JOURNAL OF CHEMICAL EDUCATION

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# Chemical Information Literacy: p$K_a$ Values—Where Do Students Go Wrong?

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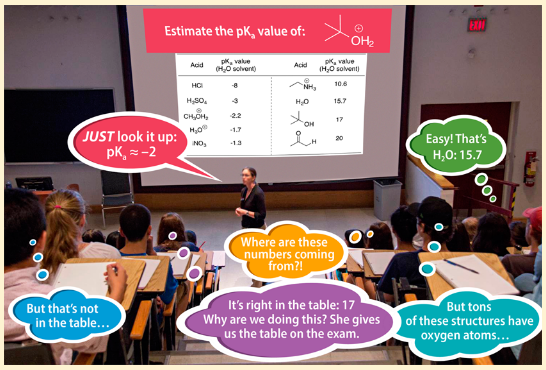
Ⓢ *Supporting Information*

**ABSTRACT:** Chemical information literacy is an essential skillset for navigating, evaluating, and using the wealth of print and online information. Accordingly, efforts are underway to improve students' acquisition and mastery of this skillset. However, less is known about students' abilities related to finding and using chemical information to solve problems. We studied students' abilities in one area of chemical information literacy: finding, estimating, and using p$K_a$ values in organic acid−base problems. We identified areas of student difficulty related to these skills, implemented instruction aligned with desired learning outcomes, and then studied students' success rates after instruction. Our results revealed improvements in some areas but not in others. In particular, students still struggled when the desired information was not directly available in the literature (i.e., data had to be estimated) or when students had to use the information in more complex contexts.



**KEYWORDS:** *First-Year Undergraduate, Second-Year Undergraduate, Organic Chemistry, Humor/Puzzles/Games, Distance Learning/Self Instruction, Acids/Bases, Chemical Education Research*

**FEATURE:** Chemical Education Research

## ■ INTRODUCTION

Information literacy is an essential 21st century skill.[1,2] The Association of College and Research Libraries (ACRL) has defined a set of competency standards for information literacy in higher education[3] with a related set specific to Science and Engineering/Technology,[4] and an updated framework in 2015.[5] According to the higher education standards,[3] the information literate student:

1. Determines the nature and extent of the information needed
2. Accesses needed information effectively and efficiently
3. Evaluates information and its sources critically and incorporates selected information into his or her knowledge base and value system
4. Uses information effectively to accomplish a specific purpose
5. Understands many of the economic, legal, and social issues surrounding the use of information and accesses and uses information ethically and legally

One example of chemical information skills specifically related to organic chemistry is being able to find and estimate p$K_a$ values.[6] These experimentally determined values quantify the strengths of acids on a practically useful logarithmic scale: the lower the p$K_a$ value, the stronger the acid.[7] Most often (99% of the time), an organic chemist or biochemist needs an estimate of the p$K_a$ value, rather than the exact value. As such, professional chemists use p$K_a$ tables assembled from experimental data (i.e., from the primary literature); the Bordwell[8] and Evans'[9] tables are the sources most often used by the organic chemistry community. In the cases when very specific p$K_a$ data are required, other sources may be used, including the CRC Handbook of Chemistry and Physics,[10] Reaxys,[11] ChemIDPlus,[12] SciFinder,[13] and more,[14−16] although such sources are typically more useful for finding experimental procedures or spectroscopic or other types of data.

These p$K_a$ values can be used in many ways, including identifying the most acidic proton or most basic atom, determining the direction of an acid−base equilibrium, and determining the predominant species at a given pH.[6] Acid−base chemistry is also integral to most reactions later in organic chemistry[17] and biochemistry.[18] To solve many acid−base problems, one must determine when to use p$K_a$ values (ACRL Standard 1), access them efficiently (ACRL Standard 2, ACS skill 1[2]), evaluate the information (ACRL Standard 3), and use them appropriately (ACRL Standard 4).

As students worked toward acid−base learning outcomes (LOs),[6] we realized that they had difficulty finding or estimating p$K_a$ values; that is, they struggled with this type of information literacy. Many students asked when it was necessary or appropriate to find p$K_a$ values (Standard 1[3]). Other students asked how to find "simple" p$K_a$ values, such as that of an alcohol or carboxylic acid (Standard 2[3]). Still others

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DOI: 10.1021/acs.jchemed.5b00420

used values from unreliable sources (Standard 3[3]) or used the values incorrectly (Standard 4[3]).

