36 ($p < 0.05$) and 0.49 ($p < 0.01$) between a general self-report questionnaire and concurrent metacognition as measured using two different general chemistry think-aloud problem-solving tasks. When considering comparisons between task-specific questionnaires and think-aloud protocols more specifically, our observed correlations are on the low end compared to prior studies, in which correlations between these measures ranged from 0.10 to 0.63 (Craig et al., 2020; Van Hout-Wolters, 2009).

There are several possible reasons for the observed discrepancies between the two measures of metacognitive behavior. Students may have reported using a greater number of strategies than they actually used due to social desirability bias, which is the tendency of survey or interview respondents to give answers that they believe will be viewed favorably by others (Paulhus, 1991). The mismatch between self-reported and observed metacognitive strategy usage might also be partially attributed to the Dunning–Kruger effect, which describes the finding that poor performers tend to overestimate their competence, leading to inflated self-assessments (Dunning, 2011; Kruger and Dunning, 1999). Students' interpretation of the strategies described by the self-report items also may have differed from the definitions used by the researchers when coding the think-aloud protocols. Students were not asked to explain how they interpreted the items on the self-report measure used in this study, but studies on the response process validity of metacognitive self-report items in high school students have shown that some students find some items confusing or ambiguous, especially items related to planning skills (Berger and Karabenick, 2016) or items with more abstract terms or phrases such as "concepts," "drawing conclusions," or "finding information" (Schellings, 2011). It is also possible that some of the students' thought processes were not included in their verbalizations. This is more likely when processes are highly automated or when a task is particularly difficult or requires a lot of effort (Ericsson and Simon, 1993; Veenman, 2016). When working on more difficult tasks, like the problems students were asked to solve in this study, learners are more likely to occasionally fall silent instead of continuously verbalizing their thoughts (Ericsson and Simon, 1993). These occasional silences were observed in most of the interviews we conducted, despite urging students to continue verbalizing their thoughts. Students' use of metacognitive strategies may be overestimated by their responses to the self-report survey and underestimated by coding of their verbalized thought processes, which means that the true number of strategies they made use of while solving the interview problems is likely somewhere between the two values.

**Table 5. Comparison of Strategies (Mean ± SD) Students Self-Reported Using or Were Observed Using While Solving At Least One Interview Problem, Grouped by Course**

| Group of Students | *N* | # Strategies Used During Interview | | Self-Reported vs. Observed % Agreement |
|---|---|---|---|---|
| | | Self-Reported | Observed | |
| Organic I | 10 | 16.3 ± 1.5 | 8.7 ± 2.4 | 53.8 ± 14.3 |
| Organic II | 16 | 14.4 ± 2.9 | 9.1 ± 1.9 | 56.1 ± 9.7 |
| Graduates | 12 | 15.6 ± 1.4 | 9.8 ± 2.3 | 59.8 ± 6.7 |
| All Students | 38 | 15.3 ± 2.3 | 9.2 ± 2.2 | 56.7 ± 10.4 |

There were particularly low levels of agreement between the two measures for several of the individual metacognitive strategies. In each of these cases, many more students self-reported using these strategies than were observed using these strategies. For instance, the percentage of students who stated that, during the think-aloud portion of the interview, they had tried to relate an unfamiliar problem to previous problems they had encountered ranged from 80-100% depending on the course, but usage of this strategy was only detected in 0-10% of interview transcripts. This could be because students were more likely to verbalize that they were trying to relate a problem to previous problems they had encountered if they did in fact recall some similarity to a problem they had seen before. The use of the strategy itself may be less conscious, and it is only when using this strategy leads the student to notice something useful or unexpected that it surfaces in students' verbalizations. Veenman (2006) noted that "many evaluation and self-monitoring processes run in the 'background' of the cognitive processes that are being executed. Only after an error is detected, rightfully or not, the system becomes alerted" (Veenman et al., 2006, p. 6). This could also explain the large differences that were seen with the "check if answered question" (self-reported: 88-100%, observed: 10-31%), "check if agreed with prediction" (self-reported: 44-80%, observed: 0-6%), and "monitor progress toward goals" (self-reported: 75-100%, observed: 8-13%) strategies. Students may be more likely to verbalize thoughts related to these strategies if, in using these strategies, they notice a problem with their answer or their progress. If certain strategies were more difficult to discern from the think-aloud protocols than other strategies, this supports the importance of using multiple methods to determine which strategies students use during the problem-solving process.

*Research Question 2: How do students who are more and less successful at solving organic chemistry problems differ in their use of metacognitive regulatory strategies?*

We hypothesized that students who scored higher on an interview problem would tend to engage in more metacognitive behaviors during the process of solving that problem, as measured by the number of strategies they self-reported or were observed using. In order to test this hypothesis, we first had to evaluate the correctness of students' responses to each interview problem. Students' average scores on these problems are shown in Table 6. Within each group of students, paired t-tests showed no significant differences when comparing performance on Problem A with Problem B (Organic Chemistry I: $p = 0.53$), Problem C with Problem D (Organic Chemistry II: $p = 0.80$, graduate students: $p = 0.63$), or the first problem students completed with the second problem they completed (Organic Chemistry I: $p = 0.10$, Organic Chemistry II: $p = 0.61$, graduate students: $p = 0.63$). This demonstrates that the two problems each student completed were of similar difficulty and that the randomized order in which students completed the problems did not affect their performance. For this reason, rather than forming comparison groups for each individual problem, we chose to look at more and less successful solutions across all 76 problems solved by the 38 participants.

**Table 6. Performance Scores (% of Possible Points) on Think-Aloud Problems, Grouped by Course**

| Group of Students | *N* | Performance Score on Problems: Mean (SD) | | | | | |
|---|---|---|---|---|---|---|---|
| | | First Problem | Second Problem | Problem A | Problem B | Problem C | Problem D |
| Organic I | 10 | 50.0 (25.0) | 37.5 (16.7) | 46.3 (21.3) | 41.3 (22.9) | - | - |
| Organic II | 16 | 46.1 (20.3) | 49.2 (23.9) | - | - | 46.9 (21.2) | 48.4 (23.2) |
| Graduates | 12 | 81.3 (22.3) | 78.1 (29.3) | - | - | 78.1 (20.7) | 81.3 (30.4) |

Due to the difficulty of the problems, only 12 solutions were fully correct, and most of these solutions were generated by graduate students. Therefore, we chose to consider any solution that received a score greater than 60% to be “more successful,” which corresponded to 20%, 25%, and 83% of the solutions generated by Organic Chemistry I, Organic Chemistry II, and graduate students, respectively. The number of metacognitive strategies students used in the process of generating more and less successful solutions is displayed in Figure 4. When comparing all interview participants, those who generated more successful solutions self-reported using a significantly greater number of strategies related to metacognitive regulation than those who were less successful ($p = 0.003$, Cohen’s $d = 0.67$). Because the distribution of solutions that were considered more successful heavily favored graduate students, we also made comparisons that only considered undergraduate participants. Similar results were observed; undergraduates whose solutions were considered more successful self-reported using more metacognitive strategies while solving these problems ($p = 0.015$, Cohen’s $d = 0.83$). Among undergraduate participants and participants as whole, observed strategy usage trended in the same direction, but these differences were only approaching statistical significance ($p = 0.053$ and $p = 0.067$, respectively).

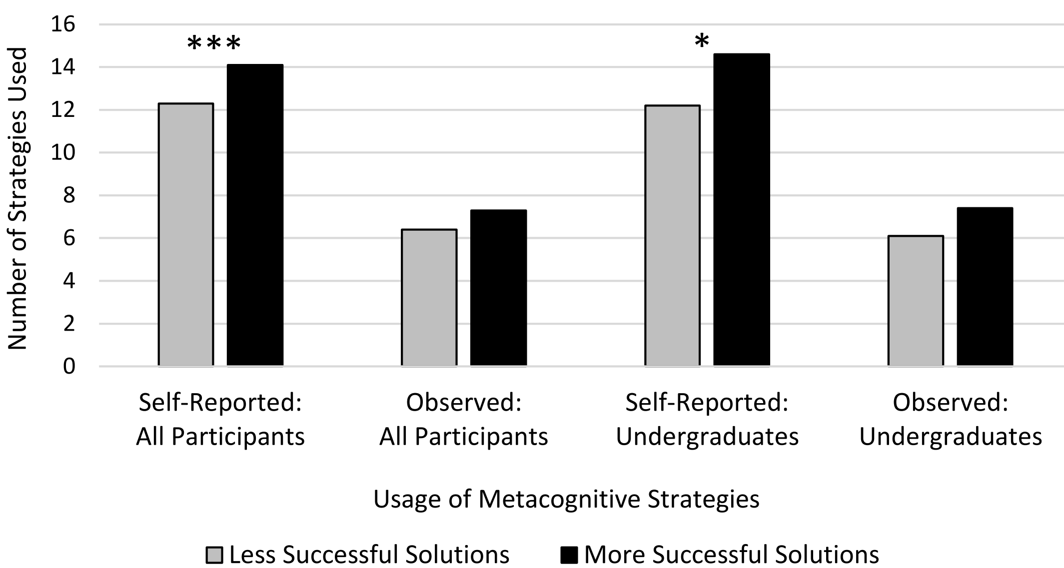

**Figure 4.** Metacognitive strategies used by participants during the process of generating more and less successful solutions (* $p < 0.05$, ** $p < 0.01$, *** $p < 0.005$). More successful solutions were defined as those receiving scores greater than 60%.

The finding that students who generated more successful solutions to organic chemistry problem-solving tasks also reported using a significantly greater number of strategies related to metacognitive regulation is consistent with our hypotheses as well as with previously published research conducted with general chemistry students. Prior research has shown that students who scored higher on measures designed to assess metacognitive strategy usage performed better on specific problem-solving tasks (Cooper et al., 2008; Wang, 2015). Specifically, in their study involving students enrolled in a general chemistry laboratory course, Cooper et al. (2008) found that students with a higher level of metacognition usage according to their scores on a concurrent measure scored significantly higher on a metacognitive self-report instrument and also showed a significantly higher ability to solve ill-defined problems. Wang (2015) observed significant positive correlations between students' performance on challenging problem-solving tasks related to thermodynamics and molecular polarity and their metacognitive regulation according to both a self-report questionnaire and analysis of think-aloud interview transcripts. These two studies are most directly comparable to our research methodology, as metacognition was assessed by both concurrent and self-report methods and performance was measured in terms of students' ability to solve relatively complex problems.

