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Teaching abductive reasoning for use as a problem-solving tool in organic chemistry and beyond

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The second-year undergraduate Organic Chemistry course sequence is often cited as one of the most, if not the most, challenging for students in the US. Thus, a persistent question remains: What is it about Organic Chemistry that makes the course so difficult for students? Herein, we put forward the hypothesis that a new mode of thinking and problem solving is expected of the students; these skills have not yet been developed in their prior scientific coursework and are often not deliberately taught in Organic Chemistry. This form of reasoning and problem solving, known as abductive reasoning, is highlighted for its connection to medical diagnosis and scientific thinking. We provide examples to showcase how instructors could explicitly foreground the reasoning process in their classroom. Ultimately, we argue that teaching how to reason using abduction may benefit students in both the short term (in the course) and the long term (in their careers as scientists and medical practitioners).

KEYWORDS

abduction, abductive reasoning, organic chemistry, diagnosis, metacognition, problem solving, pre-health education

> “What changes must be made in the *kind* of science that we teach and the way that we teach it so that the fundamental ideas of our discipline can be used outside the classroom?” – Herron & Greenbowe

1 Introduction

1.1 Background

Organic Chemistry, as traditionally taught in the US as a primarily second-year undergraduate course sequence, is often considered a course for “weeding out pre-meds” (Moran, 2013) that “strik[es] fear in the hearts of students” (Garg, 2019). This socially constructed barrier adds an additional level of pedagogical challenge for instructors. We, the authors, are instructors of Organic Chemistry and also write and review questions for standardized exams that are required for entrance into specialized medical programs;[1] thus, we are at a position in both the content delivery and assessment where we find ourselves continually asking the question: What do we want students to learn in the Organic Chemistry course sequence?

While some students may think the answer to this question is "to know, understand, and recite back the course material," this is an unsatisfying response for a number of reasons. First, such a response would imply that only memorization and algorithmic problem-solving skills are necessary for success in Organic Chemistry (Stowe and Cooper, 2017).[2] However, expert organic chemists recognize that the interconnected complexities within chemical systems means that simply following basic rules (i.e., deductive inference) will not necessarily lead to a set outcome (e.g., bulky bases do not *always* react via E2) (Achet et al., 1986). Second, while the students enter our classrooms as novices, some of them will go on to become practicing, expert organic chemists. We owe it to them, and the future of scientific discovery, to build a sound foundation of both fundamental (e.g., understanding the aldol condensation) and higher order (e.g., performing retrosynthetic analysis) skills within the discipline. Third, most US health professions (e.g., MD, DO, PA, DDS, DMD, OD, PharmD) require this course to be taken as a prerequisite for admission into their graduate programs (Kovac, 2002). These students should be presented, within their undergraduate education, the chance to improve their scientific reasoning and critical thinking skills. We think that these three features, which might not be clear to all students entering the course, illustrate that students are expected to learn and problem solve in new ways—essentially to begin to "think like a chemist" (e.g., Platt, 1964).

While certain ideas within this article were presented in a preceding paper (Wackerly, 2021), we intend to flesh out and expand upon some of those initial assertions in this manuscript and craft a more detailed hypothesis that the use of abductive reasoning is critical in the learning of organic chemistry concepts. Herein we provide support for this hypothesis by viewing it from a few different conceptual angles. First, we provide a science education overview on why learning certain organic chemistry concepts is considered challenging for students. Then, we briefly summarize the medical education viewpoint on the teaching of diagnosis and why this is important to many students in Organic Chemistry. Finally, using the lens of the Organic Chemistry curriculum we provide problem-solving examples of how abductive reasoning can assist in the teaching and learning of organic chemistry.

1.2 Why is science difficult to learn?

Johnstone asked this titular question in his seminal 1991 paper (Johnstone, 1991). One conclusion that he drew, which has since been supported by a variety of other work (e.g., Graulich, 2015; Tiettmeyer et al., 2017; Reid, 2020; Dood and Watts, 2022), is that the nature and complexity of scientific concepts strain the working memory of students. To assist instructors in conceptualizing the strain of a given concept, he created the "triangle model" which illustrated three levels of thought (Figure 1). He argued that the more levels a concept included the more cognitive load was placed on students.