Students' difficulties became apparent in class—via the classroom response system[19]—for example, when they estimated $\mathrm{p}K_a$ values of carbonic acid and diisopropyl amine in Organic Chemistry I and II courses, respectively (Figure 1).

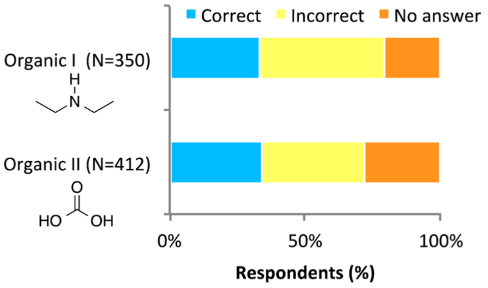

**Figure 1.** Low scores on "Estimate the $\mathrm{p}K_a$ value" questions demonstrate barriers to chemical information literacy. Accepted $\mathrm{p}K_a$ ranges were 36−40 for the amine (Organic I) and 4−7 for the carbonic acid (Organic II).

The low percentage of correct answers (33% in each group) suggested a barrier to chemical information literacy. This difficulty is consistent with our previous work that revealed that students were not proficient at finding desired information even when they had direct access to it, such as in a summary of reactions or a textbook.[20] Efficiently locating chemical and physical properties of substances is the first of the American Chemical Society's key chemical information skills.[2]

A number of reports have described teaching methods, resources, and courses to develop students' information literacy skills.[21−29] Some also describe assessment strategies to monitor students' progression toward the desired learning outcomes, including using pre/post tests and web-based assessments.[30,31] Typically, these assessments target students' ability to find information and evaluate the quality of the sources.[32] However, to our knowledge, none have studied the type of data that students find using information literacy skills and to what extent they successfully incorporate that data into conceptual chemistry problems.

Given the indications of student difficulties and the importance of developing chemical information skills, we sought to quantify the extent and nature of students' difficulties, develop associated learning activities, and analyze the impact on student success that followed. Our research questions (RQs), which related to specific competency standards for information literacy, were:

1. How prevalent were students' errors and what types of errors were made related to:
   a. Finding or estimating the correct $\mathrm{p}K_a$ values? (Standard 2[3])
   b. Using $\mathrm{p}K_a$ values when appropriate? (Standard 1[3])
   c. Applying $\mathrm{p}K_a$ values correctly in the solution to a problem? (Standard 4[3])
2. What was the effect on students' skills after explicit instruction on finding or estimating $\mathrm{p}K_a$ values and introducing online $\mathrm{p}K_a$ games?

We studied students' skills on only some information literacy skills (i.e., from Standards 1, 2, and 4) to isolate areas of student difficulties. For example, we did not analyze students' ability to select sources of information; the data (i.e., $\mathrm{p}K_a$ values) were provided in a table. This was done to allow us to target instruction in areas of student difficulty identified in the study, to scaffold (or break down) instruction into manageable components.

## METHODOLOGY

### Course and Setting

Students were enrolled either in a first (Organic I) or second (Organic II) semester of a four-semester organic chemistry course sequence. Organic I is taught in the winter semester, and Organic II is taught in the summer and fall semesters. The courses were taught in an active lecture format in 2011−2012 and a flipped course format[33] from 2013 onward. A standard organic curriculum[34] was used in 2011, and a new organic curriculum was introduced in 2012.[17] Students answered in-class questions on paper or using Top Hat,[19] a classroom response system (CRS). Assessments included weekly preclass tests and assignments,[35] two midterms, and a final exam. This research was conducted at a large, Ph.D. granting institution in Ontario, Canada.

Prior to the fall of 2014, students were taught to use $\mathrm{p}K_a$ values to solve organic chemistry problems but were not explicitly taught how to find or estimate $\mathrm{p}K_a$ values (Figure 2). In the fall 2014 semester (Organic II), instruction (in-class and video) explicitly included how to find $\mathrm{p}K_a$ values from a standard textbook,[34] professionally created tables,[9] or other sources.[10] We also provided an optional problem set and answers (separately).