The positive relationship between metacognition and problem-solving success observed in our study can additionally be compared to studies that investigate connections between student metacognition and course grades, though it is important to consider that a student's ability to solve complex problems is one of many potential influences on their grade. González and Paoloni (2015) found correlations of 0.64, 0.67, and 0.68, respectively, between students' planning, monitoring, and evaluation scores on the Physics Metacognition Inventory and their final grades in introductory chemistry. Cooper and Sandi-Urena (2009) reported that students who received A grades in a general chemistry course scored significantly higher on the Metacognitive Activities Inventory (MCAI) compared to students who received lower grades in the course. Dianovsky and Wink (2012) observed a correlation of 0.56 between students' scores on the MCAI and their numerical grades in a general education chemistry course. Several studies have also linked interventions designed to promote metacognition to improved performance in general chemistry courses. Cook et al. (2013) found that general chemistry students who attended a 50-minute lecture on metacognitive learning strategies received an average final grade that was a full letter grade higher than those who did not attend this lecture. Casselman and Atwood (2017) reported that students who engaged in homework-based metacognitive training that involved predicting their scores on assignments and making study plans received higher scores on midterm and final exams than those who did not. Mutambuki et al. (2020) noted that students exposed to instruction on metacognitive learning and study strategies in combination with active learning scored significantly higher on the final exam than those who were exposed to active learning alone, with a mean difference of 5%. Using the same metacognitive instructional model described in Mutambuki et al. (2020), Muteti et al. (2021) found that students who reported that this metacognitive lesson had a positive impact on their study strategies were more likely to receive A/B grades and less likely to receive D/F grades on the final exam than students who reported no influence. Overall, the connection between metacognition and performance that we observed in organic chemistry students is consistent with numerous studies conducted with general chemistry students, which reinforces the importance of assessing and promoting metacognitive strategy use in chemistry courses across sub-disciplines.

Metacognition and Success: Individual Problem-Solving Cases

Thus far, we have presented aggregate data on the relationship between use of metacognitive regulatory strategies and task performance. To illustrate how metacognitive regulation can be connected to task performance in a more descriptive, qualitative manner, we have selected four individual problem-solving cases that serve as examples of more and less successful solutions for problems A-D generated by students who exhibited a larger or smaller number of metacognitive behaviors during the process of solving these problems. A summary of these four cases is provided in Table 7, and a chart that shows which strategies each student self-reported and was observed using is included in Appendix S6.

**Table 7. Summary of Four Students' Scores on Selected Interview Problems and their Use of Metacognitive Strategies During the Problem-Solving Process**

| Student Pseudonym | Problem Solved | Performance Score on Problem (% of Possible Points) | # of Strategies Used While Solving Problem | |
|---|---|---|---|---|
| | | | Self-Reported | Observed |
| Andrew | A | 38 | 10 | 4 |
| Lily | B | 50 | 18 | 11 |
| Ben | C | 75 | 14 | 4 |
| Marta | D | 100 | 15 | 10 |

Less Successful Solution, Fewer Metacognitive Strategies Used:

Andrew received a relatively low score (38%) on Problem A and also exhibited fewer metacognitive behaviors than average according to both self-reported and concurrent measures. Andrew began the problem by reading the directions aloud. He then stated that the first thing he was looking for was the reactive site, and he noted that there was an alkene and an epoxide present in the starting material (*Code: Sort Relevant Info*). He predicted that the epoxide "is what would be breaking in this example" (*Code: Make Predictions*). He identified that the "$H_2SO_4$" present in the reaction conditions was an acid, which would protonate the epoxide and cause the epoxide to break apart to form a tertiary carbocation at the more substituted position of the epoxide *(Code: Reflect Relevant Knowledge)*. He then stated that a water molecule would attack this carbocation, and that he was "pretty sure this is anti addition." After drawing his final products (shown in Figure 5), he looked back over what he had done to "make sure the stoichiometry and the equation is balanced" *(Code: Check for Mistakes)*. In addition to the behaviors that were observed in his transcript according to the coding scheme, Andrew also reported that he had set goals, looked for reactions he recognized, related the problem to a previous problem he'd encountered, considered if his proposed steps were reasonable, considered if his answer was reasonable, checked if he'd answered the question, and checked if his answer agreed with his prediction. Andrew's final answer was partially correct in that he performed the hydration of the epoxide with the correct regioselectivity. However, he did not propose any reaction involving the alkene, and he drew an additional unreasonable stereoisomeric product.

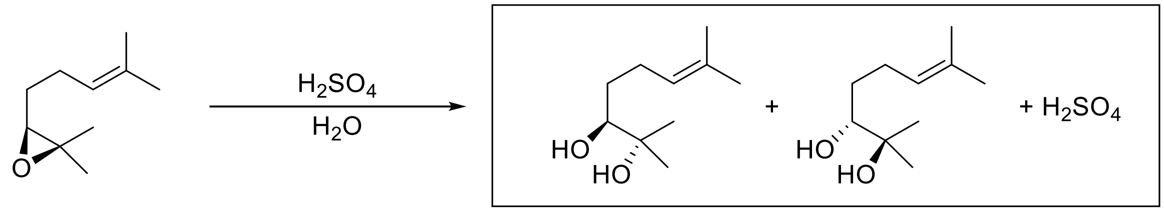

**Figure 5.** Final products proposed by Andrew for Problem A.

Less Successful Solution, More Metacognitive Strategies Used:

Lily received a score of 50% on her response to Problem B, which was categorized as "less successful," but she was above-average in terms of the number of metacognitive strategies she reported and was observed using while solving this problem. Lily started by reading the directions aloud and stating that she noticed there was a bromide present in the starting material, which she predicted would act as a leaving group at some point during the reaction (*Codes: Sort Relevant Info, Make Predictions*). Drawing on her knowledge of nucleophile strength and substitution reactions, she proposed that the potassium ethoxide would react with the alkyl bromide in an SN2 reaction *(Codes: Reflect Relevant Knowledge, Look for Reactions Recognized)*. After completing this SN2 reaction, she stated that she was now stuck because she didn't know what to do with the ethanol that was also present in the reaction conditions, and she wanted to use every listed reagent in the reactions she proposed *(Code: Note Uncertainty)*. She considered using the potassium ethoxide to deprotonate the ethanol, but she didn't think this made sense, and she questioned whether the SN2 reaction was the correct path *(Code: Monitoring Correctness)*. She considered carrying out an E2 reaction in step 1 instead, but realized that she had still not met her goal of using every listed reagent, since the ethanol did not participate in her proposed E2 reaction either (*Codes: Consider Another Way, Monitor Progress Toward Goals*). In the end, she returned to her initial proposed SN2 reaction because she thought she had seen potassium ethoxide act as a strong nucleophile more often than as a strong base.

Moving on to the second set of reagents, Lily proposed that the ethoxy group on her SN2 product could be protonated by the sulfuric acid because she had seen something similar happen in a previous problem, but she wasn't sure what to do after this protonation *(Code: Relate to Previous Problems)*. At this point, Lily went back over her previous work and again thought about whether her product for step 1 was reasonable *(Code: Periodically Check if Reasonable)*. Her conclusion was "I still think the final product of reaction one is not correct, but I have no other way. I need to base it on that to solve the next question." She then proposed a second SN2 reaction between methanol and the protonated ethoxy group of her intermediate product, and stated that the resulting final product (shown in Figure 6) "looks fine" and that there would be no further reactivity *(Code: Consider if Answer Reasonable)*. Other strategies that Lily reported using included setting goals, brainstorming multiple ways to approach the problem before she started working, considering whether her proposed steps were reasonable, checking if she had answered the question, checking for mistakes, checking that her answer agreed with what she had predicted, summarizing the main takeaway lesson, and considering how she could change her approach for the future. Lily's final answer received some partial credit because, though she had proposed SN2 reactions rather than the more favorable E2 and SN1/E1 reactions for each step of the problem, she carried out the reactions that she did propose with correct stereochemistry and regioselectivity.

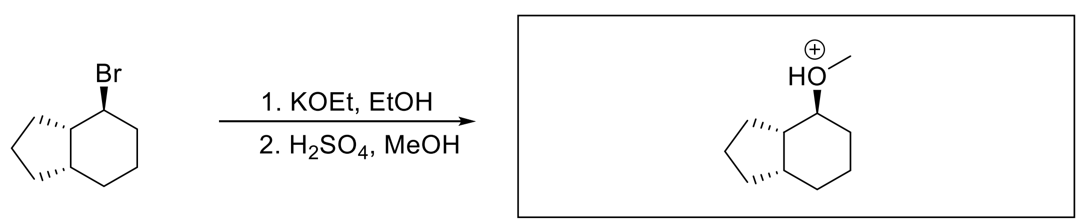


**Figure 6.** Final product proposed by Lily for Problem B.

More Successful Solution, Fewer Metacognitive Strategies Used:

Ben's solution to Problem C received a score of 75%, and was therefore categorized as "more successful." According to his response to the self-report survey, he used an approximately average number of metacognitive strategies, but the number of strategies he was observed using was below average. At the beginning of the problem-solving process, Ben noted that the conditions were acidic and that there were several sites on the starting materials that could potentially be protonated (*Code: Sort Relevant Info*). He considered protonating each of these sites *(Code: Brainstorm Multiple Ways)*. He then determined that protonation of the aldehyde would be the most productive option because he knew that the amine would most likely function as a nucleophile, and the aldehyde was the most electrophilic functional group present *(Code: Reflect Relevant Knowledge)*. Once he had decided on the nucleophile and electrophile, he drew out the mechanism for forming an imine from the aldehyde. After he reached this product (shown in Figure 7), he questioned whether the geometry of the imine was correct, but decided that the major product would be the one he had drawn and that he was done with the problem *(Consider if Answer Reasonable).* In addition to the behaviors that were observed in his transcript, Ben also reported that he had set goals, looked for reactions he recognized, related the problem to a previous problem he'd encountered, made predictions, considered if his proposed steps were reasonable, considered if there was another way to solve the problem, monitored his progress toward his goals, considered whether what he was doing was correct, noted what he was uncertain about, checked if he'd answered the question, and checked if his answer agreed with his prediction. Because Ben did form an imine by reacting the amine with the more reactive of the two carbonyls, did not make any stereochemical errors, and did not propose any additional unreasonable reactions, his answer was considered "more successful." He was not fully successful, however, because he did not consider whether any additional reactivity was possible after forming the imine, such as the Mannich reaction or an amine-catalyzed aldol reaction.