One feature that might make learning science difficult is that the instructor, or expert, may not be aware of the extent of cognitive load they are placing on students, or novices. When "multicomponent phenomena that are invisible, dynamic, and interdependent" are presented to students, a large demand is placed on the working memory of novices (Hmelo-Silver et al., 2007). However, experts are able to easily connect two or more cognitive components by "chunking several pieces of information together" (Overton and Potter, 2008) and through years of practice (Randles and Overton, 2015). Specialization within a discipline that requires connecting multiple levels will lower cognitive load for such repetitive tasks over time (Tiettmeyer et al., 2017; Price et al., 2021). However, students have typically not been exposed to such tasks, let alone have the opportunity to consistently repeat them, and thus instructors need to disentangle new concepts that might cause cognitive overload for students so they can process and incorporate new material starting from their present knowledge base and scientific models.[3]

> "[R]easoning [is the] knowledge of some facts [which] leads to a belief in others not directly observed." – C. S. Peirce

1.3 Why is organic chemistry so difficult to learn?

Here we argue that it should come as no surprise when former and current students of organic chemistry cite that organic chemistry is difficult to learn, because they are asked to problem solve and reason in new ways utilizing new content without prior exposure to, or repetition of, these scientific tasks.[4] Naturally, when a student enters a course they are expected to be ignorant of the course content since they enroll to learn it. However, students might feel that a bait-and-switch has occurred in Organic Chemistry because not only is the content new, but the logical processes required to be successful are also typically new to the students as well.

In prior scientific courses, which for most pre-health (*vide infra*) US students are two courses in general biology and two in general

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[1] We wish to keep the focus of this manuscript on the relevant student population of the Organic Chemistry course sequence. Students intending to pursue medically relevant careers which require advanced degrees (e.g., medical, dental, optometry, pharmacy, etc.) are a large portion of this population. However, if the reader is curious, we specifically write for the dental and optometric admissions exams.

[2] In this manuscript we attempt to provide the reader a broad overview of important chemical education and philosophy of chemistry publications. Since this is not a review article and the scope is quite a bit smaller, all possible relevant literature has not been cited.

[3] Cognitive overload could also stem from misconceptions and oversimplified concepts, such as the oft-stated "breaking bonds in ATP releases energy" from introductory biology courses.

[4] This can be contrasted with General Chemistry which repeats some of the content of the high school chemistry.

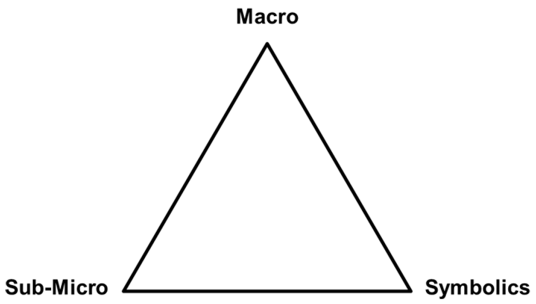

FIGURE 1
Reproduction of Johnstone's model: "Triangle of Levels of Thought".

chemistry, students are typically required to perform recall (memorization) or reason algorithmically on summative assessment items (Raker and Towns, 2010). While these skills hold value in organic chemistry, current organic chemistry education research shows that skills such as multivariate (Kraft et al., 2010; Christian and Talanquer, 2012) and mechanistic reasoning (Bhattacharyya, 2013) are more important.[5] Thus, inspired by the work in chemistry education research, the philosophy of science, and Johnstone's seminal triangle, here we propose a tetrahedron model of layered reasoning strategies that are important for consideration by instructors when teaching novice organic chemistry students.

The bottom-most point of the tetrahedron (Figure 2) was chosen to be memorization because it is not a reasoning skill. However, terms and chemical facts still need to be learned by students, which is often not a problem because they have developed this skill during their general biology and chemistry coursework. Algorithmic reasoning is a skill many students leaving General Chemistry assume they will utilize in Organic Chemistry because it was employed so frequently in that course. For example, if a student knows the pressure, temperature, and number of moles of an ideal gas, these students will likely be able to provide the volume of the gas's container. While these mathematical and deductive reasoning skills remain relevant in the laboratory portion of Organic Chemistry and even for the IUPAC naming of organic molecules (i.e., there is a definitive rule set), they start to break down when chemical systems become more complex and chemical formulas evolve to contain more meaning in the form of chemical structures.

The right corner of the tetrahedron is for the set of competencies required to interpret diagrams in organic chemistry, such as visualization (Gilbert, 2005), visuo-spatial reasoning (Pribyl and Bodner, 1987; Habraken, 1996), and representational competence (Kozma and Russell, 1997). In lieu of individually listing these skills, we designate this corner as perceptual learning, which integrates conceptual knowledge with a broad set of skills, including those related to visualization and representational competence (Van Dantzig et al., 2008; Kellman and Massey, 2013). Perceptual learning "refers, roughly, to the long-lasting changes in perception that result from practice or experience" (Connolly, 2017), and is beginning to be more deeply explored in organic chemistry pedagogy (e.g., Kim et al., 2019).

