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Activity

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Determining Synthetic Routes to Consumer Product Ingredients through the Use of Electronic Resources

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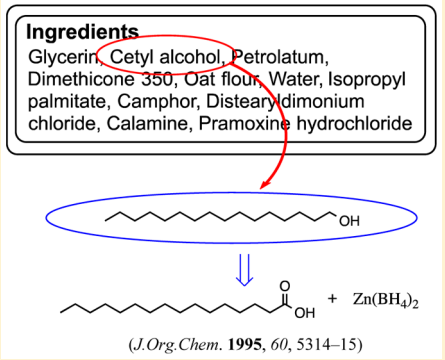
Supporting Information

ABSTRACT: An activity is described in which students in the first semester of a two semester organic chemistry laboratory class are introduced to the use of SciFinder. Students are required to determine the structures of three compounds as well as additional information regarding the synthesis of one of them using some of the features available in SciFinder.



KEYWORDS: *Second-Year Undergraduate, Organic Chemistry, Internet/Web-Based Learning, Nomenclature/Units/Symbols, Synthesis*

There can be little doubt that SciFinder is an indispensable tool for searching the chemical literature. Numerous articles have appeared in this *Journal*[1−6] and others[7] describing either the use of this resource or exercises in which students are required to use it to locate chemical information. While some of these exercises were designed for upper level undergraduate students, others were carried out as part of a second year organic chemistry course. This earlier introduction is beneficial in that it not only teaches this skill to a larger number of students with more varied backgrounds and majors, but also allows students to use this resource in much of their later coursework and/or research.

For many years now we have incorporated use of SciFinder into the first semester organic chemistry lab curriculum in the form of an "out-of-lab" exercise. The exercise is typically introduced midway through the first semester of the two semester sequence, after students have been introduced to the basics of organic nomenclature and reactions.

NATURE OF THE EXCERCISE

In this exercise, SciFinder is used to help students "decipher" the chemical names listed as ingredients in a number of commercial products. Use of ingredient labels to teach chemical nomenclature has been described previously[8] and has the advantage of relating the chemical concepts to "everyday life". Each student is assigned a different commercial product, and the ingredients found in that product (according to the label) are listed. Three of the ingredients (all organic compounds) are highlighted in boldface font for special consideration. For example, the ingredients found in Aveeno Anti Itch concentrated lotion are listed as Glycerin, **Cetyl alcohol**, Petrolatum, Dimethicone 350, Oat flour, Water, **Isopropyl palmitate**, **Camphor**, Distearyldimonium chloride, Calamine, Pramoxine hydrochloride. (For a full listing of all the commercial products featured in this exercise and their ingredients, see the Supporting Information.)

Students are asked to determine the structures of all three of the compounds listed in boldface via a "substance identifier" search using SciFinder. They are then asked to find additional information regarding one of these three compounds, which is then designated their "main compound". The additional information they must provide consists of the following:

(a) A complete bibliographic reference to a journal article in which a synthesis of the "main compound" is described.
(b) A synthetic scheme showing what starting materials and reagents are used to prepare the "main compound".
(c) An experimental procedure describing how the "main compound" is prepared and any characterization data presented in the journal article.

We have verified that this "additional information" is available for at least one of the three compounds shown in boldface, though in many cases it is not readily available for all three (students are alerted to this fact). Students are also advised against choosing the simplest compound of the three as their "main compound", as location of journal articles describing the synthesis of simple compounds is often more

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challenging than finding articles on the synthesis of more complex molecules.

Students are typically given 1 week to complete the project, and are asked to consult with the instructor if any difficulties are encountered either accessing or locating information within SciFinder. At the completion of the exercise, they turn in a "write-up sheet" containing the information requested and/or photocopies of the journal articles with the relevant information highlighted.

CONCLUSIONS

We have found that this is a useful way to introduce SciFinder to students, and it helps prepare them for more advanced applications of SciFinder (such as structure searching) which are utilized in a later experiment. Just by completing this exercise, however, they will have learned how to locate a synthetic method that, in theory, they could use to prepare a compound of interest. This exercise, thus, not only exposes students to one of the many uses of SciFinder, but also provides them with a skill that could be useful should they be engaged in a research project in the future. There are benefits to be gained by those not destined to pursue chemical research projects as well. Product labels are "demystified" somewhat by the demonstration that one can easily obtain structural and other information about any ingredient listed in a commercial product. In this way, it is hoped that this exercise may also help students to become more informed consumers.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.5b00391.

The background information on SciFinder provided in our student "course pack," the description of the required elements of the exercise, and the "write-up sheet" used to report results for this activity (PDF, DOCX)

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Notes

The authors declare no competing financial interest.

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