In the winter 2015 semester (Organic I), the same explicit instruction was provided, and four $\mathrm{p}K_a$ games were also created and delivered through the courses' learning management system, Blackboard Learn.[36] Games might have a positive impact on student engagement and learning, although the evidence for their impact on student achievement is not well-

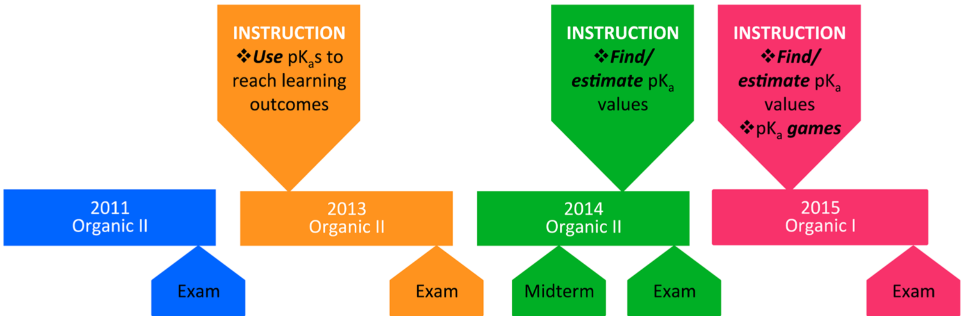

**Figure 2.** Timeline of instructional interventions and assessments.

DOI: 10.1021/acs.jchemed.5b00420
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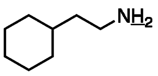
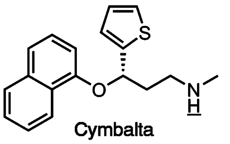
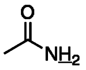
established.[37−40] The p$K_a$ games were created to encourage and scaffold student learning of this information literacy skill: finding or estimating p$K_a$ values. In the games, students were presented with organic structures and a p$K_a$ table (the games and table are available in the Supporting Information). The games had a gradient of difficulty: Level 1 (29 questions) had the exact structures as in the p$K_a$ table;[34] Level 2 (29 questions) had small organic molecules with functional groups that were present in the p$K_a$ table, but were not exact matches; Level 3 had complex structures that had functional groups represented in the p$K_a$ table; Level 4 had functional groups that were not in the table but that could be estimated using chemical principles learned in the course (examples in Box 1). Students had 10 min to complete each level by clicking on the p$K_a$ value of each compound. The games were worth a 1% bonus on students' final grades.

**Box 1. Examples of questions at each level of the p$K_a$ games. Question statement: Find or estimate the p$K_a$ value for the indicated proton in each compound.**

| Level 1 | Level 2 | Level 3 | Level 4 |
|---|---|---|---|
| $NH_3$ |  | <br>Cymbalta (Duloxetine)<br>Serotonin-norephedrine reuptake inhibitor |  |

## DATA SOURCES

Data sources included students' answers to questions in class via the CRS (Figure 1), on midterms, and on final exams. In some questions, students were directly asked to find or estimate the p$K_a$ value of specific protons; in other questions, it was necessary to find or estimate a p$K_a$ value to answer a larger question. For the purpose of this study, these larger questions included identifying a suitable base to quantitatively deprotonate a given acid (and justifying the answer) and drawing the predominant species of a given compound at a specific pH. The students were seeing all the questions for the first time; no questions were repeated with the same population. The university's Institutional Research Board approved this study.

## RESULTS AND DISCUSSION

### Before Instruction

The indications of students' difficulties (Figure 1) were confirmed with a summative midterm evaluation. Scores were low (55% average) on a question that *directly* asked students to estimate p$K_a$ values (Figure 3). Students had not received explicit instruction on the topic of finding or estimating p$K_a$ values at this point, although they had been taught to use these values in more complex questions. No correlation existed between students' ability to give the correct p$K_a$ value and their grade on the midterm ($R^2$ = 0.12), which indicates that all student types can struggle with this type of information literacy (ACRL Standard 2, RQ1a).

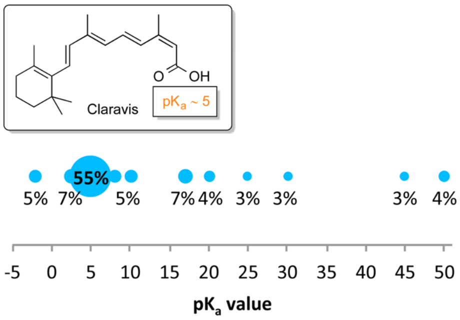
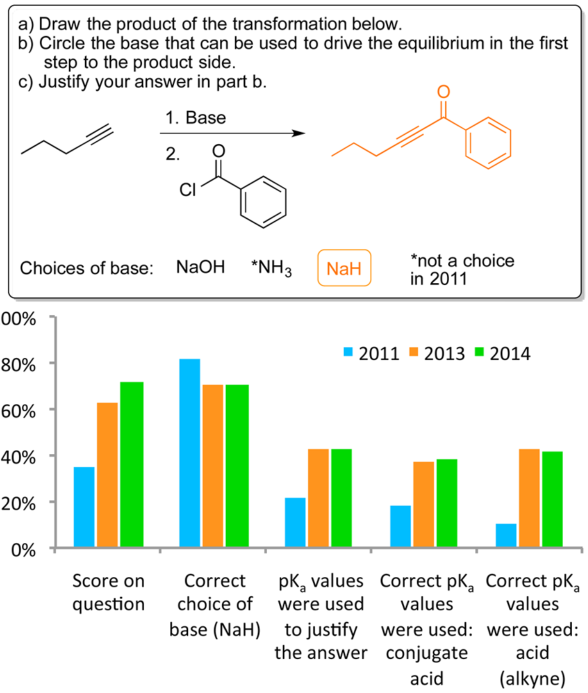


Figure 3. Distribution of answers on a question that *directly* required estimating the p$K_a$ value of a carboxylic acid (in Claravis) *before* instruction. Course: Organic II, midterm 2, 2014 ($N$ = 129). Correct answer in orange.

Many questions *indirectly* required the use of p$K_a$ values but did not explicitly ask students to find or cite p$K_a$ values (ACRL Standards 1, 2, and 4). For example, students in Organic II were asked to identify a base that could quantitatively deprotonate an alkyne and justify their answer (Figure 4).



a) Draw the product of the transformation below.
b) Circle the base that can be used to drive the equilibrium in the first step to the product side.
c) Justify your answer in part b.

Choices of base: NaOH *$NH_3$ NaH

*not a choice in 2011

Figure 4. Question that *indirectly* required finding or estimating p$K_a$ values. Answers in orange. Course: Organic II, final exam ($N$ = 386).

The average score on this question was only 36% in 2011 even though 82% of students correctly identified NaH as being a sufficiently strong base to deprotonate the alkyne. In their explanation, only 22% of students stated p$K_a$ values (or analogous chemical principles); only 11% used these values or principles correctly in their explanation. The scores increased after deliberate instruction in how to use p$K_a$ values to solve such a problem (Figure 2), although less than half of students used p$K_a$ values in their justification.

In another question type, students were asked to predict the predominant form of a compound at a given pH. In the 2011 version, the compound was phosphoric acid in a solution at pH 7.4 and the four answer choices were provided (Figure 5). Only 24% of students gave the correct answer, $HPO_4^{2-}$.

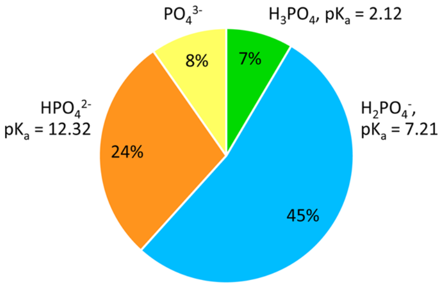


**Figure 5.** Question that *indirectly* required finding or estimating p$K_a$ values—before instruction: What is the predominant form of phosphoric acid, $H_3PO_4$, at pH 7.4 (i.e., the pH of blood)? p$K_a$ values were provided. Answer in orange. Course: Organic II, final exam, 2011 ($N$ = 386).

The low scores on the direct and indirect p$K_a$ questions signaled a need for explicit instruction in this specific type of information literacy. As of 2013, acid–base learning outcomes were developed and explicitly communicated to students;[6] however, students were not explicitly taught to find p$K_a$ values at that point. In 2014 and 2015, additional instructional supports were introduced, including (i) a video to explain how to find various p$K_a$ values in the table, (ii) videos that explained how to use p$K_a$ values to solve more complex problems, (iii) a problem set—with answers provided separately—for students to practice, and (iv) in 2015, p$K_a$ games.

The average scores on these games were fairly high—over 85%—except for the final level, which had an average score of 62% (median score 83%) (Figure 6). In the fourth level, p$K_a$ values had to be identified for functional groups that were not in the p$K_a$ table provided (Box 1).[34] Students could look up the values using another resource or could estimate the values based on the chemical principles learned in the course. This added level of difficulty is reflected in the lower average scores for that question.

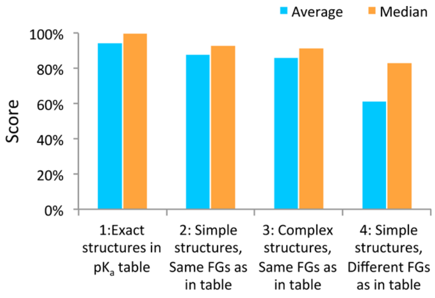


**Figure 6.** Average and median scores on p$K_a$ games for students who completed all four. Course: Organic I, 2015 ($N$ = 137).

## After Instruction: Direct Questions

After the explicit instruction on finding and using p$K_a$ values, students' answers were analyzed on related exam questions. In Organic II (2014), students were *directly* asked to estimate the p$K_a$ values of the hydrogen atoms on common functional groups. The scores were higher than before instruction, but still surprisingly low (Figure 7). In particular, students still seemed to be confusing the p$K_a$ values of phenols (p$K_a$ ≈ 10) and alcohols (p$K_a$ ≈ 16), and the various forms of nitrogen-based functional groups (e.g., amine, p$K_a$ ≈ 38 and ammonium, p$K_a$ ≈ 10).

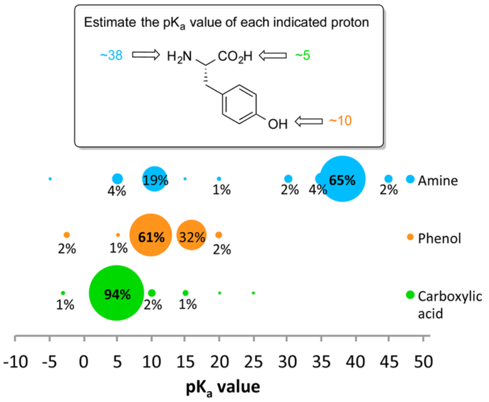


**Figure 7.** Distribution of answers on questions that *directly* required finding or estimating p$K_a$ values, after instruction. Course: Organic II, final exam, 2014 ($N$ = 391).

An inability to interpret or translate between types of chemical symbols is likely a major reason for the incorrect p$K_a$ values given for compounds that are directly listed in the p$K_a$ table. For example, phenol was represented as the condensed formula ($C_6H_5OH$) in the p$K_a$ table available on the exam[34] but as the line structure in the question. Other studies have emphasized students' difficulties related to chemical symbolism and interconverting between symbolic forms.[41,42]

Students also seemed to struggle to identify functional groups. Students might not have realized the effect of the positive charge on the ammonium in the p$K_a$ table and "saw" only the nitrogen atom. Students frequently see "complex" functional groups as being constituted of their individual and independent parts (e.g., seeing carboxylic acid as a ketone and an alcohol). Students do not realize the effect of those "combined" functional groups on their emergent properties,[43−45] which could be the cause of 32% of students identifying the phenol as having the p$K_a$ value of an aliphatic alcohol.

Students in Organic I answered direct p$K_a$ questions after receiving the explicit instruction and completing the p$K_a$ games (Figure 8). The scores were high for identifying the p$K_a$ value of the common alcohol functional group, as had been the case

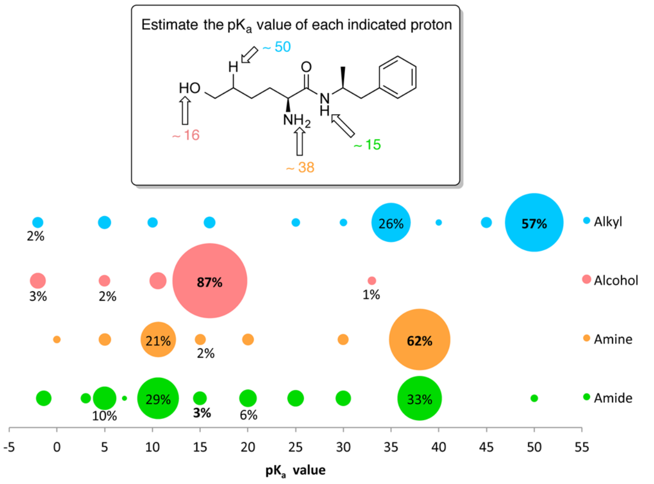


**Figure 8.** Distribution of responses on questions that *directly* required finding or estimating p$K_a$ values, after p$K_a$ games. Course: Organic I, final exam, 2015 ($N$ = 344).

DOI: 10.1021/acs.jchemed.5b00420
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for the carboxylic acid question in Organic II (Figure 7). Still, there were low scores for other common functional groups. Students' errors still seem related to difficulties mentioned earlier: (i) interpreting chemical symbols (amine/ammonium, 62% correct; not significantly different from the Organic II group); (ii) recognizing functional groups (26% of students gave the $pK_a$ of $H_2$—35—for that of the alkyl proton, and only 57% of students provided the correct answer); or (iii) estimating $pK_a$ values.

The $pK_a$ value of an amide was not listed in the $pK_a$ table provided on the exam. To estimate such values, students had to consider the factors that affect acidity and basicity (e.g., electronegativity, resonance)[6] and relate those factors to functional groups whose $pK_a$ values were listed in the table. For the amide example, one had to predict that the amide's $pK_a$ value would be less than that of a C−H $\alpha$ proton ($pK_a \sim 20$) and greater than that of a carboxylic acid ($pK_a \sim 5$). The low success rates on Level 4 of the $pK_a$ game (61%) and on the exam question in which students were asked to identify the $pK_a$ value of an amide (3% correct, 30% of answers in an acceptable range: 5−20) provided strong evidence of students' difficulties making use of information (ACRL Standard 4). The exact answer will frequently not be available in the literature, and one has to critically analyze the available data to make a best estimate. While not the first time such an issue has been described—that students do not link symbols, data, and meaning (chemical principles)[17,44] —this result highlights a significant concern in terms of science information literacy.

### After Instruction: Indirect Questions

After instruction, students' difficulties estimating $pK_a$ values still affected their ability to solve more complex, *indirect* $pK_a$ problems. The question in which students identified the appropriate base to quantitatively deprotonate an alkyne (Figure 4) was more successfully answered after instruction (63% in 2013 and 72% in 2014) than before instruction (36% in 2011); all improvements are statistically significant ($p < 0.001$). Twice as many students used $pK_a$ values in their answers in 2013 and 2014 (~43%), compared to 2011 (22%). Of the students who used $pK_a$ values in their answers, the majority in all groups described the meaning of the conjugate acid's $pK_a$ value correctly, but few in the preinstruction group (11%) incorporated the $pK_a$ of the alkyne in their response. The majority of organic and biochemical reactions involve acid−base steps, and the difficulty demonstrated here signals a major barrier to learning more complex reactions.

In another *indirect* $pK_a$ question, students were asked to draw the predominant form of alanine (2013) and tyrosine (2014) at pH 7.4 (Figure 9). The average scores improved significantly ($p < 0.001$) between 2013 and 2014, going from 6% to 24% correct for identifying the ammonium and from 24% to 64% correct for identifying the carboxylate as the major forms at pH 7.4. The major difference in instruction for this problem type was related to finding the appropriate $pK_a$ values and using them in problems. Still, there remained very low scores for questions that involved identifying the predominant form of an amine (highest average score: 24%). This amine/ammonium confusion could be symbol-related as described above or caused by another reason. For example, students might not have realized that compounds can bear two charges. Given the importance of the various forms of functional groups in chemical and biochemical contexts, carboxylic acid and phenol scores (64% and 71%, respectively) also signal a barrier to further learning.

