A multi-institutional study investigating the teaching and learning of organic chemistry

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List of Abbreviations

EPF	Electron Pushing Formalism
EFA	Exploratory Factor Analysis
CERP	Chemistry Education Research and Practice
ILO	Intended Learning Outcome
JCE	Journal of Chemical Education
KMO	Kaiser-Meyer-Olkin measure of sampling adequacy
LO	Learning Outcome
OCI	Organic Chemistry one
OCII	Organic Chemistry two
ORQ	Organic Reactivity Questionnaire
PoM	Patterns of Mechanisms
REB	Research Ethics Board
SPSS	Statistical Package for the Social Sciences
SEBOC	Self-efficacy beliefs organic chemistry
STEM	Science Technology Engineering Math
TCPS	Tri-Council Policy Statement

Abstract

Undergraduate students are completing organic chemistry courses without gaining a firm comprehension of the material (T. L. Anderson & Bodner, 2008; Bhattacharyya & Bodner, 2005, 2014). Traditional organic chemistry curricula have critical drawbacks for students' learning (Cooper & Stowe, 2018; Flynn & Ogilvie, 2015; Stowe & Cooper, 2017). New curricula have been proposed and implemented to address drawbacks but tools are needed to measure the different learning aspects of these curricula. Herein, I describe the development and implementation of two such educational measurement tools to assess different aspects of organic chemistry curricula.

My research consisted of two main projects: 1) exploring undergraduate students' understanding of reactivity principles in organic chemistry by developing and implementing a questionnaire and 2) assessing students self-efficacy beliefs in organic chemistry by developing a quantitative survey. Through my projects we created measurement tools that can be used to assess different aspects of organic chemistry curricula. Both tools place heavy emphasis on reactivity principles in organic chemistry as the key to mastering the subject.

Project 1: Exploring undergraduate students' understanding of reactivity principles in organic chemistry using the Organic Reactivity Questionnaire. A key skill in mastering organic chemistry is recognizing how different chemical concepts, like resonance or electronegativity, influence a reaction's outcome. Undergraduate students often struggle to apply reactivity principles to solve reaction mechanisms. Research has been done on how students interpret mechanistic arrows; however, less is known about how students interpret different chemical concepts when reasoning about reactivity. No measurement tools existed that explicitly examine how undergraduate students interpret different chemical concepts with respect to reactivity. Therefore, we developed an educational tool to measure how undergraduate organic chemistry students interpret chemical concepts and apply reactivity principles, called the Organic Reactivity Questionnaire (ORQ). We administered the ORQ to undergraduate students in Organic Chemistry I and Organic Chemistry II at universities across Canada. We recruited students from four different universities across three provinces to complete the ORQ online.

We analyzed the data to identify themes related to how undergraduate students at the end of Organic Chemistry I interpret reactivity principles. Students' definitions of nucleophilicity and electrophilicity largely aligned with expectations. Students often used electronegativity in their explanations of reactivity even though it was never the most relevant factor for answering the questions. Students struggled to correctly reason using inductive effects and steric hindrance. Students were more successful in determining the direction of an acid–base equilibrium when given pK_a values and would incorrectly associate charge with instability. Participants were largely successful in determining the better leaving group when atom size was the most relevant factor but would still often resort to using electronegativity. Findings from this study can help educators identify where students misinterpret chemical concepts and how educators can then adapt their teaching to address these misinterpretations. From these results, we have identified potential modifications for future implementations of the ORQ such that it could be used as a formative assessment and research tool.

Project 2: Developing the Self-Efficacy Beliefs in Organic Chemistry survey to assess undergraduate students' self-efficacy beliefs in organic chemistry. Self-efficacy beliefs are an individual's beliefs in their ability to succeed at a given task or obtain a certain goal (Bandura, 1977, 2006). Self-efficacy beliefs are correlated with students' achievement in various STEM fields, where students with high self-efficacy in a certain discipline often perform well (Flaherty, 2020). In contrast, low self-efficacy beliefs are associated with high attrition rates and lower student success in STEM courses (Chen, 2014). Organic chemistry has an infamous reputation for being a difficult, content heavy course with high attrition rates (Chen, 2014; Gilstrap, 2020). Little is known about how self-efficacy beliefs in organic chemistry might be related to student success in organic chemistry courses. We developed the Self- Efficacy Beliefs in Organic Chemistry survey (SEBOC) to measure undergraduate students' self-efficacy beliefs in Organic Chemistry I and II. We aligned the SEBOC with the *Patterns of Mechanisms* curriculum at the University of Ottawa and focused its content on reactivity. This study focused on collecting validity and reliability evidence for use of the SEBOC in Organic Chemistry I. Validity is analogous to an instrument's accuracy and is a gauge of whether the instrument is measuring

what it was intended to; reliability is analogous to an instrument's precision and gauges the consistency of the instrument's measurements. We collected validity evidence for face, test content, response process, and internal structure. Validity evidence checks the accuracy of the SEBOC and ensures that it measured what we intended it to. We consulted experts in the fields of organic chemistry, education, and chemistry education to collect validity evidence related to test content. We administered the SEBOC to students in Organic Chemistry I courses that followed a Patterns of Mechanisms curriculum and conducted an exploratory factor analysis to probe the internal structure of the SEBOC. Herein we propose a three-factor structure with 18 items to evaluate undergraduate students' self-efficacy beliefs in organic chemistry. All items possessed strong internal reliability with all Cronbach's α values ≥0.8. The results from the validity and reliability analysis suggest that the SEBOC could be used to accurately assess students' self-efficacy beliefs in introductory organic chemistry courses. Future work using the SEBOC will be to conduct a confirmatory analysis of the proposed model. A confirmatory analysis would provide greater evidence that the SEBOC generates valid data by testing the proposed factor model on the target population (i.e., OCII). Researchers could then use the SEBOC to assess and draw conclusions about the self-efficacy beliefs of the target population.

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Statement of contributions

I would like to acknowledge the work of Keith Lapierre who I worked with to develop the SEBOC (Chapter 4). Keith developed the initial item pool, conducted the pilot study, and conducted the first iteration of exploratory factor analysis.

Chapter 1. Introduction

Chemistry starts with chemistry education. The world currently faces multiple complex socio-scientific issues that impact all life, including climate change, plastic pollution, and an ongoing pandemic (Allen et al., 2022). The chemical sciences offer potential solutions to these problems, but there is currently a decline in students interested in pursuing a career in chemistry (Chen, 2014). Organic chemistry, in particular, is known as a “gatekeeper course” and has a reputation for being content heavy and difficult to understand (Elbulok-Charcape et al., 2021; Shah & Garg, 2017). This reputation, in part, is associated with the idea that organic chemistry requires vast amounts of rote memorization and that many of the concepts are isolated and lack context (Cooper & Stowe, 2018; Grove, Bretz, et al., 2012). Educational reform and curricular change need to be explored to address low attrition rates, develop critical thinking skills in graduates, and produce the next generation of scientists (States et al., 2013). Traditional organic chemistry curricula do not effectively develop students’ critical thinking skills nor aid students to think like experts (Cooper & Stowe, 2018; Flynn & Ogilvie, 2015; Stowe & Cooper, 2017).

1.1.1 The traditional organization of organic chemistry curricula promotes rote memorization

Organic reactions have traditionally been organized based on functional groups in most organic chemistry curricula. For example, reactions related to alcohols are often grouped into one module for teaching. This style of organization is the result of how organic chemistry evolved over time; chemists began categorizing molecules based on their functional groups as new functional groups were discovered through more advanced detection techniques, (Flynn & Ogilvie, 2015). Categorizing molecules based on functional groups can be beneficial when determining molecular structure (e.g., knowing what atoms might be present), but this arrangement does little to explain how reactions take place or the reaction pathway a molecule might follow (Lewis, 2010).

The goal of organic chemistry curricula is to develop expert-like thinking in learners(Chi, 2006; Randles & Overton, 2015). Organic chemistry experts use a mechanistic approach when proposing mechanisms for new reactions. A mechanistic approach looks at the elementary steps involved in a reaction and uses experimental or computational data to identify the most plausible reaction pathways. Experts rely on critical thinking and their knowledge of reactivity principles to propose possible pathways and then test their hypothesis through experiments. The mechanistic approach is a powerful and now commonly used method among practicing organic chemists because it guides the creation of viable hypotheses when predicting mechanisms for unknown reactions (Bhattacharyya, 2013, 2019; Bhattacharyya & Bodner, 2005; Flynn & Ogilvie, 2015). Experts communicate their hypothesis and findings by using the electron pushing formalism (EPF), which can be considered organic chemistry's language.

The electron pushing formalism, first introduced by Kermack and Robinson in 1922 (Flynn & Ogilvie, 2015; Kermack & Robinson, 1922), is a practical tool for communication that aids in visualizing possible reaction pathways. This approach uses arrows to depict the flow of electrons from source (electron-dense regions) to sink (electron-deficient regions) (Bhattacharyya, 2013).. Organic chemists use the EPF to efficiently communicate macroscopic and microscopic processes but learners often struggle to comprehend the EPF's symbolism (Galloway et al., 2017).

Despite the prevalence and benefits of using the EPF in organic problem solving, there is an abundance of research that shows undergraduate (and even graduate) students struggle to use the EPF effectively or do not use it at all (Bhattacharyya, 2013, 2014, 2019; Bhattacharyya & Bodner, 2005; Bodé et al., 2019; Farhat et al., 2019; Flynn & Featherstone, 2017). In a qualitative study, Bhattacharyya and Bodner (2005) interviewed fourteen graduate students in a graduate level Advanced Organic Chemistry course and asked them to propose mechanisms for sets of starting materials and products. They noted that "the curved arrows used in the electron-pushing formalism held no physical meaning for the graduate students involved with this study". To take this finding a step further, Bhattacharyya (2014) reviewed publications relating to graduate students' understanding of reactivity and proposed a model of how graduate students approach mechanistic tasks. In this model, Bhattacharyya suggests that graduate students add electron-pushing arrows only after they identify and recall known functional group transformations or learned reactions (i.e., E1, E2, S_N1, and S_N2 reactions). While this approach may work with problems involving familiar reactions, it becomes less useful when students are faced with novel reactions (Webber & Flynn, 2018). Furthermore, even if a student successfully draws a plausible mechanism, the student may have simply memorized the mechanism without thinking about reactivity (Crandell et al., 2020). There is a disconnect between how experts use the EPF in practice, how the method is taught at the undergraduate level, and how students learn organic chemistry (T. L. Anderson & Bodner, 2008; Bhattacharyya, 2013).

Students must first develop strong content knowledge of core reactivity principles before being able to use the EPF effectively. One large scale study surveyed organic chemistry faculty members across the United States and asked participants: "what skills does one require to develop proficiency in proposing and interpreting electron-, or arrow-pushing mechanisms?" (Bhattacharyya, 2013). Bhattacharyya proposed a list of skills and content knowledge, based on the responses from chemistry faculty, required for the effective use of mechanistic reasoning in practice. Among the list of skills is the ability to identify nucleophiles and electrophiles. A different qualitative study saw undergraduate students being asked to identify nucleophiles and electrophiles for a set of reactions during an interview. That study found that "students feel they need to know the mechanism of a reaction in order to evaluate whether the species involved are nucleophiles or electrophiles" (Anzovino et al., 2015). There is a gap between experts' and novices' beliefs about what prior knowledge is required to understand reactivity principles in organic chemistry (Figure 1.1). Galloway et al. (2018) interviewed OCII undergraduate students and organic chemistry faculty members about how they organized different organic chemistry reactions. They found that professors focused on mechanism type and deeper features (such as electron densities) when sorting reactions, whereas students tended to focus on surface features (such as organic structure and functional groups). Organizing organic chemistry curricula around functional groups can misguide students into using surface features as an effective strategy for interpreting reactions (Flynn & Ogilvie, 2015). The functional group organization also does not reflect the way of thinking of organic chemistry experts, who tend to think about chemical structures in terms of their reactivity and the mechanistic paths shared among different chemical species (Galloway et al., 2018). If the goal of an organic chemistry course is to teach students to think like experts, then we need to give students the tools to reason through a reaction beyond just surface features. This way, students can reasonably predict the mechanism of unknown reactions, and use chemical reasoning like that of experts (Figure 1.1). One potential way of teaching students to think like organic chemistry experts sooner (during an undergraduate degree as opposed to starting during graduate school) is to rearrange the organic chemistry curriculum based on patterns of reaction mechanisms (Cooper & Stowe, 2018). In this way, reactions can be categorized based on reactivity behaviour, rather than focusing on surface features to characterize reactivity (Anzovino et al., 2015, 2016).

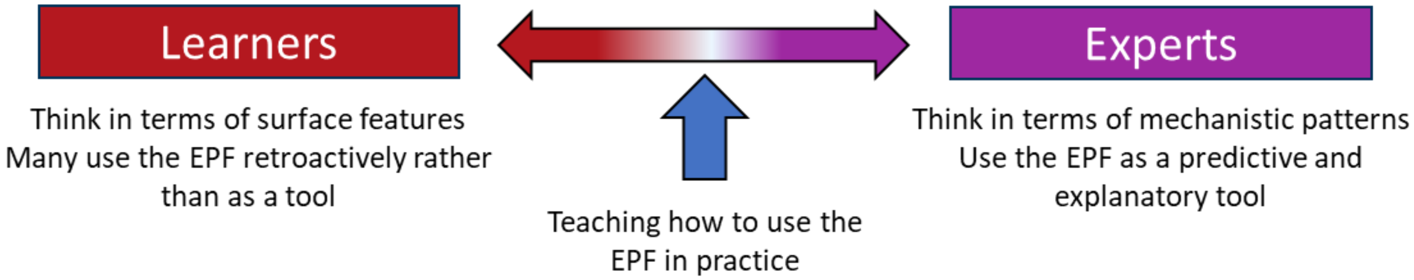


Figure 1.1. Differences between learners and experts using the EPF.

1.2 Several curricula have been proposed to promote meaningful learning

Several new organic chemistry curricula have been proposed and implemented in the United States and Canada with the goal of promoting critical thinking in students. Here we describe the objectives and organization of some of these new curricula.

Traditional organic chemistry curricula that are organized around functional groups lead students to use rote memorization when problem solving (T. L. Anderson & Bodner, 2008; Flynn

& Ogilvie, 2015; Grove, Bretz, et al., 2012). Students progress through a traditional curriculum by studying each individual functional group and examining the possible reactions they can undergo. This approach promotes the rote memorization of functional groups and reactions without understanding the underlying principles of reactivity (Flynn & Ogilvie, 2015). Novel organic chemistry curricula have been implemented to address these shortcomings; Recent curricular reforms include the Spiral organic chemistry curricula (Grove et al., 2008), Organic Chemistry Life the Universe and Everything (Cooper et al., 2019), and the Patterns of Mechanisms curriculum (Flynn & Ogilvie, 2015).

The spiral organic chemistry curriculum implemented at Miami university uses a two semester sequence where the first semester covers a wide range of organic chemistry topics and the second semester revisits the covered topics in greater depth (Grove et al., 2008). The spiral organization aims to promote meaningful learning by having students revisit topics in depth rather than learn difficult concepts based on little-to-no background knowledge. By using qualitative interviews and essays, they found that students appreciated the change to the spiral curriculum and made more sense of the material's layout (Grove et al., 2008); Attrition rates during the implementation of the spiral curriculum were also lower compared to previous years. The OCLUE curriculum was first enacted at Michigan State University and emphasizes causal mechanistic reasoning (Cooper et al., 2019). The first semester of OCLUE introduces students to organic structure-function relationships, spectroscopy, and arrow-pushing while the second semester goes into detail about mechanisms involving π-bonds. In a large scale study, Houchlei et al. (2021) found that students in the OCLUE curriculum were more likely to draw mechanistic arrows, produce mechanistically reasonable steps, and produce plausible products for an unfamiliar reaction compared to non-OCLUE students. The spiral and OCLUE curricula demonstrate that reorganizing an organic chemistry curriculum away from the traditional approach can aid students to develop more expert-like thinking.

1.3 The Patterns of Mechanisms curriculum at the University of Ottawa aims to promote expert-like thinking in students

The Patterns of Mechanisms curriculum is based on four guiding ideas 1) teaching the electron pushing formalism before any reactions, 2) using patterns of reactivity to teach reactions, 3) teaching concepts that can be transferred to other disciplines, 4) promoting self-efficacy in organic chemistry (Flynn & Ogilvie, 2015; Ogilvie, 2017). Figure 1.2 depicts the reactivity portion of the PoM curriculum organized by mechanistic categories. The PoM approach explicitly teaches students about the electron-pushing formalism before introducing any reactions or specific mechanisms.

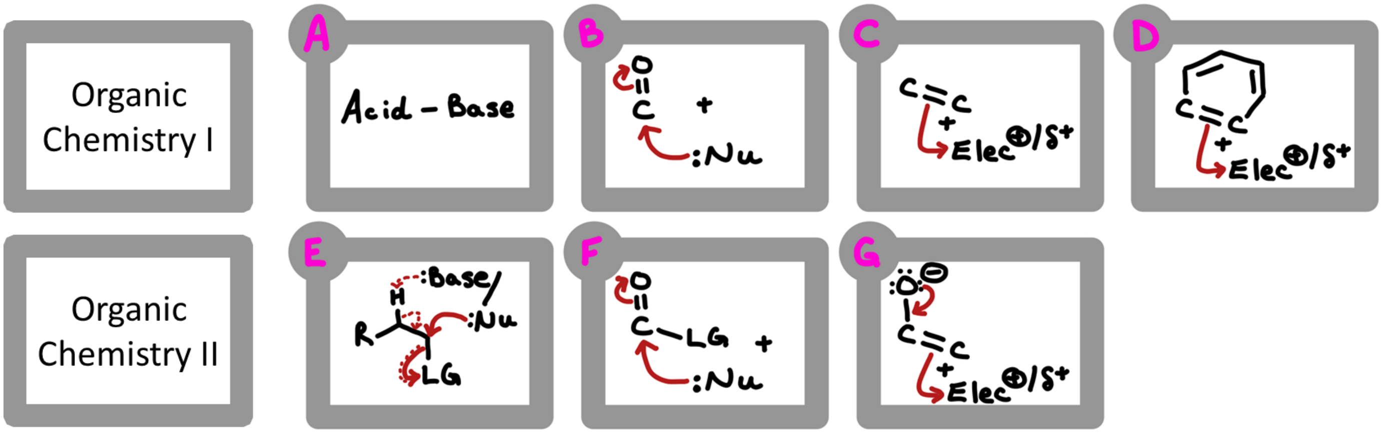


Figure 1.2. Overview of the reactivity aspect of the Patterns of Mechanisms curriculum at the University of Ottawa organized by mechanistic categories. Students progress from simple (acid-base) to more complex reactions (enolates). Each mechanistic category pictured here was used as part of the organic card-sort assessment tool (Galloway et al., 2019, Lapierre and Flynn 2020).

The EPF is organic chemistry's language and has its own distinct set of rules and symbols. Students are initially taught the EPF so they can later focus on understanding mechanisms rather than decoding the symbols of the EPF. Once students have been taught the formalism, they are taught how to use it in the context of acid-base reactions before moving into more complex mechanisms that involve π-bonds (Figure 1.2). Reactions are organized based on mechanism type rather than functional group because it reflects how experts think about reactivity. The PoM curriculum also covers structure-function relations specific to stereochemistry and conformational analysis; molecular orbital theory is taught throughout with each new reaction and students are taught spectroscopy in OCII (Figure 1.3). Organic chemistry is not an isolated field and the way of thinking used in organic chemistry can often be applied to other sciences such as biochemistry (Allred et al., 2021; Bell et al., 2019) and medicine. OCI and OCII are prerequisite courses at the University of Ottawa; as such, the organic chemistry curriculum should be organized and taught in a way that is transferable to concepts in biochemistry (Shaffer et al., 2016).

An impactful curriculum emphasizes not only content knowledge but also promotes a meaningful understanding of affective skills, such as high self-efficacy beliefs (Bandura, 1977). Self-efficacy, a person's belief that they can be successful (Bandura, 1977), is a prominent component that contributes to how students learn chemistry (Gibbons & Raker, 2019; Vogel & Human-Vogel, 2016).

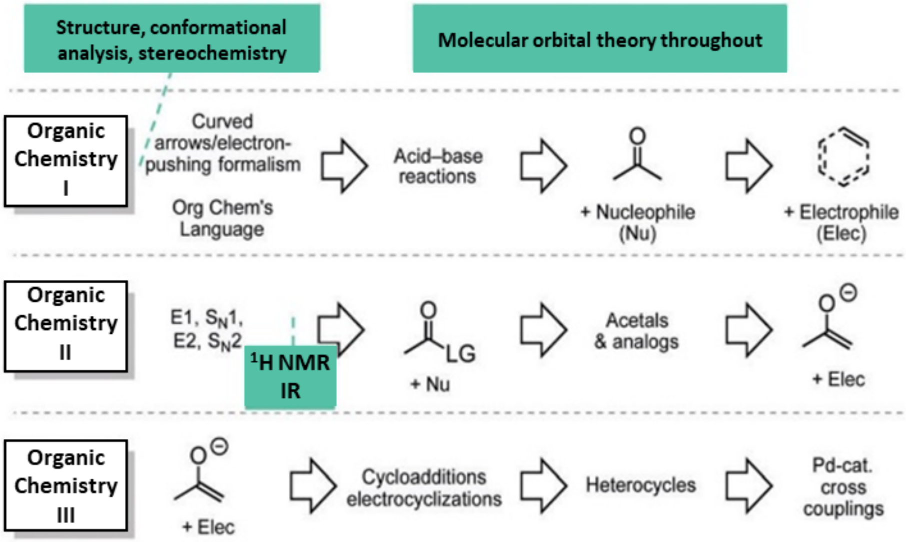


Figure 1.3. Overview of the Patterns of Mechanisms curriculum.

1.4 Curriculum evaluation is necessary to ensure that curricula are effective

Curricular evaluation is necessary because we are unable to tell if curricula are meeting the learning goals set out by educators without measuring students' achievement of the established learning outcomes.

The structure and organization of a curriculum should be based in theory with the goal of promoting meaningful understanding of concepts. A guiding theory for a curriculum can include theories of learning (e.g., social cognitive theory or information processing theory), as well as curricular frameworks containing broad and specific learning outcomes (Towns, 2010). The content and the learning environment in which the material is taught can be as important as how it is taught with respect to student learning (Ralph et al., 2022). As such, an effective organization of the material that promotes meaningful learning is essential in the knowledge acquisition process. The curriculum must then be evaluated for effectiveness once a theory or curricular framework has been established. Curricular evaluation is a very vague term that encompasses multiple aspects of learning that are often too numerous to measure in their entirety. It is much more practical to evaluate aspects of a curriculum directly related to its learning outcomes and theory rather than attempt to measure every possible aspect related to learning. Curricular evaluation "offers an opportunity for data-supported reflection and discussions on the current curriculum, as a first step towards change" (Raycroft & Flynn, 2020).

1.5 Evaluating the patterns of mechanisms curriculum: support for meaningful learning

An evaluation of the Patterns of Mechanisms curriculum has been underway at the University of Ottawa to discern what connection the new curriculum has with students' understanding of organic chemistry (Figure 1.4). Curricula encompass more than just cognitive knowledge, as such multiple measures and assessments of different domains are necessary to evaluate how a curriculum is connected to student learning. Flynn & Featherstone (2017) conducted an exam analysis looking at how students in the PoM curriculum solve and interpret questions involving the EPF, such as the strategies students used and errors students made. They sampled OCI and OCII students on "draw the arrow" and "draw the product" questions for reactions the students had never seen before. Students were given all the information required to solve the question (i.e., all the students needed to do was interpret the EPF) without needing to know the mechanism. Students performed better on "draw the arrow" questions; however, students in the PoM curriculum drew few reverse or illogical arrows, an error more commonly seen from students in functional group curricula (Flynn & Featherstone, 2017). Exams were analyzed in a separate study to compare the success rates on mechanistic-type questions before and after the PoM curriculum change. Success rates in that study were higher on unfamiliar questions for students in the PoM curriculum compared to students in a traditional curriculum ($U = 14{,}104.5$, $p < 0.001$ with a medium effect size (Cohen's $d = 0.38$)) (Webber & Flynn, 2018). The results from these studies suggest that students within the PoM curriculum are better prepared to correctly use the EPF when problem solving in organic chemistry. Galloway et al. (2017) investigated students' interpretations of mechanistic language through qualitative interviews, where students in the PoM curriculum were asked to describe their thought process as they solved unfamiliar reactions. They found that OCI students in that sample ($N = 29$) thought about arrow-pushing and bond-breaking as the movement of electrons, before formally being taught specific reactions. This result was encouraging since students in the PoM curriculum are explicitly taught the EPF and the meaning of arrows before learning specific reactions (Galloway et al., 2017). Other aspects of the PoM curriculum, in addition to the previous studies on students' interpretations of organic chemistry's language, have also been investigated. Galloway et al. (2018a) compared how experts and students in the PoM curriculum organized organic reactions and found that experts would often sort by mechanism type (deep features), whereas undergraduate students would often sort by functional group (surface features). This observation led to the creation of a summative card-sort task (Galloway et al., 2019; K. R. Lapierre et al., 2022; K. R. Lapierre & Flynn, 2020) to evaluate students' mechanistic thinking via the categorization of different reactions (Figure 1.2). 24 students participated in a card-sort task study and completed both an early (beginning of the course) and late (end of the course) administration of the card-sort task during OCII. There was a significant change in how students sorted reactions from the early to late administrations, with an increase in the number of students sorting by reaction type (37% early administration to 58% late administration, $W= 38$, $p = 0.022$, $r = 0.332$) and a decrease in students sorting by structural features (45% early administration to 21% late administration, $W = 20$, $p = 0.007$, $r= 0.386$) (K. R. Lapierre & Flynn, 2020). The card-sort task was found to produce valid and reliable data for evaluating OCI and OCII students' understanding of mechanistic patterns within the PoM curriculum (K. R. Lapierre et al., 2022). Other studies within the PoM involve mechanistic reasoning and its associated reasoning skills. In a qualitative study, Bodé et al. (2019) noticed that students in the new curriculum often used causal arguments when reasoning about the most likely mechanistic pathway on an OCII exam question. Only one of these studies (Webber & Flynn, 2018) directly compared assessment results between the old curriculum and the redesigned PoM curriculum using an exam analysis. The exam analysis found that students performed better on familiar and unfamiliar exam questions in the PoM curriculum compared to the old curriculum (Webber & Flynn, 2018). While the results were encouraging, this single comparison does not provide sufficient evidence to demonstrate that the PoM curriculum benefits student learning more than traditional curricula. Furthermore, mechanistic problem solving, while very prominent in organic chemistry, does not represent the full extent of knowledge students gain in OCI or OCII. More evidence with a broader context is needed to establish the relationship between the PoM curriculum and how students learn organic chemistry. There is currently a lack of quantitative studies and quantitative instruments for assessing cognitive skills in organic chemistry based on the PoM curriculum as well as a lack of assessment tools for the affective domain (e.g., self-efficacy). Furthermore, comparison studies between the PoM curriculum and other Canadian curricula could provide evidence that the PoM organization promotes meaningful learning in students compared to traditional curricula. My projects aimed to create measurement tools to investigate other areas of organic chemistry curricula, specifically reactivity principles and self-efficacy beliefs.

