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Chemistry By Design: A Web-Based Educational Flashcard for Exploring Synthetic Organic Chemistry

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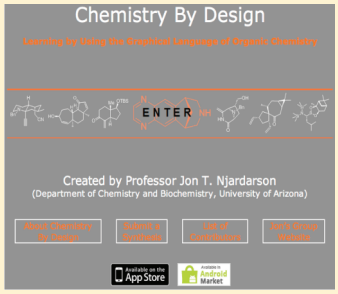
ABSTRACT: Chemistry By Design is a new educational Web site that contains a continuously growing database of natural product and pharmaceutical syntheses. It focuses on providing visitors with an opportunity to learn about the wonders of synthetic organic chemistry by browsing published sequences and viewing each synthetic step individually. Emphasis has been placed on exploiting the wonderful graphical language of organic chemistry to most effectively communicate the educational content as well as to allow visitors to test their knowledge in a variety of different ways. Chemistry By Design is also available as a free application for both Apple iOS and Android devices.



KEYWORDS: *General Public, Graduate Education/Research, Upper-Division Undergraduate, Organic Chemistry, Computer-Based Learning, Internet/Web-Based Learning, Problem Solving/Decision Making, Drugs/Pharmaceuticals, Synthesis*

Following the successful launch of our Top200 pharmaceutical posters a few years ago,[1] we started thinking about creating more sophisticated, free, Web-based educational tools that would take advantage of the graphical language of organic chemistry to connect to and educate students, professionals, and the public. Toward that end, we chose to first tackle educational challenges in our own field of research, namely, natural product synthesis and new method development.

The original educational concept was to create an interactive Web-based virtual flashcard database that would allow students to test their knowledge of organic chemistry using published natural product and pharmaceutical synthetic sequences. This idea was initially inspired by a desire to aid first-year graduate students in having a smoother and more enjoyable transition in starting to routinely read the synthetic literature, while also effectively absorbing as much content as possible. Journal space limitations naturally lead to very concise graphical representations of synthetic sequences. These limitations mean that you cannot effectively test your skills because you already see the structures of both starting materials and products. Furthermore, the fact that synthetic steps in publications are routinely bundled and starting material syntheses are not shown, but generally buried in the supplementary information section or an earlier publication, means a wealth of valuable synthetic knowledge is easily missed when not analyzed very closely. We concluded that a Web-based database of published natural product and pharmaceutical sequences that captured every single step associated with constructing these complex structures from commercially available building blocks would address such limitations.[2] Most important to our educational mission was that this new product, which aims to reach both the professionals and curious minds alike, would be free and readily accessible to anyone with access to the Internet.

These ideas have now been realized in the form of our latest educational product, Chemistry By Design (Figure 1), which was launched June 2011.[3] When visiting the Web site (Figure 1, image on left) you can start browsing and learning by pressing ENTER, which will take you to a window similar to the image shown to the right side of Figure 1. On the front page, we have additional active buttons that allow you to (1) learn about the origins of the site, (2) get instructions on how to participate in this educational project by submitting any sequences of your choice to the site, (3) view a list of contributors to the site, and (4) direct Web links to the app versions of the site. Anyone who submits a sequence(s) to the Web site will have their name added to the online list of contributors. These features will ensure that the greater organic community can aid in expanding this educational database while also providing opportunities for teachers and research groups to submit sequences to the site as part of class or group meeting projects.

Once you enter the site (Figure 1, image on right) you can browse the database by various categories such as natural products, pharmaceuticals, years, and authors. Alternatively, you can use the smart search box to find sequences of interest or simply click on the "dice" logo and have the program randomly select a sequence for you to view. On the bottom right, you are provided with two additional options. You can choose to view the sequence you have selected as is (Figure 2, image on left) or you can view it in "quiz" mode (Figure 2, image on right).

Once you have selected a synthetic sequence to view, you have a number of useful functions at your disposal. For example, you can at any time (1) switch between quiz and normal mode (Q↔S); (2) use the magnifying glass logo to look up the name and structure of any chemical abbreviation that appears in the database; (3) view the target structure by clicking on the box in the top right corner; (4) move back or forward using the next or previous buttons, the ruler on the

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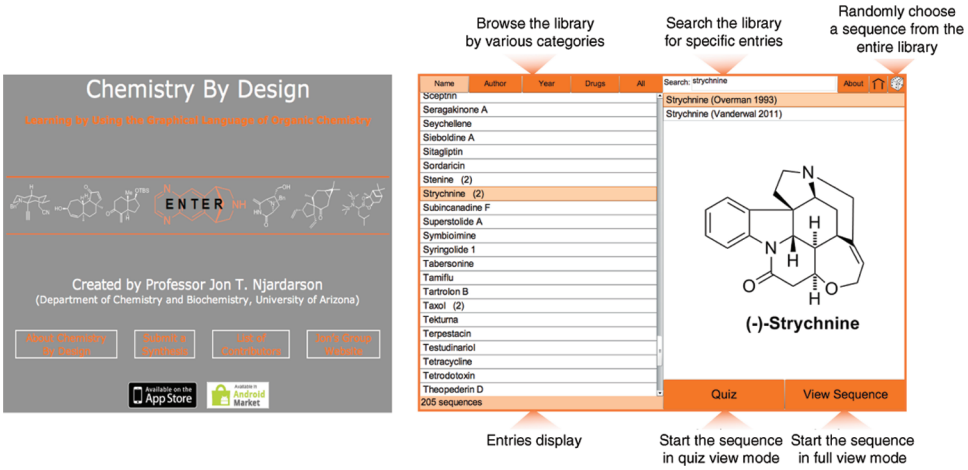

Figure 1. Homepage and first entry page for Chemistry By Design.

