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ARTICLE

The Role of Authentic Contexts and Social Elements in Supporting Organic Chemistry Students' Interactions with Writing-to-Learn Assignments

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Student affect is an important factor in the learning process and may be especially important in gateway courses such as organic chemistry. Students' recognition of the relevance of the content they are learning and interactions with their peers can support their motivation to learn. Herein, we describe a study focused on how Writing-to-Learn assignments situate organic chemistry content within relevant contexts and incorporate social elements to support positive student interactions with organic chemistry. These assignments incorporate rhetorical elements—an authentic context, role, genre, and audience—to support student interest and demonstrate the relevance of the content. In addition, students engage in the processes of peer review and revision to support their learning. We identified how the authentic contexts and peer interactions incorporated into two Writing-to-Learn assignments supported students' interactions with the assignments and course content by analyzing student interviews and supported by feedback survey responses. Our results indicate that assignments incorporating these elements can support student affect and result in students' perceived learning, but that there should be careful consideration of the relevance of the chosen contexts with respect to the interests of the students enrolled in the course and the complexity of the contexts.

Introduction

The science education research community has long acknowledged the importance of affect on learning. Affect, which describes a student's feelings towards a given task, encompasses constructs such as motivation, attitudes, beliefs, and self-concept (Simpson et al., 1994). Over the last 20 years, research in chemistry education has focused on the relation between the affective domain of learning and student knowledge acquisition (Flaherty, 2020), and various studies have demonstrated the ties between student performance and affect within introductory chemistry courses (Brandriet et al., 2011; Ferrell et al., 2016; Galloway & Bretz, 2015; Galloway et al., 2016; Ramnarain & Ramaila, 2018; Zusho et al., 2003). Supporting positive affective learning experiences may be especially important in introductory chemistry courses, such as organic chemistry, that are known to cause difficulties for students. Additionally, researchers have called for learning interventions that elicit more positive affective experiences in laboratory courses (Galloway et al., 2016; Hensen et al., 2020). With the tie between performance and affective domain of learning, it is important to examine how pedagogical interventions may impact student affect. The present study qualitatively investigates the potential for context-based writing assignments that incorporate social interactions to support positive student affectual experiences in a laboratory setting.

Role of motivation in learning within STEM

One of the constructs contributing to the affective domain of learning is motivation, and education research has revealed the importance of student motivation in learning within STEM specifically (Glynn & Koballa, 2006; Schunk & Pajares, 2002; Simpson et al., 1994). Recognizing the importance of motivation for learning, several studies within chemistry have focused on evaluating and increasing student motivation (Austin et al., 2018; Ferrell et al., 2016; Juriševič et al., 2012; Liu et al., 2017; Liu et al., 2018; Ward & Bodner, 1993). Motivation is a complex construct that has been related to learning in a variety of ways. Keller (1983) describes motivation as a multi-component construct made up of interest, relevance, expectancy, and satisfaction. Based on this conceptualization, they suggest that motivation can be supported by addressing student attention, recognizing relevance, building confidence, and satisfaction (Keller, 1983, 1987). Alternatively, Turner and Paris (1995) present the Six C's Model of Motivation that points to the significance of agency, constructing meaning and relevance of content, and social interactions. Therefore, interventions that appeal to the aspects of the various conceptualizations of motivation could support the affective domain of learning.

As relevance is a component across models of motivation, demonstrating the relevance of course content is an important consideration within science education. However, within chemistry, Gilbert (2006) identified the lack of relevance as one of the four major problems facing the chemistry education

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community in the twenty-first century. For students, when chemistry lacks relevance it is not seen as something worthwhile. Gilbert (2006) argues that if chemistry instruction appeals to students' present and anticipated interests, students will be more inclined to engage with the chemistry curriculum. This is seen in a study by Habig et al. (2018) which showed that students who might otherwise be uninterested in chemistry showed increased interest when the subject matter was made relevant to their everyday lives. Gilbert (2006) suggests that incorporating context into instruction is a fruitful way to demonstrate the relevance of chemistry to students. In one such effort within chemistry, Stuckey and Eilks (2014) implemented a context-based curriculum centered on tattooing to illustrate the relevance of chemistry content; student survey responses indicated that the context-based curriculum "significantly increased" student motivation levels. In another study, Vaino et al. (2012) found evidence that incorporating context-based lessons resulted in higher student motivation to learn chemistry content. While there have broadly been efforts to support student perceptions of relevance in science education, additional efforts are merited (Stuckey et al., 2013).

Social elements can also play a role in fostering students' motivation to learn. Social contexts can either encourage or discourage engagement, which in turn impacts motivation (Vansteenkiste et al., 2006). In the classroom, social interactions may take the form of feedback and collaborations among peers, which can shape motivation (Weinstein, 2014). Despite the importance of social elements, we know very little about the relationship between these elements and motivation in chemistry classrooms. Liu et al. (2018) found that organic chemistry students in a flipped classroom using peer-led team learning had higher motivation at the end of the semester than those in a traditional classroom. With the key role that peer interactions can play in supporting student learning, it is important to understand the role that it plays when it is an element of a pedagogy.

The role of writing in supporting the affective domain of learning in STEM

Writing has previously been used as a way to promote student interest in STEM content (Bernacki et al., 2016; Garza et al., 2021; Hulleman et al., 2010; Watts et al., 2021). For example, Hulleman et al. (2010) described a writing assignment that encouraged students to contextualize course content in their own lives and found that it augmented students' value perception of the content. Similarly, Bernacki et al. (2016) found that students who wrote about their competence and interest following individual science lessons reported higher interest in the content following the intervention than students who just wrote summaries of the lessons.

Focused on promoting conceptual learning and disciplinary thinking, Writing-to-Learn (WTL) is writing pedagogy that may also be effective at engaging the affective domain of learning as they can appeal to relevance and incorporate social elements. A series of WTL studies involving students writing about socio-scientific issues—societal issues related to science—found increased scientific literacy and use of scientific concepts in crafting arguments (Balgopal et al., 2018; Balgopal & Montplaisir, 2011; Balgopal et al., 2017). Additionally, several studies have described the use of WTL assignments that are context-based (Moon et al., 2019; Wilson, 1994), incorporate social elements through peer interactions (Cox et al., 2018; Russell, 2013), or both (Finkenstaedt-Quinn et al., 2017; Finkenstaedt-Quinn et al., 2020; Finkenstaedt-Quinn, Polakowski, et al., 2021; Finkenstaedt-Quinn et al., 2019; Gupte et al., 2021; Moon et al., 2018; Schmidt-McCormack et al., 2019; Shultz & Gere, 2015; Watts et al., 2020) to increase students' understanding of a topic. Further analysis into how WTL assignments that are context-based and incorporate social elements appeal to the affective domain of learning is warranted, especially as such assignments have been shown to shift student thinking away from memorization towards conceptual meaning making (Gere *et al.*, 2019).

This study investigates how the WTL design described by Finkenstaedt-Quinn, Petterson, et al. (2021), which is context-based and incorporates social elements (i.e., role, audience, peer review), may support students' interactions with the assignments and their perceptions of learning the course content, thereby impacting their motivation to learn the content. The WTL assignment design utilized in this study incorporates rhetorical elements—an authentic context, role, genre, and audience—that students must consider as they engage in a writing process that includes peer review and revision. Previous research demonstrates that this assignment design is effective at supporting conceptual learning and disciplinary thinking in STEM courses (Finkenstaedt-Quinn et al., 2017; Finkenstaedt-Quinn et al., 2020; Finkenstaedt-Quinn, Polakowski, et al., 2021; Gupte et al., 2021; Halim et al., 2018; Moon et al., 2019; Moon et al., 2018; Schmidt-McCormack et al., 2019; Shultz & Gere, 2015; Watts et al., 2020). While these studies have demonstrated that students interact with the content as intended, there is little research focused on how the different elements of the assignments may influence the affective domain of student learning. Initial research by Gupte et al. (2021) identified that students engaged in meaningful learning when completing the form of WTL assignments that are the focus of this study in an organic chemistry course. However, more research is warranted, specifically focused on how the context and social elements of the WTL assignments appeal to the affective domain of learning.