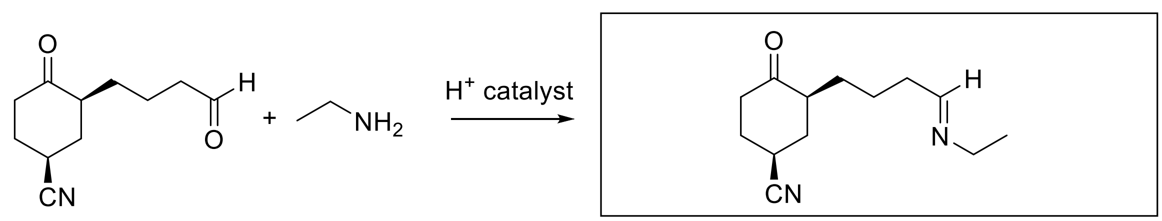


**Figure 7.** Final product proposed by Ben for Problem C.

More Successful Solution, More Metacognitive Strategies Used:

Marta received a score of 100% on Problem D, and she used an above-average number of metacognitive strategies according to both self-report and concurrent measures. Upon first seeing the problem, she noted the presence of a phosphorus ylide as well as the acidic conditions *(Code: Sort Relevant Info)*. She then predicted that the first step of the reaction would reveal a carbonyl, because she recalled she had typically seen this type of phosphonate reagent reacting with carbonyls (*Codes: Make Predictions, Reflect Relevant Knowledge*). She stated that she was not sure which acetal oxygen she should protonate first, but she decided to choose the one in the ring, keeping in mind that she could try the oxygen that was part of the isopropoxy group as well if her first idea did not work *(Code: Brainstorm Multiple Ways)*. As she worked on cleaving the acetal, she recalled that she would need to indicate stereochemistry in her answer, so she made sure that she had considered this while drawing intermediate structures *(Code: Monitor Progress Toward Goals)*. Once she generated the correct aldehyde product of step 1, she looked back over her work to consider whether what she had done was reasonable and then decided to go back to the beginning and try protonating the isopropoxy group first instead *(Codes: Periodically Check if Reasonable, Consider Another Way)*. She erroneously determined that this path was incorrect and would not lead to the desired carbonyl product *(Code: Monitor Correctness)*.

Marta then continued on to the second step of the reaction. As she drew out the mechanism for the HWE reaction, she stated that she was not sure about one step of the mechanism and would want to look it up if she had access to an answer key *(Code: Note Uncertainty).* After she reached her final answer (shown in Figure 8), she repeatedly counted the atoms present in her answer and in her intermediates to make sure she had drawn the product correctly *(Code: Check for Mistakes)*. Marta also reported that she had set goals, looked for reactions she recognized, related the problem to a previous problem she'd encountered, considered if her proposed steps were reasonable, considered if her answer was reasonable, checked if she'd answered the question, and checked if her answer agreed with her prediction. Marta's answer was fully correct and was considered "more successful."

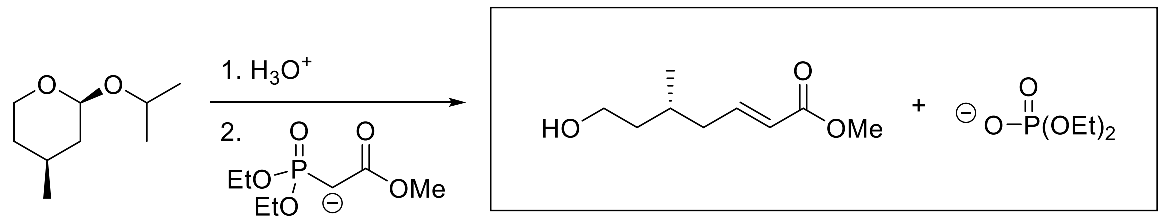


**Figure 8.** Final products proposed by Marta for Problem D.

Considering the interview participants as a group, students who generated more successful solutions tended to use a greater number of metacognitive regulatory strategies. From our analysis of the individual problem-solving pathways of Andrew, Lily, Ben, and Marta, however, it is clear that the relationship between metacognition and problem-solving success is more nuanced. Andrew and Ben both used a below-average number of metacognitive strategies in their approach to Problems A and C, respectively. Neither student received full points for their solutions because, after identifying a reasonable starting point with the use of planning strategies, they did not consider the potential for further reactivity. Had these students engaged in monitoring strategies such as pausing to consider whether there was another way to solve the problem, they may have received higher scores. Andrew's solution to Problem A received a lower performance score than Ben's solution to Problem C and was ultimately categorized as less successful because Andrew's solution contained stereochemical errors that point to a gap in his understanding of this concept. This difference in task performance between students with a similar level of metacognitive strategy usage was also seen when comparing the approaches of Lily and Marta. Lily and Marta both displayed an above-average number of metacognitive behaviors, yet Marta's solution to Problem D received full points, while Lily's solution to Problem B was considered less successful. Based on her verbalized thoughts, Lily seemed to be unsure about the role of the solvent and the favorability of different substitution or elimination reactions under the given reaction conditions, which led her to struggle to generate a reasonable solution. However, Lily's use of planning and monitoring strategies did help her to identify, consider, and dismiss several potential types of reactivity. Overall, these four cases suggest that when solving complex organic chemistry problems, a solid foundation of conceptual knowledge and metacognitive problem-solving skills can both be major contributors to success.

*Research Question 3: What reasons do students have for using or not using metacognitive strategies while solving organic chemistry problems?*

Based on data from self-report surveys and think-aloud interview coding, it is clear that some of the listed metacognitive strategies were used by the vast majority of interview participants, while others were hardly used by any. We believed that each of these strategies could be helpful for students to use while solving organic chemistry problems and were therefore interested in learning why students used certain strategies but chose not to use others. Understanding how and why students find certain strategies useful when solving problems could help instructors teach and encourage these behaviors in their own students. During the interviews, students were asked about their reasons for using or not using certain metacognitive strategies, either on the problem they had just worked on during the interview or in their organic chemistry course in general. A summary of how often each of the types of reasoning included in our coding scheme came up in reference to strategies classified as planning, monitoring, and evaluation skills is displayed in Table 8. A complete listing of what reasons students gave for using or not using each individual strategy is included in Appendix S7.

**Table 8. Frequencies with which Interview Participants Gave Certain Reasons for Using or Not Using Planning, Monitoring, and Evaluation Strategies. Increased Color Saturation Indicates Higher Frequency.**

| Themes | Codes | Type of Strategy | | |
|---|---|---|---|---|
| | | Planning | Monitoring | Evaluation |
| **Reasons for Using Strategies** | | | | |
| Using strategy helps them solve the problem efficiently | Avoid wasting time/effort | 8 | 12 | 2 |
| | Get started/narrow focus | 57 | 1 | 0 |
| | Builds confidence | 6 | 1 | 2 |
| | Many reactions to consider | 9 | 4 | 0 |
| | Keeps them from forgetting | 9 | 3 | 2 |
| Using strategy helps them solve the problem correctly | Keeps them on right track | 9 | 19 | 0 |
| | Helps avoid mistakes | 9 | 19 | 33 |
| Someone encouraged use | Someone encouraged use | 17 | 0 | 5 |
| Helps them learn/improve | Helps them learn/improve | 7 | 6 | 17 |
| **Reasons for Not Using Strategies** | | | | |
| Using strategy is detrimental to success | Prevents success – distracting | 13 | 8 | 0 |
| | Prevents success – other | 8 | 3 | 0 |
| They are not able to use the strategy | Issues with timing | 23 | 13 | 30 |
| | Unable to use effectively | 29 | 8 | 16 |
| Using the strategy is unnecessary | Unnecessary – have answer | 7 | 4 | 14 |
| | Unnecessary – redundant | 4 | 6 | 9 |
| | Unnecessary – other | 27 | 10 | 19 |

<u>Students used certain metacognitive strategies because this helped them solve the problem efficiently.</u>

Several of the reasons students stated for using metacognitive strategies related to their desire to approach problems in an efficient manner. Students very commonly mentioned that they used planning strategies such as sorting through the information in the problem statement and looking for reactions they recognized because this helped them find a starting point or narrow their focus to a more manageable set of potential reactions to consider. One participant remarked that they sorted through the information in the problem statement to determine what was relevant because it was “the best way to figure out what are the nucleophiles, what are the electrophiles, good leaving groups, acidic protons or basic sites. And then usually if there's a pair like a good nucleophile and electrophile like we had here, that would dictate a good starting point. And then I can maybe figure things out from there.” Students used other planning strategies such as jotting down their ideas and monitoring strategies like taking note of anything they were uncertain about because they didn’t want to lose their train of thought or forget something important as they were working through the problem. Several students also stated that they used metacognitive strategies because they wanted to avoid wasting time or effort while working on problems. Typically, students mentioned this reasoning when justifying their use of monitoring strategies such as pausing to consider whether they were making progress towards their goals or whether what they were doing was correct.

<u>Students used certain metacognitive strategies because this helped them solve the problem correctly.</u>

Other reasons students gave for using metacognitive strategies were more linked to wanting to solve problems correctly. Students stated that they used monitoring and evaluation strategies like considering whether their approach was correct, periodically checking if their overall approach was reasonable, or checking if they actually answered the question because they wanted to avoid making mistakes or they wanted to make sure that they stayed on the right track throughout the problem-solving process. For instance, a student said that they periodically checked if their overall approach was reasonable because it helped with “making sure you going down the right path, making sure you're getting the right steps.” A few students additionally brought up that now they always make sure to check for mistakes or make sure their answer actually answered the question because they learned from past experiences in the course that if they didn’t check their answers, they’d get lower grades on assignments: “I've lost so many dumb points [on graded assignments] for not [making sure my solution actually answered the question]. If I'm being perfectly honest, I'll get through it and I'll miss one little thing at the end and I won't completely answer it. I've done it enough that I have to be super on myself to do that.”

<u>Students used certain metacognitive strategies at the encouragement of someone else.</u>

Some students mentioned that they used certain strategies because another person, often an instructor or tutor, had suggested that they use this strategy. This usually came up in reference to planning strategies such as setting goals and sorting through information in the problem statement. For example, one student stated: “I definitely always look at what bond I need to make and what functional group I need to make if there is a product written out for me, because not only [my professor], but also my [graduate teaching assistant] reiterated that a lot.”

<u>Students used certain metacognitive strategies because this helped them learn or improve.</u>

Students reported using some strategies, particularly evaluation strategies such as summarizing main takeaway lessons or considering changes they could make to their problem-solving approach, because using these strategies helped them learn or would help them become better at solving problems. For instance, when explaining why they summarized the main takeaway lessons after finishing a problem, a student stated “I thought it was important for me to summarize what did I learn from the solution...because that'll help me in the future when I encounter this type of problem.”

Students decided not to use certain metacognitive strategies because they thought it was unnecessary.