We briefly illustrate how changes associated with perceptual learning might take place with students. Consider, for example, that in General Chemistry students might be asked to calculate the heat of combustion of hexane (denoted at C_6H_{14}). For most students at that stage, the sole association they would have with the compound's name is its molecular formula, whereas its "zig-zag" structure might represent nothing more than a crooked line. As these students progress into Organic Chemistry and learn about different representational systems and constitutional isomers, the verbal representation "hexane" changes, this is because the term is now associated with five unique isomers each with unique connectivity, properties, and reactivity (e.g., radical reaction with Br_2). Through this process, the students' *perception* for the term "hexane" changes from representing a single molecular formula to representing a family of five constitutional isomers each with a unique bond-line structure. This process continues as students advance to more complex structures (e.g., stereochemistry) and learn additional concepts like three-dimensionality, IMFs, physical properties, etc. We propose that the three corners of the tetrahedron discussed thus far are often directly connected to abductive reasoning which focuses on solving problems by generating the most likely most likely outcome of a chemical situation.

Our hypothesis includes the postulation that abductive reasoning is a complex reasoning skill for students in Organic Chemistry and should explicitly be taught in the classroom. While this idea has been presented by us previously (Wackerly, 2021), here we will just provide a brief overview so we can move on to discuss the relevance of this reasoning skill within the Organic Chemistry classroom and to highlight some examples. Firstly, the term "abduction" (Douven, 2021) is often used interchangeably with the terms "inference to the best explanation" (Lipton, 2017) and "scientific hypothesis"—and below we will argue "diagnosis." All of these terms hold common ground in that they use reasoning that connects various (similar or dissimilar) pieces of evidence/observations together in a way where a plausible conclusion can causally describe the collection of phenomena.[6] For example, say you are inside of grain windmill by the grindstone, and then you begin to see the stone rotating and producing flour. You will abduce that the weather outside has become windy. While this is a simple example only requiring you to understand that outside wind turns the sails and the sails, via a series of machinery, turn the grindstone, it is similar to the reasoning employed by expert organic chemists. Leaving the windmill and heading into your synthetic laboratory, let us say you wish to publish a new compound in the *Journal of Organic Chemistry*. According to the journal, to conclude that you have made this new compound you must "establish both identity and degree of purity." Minimally, this means you will need to obtain a ^{1}H NMR spectrum, ^{13}C NMR spectrum, and HRMS spectrum then interpret the data present in the spectra to abduce the molecular

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[5] Multivariate and mechanistic reasoning are highlighted as examples because they often require combining features from all four points of the tetrahedron.

[6] The conclusion need not explain the entire collection of evidence as some may be irrelevant, and they are unrelated to the conclusion. However, the entire collection may not contain a piece of evidence that refutes the conclusion. Thus, abductive reasoning can be useful in differentiating science from non-science and pseudoscience.

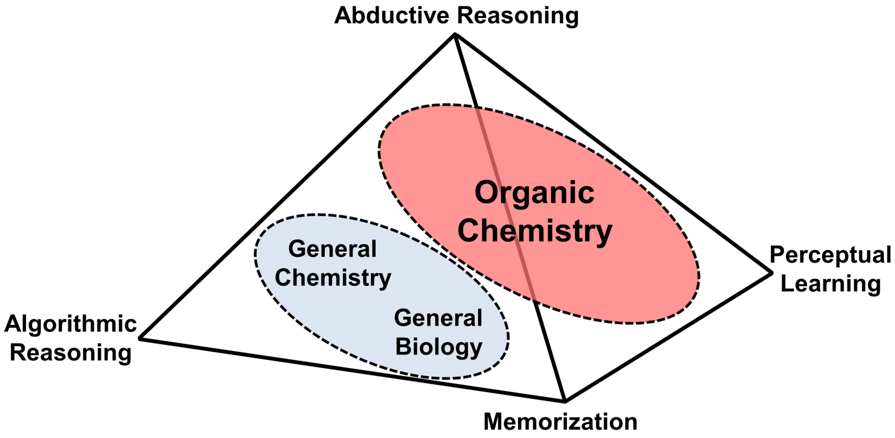


FIGURE 2
Tetrahedron model of problem-solving in Organic Chemistry.

structure of your new compound. This exact same skill that is required of expert organic chemists, is typically required of students in Organic Chemistry (Stowe and Cooper, 2019a). Thus, these students should be taught how to reason like expert scientists in order for them to develop into scientists (Cartrette and Bodner, 2010). Just as the spectroscopic analysis example highlights, instructors of Organic Chemistry often profess a goal is for students to develop critical thinking and scientific problem-solving skills: Our hypothesis presented here is that instructors must explicitly utilize the abductive reasoning process within their teaching and assessment.

