Reaction101 and **Yield101**:

Two mobile apps for chemistry with pedagogical value

Authors:

Alex M. Clark (corresponding author)

Molecular Materials Informatics, Inc.

Montréal, Québec, Canada H3J2S1

aclark@molmatinf.com

http://molmatinf.com

Maurizio Bronzetti, Steven M. Muskal

Eidogen-Sertanty, Inc.

3460 Marron Road, Suite 103-475, Oceanside, CA 92056

mbronzetti@eidogen-sertanty.com

smuskal@eidogen-sertanty.com

http://eidogen-sertanty.com

Abstract:

We describe the use of two mobile apps, *Reaction101* and *Yield101*, in the context of a learning environment. *Reaction101* includes features for learning to balance reactions. *Yield101* assists with calculating quantities that are relevant for a laboratory preparation. While both apps have capabilities that are useful to synthetic chemists at all stages of career development, they have been designed to be specifically useful to students learning chemistry at high school and undergraduate level. These mobile apps also facilitate communication of chemical data, in both digitally interpretable forms and presentation-ready formats.

Introduction

Mobile apps have become prevalent within an incredibly broad segment of the population, including education at all levels. A modern smartphone, music player or tablet computer the size of a small book now delivers high performance graphics, storage, computational capacity and access to the Internet. A growing number of educational institutions are adopting mobile devices as classroom tools (*1*). There are an increasing number of apps designed for chemists at varying stages of professional development, from high school students to graduates and beyond (*2*).

A recent review (*3*) describes a large number of mobile apps for chemistry, many of them focused on education. There are also online resources, such as SciMobileApps (*4*), which provides a living resource that is regularly updated by the community.

In this article we describe two apps: *Reaction101* (*5*) and *Yield101* (*6*), which were created with the needs of students in mind. Both of these apps are available for iOS based devices, specifically the iPhone, iPod and iPad (*7*).

Reaction101

Reaction balancing is a vital skill for students who intend to pursue any branch of chemistry, and it has traditionally been practiced by drawing out reactions on paper. Verifying whether a reaction is balanced is a relatively tedious calculation, and is prone to mistakes. Complementing this approach with a computer-assisted solution that provides real-time feedback adds an important and valuable extra dimension to learning.

Addressing this challenge is one of the primary motivations for designing *Reaction101*, a mobile app centered around the drawing and rendition of a single chemical reaction. A reaction is represented as a set of reactants, reagents and products, each of which is a distinct component. Reaction components consist of a chemical structure sketch, name, and in the case of reactants and products, stoichiometry. The reaction editor is derived from the Mobile Molecular DataSheet app (*8*), and the structure diagram sketcher is described in detail in the literature (*9*).

Reaction101 is supplemented by useful reaction aids that are provided by server side content from Eidogen-Sertanty. A public collection of common generic reactions, organized by name, is available, and any one of them can be viewed for reference purposes, or used as a starting point for drawing a new reaction. Also, individual reaction components can be obtained by searching the *Mobile Reagents* (*10*) database. Searching can be done by name, formula, exact structure, substructure, and structural similarity.

When a reaction is displayed onscreen, it is checked to verify whether it is balanced. Both sides of the reaction - reactants and products - are tallied up by multiplying the molecular formula for each component by its stoichiometry. For each element whose counts are not equal on both sides, the excess is added to the opposite side. In this way, it is made very clear at a glance that a reaction is not balanced. When a reaction is not balanced, it is because of some combination of missing components, incorrect stoichiometries, or incorrectly drawn reactants or products. Figure 1 and Figure 2 show screen captures for two reactions, where 1(a) and 2(a) are not balanced, and the display is annotated with the excess atoms on either side. The screen captures shown in Figures 1(b) and 2(b) show the analogous reactions, with all the components included, and balanced. In these cases, the element counts match, and so no excess atoms are denoted.