The most common reason students gave for not using a strategy was that they thought it wasn't necessary. This type of reasoning was used particularly often when students explained why they didn't jot down their ideas before they started working on a problem or summarize the main takeaway lessons after finishing a problem. Sometimes, this was because the student had already found an answer at the point they would have used the strategy, and after finding an answer they just wanted to move on to the next problem. Students also considered the use of some strategies to be unnecessary and redundant because they preferred to use another strategy for a similar purpose. For example, several students either stated that they didn't pause to consider whether what they were doing was correct or whether their approach was reasonable while working on the problem because they preferred to wait until after they had reached an answer to check their work, or that they didn't check their work after solving the problem because they had already done so repeatedly while solving the problem.

Students reported that they were unable to use certain strategies.

Students also mentioned that they were unable to use some strategies, especially evaluation strategies that would be used at the end of the problem-solving process such as checking for mistakes, because they typically did not have enough time or they thought that using the strategy would take too much time. Some students stated that they didn't use certain strategies, particularly planning skills such as setting goals and making predictions, because they did not feel that they were experienced enough with organic chemistry to be able to use the strategy effectively.

Students believed using certain strategies would be detrimental to their success.

A smaller number of students believed that using particular strategies was not just unnecessary or unfeasible; these students believed using these strategies would actively prevent them from successfully solving the problem, often because they deemed their use to be distracting. For example, some students mentioned that they didn't set goals before they started working on the problem because this could close their mind to other possibilities: "I think [setting a goal] just locks me in and keeps me focused on making that thing...since it's a predict the major product I feel starting from the end and going backwards would limit me and kind of blindfold me to think about one thing and not consider the other possibilities." Others mentioned that they didn't jot down their ideas or pause to consider whether there was another way to solve a problem because they found these strategies to be too distracting.

The reasons students gave for using metacognitive planning, monitoring, and evaluation strategies mostly aligned with our expectations and showed that students used these strategies for their intended purposes. As expected, students generally used planning strategies to help identify and explore possible options, monitoring strategies to keep them on track and avoid making mistakes or wasting time or effort, and evaluation strategies to assess the merits of their answer and approach as well as to learn from their experience of solving the problem. Though we are not able to compare our findings to any existing studies on student reasons for using metacognitive strategies in the context of problem solving, students have been found to give similar reasons for using or not using metacognitive strategies while reading academic texts (Andriani and Mbato, 2021; Thuy, 2020). One interesting observation is that many students mentioned being encouraged by their instructors or tutors to use certain planning strategies, but this reasoning was mentioned less often in regard to monitoring or evaluation strategies. If instructors typically concentrate on teaching planning strategies, it would be useful to additionally introduce and model the use of various monitoring and evaluation strategies during class. Students' reasons against using metacognitive strategies, especially those related to feeling unable to use certain strategies effectively, point towards opportunities for instructors to provide students with additional guidance and support in implementing these strategies. It is important to note that our goal in advocating that instructors teach students about metacognitive regulation is not for students to use every strategy listed in Table 2 when working on every organic chemistry problem they encounter. Students may rightfully not find some strategies useful in every situation, especially for more straightforward problem-solving tasks. Instead, we believe it is beneficial to introduce these skills and give students the tools to use them when needed.

## Limitations

There are several limitations associated with this study. Any student who responded to the recruitment announcements was invited to participate in this study, which introduces the risk of self-selection bias. As shown in Figure 1, the majority of the undergraduate study participants received final grades that were at least half of a standard deviation above the mean in their organic chemistry course. Understandably, it appears that students who were not performing as well in these organic chemistry courses were not as likely to volunteer to be observed while working on organic chemistry problems. Several factors also affect the generalizability of the outcomes of this study. Because the number of participants was relatively small, the results of this study should be interpreted from a primarily qualitative perspective, and statistical results should be interpreted with caution. This study was also focused on students' use of metacognitive strategies when approaching a specific type of organic chemistry problem. The problems that students were asked to solve were all relatively complex predict-the-product problems. It is likely that students' use of metacognitive strategies would differ for more straightforward exercises or for problems related to proposing mechanisms or syntheses.

Lastly, it is important to consider how our positionalities as instructors, researchers, and students influenced our analysis and interpretation of the data collected in this investigation. At the time this work was conducted, the first and fifth authors were doctoral students studying organic chemistry and chemical education at the same institution as the interview participants. The second, third, and fourth authors are current or former undergraduate students who had recently taken organic chemistry courses at this institution. The corresponding author is a professor who has taught organic chemistry courses at this institution for over a decade. Though none of the authors have taught or taken organic chemistry courses with any of the study participants, each author is either a product of or is involved in the teaching of the organic chemistry curriculum at this institution. Each of us is therefore experienced with solving organic chemistry problems similar to those investigated in this study, and we all have our own ideas about what metacognitive strategies work well for us or our students and why we choose to use or not use certain strategies. These personal experiences may have influenced our interpretation and understanding of students' words and actions while coding the interview transcripts. For example, a researcher may have more readily noted a student's usage of strategies that more closely matched their own problem-solving approaches. To mitigate potential bias and ensure that both student and instructor perspectives were taken into account, each interview was coded by at least one member of the research team who had recently taken an organic chemistry course and one who had recently taught an organic chemistry course, and any differences in interpretation were discussed until agreement was reached.

## Conclusions and Implications

The goal of this study was to investigate the behaviors related to metacognitive regulation that students engage in when approaching difficult organic chemistry predict-the-product problems. Very few studies have focused specifically on metacognition in students' approaches to solving organic chemistry problems, which involve very different skills than the more quantitative problems typically encountered in general chemistry courses. We therefore sought to link the existing literature on problem solving in organic chemistry and metacognition by providing a thorough description of metacognitive regulation in the context of solving complex organic chemistry problems. This analysis includes not only what students say they do, but also what we've observed them doing and what their reasons are for doing what they're doing.

Our analysis focused on three main research questions. First, what metacognitive strategies do students use when solving complex predict-the-product problems? Analysis of think-aloud problem-solving interviews and task-specific self-report questionnaires led us to conclude that the strategies most commonly used by students were those related to identifying relevant information, recalling prior knowledge, and monitoring or evaluating the correctness of one's progress or products, whereas far fewer students engaged in evaluation strategies that involved reflecting and learning from the experience of problem solving. When comparing the approaches of graduate and undergraduate students, one trend we observed was the higher prevalence of forward-thinking strategies, including setting goals and making predictions at the beginning of the problem, among graduate students. When examining students' use of metacognitive regulation strategies measured concurrently during think-aloud interviews as compared to their self-reported use of these same strategies, significant discrepancies between these two measures were found. Our second research question asked whether students who are more and less successful at solving organic chemistry problems differ in their use of metacognitive regulatory strategies. We found that students who generated more successful solutions self-reported using a significantly greater number of metacognitive strategies during the problem-solving process, and comparisons of observed strategy usage trended in the same direction. Analyzing individual examples of student problem-solving pathways showed that, while the use of a greater number of metacognitive strategies does not always lead to greater success on non-trivial organic chemistry problems, using these strategies can help students generate possible ideas, ensure that they are making progress in the right direction, and determine whether their answer is reasonable and complete. Our final question involved the reasons students have for using or not using metacognitive strategies. Students stated that they found many of the strategies described herein to be useful for helping narrow down options, avoid mistakes, and keep themselves on track during the process of problem solving. Yet students also had several reasons for not using these strategies, such as believing that using a strategy was unnecessary or distracting or that they were not capable of using the strategy effectively. Each of these findings suggests specific implications for research and practice.

When considering implications for research, the significant discrepancy observed between concurrent and self-report measures emphasizes the importance of using multiple measures to detect metacognitive regulation in students, as the use of a single measure may result in an incomplete understanding of students' cognitive processes related to this complex construct. The reasons for the observed discrepancies are not entirely clear; however, possible factors include social desirability bias (Paulhus, 1991), differences in students interpretation of the strategies described by the self-report items compared to the definitions used by the researchers when coding the think-aloud protocols, or a lack of inclusion of some of student's more automated cognitive processes in their think-aloud interview verbalizations (Ericsson and Simon, 1993). We suggest that future studies that rely upon self-report assessments of metacognitive regulation could make use of cognitive interviews where students are asked to explain their thought process as they answer each item of the questionnaire (Berger and Karabenick, 2016; Schellings, 2011). Analysis of these interviews could help explain the reasons for any disagreement between self-reported and observed metacognition as well as point to ways in which survey items or coding definitions could be modified to better assess strategy usage in students.

There are several teaching strategies instructors can use to enhance students' use of metacognitive regulation strategies. Instructors of introductory organic chemistry courses could introduce metacognitive strategies by modeling the use of planning, monitoring, and evaluation strategies while explaining their thought process as they go over example problems during class. Rather than only presenting polished, linear solutions, instructors could also showcase the false starts and dead ends involved in real problem solving as well as how to recover from them. For example, when presenting a solution to a problem, the instructor could begin by setting goals, making predictions, and brainstorming potential approaches, either on their own or with input from the class. As they work through the problem, they could pause to ask themselves or their students whether they are making progress towards their goals. If they determine that they are not in fact making progress, they could backtrack and try another method. After reaching an answer, they could model the use of evaluation strategies such as checking for mistakes or checking whether their answer agreed with their prediction. Instructors could also give students opportunities to practice using metacognitive strategies with the help of problem-solving workflows. Examples of problem-solving scaffolds that could promote discipline-specific metacognition in students include the "Goldilocks Help" workflow, developed by Yuriev et al. (2017) in order to scaffold the development of metacognitive self-regulation and problem-solving skills in general and physical chemistry courses, and a problem-solving workflow designed for predicting organic reactivity that was developed by our research group (Helix et al., 2022). Instructors could also provide students with an opportunity to practice using these strategies on scaffolded homework or in-class assignments that include explicit prompts that would, for example, ask students to write down goals or predictions before solving a problem or to write down "main take-away lessons" after completing a problem. Students' prior experiences with using metacognitive strategies and their memories of their past successes and failures influence their subsequent metacognitive and self-regulatory strategy choices (Finn, 2020), so having the opportunity to practice using these strategies with the help of problem-solving workflows or scaffolded assignments could enable students to feel more confident in their ability to use these strategies effectively, including in situations where they are constrained for time.

Drawing on these suggested teaching methods, we have recently piloted a series of problem-solving workshops with a small number of organic chemistry students at our institution based on the results of this investigation. According to Arslantas et al. (2018), metacognitive instruction should include "explicit instruction, modeling, integration of metacognitive skills with course content, and opportunities for practice and reflection" (Arslantas et al., 2018, p. 59). These workshops therefore begin with explicit instruction on metacognition and its importance, drawing on data collected during this study on the reasons students use certain strategies. This is followed by instructor modeling of strategies that we identified as particularly underused among undergraduate students, such as making predictions or summarizing main takeaway lessons. Students then complete scaffolded worksheets in which they are asked to write down their answers to prompts related to these strategies before, during, and after working on organic chemistry problems. Preliminary data suggests that these workshops were helpful to students, though additional research is needed to determine their efficacy in a larger classroom setting.