The present study expands on the work of Gupte et al. (2021). In their analysis of student feedback responses, Gupte et al. (2021) found that the WTL assignments supported students' meaningful learning by appealing to both the cognitive and affective domains. The assignments led students to appeal to prior knowledge, apply course content, and apply content from a related course. Thus, students connected content and had to extend existing knowledge. Gupte et al. (2021) found that students identified engaging in problem solving, the rhetorical components of the assignments, clear expectations and external supports, and the peer review process as supporting their learning of course content. The current study further examines how the WTL assignments engage the affective domain of student learning by closely examining the role of authentic context and social elements in students' interactions with the assignments. We do so via an in-depth qualitative analysis of student interviews, which also addresses the dearth of qualitative studies on the ties between student affect and learning chemistry (Flaherty, 2020). This study aims to provide insight into designing and implementing WTL assignments that positively appeal to the affective domain of learning by analyzing student interviews about two WTL assignments implemented into an organic chemistry laboratory course. Two research questions guided the analysis:

1. How does the authentic context of the WTL prompts support students' interactions with the assignments?
2. How do the social elements of the WTL process support students' interactions with the assignments?

Theoretical Framework

This study is guided by the relevance framework described by Stuckey et al. (2013) and the sociocultural theory of writing (Prior, 2006). The relevance framework allows us to conceptualize how the rhetorical elements of the WTL assignments supports students' abilities to recognize the relevance of chemistry content to personal goals and issues of societal importance. The sociocultural theory of writing provides insight into the process by which the socially mediated act of writing engages students with the content they are writing about.

Based on a review of the science education literature focused on relevance, Stuckey et al. (2013) developed a scheme encompassing the various ways that the science curriculum can be relevant for students. Stuckey et al. (2013) conceptualize relevance in the context of science education as encompassing both what students identify as interesting and the knowledge or skills they need to progress through their education and contribute meaningfully to society. Key to this conceptualization is that it incorporates both what the individual deems as relevant, intrinsic relevance, and what educators or society deem as relevant, extrinsic relevance. Complementary to this, there is also a temporal aspect, spanning what is relevant in the moment to what will be relevant for students as they progress through their education and lives.

The temporal aspect and considerations of intrinsic versus extrinsic relevance are spread across three dimensions—individual, vocational, and societal—that are not mutually exclusive or hierarchical in nature (Stuckey et al., 2013). The individual dimension captures what students find personally interesting and knowledge or skills important for their development and success in daily life. The vocational dimension moves beyond success in daily life by appealing to students' intended vocations, exposing them to new vocational opportunities, and supporting their future vocational success through knowledge and skill development. The societal dimension focuses on knowledge and skills that are important for the individual to interact meaningfully with society in a constructive, socially conscious way and makes visible the connections between science and society. The rhetorical elements of the WTL assignments can appeal to these different dimensions of the relevance framework by making the relevance of the content students are writing about explicit, thereby supporting students to interact with the content and engage in reasoning key to organic chemistry.

Using the sociocultural theory of writing, we can conceptualize how students may be interacting with and identifying the relevance of what they are learning in a course through the social process of writing. The sociocultural theory of writing describes writing as an activity that is mediated by the social and cultural contexts within which the writer is situated (Prior, 2006). For the individual writer, writing is a social and collaborative act guided by cultural contexts (e.g., classroom, disciplinary, institutional, historical) and resources (e.g., peers, class notes, textbooks). Each of these may influence how the writer approaches and crafts their text. Furthermore, the writer's response is influenced by the genre in which they are writing, which is mediated by their past experience with that genre and their past experiences writing in a particular context (e.g., a student may associate writing in science courses with lab reports) (Bazerman, 2009). For the WTL assignments, students must negotiate writing in the genre given for each assignment and consider the rhetorical context to which they apply their understanding of organic chemistry.

The sociocultural theory of writing also captures how interacting with other people can shape the writing process and final text. Students may engage in several forms of interactions as they proceed through the WTL assignments. Most obvious, students are required to interact with their peers during the peer review process incorporated into the WTL assignments. Students may also engage in non-imposed interactions with their peers, such as working through reactions or developing their reasoning prior to or during the process of writing. Additionally, they may interact with near-peers, called writing fellows, as they respond to the assignments. Beyond these explicit social interactions, students must consider the given audience of each assignment and the implicit audience of the instructor. With this conceptualization of writing, when writing is situated in and moderated by social and cultural elements, it can lead to the internalization of knowledge. Utilizing relevance and the sociocultural theory of writing allows us to conceptualize how the WTL assignments may impact students' motivation to learn and thus appeal to the affective domain of learning as they engage in the writing process.

Methods

Guiding research paradigm

The aim of this study is to capture how students viewed the WTL assignments as influencing their construction of knowledge (e.g., students' lived experiences with the WTL assignments). As such, we proceeded using an interpretivist paradigm that centered around collecting qualitative data from students about how they conceptualized their experiences. The use of qualitative data (i.e., interviews and feedback surveys) allowed us to capture the understanding that students attributed to their experiences with WTL. In addition, by utilizing both interviews and open-response feedback surveys, we sought to capture rich data from the interviews and substantiate those findings through examination across a broader population of students via the feedback survey responses. The theoretical frameworks chosen for this study also reflect our interpretivist approach in that the relevance framework emphasizes value as identified by the students, as well as values dictated by society, and the sociocultural theory of writing acknowledges the social and cultural influences surrounding students' writing experiences.

Context and Setting

This study aimed to develop a qualitative understanding of how the rhetorical elements—authentic context, role, and audience—and social interactions incorporated into the WTL assignments impacted student motivation to learn the organic chemistry content. This study was based on the qualitative analysis of student interviews about WTL assignments implemented into a second semester introductory organic chemistry laboratory course at a large research-intensive university in the midwestern United States. The laboratory course consists of a one-hour lecture component and a four-hour lab session once a week. Throughout the course, students completed a weekly lab assignment based on the experiment for the week. In addition, two quizzes were given during the term to assess learning on organic mechanisms and spectral analysis. Students also completed three WTL assignments wherein they completed a first draft, participated in peer review, and then made revisions.

Data collection for this study took place during a mandatory stay-at-home order resulting from the coronavirus pandemic. The majority of the students who take the course are second- and third-year students at the university. The class is a prerequisite for a range of majors and pre-professional, primarily pre-health, pathways. During the semester from which we recruited students, the most represented fields of study included neuroscience, biomolecular science, biochemistry, and molecular, cellular, and developmental biology. Other common majors included public health, movement science, and biomedical engineering. Study data included student interviews and feedback survey responses. Institutional Review Board approval was obtained to recruit students and gather student data. All students included herein agreed to participate in the study. Analysis was performed on de-identified data and pseudonyms are used when we present student data below.

WTL Assignment Design

The WTL assignments that are the focus of this study follow the structure outlined by Finkenstaedt-Quinn, Petterson, et al. (2021) and were designed by a group of faculty, graduate students, and an undergraduate student experienced in the organic chemistry curriculum. The assignment design team discussed the contextual relevance of the WTL assignments and decided to align the contexts of the assignments to match the pre-health interests of the majority of students enrolled in the organic chemistry course.

The first WTL assignment administered in the course asked students to explain the mechanism for the racemization and acid hydrolysis of thalidomide and design an analog of thalidomide that would not undergo such mechanisms (Appendix 1A). Students were asked to imagine themselves as experts in the chemical pathways that lead to congenital disabilities and write an email to a colleague in obstetrics and gynecology explaining the mechanisms above and suggesting why their analog would prevent them from happening.

The second WTL assignment focused on forming an ylide using a base-free mechanism as part of a general Wittig reaction (Appendix 1B). The prompt provided students with information on the medical relevance of the mechanism used in manufacturing Benzoxepine, a therapy used to treat tuberculosis and some cancers. It then instructed students to write the section of an NIH grant proposal from the perspective of a medicinal chemist conducting research on the base-free Wittig reaction.

The final WTL assignment focused on intramolecular aldol reactions (Appendix 1C). It instructed students to assume the role of a lab technician for Doctors Without Borders (MSF) who is collaborating with researchers from the University of Ghana to develop a more effective synthesis pathway for Ivermectin, a drug that treats river blindness. Students were asked to write a summary comparing two possible reaction pathways, incorporating the mechanisms and reaction coordinate diagrams for each in their response, and provide an argument for the most likely pathway.