Solving problems that require abductive reasoning will also require skills from the three other points of the tetrahedron, which will render them cognitively complex. Teaching abductive reasoning in the classroom should not require additional formal training for instructors/experts since abductive reasoning skills have already been developed over the course of their careers. Further, philosophers have long held (Harman, 1965) that humans utilize abductive reasoning as a matter of course in their day-to-day lives. Paralleling human logic, abductive reasoning has likely been utilized (Pareschi, 2023) and will continue to be (Dai and Muggleton, 2021) an integral part of artificial intelligence. This reasoning skill is particularly important for students required to take Organic Chemistry. It might be obvious that future scientists will need the skills to create new hypotheses and design experiments that could potentially refute current hypotheses, but in our experience, it seems less obvious to pre-health students that using abductive reasoning for problem solving in Organic Chemistry will play a critical role in their desired careers.

2 Framing for pre-health students (diagnosis)

2.1 Why is organic chemistry relevant for pre-health students?

In a post-COVID world where test-optional admissions are on the rise and the future of post-graduate education feels increasingly uncertain, convincing students of the importance of Organic Chemistry goes beyond just passing the course. This is especially true for the majority of students taking Organic Chemistry who are pre-health majors. Instructors need to show students the connection between organic chemistry and the health field.

Thus, problem solving in Organic Chemistry can be framed as a diagnostic problem-solving tool–similar to what medical practitioners do when making a diagnosis (Stowe and Cooper, 2019b). By overtly showing students the parallels between medical diagnosis and organic chemistry problem solving, instructors demonstrate that students are not just being taught a bunch of facts–they are developing critical thinking skills they can use in the real world. Bridging the gap between theory and practice helps students see the bigger picture and gives them the tools they need to succeed in both their studies and future careers.

The parallels between medical diagnosis and organic chemistry problem solving should be readily apparent (Table 1). Both involve analyzing complex systems (human body/chemical reactions) to identify patterns and relationships, emphasizing the importance of critical thinking and logic-based problem-solving skills, as well as using evidence. Both fields rely on the use of abductive reasoning (Wackerly, 2021; Martini, 2023), although typically neither field explicitly states it to students. Table 1 uses simplified language accessible to students that describes the abductive theory of method (ATOM) in clinical diagnosis (Vertue and Haig, 2008), and its parallel to expert thinking in organic chemistry.

For example, to "diagnose" the product of an organic chemistry reaction, first the background information, including structure, reactivity, and stability of the starting materials and reagents must be analyzed, which is similar to how medical professionals take patient history. Abductive reasoning is then used to generate the most likely answer. Finally, the hypothesis is tested through gathering evidence such as utilizing spectroscopic analysis which is similar to a physician ordering lab work or imaging. This is an iterative process, wherein multiple pieces of spectroscopic evidence are needed to point to the same answer. Similarly, a physician may order additional studies or perform physical exams to support or refute their medical diagnosis. Although the goals appear different, the same skills are developed such as drawing hypothesis based on empirical evidence. By explicitly demonstrating how these thought processes are parallel, instructors of Organic Chemistry may help students to appreciate the mental training they are receiving in the course.

TABLE 1 Comparison of medical diagnosis to skills developed in Organic Chemistry.

	Medical diagnosis	Parallel to organic chemistry
Background information	Involves gathering patient history, physical exams, and tests	Requires analysis of structure and reactivity of molecules
Initial hypothesis	Utilizes abductive reasoning to form a preliminary diagnosis	Involves abductive reasoning to propose plausible mechanisms or structures
Iterative nature	Hypotheses are continuously revised based on feedback from other clinicians and tests	Hypotheses are tested and revised through experimentation
Goal	To identify the underlying cause of symptoms and provide treatment	To generate plausible mechanisms and/or structures from observed data
Skills developed	Critical thinking, pattern recognition, hypothesis refinement	Critical thinking, analytical skills, hypothesis refinement
Importance of evidence	Relies on empirical data and patient feedback	Relies on experimental data and spectroscopic analysis
Real-world application	Used by physicians to generate positive health outcomes for patients	Used by chemists to create new medicines, materials, etc.

Organic Chemistry has been deemed essential as a prerequisite for medical school by a panel of medical school professors of biochemistry (Buick, 1995). While many current medical students do not think that the material covered in Organic Chemistry was a valuable part of their undergraduate curriculum, the majority agree that the critical thinking skills learned in the course were valuable (Dixson et al., 2022). While there are those in the field of medicine who think that Organic Chemistry should be de-emphasized in the pre-med curriculum, those that defend Organic Chemistry do so for some of the same reasons we discuss herein, namely that the critical thinking and problem-solving skills in the course directly align with patient diagnosis (Higgins and Reed, 2007).