## Conflicts of Interest

There are no conflicts to declare.

## Acknowledgements

K.A.B. would like to thank the NSF for a graduate research fellowship (NSF-GRFP 2018241803) as well as the UC Berkeley College of Chemistry for additional research funding. We additionally appreciate the contributions of Zachary Firestein and Katarina Gibson during the pilot stage of this work. Finally, we would like to thank the participants of this study for their willingness to share their valuable time.

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# Electronic Supplementary Material (ESI) for:

# Metacognitive Regulation in Organic Chemistry Students: How and Why Students Use Metacognitive Strategies When Predicting Reactivity

Authors: Katherine A. Blackford, Julia C. Greenbaum, Nikita S. Redkar, Nelson T. Gaillard, Max R. Helix, Anne M. Baranger

## Appendix S1: Interview Protocol

**Introduction and Background Questions:**
Thanks so much for coming, I really appreciate your help. First, I just want to start off with a couple background questions and some general questions about your experience with organic chemistry.

Undergraduates:
1. What organic chemistry courses have you taken so far?
2. What is your year in school and intended major?

Graduate Students:
1. What year are you in your program?
2. Which research group are you in?
    - How long have you been working with them?
    - Can you briefly (~1-2 min) describe your project?
3. Have you taken any organic courses in graduate school?
    - If yes, what were they?
    - If no, when was the last organic course you took?
4. Have you taught any organic chemistry courses?
    - If yes, what were they?

**Instructions for Think-Aloud Portion:**
Part of what I'm trying to study is the detailed thought processes that go on in people's minds while they are working on solving typical organic chemistry problems. What I'm going to have you do is work through a predict-the-product organic problem, and I want you to vocalize your thoughts as you have them, to the best of your ability.

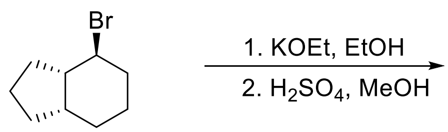
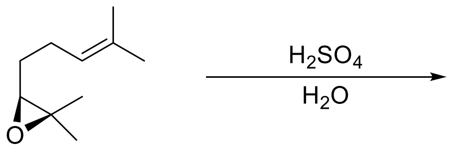
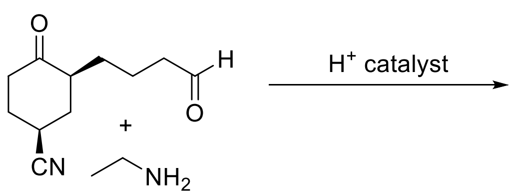
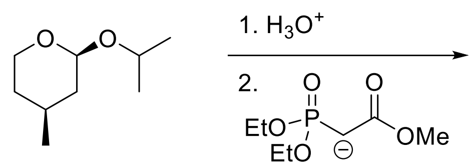
You are not being evaluated on whether you get the "right" answer – there might not even be one specific "right" answer. Mainly what I'm hoping to get insight into is how people end up at a variety of answers, what the thought processes are that lead to those answers, and what kinds of things people are considering that don't make it onto the page or into their "final answer."

Do you have any questions for me?

Please vocalize your thoughts as you have them, and let me know when you have finished working on the problem. If you are completely unsure and don't have thoughts on how to proceed further, just give me your best guess. We're trying to get at the best approximation of the thoughts you'd have if you were sitting alone, working on this problem without any cameras. Please try to keep talking, even if your thoughts aren't fully formed yet.

**First Think-Aloud Problem:**

*Each student works on two problems over the course of the interview. They work on the first problem before the discussion portion of the interview. The order of the problems is chosen randomly prior to the interview.*

| Problems Completed by Organic Chemistry I Students | |
|---|---|
|  |  |
| **Problems Completed by Organic Chemistry II Students and Graduate Students** | |
|  |  |

**Survey Completed After the Student Finishes the First Problem:**

Great job! The next thing I'd like you to do is fill out this short survey. After you've filled out the survey, we'll discuss your answers and then talk more about how you approach organic chemistry problems.

*The student is sent a link to a survey hosted on Qualtrics. Once they finish it, they engage in a guided discussion about their problem-solving strategies.*

**Discussion Questions:**

- There are many different strategies mentioned on this survey.
  - Can you explain why you do use [strategies the student said they used often]?
  - Can you explain why you don't use [strategies the student said they did not often use]?
- Are there some strategies you use all the time, and some you only use when you're having trouble with a problem?
- What is your strategy when solving a problem on an exam?
- Would your strategy change at all if it was a problem on a homework assignment?
- Does time pressure lead you to change your strategy? What about access to notes?
- How did you come to use the strategies you use?

**Second Think-Aloud Problem and Accompanying Survey:**

*The student completes a second problem while vocalizing their thoughts. After they finish, the student is sent a link to a second survey hosted on Qualtrics.*

Thank you so much for completing that survey and for participating in this interview. Please let me know if you have any questions for me before we end the interview.

## Appendix S2: Survey Taken on Qualtrics after Interview Problems

*Notes:*

- *The answer choices were the same for each question in Part 1. For brevity, these answer choices are only displayed for the first item in this Appendix.*
- *After the first interview problem, students completed both Part 1 and Part 2. After the second interview problem, students completed only Part 2.*

**Part 1:** Please indicate how frequently you used the following strategies when solving organic chemistry problems on homework and on exams for the most recent course you have taken that was related to organic chemistry. Choose the option that best represents your actual behavior when solving problems, not what your behavior would have ideally been if you had more time, had studied more, etc.

1. I set goals (ex. "I need to make this bond," or "I want to make this functional group") before attempting a solution.

| | Always | Most of the time | Sometimes | Rarely or Never |
|---|---|---|---|---|
| While working on homework | ○ | ○ | ○ | ○ |
| While working on exams | ○ | ○ | ○ | ○ |

2. Before I start working on a problem, I sort through the information in the problem to determine what is relevant.
3. Before I start working on a problem, I look for any reactions I recognize.
4. I reflect upon things I know that are relevant to a problem before I start working.
5. I try to relate unfamiliar problems with previous problems I've encountered.
6. I jot down my ideas or things I know that are related to the problem before attempting a solution.
7. I make predictions about what will happen before I start working on a problem.
8. I brainstorm multiple ways to solve a problem before I actually start solving it.
9. I consider whether my proposed steps are reasonable before I actually start solving a problem.
10. When I'm the middle of working on a problem, I pause to consider whether there is another way to solve it.
11. While I'm working on a problem, I pause to consider whether I am making progress towards my goals.
12. I pause to consider whether what I am doing is correct while I'm working on a problem.
13. I take note of what I am uncertain about as I work on a problem.
14. As I work on a problem, I periodically check back over what I have done so far to make sure my overall approach is reasonable.
15. I think about whether my answer is reasonable after I finish a problem.
16. I make sure that my solution actually answers the question.
17. I check back over my work once I finish a problem to make sure I didn’t make any mistakes.
18. Once I reach an answer, I check to see that it agrees with what I predicted.
19. Once I finish a problem, I summarize the main take-away lesson I have learned.
20. After I finish a problem, I consider how I might change my approach for future problems.

**Part 2:** Please indicate whether you used these strategies when working on the interview problem.

| | Yes | No |
|---|---|---|
| I set goals (ex. "I need to make this bond," or "I want to make this functional group") before attempting a solution. | ○ | ○ |
| Before I started working, I sorted through the information in the problem to determine what is relevant. | ○ | ○ |
| Before I started working, I looked for any reactions I recognized. | ○ | ○ |
| I reflected upon things I know that are relevant to the problem before I started working. | ○ | ○ |
| I tried to relate unfamiliar problems with previous problems I've encountered. | ○ | ○ |
| I jotted down my ideas or things I know that are related to the problem before attempting a solution. | ○ | ○ |
| I made predictions about what would happen before I started working on the problem. | ○ | ○ |
| I brainstormed multiple ways to solve a problem before I actually started solving it. | ○ | ○ |
| I considered whether my proposed steps were reasonable before I actually started solving the problem. | ○ | ○ |
| When I was in the middle of working on the problem, I paused to consider whether there was another way to solve it. | ○ | ○ |
| While I was working on the problem, I paused to consider whether I was making progress towards my goals. | ○ | ○ |
| I paused to consider whether what I was doing was correct while I was working on the problem. | ○ | ○ |
| I took note of what I was uncertain about as I worked on the problem. | ○ | ○ |
| As I worked on the problem, I periodically checked back over what I had done so far to make sure my overall approach was reasonable. | ○ | ○ |
| I thought about whether my answer was reasonable after I finished the problem. | ○ | ○ |
| I made sure that my solution actually answered the question. | ○ | ○ |
| I checked back over my work after I finished the problem to make sure I didn’t make any mistakes. | ○ | ○ |
| Once I reached an answer, I checked to see that it agreed with what I predicted. | ○ | ○ |
| Once I finished the problem, I summarized the main take-away lesson I learned. | ○ | ○ |
| After I finished the problem, I considered how I might change my approach for future problems. | ○ | ○ |

Appendix S3: Metacognitive Strategies Coding Scheme

General Notes on Usage of Planning, Monitoring, and Evaluation Codes:

- Planning Codes: These should only be assigned before the student draws their first new chemical structure. If the problem consists of multiple steps, planning codes can also be assigned when the student begins talking about the second step of the reaction.
- Monitoring Codes: These should only be assigned after the student has started drawing their first new chemical structure, but has not yet reached an answer.
- Evaluation Codes: These should only be assigned after the student has reached their final answer, or what they initially stated was their answer if they then changed their mind about their answer.

