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Using Structure-Based Organic Chemistry Online Tutorials with Automated Correction for Student Practice and Review

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Ⓢ *Supporting Information*

ABSTRACT: This article describes the development and implementation of an open-access organic chemistry question bank for online tutorials and assessments at University College Cork and Dublin Institute of Technology. SOCOT (structure-based organic chemistry online tutorials) may be used to supplement traditional small-group tutorials, thereby allowing students to develop essential problem-solving skills in organic chemistry. This online approach may be used for both formative and summative assessment. Students complete one problem set weekly or fortnightly, which consists of a number of questions of varying difficulty. A wide range of question types is possible; for example, prediction of reaction products, identification of reaction intermediates or reagents, and retrosynthetic analyses. Questions involving stereochemistry may be also be incorporated. The implementation is described, along with several sample questions and advice for creating questions. This approach is suitable for all levels of undergraduates, from introductory nonmajors to final-year chemistry students. Student feedback was overwhelmingly positive, and in particular, students found SOCOT to be a quite useful tool for review purposes. Our approach uses MarvinSketch, which is free for academic purposes, and the SMILES algorithm, which converts chemical structures into a text string and is compatible with any learning management system.

KEYWORDS: *First-Year Undergraduate/General, Upper-Division Undergraduate, Organic Chemistry, Internet/Web-Based Learning, Reactions, Synthesis, Mechanisms of Reactions*

■ INTRODUCTION: THE CASE FOR ONLINE ORGANIC CHEMISTRY TUTORIALS

The use of technology in the teaching and assessment of undergraduate chemistry has been widely reported. Common examples include online quizzes, prelecture resources, post-lecture resources, preparative work for laboratory practicals and laboratory feedback.[1−4] A web-based approach to assessment in organic chemistry has a number of benefits including considerable time and labor savings, scalability to larger classes, and importantly provides regular problem-solving practice to students coupled with automatic feedback which may be used for both summative and formative assessment.[5] It has been previously asserted that there is a correlation between the completion of assigned homework problems and student success.[6,7] It has also been found that students view quizzes as valuable learning tools.[8]

One major limitation exists for the organic chemistry subdiscipline where the drawing of chemical structures and interpretation of mechanisms is a key skill.[9−11] Traditionally, this skill has often been developed by the use of problem sheets which are submitted and assessed by a tutor or instructor and feedback is given at a later date in small group tutorials. More recently, clickers have been used as a method of assessing student understanding of mechanisms.[12] We wished to develop an approach which more closely mimics the traditional tutorials and offers students the opportunity to work through questions on their own time and later receive feedback. Commercial e-learning packages for chemistry offer many benefits, including the ability to draw structures. Our own experience with these packages, coupled with student feedback, points to a number of distinct drawbacks, including the following:

- An additional access cost which must be borne either by the institution or the student.
- The breadth of material available which may not include relevant examples for nonchemistry major students, e.g., pharmacy or food science students.
- The difference in emphasis on particular topics which may not be suitable for a particular course.
- The level of difficulty may not match course requirements.

We, therefore, sought to develop an online resource which would allow students to draw chemical structures within a standard learning management system (LMS) such as Blackboard or Moodle. The other requirement of this project was that the questions would be made available on the Internet via an open-access question bank. Problems could be selected by the instructor who would have total control over the breadth, difficulty and emphasis of the individual assignments. Structure-based Organic Chemistry Online Tutorials (SOCOT) is our attempt to mimic the traditional tutorial using an online approach while maintaining flexibility and controlling costs.

■ DEVELOPMENT OF SOCOT

We initially designed a system which integrates with commonly used LMS systems such as the commercial product "Blackboard" or open source "Moodle". As many institutions already have such LMS systems in place on a campus-wide level, an approach which builds upon an existing LMS could be implemented at little or no additional cost to the instructor or students. While these packages have an inbuilt assessment system, they obviously are not chemically aware and do not support the drawing or checking of chemical structures.