Each WTL assignment consists of three stages: first, students completed a draft in response to the assignment prompt (Appendix 1). After submitting their first draft, students participated in an anonymous peer review process mediated by an automated tool through the university's online learning management system. In the peer review process, students were tasked with providing feedback about their peers' drafts in response to content-focused rubric criteria. Students were given five days to review their peers' drafts. After giving and receiving three peer reviews on average, students were given one week to revise their first draft and submit a second draft. Grading for the first draft and peer review was based on effort and completion. The second draft was graded based on two content-focused criteria pulled from the peer review criteria. Throughout each of the WTL assignment stages, students were encouraged to seek out near-peer writing fellows associated with the WTL component of the course if they needed help with the reaction mechanisms or writing. Writing fellows are former students who succeeded in the course and serve as teaching assistants for the WTL portion of the course, where they are a resource for students and support the instructor by grading the assignments.

Student Interviews

Convenience sampling was used to recruit students for the interviews, where students indicated their willingness to participate in an interview about the WTL assignments on a survey administered to the class. Ten students agreed to be interviewed and all data collection took place over Zoom, a video-conferencing software that allows one or more parties to meet virtually. One of the first authors (MP) did the interviews in an effort to enhance the potential for rapport with the students, as MP had previously taken the course during an iteration that used WTL and served as a near-peer writing fellow for the course during the semester during which data was gathered. Students were interviewed about their experiences with the first two WTL assignments and were provided with copies of their final drafts of those assignments prior to the interviews. The interviews were semi-structured and focused on how students interacted with the rhetorical elements of the WTL prompts, the peer review portion of the assignment, and the resources they used when working on the assignments. Audio-visual data was collected via Zoom recording software in addition to audio data recorded on an external device. The interviews were transcribed for analysis.

Nine of the ten interviewees were first or second-year students, and one was a graduating fourth-year student. Each had a declared or intended major in a biological sciences field, and six of the ten participants reported intentions to pursue a pre-medical or pre-health track. The students reported that their primary reason for taking the course was that it is a prerequisite for their major or pre-professional track of choice. All of the students reported that they had some academic writing experience prior to taking the course, ranging from primarily scientific writing through research experiences and other STEM courses to writing in their humanities courses, including college-level English and writing courses and AP courses in high school. Two students also reported prior experience in other courses with the WTL assignment design that is the focus of this study.

After an initial review of the transcripts, one researcher developed the coding scheme through inductive coding. Two of the researchers then met to discuss the initial coding scheme and agreed on codes and definitions. The team then independently coded two transcripts using the coding scheme. Adjustments were made to the scheme, including the addition of codes and modifying the definition of others to reach a final coding scheme (Appendix 2) in keeping with inductive coding methods (Miles et al., 2014). The two researchers applied the final coding scheme to the remaining interviews and discussed any disagreements until consensus was reached (Watts & Finkenstaedt-Quinn, 2021). Once full agreement was met, the research team organized the codes based on their relation to the research questions and performed thematic analysis (Braun and Clarke, 2006). In this process, the research team equally divided the codes from the codebook. Each researcher then wrote a summary of the common themes arising from each code. The team then met to discuss and present their findings from the thematic analysis, and these findings became the foundation for the results and discussion section. Discussions between the two researchers during development of the coding scheme and about the results of the thematic analysis support the dependability of the analysis (Lincoln & Guba, 1985).

Feedback surveys

To gather additional information on students' experiences with the WTL assignments, Qualtrics surveys were administered to the class after each WTL assignment. The aim was to elicit students' general experiences with each of the WTL assignments, and the surveys contained questions that asked students to describe what parts of the assignment they enjoyed, did not enjoy, and what was clear or unclear about the directions in the assignment. We applied the same coding scheme as that used to analyze the interviews to responses to the question, "what did you like about the assignment?". We followed a similar coding procedure whereby each researcher coded each feedback survey response, and any discrepancies were discussed to reach complete consensus in the coding. These results served as a secondary data source to corroborate our findings from the transcripts and add to the credibility and dependability of our study (Lincoln & Guba, 1985).

Results and Discussion

This study sought to determine how the rhetorical and social elements built into the WTL assignment design impacted students' interactions with the chemistry addressed in the WTL assignments by appealing to the affective domain of learning. These elements include the authentic context that students responded to when writing, the peer interactions built into the assignment through a structured peer review process, and the available support of near-peer writing fellows. Guided by the relevance framework and sociocultural theory of writing (Prior, 2006; Stuckey et al., 2013), this study presents the results of our analysis of interviews with students focused on the WTL assignments.

RQ1 findings: The authentic context incorporated into the WTL assignments supported students' interaction with the assignments and helped them draw connections between organic chemistry content and medically relevant applications

The context supported students' interactions with the assignments by making the relevance of the content explicit and appealing to personal interests. We found that the majority of the interviewed students had positive perceptions about the authentic contexts given in the WTL assignments and of the assignments' integration into the lab setting. Students' perceptions were reflected by their discussion of how the contexts around which the assignments were structured were interesting or made the content appear relevant. They noted this by either broadly discussing how the context enabled them to identify the relevance of the content targeted by the assignment or describing how the context related directly to their personal interests as intrinsically interesting or tied to their aspirational goals.

Students showed interest in the applicability of the chemistry content to the authentic contexts presented in the assignments. They stated that the authentic contexts they wrote in response to were more interesting than a "made up" example. Laurel stated,

> "*I definitely think as with any of the prompts when they frame them in terms of how this molecule's been applied in the real world and frame it as a real-world problem or something like that definitely makes it a lot more interesting.*"

As described by Rose, writing about chemistry in response to an authentic context that they viewed as relevant also made students more motivated to complete the assignment:

> "*...getting the context and a relevant one, make it seem more*

interesting, makes it seem more relevant and worth doing then."

This response indicates that including authentic contexts in prompts helped motivate students to complete the WTL assignments, and attend to the chemistry content targeted by the assignments. This finding is in keeping with Gilbert's (2006) claim that the chemistry curriculum should be made relevant to the students' lives to promote more voluntary chemistry learning.

A majority of the participants also identified the prompts' contexts as intrinsically relevant to their lives at the individual and vocational dimensions. Fern's interest in the context was grounded in their identity as a biochemistry major. They liked that the chemistry outlined in the assignments was relevant not only to themselves as a biochemistry student but also relevant to life outside the lecture hall and laboratory. Fern said,

"I *think it made me more engaged, because it is more relevant to my major as a biochem student. I do think it's cool, though, to actually apply what we're learning in [class], and what we're learning in lab, to actual real-world examples and what they do in the medical field.*"

In addition, the medical relevance of the chemistry presented in the prompts promoted positive interactions in most of the interviewed students. Poplar, one such pre-health student, described how the second WTL prompt, which targeted the Wittig reaction, supported their recognition of the importance of chemistry at the vocational level, saying,

"It was the Wittig one, I believe, had something to do with cancer and how did the drug we were dealing with had effects that could be helpful for fighting cancer. In that way, I was like, "Okay, well, yeah, chemistry is very important if I was going to be trying to research cancer."

Hazel is a pre-med student who also expressed a personal interest in the chemistry targeted by the thalidomide prompt, and found the connection compelling. Hazel said,

"I mean [racemization and acid hydrolysis of thalidomide] felt like a very relevant issue that I wanted to attack."

Hazel's desire to "attack" the issue outlined in the prompt demonstrates how incorporating authentic contexts into the WTL assignments that appeal to students' personal and vocational interests can support their motivation to learn.

Lastly, students also appreciated the extrinsic relevance of the assignments to the content covered in the laboratory course, whereby they applied concepts from lecture to the WTL assignments. A few of the students mentioned finding the assignments relevant because they focused on chemistry from the course. As Fern described,

"I do think it's cool, though, to actually apply what we're learning in [organic chemistry II lab]..."

This sentiment was also present among feedback survey responses. In the feedback survey responses, students described positive perceptions of the assignments, as they could draw on their prior knowledge or content pertinent to the course. For example, one student wrote about the thalidomide assignment,

"A good review of [organic chemistry I lab], and at the same time introduced carbonyl reactivity that was being covered in [organic chemistry II lecture and lab]."