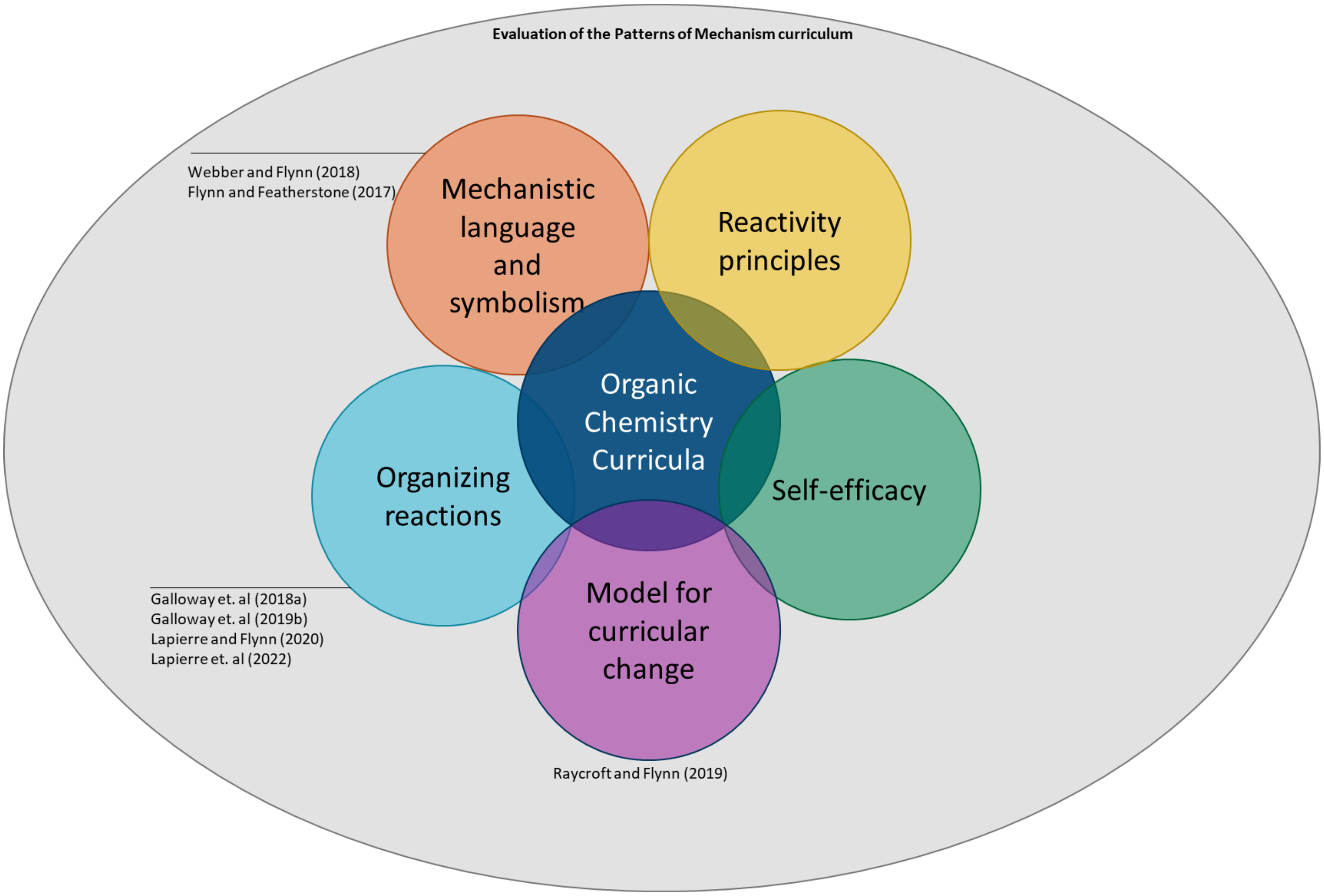


Figure 1.4. Evaluation of the Patterns of Mechanisms curriculum.

1.6 Research Questions and goal for this thesis

The goal of this thesis is to design and validate instruments for the Canada-wide curricular evaluation. This work builds on previous studies with the goal of further evaluating the PoM curriculum and its connections to student learning. Specifically, this work investigates less explored aspects of the PoM curriculum: how students in the PoM curriculum interpret reactivity principles and students' self-efficacy beliefs in organic chemistry. Herein, we describe the development of two chemistry education questionnaires, known as educational research instruments, that can be used to investigate these two aspects of the PoM curriculum.

The first project (Chapter 3) describes the development and implementation of the Organic Reactivity Questionnaire (ORQ) to qualitatively assess students' understanding of reactivity principles. The specific research questions for this project were: *How do undergraduate students interpret reactivity principles with respect to nucleophilicity and electrophilicity? What factors do undergraduate students consider when determining the direction of an acid-base equilibrium? What factors do undergraduate students consider when determining leaving group stability?*

The second project (Chapter 4) describes the development of the Self-Efficacy Beliefs in Organic Chemistry (SEBOC) survey which can be used to assess students' self-efficacy beliefs in organic chemistry with a focus on reactivity principles. The goal of this project was to collect validity and reliability evidence for the SEBOC in the context of OCI and OCII courses.

Once established, we can use these instruments to efficiently assess undergraduate students' interpretations of reactivity principles and their self-efficacy beliefs towards organic chemistry. These instruments can give educators a better idea of where students struggle or excel within a specific curriculum. Educators can then design new teaching interventions or make changes to specific aspects of the curriculum to better aid student learning.

Chapter 2. Theoretical Frameworks and Positional Statement

2.1 Intended, Enacted, and Achieved curriculum

A curriculum is more than just an outline of information that students are expected to learn over several courses. Curricula encompass educators' expectations of students, students' acquisition of knowledge and skills, and students' abilities to demonstrate what they have learned. We used the Intended, Enacted, and Achieved curricular framework (Raycroft & Flynn, 2020) to guide this curricular investigation. Within the intended curriculum there are intended learning outcomes (ILOs), the "knowledge, skills, and values students are expected to demonstrate by the end of a course (Biggs & C., 2011; Krathwohl, 2002; Towns, 2010) and inform how a curriculum is enacted. The enacted curriculum encompasses all aspects of a course that help students achieve the intended learning outcomes. The enacted curriculum can be categorized into three main components: taught, practiced, and assessed. The taught component communicates the intended learning outcomes to the learners (Carle & Flynn, 2020) and includes lectures, videos, textbooks, and class notes. The practiced component gives learners an opportunity to consolidate what they have been taught through formative assessments and homework. The assessed component includes summative assessments such as midterms, exams, and final projects. Finally, the achieved curriculum encompasses the degree to which each ILO has been reached. To determine if the ILOs have been reached by the learners one could look at their answers to specific questions on exams and performance on extracurricular evaluation tools (such as instruments designed to probe specific LOs). The current research investigates the achieved component of the curriculum by analyzing students' answers on chemistry education instruments.

2.2 Self-efficacy beliefs

Self-efficacy beliefs is an aspect of social cognitive theory defined as an individual's beliefs in their ability to successfully perform a task or complete a goal (Bandura, 1997). Self-efficacy beliefs are directly related to an individual's ability to perform a given task and influence learning (Schunk & Usher, 2012). Bandura (1997) theorized four sources contributing to an individual’s self-efficacy beliefs: mastery experiences, vicarious experiences, verbal persuasion, and emotional/physiological states. Mastery experiences are thought to possess the most influence over a person’s self-efficacy beliefs, as an individual’s experiences and past performances act as a tangible indicator of their capabilities. For example, an individual who has viewed their experience in general chemistry as successful may have an increased self-efficacy belief toward chemistry as they transition to organic chemistry courses. Self-efficacy has been found to be positively correlated to achievement outcomes in many studies, as well as adaptive motivational processes, effort, and persistence (Pintrich and De Groot, 1990; Multon et al., 1991; Pajares and Miller, 1994; Zusho et al., 2003). Self-efficacy has been found to correlate moderately with other affective measures directly related to chemistry such as chemistry identity (Hosbein & Barbera, 2020; Kurbanoğlu & Akin, 2012), chemistry self-concept (Gibbons & Raker, 2019), and chemistry mindset (Santos et al., 2022).

2.3 Positional Statement

A positional statement describes the researcher’s beliefs, experiences, perspectives that may influence how they conduct a study and draw conclusions (Holmes, 2020). All researchers bring bias into research based on their personal views and experiences; as such, the purpose of a positional statement is to identify and acknowledge the biases brought in by the researcher.

I have a Bachelor’s degree in Biomedical Sciences from the University of Ottawa. I went through the same organic chemistry curriculum as the participants in the studies presented here. My experience with this curriculum differed substantially then the participants in this study in that I did not take organic chemistry online during a pandemic and so I analyzed participants’ responses from the point of view of someone who did not learn organic chemistry in an online setting. I am a strong believer in evidence-based teaching and have conducted previous work in chemistry education during my undergraduate degree. My experiences and beliefs may introduce bias in my research; as such, the purpose of this positional statement is to clarify the point of view from which I conduct chemistry education research.

Chapter 3. Exploring undergraduate students' understanding of reactivity principles in organic chemistry using an Organic Reactivity Questionnaire

3.1 Introduction

Organic chemistry has a reputation for a being a difficult and demanding course and is often considered a gatekeeper to the sciences (Elbulok-Charcape et al., 2021; Shah & Garg, 2017). Students perceive organic chemistry as daunting because of the deceptively vast amounts of memorization required to learn the multitude of reactions each functional group can undergo (Grove, Bretz, et al., 2012). Furthermore, students are required to simultaneously learn the nuances of the electron pushing formalism, organic chemistry's language, to produce viable mechanisms for the reactions they just learned. Organic chemistry experts use the EPF as a problem solving tool and will often conceptualize reactions based on their mechanisms rather than surface features (Galloway et al., 2018); conversely, students will often rely on rote memorization of mechanisms for specific reactions taught in class rather than using the electron pushing formalism as a problem solving tool (Bhattacharyya, 2014; Bhattacharyya & Bodner, 2005; Grove, Cooper, & Rush, 2012; Houchlei et al., 2021). Graulich notes that "understanding the embedded basic concepts in organic chemistry and using this knowledge as a source of prediction are huge challenges for students" (Graulich, 2015). Organic reactivity principles are inherent to reaction mechanisms and students need to be able to reason between the different reactivity principles involved to predict a viable mechanism (Bhattacharyya, 2013, 2014). An abundance of research has been done on students' abilities (or lack thereof) to use mechanistic reasoning and the EPF to solve mechanistic problems (Bodé et al., 2019; Caspari, Kranz, et al., 2018; Flynn & Featherstone, 2017; Graulich & Bhattacharyya, 2017; Grove, Cooper, & Cox, 2012; Grove, Cooper, & Rush, 2012; Houchlei et al., 2021; Lieber & Graulich, 2020). Much less is known about what chemical concepts students leverage and compare when making decisions about reactivity. Chemical concepts that influence reactivity can include, but is not limited to resonance/delocalization, atom size, electronegativity, pK_a values, charge, and steric hindrance.

3.1.1 Prior research on students’ understanding of chemical concepts related to reactivity

Students will often use a single parameter when making decisions about reactivity rather than weighing different chemical properties to derive causal explanations (Bhattacharyya, 2014; Eckhard et al., 2022). Students must be able to use multivariable reasoning to effectively solve reactivity tasks as there are often multiple factors simultaneously involved in determining reactivity (Eckhard et al., 2022). Students’ must use their reasoning skills to make viable judgements about which chemical concept(s) are most relevant for a given context and how they might influence reactivity.

3.1.1.1 Resonance

Several studies have explored undergraduate students’ ideas about resonance and all unanimously cite resonance as an essential concept for understanding reactivity in organic chemistry (Betancourt-Ṕerez et al., 2010; Brandfonbrener et al., 2021; Carle & Flynn, 2020; Kim et al., 2019; Xue & Stains, 2020). One quantitative study identified medium significant correlations between students’ grade in organic chemistry and their ability to 1)draw curved arrows to represent electron movements between adjacent atoms in resonance structures; 2) draw alternate Lewis structures to represent a given ion or molecule (Betancourt-Ṕerez et al., 2010). An exploratory study investigated how students interpreted resonance and resonance structures in general (Xue & Stains, 2020). They found students in the first semester of organic chemistry often demonstrate alternative concepts about resonance and have difficulty in identifying underlying features of resonance structures. Another qualitative study analyzed students’ responses to a Writing to Learn assignment designed to elicit students’ explanations of resonance and its influence on reactivity to a general, non-scientific audience (Brandfonbrener et al., 2021). Most students in that study associated resonance with an increase in stability but often did not consider the context of comparing multiple structures. Their findings suggest that the students in their study “may hold a rule-based understanding of the relationship between resonance and stability” (Brandfonbrener et al., 2021). Ten essential learning outcomes for delocalization have been identified and four of them directly relate resonance and reactivity: LO7 use delocalization concepts to determine to determine and justify the relative stability/energy/reactivity of ions; LO8 use delocalization concepts to explain relative acidity/basicity; LO9 determine and justify the electrophilic and nucleophilic sites on a molecule using delocalization concepts; LO10 use delocalization concepts to predict and justify the course of a reaction (Carle & Flynn, 2020).

3.1.1.2 Acid–base reactions and pK_a values

Acid–base mechanisms are one of the most common mechanism types found in biological systems, enzyme interactions (Holliday et al., 2007; Nath et al., 2014), and biochemistry in general (Bell et al., 2019). Students need to have a solid understanding of acid-base mechanisms because it will likely be the most applicable skill in their future careers. Students' understanding of acid–base reactions and pK_a values have been a large focus of the CER community over the past ten years (Bretz & McClary, 2015; Cooper et al., 2016; Flynn & Amellal, 2016; McClary & Bretz, 2012; Petterson et al., 2020; Schmidt-McCormack et al., 2019; Stoyanovich et al., 2015; Yik et al., 2021). Researchers in one study administered a pen and paper concept inventory on acid strength to second semster undergraduate students (*N*=89) in a spiral organic chemistry curriculum (Bretz & McClary, 2015). Of the students, ~30% of students in their study held alternative conceptions about acid strength where students relied on functional groups and stability to determine acid strength. Students primarily focused on structural features without considering underlying electronic features. In their follow-up study, Bretz & McClary (2015) expanded their sample to Organic Chemistry II classes from two universities using different curriculla (N=342) and used a pre/post test design to identify changes in conceptions. They identified no changes after an additional semster of organic chemistry and observed that their results were independent of curricullum type (Bretz & McClary, 2015). Cooper et al. (2016) investigated students' reasoning skills about acid–base reactions and found that students who elcited causal reasoning on acid–base questions tended to have higher success on drawing mechanisms for acid–base reactions, providing further evidence of the importance of acid–base knowledge to solving mechanistic tasks. Stoyanovich et al. (2015) developed acid–base learning outcomes for the Patterns of Mechanisms curriculum and identified essential knowledge required for 28 commonly taught reactions. Resonance, electronegativity, and inductive effects were the most prominent factors required to understand the 28 reactions, with >40% of all reactions requiring at least one of them to understand. Petterson et al. (2020) interviewed 13 undergraduate students and asked them to solve three different acid–base mechanisms. The students in ther study were split into two groups, one group solved the problems using pencil and paper while the other used a mechanisms app. Students would often focus on explicit features with little consideration for electronics. The students in their study who were aided by a mechanisms app would more often consider alternative reaction pathways compared to stuents who used pencil and paper.

Overall, research on undergraduate students' understanding of acid–base chemistry reveals that students often focus on surface features when problem solving and that there exists a relationship between students' success with acid–base reactions and their understanding of mechanisms. The focus of previous studies has mainly been on students' interpetations of acid–base mechanisms and their ability to correctly use pK_a values. It is still unknown what reactivity principles students leverage when solving acid–base reactions.

3.1.1.3 Steric hindrance

Steric hindrance is a topic essential to reactivity that often determines the mechanistic path a reaction will take (Anslyn & Dougherty, 2006; Clayden et al., 2001; Ogilvie, 2017). Steric hindrance is "the repulsive force experienced by large substituents" (Clayden et al., 2001) where molecules with larger steric bulk tend to be less reactivity. Much less is known about students' understanding and interpretations of steric hindrance in the context of reactivity despite its omportance in determiming mechanistic paths. In a qualitative study analyzing students' reasoning about mechanisms, Finkenstaedt-Quinn et al. (2020) observed students' problematic reasoning where using sterics to justify carbocation stability in the products rather than focusing on the effects sterics has on the reactants. (Bodé et al., 2019) conducted an exam analysis to examine how students in OCII used mechanistic reasoning when determining the likelihood of an S_N1 reaction to proceed. Students in their study who selected the incorrect claim would often use steric hindrance as a relevant factor when it was irrelevant to answering the question. Students appear to make the most errors around steric hindrance because they are sometimes unsure about when it is a relevant factor. We still do not have a firm understanding of how students' interpret steric hindrance and more work needs to be done to investigate students' interpretations.

3.1.1.4 Electronegativity

An exam analysis conducted in a Patterns of Mechanisms curriculum found that students would often consider electronegativity in solving mechanism style questions (Webber & Flynn, 2018). DeFever et al. (2015) observed that students would often focus on the atomic scale rather than the molecular for concepts such as electronegativity. (Talanquer, 2018b) notes that students' difficulties with reaction may arise from over-focusing on atomic properties like electronegativty rather than considering molecular properties. Furthermore, electronegativity is often used as a heuristic by students to quickly weigh chemical properties based on memorized rules (Maeyer & Talanquer, 2013; Talanquer, 2014). Heurisitcs are problem solving techniques that use "rules of thumb" to arrive at a solution quickly. Heuristics can be useful when working through time sensitive tasks, like writing an exam, but may cause systematic errors in judgement if overrelied on (Talanquer, 2014).

3.1.1.5 Charge

In a qualitative interview study, Anzovino and Bretz (2015) observed that students would often mention charge when defining nucleophiles and electrophiles, refering to electrophiles as (usually) having a full positive charge and nucleophiles a full negative charge. Charge is an explicit strucutural feature and does not encompass the functional aspect of nucleophiles and electrophiles. Only a single student in their study defined nucleophies and electrophiles in terms of functionality, where nucleophiles donate electrons and electrophiles accept electrons. Galloway et al. (2017) interviewed 29 OCI students and asked them to work through organic mechanism tasks to investigate how undergraduate students interpreted organic chemistry's symbolism. Students frequently discussed charge during all tasks and would often emphasize charge over electron movement. Students sometimes discussed charge as if it were an object that could be moved or placed, which could hinder their thinking about electron movement and would often focus on neutralizing chrage when working through reactions (Galloway et al., 2017).

3.1.2 Patterns of Mechanisms curriculum

A redesigned organic chemistry curriculum, organized around mechanistic patterns, was implemented at the University of Ottawa with the goal of helping students to problem solve like organic chemistry experts and reduce cognitive load. A big part of teaching students to think like organic chemistry experts involves comparing chemical concepts to determine reactivity.

3.2 Theoretical framework

3.2.1.1 Claim-Evidence-Reasoning

Traditional organic chemistry assessments of mechanistic tasks, where students are given starting materials, reactants, and products, may not be accurate evaluations of students' mechanistic reasoning abilities (DeCocq & Bhattacharyya, 2019). Chemistry assessments that emphasise the recall of facts and rote memorization may not be an accurate representation of students' understanding if they are not prompted to use their knowledge meaningfully (Cooper & Stowe, 2018). Encouraging students to explain their reasoning on both formative and summative assessments allows them to practice their reasoning skills, instead of focusing on rote memorization and recall, and provides a stronger assessment tool for students to demonstrate their understanding of organic chemistry concepts (Crandell et al., 2020). Bretz & McClary (2015) recommended that students be prompted to explicitly state *why* they made their decisions when answering questions about reactivity (I.e., which species is the acid/base, nucleophile/electrophile). Several calls to action have suggested benefits for prompting students to practice scientific reasoning (Cooper, 2015; Talanquer, 2018a) and it has also been suggested that prompting students to use their knowledge to construct explanations provides stronger evidence of students' knowledge coherence (Cooper & Stowe, 2018). Assessment tasks should be designed using theory and evidence based practices to effectively scaffold students’ use of scientific reasoning (Caspari & Graulich, 2019; Crandell et al., 2020). The claim-evidence-reasoning framework for scientific argumentation has been used to design tasks to elicit students’ reasoning in different chemistry education contexts (Becker et al., 2013) including undergraduate organic chemistry courses (Bodé et al., 2019; Deng & Flynn, 2021; Lieber & Graulich, 2022). We used the claim-evidence-reasoning framework (Figure 3.1)in the current study to scaffold students’ responses and gain a better understanding of why they chose their answer. We first asked students to state a claim (select an answer from the options given), select evidence to support the claim (factors involved in reactivity), and then provide reasoning to explain why they chose the claim and evidence (open-ended response).

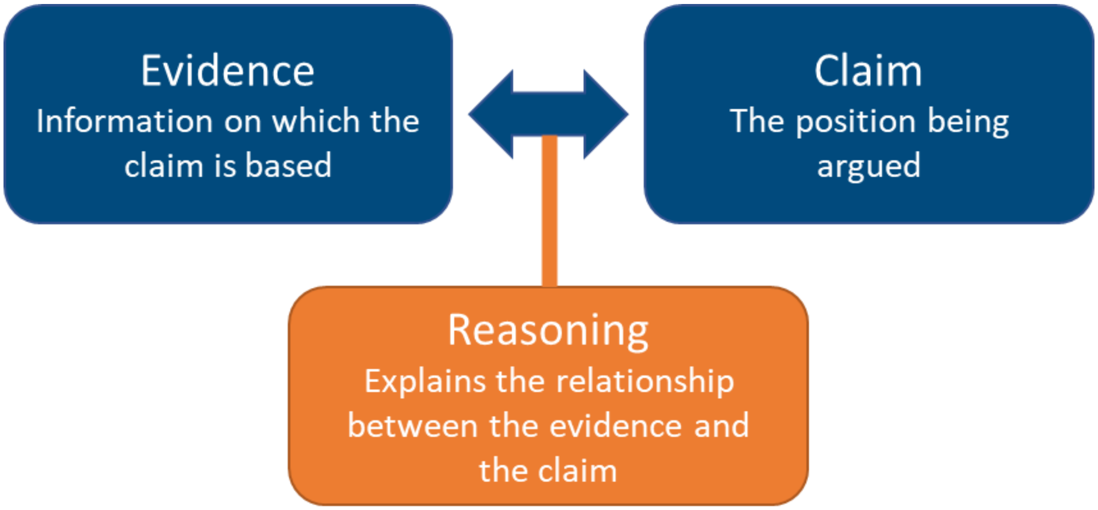


Figure 3.1. Claim-evidence-reasoning framework.

3.3 Goals and Research Questions

The goal of the current study is to propose an evaluation model for reactivity principles in organic chemistry and to create a questionnaire based on this model to evaluate students’ understanding of reactivity principles. The research reported herein is part of a broader study to evaluate the *Patterns of Mechanisms* curriculum with respect to other organic chemistry curricula at Canadian institutions. Identifying a set of core reactivity principles would help identify part of what students would benefit from knowing by the end of an organic chemistry course. Ideally, those core principles would also be transferable to and applicable in related disciplines, such as biochemistry. In principle, students who are proficient in analyzing and applying these principles would be able to more readily apply their knowledge in new contexts (within organic chemistry or in related disciplines such as biochemistry). We can then use this model to build assessment tools and, using the results from those tools, inform the refinement of curricula. The following research questions guided our analysis:

RQ 1: How do undergraduate students interpret reactivity principles with respect to nucleophilicity and electrophilicity?

RQ 2: What factors do undergraduate students consider when determining the direction of an acid–base equilibrium?

RQ 3: What factors do undergraduate students consider when determining leaving group stability?

3.4 Methods

3.4.1 Ethics

Ethics approval (or exemption) from an internal Research Ethics Board (REB) is required before conducting any research with humans in Canada (Canadian Institutes of Health Research et al., 2018). We obtained ethics approval from our host institution's REB before proceeding with this study; we also obtained ethics approval from all other institutions from which we recruited participants as outlined by the tri-council policy statement (Canadian Institutes of Health Research et al., 2018). We followed a *Reciprocal Research Ethics Board Review model* where we received clearance from each individual institution's REB based on the full ethics review of this study, conducted at our own institution (Figure 3.2). This project was granted allowance for a truncated review by each REB because it was categorized as a minimal risk study. Each institution's ethics office had their own internal requirements for reviewing studies hosted by external researchers.

3.4.1.1 Review procedure

We contacted the ethics office for each university we intended to recruit from and provided them with our full ethics review application and certificate of ethics clearance (# H11-18-1363). The ethics officers from each university replied with next steps for clearing our study at their institutions. One institution required an informal review of our ethics application and clearance by the Chair of their REB; The Chair reviewed our ethics documents and gave us clearance. A different university required us to have a local PI and for their REB to conduct a formal, truncated review of the study; We enrolled a local professor from that university and the REB gave us clearance after conducting a review. Two other universities conducted truncated reviews, based on our ethics application and clearance certificate, and issued us Letters of Acknowledgement. The Letters of Acknowledgment confirmed that the local REBs reviewed and cleared our study while allowing our REB to maintain primary responsibility for our project.

Figure 3.2. Steps to obtain ethics approval from external universities.

3.4.2 Participants and context

The local administration for this research was conducted in Organic Chemistry II courses taught at a large, research-intensive Canadian university. "OCII is the students' second semester of organic chemistry. OCI is offered in the winter semester of students' first year of their studies, and OCII is offered in the summer and fall. Students can take these courses in English or French. OCII is a 12-week course consisting of two weekly classes (200−400 students total, 1.5 h each, mandatory, lecture or flipped format) and a tutorial session (1.5 h, optional, also called a recitation or discussion group). Assessment for the course is composed of two midterms, a final exam, online homework assignments, and class participation using a classroom response system. The general topics covered in OCII include reactions with σ electrophiles (e.g., $S_N1/S_N2/E1/E2$, and oxidation reactions), introduction to 1H NMR and IR, reaction of π electrophiles with leaving groups, and reactions with π nucleophiles (e.g., aldol reaction)" (Flynn & Ogilvie, 2015).

All other participants were recruited from large, research-intensive Canadian universities. Two universities were located in Atlantic provinces (A), two were located in Central Canada (C), and one was located in the Prairie provinces (P). This convenience sample was selected based on course type, as all these universities offered OC I during the Fall semester. All schools followed a traditional organic chemistry curriculum where reactions with σ electrophiles (e.g., S_N1/S_N2/E1/E2) were taught in OC I. Participant information is summarized in Table 3-1.

Table 3-1. Summary of participants recruited for this study.