This process of abductive reasoning coupled with framing for the medical field may serve the students better in both the short term and long term. Students who employ more metacognitive strategies such as the type we are advocating for here are better able to solve problems in Organic Chemistry (Blackford et al., 2023). Connecting course material to students' future career aspirations also leads to better engagement and course performance (Hulleman et al., 2010). Additional benefits of this diagnostic reasoning process include students' ability to apply this metacognitive strategy in other courses in their majors, such as biology (Morris Dye and Dangremond Stanton, 2017), and their future medical careers (Friel and Chandar, 2021). Therefore, diagnostic reasoning should be explicitly modeled and assessed in Organic Chemistry courses.

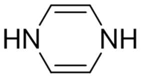
2.2 Using "diagnosis" in examples for students

While there are a variety of ways to teach students how to approach organic chemistry problems like an expert, we would like to present how to do this through the lens of "diagnosis." Other ways of describing argumentation and the process of problem solving have been discussed in the chemical education literature (e.g., Cruz-Ramírez De Arellano and Towns, 2014; Stowe and Cooper, 2019a; Walker et al., 2019) as well as the philosophy of chemistry literature (e.g., Kovac, 2002; Goodwin, 2003). While they differ in the number of steps and what those steps are called, the processes have a similar logical flow. First, gather evidence and make observations (*What you see*), link this to previous knowledge (*What you know*), and finally make a reasoned conclusion (*Hypothesis*) which is a logical consequence—often via abductive inference.

The following examples (Figures 3–6) are designed to highlight the use of these three steps to explicitly diagnose problems from across the two semester Organic Chemistry sequence. This process can be used in the classroom as a model to guide students through the abduction process and could be used to explicitly scaffold problems. Moreover, instructors can use this model to ascertain the complexity of their assessments including the required prerequisite factual knowledge and the multiple steps required. The complexity of organic chemistry questions is determined by the number of "subtasks" the student must complete (Raker et al., 2013), factual knowledge required, and facets of perceptual learning (*vide supra*). A number of explicit decisions were made in formulating the below questions. The discussion points are certainly not exhaustive, and practitioners should adapt questions to their own students and situations. The amount of information provided or not provided, such as the exclusion of lone-pairs and inorganic by-products, was chosen to be consistent with the information provided by practicing organic chemists and one goal of teaching organic chemistry is to facilitate the development toward expert-level practice. We intentionally included one example of additional information, Figure 4 entry marked with a *, to highlight that there are many more subtasks that could be utilized to assist with arriving at a probable conclusion, but we tried to exclude all other non-essential explanations. We do not suggest that all students should solve each problem from top to bottom as outlined here; in reality expert chemists often take different routes, based on the same evidence and premises, to reach similar conclusions. Although these problems are multiple-choice, we have modeled how to solve them as either multiple-choice or open format. The complexity of these questions can also be adjusted, for example in Figure 4 the mechanistic arrows could be included in the distractors and answer instead of in the stem. This type of alteration can allow for the assessment of mechanistic thinking (e.g., Bodé et al., 2019; Finkenstaedt-Quinn et al., 2020; Watts et al., 2020; Dood and Watts, 2022). The following examples demonstrate that when the diagnosis/abduction process is utilized, students can develop and enhance their problem-solving skills.

The first example shown in Figure 3 is a case of aromaticity (Jin et al., 2022). Students will typically memorize the requirements and check the structure for being cyclic, planar, containing Huckel's number ($4n+2$) electrons, and a p orbital at every vertex (i.e., conjugated). However, this problem does not ask for a simple definition of aromaticity, but an application of the ruleset to a structure students would not have typically encountered. The diagnosis requires observations about the structure including

Which best explains why this molecule is non-aromatic?



A) The ring has 8 π electrons
B) The molecule is not planar
C) The molecule has no conjugation
D) The molecule is acyclic

Evidence & Observations (What you see)	**Premises (What you know)**	**Reasoned Conclusion (Hypothesis)**
A six-membered ring	Cyclic systems are a requirement for aromaticity (low energy)	This molecule meets the cyclic requirements for aromaticity
Two nitrogen atoms adjacent to two π bonds	A lone pair of electrons on a second-row atom adjacent to a π bond will typically be conjugated and sp^2 hybridized (vinylic)	The lone pairs on nitrogen atoms can be conjugated to the π bonds, making a fully conjugated system
There are 2 π bonds and 2 lone pairs in the cyclic system (8 π electrons)	If a cyclic, conjugated, planar system contains an even number of π electron pairs, the molecule is antiaromatic (high energy)	If the molecule is planar, it will be antiaromatic
The problem states the molecule is non-aromatic	Cyclooctatetraene adopts a non-planar "tub" conformation to avoid antiaromaticity	This molecule is not planar to avoid antiaromaticity
Diagnosis: The molecule is non-aromatic because the ring is not planar.		