SMILES (Simplified Molecular Input Line Entry Specification) is an algorithm for converting chemical structures unambiguously to ASCII strings which are machine readable.[13] Accordingly, a LMS system, in conjunction with a software module which allows students to draw structures and generate the corresponding SMILES string, provides an inexpensive alternative to commercial packages.

MarvinSketch is an advanced chemical editor for drawing chemical structures, queries and reactions.[14] It can generate SMILES strings for a given structure or reaction intermediate. The package is free to use for academic purposes. Importantly, MarvinSketch, which is written in Java, is cross-platform compatible and can be delivered over the web. A student may use MarvinSketch on a Windows or Apple computer from anywhere that has an Internet connection, and is not restricted to a specific PC laboratory. Browser incompatibilities have not been reported by our students over the course of this project.

Implementation

Implementation is straightforward, with the lecturer drawing the problem in MarvinSketch or in another molecular drawing package such as Chemdraw. The scheme is saved directly or screen captured to a graphics files. In Blackboard or Moodle, a "fill in the blank" type question is selected and the appropriate instructions added (e.g., "Draw the product of the following reaction in MarvinSketch and copy the SMILES string to the box below"). The graphics file is then uploaded to the LMS and is displayed as part of the question. The SMILES string for the correct structure is generated using MarvinSketch and pasted into the LMS as the correct answer. Additional feedback may also be included for an incorrect answer, such as the correct structure, incorporated as a graphics file.

The MarvinSketch applet may be hosted on a Web server or for convenience, the applet can also be uploaded directly to the LMS system. In the case of Blackboard, the set of files is uploaded as a single zip archive, from which the URL which loads the applet can then be obtained. This URL may be used for all subsequent assignments. A step-by-step guide on how to incorporate questions of your own design into Blackboard is provided in the Supporting Information.

On successful completion of the above, students will be presented with a set of problems and a hyperlink to the MarvinSketch applet. Clicking the link will open the applet in a new browser window, where the structure can be drawn and the SMILES string generated. Alternatively, students may download the MarvinSketch software and install the application on their own personal computer. Copying and pasting of the SMILES string allows the answer to be submitted to the LMS and the student can then proceed to the next question.

In a typical example, the student is asked the identify the product of the reaction of 1-methylcyclohexene with hydrochloric acid; this question not only checks the student's ability to identify a chloroalkane as the product, but also tests their ability to apply Markovnikoff's rule. On drawing the product in MarvinSketch, the correct SMILES string (CC1(Cl)CCCCC1) is generated (Figure 1). This string is then submitted to the LMS which checks the student's answer against that predefined by the instructor and awards a mark if both match. In those cases where there may be multiple solutions to the same question, the instructor can configure the LMS to accept multiple answers.

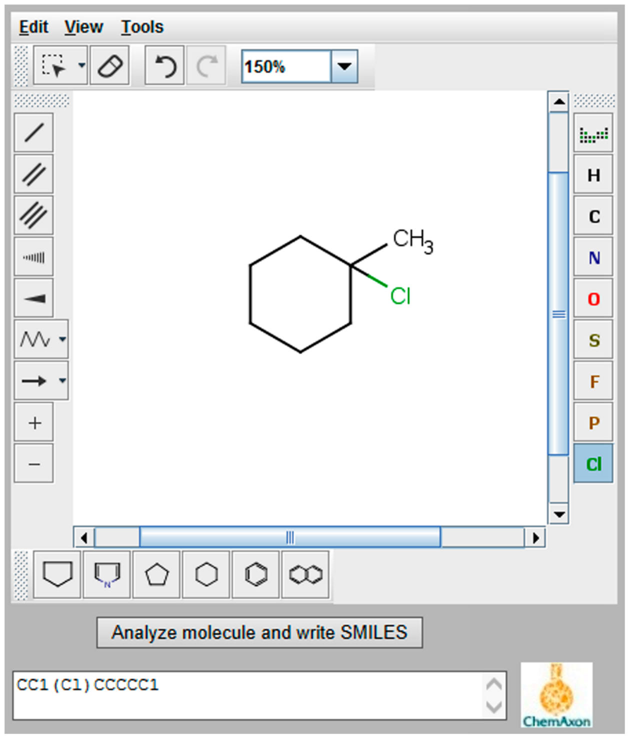

Figure 1. Screenshot of the MarvinSketch interface in Internet Explorer. The student draws the structure and clicks the button to generate the SMILES string in the lower panel, which is then copied and pasted into the LMS.