Tied to relevance, students appreciated that they were applying their content knowledge to an authentic context. These results also substantiate the findings by Gupte et al. (2021) by providing evidence from a different semester, and different group of students, that the assignments led students to draw on prior and course knowledge. Additionally, they may indicate a way to address the potential disconnect for students between what they learn in laboratory courses and its importance beyond the lab (DeKorver & Towns, 2016).

The contexts helped guide students to focus on the organic chemistry content targeted by the assignments and led to student perceptions of knowledge gains. The data from these interviews also suggest that the context presented in the prompts helped guide students to consider the chemistry content targeted by the assignments. This is important as the aim of each WTL assignment is to increase student knowledge or disciplinary thinking for a particular aspect of organic chemistry (e.g., acid-base chemistry, reaction mechanisms, reaction coordinate diagrams) and we posit that as students write about the target concepts their understanding of the concepts may develop (Finkenstaedt-Quinn, Petterson, et al., 2021). All of the participants reported perceived learning of organic chemistry content as a result of completing the WTL assignments. For example, participants said that the thalidomide assignment taught them about racemization and acid hydrolysis, which were previously novel concepts. Rose said they learned about the chemical components of thalidomide when completing the first WTL assignment, saying,

"Definitely before that, we hadn't gone over racemization in my class. I mean, I had known the historical things about thalidomide, but I didn't know the science behind it."

Virginia also said they learned the mechanism of racemization by completing the first WTL assignment. They also learned the definition of a chemical analog, telling the interviewer

"And then I learned about analogs. I didn't really know what that specifically was. I knew what it was, but then they defined it as, "This is an analog," and I'm like, "Oh, okay, cool."

Virginia used this new knowledge to propose an analog for the thalidomide molecule that was resistant to both acid hydrolysis and racemization. For the Wittig assignment, students described chemical concepts introduced in lecture, then practiced in the lab. Cheri said

"*...I definitely just, like I said, learned more about the mechanism of ylide formation and then using the ylide to go and make those bonds."*

Students also described gaining a better understanding of the chemistry in several feedback survey responses for both the thalidomide and the Wittig WTL assignments, particularly when the prompts asked students to derive a curved-arrow mechanism for the thalidomide acid hydrolysis/racemization and Wittig reactions. One student wrote about the Wittig WTL assignment,

"I liked how this assignment made me explain why the base-free [Wittig] reaction did not need an additional base as opposed to the traditional [Wittig] reaction. This helped me understand [Wittig] reactions deeper."

Gupte et al. (2021) reported similar findings, where students reported developing knowledge from completing the same assignments in an earlier semester. When considered in alignment with Schmidt-McCormack et al. (2019), which demonstrates that WTL can support students to develop acid-base knowledge in an organic chemistry context, and Watts et al. (2020), which demonstrates that students can reason mechanistically when responding to a WTL assignment, our findings indicate that not only can WTL support students' learning but that students also perceive they are learning. In addition, the ability of the contexts to support student learning is also in alignment with one of the models that Gilbert (2006) presents for successfully incorporating contexts into chemistry education, where the concepts and application help give meaning to one another.

Students described primarily positive affect about the WTL assignments, where the contexts were important in supporting positive interactions. Students primarily described positive affective responses to the contexts presented in the WTL assignments. Ash and Elm both reported positive affect specifically for the context of the second WTL prompt. Ash said,

> "*I also like how there's been a lot of focus on natural products and pharmaceuticals.*"

Elm, similarly, said,

> *"I really liked it. Yeah, I really liked it because it made me take a step back and realize, all right, I guess orgo has a place in the medical field, it's not totally pointless to me."*

Feedback survey responses also indicated that students generally had positive affective emotions about the contexts incorporated into the WTL prompts. They liked that the prompts were applicable to their personal endeavors and the greater society, in keeping with Stuckey's (2013) vocational and societal domains of relevance. A few students, however, did not like the focus on medically relevant contexts across all three WTL assignments. Two of the students who disliked the medically relevant contexts of the WTL assignments still expressed positive affect about the WTL assignments. For Bruce and Virginia the contexts helped contextualize why WTL is used in their laboratory course. Virginia said,

> *"...I can see what the actual positives are now…looking at it, it is definitely useful."*

While the contexts did not intrinsically appeal to Virginia, they could still identify the extrinsic relevance of the medical contexts to the course content.

The feedback surveys also indicated that the prompts' creative aspects led to a positive response from students. The overall positive emotions towards WTL assignments due to the contexts and students recognizing their purpose may promote positive interactions with the assignments. This finding is supported by a study by Hulleman et al. (2010) where they claim that the extent of student engagement with an assignment is predicated on the student's perceived value of the assignment and the extent to which the student can think positively about the assignment.

RQ 2 findings: The social elements of the WTL assignments support student interactions with the assignments and their development of chemistry knowledge

The sociocultural rhetorical elements given in the prompt supported positive student interactions with the assignments. The role, genre, and audience are also key components of the prompts that, in alignment with the sociocultural theory of writing (Prior, 2006), impacted students' perceptions of the WTL assignments. Ash, Hazel, and Rose all mentioned that they appreciated the background information about the scenarios that were provided in the prompts. More specifically, Elm and Rose discussed how the role they were given in the prompts made the assignments more engaging. Elm said:

> *"Yeah, just setting the stage if you will for what we are in the thing, like by saying that we're working with Doctors Without Borders or something, […] I remember reading that and being like, okay, this is like a real-life scenario, I can appreciate that."*

Laurel and Elm also described how the genre in which students were writing for the assignments, an email and a grant proposal, added to the authenticity of the assignment. For Laurel, writing in the form of a grant proposal also impacted how they viewed the relevance of the assignment:

> *"I think one of them we wrote as like a draft proposal and stuff like that definitely made it seem more relevant in terms of what I might encounter in the future or just more interesting for now."*

This demonstrates how incorporating the sociocultural elements of role and genre into the prompt can also support the authenticity and relevance of the WTL assignments.

The audience was also important for Hazel and Laurel. They both appreciated writing about the organic chemistry content to a less knowledgeable audience, discussing how the audience allowed them to provide more fundamental chemistry explanations. Hazel described this as:

> *"I also liked that they've targeted it towards an audience that didn't know a lot about chemistry because I like that you can strip it down to the basics when you want to explain something."*

Relatedly, all of the students discussed how they view explaining as part of their learning process, and four students explicitly extended this to the WTL assignments. Elm said:

> *"But with the [WTL] assignments where you have to... it's easy to write and be like, yeah, the carbonyl goes and gets deprotonated or whatever. Like where you have to go back and be like, okay, what does that actually mean? [...] it makes you think about it in a simple way so that you can like it's easier to retain and understand."*

This sentiment was also present in the feedback surveys, where students identified that writing out explanations helped them better understand the reactions. One student wrote,

> *"I will always have a strong grasp on the Wittig reaction do [sic] to the need of having to explain the reaction through words."*

While Gupte et al. (2021) found that students reported difficulty balancing the audience with the level of explanation they should give, our findings indicate that incorporating an audience besides the instructor into the WTL assignments supports students' interactions with and learning of organic chemistry content.

The ways that students described their perceptions of the sociocultural elements incorporated into the assignment description (i.e., the role, genre, and audience) indicates that they supported positive interactions with the authentic context. In addition, writing to an audience led students to reflect on their explanations and own understanding of the chemistry.

The peer review and revision stages positively impacted student affect towards the assignment. Students expressed both positive and negative affective responses related to the act of writing. When the first WTL assignment opened, all but one of the students reported negative feelings towards it. This perception was because they simply did not want another assignment to do or because they had anxiety about the WTL process—either because they were unfamiliar with the process or did not like writing. Elm said,

> *"at the beginning, I really hated the [WTL] assignments, they made me really upset because I don't like writing."*

This indicates additional reasons behind negative affective responses toward the WTL assignment beyond those identified in Gupte et al. (2021), which were primarily due to the content targeted by the assignments. The negative affective responses our study identified may be due to students' lack of experience with writing in STEM classrooms that is not in the form of a laboratory report and indicates that familiarizing students with the WTL process prior to the assignments could help alleviate negative responses.