Location	Course	n*	n
Atlantic	Organic Chemistry I	4	1
Central (a)	Organic Chemistry I	12	10
Central (b)	Organic Chemistry I	9	6
	Introduction to Biochemistry	7	5
Prairie	Organic Chemistry I	10	8
University of Ottawa	Organic Chemistry II	67	45
Total		109	75

n* the number of participants who consented and completed at least one question.

n the number of participants who completed all questions.

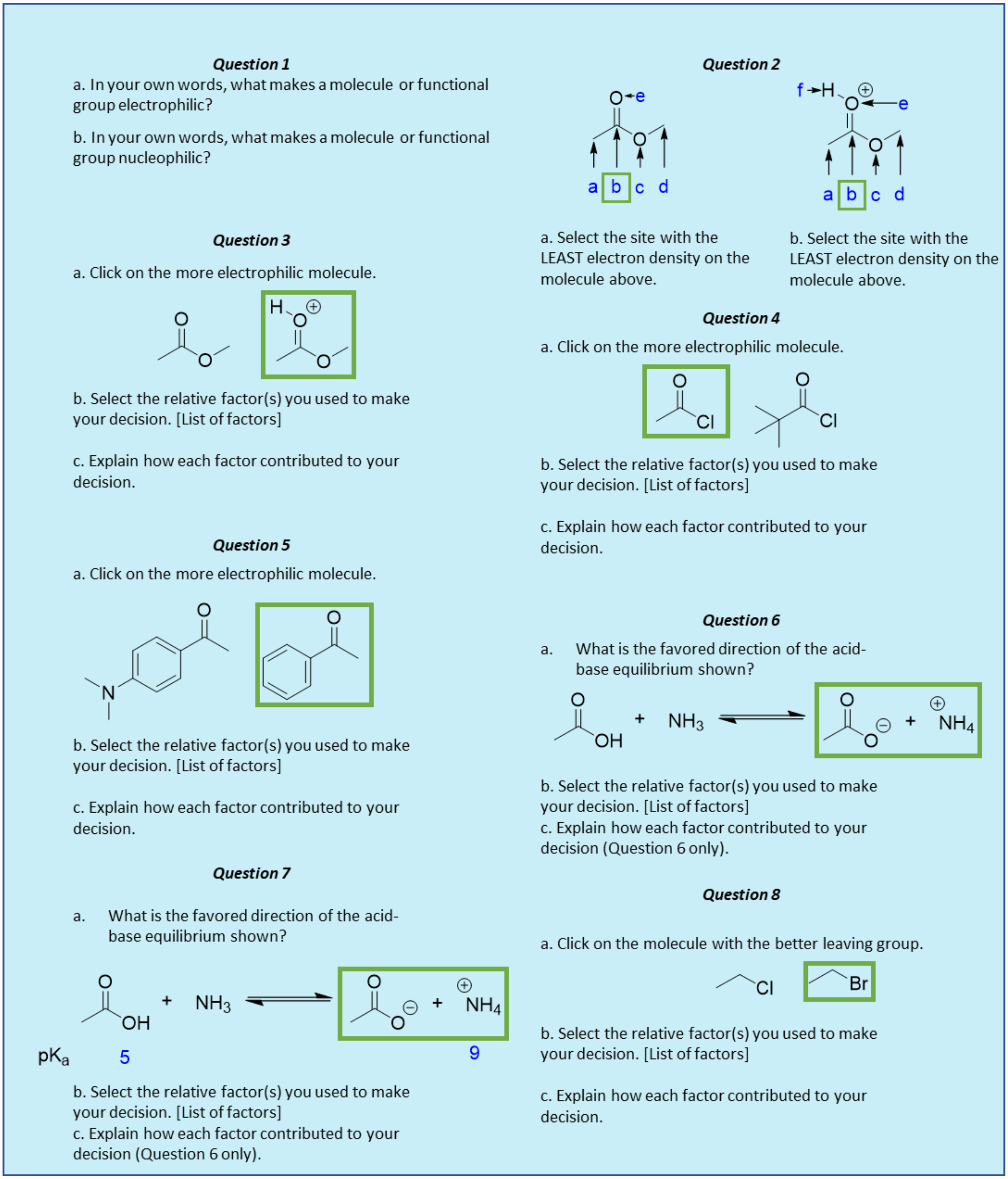
3.5 Questionnaire Development

We designed the ORQ based on learning outcomes from the *Patterns of Mechanisms* curriculum. Specifically, question development was guided by the following learning outcome: Rank electrophilic and nucleophilic sites in increasing/decreasing order of reactivity and justify your answer. We developed an initial question pool of nine items related to nucleophilicity and electrophilicity in organic chemistry and the factors that may influence them (Figure 3.3).

Figure 3.3. ORQ development timeline.

3.5.1 Questions on the ORQ

The ORQ contains a combination of closed-ended multiple choice questions, where students are asked to select a claim or evidence, and open-ended free response questions, where students can provide the reasoning for their claim with more context (Figure 3.4). Scaffolding has been recommended to help students elicit deeper comprehension of chemical phenomena (Crandell et al., 2020). A scaffold is an educational aid or instructional tool that "often addresses anticipated difficulties that a student might have" (Puntambekar, 2022). Scaffolding can be done in a chemistry context to elicit students' reasoning, by separating the prompts for the initial question and the explanation of why that phenomenon occurred (Crandell et al., 2020). We scaffolded participants' thinking by providing a list of possible factors contributing to the reactivity of the given molecules (electronegativity, resonance, etc.) and gave a separate prompt asking students to explain their answer. The structure of the ORQ is based on our proposed model for reactivity principles in organic chemistry consisting of four main categories: nucleophilicity/electrophilicity, electron density, acid–base reactions, and leaving group.



Question 1

a. In your own words, what makes a molecule or functional group electrophilic?

b. In your own words, what makes a molecule or functional group nucleophilic?

Question 3

a. Click on the more electrophilic molecule.

b. Select the relative factor(s) you used to make your decision. [List of factors]

c. Explain how each factor contributed to your decision.

Question 5

a. Click on the more electrophilic molecule.

b. Select the relative factor(s) you used to make your decision. [List of factors]

c. Explain how each factor contributed to your decision.

Question 7

a. What is the favored direction of the acid-base equilibrium shown?

b. Select the relative factor(s) you used to make your decision. [List of factors]
c. Explain how each factor contributed to your decision (Question 6 only).

Question 2

a. Select the site with the LEAST electron density on the molecule above.

b. Select the site with the LEAST electron density on the molecule above.

Question 4

a. Click on the more electrophilic molecule.

b. Select the relative factor(s) you used to make your decision. [List of factors]

c. Explain how each factor contributed to your decision.

Question 6

a. What is the favored direction of the acid-base equilibrium shown?

b. Select the relative factor(s) you used to make your decision. [List of factors]
c. Explain how each factor contributed to your decision (Question 6 only).

Question 8

a. Click on the molecule with the better leaving group.

b. Select the relative factor(s) you used to make your decision. [List of factors]

c. Explain how each factor contributed to your decision.

Figure 3.4. Questions on the ORQ.

3.5.2 Pilot administration

A pilot administration in education research refers to a small-scale version of the study that is used to test specific features like the study's design, participant recruitment strategies, measures, and data analysis methods(Moore et al., 2011).

We conducted a pilot study of the ORQ with upper-year science students to identify potentially confusing or problematic items (Figure 3.3). Three chemistry graduate students and two fourth year science undergraduate students (*N* = 5) completed the ORQ and were asked to provide written feedback on the questions. Specifically, we wanted to know if the questions were being interpreted as intended by participants and if any items were tricky or confusing (Deng et al., 2021). We re-worded the structure of some of the questions based on feedback from this pilot to ensure clarity and comprehension. Minor wording changes were made and open-ended, "Explain how each factor contributed to your decision" prompts were added to two of the items. We then sent the ORQ to three experts in organic chemistry and asked for written feedback on each item to acquire evidence of content validity. Two of the experts actively conduct research in chemistry education while the third is a practicing organic chemist. We asked each expert: 1) Based on your knowledge, do the questions being asked of students ascertain the core principles of reactivity? 2) What else do you think we should include in this instrument? (is there something important that you feel is missing?) 3) Are these questions appropriate for the level of the students? 4) Other suggestions? The responses from experts aided in expanding the scope of the ORQ to include questions specific to acid–base, electron densities, and leaving group. The experts on our panel stated that, while essential, nucleophilicity and electrophilicity do not encompass a complete picture of core reactivity principles in organic chemistry. We then verified the changes made to the ORQ via an interview with one of the previously consulted experts in organic chemistry and an expert in education research. We identified a potential bias in the ORQ during this meeting. Since the ORQ was based on learning outcomes from the *Patterns of Mechanisms* curriculum, there exits the possibility that students from our host institution perform better on the given tasks because they are explicitly taught the skills in that it was based exclusively on learning outcomes from the University of Ottawa. If we wanted to survey only uOttawa students this would not be an issue; however, since we wanted to administer the ORQ to multiple institutions, we needed to minimize bias from the PoM curriculum and ensure that the ORQ encompassed learning outcomes on reactivity from other schools.

We consulted a fourth expert in organic chemistry, from a different institution within the same province, to see if the questions on the ORQ aligned with the content they teach in organic chemistry I and II. Specifically, we asked this expert: 1) Would you expect your students to be able to answer these questions? 2) Do you have any suggestions for a question that better reflects the curriculum at your institution or the way you teach organic chemistry? 3) Is there a question here that you would not expect your students to be able to answer, based on what you teach? 4) Based on the teaching approach you take, is there a question here your students wouldn't be expected to answer because it's not taught? We determined that the questions on the ORQ were in line with what was expected of students at a separate institution using a curriculum different from the *Patterns of Mechanisms*. We also revised the instrument based on this feedback such as adding a question explicitly asking students to identify areas of high/low electron density and minor changes to wording for clarity. The final version of the ORQ contained 11 items, 7 of which were multi-tiered based on the claim-evidence-reasoning framework.

3.5.3 Administration to undergraduate students

Participation was completely voluntary and if participants no longer wanted their data used for research after giving their consent, they could opt-out of the study (via an exit button). Participants were not required to complete the entire questionnaire; we removed all data from any students who opted-out and retained data from participants who did not complete the entire questionnaire without opting-out (this information was outlined in the consent form given to participants). Participants could also choose to have their data removed from the study by contacting the Primary Investigator or student researcher post data collection (see **Error! Reference source not found.** for administration timeline).

3.5.3.1 Local administration

We administered the ORQ with undergraduate students in OCII during a review workshop in September 2021, Fall semester, at the University of Ottawa. The workshop was conducted virtually over Zoom and students from all course sections were invited to participate. We asked students to complete the ORQ during the first half of the workshop to gauge their understanding of reactivity principles. The course instructor then reviewed questions like those found on the ORQ with the students. Completion of the ORQ was optional and participants were required to “opt-in” via a consent form on SurveyMonkey for their data to be used in research. The student researcher and primary investigator were both present during the workshop to answer questions. We used the results from the local administration to identify potentially problematic or confusing questions.

3.5.3.2 Multi-institutional administration

This study seeks to broaden the scope of organic chemistry education research in Canada by including undergraduate students from multiple Canadian universities each using a different organic chemistry curriculum. We contacted organic chemistry instructors at five different Canadian universities to aid in student recruitment. Students were recruited with help from course instructors via class announcements on a virtual learning platform (Brightspace, Blackboard, institutional email, etc.). Four of the five instructors accepted our invitation to participate and agreed to share the recruitment message and survey with students in their course(s). We recruited students from four different Canadian Universities during the 2021 Fall semester. Students were incentivised to participate with the option to be entered into a draw to win one of two Amazon gift cards (values of $20 and $100). Participation was completely voluntary and online via SurveyMonkey; students could complete the questionnaire at their own leisure and were asked not to consult any external resources (e.g., textbook, class notes, etc.). We started our recruitment during the 2021 winter term in mid-November because we wanted to ensure participants had obtained enough knowledge of organic chemistry to understand the concepts presented in the Reactivity questionnaire. At the University of Ottawa, students take OCII in the Fall semester whereas most other Canadian institutions, including those sampled, teach OCI in the Fall and OCII in the Winter. All participants were recruited from OCI courses except for an introductory biochemistry course at C2a.

3.5.4 Data Analysis

We developed the Organic Reactivity Questionnaire (ORQ) as a method to assess students' interpretations of essential reactivity principles in organic chemistry. This study was exploratory in nature and used qualitative methods to see how undergraduate students studying at Canadian institutions interpret reactivity principles in organic chemistry. Specifically, we used thematic analysis to categorize students' responses and identify patterns within the data. We used the quantitative data from closed-ended, multiple choice questions to guide our analysis of students' open-ended responses.

3.5.4.1 Thematic analysis and coding

Thematic analysis is a qualitative method of analysis that identifies patterns from rich, detailed data (e.g., an interview transcript or written response); We refer to the identified patterns as themes (J. Creswell & Guetterman, 2021; J. W. Creswell & Miller, 2000). Themes emerge from the data after conducting multiple rounds of sorting and labelling the data (Figure 3.5). The process of systematically labelling the data in this way is called coding. A code is a meaningful label or category assigned to a piece of data by the researcher; Codes can be assigned before the analysis (deductive approach) or they can be created during the analysis (inductive approach). Thematic analysis is an iterative, systematic process of coding the data over multiple rounds to reduce it into a set of themes (Carle, 2022; Saldaña, 2013).

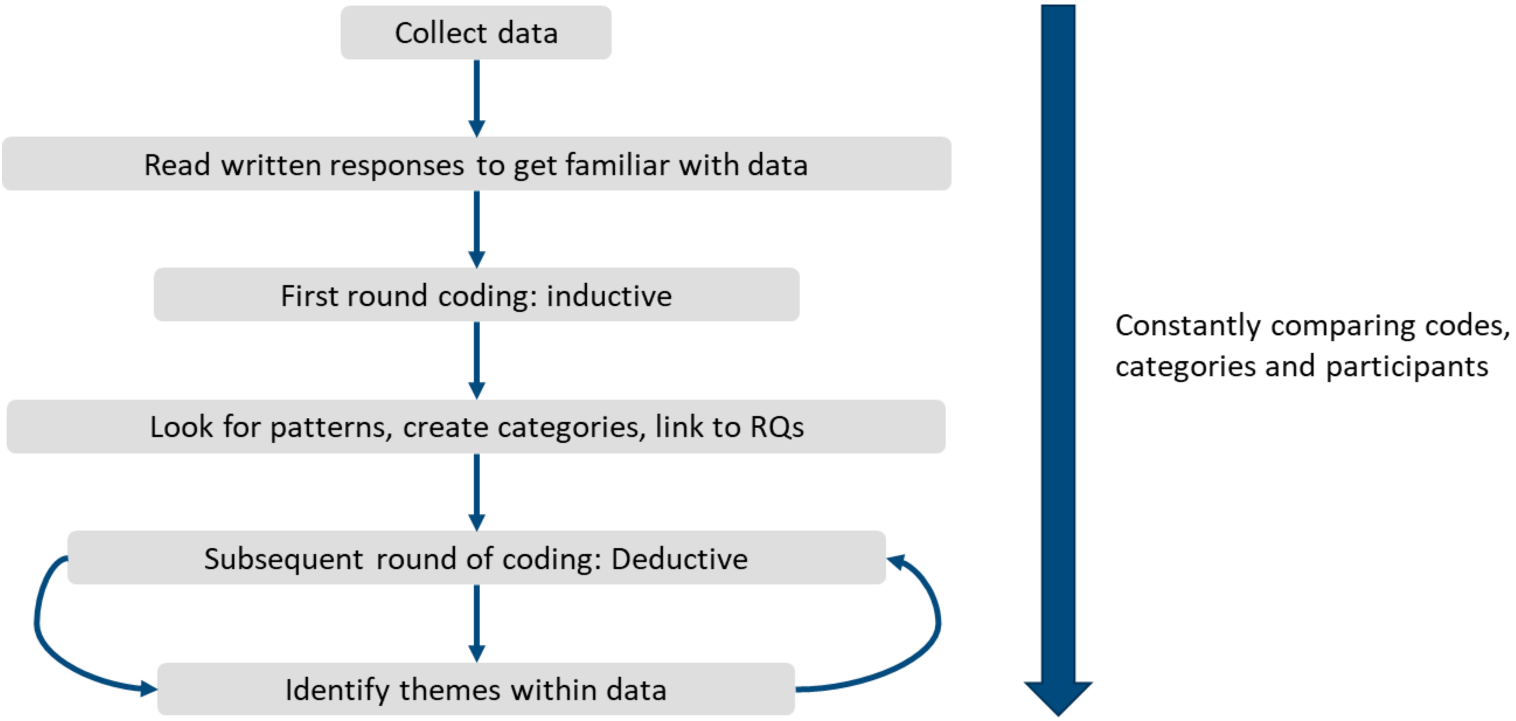


Figure 3.5. Workflow of thematic analysis (Carle, 2022).

We removed two questions from the ORQ before conducting a full data analysis; One question involved ranking nucleophilic sites on a larger molecule and the other asked students to select the most nucleophilic sites on a pair of molecules. We removed these questions because they lacked a reasoning component and very few students (<10%) answered the questions correctly. A low amount of correct answers could indicate that the question was simply more difficult but we cannot conclude this without further investigating item discrimination or item difficulty (Steyer, 2001). We conducted several rounds of coding for all open-ended response items using constant comparative analysis (J. Creswell & Guetterman, 2021). We used an inductive, open-coding approach to assign meaning to individual responses and then grouped the codes into categories and created a codebook based on the created categories. We then used a deductive coding approach to place participants' responses within the developed categories. We did not seek to categorize students' types of reasoning as was done in previous work (Bodé et al., 2019; Deng & Flynn, 2021). Instead, we used qualitative analysis of students' explanations to provide deeper insight into their thought processes and reasoning for their claim selection. Closed-ended questions were multiple choice, such as when making a claim, or selecting factors as evidence for a claim. Codebook reliability for each question was determined using Krippendorff's α. A second rater independently coded a subset of 20% of responses and Krippendorff's α was calculated based on this subset. Reliability data is summarized in Table 3-2. A threshold value of 0.67 is considered an acceptable agreement and values between 0.67-0.79 indicate that the results can be used to draw tentative conclusions; A value of 0.8 is considered a definitive agreement (Hayes & Krippendorff, 2007; Watts & Finkenstaedt-Quinn, 2021). Three out of the six questions analyzed met the threshold for an acceptable agreement after a single round of coding. Codebook reliability for questions 3, 4, and 5 did not initially meet the threshold for an acceptable agreement. Both raters met to discuss disagreements and revised the codebook until the acceptable cut-off was met. Questions 3, 4, 5, and 8 met the threshold for tentative conclusions, as such, we proceeded with caution when interpreting our findings for these questions.

Table 3-2. Reliability data for each question on the ORQ.

Question	**Percent agreement**		**Krippendorff's α**	
	Round one	Following discussion with rater	Round one	Following discussion with rater
1a	95	-	0.82	-
1b	97	-	0.87	-
3	90	96	0.45	0.78
4	90	95	0.41	0.74
5	93	96	0.54	0.72
8	96	-	0.77	-

3.6 Results and Discussion

We began our analysis by looking at each question individually and then organized the themes based on the study's RQs. The first section covers students' interpretations and definitions of nucleophilicity and electrophilicity; the second section looks at what chemical concepts students focus on when solving acid-base problems; the last section touches on the chemical concepts students use to interpret leaving group stability.

3.6.1 RQ 1: How do undergraduate students interpret reactivity principles with respect to nucleophilicity and electrophilicity?

Students' definitions of nucleophilic and electrophilic

Students' definitions largely aligned with expectations and often connected structural and functional aspects of nucleophilicity and electrophilicity. Students most consistently stated that a functional group or species is electrophilic if it accepts electrons, is electron deficient, and (often) has a full or partial positive charge (Figure 3.6). Students most consistently stated that a functional group or species is nucleophilic if it donates electrons, is electron rich, and (often) has a full or partial negative charge. These results were consistent with those from interviews done by Anzovino & Lowery Bretz (2015) where the students in their sample would often identify charge and the ability to accept/donate electrons in their definitions. In our current sample, many students also identified that the availability of electrons, either as electron rich or electron deficient, contributed to the nucleophilicity and electrophilicity of a molecule. These results are encouraging because it indicates that students are often thinking about the functional aspects of nucleophiles and electrophiles (e.g., reactivity) rather than just structural features, at least in their definitions.

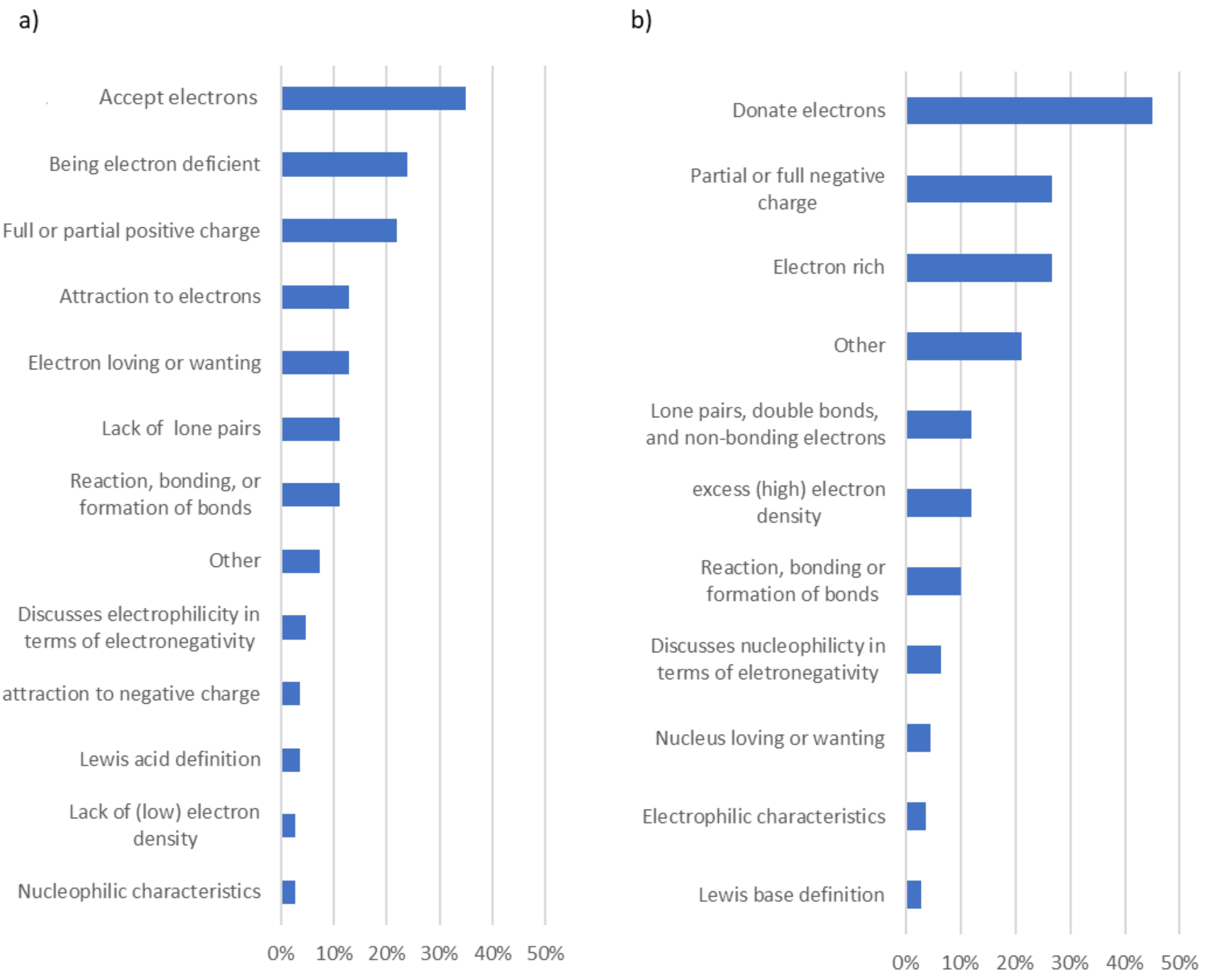


Figure 3.6. Students' definitions of what makes a molecule or functional group a) electrophilic and b) nucleophilic (N=109).

Students' interpretations of electron density

Question 2: Many students were misled by a charge cue when identifying areas of low electron density. Of the students, 45% correctly selected *site b,* the carbonyl carbon, as the site of least electron density on the unprotonated ester whereas 35% selected *site a*, the alpha carbon (Figure 3.7). This answer distribution was surprising given that the α carbon on methyl ethanoate does not participate in resonance, does not have a full positive charge, and is not immediately adjacent to a very electronegative atom. The distribution of responses changed when students were asked to select the site of least electron density for a protonated version of the same ester (Figure 3.7). Fewer students selected the correct answer (site b); Instead, 41% of students selected *site f* and 30% selected *site e* when shown the protonated ester. While not the expected answer, site f, a hydrogen bonded to a charged carbonyl oxygen, can be considered a site of very low electron density since it is directly bonded to oxygen, a very electronegative atom, and can readily participate in an acid–base reaction as an acid. What may be concerning is that *site e*, the charged oxygen, was the second most selected site by students. This result indicates that many students were likely using surface features to answer this question (charge in this case) and, based on their definitions (Figure 3.6), likely associated the positive charge with a lack of electrons and low electron density. The positive formal charge in this case does imply that the carbonyl oxygen donated electrons; however, it is still not the site of least electron density.

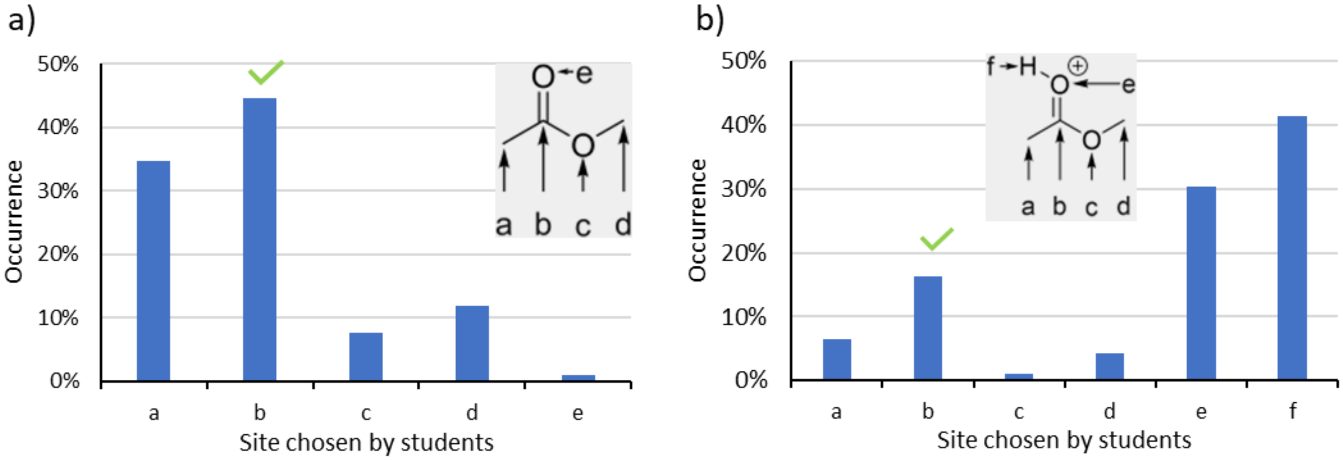


Figure 3.7. Distribution of student responses for selecting the site of least electron density on a) an unprotonated ester and b) a protonated ester (N= 92).