Following the deadline for each assignment, a percentage grade was automatically returned to each student. In addition, feedback was provided for any incorrectly answered problem in the form of a full solution. Feedback may be as detailed as the instructor requires but would generally include a full solution to the question, along with a brief description of the reaction mechanism, e.g., the alkene is unsymmetrical, so HCl adds in a Markovnikoff fashion under ionic conditions, i.e., H to the less substituted carbon and Cl to the more substituted carbon.

Problem Styles

Introductory Level: For each assignment, a group of 70, first year BPharm students were presented with 12 problems. Typically, the problem set was divided into two groups with the first six questions aimed at beginners or intermediate level, while the final six were more challenging and more deeply probed the student's understanding. Each subset of six questions was presented to students in random order and backtracking was disabled so as to minimize the possibility of plagiarism. In the most common style of problem, the student is presented with both the starting material and reagents and is then required to draw the product (Figure 2).

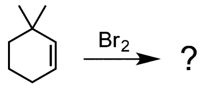

Figure 2. This question requires the student to draw the product of a bromination reaction and to show the correct relative stereochemistry.

A more difficult variation on this problem type requires the student to identify the major product of a reaction, e.g., what is the major product of the dehydration of an unsymmetrical alcohol? Alternatively, a series of reactions may be presented and the students must work their way through the synthetic scheme and identify the final product (Figure 3). This style of question is considerably more challenging, requiring students to work through each of the reactions in turn, before finally submitting their proposed structure for the final product. The feedback provided for this multistep sequence includes the structures of each of the intermediates along with a description of what is occurring in each of the steps.

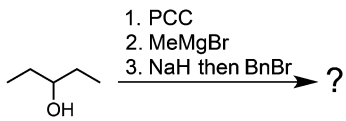

Figure 3. In this more challenging question, the student is asked to identify the compound which results from a sequence of three reactions.

Problems involving "curved arrow" mechanisms are not easily implemented on a computer-based system. As an alternative, we ask students to interpret "curved arrow" mechanisms and to draw the resulting reaction intermediates (Figure 4). We have previously found that some students tend to rote learn mechanisms without necessarily understanding the chemical meaning of the arrows. Therefore, problems which require students to figure out which bonds are being broken and where charges should be distributed are of some considerable benefit.

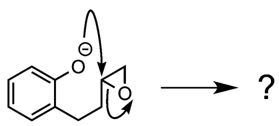

Figure 4. Here the student must interpret the "curved arrow" mechanism and draw the resulting anionic intermediate.

Questions may also be adapted for nonchemistry majors, e.g., the incorporation of questions on active pharmaceutical ingredients (APIs) for pharmacy students (Figure 5). Equally, feedback may be tailored for a particular audience, e.g., the inclusion of the generic name, trade name and biological activity of a drug compound which are of particular interest to pharmacy students.

Advanced Undergraduate Level

For each assignment, 8 fourth year undergraduate students studying medicinal chemistry were presented with three advanced problems based on material covered in the previous lecture. Two problem styles were utilized, which either involved the student predicting the missing product from the reaction scheme, or a retrosynthetic analysis requiring the student to identify the starting material used in the preparation of a given product (Figure 6).

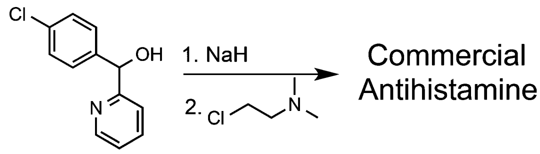

Figure 5. Pharmacy students are required to identify the product of an alkylation reaction, which also happens to be a commercially available antihistamine.