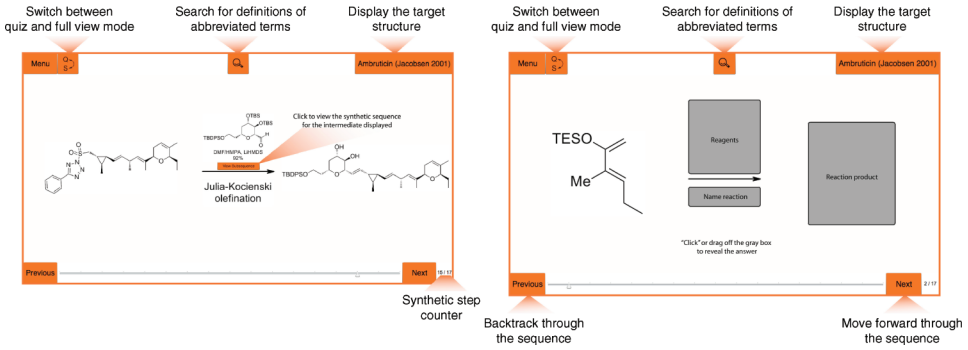

Figure 2. Normal (left) and quiz (right) viewing modes.

bottom, or simply swiping away the virtual flashcard; (5) view the step number you are viewing in the longest linear sequence; and (6) return to main menu.

The Web site contains a number of other useful features. We have designed the quiz mode in such a way as to maximize choices and flexibility. You can choose to first reveal either the product or the reagents or, alternatively, by going backward in a sequence, you can instead choose to reveal first either the starting material or reagents. This built-in flexibility means that you are never locked into continuing the original line of questions you chose in the beginning for the rest of the sequence. Additionally, bonus "name reaction" questions are scattered around the sequences.

One of the challenges we faced was how to display every single synthetic step for convergent (branched) sequences. This issue we solved by providing "view subsequence" buttons (Figure 2, image on left) at every branch point in which a main sequence is merged with another sequence. By clicking on this link, you are taken into a loop that shows you how the new structure that is being merged is made. All other functions of the site remain the same for these loops. This solution allowed us to capture every single reaction used in constructing a given target structure, which in turns provides an easy opportunity to count the total number of steps used in a sequence (number of steps in longest linear sequence and the number of steps in subsequences used). Finally, when you reach the target structure at the end of the sequence, you are provided with a hyperlinked journal citation link.

In developing Chemistry By Design, we envisioned it as especially well matched as an educational supplement for graduate and advanced undergraduate organic chemistry courses while also serving the curiosity and knowledge thirst of the professional chemistry community.[4] It is our hope that the site's simple design philosophy[5] and strong emphasis on graphics over text will be appealing and intriguing to those not already exposed to the wonders of organic chemistry. In addition to the new content we continuously add to the site, we are extremely grateful for all the outside submissions of synthetic sequence we have received to date. The educational value of the site will continue to grow as its database of natural product and pharmaceutical sequences grows.

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(1) McGrath, N. A.; Brichacek, M.; Njardarson, J. T. *J. Chem. Educ.* **2010**, *87*, 1348. Our Top200 drug posters can be found at http://www.cbc.arizona.edu/njardarson/group/top-pharmaceuticals-poster (accessed May 2012).

(2) Professor Hans Reich has made important contributions towards this goal. His Web site (http://www.chem.wisc.edu/areas/reich/syntheses/syntheses.htm) features hundreds of syntheses, all of which display each sequence on a single page. Although packed with valuable information and helpful search features, this site does not offer the same type of interactive educational experiences our site does. Recently, a new Web site called SynArchive (http://www.synarchive.com) was launched that follows a very similar presentation path to that of Professor Reich's site (accessed May 2012).

(3) Chemistry By Design http://www.chemistrybydesign.oia.arizona.edu (accessed May 2012).

(4) As of May 20, 2012, there have been more than 150,000 visits to Chemistry By Design Web site along with tens of thousands of downloads of the iphone or ipad and android app versions of the Web site since its June 26, 2011, launch. Google Analytics data monitoring of the site shows that individuals from most countries in the world, every state in the union, and countless cities around the globe have used Chemistry By Design. We are pleased to report that many students, professors, and industrial chemists have taken time to submit a synthetic sequence of their choice to the site. By following the instructions for sequence submission provided on the Chemistry By Design Web site, more than 80 new syntheses have been added to the site since its launch. The names of those individuals have all been added to the online acknowledgement roster. This last fall semester (2011), Professors Gregory B. Dudley (Florida State University), Uttam K. Tambar (UT Southwestern Medical Center), and Aaron Aponick (University of Florida) successfully used the site as a supplement to the graduate organic chemistry course. The names of the students in their classes that participated by submitting a sequence are also part of the continuously growing acknowledgement list.

(5) For recent references related to the use and educational value of virtual flashcards consult (a) Nakata, T. *Comput. Assisted Language Learn.* **2011**, *24*, 17−38. (b) Lin, F.-Y.; Liu, Y.-H. *Proceedings of the 2009 International Conference on Computing, Engineering and Information* **2009**, 265−268, DOI: 10.1109/ICC.2009.20.