Despite the initial negative affect about the assignments, the majority of the students in this study described a positive affective shift as they gained experience with the assignments. Both Bruce and Hazel explained that by the second WTL assignment, they understood the expectations, and this understanding created a more positive experience. Bruce said,

> *"I think part of my reluctance was that I felt like it was going to be hard to write chemistry in a way that felt interesting and worthwhile. And so, by the end, I think that part was easier…"*

This shift in affect aligns with how students experience genres in the sociocultural theory of learning, where the writer may first need to learn how to write in a specific genre before they can fully engage with it (Bazerman 2009). It implies that instructors should carefully consider genre when incorporating writing assignments into chemistry classrooms that deviate from traditional genres that students experience.

In addition, almost all of the interviewed students reported that the structured interactions with their peers and the chance to revise served to reduce negative emotions, such as stress and anxiety, affiliated with the WTL assignments. They appreciated having the opportunity to revise and resubmit a second draft after receiving peer review comments. Hazel said:

> *"[The peer review process] just took some of the stress away of having to write this assignment."*

The majority of the students who were interviewed also noted that they felt some reassurance knowing that they had an opportunity to revise their initial drafts. When asked about the opportunity to revise, Bruce said,

> *"I felt more confident to write something that I wasn't sure was the way I wanted it to be in the final paper because I knew I'd get some comments on it that maybe would help me find a better way to say what I was saying."*

Conversely, a few students mentioned that they put more effort into completing the initial draft because they did not want their peers to tell them they had described the organic chemistry content incorrectly and then have to spend more time revising their final draft.

The positive affect affiliated with peer review might also address negative affect due to student difficulty with the content targeted by the assignments, such as that expressed by Cheri and Fern, and seen in Gupte et al. (2021). For example, Cheri expressed negative feelings towards the thalidomide WTL assignment, in which students were asked to describe the mechanism by which thalidomide undergoes racemization and acid hydrolysis and propose an analog that is not susceptible to the reactions. Cheri said,

> *"I feel like [the thalidomide] one I was the most disconnected with, to be honest, because I didn't totally understand it still even when I submitted my final…"*

Their lack of assuredness instilled a negative affect towards the assignment. However, the peer review process could serve to mitigate negative affect arising from content difficulty. For example, Cheri and Virginia both discussed how they could rely on their peers to correct them if they did not understand a concept or thought they were describing it incorrectly and, thus, incorporate the content they felt unsure about into their initial drafts. Cheri said:

> "*I was like, you know what? This might be wrong, but my peer reviewers are going to tell me. And so then I can just fix it and like make it better."*

Thus, the social interactions can support positive student perceptions by reducing potential negative affect about experiencing a new genre of writing and the difficulty of the content targeted by the assignments. This, in turn, could foster a better learning environment as interactions with peers can improve students' confidence and support students' motivation to learn (Schunk, 1991; Vansteenkiste et al., 2006).

Peer review and revision incentivized student interactions with the WTL assignments and supported the learning process. Students described the peer review and revision stages of the assignments as incentivizing them to fully interact with the assignments and helping them to develop their understanding of the chemistry content. A majority of the students discussed how the peer review and revision processes led them to put more effort into the initial drafts of the WTL assignments. Students primarily expressed that this was because they knew their peers would be reading their drafts. However, they differed in their reasons for why this incentivized them. Cheri, Poplar, Ash, and Virginia all discussed that they felt having a good initial draft would allow them to get more beneficial feedback from their peers that they could then use to revise their initial draft. Cheri said:

> "*Well it definitely made me want to write a better, more coherent full version of what I was trying to say. Because I feel like I could get the most out of it if I had my full best shot on the paper when I submitted it versus just this, crappy write.*"

Bruce provided an alternate perspective for how peer review may have incentivized students to put additional effort into the initial draft. Bruce recognized that they themselves learn from reading their peer's work and thus wanted to submit a good initial draft that might benefit the reviewer reading it,

> *"Knowing that I got a lot of out of reading other people's papers, I think it encouraged me to write in a way that I think somebody else could get something out of reading mine.*

Fern more broadly discussed how the peer social interactions led them to put more effort into the assignment. Specifically, Fern described spending time carefully reading their peers' drafts and providing meaningful feedback. This careful reading may benefit students like Fern as well, as it allows students more time for reflection on their writing.

Students also discussed how interacting with their peers during peer review supported their learning and identified that they liked the peer feedback aspect of the assignments. Ash said:

> *"I like the idea of not only learning and being able to fix it but also that I was learning from peers."*

Students ranged in how they talked about the peer review process supporting their learning. Similar to the results found by Gupte et al. (2021), students discussed the benefits of both reading their peers' drafts and receiving feedback but provided greater insight into how both elements of the peer review process benefited them. Almost all of the students discussed feeling that they benefited from reading their peers' work. This aligns with findings indicating that reading their peers' work is more beneficial to student learning than receiving peer feedback for learning-to-write style assignments (Cho & MacArthur, 2012; Cho & Cho, 2011; Lundstrom & Baker, 2009; Nicol et al., 2014) and WTL assignments (Finkenstaedt-Quinn, Polakowski, et al., 2021). The majority of the students mentioned that by reading their peers' drafts they were able to see the organic chemistry content presented in different ways and at different levels of complexity. Laurel said:

> *"Yeah. I definitely think sometimes reading the peer reviews made me look at things from a different perspective, especially if they had a mechanism that was different than mine or completely disagreed with which carbon something would end up on or something that counteracted my initial thoughts. That was definitely really helpful because [...] it definitely helped me re-evaluate my own thinking."*

Students also described how reading their peers' work helped them gauge their own responses and whether they had provided enough detail in their mechanistic descriptions. Ash, Cheri, Elm, and Poplar discussed how peer review helped clarify content for them or identify content that was missing from their own drafts, primarily from reading. These students' sentiments are similar to the findings of Nicol et al. (2014), focused on learning-to-write, where they found that reviewing their peers' work led students to engage in reflective, evaluative thinking about their own work through the process of comparing their work and the work of their peers.

The majority of the students also explicitly discussed how they found receiving feedback from their peers to be beneficial. Students primarily described receiving feedback in which their peers identified incorrect content in their initial drafts and how that was helpful. Cheri explained how it was beneficial on the base-free Wittig WTL assignment.

> *"And then I also use the peer reviews a lot because, like I said, for the Wittig one, my first draft was wrong, so I had to change it and all of their suggestions were helpful."*

Cheri's sentiment aligns with findings by Halim et al. (2018), which demonstrated that students made content-focused revisions based on peer feedback on WTL assignments implemented in an introductory biology course. Relatedly, Bruce, Cheri, Hazel, and Virginia described how they used the peer review process to get feedback on content descriptions they weren't confident about. Hazel said:

> *"Like I took more risks in what I was doing and if it's not right, maybe I'm on the right track. Someone will help me along the way. It helps."*

Similar responses to the peer review process were present in responses to the feedback surveys, in which students specifically mentioned the benefits of both reading their peers' work and receiving feedback on their own initial drafts.

Our results indicate that the peer review process supported student interactions with the assignments and led to perceived learning benefits. Knowing that they would be interacting with their peers led students to put more effort into their initial drafts. Students also recognized the learning benefits associated with both reading their peers' draft and receiving feedback from their peers. This perception, in turn, prompted students to closely read and consider the drafts they read and peer reviews that they gave, in addition to considering the feedback they received from their peers. This finding demonstrates a metacognitive approach to the peer review stage, which is thought to be especially important for meaningful engagement in both peer feedback processes and successful WTL (Gere et al., 2019; Klein, 2015; Nicol et al., 2014).