FIGURE 3
Diagnosis of an aromaticity problem.

recognition of the implicit lone pairs on the nitrogen atoms and the carbon–carbon π bonds, recall of the requirements of aromaticity, and then application of abductive reasoning to the concepts learned (e.g., in class) and perceived by the structural representation. It is easy to see that the 1,4-dihydropyrazine is cyclic, has 8 π electrons, and a *p* orbital at each vertex. However, this simple analysis would result in the structure being anti-aromatic, so the student must recognize that in order for it to be non-aromatic as the problem states, planarity must be disrupted.

The second example shown in Figure 4 is a curved arrow mechanism problem for a reaction not typically covered in the Organic Chemistry course sequence (Sarode et al., 2016). Students must apply the rules of curved arrows and properly atom map to diagnose the correct product.[7] The pre-existing conditions for a mechanism question with arrows shown include the nature of curved arrows and the examination of the scheme will require atom mapping and keeping track of which bonds are broken and formed.

The third example shown in Figure 5 is a substitution/elimination problem (Brown et al., 1956). Students frequently find these reactions challenging and may employ a variety of heuristic models to approach them. Just as medical diagnosis begins with gathering information (taking patient information), solving this problem begins with direct observation and application of what is known about the structure and reactivity of these molecules. The alkyl halide has a good leaving group and has tertiary electrophilic carbon classification while the *t*-butoxide reagent is electron-rich, bulky, and reactive. Students must reason abductively how these characteristics interact with each other. This iterative process first eliminates S_N2 due to the nature of the alkyl halide, then identifies E2 as the mechanism with the bulky alkoxide. Next, an understanding of thermodynamics vs. kinetics to differentiate the two possible E2 pathways. Finally, a re-examination of the problem indicates the less stable product is formed preferentially; this is *best explained* by steric crowding in the transition state of the reaction between the alkyl halide and alkoxide.

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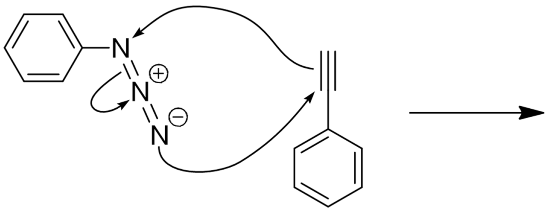
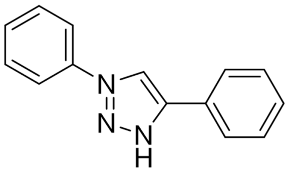
[7] While one could argue that the diagnosis/answer to the problem presented in Figure 4 does not require abductive reasoning, we have included it because the skills required here can be applied to more complex problems that, for example, include mechanistic reasoning (*vide infra*).

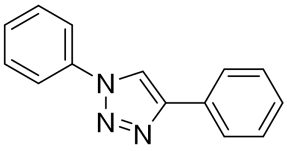
Which of the following is the product of the reaction mechanism (curved arrows)?



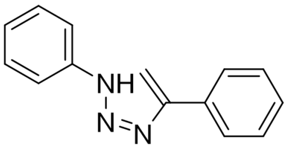
A)



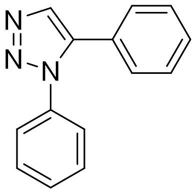
B)



C)



D)