Students' interpretations of electrophilicity

Question 3: Most students correctly identified the more electrophilic species when a positive charge was the major differentiating factor. The majority of students (87%) correctly selected the protonated ester as being more electrophilic (Figure 3.4) compared to the unprotonated ester. Of the students, 82% identified charge as evidence for selecting Claim B. The students here connected a positive formal charge to electrophilicity, as many did in their definitions of electrophilicity (Figure 3.6). Charge is a structural feature (Anzovino et al., 2015) and may incorrectly cue students about which sites of a molecule are nucleophilic/electrophilic if they do not understand the underlying meaning symbolized by charge. Furthermore, using charge as a cue without realizing the functional aspects of nucleophiles and electrophiles does not demonstrate a thorough understanding of the concepts. We expected students to connect a positive formal charge to a lack of or lower electron density and align this with the given definition of electrophilicity. One example of the expected answer came from Participant 120 who selected Claim B:

"*The addition of the hydrogen molecule and the positive charge on the oxygen makes molecule [B] more electrophilic as the electron density is less than that of molecule [A] and it is more open to accepting electrons*."

Many students connected positive charge with a lack/ deficiency of electrons in their written responses. However, an equivalent number of students did not explicitly make the connection between positive charge and electron deficiency, instead using the positive charge as a heuristic cue to identify electrophilicity. A heuristic is a mental shortcut that uses cues to quickly come to an answer based on memorize "rules". Using charge as a heuristic is quick when comparing two molecules but may lead to misinterpretations about reactive sites, as seen in Figure 3.7. Answers were considered partially correct if a student simply stated that Molecule B was more electrophilic because it has a positive charge. An explicit connection needed to be made between positive charge and electron deficiency for the reasoning to be considered correct. Resonance/delocalization was identified mainly because the π bond in the carbonyl could be delocalized.

Question 4: Students were near evenly divided on which molecule was more electrophilic given different degrees of steric hindrance. Students were near evenly split in their selection of a claim with 51% correctly selecting Claim A and 49% selecting Claim B (Figure 3.8), suggesting they were guessing at the answer. We expected students to use the difference in molecular structure, a surface feature, to make their decision and identify steric hindrance as evidence for their choice. However, only 26% of students selected steric hindrance as evidence to support Claim A despite being the most relevant factor in determining electrophilicity for this question. Few students (11%) used steric hindrance as evidence to support Claim B, the incorrect answer. Inductive effects was the second most prevalent piece of evidence selected by students.

We expected the following argument in students' responses to suitably answer Question 4: *Molecule B has more steric hindrance due to the tert-butyl group; greater steric hindrance makes it more difficult (greater energetic barrier) for a nucleophile to access the most electrophilic site. Therefore molecule A is more electrophilic*.

Successful students on Question 4 connected steric hindrance with the accessibility of the electrophilic site. A students' reasoning was considered correct for this question if they connected steric hindrance with accessibility, energy of the reaction, or favourability, and selected Claim A. Ten students gave responses aligned with the expected answer and selected the correct molecule; For example, participant 115 described why steric hindrance was present and connected it to the accessibility of the active site:

> "*…The tert-butyl group adds physical bulk steric to the carbonyl, introducing steric hinderance. This will prevent nucleophiles from attacking the carbonyl thus decreasing its electrophilicity*."

If students identified steric hindrance in their argument but did not connect steric hindrance to the accessibility of the reactive site then their answer was considered partially correct. For example, Participant 27 selected Claim A and stated:

"*I assume the t-butyl group has something to do with hinderance but haven't memorized that rule yet*"

This participant could recognize that molecule B has greater steric hindrance compared to Molecule A but was unable to correctly connect an increase in steric hindrance to a decrease in electrophilicity (weaker electrophile) in their response. This participant also may have been trying to apply memorized rules instead of understanding the reasoning behind each principle. We emphasize the drawbacks of rule-based reasoning later in this section. Another example of partially correct reasoning came from participant 134 who made a direct association between "bulkiness" and electrophilicity without explicitly describing active site accessibility:

"*The larger and more bulky the electrophile, the weaker it is.*" (correctly selected Molecule A)

Inductive effects was selected by 21% of students to support Claim B and 13% to support Claim A. Inductive effects was the second most prevalent factor selected by students; Students would often discuss inductive effects in terms of the tertbutyl group having either a stabilizing or destabilizing property on the rest of the molecule. The definition of electrophilicity that we gave to participants did not include any mention of structural features that could lower the likely hood of a molecule reacting (the definition does not mention the accessibility of the nucleophile to the electrophilic site). Students would have to have been taught about steric hindrance to answer this question. A few students stated that the *tert*-butyl group could be involved in resonance. Resonance is often taught in OC I and II as a phenomenon specific to π bonds. This makes sense given that the IUPAC definition of resonance (delocalization) focuses on π bonding in a conjugated system(IUPAC, 2019). However, σ bonds can participate in resonance, just not in the traditional sense (Olah, 2005). It may be beneficial for instructors to mention Georg Olah's work on non-classical carbocations during class to help further clarify resonance to students.

Question 5: Students were near evenly divided on which molecule was more electrophilic when interpreting resonance and inductive effects were necessary to select the

correct claim. Students were near evenly split in their selection of a claim with 49% of students correctly selected Claim B and 51% of students selecting Claim A (Figure 3.8). The most prominent pieces of evidence selected by students were resonance, inductive effects, and electronegativity, no matter if they selected the correct claim.

Overall, the most prominent incorrect idea about resonance was that a molecule that could form more resonance structures is more reactive or electrophilic. One student stated that:

> *"The NR2 [sic] group on the first molecule is a strong activation group because it can help the molecule through resonance structures during a reaction and lower the activation energy."*

Here it appears that the student was suggesting an electrophilic aromatic substitution and did not identify the carbonyl as the most reactive site. Furthermore, this illustrates a possible misinterpretation about how resonance relates to the thermodynamics of a rection. Participant 21 stated that "[Molecule A has] *more resonance which means more charge, oxygen pulls electron density from nitrogen*" suggesting that they believe resonance (delocalization) actively produces charge rather than delocalizes it, which is incorrect. Of the students, five associated a higher electronegativity with greater electrophilicity, based on the idea that a more electronegative atom will attract electrons. Some participants associated nitrogen with electrophilicity but gave no further reasoning such as:

> "*The N allows the chosen molecule [Molecule A] to be more electrophilic*."

Many students could identify that resonance and inductive effects were both involved in determining which molecule was more electrophilic but struggled to explain how they were involved. Previous research has found that students often struggled when multiple chemical concepts were involved in determining reactivity (Caspari, Weinrich, et al., 2018; Caspari & Graulich, 2019; Eckhard et al., 2022). Students are required to use multivariate reasoning when solving problems with multiple relevant factors involved; that is, students need to identify different factors, identify which ones are relevant to the problem, compare the factors, and decide which factor influences reactivity the most. Understanding resonance was essential to answering this question correctly; however, eight students had incorrect ideas about the role resonance played in determining the overall reactivity of a molecule. Participants would often consider the electronegativity of nitrogen or the lone pairs present on nitrogen when determining electrophilicity. Those who considered the lone pairs on nitrogen often reasoned that the lone pairs overall made the molecule more nucleophilic. Those who considered electronegativity often reasoned that the nitrogen would make Molecule A more electrophilic because it would pull electron density towards itself. Individuals who considered nitrogen as a nucleophilic atom selected the correct claim but used incorrect reasoning. Some students intuitively knew that nitrogen is often a good base and good nucleophile, while others considered the lone pair present on nitrogen and used it to identify nitrogen as a nucleophilic atom. Eight students associated the nitrogen on Molecule A (and its lone pair) as being nucleophilic and used this to determine that Molecule A was overall less electrophilic than Molecule B. This type of reasoning helped students to select the correct claim (Claim B) but uses a heuristic cue to solve a multilayered question about reactivity. Using heuristic cues rather than comparing chemical concepts demonstrates limited knowledge of the underlying principles involved (See *Rule-based reasoning and heuristic cues* later in this section).

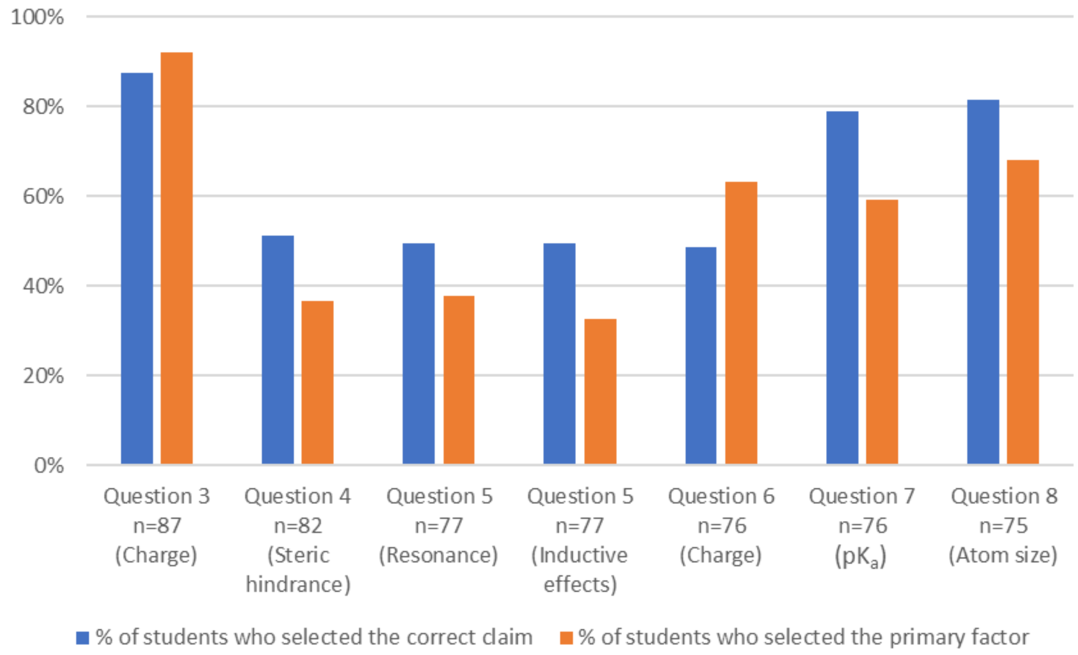


Figure 3.8. Summary of responses for closed ended question on the ORQ. Brackets denote the primary factor for that question.

Electronegativity was used often in students' responses despite never being the primary factor for answering the questions. Electronegativity was selected by >15% of students for each question (Figure 3.9). Electronegativity was never the primary expected factor for answering the questions, but it was chosen more often across different questions then hybridization or orbitals (which were also not primary factors). There was often a direct association made between electronegativity and electrophilicity in students' reasoning, especially when different heteroatoms were present (questions Question 4, Question 5, QUESTION 8). Students who selected electronegativity would often reason that there was a linear relationship between electronegativity and electrophilicity. Some students described this as a positive relationship (as electronegativity increases, electrophilicity increases) or negative relationship (as electronegativity increases, electrophilicity decreases). Participant 156 selected the correct answer for Question 5 and reasoned that a greater electronegativity resulted in a more electrophilic species:

"*Nitrogen adds a certain level of electronegativity that attracts electrons*"

The positive relationship seems to be that something that can better attract electrons is more electrophilic (based on electronegativity alone). In contrast, Participant 163 selected the incorrect answer for Question 5 and reasoned that the species with less electronegativity overall will be more electrophilic:

"*N is another electronegative molecule and while both are resonance stabilized and have very big, electronegative O, the second will be more electrophilic as it does not have that extra N*."

This type of linear relationship between electronegativity and electrophilicity appeared more often when students were provided with differing heteroatoms between answer choices (Question 5, Question 8) but was also present when species were charged (Question 3, AB i, AB ii). Some students' reasoning involved the favourability of charge on an electronegative atom where they associated positive charge on a highly electronegative atom with being unstable or unfavourable. Participant 23 selected the correct answer for Question 3 and reasoned that the charged species was more electrophilic:

"[The charged species] *violates octet rule, positive charge is unstable on oxygen since it is an electronegative atom.*"

Presumably, this participant was following a rule that the most electronegative atom should carry any negative charge. Here the participant used the octet rule heuristic (Taber, 2009) alongside electronegativity (Talanquer, 2014) and determined that the charged molecule was unstable, rather than considering that it was electron deficient. For question 8, seven students considered Br as a better leaving group compared to Cl because it was less electronegative, such as Participant 159:

"When the only difference is the leaving group and the two are on the same row the least electronegative is the most nucleophilic and as such the best leaving group"

This explanation made sense given that the options for leaving groups were both halogens but this rule-based reasoning using electronegativity does not account for why the less electronegative atom is considered the better leaving group. Students can be led to incorrect answers if they misunderstand given rules when using rule-based reasoning. Eight students believed that the more electronegative atom was the better leaving group and incorrectly chose Cl as the better leaving group based on this rule:

"*The more electronegative atom is the leaving group*" (Participant 28).

Our results here are similar to those from Popova & Bretz (2018), who found that the students in their study "used the concept of electronegativity as the primary, or only, factor to explain why halides are good leaving groups.” We echo their point here that “while electronegativity can be used to draw inferences about some leaving groups, it is not the most appropriate criterion when discussing leaving group ability of leaving groups of very different sizes, as in the case with halides” (Popova & Bretz, 2018). Overall, students refer to electronegativity for quick, rule-based decisions about reactivity of heteroatoms. Electronegativity is a straightforward factor to identify and compare but students should not rely too heavily on electronegativity before considering other factors that may be involved.

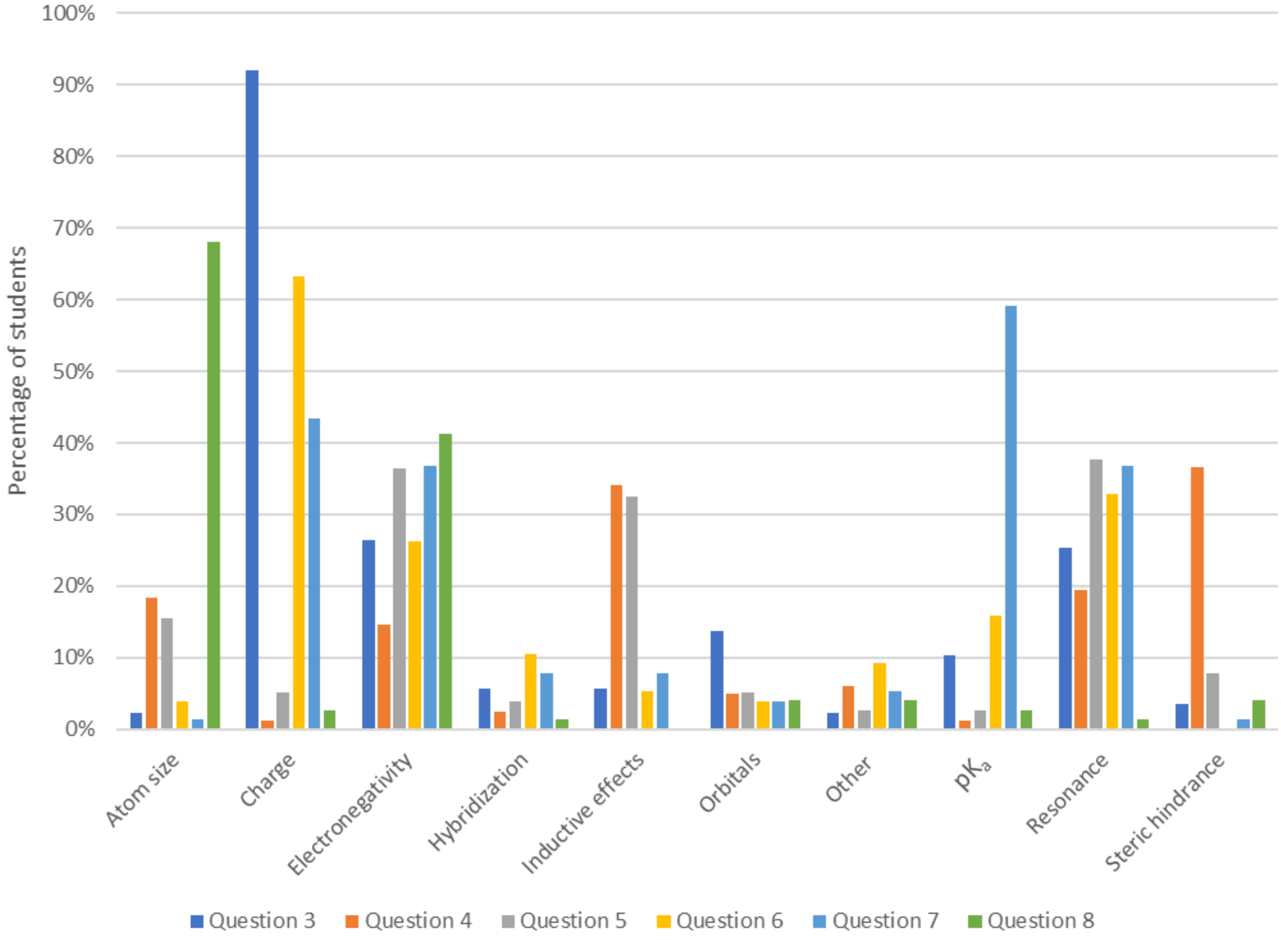


Figure 3.9. Percentage of students per selected factor used for each question on the ORQ.

The role of inductive effects was not evident across students’ responses.

Inductive effects appeared often in students’ responses for questions Question 4 and Question 5 (Figure 3.9) where the tert-butyl group or amine were discussed in terms of their electron withdrawing/donating properties. The role of inductive effects in determining electrophilicity seems to be unclear to students, they can identify when inductive effects are present but have difficulty connecting how inductive effects connect to stability. Students considered the tert-butyl group as either a stabilizing or destabilizing property but in both cases there was a mix of answers about whether the tert-butyl group was electron withdrawing or electron donating.

Participant 72 claiming that Molecule B with the tert-butyl group is more electrophilic: "*only diff [sic] is the tertbutyl, causes tertiary carbon to be induced negatively, therefore stealing the alpha carbons electron even more*."

Participant 11 claiming that Molecule A is more electrophilic: "*alkyl groups are EWG and makes second structure more stable, hence weaker electrophile*."

Both participants selected inductive effects as evidence and both considered the tert-butyl group as electron withdrawing, but participant 11 correctly identified this property as stabilizing. The tertbutyl group does not cause any permanent dipoles within Molecule B, as such what most students were likely referring to was hyperconjugation. We did not include hyperconjugation on the list of possible factors given to students, however two students explicitly identified that hyperconjugation was present in Molecule B and reasoned that hyperconjugation from the tertbutyl group contributed to the stability of Molecule B:

*"Extra methyl donates electrons to carbocation, reducing the charge on the electrophilic site (hyperconjugation) and making it weaker." (*Participant 5 selected the correct claim A for Question 4)

"*…This carbocation is highly unstable but the first molecule is more electrophilic due to having a low amount of alkyl groups (that donate electron density toward the carbocation by hyper conjugation). The second molecule has three electron donating groups which stabilizes the carbocation better making it less electrophilic. In both molecules the chlorine produces inductive effects pulling electron density away from the carbocation further destabilizing it but* *the alkyl groups push electron density into the carbocation contracting the affect*." (Participant 32 selected the correct claim A for Question 4)

15 students considered the tert-butyl group to have a stabilizing effect on Molecule B (Question 4) via inductive effects. Responses describing this varied but in general described more branching to be more stable because it could spread out charge. 4 students reasoned that the tertbutyl group caused a destabilizing effect in Molecule B (Question 4) and claimed that it was the more electrophilic molecule (Claim B). Participant 161 illustrates this idea by suggesting that the tertbutyl group makes Molecule B more electrophilic by withdrawing electrons:

"*the inductive effects reduces the carbon stability and in order to regain the atom has to attract electrons thus making more electrophilic*"

Inductive effects was not a primary factor in determining electrophilicity in Question 4. It is possible that many students selected inductive effects because hyperconjugation was not given as an option for evidence and that inductive effects was the next closest idea, as they both involve bond polarization. However, two students correctly identified and described hyperconjugation in their responses, indicating that some students may not be clear on the differences between the two concepts. Furthermore, steric hindrance was the primary factor in determining electrophilicity for Question 4, not hyperconjugation or inductive effects. Students' who selected inductive effects for Question 4 likely produced incorrect reasoning because they did not identify the relevant factor (steric hindrance in this case). Previous work has found that students may use an incorrect argument because they did not identify relevant factors. One study conducted with students in the PoM curriculum found that students in OCII would incorrectly identify steric hindrance as a relevant factor when selecting a mechanism for an SN1 reaction (Bode et al., 2019). Students who selected steric hindrance as evidence often selected the incorrect claim because steric hindrance was less relevant to their context compared to carbocation stability and hyperconjugation (Bodé et al., 2019). In the current work, we gave no explicit information about the reactions the given molecules would undergo and assumed that students would identify the carbonyl carbon as the primary electrophilic site. Participant 116 selected Claim B (Question 4) and stated:

“*Molecule on the right can stabilize a (+) charge better when the Cl leaving group leaves*.”

This participant was completing Organic Chemistry I in a curriculum where reactions with carbonyl compounds may not have been taught extensively in the first semester of organic chemistry. In the PoM curriculum reactions involving leaving groups are taught early in Organic Chemistry II (students second semester of organic chemistry. This participant considered the possibility of the chlorine acting as a leaving group before a reaction with a nucleophile (S_N1/E1 mechanisms) and considered the stabilities of molecules A and B after the chlorine left to compare their relative electrophilicities. Only 32% of students identified inductive effects as one of the primary factors involved in Question 5. Seven students reasoned using inductive effects but none of them went in depth about how inductive effects influenced electronegativity. Most of these students focused instead on associating nitrogen with inductive effects, where the nitrogen atom “turned on” inductive effects:

(Participant 38, selected the incorrect claim A for Question 5) “*The selected one [Molecule A] is less stable due to not having the inductive effects of N, and therefore would be more nucleophilic.*”

This individual may have accidentally selected the wrong claim as their explanation states that the molecule without nitrogen is more nucleophilic, yet they selected Molecule A, which contains nitrogen. Similarly, Participant 57 selected the correct claim B for Question 5 and made a direct association between inductive effects and electrophilicity:

“*The absence of the inductive effect allows for a more electrophilic molecule*.”

This type of reasoning is surface level as it doesn’t explain how the lack of inductive effects contribute to greater electrophilicity while assuming that the relationship between inductive effects and reactivity is linear. The relationship between inductive effects and reactivity is often nuanced and context dependent as the type of substituent and its location will have differing effects. Participant 55 gave a more implicit explanation suggesting that inductive effects from the nitrogen influence the charge on oxygen:

(Participant 55 selected the incorrect claim A for Question 5 and selected inductive effects as evidence) *"Nitrogen would induce the negative charges on oxygen"*

For this response, it was difficult to determine if the participant was referring to resonance rather than inductive effects. For future administrations of the ORQ it may be worth adjusting Question 5 such that only one primary factor is involved (such as by making the substituents meta, which would result in each molecule having the same number of resonance structures, making inductive effects the primary factor). We are also unsure how the type of substituent (in this case an amine) connected to students' responses and if their responses would have differed with a different substituent. Our findings suggest that inductive effects may need to be explicitly differentiated from hyperconjugation while teaching and the role of inductive effects clarified in the context of reactivity. Many of the students in this study may have had less exposure to inductive effects as a concept if they did not cover relevant reactions such as electrophilic aromatic substitutions, as such we interpret these results with caution and will use them to guide future modifications of the ORQ.

Students could identify when resonance was present but not necessarily what effect it had. Resonance was consistently selected by participants for questions where a π–bond was present. Most of the questions on the ORQ involved resonance, even if it was not always the most relevant factor in determining reactivity. A sound understanding of the concept of resonance and how to use it in practice was required of students to fully understand several of the questions. Based on the learning outcomes from Carle & Flynn (2020), participants in this study were required to 1) determine and justify the electrophilic and nucleophilic sites on a molecule using delocalization concepts, and 2) use delocalization concepts to predict and justify the course of a reaction, which in our context meant selecting the more electrophilic species (more likely to react). Greater than 15% of students selected resonance as a relevant factor for all questions except Question 8. Question 8 was the only question that contained species without π-bonds. For Question 3, only eight participants discussed resonance in their open-ended responses despite 38 students selecting it as a relevant factor. Two participants gave similar reasoning but selected different claims for Question 4. Both incorrectly stated that molecule B, containing a tert-butyl group, has a greater possibility for resonance:

Participant 18 selected Claim A and stated: "*there is more possibility for resonance in the other molecule, making it more stable and less likely to react with a nucleophile*"

Participant 21 selected Claim B and stated: "*more opportunity for resonance with the more carbons*"

The incorrect idea that σ-bonds could form resonance structures was not prominent among participants' answers, but these responses give a better idea about participants' understanding of resonance. These participants, likely, either did not attempt to draw resonance structures or drew incorrect resonance structures when answering Question 4. Resonance was not the primary factor involved in determining reactivity for Question 4 but if students could not identify correct resonance structures for both molecules, then their reasoning was incorrect. Context is important, the assumption was that students could identify the most electrophilic or nucleophilic site, and they were not given more than a single reactant because we did not want participants to have to consider competing reaction pathways. However, the contexts students had in mind may have led them to a different answer. For example, the participants above, who claimed that molecule B had a greater possibility to form resonance structures, may have been considering if the tert-butyl group had a carbocation, as some previous studies observed that students may focus on carbocation stability (Eckhard et al., 2022). Other incorrect ideas about resonance included the idea that resonance produces charge, that more resonance structures means that a nucleophile has more places to attack, and that more opportunity for resonance means the molecule is more electrophilic. Brandfonbrener et al. (2021) observed that the students in their study would often associate resonance with stability. Students should be able to use resonance to infer reactivity(Carle & Flynn, 2020). We observed that students can identify resonance but have a harder time correctly applying it in context. Instruction should focus on giving students examples on how resonance might influence reactivity and using resonance in context.

Explicit use of heuristics and rule-based reasoning

Rule based reasoning involves using a memorized rule or algorithm to solve a problem (Bhattacharyya, 2008; Bongers et al., 2020; Maeyer & Talanquer, 2013; Talanquer, 2014). One common example of a rule students learn early in their education is the "octet rule". Rule-based reasoning functions similarly to heuristics in that it can be used to get to an answer quickly; however, rule-based reasoning suffers from similar drawbacks in that the "rules" can be overgeneralized by students and lead them to incorrect ideas (Taber, 2009).