(a) (b)

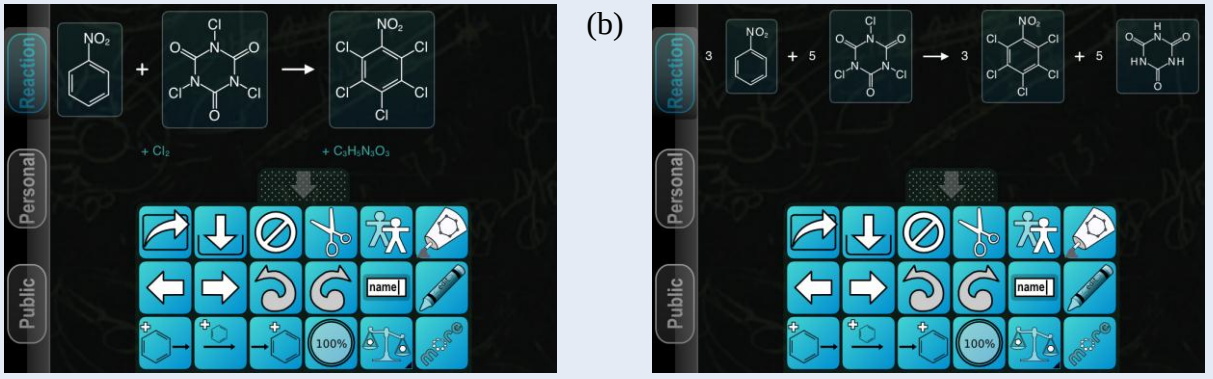


Figure 1. Unbalanced (a) and balanced (b) representations of a perchlorination reaction (*11*)

(a) (b)

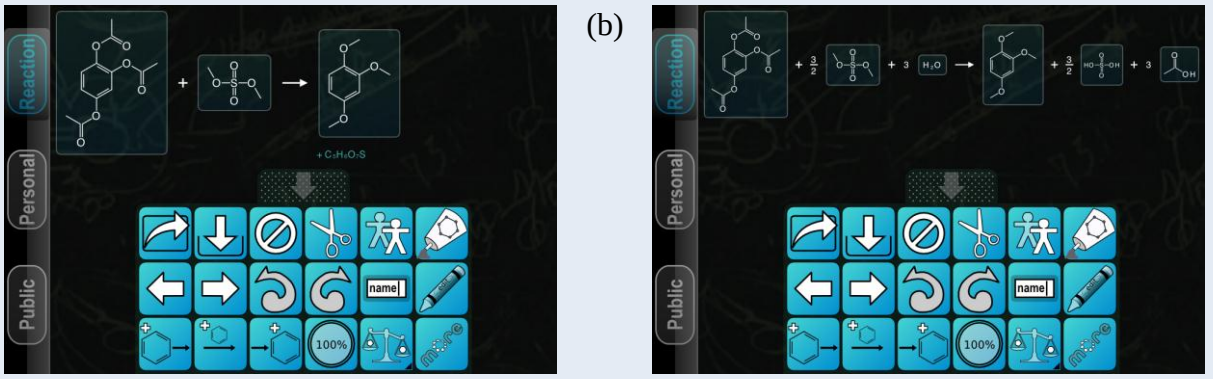


Figure 2. Unbalanced (a) and balanced (b) representations of a deacylation/methylation reaction (*12*).

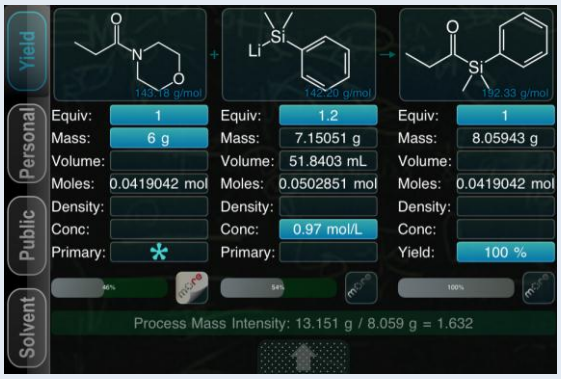
This concise feedback can be thought of as a kind of checksum for the correctness of a reaction, i.e. a balanced reaction is not necessarily correct, but a non-balanced reaction is definitely wrong or incomplete. Often the leftover element counts make missing components quite obvious, for example elimination of small molecule byproducts such as water. The student is free to experiment by tinkering with the reaction components and stoichiometric equivalents, and obtain real-time feedback as to the extent to which the reaction is balanced.