| Code | Description | Example(s) |
|---|---|---|
| Set Goals | *"I set goals (ex. "I need to make this bond" or "I want to make this functional group") before attempting a solution."*<br>The student states something they want or think they'll need to do to answer the question. | • "So somehow... I guess I have to make that into a carbonyl"<br>• "I have to figure out where it would attack and why this acid would make it attack there." |
| Sort Relevant Info | *"Before I started working on the problem, I sorted through the information in the problem to determine what was relevant."*<br>The student verbally identifies, highlights, or circles instructions, reagents, functional groups, etc. that they notice in the problem statement. | • "Ok so I see a lot of carbons here"<br>• "I see a double bond"<br>• *Student circles aldehyde*<br>• *Student highlights "stereochemistry" in problem statement* |
| Look for Reactions Recognized | *"Before I start working on a problem, I look for any reactions I recognize."*<br>The student identifies or states that they are looking for known reactions. | • "This is kind of like a Wittig"<br>• "The first thing I would say...is does it look like anything I'm immediately familiar with, anything I know how to do without working it out." |
| Reflect Relevant Knowledge | *"I reflected upon things I know that are relevant to the problem before I started working."*<br>The student states what they know about reactions or structural features they've identified in the problem. | • "The Wittig-type would give the double bond here"<br>• "I know oxygen is a pretty good nucleophile"<br>• "We learned this is the trans" |
| Relate to Previous Problems | *"I tried to relate unfamiliar problems with previous problems I've encountered"*<br>The student refers back to a problem they had previously solved and compares it to the problem they are currently working on. | • "My first prediction is that this oxygen right here is going to get a hydrogen from the sulfate. And why I did that is because I think I've seen this in a past question." |
| Make Predictions | *"I made predictions about what would happen before I started working on the problem."*<br>The student makes a prediction about what reactivity will occur beginning from the starting material (or an intermediate product in the case of a multi-step reaction). | • "This presumably would hydrolyze the acetal to get back to either a hemiacetal or an aldehyde"<br>• "You're probably making an alkene"<br>• "First this will make an imine" |

| | | |
|---|---|---|
| Jot Down Ideas | *"I jotted down my ideas or things I know that are related to the problem before attempting a solution."*<br>At the beginning of the problem, the student writes downs things they know or adds other written annotations to the problem. | • *Student writes "strong acid" beside $H_2SO_4$*<br>• *Student writes "1. open the epoxide 2. methyl shift"*<br>• *Student writes "6 memb ring?"* |
| Brainstorm Multiple Ways | *"I brainstormed multiple ways to solve the problem before I actually started solving it."*<br>The student proposes multiple possible ways to solve the problem, at the beginning of the problem-solving process. | • I feel like there's many things I could do here. I feel like I could do either like maybe open the epoxide, or I could maybe do a methyl shift |
| Consider If Plan Reasonable | *"I considered whether my proposed steps were reasonable before I actually started solving the problem."*<br>The student makes a judgement about whether their proposed steps are correct or likely, before they draw their first new structure. | • "Right away I think 'it's acid so it's going to protonate the amine'…but that's not really a useful reaction because it's just going to sit there." |
| Consider Another Way | *"While I was working on a problem, I paused to consider whether there was another way to solve it."*<br>After they have started down one path, the student considers an alternate chemical path or an alternate problem-solving approach. | • "Maybe I'll just try to do the protonation of the other one and see what happens"<br>• "Hm, maybe I should think more about the mechanism" |
| Monitor Progress Towards Goals | *"I paused to consider whether I was making progress towards my goals as I worked on the problem."*<br>The student considers whether what they have done so far has gotten them closer to a goal they had previously stated or considers what they still need to do in order to achieve their goals/continue making progress. | • "Ok so now we're catalytic in acid" (Note: Student previously set a goal to find a way to make the reaction catalytic in acid, and they're confirming that they've done that)<br>• "I'm just trying to make a carbonyl group, so would that help?"<br>• "That's probably not going to get me anywhere useful for this." |
| Monitor Correctness | *"I paused to consider whether what I was doing was correct as I worked on the problem."*<br>The student asks themselves whether something is correct, or states that something they've done or are proposing to do is right/reasonable or wrong/unreasonable. | • "That leaves a positive charge there, so you don't want to do that"<br>• " This looks so wrong"<br>• "This is kind of reasonable"<br>• "I think this works" |
| Note Uncertainty | *"I took note of what I was uncertain about as I worked on the problem."*<br>The student states what they are not sure about or what they do not know. | • "And then I am a little stuck on what to do with the second solvent in this first step."<br>• "I don't have a periodic table so I'm not exactly sure if sulfur is the one that would be donating electrons." |

| | | |
|---|---|---|
| Periodically Check If Reasonable | *"As I was working on the problem, I periodically checked back over what I had done so far to make sure my overall approach was reasonable."*<br>The student looks back over what they've done so far to confirm that their steps were reasonable. | • "I like that step, and I like that step. I'm a little iffy about these steps."<br>• "Ok, let's see. Do I like this? Let me think. Uh-huh. Am I forgetting anything?" (Note: They are checking back on what they've done so far, in the middle of the problem) |
| Consider If Answer Reasonable | *"I thought about whether my answer was reasonable after I finished the problem."*<br>Once they have reached an answer, the student states whether they think their answer is correct or reasonable. | • "It doesn't look that bad, hm, ok I think I'm happy with it"<br>• "I don't agree with the product. Because that looks off." |
| Check if Answered Question | *"I made sure that my solution actually answered the question."*<br>The student refers back to the question statement to make sure that they followed the directions or that their answer fulfills all components of the prompt. | • "So am I happy with that? Let's look. Major products. I want to say this is the major product." (Note: They refer back to the instructions, which said to predict the major products.) |
| Check For Mistakes | *"I checked back over my work after finishing the problem to make sure I didn't make any mistakes."*<br>The student goes over what they've done to make sure their answer is correct and free of mistakes. | • "Then count my atoms just to make sure I didn't miss anything. This one's here, this one's right here."<br>• "Is there anything else that I'm missing? Charges? Oxygen has a good charge, all the other ones have a good charge. Ok." |
| Check If Agreed With Prediction | *"Once I reached an answer, I checked to see that it agreed with what I predicted."*<br>After reaching an answer, the student refers back to a prediction that they had made during the problem and considers whether their answer agrees with that prediction. | • "So I think this is my final answer. I also said there would be no acid-base, but water is there so maybe?" (Note: This student had predicted there would be no acid-base chemistry involved in the reaction. They are referring back to this prediction.) |
| Summarize Main Takeaways | *"Once I finished the problem, I summarized the main take-away lesson I learned."*<br>After reaching an answer, the student considers what they learned from the problem. | • "There's a divergence that could give you that product, but I just kept going with mine. I see that you have to draw your product and then really sit and think about it." |
| Consider Changes For Future | *"After I finished the problem, I considered how I might change my approach for future problems."*<br>The student suggests a way that they could change or improve the way they approach problem solving in the future. | • A possible example would be a student stating that they should check their work more in the future. |

Appendix S4: Reasons for Using or Not Using Metacognitive Strategies Coding Scheme

Reasons for Using Strategies:

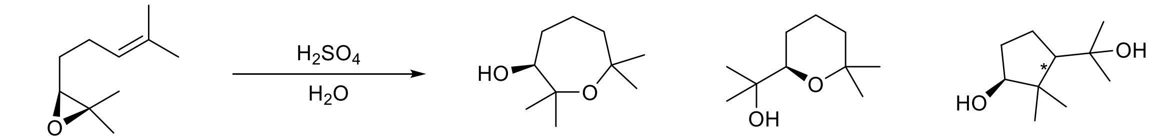
| Code | Description | Example |
|---|---|---|
| Builds confidence | The student uses this strategy because it helps them feel more confident in their answer or thought process. | "If I see something unfamiliar and I think, you know, how is this similar to something I've done before...that'll make me feel a lot more confident." |
| Many reactions to consider | The student uses this strategy because they recognize that a wide variety of reactions or types of reactivity exist and could possibly be relevant to the problem. | "The more organic chem classes you take, you learn a lot more reactions, and I think having that much information to go through is kind of a lot. And so being able to break it down into smaller chunks I find very useful." |
| Helps them learn/ improve | The student uses this strategy because it helps them learn or improve their knowledge or problem-solving skills. | "I thought it was important for me to summarize what did I learn from the solution...because that'll help me in the future when I encounter this type of problem." |
| Avoid wasting time/effort | The student uses this strategy because it helps them avoid wasting time or effort during the problem-solving process. | "If I'm not certain about something, I don't want to waste too much time on it. And so I'll star it, try to guess something, and then come back to it at the end if I have time." |
| Get started/ narrow focus | The student uses this strategy because it helps them get started on the problem or narrow their focus to certain pathways. | "Identifying specifically the bonds that need to be made or broken really helps you narrow the focus of a 1000 molecular weight molecule down to the 5 or 6 atoms that are actually relevant to the question and that takes out a lot of options." |
| Keeps them on right track | The student uses this strategy because it helps them stay on the right path and continue making progress towards an answer. | "It helps with making sure you're going down the right path, making sure you're getting the right steps. Especially when I get stuck, I think just looking at what I need to get to is a key thing I do." |
| Keeps them from forgetting | The student uses this strategy because it helps prevent them from forgetting an idea or piece of information. | "Yeah, I would sometimes do that because I don't want to just rely on my brain to remember everything." |
| Someone encouraged use | The student uses this strategy because another person, such as an instructor or tutor, encouraged them to use this strategy. | "I definitely always look at what bond I need to make and what functional group I need to make if there is a product written out for me. Because not only [my professor], but my [teaching assistant], reiterated that a lot. So that's just how I learned o-chem." |
| Helps avoid mistakes | The student uses this strategy because it helps them avoid making mistakes. | "One of my biggest mistakes could be with forgetting atoms or incorrect stereochemistry. So I made sure, for this example, to double check my stereochemistry, and I was trying to count the carbons in one of the chains in the ring that opened." |

Reasons for Not Using Strategies:

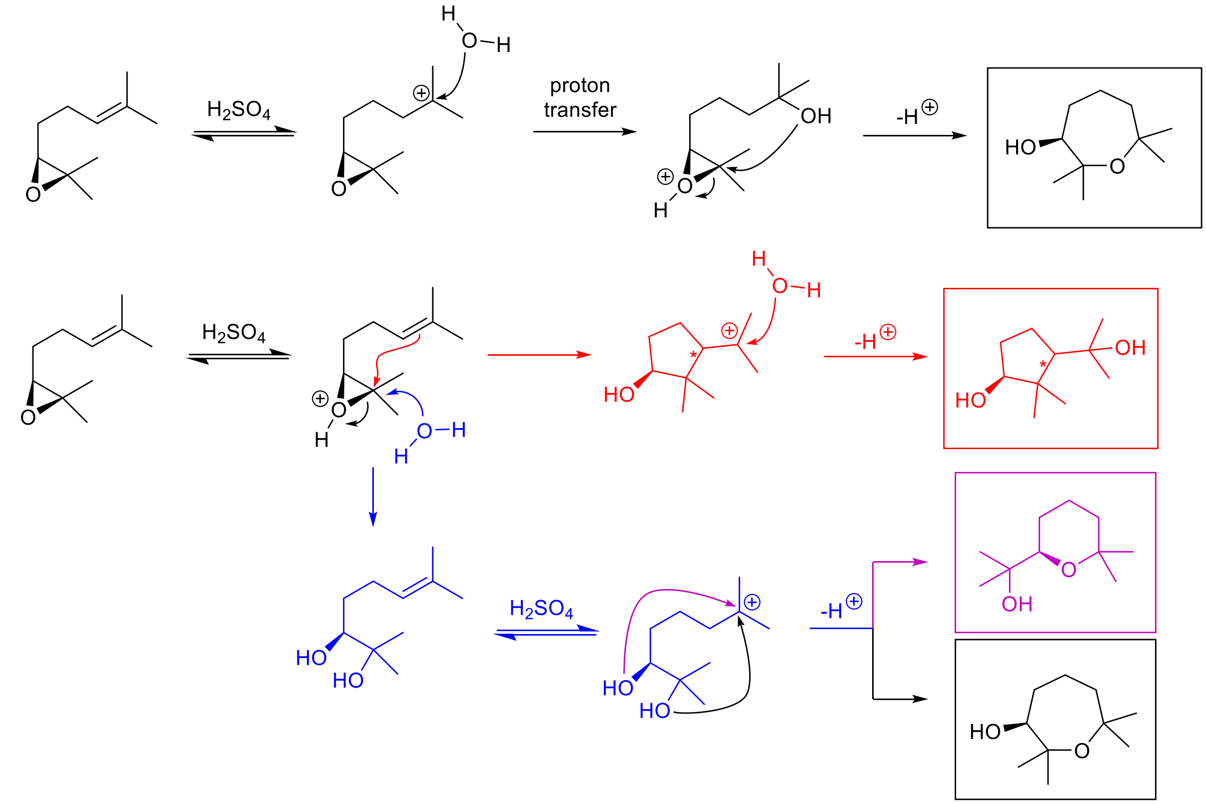
| Code | Description | Example |
|---|---|---|
| Prevents success: distracting | The student does not use this strategy because it distracts them and they therefore consider it to be detrimental to their success in solving the problem. | “So that one is mainly just because I tend to work things out to the end and then I go back to evaluate whether what I got was reasonable so when I'm working on something I'm not as distracted by what other things could be happening.” |
| Prevents success: other | The student does not use this strategy because they consider it to be detrimental to their success in solving the problem for another reason, or they state that it is detrimental without stating a specific reason. | “I think the setting goals could be potentially dangerous if it leads you down a wrong path. Especially when approaching certain problems like mechanism or predict-the-products you kind of have to be open-minded until you've at least narrowed it down.” |
| Issues with timing | The student does not use this strategy because there is not typically enough time for them to use it. | “Yeah, I think just because of the time constraints, I don't normally do that...I don't really have time to list it out.” |
| Unable to use effectively | The student does not use this strategy because they believe they are unable to use the strategy effectively, often because they do not feel experienced enough to do so. | “I never really predict products because it's really hard for me to visualize what's going to happen.” |
| Unnecessary: have answer | The student does not use this strategy because they consider it to be unnecessary when they have already found an answer to the problem. | “But like brainstorming other ways to solve it, I feel like in some cases that would kind of be a waste of time or unnecessary since if you're already doing it in your way and that's going to lead to the desired product and you already know that, then you don't really need to brainstorm ways to do it...you're just trying to get to the answer or something.” |
| Unnecessary: redundant | The student does not use this strategy because they consider it to be unnecessary because they either use a different strategy for the same purpose or use a similar strategy at a different time in the problem. | “After I finish a problem I usually immediately get to the next problem, so that's why I marked "no" on a lot of those, like after the problem checked to see if it made sense, checked to see if you answered the question, I feel like I double-check myself enough times each step if I could actually get to an answer that there's no need to go past that.” |
| Unnecessary: other | The student does not use this strategy because they consider it to be unnecessary for another reason, or they state that it is unnecessary without stating a specific reason. | “I just don't find it very helpful. I know some people like to make lots of thought maps to understand where the initial reactant could lead them to, but to me, that just seems like a waste of brainpower.” |

## Appendix S5: Accepted Answers, Mechanisms, and Grading Rubrics for Problems A-D

**Accepted Answer(s): Problem A**




**Mechanism:**

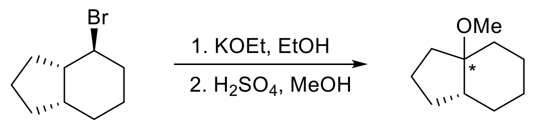



**Grading Rubric:**

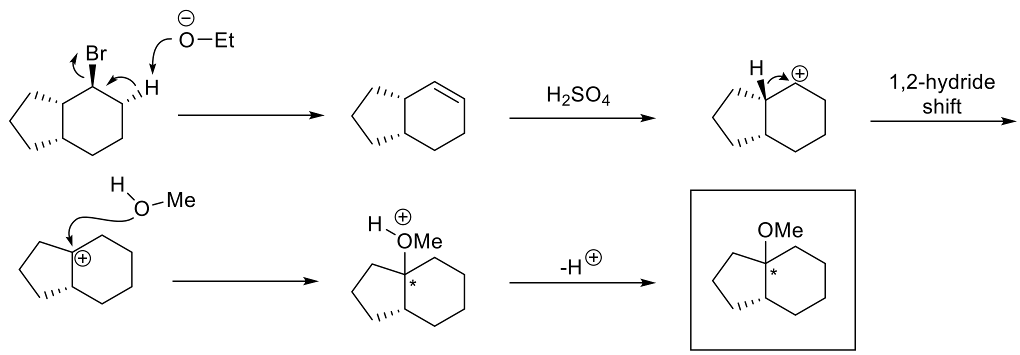
Minimum score: 0 (fully incorrect answer; no partial credit possible)
Maximum score: 4 (fully correct answer)
Partial Credit Options and Point Deductions:

| | |
|---|---|
| +2 points | Student's product involved a reasonable reaction between the epoxide and the given reagents, but there was no involvement of the alkene |
| +2 points | Student's product involved a reasonable reaction between the alkene and the given reagents, but there was no involvement of the epoxide |
| +3 points | Student's product involved reasonable reactions between both the alkene and the epoxide with the given reagents, but no intramolecular cyclization |
| -0.5 points | Student's product included the result of unreasonable further reactivity |
| -0.5 points | Stereochemical errors or minor drawing errors are present in the product(s) the student drew. *Note: these errors should not be considered when determining whether an answer qualifies for other partial credit options.* |

**Accepted Answer(s): Problem B**




**Mechanism:**

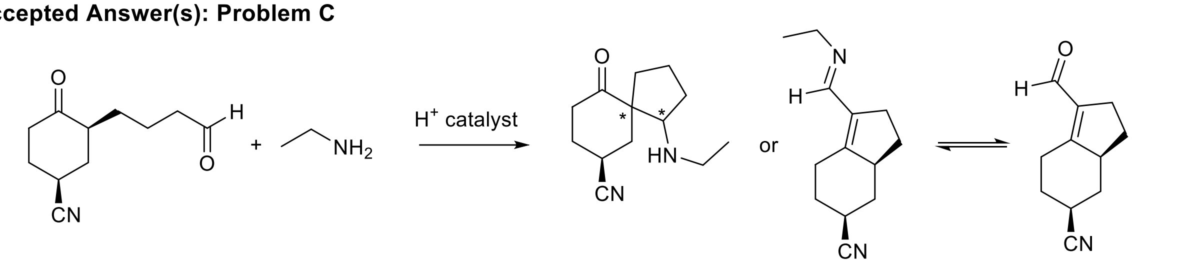



## Grading Rubric:

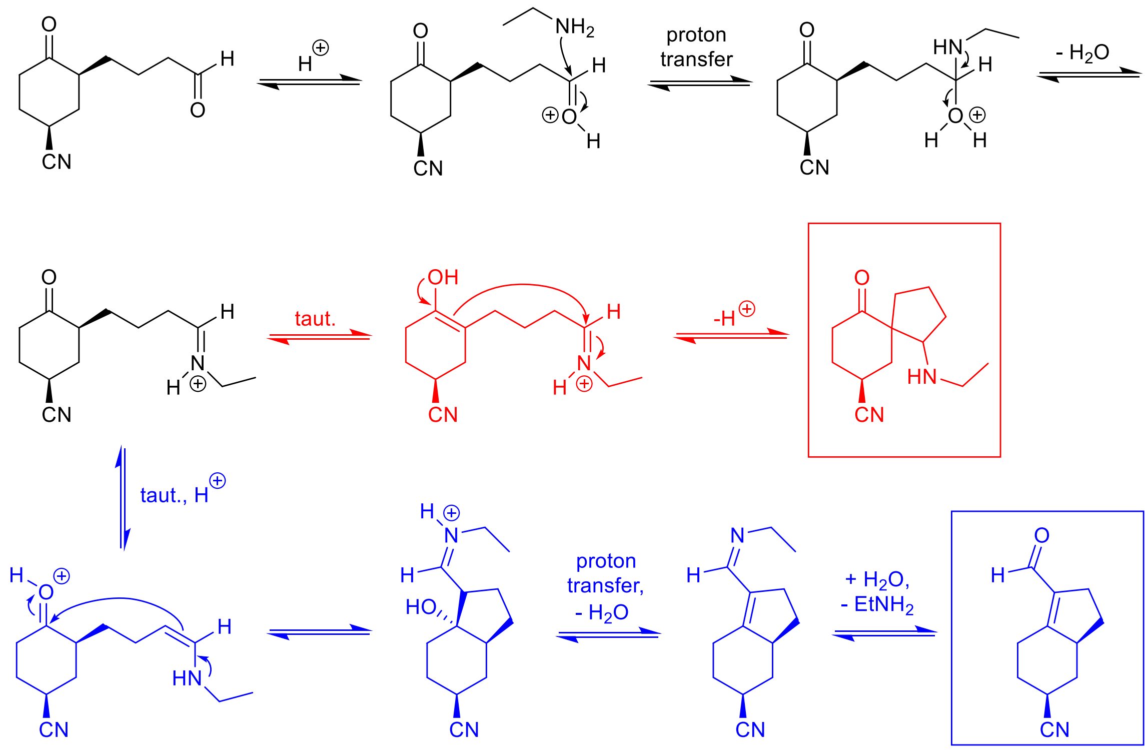
Minimum score: 0 (fully incorrect answer; no partial credit possible)
Maximum score: 4 (fully correct answer)
Partial Credit Options and Point Deductions:

| | |
|---|---|
| +1 point | Student chose incorrect reaction type (i.e. E1, SN1, or SN2 instead of E2) for step 1, but completed chosen reaction correctly, OR chose correct reaction type (E2) but completed chosen reaction incorrectly |
| +2 points | Student completed step 1 correctly |
| +1 point | Based on their answer to step 1, student chose incorrect reaction type for step 2, but completed chosen reaction correctly, OR chose correct reaction type for step 2 but completed chosen reaction incorrectly |
| +2 points | Student generated correct product in step 2 based on the product they generated in step 1 |
| -0.5 points | Stereochemical errors or minor drawing errors are present in the product(s) the student drew for step 1 and/or step 2. *Note: these errors should not be considered when determining whether an answer qualifies for other partial credit options.* |