One participant explicitly used rule-based reasoning and wrote "ARIO" in their open-ended responses for questions 3, 4, and 5. ARIO is a "rule" that you look at the atom (e.g., oxygen vs nitrogen) then the factors that dominate are resonance, then inductive effects, then orbitals/hybridization. This participant was able to select the correct answer for questions 3 and 4 using ARIO but chose the incorrect answer for question 5 showing that "rules" like ARIO may break down when there are multiple relevant factors. Furthermore, this participant did not select steric hindrance as a relevant factor for question 4 as ARIO does not account for steric hindrance. ARIO also breaks down when used for more advanced reactions like cycloadditions or predicting stereoselective outcomes. Educators have good intentions when teaching "rules" like ARIO; ARIO simplifies complex problems and helps students reach conclusions faster, which can be useful on tests. The problem is that students relying on the "rule" focus on memorizing rather than learning the science and comparing chemical concepts.

Another participant explicitly stated that they were unsure how to answer question 8 because they did not know what rule to apply:

"*i havent [sic] memorized this rule yet but in an aprotic solution the atom with a smaller size is a better leaving group?"* (Participant 27 Claim B).

No reaction conditions were given to students, as such students were required to reason using only the chemical concepts they were given. This participant likely assumed certain reaction conditions and tried to apply rule-based reasoning but selected the incorrect choice because the rule they applied was inappropriate to the context of the question. Students were not required to complete the ORQ under a time restraint, so it is unlikely that they used rule-based reasoning just to move on to the next question faster. The ORQ was a low-stakes assessment, with no credit or grade connected to it, and students were allowed to spend an unlimited amount of time to complete it. Rule-based reasoning may help students quickly choose an answer on tests and reduce cognitive load, but students should not over-rely on it for solving complex tasks. Teaching students when and how to avoid using rule based reasoning could be a goal for instructors during introductory organic chemistry courses (Bodé et al., 2019; Maeyer & Talanquer, 2013).

3.6.2 RQ 2: What factors do undergraduate students consider when determining the direction of an acid–base equilibrium?

Students were more successful using pK_a values then relative stability rules when determining the direction of an acid base equilibrium. Students were equally split on the favored direction of an acid–base equilibrium when not given pK_a values. 49% of students correctly selected that the equilibrium favors products and 49% of students selected that the equilibrium favors starting materials (Figure 3.10). Most students who selected that the equilibrium would favour the starting materials selected charge as evidence. Seven students used pK_a values to answer question 6 even though the values were not given, and participants were asked not to consult outside sources. 79% of students correctly selected that the equilibrium will favour the products after being given pK_a values. pK_a values are experimentally derived and are the most consistent way to identify the direction of an acid–base equilibrium. We expected students to be able to identify relevant factors but ultimately rely on pK_as to answer this question correctly. One participant compared relevant factors to determine equilibrium direction and then confirmed their reasoning using pK_a values:

(Participant 104, selected favours products, question 6)“*Firstly, the conjugate base of the carboxylic acid can delocalize that negative charge easily using resonance, making it stable. Then the Nitrogen can easily delocalize the positive charge making it also stable. So there is no reason as to why it wouldn't favor the products. Then we can look at Pka, and it supports my thought, where the product acid has a higher pka than the reactant.*”

This individual demonstrated that they could compare relative factors, going beyond rule-based reasoning using charge, and used data (pK_a values) to support their claim. The correct answer to this question went against some of the reasoning seen in Question 3. Several students initially considered charge as being unstable and that charged molecules are more reactive and will often "want" to become neutral to obtain stability. In this case, charge was a misleading cue to students since the acid–base equilibrium favoured the side with the charged species. Here students may be showing an overreliance on charge cues where charged species are intuitively considered unstable or unfavourable. We noticed responses similar to those observed by Galloway et al. (2017) where students in their study stated that charges needed to be neutralized in a reaction. 10 of 30 participants who responded to the open-ended part of question 6 stated that charged species were more reactive (or less stable) compared to neutral species, and therefore selected that the reactants were favored because they were not charged. pKa values are experimental evidence that indicates the direction of an equilibrium. We want students to be able to interpret pKa values to problem solve but we also want students to explain why a phenomenon occurs using othe possible factors. Some essential aspects of reactivity were missing from this question that were elucidated after data analysis; solvation plays an important role in acid–base equilibria but was not explicitly present in the question and thermodynamics and kinetics were not addressed. The presented acid–base question implicitly assumes that water is the solvent, but this is not always the case in organic chemistry problem solving. The properties of different solvents can influence the direction of the equilibrium. Thermodynamics and kinetics, while not explicit here, are concepts experts use often to determine the likeliness of a reaction occurring and why. Future iterations of the ORQ will include other essential concepts beyond nucleophilicty and electrophilicty; specifically, we would include questions on solvation and explicitly address the idea of thermodynamics versus kinetics.

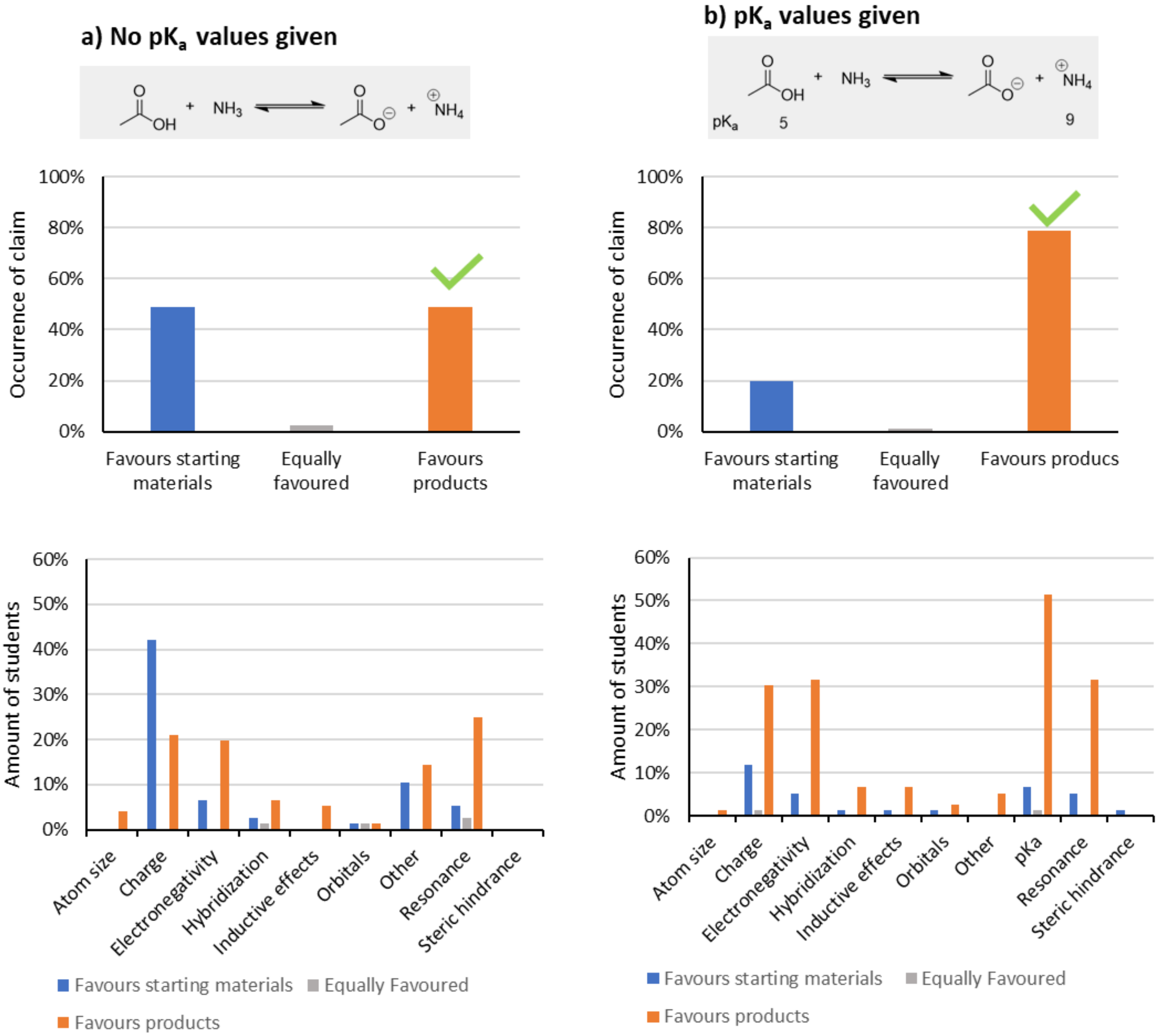


Figure 3.10. Claims and evidence selected by students for the direction of an acid-base equilibrium. Participants were asked to select the favored direction and select the evidence they used to make their claim. Students were not given pKa values at first but were provided with them after completing the first acid-base question. The expected answer (✓) was that participants would select Claim B because of the charge present (N= 76) Note that pK_a was not given to students as an answer choice for evidence, all counts of pK_a as evidence here is taken from students' open-ended responses in the "other" option.

3.6.3 RQ 3: What factors do undergraduate students consider when determining leaving group stability?

Most students correctly identified the better leaving group when atom size was the primary factor involved. 81% of students selected the correct claim, that the alkyl bromide contains the better leaving group (Figure 3.8). 19% of students selected the incorrect claim, the alkyl chloride, suggesting chlorine as a better leaving group than bromine. 70% of students overall selected atom size as evidence when making their claim (Figure 3.9).

We observed several cases where students used rule-based reasoning without further explanation such as: a larger atom is a better leaving group, a weaker base is a better leaving group, and a more/less electronegative atom is a better leaving group. This type of reasoning is similar to findings from Popova & Bretz (2018) where they found that ~30% of participants in that study were limited to making assertions about which leaving groups were good rather than explaining why they were considered good. Twenty students in our study went beyond rule-based reasoning and explained why a larger atom was a better leaving group:

"*Br is bigger than Cl and can better stabilize charge, which makes it a better leaving group*" (Participant 18).

The connection between atom size and the stability of charge shows a deeper level of reasoning compared to associating atom size with leaving group stability without further explaining how atom size influences leaving group stability. Seven students demonstrated a deep understanding of how atom size influences leaving group stability by discussing electron density in terms of atomic structure:

"*Bromine is bigger than chlorine - bond is farther from nucleus as it is in a higher valence ring, therefore it is easier to remove*" (Participant 128).

Students were generally successful in selecting the correct leaving group and identifying atom size as the most relevant factor. Few students from the current study went beyond rule-based reasoning when completing this task, often citing a rule that a bigger atom is a better leaving group. This rule worked well in the current context but demonstrated a limited understanding of why leaving group stability is affected by atom size. Future implementations of the ORQ will include more leaving group questions to further assess students' comprehensions of leaving group stability and its relation to reactivity principles.

3.7 Limitations

This was a single time point with a limited sample from each individual university. Since each curriculum may teach different topics at different times (ex. teaching substitution/elimination reactions in ORG I vs. ORG II) we cannot confirm that all students were taught content relevant to every question on the ORQ. The acid–base question used on the ORQ did not explicitly have solvent effects as a factor influencing reactivity. Solvation is a concept used by experts that students may not always take into consideration but it was not explored here. This work was largely exploratory in nature so we cannot suggest any connections between curricula and students' abilities to reason with reactivity principles within the current study. Previous studies have found that students would often discuss polarization when giving explanations about reactivity (Anzovino et al., 2015; Eckhard et al., 2022). This study did not explicitly look for if students were discussing reactivity using polarization. This was a voluntary assessment (not high stakes) so there may have been limited depth to students' explanations. We did not ask questions related to demographic information (program of study, age, gender, etc.) to keep the ORQ concise and avoid survey fatigue. However, without this information we are unable to identify underlying variables that may connect to students' responses. This was an exploratory study that attempted to use a mix quantitative (multiple choice) and qualitative questions (open-ended explanations) to elicit students' coherence with reactivity principles. Most of the questions involved resonance and many students brought up resonance in their answers but we are unable to identify if students were actually drawing resonance structures while answering the questions and if they were drawing resonance structures correctly. The role of energetics in the context of reactivity and energetics in students' arguments was not explored through this study. Energetics is inherent to mechanistic reasoning and is the driving explanation of all reactions. This study was limited to students completing Organic Chemistry I or just beginning Organic Chemistry II, as such we are unable to make claims about how students would perform on the ORQ after completing Organic Chemistry II. Further evidence is needed to establish the response process and external validity of the ORQ to ensure that items are interpreted as intended and that they correlate with summative assessment scores.

3.8 Conclusions

A key skill in mastering organic chemistry is recognizing how reactivity principles, like resonance or electronegativity, influence a reaction's outcome. However, students often struggle to identify or compare chemistry concepts related to reactivity and little is known about students' interpretations of these concepts. Herein, we explored undergraduate students' interpretations of reactivity principles in organic chemistry using an Organic Reactivity Questionnaire (ORQ). We recruited students from four different universities across Canada to complete the ORQ

We scaffolded students using the claim-evidence-reasoning framework to better elicit why they chose a certain answer. We attempted to expand the context of this study by including students from multiple Canadian institutions and different organic chemistry curricula such that our results incorporated perspectives from outside our host institutions.

Students met expectations when asked to provide a definition of nucleophilicity and electrophilicity and actively connected aspects of structure and function. The students in the current study sample were largely successful in identifying the more electrophilic molecule when given a surface level cue, in this case a positive formal charge. Students were less consistently able to compare the electrophilicity of molecules when a surface feature cue, such as a formal charge, was not given, as shown in the near even split in answers for questions 4 and 5. Less than half of the students identified steric hindrance as a relevant factor in question 4. Students showed a slightly higher tendency in selecting inductive effects as a relevant factor when different alkyl chains or heteroatoms were present, such as in questions 4 and 5. Participants had a tendency overall to focus on electronegativity and directly associate electronegativity with electrophilicity or leaving group stability. Students were able to identify when resonance was present but were more rarely able to correctly explain how resonance contributes to electrophilicity. Students were more successful on determining the direction of an acid–base equilibrium when given pK_a values and would incorrectly associate charge with instability.

3.9 Implications for teaching

Giving students the opportunity to practice their reasoning skills to compare chemical concepts can help them develop a deeper understanding of the material (Cooper & Stowe, 2018; Noyes et al., 2022). Educators can design formative assessment tasks like the three-part questions seen on the ORQ as both practice and a diagnostic tool for students. This way, students can see where they may be misinterpreting concepts related to reactivity. One participant indicated that the ORQ helped them identify their misinterpretations:

"I think the nitrogen introduces more resonance structures and more electrons means less electron deficiency**. I think doing this exercise is exposing my misunderstandings"**

Actively scaffolding students during practice or summative assessments may help them identify gaps in their knowledge or understanding and assist them in building reasoning skills for organic chemistry. Helping students understand *why* reactions follow certain pathways makes them better prepared problem solvers. Talanquer (2017) found that asking students to consider the incorrect answer showed a positive impact on their own answers. Herein we identified and described some of the common errors made by students from Canadian universities when reasoning about reactivity. Instructors can illustrate these potential errors to students while teaching to further aid students' understanding of reactivity principles and improve their reasoning. Many students in our study were unable to differentiate between inductive effects and steric hindrance as the most relevant factor in determining reactivity; Educators could emphasize the role of each factor and explicitly differentiate the contexts for when one is more relevant to the reaction.

Students in our study often considered the “stability” of a molecule when making their decisions but more rarely leverage ideas related to reaction kinetics or thermodynamics. Indeed, even with an active scaffold, students have been reluctant to discuss reactivity in terms of thermodynamics (Eckhard et al., 2022). While the stability argument is not inherently wrong, it lacks some depth in terms of causal reasoning. Emphasising thermodynamics during in class discussions can help students to develop a deeper understanding of why mechanistic steps occur. Students in this study were sometimes unable to identify the primary factor involved in determining reactivity.

3.10 Implications for research

We allowed participants to click on an image in SurveyMonkey so that they did not have to look back and forth between images and the answer choices, however since the species were not labelled it made it more difficult to interpret which molecule participants were referring to in their open-ended responses. There has been consistent research out put on undergraduate students’ understanding of resonance and delocalization in the last ten years but very little is known on students’ understanding of the other factors explored in this study, specifically steric hindrance and inductive effects. More research is needed to understand any misinterpretations or difficulties students have with these concepts.

3.11 Future work

The ORQ contained a limited diversity of questions about acid–base chemistry and leaving groups. We hope to add more acid–base and leaving group questions to future versions of the ORQ to gai a more robust idea of how students interpret these concepts. Most of the participants in this study had either recently completed their first semester of organic chemistry or were near completion. It would be interesting to see how students’ understanding changes (if at all) throughout several semesters of organic chemistry by collection data at multiple timepoints. (End of ORG I and end of ORG II). In theory, all students should have similar knowledge of organic chemistry at the end of ORG II. Cognitive interviews to collect evidence of response process validity, some of the students’ responses suggest that they misinterpreted what the questions were asking (such as explaining why a species was nucleophilic rather than electrophilic). It is possible that our examples were too vague and required more context, such as the reaction or mechanisms most likely to occur, this information can also be obtained by conducting cognitive interviews with participants. Evidence for external validity could further strengthen trust that the ORQ is measuring relevant knowledge about reactivity. External validity evidence can be collected by comparing students' responses and scores on the ORQ with exam scores or final grade. The students in our study had differing knowledge of organic reactions because our sample came from multiple institutions, using different organic chemistry curricula. Some students may not have had exposure to all the concepts presented as many had yet to complete their first semester of organic chemistry. We will include a demographic survey with future administrations of the ORQ that will also ask students about the types of reactions, relevant factors (e.g., steric hindrance, inductive effects, etc.) and organic mechanisms they have learned so far. This way, we can gain further insight into participants open-ended responses. The results from this study will be used to further revise the items on the ORQ for clarity and to improve upon the depth of our results. The eventual goal of this work will be to make quantitative comparisons between the efficacy of different Canadian organic chemistry curricula on student reasoning and understanding of reactivity. This way, we can identify aspect of different curricula that aid students in understanding reactivity principles.

Chapter 4. A Self-Efficacy Beliefs Scale in Organic Chemistry Based on a Patterns of Mechanisms (Reactivity) Curriculum

4.1 Introduction:

Organic chemistry has an infamous reputation for being a difficult, content heavy, “gatekeeper” course with high attrition rates (Elbulok-Charcape et al., 2021; Shah & Garg, 2017). The majority of students who make up organic chemistry classes are not chemistry majors and may not consider themselves as being “a chemistry person” or being good at chemistry (Brown et al., 2012; Hosbein & Barbera, 2020). Even students who consider themselves as being “good at chemistry” after being successful in previous chemistry courses may have negative beliefs and outcomes when entering organic chemistry (T. L. Anderson & Bodner, 2008). These negative beliefs can have adverse effects on students’ learning and performance in organic chemistry courses which may discourage them from completing their degree (Luo et al., 2021). Educators must look beyond content knowledge and cognitive skills if they want students to be successful in organic chemistry and beyond.

4.1.1 Affect and self-efficacy beliefs in chemistry

Learning encompasses more than just content knowledge and the memorization of facts. Learning can be categorized into three broad domains: cognitive, psychomotor, and affective (L. W. Anderson et al., 2001). The cognitive domain focuses on content knowledge and related skills such as critical thinking and problem solving; the psychomotor domain focuses on physical tasks involving movement; and the affective domain focuses on attitudes, values, and interests (*Bloom’s Taxonomy, Centre for Teaching Excellence, University of Waterloo*, 2022).

Self-efficacy is an aspect of the affective domain known to be correlated with students’ success in multiple academic fields, including chemistry (Flaherty, 2020; Luo et al., 2021). Self-efficacy is an individual’s beliefs in their ability to perform a task or achieve a goal (Bandura, 1977). Non-chemistry majors, who make up the majority of introductory chemistry courses, are more likely to exhibit lower self-efficacy (Uzuntiryaki & Aydin, 2009). High self-efficacy has been associated with reduced attrition rates and higher rates of success in organic chemistry courses (Avargil et al., 2020; Chen, 2014) and continue in their degree. Furthermore, Self-efficacy has been found to correlate moderately with other affective measures directly related to chemistry such as chemistry identity (Hosbein & Barbera, 2020; Kurbanoğlu & Akin, 2012), chemistry self-concept (Gibbons & Raker, 2019), and chemistry mindset (Santos et al., 2022).

4.1.2 Theoretical background: Social cognitive theory

Self-efficacy beliefs stem from Social cognitive theory (Bandura, 1997). Social-cognitive theory emphasizes that much of human learning occurs in social environments and recognizes learners as active seekers and processors of information (Shunk, 2012). There is reciprocal causation between the learner, their behaviour, and the social environment in which they exist such that they each influence and change each other (Shunk, 2012). The idea of reciprocal interaction is actively demonstrated through self-efficacy; self-efficacy influences achievement behaviour, like persistence or effort, which affects self-efficacy. A student working through organic reaction mechanisms may find them confusing and frustrating at first, but if they practice effectively and use productive habits, they improve their confidence and subsequently work through more advanced reactions. Self-efficacy beliefs have been shown to influence factors such as learning, motivation, emotion, and achievement (Bong & Clark, 1999; Bong & Skaalvik, 2003; Schunk & Usher, 2012; Williams & Williams, 2010; Zimmerman et al., 1992). Additionally, an individual's self-efficacy can influence their decisions (Betz & Hackett, 1983; Hackett & Betz, 1981; Patall, 2012), effort exerted on an activity, and their resilience towards obstacles (Joët et al., 2011; Moos & Azevedo, 2009).

Bandura (1997) theorized four sources contributing to an individual's self-efficacy beliefs: mastery experiences, vicarious experiences, verbal persuasion, and emotional/physiological states. Mastery experiences are thought to possess the most influence over a person's self-efficacy beliefs, as an individual's experiences and past performances act as a tangible indicator of their capabilities. For example, an individual who has viewed their experience in general chemistry as successful may have an increased self-efficacy belief toward chemistry as they transition to organic chemistry courses. Self-efficacy has been found to be positively correlated to achievement outcomes in many studies, as well as adaptive motivational processes, effort, and persistence (Pintrich and De Groot, 1990; Multon et al., 1991; Pajares and Miller, 1994; Zusho et al., 2003).

4.1.3 Measuring self-efficacy beliefs in organic chemistry

Promoting students’ self-efficacy beliefs towards organic chemistry may improve their overall success and lower attrition rates. We need an accurate and precise measure of students’ self-efficacy beliefs to measure how these beliefs change during an organic chemistry course. Self-efficacy is a theoretical construct; It is a combination of underlying ideas and concepts that together form a set of held beliefs. Self-efficacy cannot be directly measured or observed; As such, we need to develop context specific tools, called instruments, that can measure different aspects of self-efficacy. These tools can be anything that elicit, and record, peoples’ thoughts related to self-efficacy; Examples of educational instruments include interview protocols, observation protocols, surveys, and tests. These instruments need to generate valid and reliable data to ensure that they are consistently measuring the intended construct. Validity refers to the degree to which evidence/theory support interpretations of data for proposed uses within a specific population (Deng et al., 2021); Reliability refers to an instrument’s precision and how consistently it measures the intended construct. We can then use these indirect measures of self-efficacy, once validity and reliability evidence is established for the data, to create a discipline specific model of self-efficacy beliefs. This model can then be used to identify difficult topics in a curriculum and potentially at-risk students. Ideally, students’ self-efficacy would exhibit a net positive change after a full course of instruction; a net negative change may indicate the need to change a curriculum or teaching approaches to better aid learning. Several self-efficacy beliefs instruments have been developed in a variety of STEM fields including mathematics (Williams & Williams, 2010), biology (Baldwin et al., 1999; Batiza et al., 2013), physics (Çalisçkan et al., 2007; Shaw, 2004), and chemistry (Gibbons & Raker, 2019; Liu et al., n.d.; Villafañe et al., 2016). Self-efficacy beliefs instruments should be domain specific (Bandura, 2006). General instruments, such as a self-efficacy beliefs in STEM survey, lack predictive power because self-efficacy beliefs are task specific (Choi, 2005).

One study surveyed organic chemistry II students across an entire semester and found that self-efficacy and performance in that course fit a reciprocal causation model. In other words, "students’ beliefs in completing a specific organic task at one time point predicted their confidence at the subsequent time point across the semester" (Villafañe et al., 2016). Increased achievement has been found to be directly associated with increased self-efficacy in introductory general and organic chemistry courses (Gibbons & Raker, 2019).

4.1.4 Goals:

Herein, we aim to develop a domain specific, self-efficacy beliefs instrument rooted in the principles of reactivity in organic chemistry. This work aims to provide researchers and educators with an instrument that can produce valid and reliable data to capture change in self-efficacy beliefs for introductory organic chemistry courses (i.e. OCI and OCII).

4.2 Methods

We obtained ethics approval from our institutions research ethics board before collecting or analyzing any data (ethics #H-11-18-1363).

We developed the Self-Efficacy Beliefs in Organic Chemistry survey (SEBOC), guided by the principles of self-efficacy instrument design as described by Bandura (2006) and adhering to the standards for reliability and validity put forward by the Standards of Educational and Psychological Testing (Figure 4.1) (American Educational Research Association et al., 2014).