Interactions with the writing fellows and their peers outside of the WTL process served as an additional feedback mechanism for students. In addition to interacting with their peers during the peer review process, students discussed two other social avenues that they utilized during the writing process—writing fellows and other peers. Writing fellows are near-peers who have taken the course previously and received training to support students with writing about content. They hold office hours throughout the semester when students are working on the WTL assignments and students are encouraged to attend these with questions. The majority of the students discussed attending office hours with the writing fellows, primarily specifying that they visited the fellows when working on the Thalidomide WTL assignment. Cheri, Elm, and Fern talked about how they attended office hours to check their mechanisms with the writing fellows. Each of them first attempted the mechanism and then utilized the fellows as a social resource of a more knowledgeable peer to check both their mechanism and description. Fern described how interacting with the fellows helped clarify the chemistry:

> *"I just found it really helpful to go over my thought process and talk about what I was trying to say [about acid hydrolysis]. I guess it just helped me better understand the process and that my answer wasn't wrong, but it helped me understand what the [writing fellows] were looking for and what they want me to learn from the specific process."*

Elm also mentioned discussing the style and formatting of their draft with a writing fellow. Interacting with writing fellows for support with both the content and writing style were also mentioned in the feedback survey responses, as evidenced by one student who wrote:

> *"I liked the [writing fellows]. They were very helpful in figuring out where I was going wrong chemically, and they helped me structure my paper properly."*

These responses indicate that students were interacting with the fellows in the intended ways. A few students also discussed meeting with their peers prior to or while writing their initial draft to reason through the reaction mechanisms together. These unstructured interactions with writing fellows and peers align with the sociocultural theory of writing, where the social interactions influenced what students wrote during the initial drafting and revision stage prior to peer review (Prior, 2006).

Limitations

There are several limitations associated with this study. First, the study was conducted at a large university in the Midwestern United States, with a specific social and education setting. Thus, students' experience are not necessarily transferable to another institution. Relatedly, our findings are also limited to the specific WTL prompts designed to appeal to the predominately pre-health student population of the course. Different WTL prompts used in courses with different demographics may not see similar results. Additionally, course instruction was disrupted with the onset of the COVID-19 pandemic. It is unclear how the transition to remote learning, and the added stresses of the pandemic, influenced students' motivation or engagement with the course material and thus the WTL assignments. There were also no incentives for students to participate in interviews or complete the feedback surveys, which may have led to a bias in our data collection towards students with strong positive or negative feelings about the assignments. For these reasons, the study results may not fully encompass students' motivation and interactions with the WTL assignments utilized in this study. In addition, our results are limited to student perceptions of learning and, as such, we cannot make claims about gains in student conceptual understanding from completing the assignments. However, in the context of organic chemistry, Schmidt-McCormack et al. (2019) indicate that WTL can support student learning of acid-base concepts and Watts et al. (2020) found that WTL can elicit mechanistic reasoning.

Conclusions

This study investigated how the rhetorical (i.e., authentic context, role, genre, and audience) and social aspects (i.e., peer review, revision, and interactions with writing fellows) incorporated into WTL assignments influenced how students interacted with the assignments in a second-semester organic chemistry laboratory course. Using the relevance framework outlined by Stuckey et al. (2013) and the sociocultural theory of writing by Prior (2006), we qualitatively analyzed student interviews about the WTL assignments. The results indicate that the rhetorical elements promoted positive student interactions with the WTL assignments by making the relevance of the target content explicit and supporting the authenticity of the context. The structured social interactions, specifically peer review and assistance of the writing fellows, promoted a positive affective learning experience while also allowing students to reflect on their explanations and understanding of the course material. Overall, the findings of this study further our understanding of the effectiveness of the WTL assignment design utilized herein by demonstrating how both the rhetorical elements and social interactions positively appeal to the affective domain of learning.

Our results indicate that the authentic context served to make the relevance of the content explicit at the personal, societal, and vocational levels. This finding is important, as student recognition of the relevance of course content has been tied to their motivation to learn. Students described that the contexts appealed to them, even when they were not intrinsically relevant, and supported positive affect about the assignments. The additional rhetorical elements incorporated into the WTL prompt (i.e., the genre, role, and audience) supported the authenticity of the context. Students also described how the context and audience influenced how they considered the organic chemistry content targeted by the assignments and that they perceived these aspects as beneficially supporting their learning.

The social elements, both those built into the WTL process (i.e., peer review) and more unstructured interactions (i.e., meeting with writing fellows and peers), also supported positive student interactions with the assignments and content. The peer review process led students to put effort into the first draft of their assignment and metacognitively reflect about their understanding of the organic chemistry content targeted by the assignments. Here, students reported the benefits of both reading their peers' writing and receiving feedback from their peers. Students found both of the available feedback mechanisms, peer review and interactions with the writing fellows, beneficial to complete the assignments.

Our findings have several implications for incorporating WTL assignments into chemistry classrooms. Our findings suggest that incorporating rhetorical elements, and specifically authentic contexts, into WTL assignments can facilitate student learning of chemistry content. However, some of the interviewed students felt that there was too much emphasis on medically relevant contexts. As such, we suggest that instructors consider surveying their course, then tailoring the WTL contexts to students' interests or selecting a range of contexts to appeal to a variety of personal, societal, and vocational interests. Future research on WTL could focus on how different contexts, roles, genres, or audiences may influence students' interactions with the assignments. Our results also indicate that instructors should consider implementing peer review and revision when incorporating WTL assignments into their courses, as students primarily perceived these processes as beneficial to their learning. Future research could further explore the role that peer review can play in reducing negative affect affiliated with student difficulty with the content targeted by assignments such as the WTL assignments described herein. Lastly, many students demonstrated an initial negative affective response to the WTL assignments. This response could be mitigated by instructors explaining to students the process and purpose of WTL assignments prior to students experiencing them in the course. This approach would help familiarize students with how to do the WTL assignments while also providing context for how the assignments improve learning and why they are included in the course.

Conflicts of interest

There are no conflicts to declare.

Acknowledgements

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ARTICLE

Appendix 1: Full text of the WTL assignments

1A – Developing a Therapeutic Analog for Thalidomide

Thalidomide was widely used after World War II as a sedative and later as a treatment for morning sickness. Unfortunately, after its widespread use, it was discovered that thalidomide causes very serious side effects—in particular, birth defects such as phocomelia (limb malformation). The drug was banned in 1962, and these events resulted in important changes to the way the FDA approves drugs. Now, despite the inherent dangers, thalidomide is used for treatment of nausea related to chemotherapy, where benefit of treatment outweighs the inherent dangers.

It is understood that thalidomide exists as two **enantiomers**; one is a teratogen that causes birth defects, while the other has therapeutic properties. Rapid **racemization** occurs at neutral pH, so both enantiomers are formed at roughly an equal mixture in the blood, which means that, even if only the therapeutic isomer is used, both will form once introduced in the body. The racemization is illustrated below in **Figure 1**.

Figure 1: The rapid racemization of thalidomide.

Furthermore, both enantiomers are subject to **acid hydrolysis** once in the stomach at lower pH, which could produce products that are teratogens. The structure of thalidomide and two thalidomide hydrolysis products are shown below in **Figure 2**. For these reasons, it is important to prevent both the racemization and the subsequent hydrolysis of thalidomide.

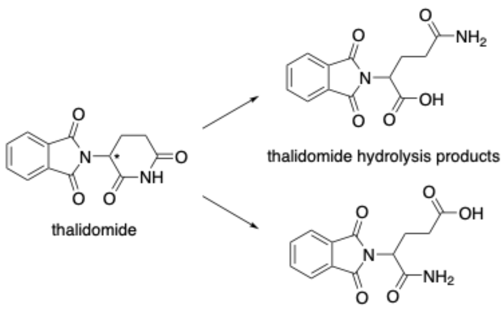


Figure 2: Thalidomide and two thalidomide hydrolysis products. The stereocenter is shown (*). You are an OB-GYN at the Mayo Clinic. A colleague, who is an oncologist at the University of Minnesota, has approached you about a potential collaboration on a human clinical trial. This trial will propose and test the efficacy of thalidomide **analogs** for the treatment of nausea in cancer patients. (See note on the third page for an explanation of an analog.)

As an organic expert in the chemical pathways that lead to birth defects, you are writing an email to your collaborator. Your goal will be to propose a structural difference that will make the thalidomide analog unreactive toward both racemization and hydrolysis. You must provide descriptions of the structure and reactivity of thalidomide toward racemization and hydrolysis as well as descriptions of the structural differences in the proposed analog that will make it unreactive to both of these processes. The oncologist is not an expert in organic chemistry. Therefore, carefully consider which organic chemistry terms to use and when to define or explain them. Use clear and concise language, striking a balance between organic jargon and oversimplified explanations.