The app also features an automatic balancing feature, which attempts to guess the stoichiometry of each component by picking the coefficients that lead to the most balanced result. While this may seem like a way to shortcut the learning process, it is only effective if the actual components are correctly specified.

Yield101

When setting up a reaction in a lab, the calculations that go into adding up molecular weight, interconverting mass and volume by density or concentration etc., are not particularly difficult, but they must be learned by repetition. Students need to focus on observing the experiment as it progresses, learning how to use the equipment, thinking about the actual chemistry that is occurring, recording experimental notes legibly, scheduling timing in order to workaround availability of shared resources, getting the experiment finished

(a)



(b)

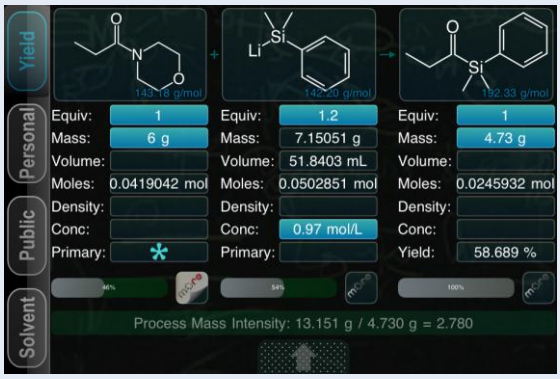


Figure 3. Yield scheme for a silylation reaction (*13*). Values that are highlighted in turquoise are *actual* values, provided by the user, while non-highlighted values are calculated. (a) shows the scheme before the reaction is complete, where the yield has been set to 100% in order to trigger calculation of the mass of the theoretical maximum (8.06 g). (b) shows the scheme after the reaction is complete, with the actual yield specified explicitly (4.73 g, 59%).

before the deadline, and all the while paying attention to laboratory safety protocols. Devoting too much time to quantity interconversion may take attention away from the learning experience. As with reaction balancing, introducing a tool that performs these interconversions automatically provides a real-time answer key. It can be used in conjunction with a manual calculation, to confirm the answer and build confidence.

The *Yield101* app has a similar interface to *Reaction101*, as both apps present an individual reaction as the central object, but its focus is on the physical quantities that make up an individual laboratory preparation. Each of the reactants and products are characterized by, in addition to structure, stoichiometric equivalents, mass, molar mass, volume, density and concentration. The purpose of the app is to make use of the relationships between these properties. The user needs to provide the actual measurements. The algorithm will then calculate any of the missing quantities that are implied by actual data.

Within an individual component, the following relationships apply:

- molecular weight is derived from structure
- mass and molar mass are related via molecular weight
- mass and volume are related by density (for pure substances)
- mass and volume are related by concentration (for diluted substances)

When there is more than one reactant, one of them should be marked as being *primary*. By using the primary reactant as a reference point, the following relationships between components apply:

- molar mass of reactants and products can be derived from the molar mass of the primary reactant, scaled by the ratio of their stoichiometry
- yield of products can be derived from the expected molar mass (from stoichiometry) relative to the observed molar mass

By applying these relationships iteratively, a few key experimental measurements provided by the user can allow many of the remaining quantities to be derived, ultimately providing a percentage yield for the reaction, once the products have been measured.

The app can be used to enter actual values as they become available, or it can be used in a more speculative way, e.g. by entering a value of 100% for a yield, the calculations will be done in reverse, and the theoretical maximum quantities will be filled out instead, as is illustrated in Figure 3(a). In Figure 3(b), the actual yield for the reaction has been entered.

Some quantities can be codependent, e.g. providing mass, volume *and* density is allowed, but it introduces the possibility of inconsistency. If the calculated and provided values do not match up, they are all highlighted in red, indicating that a mistake has been made, and some correction is required.

The app also has the ability to print out a quantity scheme (or create a PDF file), which is a useful pre-laboratory exercise (see Figure 4). Prior to beginning the experiment, the known quantities and properties can be entered, which provides information on quantities of reaction equivalents and theoretical yields. Once the experiment is completed, actual values can be applied to produce a second scheme, either or both of which can be attached to the laboratory report, if this is allowed as part of the exercise.