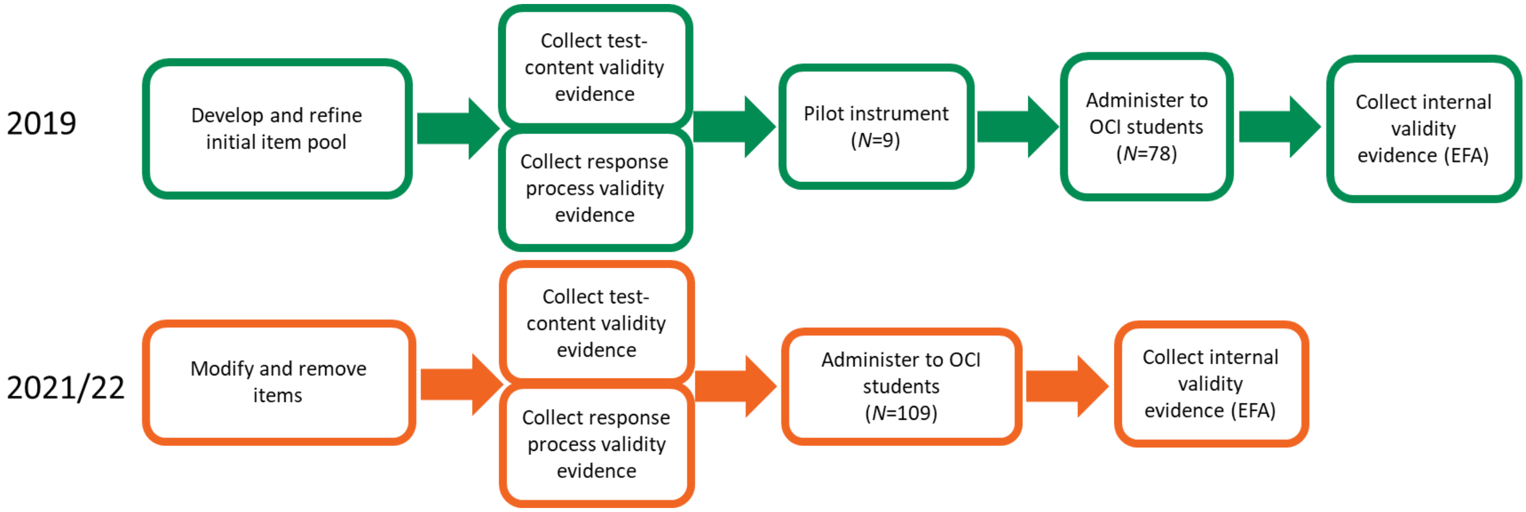


Figure 4.1. Development process of the SEBOC

4.2.1 Instrument development:

4.2.1.1 *Phase 1: instrument development and pilot study*

Two lenses guided the selection of the intended dimensions within the SEBOC: 1) learning outcomes from the *Patterns of Mechanisms* Curriculum (Carle & Flynn, 2020; Flynn & Ogilvie, 2015; Stoyanovich et al., 2015) and 2) previously constructed instruments used for assessing self-efficacy beliefs in chemistry (Dalgety et al., 2003; Uzuntiryaki & Aydin, 2009; Villafañe et al., 2016; Winkelmann et al., 2015) as well as other STEM-related disciplines (Baldwin et al., 1999; Çalisçkan et al., 2007; Shaw, 2004). The dimensions included within the SEBOC aimed to target three separate but highly interrelated dimensions of self-efficacy beliefs in organic chemistry that instructors often aim to promote: *cognitive skills, everyday applications, and experimental practices.*

The SEBOC places a strong focus on the dimension of *cognitive skills relating to organic chemistry*. The items included within this dimension include domain-specific tasks relating to the essential conceptual knowledge novices in the field typically learn at the beginning of their Introductory Organic Chemistry curriculum. Essential conceptual tasks such as understanding representation in organic chemistry, the symbolic language of organic chemistry, and principles of reactivity serve as the foundational knowledge in organic chemistry and underpin the entire curriculum.

The second intended dimension included within the SEBOC, *self-efficacy towards everyday application of organic chemistry* is modified from the College Chemistry Self-Efficacy scale (Uzuntiryaki & Aydin, 2009). Students' attitudes towards chemistry can be influenced by relating it to everyday life (Treagust et al., 2018); Students will likely understand concepts better if they are able to make meaningful connections with the content material (Galloway & Bretz, 2015; Lowery Bretz, 2001). As such, situating chemistry in everyday life, using relevant examples, is beneficial to helping students learn. One example of this could be bridging chemistry with larger societal issues like climate change (Flynn et al., 2019; Mahaffy et al., 2018; Matlin et al., 2016).

The third intended dimension of the SEBOC instrument is rooted in *experimental practices relating to organic chemistry*. This dimension aims to extend the role of cognitive skills in organic chemistry to the knowledge required within a laboratory setting. For example, cognitive skills relating to laboratory experience could include designing an experiment and interpreting data. This third dimension does not include self-efficacy with respect to psychomotor skills in experimental settings, but rather the self-efficacy towards the cognitive skills required in experimental settings. This dimension differs from everyday applications in that students require an understanding of specific lab techniques.

We collected validity evidence with respect to face, test-content, and response process throughout the instrument design process to ensure that the SEBOC was assessing the intended construct (Arjoon et al., 2013). Face validity is often referred to as one of the weaker sources of validity evidence as it is a subjective measure based on whether the reader believes the instrument is measuring the intended construct. Face validity evidence was established through literature review as well as informal discussion between authors and colleagues in the field of chemistry education. We refined the initial item pool for clarity before moving forward to collecting evidence based on test content and response process.

Evidence based on test content acts as an indicator that dimensions, items, and instruction are appropriately rooted in the intended measure conceptually (American Educational Research Association et al., 2014). For our context, a panel of ten experts in domains ranging from Chemistry Education, Education, and Organic Chemistry were recruited to provide electronic feedback on the instrument. Specifically, we sought quantitative feedback to determine whether the items were clear and relevant to the intended dimensions and asked for experts to judge the alignment between experts' knowledge and the intended dimensions. Additionally, an open-response section was provided to allow for additional comments, questions, or areas of concern. A total of 14 items were modified where experts perceived the item differently than intended or to address potential shortcomings. For example, recurring feedback from experts asked for examples to be provided.

We conducted cognitive interviews with students who had completed Organic Chemistry I to collect evidence for response process validity. Cognitive interviews check that the target population perceived the items in the instrument as intended and helps us identify ambiguous or redundant items(Deng et al., 2021). We modified two items based on the results from the semi-structured cognitive interviews; The item "visualize a molecule in three dimensions, given the structure" was modified as the item elicited discussion regarding the use of molecular modelling kits. While an important skill, using molecular modelling kits is a psychomotor skill, while the item aimed to elicit the cognitive skills required for understanding a molecular representation. To better capture this, the item was modified to "Form a 3-dimensional mental image of a molecule."

We conducted a small pilot study to pretest the items due to the limited number of cognitive interviews (Bandura, 2006). This pilot consisted of Organic Chemistry II students *(N=9)* enrolled in the summer course of 2019 at a midsize Canadian Institution, who completed the 42-item version of the SEBOC within the week prior to their final exam. Students were incentivized to participate with an opportunity to win one of two 50$ Amazon gift cards. The objective of the pilot study was to highlight any items that lacked the ability to differentiate between participants (*e.g.,* items where all participants selected the maximum efficacy). We found no items that lacked an ability to capture gradients of challenge during the pilot study. As such, we did not eliminate any items because no single item lead to a strong majority selecting one of the seven levels of confidence (K. Lapierre, 2019).

4.2.2 Phase 2: Exploratory Factor Analysis

Exploratory factor analysis (EFA) is a statistical method used to generate a hypothesis, or propose a model, about an underlying variable that cannot be directly measured (e.g., self-efficacy beliefs) (Field, 2013). EFA groups variables based on how the target population (in this case undergraduate students taking organic chemistry) responds to different questions related to the underlying construct. For example, we can ask students about their confidence in doing specific tasks in an organic chemistry course and then conduct an EFA to identify categories of variables related to self-efficacy beliefs in organic chemistry. Some items can be complex and may cross load onto more than one category (factor). Cross loading means that an item was grouped into more than one category and may need to be further investigated, modified, or removed (Hair et al., 2014).

We were interested in identifying underlying groups of variables on the SEBOC related to self-efficacy. We conducted two separate iterations of exploratory factor analysis on the SEBOC, using IBM SPSS 28, to identify groups of variables and variables that might not be related to the targeted construct. Two iterations were necessary because the first iteration did not meet sample size recommendations. The first iteration was completed in the Summer of 2019 and was used to guide further revisions of the SEBOC. We did not use this analysis to propose a model of organic self-efficacy beliefs because it lacked the suggested sample size required for the number of instrument items. We revised the SEBOC and conducted interviews with experts to collect test-content validity evidence following the revisions. We then completed a second iteration of exploratory factor analysis in the Spring of 2022 with the goal of proposing a factor structure of self-efficacy beliefs in organic chemistry.

4.2.3 First administration

4.2.3.1 Instructional context:

Participants of the first iteration were recruited in the Summer of 2019 and had recently completed a one-semester Organic Chemistry course (Organic Chemistry I) at a large bilingual Canadian university. Participants completed the 42-item instrument online hosted on SurveyMonkey at their leisure, with an average completion time of eight minutes (“SurveyMonkey, “2019). As done in the phase 1 pilot, students were incentivized to participate with an opportunity to win one of two 50$ Amazon gift cards. The Organic Chemistry I course is a requirement for a diverse set of programs, including chemistry-focused programs (i.e., Chemistry, Biochemistry, Chemical Engineering), Biomedical Sciences, Health Sciences, Psychology, etc. Participants (*N* = 78) were recruited from all Organic Chemistry I course sections (approx. 1800 students) through their shared laboratory components after final course grades had been finalized. Demographic information was self-reported by 96% of participants, revealing the participant sample possessed a greater proportion of women (75%) to men (25%) (K. Lapierre, 2019).

4.2.3.2 Results

Our initial analysis suggested that we group the 42 items into 11 categories (factors). Each category encompassed a broader idea related to organic chemistry (e.g., mechanisms, orbitals, etc.) that together made up a percentage of self-efficacy beliefs related to organic chemistry. However, we decided to group items using only seven categories based on other categorization methods because of the sample size.

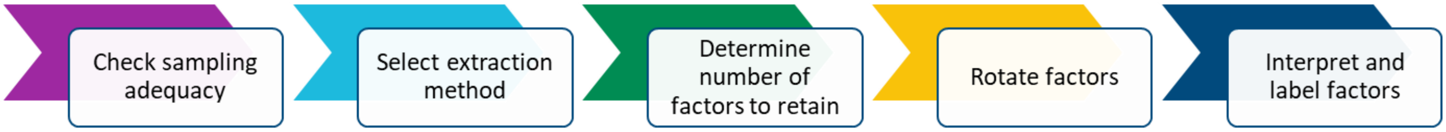


Figure 4.2. General procedure of EFA (Lapierre, 2019)

EFA generally follows the systematic procedure found in Figure 4.2. Sampling adequacy can be checked using the Kaiser-Meyer-Olkin (KMO) measure which produces a value between zero and one. Values closer to zero indicate that the sample may not be adequate for factor analysis and that the results should be interpreted with extreme caution, values closer to one indicate a good sample size for EFA and that the results will likely be meaningful (Field, 2013). Extracting factors means grouping survey items into different numbers of categories based on responses from participants. Principal axis factoring creates the simplest model possible based on the given data. Researchers must then decide how many factors (categories) the model should have based on theory (e.g., one category could be called *organic mechanisms* based on the items being related to reaction mechanism LOs). There are several methods that can be used to determine the number of factors a model should have, specifically the Kaiser criterion, the scree plot, and parallel analysis are the most common. The Kaiser criterion is an easy-to-use method but has very specific criteria where it is accurate and often overestimates the number of factors in the model (Field, 2013). The scree plot uses a graph that compares the total number of items to a possible number of factors (eigenvalues) and determines how many to retain based on inflection points of the graph. This method is somewhat ambiguous as it relies on the research to interpret where the inflection points on the graph are. Parallel analysis is a more robust method that generates random eigenvalues and compares the actual data to randomly generated samples(Patil et al., 2017). The factors are then rotated once the researcher has decided the number of factors to retain. Factor rotation is a mathematical operation that makes it easier to interpret the factor structure by maximizing the loadings of items to each factor (Hair et al., 2014). We used an oblique rotation in our analysis because it is considered to be more appropriate for modeling ideas that may be correlated (like reactivity principles) (Field, 2013). The researcher then decides if the items grouped onto each factor make sense (based on theory) and labels each factor based on the items grouped under it.

Factors were extracted using principal axis factoring, with the Kaiser criterion of the eigenvalues for the 42-item instrument indicating to retain a total of 11 factors, accounting for 67% of the variance and an average communality of 0.67 with no items below 0.4. The Kaiser criterion may not provide an accurate number of retained factors in the current context; as such, multiple methods were investigated in conjunction with the Kaiser criterion approach (Field, 2013). A Scree plot revealed multiple points of inflexion indicating to retain 2 factors, 7 factors, or 11 factors. Lastly, the parallel analysis comparing the randomly generated eigenvalues to the actual eigenvalues indicated to retain a total of 7 factors. A 7-factor structure was thus investigated, meeting the criteria for the Kaiser-Meyer-Olkin (KMO) measure of sampling adequacy (0.72) and rejecting the null hypothesis for Bartlett's test (p = 0.000). Within the 7-factor structure, three items (items 4, 6, and 18) were found to possess communalities below 0.4 and were eliminated from the factor structure before proceeding (K. Lapierre, 2019).

The sample size for this analysis (N = 78) was considered small given the number of items on the SEBOC. For a sample size of 70, factor loadings of 0.65 could be considered substantive, indicating that the proposed structure may not accurately fit the data and so should be interpreted with extreme caution (Hair et al., 2014).

4.2.4 Second administration

We modified the SEBOC based on the learning outcomes from the Patterns of Mechanisms organic chemistry curriculum and the first iteration of exploratory factor analysis before proceeding with a second iteration. The goal of this modification was to shorten the SEBOC to remove redundant items and to improve the wording and content of individual items. For example, we removed the scale related to self-efficacy beliefs towards spectroscopy. Factor loadings for both items on the spectroscopy scale were substantive (>0.75) however the scale only contained two items, so the amount of variance captured was limited (Hair et al., 2014). Furthermore, spectroscopy is taught at different times in different curricula. In the *Patterns of Mechanisms* curriculum, students are not taught about spectroscopic methods until after the first midterm of Organic Chemistry II. The participants in this sample had just completed Organic Chemistry I and would not have been taught spectroscopy in a formal course setting, which likely explains why the loading for these two items were high. A full summary of all items that were cut and reasons behind these can be found in Appendix B. We re-assessed the test-content validity evidence of these items within the proposed factor structure through qualitative interviews with a panel of three experts, two specialized in organic chemistry and one in educational psychology with a chemistry background. We conducted semi-structured interviews individually with each expert with the goals of determining 1) the extent to which the SEBOC covers key concepts/essential topics for Organic Chemistry I and II and 2) if the SEBOC was missing any essential concepts related to organic chemistry. Specifically, we asked each expert if they thought the items fit well under the labelled factor, if the topic/factor was relevant to their course, and if they found the wording for each item to be clear (or otherwise asked them to re-word the item). Overall, the experts found that the modified SEBOC covered a range of essential organic chemistry topics. One expert pointed out that the SEBOC did not include any items related to organic nomenclature. We did not include items about organic nomenclature on the SEBOC because they were not directly related to reactivity. Another expert noted that they strongly emphasise conformational analysis when they teach and that the SEBOC was missing items related to conformation and structure. Conformational analysis, structure, and stereochemistry are often essential in understanding reactivity, therefore we added items specific to conformational analysis, such as translating between different types of 2D and 3D representations based on recommendations from the expert. A full summary table of feedback from experts can be found in Appendix B. We conducted semi-structured cognitive interviews with undergraduate students (*N* = 2) to collect evidence for response process validity for the modified scale and ensure that all items were interpreted as intended. Responses from these interviews suggested that all items were interpreted as we intended by the students and that no further modifications were necessary. A summary of the interview protocol can be found in Appendix B. We expected the factor structure to group into distinct factors on mechanisms, reactivity, conformational analysis, and everyday applications based on the first iteration of exploratory factor analysis done on the 42-item instrument (see **Error! Reference source not found.**).

4.2.4.1 Instructional context

Participants for the second administration were recruited near the end of Organic Chemistry I in the Winter of 2022 at the same large bilingual Canadian university. Participants completed the 22-item instrument online hosted on SurveyMonkey at their leisure (*Surveymonkey*, 2022), with an average completion time of three minutes. Each participant was compensated for their time with a $5 Amazon e-gift card. We changed the incentive to participate from a draw to each participant receiving a gift card as compensation to try and improve participation. Participants (*N* = 109) were recruited from all Organic Chemistry I course sections (approx. 1800 students) through their shared laboratory components before course grades had been finalized. Participant data was anonymized by the student researcher before starting data analysis to ensure anonymity. Demographic information was self-reported by 99% of participants, revealing that the sample again possessed a greater proportion of women (80%) than men (17%); 2% of participants selected they would prefer not to answer and 1% identified as non-binary.

4.2.4.2 Results

Our initial analysis suggested that the 22 items should be grouped into four categories (factors). Each category encompassed a broader idea related to organic chemistry (e.g., mechanisms, orbitals, etc.) that together made up a percentage of self-efficacy beliefs related to organic chemistry. However, we decided to group items using only three categories based on parallel analysis.

Factors were extracted using principal axis factoring for the 22-item instrument with oblique rotation (direct oblimin). We ran an initial analysis to obtain eigenvalues for each factor. Four factors had eigenvalues over Kaiser's criterion of 1, which explained 52.7% of the total variance. The Scree plot showed an inflexion that also indicated to retain 4 factors. We conducted a parallel analysis to confirm a 4-factor model because our sample did not fit recommendations for the use of Kaiser's criterion and our total sample was less than 200, the minimum recommended sample for use of a scree plot (Field, 2013; Hair et al., 2014). Parallel analysis (Patil et al., 2017) indicated to retain 3 factors (Table 4-1Table 4-1. Parallel analysis results); as such, a 3-factor structure was investigated. The Kaiser-Meyer-Olkin (KMO) measure verified the sampling adequacy of the analysis with a KMO= 0.85, deemed as meritorious or excellent sampling adequacy (Hutcheson, 1999). Within the 3-factor structure, four items (items 1, 7, 15, and 16) possessed communalities below 0.4 and were eliminated from the factor structure before proceeding. Factors were extracted using principal axis factoring from the 18-item instrument with oblique rotation (direct oblimin). The 3-factor model was confirmed again using parallel analysis and explained 60.1% of the total variance. Sampling adequacy was verified again with a KMO = 0.85 with no items possessing a communality below 0.4. Table 4-2 shows factor loadings after rotation. The factor loadings suggest that factor 1 represents Self-efficacy beliefs towards reactivity and organic mechanisms, factor 2 represents Self-efficacy beliefs towards representations in organic chemistry, and factor 3 represents Self-efficacy beliefs towards applications of organic chemistry. All three factors were found to possess high internal reliability, with all values of Cronbach's $\alpha \geq 0.8$, a summary of reliability data can be found in Table 4-3.

Table 4-1. Parallel analysis results indicating to retain three factors.

Factor number	1	2	3	4	5	6	7
Randomly generated eigenvalue (parallel analysis)	1.990	1.736	1.578	1.472	1.360	1.272	1.187
Actual eigenvalue (factor analysis)	6.905	2.252	1.658	1.005	0.783	0.721	0.648

Table 4-2. SEBOC factor loadings for the second iteration of exploratory factor analysis (factor loadings <0.3 omitted, factor loadings ≥ 0.4 are bolded).

SEBOC item	Factor		
	1	2	3
Self-efficacy beliefs towards reactivity and organic mechanisms			
5. Propose a possible mechanism and the products for a reaction, given the starting materials.	**0.898**		
6. Propose a possible mechanism for a reaction, given the starting materials and products.	**0.843**		
9. Compare two potential mechanisms for a reaction and justify which is the most likely to occur.	**0.715**		
11. Identify nucleophilic or electrophilic sites in a molecule.	**0.658**		
12. Compare two nucleophilic or electrophilic sites and justify which is most likely to participate in a reaction.	**0.632**		
17. Explain how a reaction coordinate diagram describes an associated reaction mechanism.	**0.537**		
14. Identify similarities between multiple reactions based on their underlying mechanisms.	**0.482**		
Self-efficacy beliefs towards representations in organic chemistry			
21. Convert between 2D and 3D representations of a molecule (e.g., Lewis structure to Newman projection).		**0.808**	
18. Convert between 2D representations of a molecule (e.g., Lewis structure to line structure).		**0.716**	
20. Convert between 3D representations of a molecule (e.g., Newman projection to perspective diagram).		**0.619**	

3. Explain a concept learned in organic chemistry to a peer.	0.330	**0.459**	
Self-efficacy beliefs towards applications of organic chemistry			
13. Design a laboratory procedure to perform a synthesis reaction learned in your organic chemistry course.			**0.828**
19. Draw the molecular orbitals on a given nucleophile and electrophile (i.e., highest occupied molecular orbital and lowest unoccupied molecular orbital).			**0.622**
4. Propose a retrosynthetic analysis as part of a synthesis.		-0.347	**0.580**
8. Critique a news report or documentary that deals with some aspects of organic chemistry.			**0.573**
2. Visualize how molecules are interacting in 3D space as a reaction proceeds.			**0.572**
22. Apply concepts learned in organic chemistry to other sciences.		0.348	**0.553**
10. Interpret and draw conclusions from data collected in your organic chemistry lab course.		0.337	**0.431**
Omitted items			
7. Draw the resonance structures of a molecule.			
15. Explain which side of an acid-base equilibrium is favored using chemical properties (other than pKa values).			
1.Describe how organic chemistry underlies a global issue (e.g. societal, environmental), either positively or negatively.			
16. Explain how a reaction takes place using the molecular orbitals involved.			

For cognitive tests, such as asking students to select the most viable mechanism from a multiple choice, an α value of ≥0.8 is considered acceptable (Kline, 2013). The SEBOC is an ability test that measures self-efficacy beliefs specific to organic chemistry. Kline suggests that for ability tests an α value of ≥ 0.7 is acceptable due to the wide array of constructs being measured (Kline, 2013). All three factors on the SEBOC have α values ≥ 0.8 indicating that each scale is likely producing reliable data in our context. Values of Cronbach's α can be affected by the number of items in a scale, where more items can result in a higher value of α (Field, 2013). The *Applications* scale and the *Reactivity and organic mechanisms* scale have higher values of α but also contain seven items each (compared to Representations which has four). We further analysed the reliability evidence for each scale by looking at the corrected item-total correlation for each item and each scale's α value if specific items were deleted. All items for each scale were found to correlate moderately (>0.4) with the total score for that scale, further providing evidence that the scale produces reliable data. We also found that the α values for both scales would not increase if any items were deleted, indicating that no one item produced reliability issues. The Applications scale has a somewhat lower value of α compared to Reactivity and organic mechanisms despite having the same number of items (Table 4-3) indicating that the Applications scale may contain redundant or problematic items. This lower α value could be the result of the cross loaded items (items 10 and 22).

Table 4-3. Reliability evidence for the SEBOC instrument based on a 3-factor structure.

Factor	Number of items	Eigenvalues	% of variance	Cronbach's α
1.Reactivity and organic mechanisms	7	6.91	38.36	0.89
2.Representations	4	2.25	12.51	0.80
3.Applications	7	1.66	9.21	0.83

Table 4-4. Factor correlation matrix

Factor	1	2	3
1.Reactivity and organic mechanisms	1		
2.Representations	0.27	1	
3.Applications	0.54	0.21	1

Average scores for items related to *Applications* were lower than *Mechanisms* and *Representations* (Table 4-5). It is possible that students are more confident in skills related to the first two factors because they have more formal practice with them. Indeed, organic chemistry assessments have been known to focus on mechanistic tasks and conformational analysis as opposed to everyday or industrial applications. Organic chemistry assessments will often ask students to predict the products of a reaction or draw mechanisms rather than consider possible application of their organic chemistry knowledge (Cooper & Stowe, 2018). The small correlation between Representations and Applications (0.21) was unexpected given that three of the items in Applications (items 2, 4, and 19) all require spatial ability skills or the use of conformational analysis. This smaller correlation might be because other items in Applications were not directly related to representational skills. For example, item 22 (Apply concepts learned in organic chemistry to other sciences) is vague and complex, given that it cross loads, and does not necessarily involve representational competence or conformational analysis.

Table 4-5. SEBOC Factors Descriptive Statistics (N=109)

Factor	Average factor score (/7)	Standard deviation	Range
1.Reactivity and organic mechanisms	4.3	1.2	1.1–.0
2. Representations	5.1	1.1	1.3–7.0
3. Applications	3.6	0.99	1.4–7.0

4.3 Discussion:

Reactivity and organic mechanisms correlated moderately with *Applications of organic chemistry* (Table 4-4). This correlation makes sense given that many applications of organic chemistry involve mechanisms and reactions, such as synthesis (Bhattacharyya, 2004; Bodé & Flynn, 2016). Indeed, mechanistic and non-mathematical tasks are most prevalent in organic chemistry problem solving (Cartrette & Bodner, 2010; Graulich, 2015). *Organic Representations* has a small correlation with *Reactivity and mechanisms* (0.27) and *Applications* (0.21) respectively. All the factors proposed here are in line with skills required to problem solve in organic chemistry, those being “judging trends in reactivity, devising mechanisms to predict chemical change, or rationalizing spatial relationships” (Graulich, 2015). Items 3 and 10 cross-load onto two factors with differences in loading less than 0.2. These items can be considered complex and may need to be cut or further investigated for revisions. Item 10 asks students about more than one skill, “interpret and draw conclusions” as opposed to just “interpret”. The complexity of this item might be resolved by simplifying the wording, splitting the item, or through response process interviews with participants to check their interpretation of the wording. Item 3 cross-loads to both mechanisms and representations neither of which make sense for the item. Our *a priori* expectation for this item was that it would clump with *Applications* or other items not related to skills demonstrable on organic chemistry summative assessments. Items 7 (“Draw the resonance structures of a molecule”) and 15 (“Explain which side of an acid-base equilibrium is favored using chemical properties”) were omitted from the factor structure due to having low communalities but are considered essential items based on the learning outcomes for Organic Chemistry I and II (Flynn & Ogilvie, 2015). Resonance is a fundamental organic chemistry concept required to explain the reactivity of functional groups (Carle & Flynn, 2020; Duis, 2011) and acid-base reactions are present in a huge amount of mechanisms (Bell et al., 2019; Ogilvie, 2017). Further investigation of the model is needed to identify if these essential skills fit based on theory.

4.4 Conclusion

Organic chemistry is often considered a heavy and difficult course by students and has high attrition rates (Chen, 2014; Gilstrap, 2020). Students’ affect, their feelings and emotions, play a role in their persistence and achievement in chemistry courses (Flaherty, 2020; Santos et al., 2022). Research suggests that self-efficacy beliefs, specifically, may be predictive of students’ outcomes in organic chemistry courses (Villafañe et al., 2016). If we can identify students with low self-efficacy beliefs in organic chemistry, then we can better aid them to succeed through teaching interventions. We need an accurate and precise measure of students’ self-efficacy beliefs to measure how these beliefs change during an organic chemistry course.

We developed the Self-efficacy Beliefs in Organic Chemistry (SEBOC) scale to measure undergraduate students’ self-efficacy beliefs in organic chemistry. We proposed an initial 42-item instrument based in three inter-related subscales: Cognitive skills, everyday applications, and experimental practices. We collected validity evidence related to content, responses process, and internal structure and then modified items on the SEBOC based on the validity evidence collected. Modifications at this stage involved removing redundant items or items not directly related to organic reactivity. We further collected validity evidence for the SEBOC following modifications to ensure that the modified items would still produce valid data in the context of undergraduate organic chemistry courses. We collected validity evidence of test-content by conducting semi-structured interviews with experts in the fields of organic chemistry and chemistry education (*N*=4) and further adjusted the wording and structure of items. Two chemistry students participated in semi-structured cognitive interviews to collect evidence of response process validity. Finally, we administered the SEBOC to students at the end of an Organic Chemistry I course (*N*=109) and conducted an EFA to check internal structure. Results from the EFA suggest an 18-item instrument divided into 3 factors: Self-efficacy beliefs towards reactivity and organic mechanisms (7 items), Self-efficacy beliefs towards representations in organic chemistry (4 items), and Self-efficacy beliefs towards applications of organic chemistry (7 items).