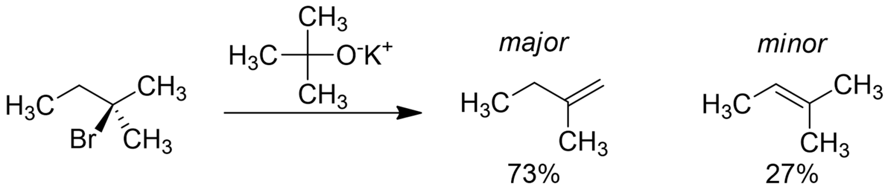


Evidence & Observations (What you see)	Premises (What you know)	Reasoned Conclusion (Hypothesis)
There are 3 curved arrows	Curved arrows represent the movement of a pair of electrons	There should be 3 bonds made/broken
Arrow 1 starts at the negative nitrogen and ends at the alkyne	Negatively charged species are good nucleophiles	The negative nitrogen is the nucleophile and the alkyne is the electrophile
Arrow 1 starts at the negative nitrogen and ends at the alkyne	If an arrow starts at a lone pair and ends at an atom, a new σ bond is formed	A bond is formed between nitrogen and carbon
Arrow 2 starts at the alkyne π bond and ends at the neutral nitrogen	If an arrow starts at a π bond and ends at an atom, the π bond is broken and a new σ bond is formed	A bond is formed between carbon and nitrogen
Arrow 3 starts at the diaza π bond and ends at the positive nitrogen	If an arrow starts at a π bond and ends at an atom, it becomes a lone pair	The central nitrogen is now neutral with a lone pair
There are 5 atoms involved in the 3 arrows	The atoms involved in bond formation need to be connected	A ring is formed
The arrows connect the 5 atoms in the ring in a specific order	Atoms in mechanisms must be mapped	The phenyl groups have a 1,3-relationship
There are no N-H bonds in the starting material*	No arrows involved hydrogen atoms	There are no N-H bonds in the product
Diagnosis: B is the correct product because it has the proper atoms and connectivity		

FIGURE 4
Diagnosis of a mechanism problem.

The final, and most complex, example shown in Figure 6 is a predict the product, addition reaction problem (Inoue and Murata, 1997) that is analogous to halohydrin formation. The problem requires separate diagnoses as it is layered where advancement to the second part is necessitated by the successful completion of the first addition step. Students would need to

Which of the following best explains the reaction?



A) The thermodynamic product predominates due to the stability of the product
B) The thermodynamic product predominates due to steric hinderance in the transition state
C) The kinetic product predominates due to the stability of the product
D) The kinetic product predominates due to steric hinderance in the transition state

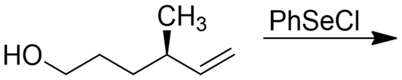
Evidence & Observations (What you see)	**Premises (What you know)**	**Reasoned Conclusion (Hypothesis)**
The organic reactant is a haloalkane	Haloalkanes typically react in substitution or elimination reactions	S_N & E reaction analyses will be needed
The haloalkane contains a bromine	S_N & E reactions require a good leaving group (i.e., I, Br, Cl, OTf, OTs, OMs)	The bromine will act as the leaving group in an S_N or E reaction
The leaving group is on a 3°, electrophilic carbon	Reactions at 3° carbons typically proceed via S_N1/E1/E2	An S_N2 reaction cannot occur
The reagent contains a negatively charged oxygen bonded to an alkane (alkoxide)	Alkoxides can react as strong nucleophiles or strong bases	An S_N2 or E2 reaction can occur
The alkane of the alkoxide is a *tert*-butyl group	Sterically bulky nucleophiles/bases will predominantly react as bases	An E2 reaction will occur
The minor product alkene is more substituted than the major product alkene	More substituted alkenes are more stable (thermodynamic product)	The minor product is the thermodynamic product
The haloalkane is tertiary and the alkoxide is bulky	The transition state will be sterically crowded	The lower energy transition state (kinetic product) leads to the major product

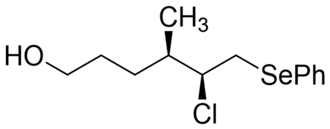
Diagnosis: The preferential formation of the less stable, major product proceeds with a lower energy of activation due to the steric bulk of the alkoxide acting as the base, thus the kinetic product is preferentially formed in this reaction.

FIGURE 5
Diagnosis of a substitution/elimination question.

differentiate between the nucleophilicity of the alcohol and π bond after recognizing them as potential nucleophiles. After using abduction to recognize the higher reactivity of the π bond, students should then reason that selenium is electrophilic, akin to bromine in Br$_2$ due to being polarizable and bonded to a leaving group. This diagnosis is supported when taking into account the stereospecificity of the transformation, which precludes carbocation intermediates. The second diagnosis requires that students recall the regioselectivity of reactions with 3-membered cationic rings at the more substituted carbon. The remaining nucleophilic oxygen atom can now react with a higher energy seleniranium ion. However, conformational analysis of

Which of the following is the major product of the reaction?



A)


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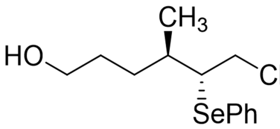
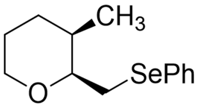
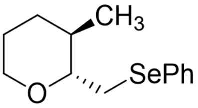
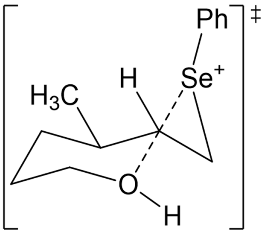


C)


D)


Evidence & Observations (What you see)	**Premises (What you know)**	**Reasoned Conclusion (Hypothesis)**
The organic reactant is an alkene	Alkenes (π bonds) can react as nucleophiles	An alkene addition mechanism may be operative
The organic reactant is an alcohol	Alcohols (lone pair) can react as weak nucleophiles	The alkene is more reactive as a nucleophile than the alcohol
The reagent is an organoselenium compound	Selenium is large/polarizable (akin to bromine) and can form cationic 3-membered rings	A cationic, 3-membered ring containing selenium (seleniranium ion) can be formed
The reagent is a chloroselenium compound	Bonds between large atoms are weak (e.g., Br-Br)	Chloride may be a leaving group in this reaction
Diagnosis: The first step of the reaction involves the formation of a seleniranium ion via nucleophilic attack of the alkene on the chloroselenium electrophile		
The seleniranium ion is formally cationic	Cations are electron poor and electrophilic (e.g., bromonium ion)	The seleniranium ion can react as an electrophile to open the ring
The alcohol remains unreacted	The alcohol is nucleophilic (e.g., halohydrin formation)	The alcohol oxygen attacks the carbon bonded to selenium
This attack will be nucleophilic substitution	Weak nucleophiles attack carbons that bear more partial positive charge	The cationic 3-membered ring will be attacked at the more substituted carbon
This attack will be intramolecular substitution	The alcohol must attack from the backside of the C-Se bond	Attack will occur with less buildup of steric strain in the transition state
Diagnosis: The molecule shown in D will result from the three-step mechanism		



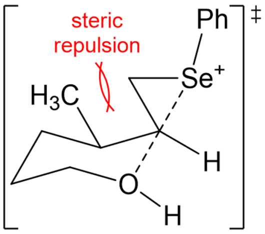


FIGURE 6
Diagnosis of a predict the product reaction.

the transition state is needed to discern the pseudo axial/equatorial approach of the oxygen atom on the seleniranium ion (Figure 6, bottom). Students would then need to apply their knowledge of chair conformations and the lower energy state when having ring substituents equatorial. Thus, the *trans*-oxacyclohexane is formed.

3 Conclusion and future work

While Organic Chemistry is often regarded as the most challenging undergraduate course in the US, we argue it has gotten a "bad rap" because students are not always prepared for the challenges that lie ahead when they enter the course. Students generally perform better on assessments when they employ metacognitive strategies (i.e., "thinking about thinking"). This has been demonstrated in a variety of courses (Arslantas et al., 2018), including Organic Chemistry (e.g., Graulich et al., 2021; Blackford et al., 2023). The consensus is that students who employ more metacognitive strategies in Organic Chemistry are more successful in problem-solving tasks and are better able to use those strategies when they are explicitly modeled and scaffolded. We have argued that instructors of Organic Chemistry should teach and demonstrate how to think and problem solve via "diagnosis" (i.e., abductive reasoning) in their classrooms. We hypothesize that students may score higher on metrics that assess scientific learning when these types of diagnostic models are utilized.

As constructors of nationally standardized exams, we fully acknowledge that a lot of growth on organic chemistry knowledge assessment still remains to be achieved. For Organic Chemistry course instructors, we hope the above insight into abductive reasoning can also be used on the assessment side of teaching requirements. Namely, that the cognitive load placed on students when solving each problem be carefully considered when constructing summative assessment items. Though this point has been frequently made previously (e.g., see Raker et al., 2013), we believe it is worthwhile for all writers of questions in Organic Chemistry to map out, step-by-step, the logic required to solve each question to determine the cognitive load. This can, in turn, help these instructors teach from a novice-focused perspective—as opposed to the "sage on the stage." The prior section provided examples with varying levels of complexity and demonstrated that cognitive load can be approximated by the number of reasoning steps (subtasks) required when the assessment piece is broken down. Further, this process could potentially also help the exam writer identify if items require little to no scientific reasoning (e.g., pure memorization questions).

The above manuscript merely outlines a hypothesis that we have generated over the course of our time teaching Organic Chemistry with this "diagnosis" method of abduction. To fully explore its validity, educational research is needed. This will be a precarious endeavor, because measuring the efficacy of teaching abductive reasoning will require assessment of scientific thinking skills in Organic Chemistry, and, as we just pointed out, there are already strong arguments that we are still quite far away from such valid assessments. However, we can be sure that if you are teaching Organic Chemistry from the perspective of your experience and expertise as an organic chemist, then opening a window for your students into how *you* think and problem solve will benefit your students. Our position is that instructors of Organic Chemistry should not only be explicitly teaching students the abductive reasoning skills to tackle complex problems, but they should also frame it as "diagnosing" the chemical situation.

Data availability statement

The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding author.

Author contributions

JW: Writing – review & editing, Writing – original draft, Conceptualization. MW: Writing – review & editing, Writing – original draft. SZ: Writing – review & editing, Writing – original draft.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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