**Accepted Answer(s): Problem C**




**Mechanism:**

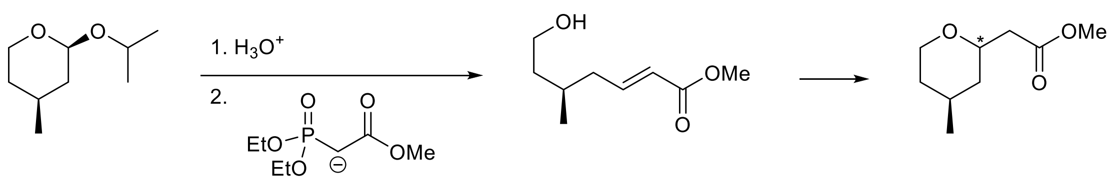



**Grading Rubric:**

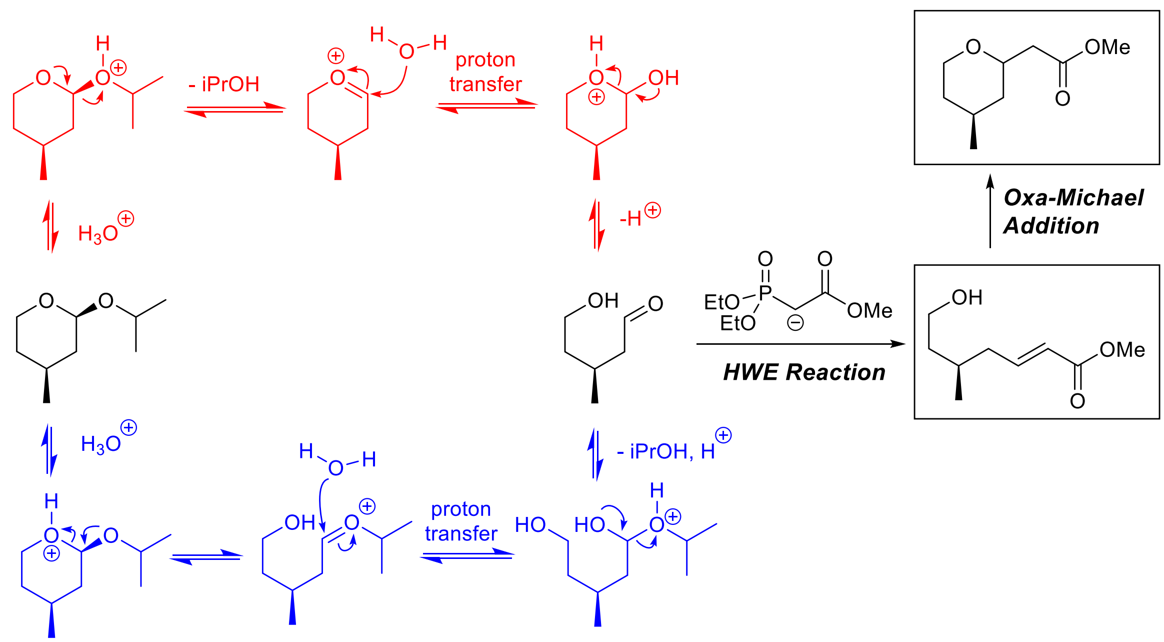
Minimum score: 0 (fully incorrect answer; no partial credit possible)
Maximum score: 4 (fully correct answer)
Partial Credit Options and Point Deductions:

| | |
|---|---|
| +1 point | Student used ethylamine as a nucleophile to react with one of the carbonyls |
| +1 point | Student chose correct carbonyl as the electrophile |
| +1 point | Student generated an imine, iminium ion, or enamine after reacting ethylamine with their chosen carbonyl. |
| +1 point | Student completed a reasonable intramolecular Mannich reaction or amine-catalyzed aldol reaction after generating an imine, iminium ion, or enamine. |
| -0.5 points | Student's product included the result of unreasonable further reactivity |
| -0.5 points | Stereochemical errors or minor drawing errors are present in the product(s) the student drew. *Note: these errors should not be considered when determining whether an answer qualifies for other partial credit options.* |

**Accepted Answer(s): Problem D**




**Mechanism: (Note - two possible mechanisms are possible for the hydrolysis of the acetal)**




**Grading Rubric:**

Minimum score: 0 (fully incorrect answer; no partial credit possible)

Maximum score: 4 (fully correct answer)

Partial Credit Options and Point Deductions:

| | |
|---|---|
| +1 point | Student completed initial steps of the acetal hydrolysis reaction in step 1, but they did not complete the overall acetal hydrolysis transformation correctly |
| +2 points | Student completed step 1 correctly |
| +1 point | Student completed first step of the HWE reaction with the product they generated in step 1, but they did not complete the overall HWE transformation correctly |
| +2 points | Student generated correct product of HWE reaction in step 2 based on the product they generated in step 1 |
| -0.5 points | Stereochemical errors or minor drawing errors are present in the product(s) the student drew. *Note: these errors should not be considered when determining whether an answer qualifies for other partial credit options.* |

Appendix S6: Strategies Used By Students During Selected Problem-Solving Cases. Shaded Cells Indicate Strategy Usage

| **Strategy** | **Andrew (Less Successful Solution, Lower Metacognition)** | | **Lily (Less Successful Solution, Higher Metacognition)** | | **Ben (More Successful Solution, Lower Metacognition)** | | **Marta (More Successful Solution, Higher Metacognition)** | |
|---|---|---|---|---|---|---|---|---|
| | **Strategy Used?** | | **Strategy Used?** | | **Strategy Used?** | | **Strategy Used?** | |
| | **SR [a]** | **OB [b]** | **SR** | **OB** | **SR** | **OB** | **SR** | **OB** |
| Set Goals | ■ | | ■ | | ■ | | ■ | |
| Sort Relevant Info | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ |
| Look for Reactions Recognized | ■ | | ■ | ■ | ■ | | ■ | |
| Reflect Relevant Knowledge | ■ | ■ | ■ | ■ | ■ | ■ | ■ | ■ |
| Relate to Previous Problems | ■ | | ■ | ■ | ■ | | ■ | |
| Jot Down Ideas | | | | | | | | |
| Make Predictions | ■ | ■ | ■ | ■ | ■ | | ■ | ■ |
| Brainstorm Multiple Ways | | | ■ | | | ■ | | ■ |
| Consider If Plan Reasonable | ■ | | ■ | | ■ | | ■ | |
| Consider Another Way | | | ■ | ■ | ■ | | ■ | ■ |
| Monitor Progress Toward Goals | | | ■ | ■ | ■ | | ■ | ■ |
| Monitor Correctness | | | ■ | ■ | ■ | | ■ | ■ |
| Note Uncertainty | | | | ■ | ■ | | ■ | ■ |
| Periodically Check If Reasonable | | | ■ | ■ | | | ■ | ■ |
| Consider If Answer Reasonable | ■ | | ■ | ■ | ■ | ■ | ■ | |
| Check If Answered Question | ■ | | ■ | | ■ | | ■ | |
| Check For Mistakes | | ■ | ■ | | | | | ■ |
| Check If Agreed with Prediction | ■ | | ■ | | ■ | | ■ | |
| Summarize Main Takeaways | | | ■ | | | | | |
| Consider Changes for Future | | | ■ | | | | | |

[a] Self-reported strategy usage: student selected "yes" when asked on the post-problem survey if they had used this strategy while solving the problem

[b] Observed strategy usage: evidence of this behavior was detected in think-aloud transcript

Appendix S7: Frequencies with which Interview Participants Gave Certain Reasons for Using or Not Using Individual Strategies. Increased Color Saturation Indicates Higher Frequency.

| | Builds confidence | Many reactions to consider | Helps them learn/improve | Avoid wasting time/effort | Get started/narrow focus | Keeps them on right track | Keeps them from forgetting | Someone encouraged use | Helps avoid mistakes | Prevents success - other | Prevents success - distracting | Issues with timing | Unable to use effectively | Unnecessary - other | Unnecessary – have answer | Unnecessary - redundant |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Set Goals | 2 | 2 | | 1 | 8 | 3 | 1 | 6 | 1 | 4 | | 2 | 5 | 3 | 1 | |
| Sort Relevant Info | | 1 | | 1 | 14 | 1 | | 2 | | | | 1 | | | | |
| Look for Reactions Recognized | 1 | 4 | | 1 | 11 | | | 2 | | 1 | | | | | | |
| Reflect Relevant Knowledge | | | 1 | 1 | 6 | 3 | 1 | 3 | 1 | | | 1 | 1 | 1 | | |
| Relate to Previous Problems | 1 | 1 | 4 | 1 | 7 | | | 1 | 1 | 1 | 1 | 1 | 1 | 3 | | |
| Jot Down Ideas | 1 | 1 | 2 | 1 | 7 | 1 | 7 | 2 | 3 | | 7 | 9 | 4 | 14 | 1 | |
| Make Predictions | 1 | | | 2 | 2 | 1 | | 1 | 2 | 1 | 1 | | 11 | 1 | 1 | |
| Brainstorm Multiple Ways | | | | | 2 | | | | | 1 | 3 | 8 | 2 | 5 | 4 | 2 |
| Consider if Plan Reasonable | | | | | | | | | 1 | | 1 | 1 | 5 | | | 2 |
| Consider Another Way | | 3 | | 1 | | 1 | | | 3 | 1 | 4 | 1 | 2 | 1 | 4 | |
| Monitor Progress Toward Goals | | | | 4 | | 4 | | | 1 | | | 2 | 3 | 1 | | 1 |
| Monitor Correctness | | 1 | 1 | 4 | | 4 | | | 8 | | 1 | 1 | | 3 | | 1 |
| Note Uncertainty | | | 5 | 2 | 1 | 4 | 3 | | 1 | 1 | | 6 | 1 | 2 | | 1 |
| Periodically Check If Reasonable | 1 | | | 1 | | 6 | | | 6 | 1 | 3 | 3 | 2 | 3 | | 3 |
| Consider If Answer Reasonable | 1 | | | | | | | | 3 | | | | 2 | 1 | 1 | |
| Check If Answered Question | | | 1 | 1 | | | | 1 | 9 | | | | | | 1 | 1 |
| Check For Mistakes | 1 | | | 1 | | | 1 | 2 | 18 | | | 14 | 1 | 2 | 1 | 2 |
| Check If Agreed with Prediction | | | 1 | | | | 1 | | | | | 2 | 8 | 2 | 1 | 1 |
| Summarize Main Takeaways | | | 12 | | | | | 2 | 2 | | | 10 | 2 | 11 | 5 | 4 |
| Consider Changes for Future | | | 3 | | | | | | 1 | | | 4 | 3 | 3 | 5 | 1 |