4.5 Implications for Teaching and Research

The SEBOC can be used as a tool to identify how students' self-efficacy beliefs change over the course of a semester or multiple semesters. It could also be used to aide in curricular reform such that students complete organic chemistry courses with higher self-efficacy beliefs from when they began. The self-efficacy beliefs in organic chemistry model we proposed through EFA suggests that the students in our study have lower self-efficacy related to applications of organic chemistry (Table 4-5). This result is not generalizable nor is it definitive; however, applications of organic chemistry may be an area for instructors to emphasize while teaching.

4.6 Limitations

The SEBOC emphasises cognitive skills related to organic reactivity and may not encompass all aspects of self-efficacy beliefs related to an introductory organic chemistry course. Our sample of participants came from a single organic chemistry course from a single institution using the Patterns of Mechanisms curriculum. The second iteration of this work was carried out during the Covid pandemic and the possible influence this had on how participants responded is unknown. Herein our sample was only large enough to propose a factor structure for self-efficacy beliefs in organic chemistry, confirmatory analysis needs to be conducted to assess the model fit on the targeted demographics (organic chemistry I and II students). We were unable to make any inferences between demographic variables and self-efficacy beliefs in the current study due to its exploratory nature. The SEBOC provides a way to identify students' self-efficacy beliefs, but it is strictly a detection instrument; Future work using the SEBOC to identify students with lower self-efficacy beliefs could focus on how to improve self-efficacy over the semester.

Chapter 5. Conclusions

Traditional organic curricula organized around functional groups tend to promote students to rely on rote memorization rather than forming a deeper understanding of concepts(Flynn & Ogilvie, 2015; Grove, Bretz, et al., 2012). New curricula have been proposed and implemented that organize the content differently to try and emphasize understanding of deeper concepts. Evidence is needed to validate that these new curricula are promoting students' deeper understanding of organic chemistry concepts. Assessment instruments can be used to assess these curricula and make comparisons between the different types of curricula (ie. Traditional vs. reformed, and between the different reformed). My Master's work aimed to develop instruments to assess two separate aspects of the Patterns of Mechanisms curriculum at the University of Ottawa: 1) Students' understanding of reactivity principles in organic chemistry and 2) Students' self-efficacy beliefs in organic chemistry.

5.1 Summary of findings from chapters three and four

5.1.1 Chapter three: The Organic Reactivity Questionnaire

Recognizing how reactivity principles, like resonance or electronegativity, influence a reaction's outcome is a key skill in mastering organic chemistry. Organic chemistry experts can weigh the different chemical concepts involved in a reaction and use the electron pushing formalism to predict possible reaction pathways. Students often struggle to correctly identify and reason using different chemical concepts. Research has been done on students' comprehension of the electron pushing formalism (Bhattacharyya & Bodner, 2005; Crandell et al., 2020; Flynn & Featherstone, 2017; Galloway et al., 2017) but very little is known about how undergraduate students' compare chemical concepts to determine reactivity. We developed the Organic Reactivity Questionnaire (ORQ) to investigate how undergraduate students interpret reactivity principles in organic chemistry. Specifically, we wanted to learn: *How do undergraduate students interpret reactivity principles with respect to nucleophilicity and electrophilicity? What factors do undergraduate students consider when determining the direction of an acid-base equilibrium? What factors do undergraduate students consider when* *determining leaving group stability?* We invited undergraduate students in organic chemistry courses from five different universities across Canada to complete the ORQ online.

Students' definitions of nucleophilicity and electrophilicity aligned with expectations and were similar to those observed in previous studies (Anzovino et al., 2015). Students often selected electronegativity as a relevant factor and would frequently discuss electronegativity in their arguments; however, electronegativity was never the most relevant factor for answering any of the questions. These results align with the findings of previous studies that noticed students would often focus on electronegativity and use it as a rule or heuristic to problem solve (Maeyer & Talanquer, 2013; Talanquer, 2014). Many students misinterpreted inductive effects and incorrectly identified it as being more relevant than steric hindrance. Furthermore, we found that many students tended to confuse the concepts of inductive effects and hyperconjugation. Students were more successful using pK_a values then relative stability rules when determining the direction of an acid–base equilibrium; We noticed that students over-relied on charge as a cue for molecules being "unstable". Half of the students predicted the incorrect direction of an acid-base equilibrium when only given the reaction; Most students changed their answer when given pK_a values. Most students correctly identified bromide as the better leaving group compared to chloride; The majority of students stated that atom size was the most relevant factor in determining leaving group stability for this question but would often use it as a heuristic (e.g., a bigger atom is always a better leaving group). Overall, students would often select the correct answer when given a surface level cue like charge; however, students were inconsistent in selecting the most relevant chemical concept required to answer the questions. Furthermore, students often used heuristics and rules rather than using reasoning to compare chemical concepts. The students we sampled had only just completed, or nearly completed, a single course in organic chemistry. It may not be realistic to expect students to think like experts after a single course of instruction. However, several students did exhibit mechanistic reasoning without the use of heuristics. This result is promising as it may indicate some success in the curriculum in elciting expert-like thinking in students earlier than before. Future studies comparing students in different curricula will be the next step in identifying learning gain differences between institutions.

5.1.2 Implications and future work for the Organic Reactivity Questionnaire

This work identified some of students' strengths and weaknesses when interpreting reactivity principles in organic chemistry. Students' comprehension of reactivity principles should include the ability to reason using different chemical concepts. Therefore, we recommend that organic chemistry educators give students the opportunity to practice reasoning using reactivity principles on formative assessments. Questions like those on the ORQ can be used in class or for practice to help students develop their chemical reasoning skills. Educators can also design their own tasks, using scaffolding, to promote students' use of causal mechanistic reasoning on assessments (Noyes et al., 2022).

5.1.3 Chapter four: Self-efficacy Beliefs in Organic Chemistry Survey

Self-efficacy beliefs are an individual's beliefs in their ability to succeed at a given task or obtain a certain goal (Bandura, 1977, 2006). Self-efficacy beliefs are correlated to students' achievement in various STEM fields, where students with high self-efficacy in a certain discipline often perform well (Flaherty, 2020). In contrast, low self-efficacy beliefs are associated with high attrition rates and lower student success in STEM courses (Chen, 2014). Organic chemistry has an infamous reputation for being a difficult, content heavy course with high attrition rates. Little is known about how self-efficacy beliefs in organic chemistry might be related to student success in organic chemistry courses. We developed the Self-Efficacy Beliefs in Organic Chemistry survey (SEBOC) to assess undergraduate students' self-efficacy beliefs in organic chemistry. We collected validity evidence related to face, test content, response process, and internal structure. Face validity evidence was gathered through literature review and discussion with colleagues; Test content validity evidence was collected by consulting a panel of experts in organic chemistry, education, and chemistry education. We conducted two, separate iterations of exploratory factor analysis on the SEBOC to collect validity evidence related to internal structure. Undergraduate students in OCI were recruited for the first iteration in the summer of 2019 (*N*=78) and an EFA was conducted on the 42-item version of the SEBOC. We modified the 42-item version based on the results from this EFA and removed any redundant items. We then recruited undergraduate students in OCI in the Winter of 2022 (*N*=109) and conducted an EFA on the revised, 22-item version. Results from the EFA suggest an 18-item instrument with a 3-factor structure*: Self-efficacy beliefs towards reactivity and organic mechanisms* (7 items), *Self-efficacy beliefs towards representations in organic chemistry* (4 items), and *Self-efficacy beliefs towards applications of organic chemistry* (7 items). All items possessed strong internal reliability with all Cronbach's α values ≥0.8.

5.1.4 Implications and future work for the Self-efficacy Beliefs in Organic Chemistry survey

Herein we developed a survey to assess undergraduate students' self-efficacy beliefs in organic chemistry. The SEBOC could help educators to identify students with lower self-efficacy and create interventions to help those students succeed in organic chemistry courses. Instructors could identify students' self-efficacy beliefs as a starting point in course design such that the aim is to improve students' self-efficacy beliefs over the course of a semester. Future work using SEBOC will involve further investigating the proposed factor structure and conducting a confirmatory factor analysis to verify the proposed model in the context of OCI and OCII courses.

5.2 Concluding thoughts

Organic chemistry curricula need to develop critical thinking in learners such that they can apply their skills and knowledge to novel situations. Students in introductory organic chemistry courses, from this study, can identify ideas and concepts related to reactivity. Students in introductory organic chemistry courses, from this study, have moderate self-efficacy beliefs in the areas of mechanisms and representations. Students are generally adept at calling on basic concepts and using it to solve simple problems; however, students often struggled to apply those concepts to complex tasks involving multivariate reasoning. Throughout this thesis, one of the constantly restated goals of organic chemistry curricula was to develop expert-like thinking in learners. Specifically, we want students to think about reactions in terms of mechanistic patterns and finish the course with overall higher self-efficacy than when they began. Our proposed model of self-efficacy beliefs in organic chemistry emphasizes reactivity as a key concept students need to master. Self-efficacy beliefs towards reactivity explained the greatest variance in organic chemistry self-efficacy, indicating it as a core area of focus for instruction. The ORQ could be used in conjunction with the SEBOC to help compare students' self-efficacy beliefs towards reactivity to students' actual knowledge and understanding of the concept. Educators can then use the results from these assessments to identify specific areas that need review, emphasize these areas in teaching, or implement teaching interventions. Both the ORQ and the SEBOC require key revisions before they are ready to be used for a large-scale curricula evaluation. The content of the ORQ could be expanded to include more nucleophile question and cover more factors used by organic chemistry experts when problem solving. Specifically, we could update the ORQ to include concepts like solvent effects and ideas about thermodynamic or kinetic influences on reactivity. The SEBOC requires further validation study through confirmatory factor analysis to check that it produces valid data in the context of Organic Chemistry I and II courses. The studies I conducted as part of this thesis were exploratory in nature and offer a good starting point to refine and design assessments for curricular evaluation studies. We need formal assessments that target specific learning goals in a curriculum that can provide robust results about student learning in organic chemistry.

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Appendix A: Organic Reactivity Questionnaire

Codebook-ORQ

Instructions: Place an x under any of the codes you believe match a participant's definition (details below). Use the notes column to memo anything you feel is necessary (possible new code, suggestions for code revisions, general notes on the data, etc). A participant's response can be coded to more than one code (i.e. there can be multiple x per row if the response covers multiple codes). LG=Leaving Group, Ele=Electrophile

If participant mentions positive or negative (without the word charge) charge can be implied.

Potential new code: disjointed reasoning where the reasons don't flow: "oxygen is more electronegative than hydrogen and carbon. double bond contributes to resonance and stabilization. oxygen is pulling electrons to itself and carbocations are very electron deficient."

Potential new code: Misinterpretation of chemistry concepts

Explicit codes: participant selects an answer (Claim A or Claim B) and clearly states in their explanation that Molecule A/B or the molecule on the left/right has certain characteristics that make it Electrophilic.

Implicit: Participant gives explanations about the molecules characteristics/ factors they chose to make their decision but does not state outright that "these things make it more electrophilic". In this case, electrophilicity is implied based on the molecule they chose. Assume that they believe their chosen molecule is more electrophilic (unless the written explanations indicate otherwise).

5.2.1

Question 3	
Code	Description
Associates neutrality with stability	Any mention of neutrality in their answer (explicit or implicit) where the driving force behind their choice is the idea that a molecule that is neutral is less reactive/more stable.
Compares nucleophilicity instead of electrophilicity	Instead of comparing electrophilic characteristics, they first look at nucleophilic characteristics and reason using nucleophilicity. Ex. "the molecule on the left is a stronger nucleophile and weaker electrophile, therefore the molecule on the right is more electrophilic." Reasoning that if a molecule is less nucleophilic then it is more electrophilic.

Question 3	
Code	Description
higher electronegativity means greater electrophilicity	Instances where there is a direct association between electronegativity and electrophilicity. This could be explicit: “molecule A has higher electronegativity so it is more electrophilic”, or implicit: participant selects molecule A but in their open responses writes “it’s more electrophilic” without other context.
Incorrect reasoning about the relationship between stability and electrophilicity	Instances where participants connect a greater electrophilicity with greater stability (which is incorrect). Could be explicit: where they state that the more electrophilic molecule is more stable, or implicit, where they select the more electrophilic molecule (correct claim) but in their response state that it is more stable.
Incorrect ideas about charge	Any ideas about charge that are incorrect. Ex. Positive charge means electron rich, negative charge means electron poor. Can also apply if the word charge is used vaguely without identifying positive/negative
Molecule B is electron deficient	Instances where participant mentions Molecule B (the charged species) being electron deficient but does not make any connection to explain why it’s electron deficient. Ex: Participant selects Molecule B as an answer and state: “lower electron density” or “electron deficient”.
positive charge means electrophilic	Any instance where a participant just states “it has a positive charge, “ positive charge”, “positive charge so it’s electrophilic”, etc. Any response that directly associates a positive charge with electrophilicity but gives no further explanation. Can be implicit, Ex. if a participant writes “it’s positive” or “positive charge” without further explanation then it would still fall under this code. This code captures when students use positive charge as a cue for electrophilicity without considering what the charge symbolizes. Mention of an empty orbital counts as meaning a lack of electrons. Must explicitly state that the charge is positive. Cation counts for this code. That means they did not give any

Question 3 Code	Description
	further explanation. IF they connect electrophilicty back to a somewheat viable explanation, then it does not fall under this code.
positive charge indicates a lack of electrons; therefore, the molecule is electrophilic	This was the expected answer. Participant connects the positive charge to a lack of electrons and then reasons that the lack of electrons indicates that the molecule is electrophilic. This code captures instances where participants understand a deeper connection between. Just because something "wants" electrons does not mean it is deficient. Must be explicit about the lacking of electrons, low electron density, empty orbital.
Positive charge means greater attraction to electrons or negative charge	Mention of a molecule attracting or having a greater attraction to electrons or negative charge (electron source). Can include statements like "more readily accepts electrons"
Positive charge on an electronegative atom is not favourable	Favourability regarding charge on an electronegative atom.
Other	Ideas not captured by current codes or may not yet have a defined category. If the explanation makes sense and is easy to follow, code it here rather than vague, unclear, or I don't know.
Vague, unclear, or I don't know	Any instance where a participant does not attempt to give an explanation and writes: "IDK", "I don't know", "I guessed", etc. Only code this if there is no other attempt at answering (question marks after an attempted answer do not count for this code). Reponses can also be coded to this if they were difficult to understand or would otherwise require more clarification from the participant.

Question 4 Code	Description
Belief that a tertbutyl group can participate in resonance	For example: claiming that Molecule B is more stable because it has more opportunities for resonance. Such a statement is incorrect because both molecules could only form 2 viable resonance structures in this case.
Compares nucleophilicity instead of electrophilicity	Instead of comparing electrophilic characteristics, they first look at nucleophilic characteristics and reason using nucleophilicity. E.g., “the molecule on the left is a stronger nucleophile and weaker electrophile, therefore the molecule on the right is more electrophilic.” Reasoning that if a molecule is less nucleophilic then it is more electrophilic.
Connects sterics with the accessibility of the electrophilic site	Expected answer. Participant must connect steric hindrance to the accessibility of a reactive site (this can include statements like "molecule A has more space for a nucleophile to attack" that describe the ability of a nucleophile to react.
Hyperconjugation	Any explicit mention of Hyperconjugation (they must use the word).
Identifies sterics as being present but does not explain a connection to accessibility of reactive sites	This code captures if a participant states that the tertbutyl / bulky/large group causes steric hindrance or that steric hindrance causes molecule A/B to be more/less electrophilic but does not include any explanation about accessibility to a reactive site.
incorrect reasoning about the relationship between stability and electrophilicity	For example: a more stable molecule is more electrophilic. If they select claim B and mention that molecule B is more stable, the response would also fall under this code

Question 4	
Code	Description
Molecule B can better stabilize a charge because it is bigger	usually with respect to inductive effects or atom size
Refer to an entire species as being an atom	Any instance where a participant refers to an entire molecule or species as being an atom
Rule based reasoning using atom size or amount	larger=more electrons (higher electron density)=more nucleophilic/ smaller=less electrons= more electrophilic, or something like this. Participants do not necessarily have to state electrophilic/ nucleophilic in their response for this code to apply (because their chosen claim mentions that their chosen molecule is more electrophilic). This code applies if the participant only uses a rule about atom size without giving further explanations.
The tertbutyl group has a destabilizing effect	Mention that the tertbutyl/extra alkyl group causes a destabilizing effect. Also applies if they mention that inductive effects have a destabilizing effect. (cannot use the word bulky, must say tertbutyl)
The tertbutyl group has a stabilizing effect	Any mention of the tertbutyl group/larger group/ larger alkyl group better distributing electrons/charge, reducing a charge, or otherwise resulting in a stabilizing effect of molecule B. Can include statements such as "a tertiary carbon is more stable". Do not need to directly reference the tertbutyl group, if they mention that molecule B/the second molecule can better spread out electrons the it would also count. (cannot use the word bulky, must say tertbutyl)
Other	Ideas not captured by current codes or may not yet have a defined category. If the explanation makes sense and is easy to follow, code it here rather than vague, unclear, or I don't know.
vague unclear or I don't know	Any instance where a participant does not attempt to give an explanation and writes: "IDK", "I don't know", "I guessed", etc.

Question 4 Code	Description
	Only code this if there is no other attempt at answering (question marks after an attempted answer do not count for this code). Reponses can also be coded to this if they were difficult to understand or would otherwise require more clarification from the participant.

Question 5 Code	Description
Incorrect ideas about resonance	ex, More possible resonance means there is more charge on a molecule, more possible resonance structures means more electrophilic
Incorrect reasoning about the relationship between stability and electrophilicity	Instances where participants connect a greater electrophilicity with greater stability (which is incorrect). Could be explicit: where they state that the more electrophilic molecule is more stable, or implicit, where they select the more electrophilic molecule (correct claim) but in their response state that it is more stable.
Molecule A can form more resonance structures than molecule B	Expected answer. Any mention that Molecule A can form more resonance structures and is more stable
The more electrophilic molecule has less electrons	Statements about the amount of electron density/number of electrons for each molecule, they can discuss either one. Ex. “the other molecule has more electrons”, “this molecule has less electrons”, “the first molecule has more electron density”. “
more electronegative atoms means the molecule is more electrophilic	Makes a positive linear connection between electronegativity and electrophilicity. Higher electronegativity=more electrophilic. Can mention that this is because one molecule has more electronegative atoms.

Question 5	
Code	Description
more electronegative atoms means the molecule is more nucleophilic (less electrophilic)	Makes a negative linear connection between electronegativity and electrophilicity. Higher electronegativity=less electrophilic (more nucleophilic). Can mention that this is because one molecule has more electronegative atoms.
Nitrogen contributes to inductive effects	Any connections between nitrogen and inductive effects. Code to this if nitrogen and inductive effects appear in the same sentence. Could also use the word "induce". Can be implicit: if they mention that one molecule has inductive effects (where the other may not) it can also be coded here.
Nitrogen is electrophilic	If they mention that the nitrogen contributes to electrophilicity but with no other explanation (or minimal explanation). Ex. "Nitrogen makes the molecule more electrophilic", then code to this
Nitrogen is nucleophilic	Any participants who selected Molecule B because they considered nitrogen as nucleophilic or described its nucleophilic characteristics (lone pairs, usually gives away electrons, vaguely states that nitrogen is nucleophilic).
Nitrogen stabilizes charge via resonance	Can either explicitly use the word stabilizes or describe the resonance structures formed from the lone pair on the nitrogen.
rule base reasoning on atom size or amount	larger=more electrons (higher electron density)=more nucleophilic/ smaller=less electrons= more electrophilic, or something like this. Participants do not necessarily have to state electrophilic/ nucleophilic in their response for this code to apply (because their chosen claim mentions that their chosen molecule is more electrophilic). This code applies if the participant only uses a rule about atom size without giving further explanations.
Steric hindrance as primary factor	Participant's explanation focuses on steric hindrance or how bulky one molecule is to determine relative electrophilicity

Question 5	
Code	Description
Other	Ideas not captured by current codes or may not yet have a defined category. If the explanation makes sense and is easy to follow, code it here rather than vague, unclear, or I don’t know.
Vague, unclear, or I don't know	Any instance where a participant does not attempt to give an explanation and writes: “IDK”, “I don’t know”, “I guessed”, etc. Only code this if there is no other attempt at answering (question marks after an attempted answer do not count for this code). Reponses can also be coded to this if they were difficult to understand or would otherwise require more clarification from the participant.

Question 8	
Code	Description
Br is a better nucleophile	Any instance where bromine is mentioned as a nucleophile
Br is less electronegative than Cl (less electronegative atom is the better LG)	Mention of Br being less electronegative then Cl or mention that the less electronegative atom is the better leaving group. Can be explicit: “Br is less electronegative so it’s the better LG”, or implicit: (participant selects claim B) “This one is less electronegative”.
discussion of electrons in terms of atomic structure	Statements about electrons in relation to atomic radius, distance from nucleus, shielding, valence shells, or other atomic properties.
Incorrect ideas about chlorine and LG stability	Participant MUST have selected claim A and given incorrect ideas about Cl as an atom. Ex: “Cl is bigger than Br” or “Cl is more reactive so it’s the better LG”.
incorrect ideas about electronegativity	See the two codes below

Question 8	
Code	Description
Bromine is more electronegative than Cl	Any mention of Br being a more electronegative atom compared to Cl
Chlorine is more electronegative so it's a better leaving group (more electronegative atom is a better leaving group)	Any statements where they mention chlorine as the more EN atom or associate a higher electronegativity with a better leaving group. Can be explicit: Cl is more electronegative therefore better leaving group or implicit: (selects claim A) “more EN atom is better LG”.
Larger atom better stabilizes charge	Can include "stabilize electrons", "stabilize" as a more general term or "spread out charge" (this one must say charge, if they talk about electrons spreading out then it should go in the atomic structure code).
Larger atom is better leaving group	This code captures instances where there are no further explanations beyond big atom = better leaving group. Can include short answers such as "Br is bigger", "Br is the bigger atom", "Br is larger than Cl" without any further explanation as to why the difference in atom size contributes to leaving group stability.
Uses periodic trends to explain leaving group stability	Statements like: “Cl is higher up in a column then Br” or any mention of columns, rows, and the periodic table.
Weaker base is better LG	Any mention of something being a weaker base or less basic being the better LG. Can include mention of a higher pKa.
Other	Ideas not captured by current codes or may not yet have a defined category. If the explanation makes sense and is easy to follow, code it here rather than vague, unclear, or I don’t know.

Question 8	
Code	Description
Vague, unclear, or I don't know	Any instance where a participant does not attempt to give an explanation and writes: “IDK”, “I don’t know”, “I guessed”, etc. Only code this if there is no other attempt at answering (question marks after an attempted answer do not count for this code). Reponses can also be coded to this if they were difficult to understand or would otherwise require more clarification from the participant.

Appendix B: SEBOC

5.3 Table of modifications

Original wording	Change recommended by first expert	Change recommended by second expert	Change recommended by third expert
Describe how organic chemistry is involved in a global issue (e.g. societal, environment), either positively or negatively.	Describe how organic chemistry is involved underlies a global issue (e.g. societal, environment), either positively or negatively.		
Compare two potential mechanisms for a reaction and justify which is the most likely to occur.			
Compare two nucleophilic or electrophilic sites and justify which is most likely to participate in the reaction		Compare two nucleophilic or electrophilic sites and justify which is most likely to participate in a reaction	Compare two nucleophilic or electrophilic sites and justify which is most likely to participate in a reaction covered in this course
Identify similarities between multiple reactions based on their underlying mechanisms			
Use chemical properties (e.g. electronegativity, atom size) to predict and justify the direction of an acid–base equilibrium	Explain which side of an acid-base equilibrium is favored using chemical properties		

Propose a synthesis for a target compound.	Propose a multi-step synthesis for a target compound.	
Justify the outcome of a reaction using orbitals.	Explain how a reaction takes place using the molecular orbitals involved.	
New Item	Draw the molecular orbitals on a given nucleophile and electrophile (i.e., highest occupied molecular orbital and lowest unoccupied MO)	
Visualize how molecules are interacting in space as a reaction proceeds	Visualize how molecules are interacting in 3D space as a reaction proceeds.	
Convert between various representations of a molecule (e.g. Lewis structure, line structure, Newman Projection)	Convert between various representations of a molecule (e.g. Lewis structure, line structure).	
New Item	Convert between various representations of a molecule (e.g. Newman Projection and Stereochemical isomers).	
Describe how organic chemistry is involved in a global issue (e.g. societal, environment), either positively or negatively	Describe how organic chemistry underlies a global issue (e.g. societal, environment), either positively or negatively	
Critique a news report or documentary that deals with some aspect of organic chemistry		Critique popular media that involves organic chemistry

Design a laboratory procedure for a reaction learned in your organic chemistry course.	Design a laboratory procedure to perform a synthesis reaction learned in your organic chemistry course.		Design a laboratory procedure to perform a reaction learned in your organic chemistry course.
Apply concepts learned in organic chemistry to other sciences		Recognize when a topic in another science requires organic chemistry to understand	Apply concepts and skills learned in organic chemistry to other sciences

5.4 Semi structured interview protocol

Preamble and introduction

Interviewer: “Thank you for taking the time to participate in this study. We are conducting this study to explore students’ confidence in organic chemistry. Please know that this study is completely voluntary; you do not have to answer any questions you do not feel comfortable answering and if you do not wish to continue at any point, we will stop the interview. Do you have any questions before we begin?”

Participant completes the SEBOC (not timed but should be completed within 30 min). Interviewer then reads out the first question and asks the participant: “why did you answer this question as you did?”