Your email should be approximately between 500-700 words (1-2 pages) in length. It should address the following points:

1. Provide thorough descriptions of the mechanisms of both racemization and acid hydrolysis, highlighting the critical structural features of thalidomide and their role in these mechanisms.
    a. When racemization occurs, what changes occur in the molecule?
    b. When hydrolysis occurs, what changes occur in the molecule?

2. Propose a thalidomide analog (one compound) that would not undergo racemization or hydrolysis. Explain what structural features are in place that would inhibit or prevent these processes.

You can and should include figures of schemes, structures, or mechanisms, if that supports your response. We suggest that you have the figure(s) in front of you—ready to color-code or mark-up in various ways—and that you use your visible thinking to guide your audience through your explanation. Any images that you include in your response, *including the figures in this prompt or those that you draw in ChemDraw or on paper*, must have the original source cited using either ACS or APA format. Given your audience, your written response should suffice so that the explanations can be understood without the figures. **You will be graded only on your written response.**

An analog is a compound that is very similar to but has small structural differences from the pharmaceutical target. For example, m-cresol (shown in Figure 3 below) is an analog of phenol.

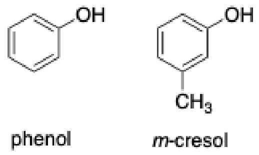


Figure 3: Phenol and m-cresol, an analog of phenol.

1B – Using the Base-Free Wittig Reaction to Synthesize Anticancer Compounds

Benzoxepine (Figure 1) is a heterocycle composed of a six-membered benzene ring and a seven-membered oxepin ring. Some benzoxepine analogs inhibit tuberculosis, and others inhibit cancers by inducing activation of the apoptosis pathway. The benzoxepine analog shown in Figure 2 is a **benzoxepinoisoxazolone** whose anticancer activity is attributed to its structure that is functualized with phenyl and azole groups.

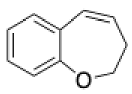


Figure 1: Benzoxepine.

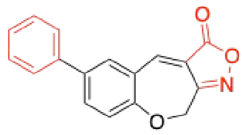


Figure 2: A benzoxepinoisoxazolone, a benzoxepine that has been modified with phenyl and azole functional groups.

However useful, isolating benzoxepine analogs from natural sources is inefficient. Benzoxepine analogs are important intermediates in the synthesis of therapeutic drugs, such as the aforementioned benzoxepinoisoxazolone. They are also important in studies that deduce structure-activity relationships to develop other medicinal treatments. Recently, German researchers synthesized benzoxepine analogs (Figure 3) using a **base-free Wittig reaction** (Figure 4). This reaction is a novel development that will synthesize therapeutic drugs on an industrial scale while producing fewer waste byproducts.

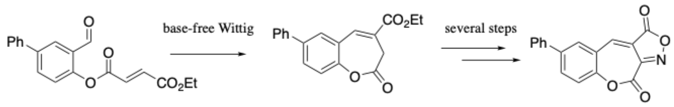


Figure 3: Synthesis of benzoxepinoisoxazolone through the base-free Wittig reaction.

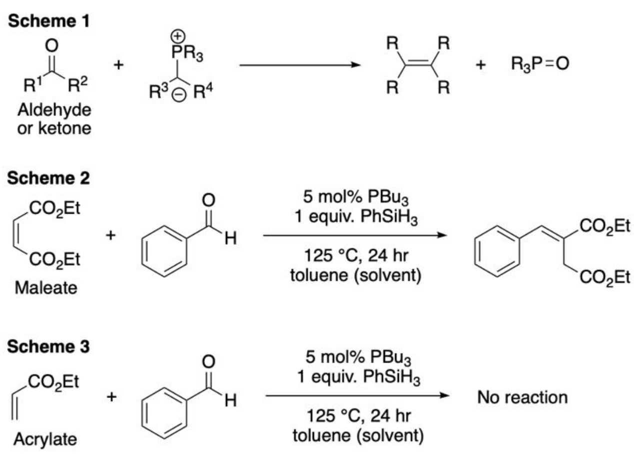


Figure 4: Generalized schemes of the base-free Wittig reaction. Scheme 1 shows the standard Wittig reaction, and Scheme 2 shows an example of the base-free Wittig reaction using a maleate starting material. Scheme 3 shows that the base-free Wittig reaction fails when using an acrylate starting material instead.

You are a medicinal drug developer in a research group that primarily studies anticancer compounds. Inspired by the benzoxepinoisoxazolone in Figure 2, the group's current goal is synthesizing benzoxepine analogs using the already developed base-free Wittig synthesis and evaluating them for anticancer activities. To do so, your research team is drafting a grant proposal for the National Institute of Health (NIH) that summarizes the group's research goals and argues for the significance, innovation, and impact. You, the organic chemist expert, must write the section of the grant proposal that explains the base-free Wittig reaction that synthesizes benzoxepine analogs. Because the reaction is critical for the success of the project, you must demonstrate to the committee that your team understands how the reaction works and why it is selective. The committee who will review the proposal is made up of scientists from many disciplines, including chemistry, biology, and medicine. Therefore, they may not be experts when it concerns mechanisms or organic-specific terms. The NIH recommends that you:

- write organized and logical paragraphs
- include figures that assist the reviewers in understanding complex information
- use clear and concise language, striking a balance between organic jargon and oversimplified explanations

Your section of the grant proposal should be approximately between 500-700 words (1-2 pages) in length. It should address the following points:

1. Explain the critical structural and electronic features and properties of the starting materials and reagents in Scheme 2 and their role in the mechanistic steps that lead to the formation of the products without the use of an external base.
   a. In describing the mechanistic steps for the reaction in Scheme 2, what changes occur within those steps to the starting materials and reagents that lead to the formation of the ylide? (Note that the ylide is not shown in this scheme.)
   b. What structural changes happen to PBu_3 at each mechanistic step?
   c. Focus on the *how* and *why* as well as the *what.*
2. When comparing the starting materials and reagents in Scheme 2 to those in Scheme 1, what structural differences are present that allow the Wittig reaction to proceed without the use of an external base?
3. Why would researchers want to synthesize benzoxepinones through the modified, base-free Wittig reaction over the traditional Wittig reaction? Focus on key aspects of the overall reaction that make it significant, innovative, and impactful for larger-scale research studies.
4. Propose a reason why the reaction works with maleate but does not work with acrylate, as shown in Scheme 3. What structural features are present or absent in the acrylate that prevent the modified Wittig mechanism from happening?

You can and should include figures of schemes, structures, or mechanisms, if that supports your response. We suggest that you have the figure(s) in front of you—ready to color-code or mark-up in various ways—and that you use your visible thinking to guide your audience through your explanation. Any images that you include in your response, *including the figures in this prompt or those that you draw in ChemDraw or on paper*, must have the original source cited using either ACS or APA format. Given your audience, your written response should suffice so that the explanations can be understood without the figures. **You will be graded only on your written response.**

1C – Exploring Possible Reaction Pathways for a Catalyzed Intramolecular Aldol Reaction

(not included in this investigation)

Ivermectin is a drug used to treat onchocerciasis, a parasitic disease commonly known as river blindness. While the disease is rare in the United States, it is especially prevalent in Ghana, where more than 15% of the population is affected. As a lab technician for Médecins Sans Frontieres (Doctors Without Borders), you have traveled to Ghana to collaborate on a study initiated by biochemists at the University of Ghana who are working to develop a more efficient synthesis of ivermectin. The biochemists you are working with have identified a new strategy to perform **intramolecular aldol reactions** that uses the catalyst triazabicyclodecene (TBD). The TBD-catalyzed aldol reaction could be used in the place of the traditional aldol reaction for an early synthetic step in the synthesis of ivermectin. Using TBD will replace the need of strong acids and bases in this synthetic step, which will limit undesired side reactions. An example of a TBD-catalyzed aldol reaction with a simplified starting material is shown in **Figure 1**.

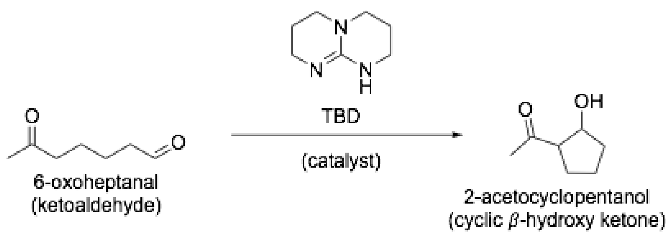
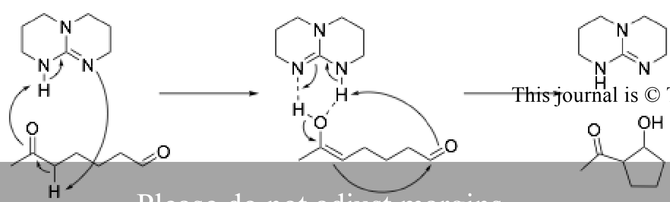
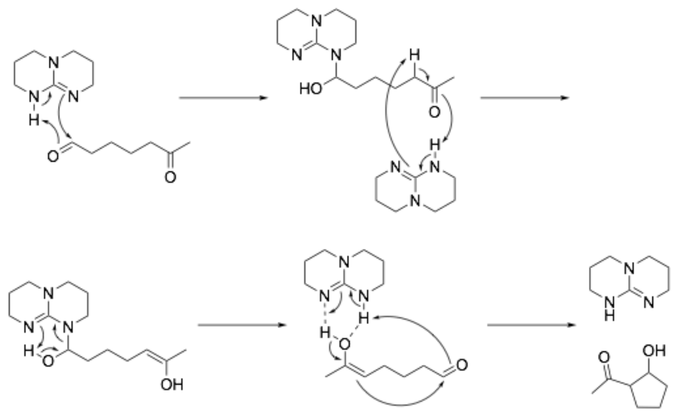


Figure 1: The intramolecular, TBD-catalyzed aldol reaction of 6-oxoheptanal produces 2-acetocyclopentanol.

The biochemists you are working for have asked you to research the mechanisms for the reaction. This will help them determine the feasibility of applying it to the synthesis of ivermectin. You have identified two potential mechanistic pathways, shown below in **Proposed Mechanism A** and **Proposed Mechanism B**.



Proposed Mechanism A



Proposed Mechanism B

For each proposed pathway, you have performed computer simulations to determine their energy profiles. The results of your calculations are shown in **Figure 2**, where each reaction coordinate diagram is presented side-by-side

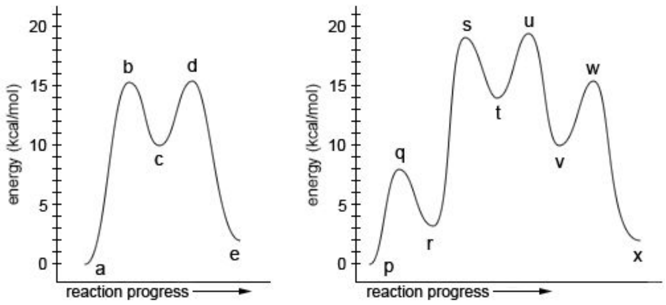


Figure 2. Reaction coordinate diagrams for Mechanism A (left) and Mechanism B (right). Note that claims about reaction times between Mechanism A and B can't be made since the units on the horizontal axes aren't specified.

At the end of the summer, you will write a brief report to summarize your findings, suggest the most likely pathway, and share your part of the project with the rest of the team. You should provide a detailed explanation of the mechanisms for both reaction pathways. Also, your argument for the most likely pathway should be supported by the mechanisms and the reaction coordinate diagrams. The report is directed toward the biochemists and other concerned parties who will use your recommendations to decide the feasibility of applying this reaction to the more complicated synthesis of ivermectin. Therefore, they may not be experts when it concerns mechanisms or organic-specific terms. Use clear and concise language, striking a balance between organic jargon and oversimplified explanations.

Your report should be approximately between 500-700 words (1-2 pages) in length. It should address the following points:

1. Discuss how each mechanism correlates with the corresponding energy diagram.
    a. Summarize the findings.
    b. Specifically, explain how the transition states and intermediates of the mechanisms correspond to features on the diagrams.
    c. Take care to translate which specific step in the mechanism corresponds to which specific feature of the associated reaction coordinate diagram.
2. Identify which reaction pathway *you think* is most likely to occur. You will be evaluated on the explanation of your choice, *not the choice itself*.
3. When discussing mechanisms, be sure to write about the structural features and electronics of the molecules involved. Include descriptions of how the molecules interact in the mechanism and how they change in structure as a result of their interactions.

You can and should include figures of schemes, structures, mechanisms, or reaction coordinate diagrams, if that supports your response. We suggest that you have the figure(s) in front of you—ready to color-code or mark-up in various ways—and that you use your visible thinking to guide your audience through your explanation. Any images that you include in your response, *including the figures in this prompt or those that you draw in ChemDraw or on paper*, must have the original source cited using either ACS or APA format. Given your audience, your written response should suffice so that the explanations can be understood without the figures. **You will be graded only on your written response.**

ARTICLE

Appendix 2 – Coding Scheme

Code	Definition	Exemplar
Assignment features		
Relevant	Students say that the relevance of the prompt is engaging or disengaging. They use language like "relevant" or "real-life example" or alike. Note: personal relevance is not coded here and should be coded as *context interest*.	*"[The context] makes it seem more relevant and worth doing."*
Context interest	Student mentions the context as relevant to their career interests/life or finds the context personally interesting	*"...definitely made it seem more relevant in terms of what I might encounter in the future or just more interesting for now."*
Understands purpose	This code applies to when a student recognizes the importance of WTL as a learning tool	*"Yeah, I understand why [WTL] is there and I think I get that WTL] is important."*
Explaining concepts as a way to learn	Student says that the idea of explaining is a part of their learning process	*"But also, I like organic chemistry, so I enjoyed explaining the concepts to my friends. I had a lot of friend study groups that I would do and I found it pretty effective in my learning to go through it because I don't have to know everything but it's still helpful when I'm teaching others or I'm trying to go through a problem with someone else."*
Role	Students find the role in the prompt engaging. This could be the audience, the format requested, or the role they've been required to play.	*"Well, definitely creating the scenario is engaging."*
Knowledge Acquired		
Chemistry-related knowledge	Student mentions chemical knowledge acquired while completing WTL. This could be knowledge about the mechanism, definition of an analog (WTL 1) or general understanding of the chemical process.	*"And then another thing... oh I learned what racemization was."*
Other knowledge	Learns something from the prompt or doing the assignment unrelated to course content or learning goals. This could include knowledge about the drug's use, the history behind a drug, side effects, etc.	*"I think I learned less. I think about maybe chemistry then about my own thinking process or something like that as I did, because like I said, it was pretty daunting at first."*
Peer Review		
Effort-focused engagement	Student says that the WTL process, usually referring to the PR element, made them put forth effort on the various stages of the assignment, usually referring to the first draft.	*"I felt that [peer review] does bring a level of expectation that you put in a good effort..."*
Reduction in stress/anxiety	Student says that the PR process reduced stress/anxiety they had toward the assignment, or boosts students' confidence	*"...it took a lot of stress off because I was writing..."*
Learning from peer review	Student says they used PR as a way to learn what was correct or compares their response to the responses of their peers.	*"I think this is right, we're going to take a guess," and then people would tell me whether I was right or not, which was very helpful."*
Relying on peer review	This is different from using it as a learning tool. This code should be applied where students say something like "it didn't matter if I was right because my PR would correct me."	*"I don't know if you didn't include this because of time or if you don't know what it is, but here's a brief explanation about it." And I was like, "Cool, that's good." Because personally I tried to write everything about the m-write in the draft because I figured if I worried about it at least and it's wrong, then someone can correct me as opposed to me not writing it at all."*
Affect		

Positive affect towards WTL	Student shows a positive affect towards WTL	*"Yeah, definitely. The Wittig one I thought was much easier...And then also I've gotten experience with the 700 words of chemistry or 216 and what the expectations are. So I feel like it got easier as the semester went on for sure."*
Negative affect towards WTL	Student's opinions towards WTL are negative.	*"I feel like that one I was the most disconnected with to be honest, because I didn't totally understand it still even when I submitted my final, I wasn't positive that my mechanism was even correct."*
Other		
Writing fellow	Student discusses visiting the writing fellows for help on the assignment	*"And then from there, in that first time, the thalidomide, I went to the writing fellows and I checked over the acid and the base mechanism to see which is right, and then I found they were both right."*

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