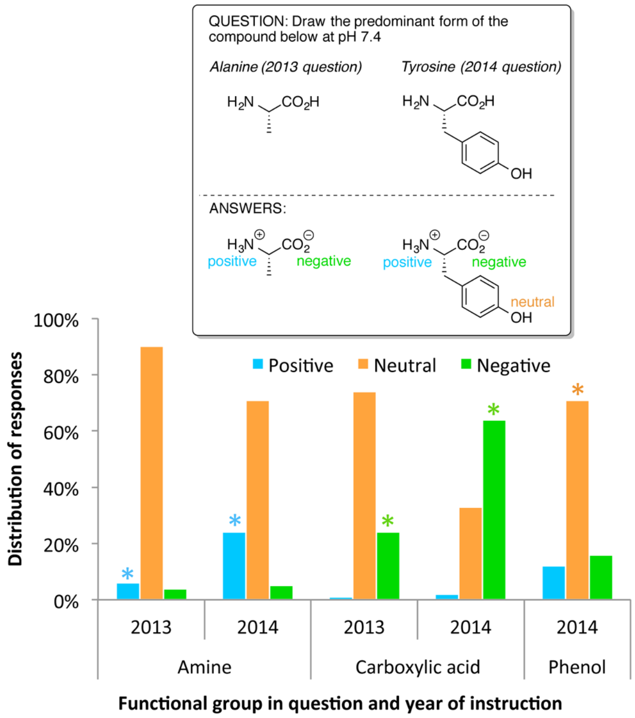

**Figure 9.** Distribution of students' responses when asked to draw the predominant form of tyrosine at pH 7.4, *indirectly* requiring use of $pK_a$ values. Course: Organic II, final exams, 2013 (before instruction) and 2014 (after instruction) ($N$ = 318 and 391). Correct answers are indicated with an asterisk (*).

Little correlation ($R^2 < 0.15$) existed between students' ability on direct and indirect $pK_a$ questions and their grade on the examination, which indicates that all student types can struggle with this type of information literacy (ACRL Standard 2, RQ1a).

## ■ CONCLUSIONS AND IMPLICATIONS FOR TEACHING AND LEARNING

Herein, we described the specific difficulties that students in the first two semesters of organic chemistry demonstrated with science information literacy: finding and estimating $pK_a$ values. Those difficulties permeated other problem types that involved using $pK_a$ values, such as identifying the predominant species at a given pH, determining the direction of an acid−base equilibrium, or selecting an appropriate acid or base to create a specific reagent (e.g., to generate an acetylide nucleophile from an alkyne). Other problem types that require using $pK_a$ values are part of the Organic I and II courses, including determining the direction of an equilibrium or determining the $pK_a$ value of a species' conjugate acid. Although those question types were not part of this study, analogous difficulties related to chemical information literacy are probable.

To help students gain science information literacy skills specifically related to $pK_a$ values, we (i) communicated the learning outcomes in the courses,[6] (ii) gave explicit instruction on finding $pK_a$ values in class and using videos (that we created), (iii) designed associated learning opportunities using problem sets and online $pK_a$ games, and (iv) gave assessments that directly probed students' knowledge and abilities and were aligned with the intended learning outcomes. The scores on exams following this instruction and learning opportunities were significantly higher than before explicit instruction, although difficulties remained. Students should be taught both to interpret and use p$K_a$ values,[7] *and* how to find and estimate them.

Students' improvements make sense from a learning theory perspective, such as the Interactive Compensatory Model of Learning.[46,47] For example, the students were extrinsically motivated with bonus marks for completing the p$K_a$ games and summative assessments (midterms and exams). They had opportunities for deliberate, scaffolded practice and immediate feedback through in-class activities and p$K_a$ games (and eventual feedback after exams). Gaining a fluency in finding and estimating p$K_a$ values likely also decreased students' cognitive load during class in related problems. Teaching through videos that explained worked examples can increase students' prior knowledge before they came to class, thereby allowing for more new learning.

Because we studied students' skills on only some information literacy skills (i.e., from Standards 1, 2, and 4), we isolated areas of student difficulties. If students had to select sources of information *and* find or estimate p$K_a$ values, we might not have discovered that students struggle *even when* the data source is provided. As a result, we could scaffold—or break down—instruction into smaller components. Future instruction will further teach students to (i) select sources of information; (ii) navigate between the macroscopic, submicroscopic, and symbolic levels to connect p$K_a$ values, structural drawings (symbols), and chemical meaning;[41,42,48] and (iii) estimate quantities or predict results when the exact information is not available. Information literacy will help students navigate and make critical use of the vast pool of available data.

## ■ ASSOCIATED CONTENT

### Ⓢ Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.5b00420.

p$K_a$ table (PDF, DOCX)
p$K_a$ game (PDF, DOCX)
p$K_a$ game answers (PDF, DOCX)

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### Notes

The authors declare no competing financial interest.

## ■ ACKNOWLEDGMENTS

We sincerely thank Gisèle Richard for graphic design assistance.

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