Participant then responds (or chooses not to) and if more information is needed the researcher can ask any of these follow up questions:

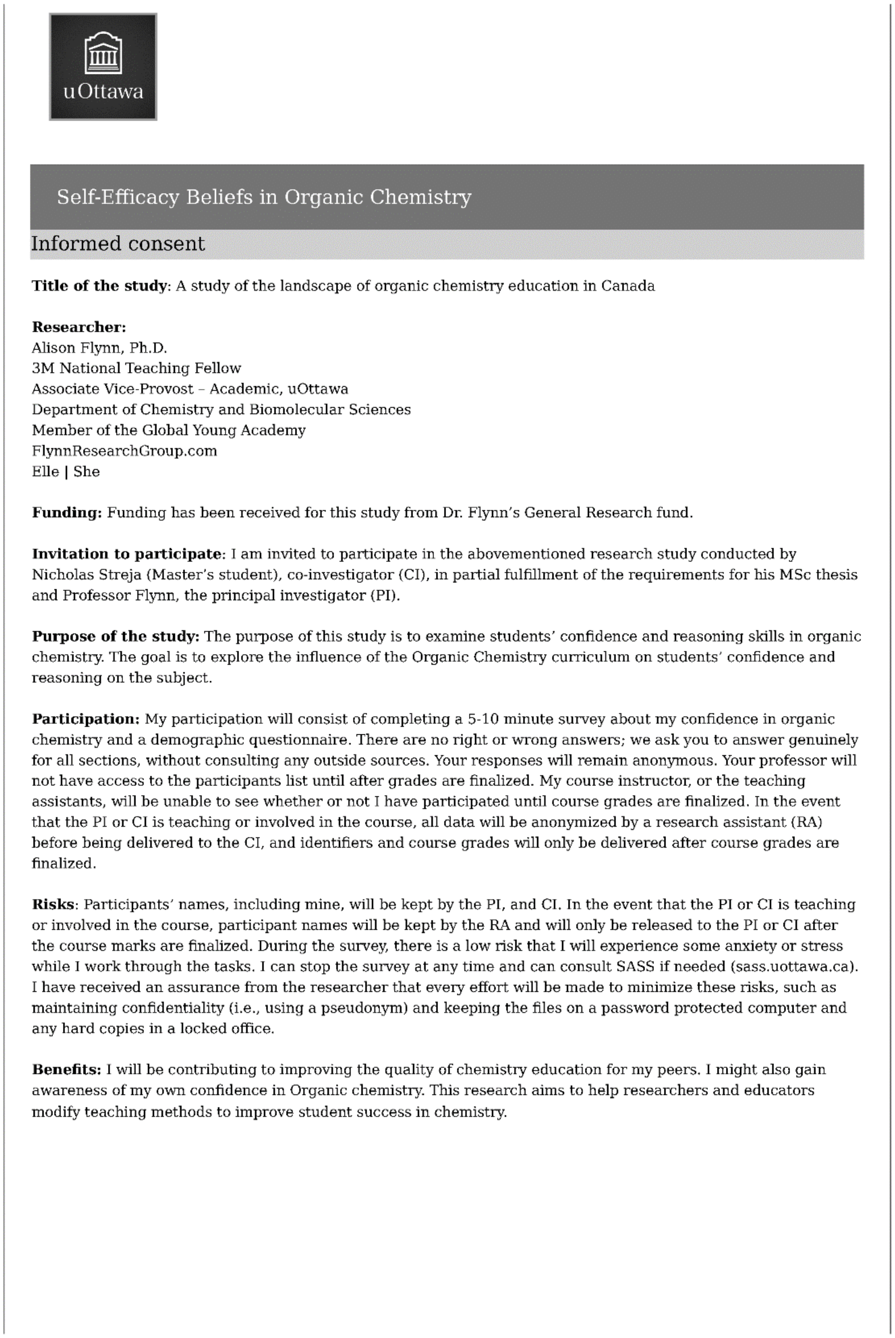
Was this question difficult to answer?

How would you describe this question/skill in your own words?

How did you interpret this question?

Is there anything you would change about how this question was worded/what it was asking?

How do you define ___



uOttawa

Self-Efficacy Beliefs in Organic Chemistry

Informed consent

Title of the study: A study of the landscape of organic chemistry education in Canada

Researcher:
Alison Flynn, Ph.D.
3M National Teaching Fellow
Associate Vice-Provost – Academic, uOttawa
Department of Chemistry and Biomolecular Sciences
Member of the Global Young Academy
FlynnResearchGroup.com
Elle | She

Funding: Funding has been received for this study from Dr. Flynn's General Research fund.

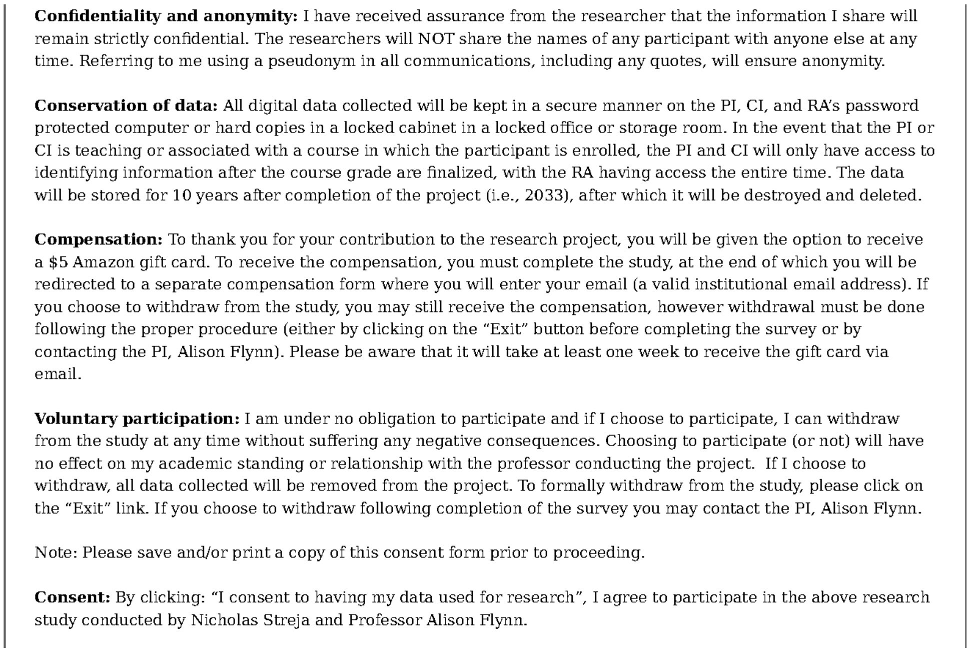
Invitation to participate: I am invited to participate in the abovementioned research study conducted by Nicholas Streja (Master's student), co-investigator (CI), in partial fulfillment of the requirements for his MSc thesis and Professor Flynn, the principal investigator (PI).

Purpose of the study: The purpose of this study is to examine students' confidence and reasoning skills in organic chemistry. The goal is to explore the influence of the Organic Chemistry curriculum on students' confidence and reasoning on the subject.

Participation: My participation will consist of completing a 5-10 minute survey about my confidence in organic chemistry and a demographic questionnaire. There are no right or wrong answers; we ask you to answer genuinely for all sections, without consulting any outside sources. Your responses will remain anonymous. Your professor will not have access to the participants list until after grades are finalized. My course instructor, or the teaching assistants, will be unable to see whether or not I have participated until course grades are finalized. In the event that the PI or CI is teaching or involved in the course, all data will be anonymized by a research assistant (RA) before being delivered to the CI, and identifiers and course grades will only be delivered after course grades are finalized.

Risks: Participants' names, including mine, will be kept by the PI, and CI. In the event that the PI or CI is teaching or involved in the course, participant names will be kept by the RA and will only be released to the PI or CI after the course marks are finalized. During the survey, there is a low risk that I will experience some anxiety or stress while I work through the tasks. I can stop the survey at any time and can consult SASS if needed (sass.uottawa.ca). I have received an assurance from the researcher that every effort will be made to minimize these risks, such as maintaining confidentiality (i.e., using a pseudonym) and keeping the files on a password protected computer and any hard copies in a locked office.

Benefits: I will be contributing to improving the quality of chemistry education for my peers. I might also gain awareness of my own confidence in Organic chemistry. This research aims to help researchers and educators modify teaching methods to improve student success in chemistry.



Confidentiality and anonymity: I have received assurance from the researcher that the information I share will remain strictly confidential. The researchers will NOT share the names of any participant with anyone else at any time. Referring to me using a pseudonym in all communications, including any quotes, will ensure anonymity.

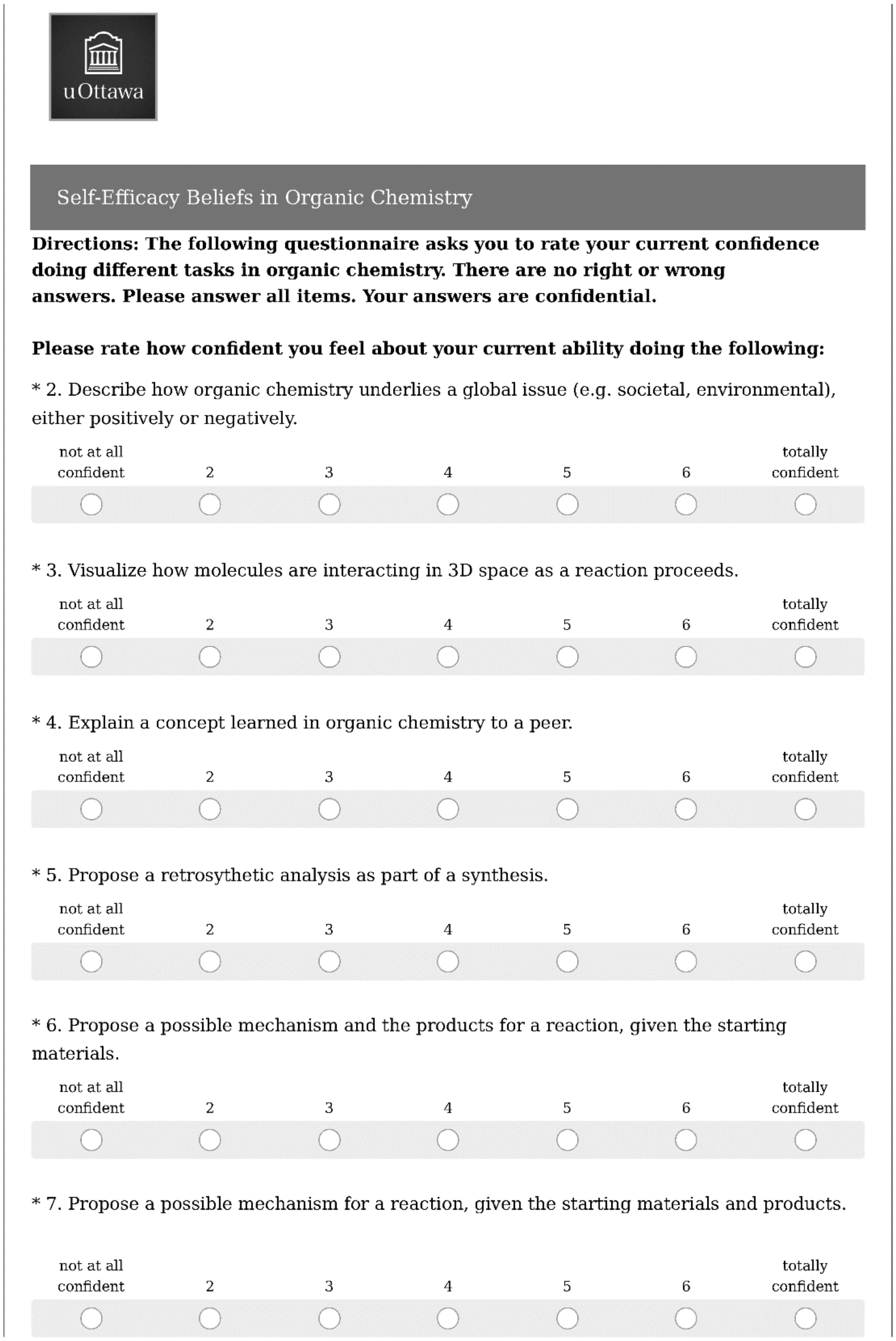
Conservation of data: All digital data collected will be kept in a secure manner on the PI, CI, and RA's password protected computer or hard copies in a locked cabinet in a locked office or storage room. In the event that the PI or CI is teaching or associated with a course in which the participant is enrolled, the PI and CI will only have access to identifying information after the course grade are finalized, with the RA having access the entire time. The data will be stored for 10 years after completion of the project (i.e., 2033), after which it will be destroyed and deleted.

Compensation: To thank you for your contribution to the research project, you will be given the option to receive a $5 Amazon gift card. To receive the compensation, you must complete the study, at the end of which you will be redirected to a separate compensation form where you will enter your email (a valid institutional email address). If you choose to withdraw from the study, you may still receive the compensation, however withdrawal must be done following the proper procedure (either by clicking on the "Exit" button before completing the survey or by contacting the PI, Alison Flynn). Please be aware that it will take at least one week to receive the gift card via email.

Voluntary participation: I am under no obligation to participate and if I choose to participate, I can withdraw from the study at any time without suffering any negative consequences. Choosing to participate (or not) will have no effect on my academic standing or relationship with the professor conducting the project. If I choose to withdraw, all data collected will be removed from the project. To formally withdraw from the study, please click on the "Exit" link. If you choose to withdraw following completion of the survey you may contact the PI, Alison Flynn.

Note: Please save and/or print a copy of this consent form prior to proceeding.

Consent: By clicking: "I consent to having my data used for research", I agree to participate in the above research study conducted by Nicholas Streja and Professor Alison Flynn.



uOttawa

Self-Efficacy Beliefs in Organic Chemistry

Directions: The following questionnaire asks you to rate your current confidence doing different tasks in organic chemistry. There are no right or wrong answers. Please answer all items. Your answers are confidential.

Please rate how confident you feel about your current ability doing the following:

* 2. Describe how organic chemistry underlies a global issue (e.g. societal, environmental), either positively or negatively.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 3. Visualize how molecules are interacting in 3D space as a reaction proceeds.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 4. Explain a concept learned in organic chemistry to a peer.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 5. Propose a retrosythetic analysis as part of a synthesis.

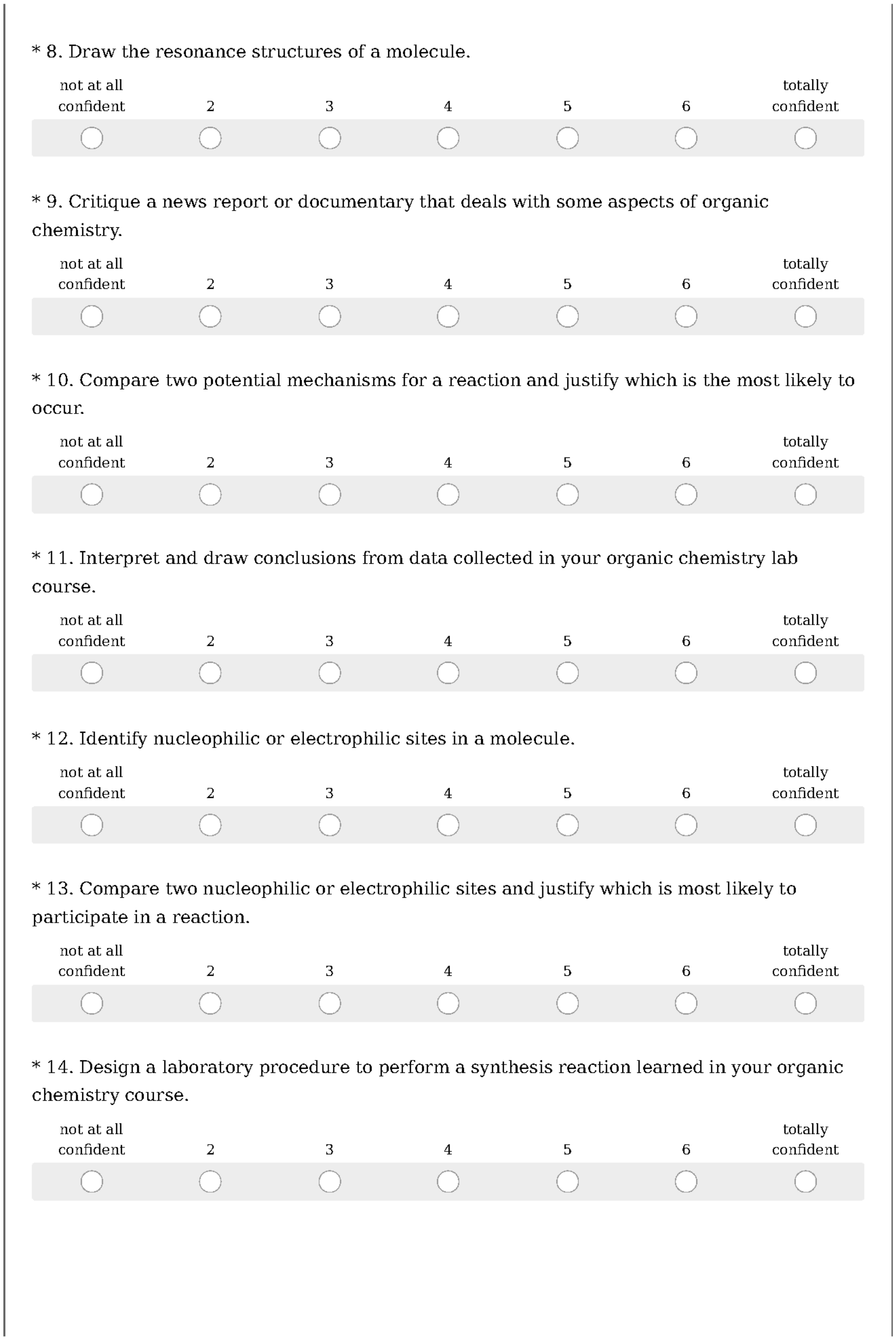
not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 6. Propose a possible mechanism and the products for a reaction, given the starting materials.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 7. Propose a possible mechanism for a reaction, given the starting materials and products.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○



* 8. Draw the resonance structures of a molecule.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 9. Critique a news report or documentary that deals with some aspects of organic chemistry.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 10. Compare two potential mechanisms for a reaction and justify which is the most likely to occur.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 11. Interpret and draw conclusions from data collected in your organic chemistry lab course.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 12. Identify nucleophilic or electrophilic sites in a molecule.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 13. Compare two nucleophilic or electrophilic sites and justify which is most likely to participate in a reaction.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 14. Design a laboratory procedure to perform a synthesis reaction learned in your organic chemistry course.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 15. Identify similarities between multiple reactions based on their underlying mechanisms.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 16. Explain which side of an acid-base equilibrium is favored using chemical properties (other than pKa values).

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 17. Explain how a reaction takes place using the molecular orbitals involved.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 18. Explain how a reaction coordinate diagram describes an associated reaction mechanism.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 19. Convert between 2D representations of a molecule (e.g., Lewis structure to line structure).

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 20. Draw the molecular orbitals on a given nucleophile and electrophile (i.e., highest occupied molecular orbital and lowest unoccupied molecular orbital).

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 21. Convert between 3D representations of a molecule (e.g., Newman projection to perspective diagram).

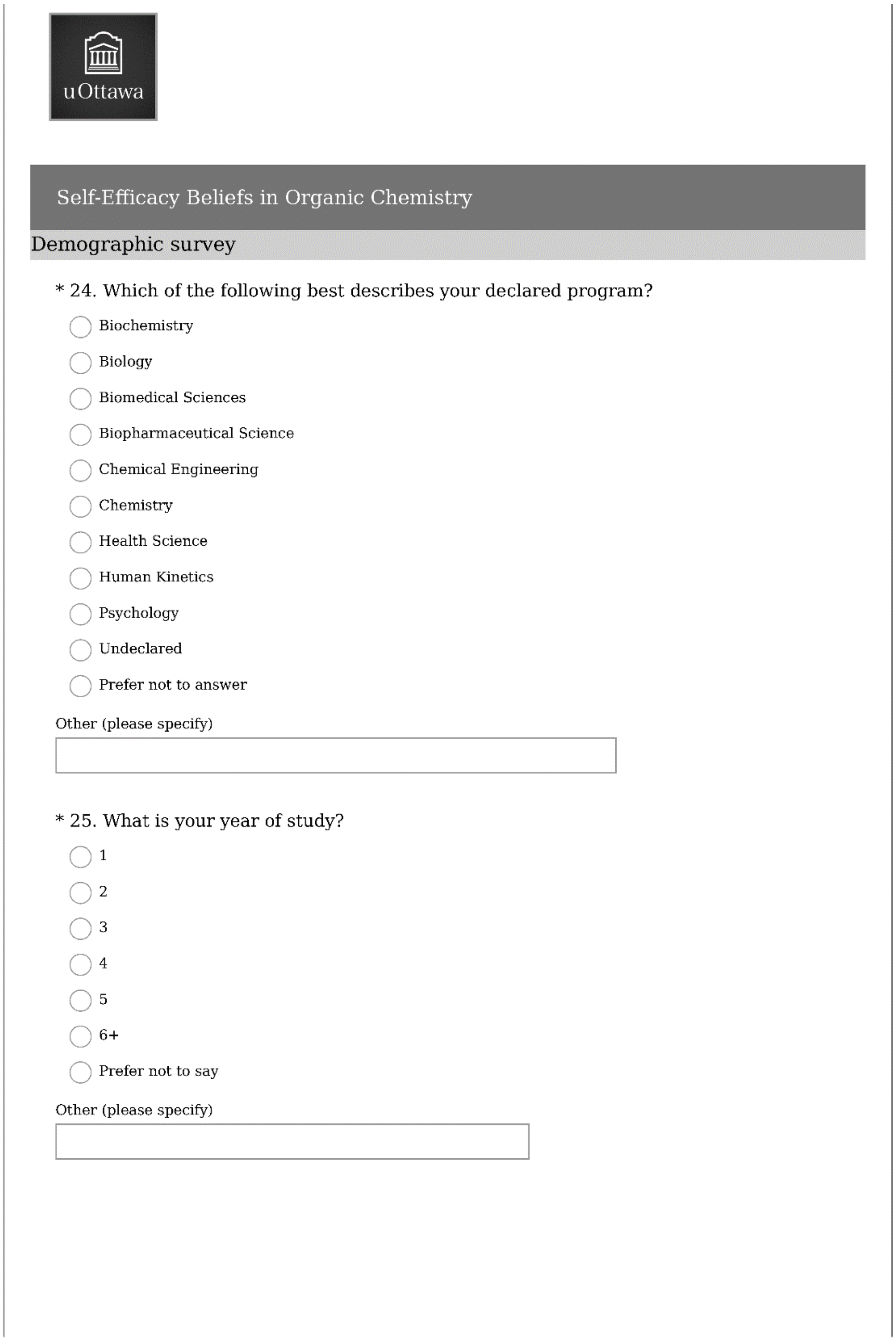
not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 22. Convert between 2D and 3D representations of a molecule (e.g., Lewis structure to Newman projection).

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○

* 23. Apply concepts learned in organic chemistry to other sciences.

not at all confident	2	3	4	5	6	totally confident
○	○	○	○	○	○	○



Self-Efficacy Beliefs in Organic Chemistry

Demographic survey

* 24. Which of the following best describes your declared program?

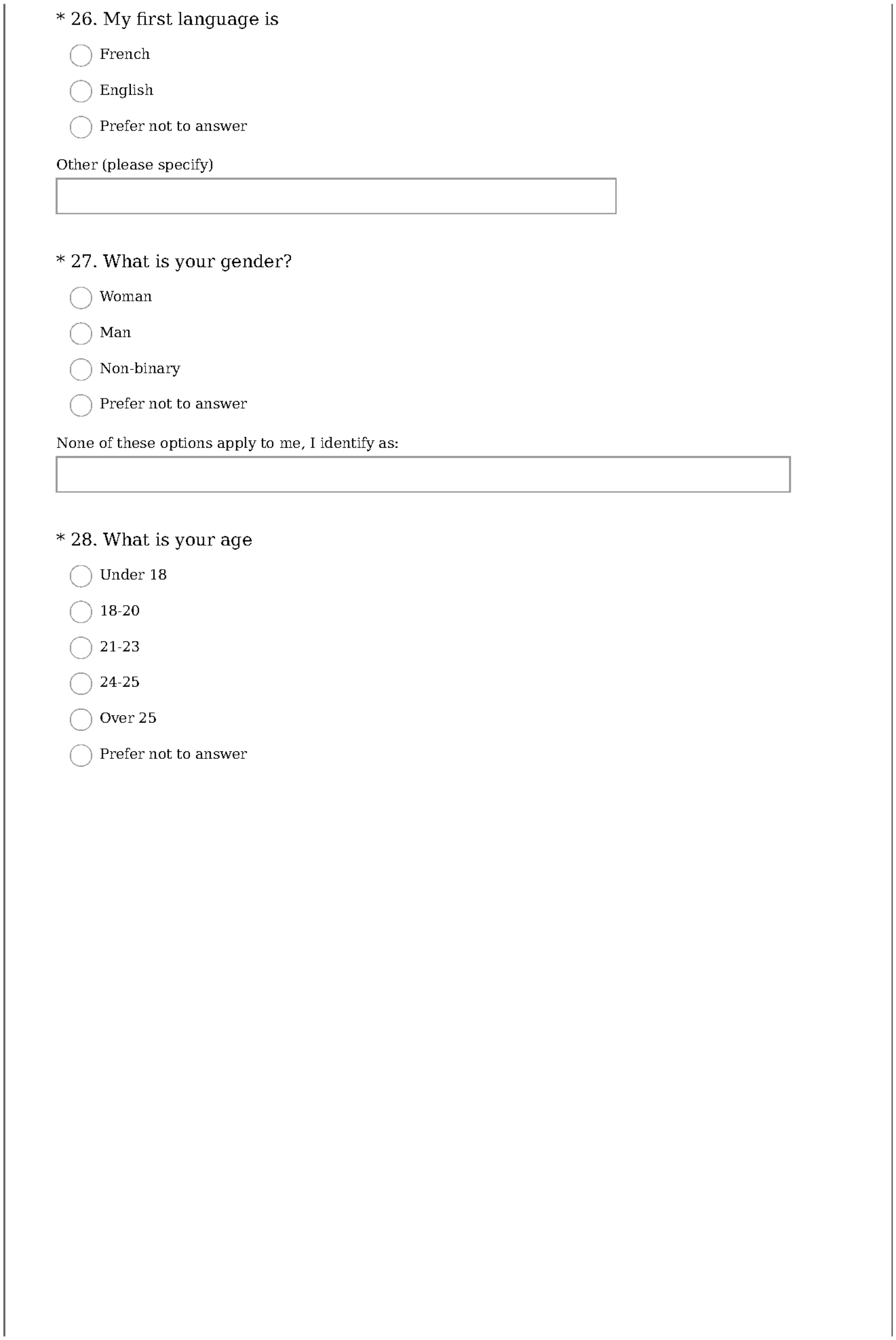
- ○ Biochemistry
- ○ Biology
- ○ Biomedical Sciences
- ○ Biopharmaceutical Science
- ○ Chemical Engineering
- ○ Chemistry
- ○ Health Science
- ○ Human Kinetics
- ○ Psychology
- ○ Undeclared
- ○ Prefer not to answer

Other (please specify)

* 25. What is your year of study?

- ○ 1
- ○ 2
- ○ 3
- ○ 4
- ○ 5
- ○ 6+
- ○ Prefer not to say

Other (please specify)



* 26. My first language is

○ French

○ English

○ Prefer not to answer

Other (please specify)

* 27. What is your gender?

○ Woman

○ Man

○ Non-binary

○ Prefer not to answer

None of these options apply to me, I identify as:

* 28. What is your age

○ Under 18

○ 18-20

○ 21-23

○ 24-25

○ Over 25

○ Prefer not to answer

* 29. Which of the following groups do you identify with? (select all that apply)

☐ Asian - East
☐ Asian - South
☐ Asian - Southeast
☐ Black - African
☐ Black - Caribbean
☐ Black - North American
☐ First Nations
☐ Indian - Caribbean (e.g. Guyanese with origins in India)
☐ Indigenous
☐ Inuit
☐ Latinx/Hispanic
☐ Metis
☐ Middle Eastern
☐ White - European
☐ White - North American
☐ Prefer not to answer

None of these apply to me, I identify with: