

JSME Molecular Editor: A Tool for creating Interactive Web-based Organic Chemistry Exercises

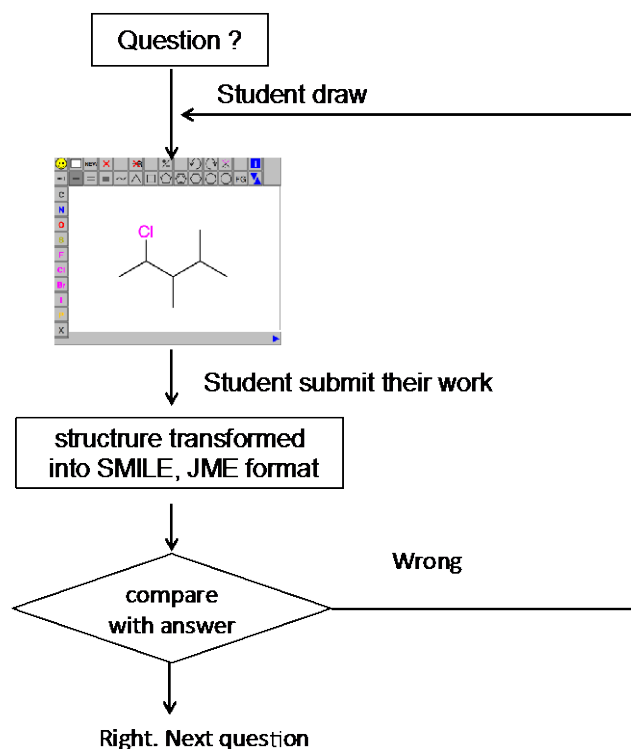
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Abstract There has been an impressive growth of open online course in recent years. However, the number of free organic chemistry courses is limited. To create an organic chemistry course online, we need a tool that can draw chemical structure and can be embedded into the web. We found that JSME Molecular Editor was a free and easy-to-use computer program for creating chemistry online course. We have developed interactive web-based organic nomenclature exercises by integrating JSME Molecular Editor into the website <http://www.ihoahoc.com/nomenclature/Enomenclature.html>. The three types of exercise were created: (i) students are given structure of an organic compound, then they have to identify a specific functional group inside this structure (ii) students are given the IUPAC name of an organic compound, then they have to draw structure of this compound (iii) students are given structures of an organic compound, then they have to write the IUPAC name of this compound. These exercises have been used for first year students at Faculty of Pharmacy, Lac Hong university, Vietnam.

Web-based organic chem exercises using JSME Editor



Keywords: first-year undergraduate/general, second-year undergraduate, organic chemistry, internet/web-based learning, distance learning/self instruction, nomenclature/units/symbols, student-centered learning

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1. Introduction

To understand organic chemistry, students need to acquire basic skills such as how to draw the structure of organic compounds or how to name an organic compound given its structure.

The learning resources for these exercises almost are from textbooks. There are some free online organic chemistry courses, but most require multiple-choice answers [1,2]. In organic chemistry, however, answers are usually structural drawings. There are limited free interactive online learning resources that allow a student to draw a chemical structure in response to a question. An important requirement to create interactive online organic exercises is to edit molecules directly within the web browser. Therefore, it is necessary to integrate a chemical structure drawing software into the website. One of the most popular commercial tools to create interactive organic exercise online is MarvinSketch from Chemaxon. In collaboration with Chemaxon, Pearson Education has integrated Marvin Sketch into an online homework, tutorial, and assessment system [3,4,5]. Another interesting cheminformatics application is Chemdoole Web Component, which is the chemistry toolkit for structure viewing and editing that is originally built using only web standard technologies, HTML5, CSS, and JS, and is accordingly supported by all modern desktop and mobile browsers [6].

In this work, we choose JSME Molecular Editor [7] to integrate into our website due to two reasons. First, it is a free molecule editor. Secondly, it is an easy-to-use tool with a very detailed instruction.

2. JSME Molecular Editor

JSME is a free molecule editor written in JavaScript, which supports drawing and editing of molecules on desktop computer, as well as on handheld devices including iPhone, iPad and Android smartphones and tablets. The editor is able to export molecules as SMILES [8] or in the compact "JME" format (one line textual representation of a molecule or reaction including also 2D

atomic coordinates). The SMILES code generated by JSME is canonical, i.e. independent on the way how the molecule was drawn. The JSME editor can communicate with other elements on the HTML page via its public functions. These functions can retrieve created molecules, programmatically display new molecules. Detailed description of JSME functions is available on-line in the JSME documentation page [9].

3. Exercises

Exercise 1. Identify a specific functional group in the molecule structure

The structural features that make it possible to classify compounds into families are called functional groups. The chemistry of every organic molecule, regardless of size and complexity, is determined by the functional groups it contains. As a result, different compounds with the same functional group often have similar chemical reactivity. For example, compounds containing R-C(=O)-H functional group have similar reactivity, called aldehyde. To learn the common reactions, it is important for a student to identify these functional groups in organic compounds.