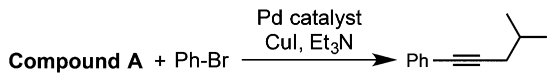

Figure 6. In this example, the student must perform a retrosynthetic analysis and identify the correct starting material.

Points To Note

As with any electronic system which lacks chemical intuition, any possible ambiguity should be avoided in questions. Occasionally, there may exist multiple solutions to a single question, e.g., several different resonance structures for the same intermediate. The instructor should always check whether the SMILES strings generated are identical or not. For example, in answer to the question in Figure 2, the correct relative stereochemistry may be represented by either (2*R*,3*R*)-2,3-dibromo-1,1-dimethylcyclohexane (SMILES = CC1(C)CCC[C@@H](Br)[C@@H]1Br) or (2*S*,3*S*)-2,3-dibromo-1,1-dimethylcyclohexane (SMILES = CC1(C)CCC[C@H](Br)[C@H]1Br). In these cases, the instructor should allow for multiple correct answers to be accepted by the LMS. More generally, instructors need to be aware of the different SMILES strings generated when hydrogen atoms are explicitly added to a structure. For the most part, hydrogen atoms are ignored when generating SMILES strings, unless they have been deliberately added. For example, the typical SMILES string for *Z*-2-butene corresponds to C\C=C/C (Figure 7). When the hydrogen atoms are explicitly added to the alkene bond, a different SMILES string is generated, i.e., [H]\C(C)=C(/[H])C. Such pitfalls can be readily avoided once the instructor preconfigures MarvinSketch to ignore explicit hydrogens when generating SMILES strings.

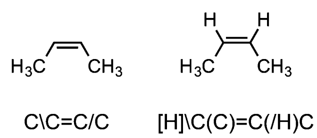

Figure 7. Comparison of SMILES for *Z*-2-butene with implicit and explicit hydrogens.

■ EVALUATION: STUDENT FEEDBACK

Having completed several assignments over the course of an academic year, 70 first year pharmacy students were surveyed on their experience with MarvinSketch to which 51 students (73%) of the class responded. Overall, the feedback from the students was extremely positive. Of the total number, 93%

either agreed or strongly agreed that it was a “beneficial learning experience”. The remaining 7% were neutral. Additionally, 84% agreed that the above approach was “a useful revision tool”, while 4% disagreed and 7% were neutral. Comments included “it gets you to review and revise notes regularly”, “it’s great for revision, helped to understand mechanisms” and “it gives you opportunity to figure out gaps in learning and work on them”. Note that use of “revision” by Irish or British students is equivalent to “review” in an American context.

Eight students from a medicinal chemistry (Year 4) undergraduate program completed assignments as part of a second semester “Advanced Synthesis for Drug Discovery” module. As with the first year students, the feedback from this cohort was also very positive. All students responded to the survey. A significant number (75%) of students found the online tutorials to be beneficial to their learning. Eighty percent of students felt they had a better understanding of their lecture notes having completed the assignments. The most telling statistic was that all students believed that online assignments during their previous three years as undergraduates would have enhanced their learning and understanding of organic chemistry. Comments included “great for revision”, “it’s useful to access the questions again for revision”, “great to be able to access the assignments from home” and “easy to figure out what you don’t know”.

■ CONCLUSIONS

Problem solving is a key skill of the organic chemist and has traditionally been developed through weekly small-group tutorial sessions. With increasing student numbers and diminishing resources, this approach may no longer be always feasible. Thus, we have attempted to mimic the traditional tutorial with an online assignment approach. Our approach has been tested with a first year group of BPharm students as well as a fourth year group of chemistry majors and feedback has been extremely positive. Future work will involve extending the problem sets to include second and third year chemistry majors and evaluating their grades in organic chemistry over the next 3 years. We also intend to enhance the feedback option, which would be capable of prompting the student or pointing out common mistakes.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information

A full, step-by-step guide on how to incorporate questions of your own design into Blackboard is provided. This material is available via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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