In this exercise, students are given the structure of an organic compound, then are required to color a specific functional group. When they submit their work, JME format (textual representation of a molecule including also 2D atomic coordinates) of that colored molecule will be compared with JME format that we set up as the answer, then the website will give the feedback whether the student has correct or incorrect answer. If students draw incorrectly, they can revise and resubmit. Some interesting facts about these compounds also are given.

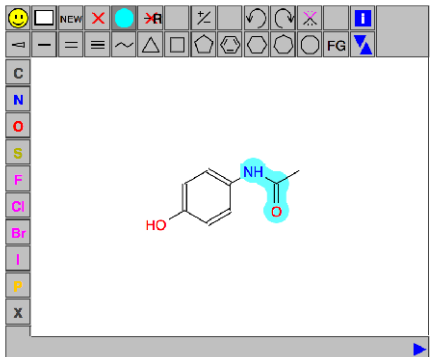
For example, students are given structure of paracetamol, then are required to identify amide functional group inside this structure. Students need to color C(=O)-NH to answer correctly. Students also can know that paracetamol is a drug for treating fever if they click on "interesting facts" button. We also add "Help" page which include all common functional groups and instruction to solve the problem.

Identify function group in organic compounds

Learning objective: Recognise and name common functional groups.

Help

Guidance: Click on blue circle, then colour the functional group.



New question
Check

Identify ' amide ' group in Paracetamol

Interesting facts

Paracetamol belongs to a group of medicines known as analgesics, or painkillers. It is used to relieve mild-to-moderate pain. It is also useful for lowering a raised temperature (fever), such as after childhood immunisation

Figure 1. This exercise ask to identify a specific functional group in a given compound structure

Draw structure of organic compounds

Learning objective: Using JSME Molecular Editor to draw an organic compound given its IUPAC name

Guide: How to use JSME (JavaScript Molecular Editor)

Select an organic compound belong to any functional group below:

Hydrocarbon
Alkyl halide
Alcohol, Phenol

Aldehyde, Ketone
Acid carboxylic
Amine

Draw the compound below:

2-Bromopentane

Click here to check

Check

Correct. This is '2-Bromopentane'

Figure 2. This exercise ask students to draw an organic compound given its IUPAC name

Exercise 2. Draw a molecule given its IUPAC name

There are millions of known organic compounds. The most widely used nomenclature system is International Union for Pure and Applied Chemistry, usually called the IUPAC system. Although many software programs can generate systematic chemical names for chemical structures in accordance with IUPAC rules or generate chemical structures from systematic names, it is important for chemists to understand IUPAC name.

In this exercise, students are given the IUPAC name of a compound, then are asked to draw structure of this molecule. When they submit the molecule, the program will compare its SMILE format with the SMILE format that we set up as the answer. If they are the same, the website will feedback that student's answer is correct. If students draw incorrectly, they can revise and resubmit.

For example, when students click on Alkyl halide, a random compound belonging to this functional group appears such as 2-Bromopentane. Students need to draw this compound in JSME Molecular Editor in order to answer this question. After drawing, they can check their result by clicking on "Check" button. We also add "How to use JSME" page which give detailed information of menu and examples to draw a chemical structure. Students should learn this before start solving these exercises.

Exercise 3. Write IUPAC name of an organic compound given its structure

Student are given structure of an organic compound categorized by its functional group, they are then required to name the compound based on IUPAC nomenclature rules. This type of exercise is more difficult than other two above. Therefore, hints and answers were provided in case the students could not answer correctly.

Name an organic compound given its structure

Learning Objective: Write IUPAC name of an organic compound given its structure

Select a functional group by double click:

Hydrocarbon
Alkyl halide
Alcohol, Phenol

Aldehyde, Ketone
Acid carboxylic
Amine

Write IUPAC name of the compound on the left:

Write here

Check

Hint
Answer

Butane

Figure 3. This exercise ask students to write IUPAC name of an organic compound given its structure

For example, if students double click on “Hydrocarbon” button, a random structure of $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ will appear inside the JSME Molecular Editor. The students need to write the IUPAC name of this compound. After writing their answer, they can check the result by clicking on “Check” button. If students want to know the hints, they need to answer at least once, or if they want to know the answer, they need to answer it at least twice.

Html source code of these exercises can be viewed by right clicking on the webpages, then selecting “View Page Source”.

4. Conclusion

A free, interactive online organic nomenclature exercise were built to support student learning. Through these exercises, students can draw structure given its IUPAC name as well as write IUPAC name of an organic compound given its structure. These exercises were essential for student to understand organic chemistry. JSME Molecular editor is promising for web-based applications in learning and teaching organic chemistry.

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