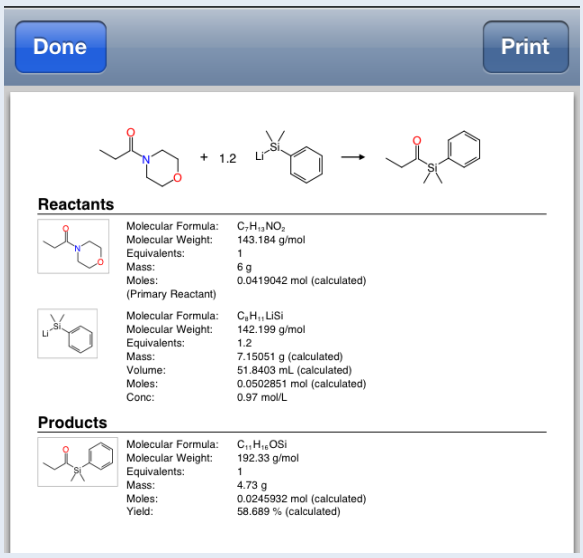


Figure 4. Print-ready display of a reaction yield scheme.

Besides calculating the quantities of reactants and products involved in an experiment, *Yield101* also introduces a calculated quantity called *process mass intensity* (PMI). This is an index that is often promoted in the context of green chemistry (*14*). The calculation is very simple: total mass of all reactants divided by total mass of desired products. Water is typically excluded from both sides of the reaction, and non-aqueous solvents are added to the product side only if they are recovered. The ideal "green reaction" has a PMI value of 1, which means that there are no unused byproducts other than water, and non-aqueous solvents were either not used or recovered, and the yield was 100%. While the PMI values for two different reactions are not usually comparable, smaller values are more desirable from the point of view of waste and environmental side effects.

Yield101 displays the PMI calculation at the bottom of the screen, as shown in Figure 5, and also displays the relative contribution for each of the components, in the form of a percentage sidebar. Calculation of these metrics is not typically a high priority in the laboratory environment, and so the always-on automatic calculation of these properties is a way to encourage students to start thinking about the environmental implications of chemical

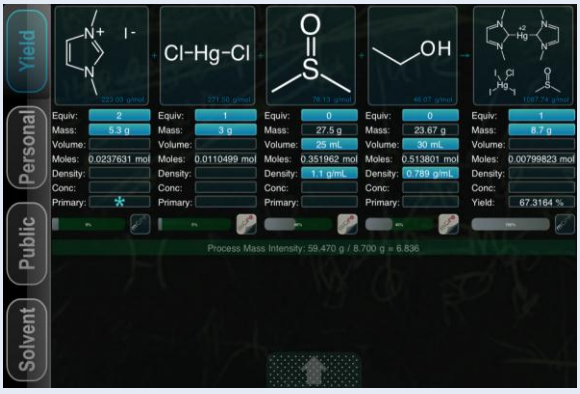


Figure 5. Yield scheme for a mercuration reaction (*15*). All solvents are included on the reaction side. The calculated PMI is 6.836.

reactions early on in their careers, which is likely to become an increasingly important skill.

Communication

Both *Reaction101* and *Yield101* have strong data sharing capabilities. App-to-app sharing can be accomplished via the *open-with* functionality: both *Reaction101* and *Yield101* are capable of sending and receiving reaction content, so they can pass reaction schemes between each other. The same applies for any other installed app that registers itself appropriately (*16*).

Both apps are capable of storing content on a cloud-hosted server, which is associated with the device. Reactions or yield schemes can be recalled for later use, and *Yield101* is capable of opening reactions stored by *Reaction101*, which binds them together in a logical workflow:

- use *Reaction101* to draw and balance a reaction
- use *Yield101* to fill in quantity data, once for each experiment

Reactions and yield schemes can be sent by email. An outgoing email message includes a picture of the reaction, and the actual data. If the recipient of the email message is running either of these apps, the content can be automatically extracted and opened within the selected app. If the recipient is using a generic email client, the attachment content can be downloaded and used by any compatible software. Incoming attachments, either originating by email or from a browser download, can be opened with either app, if they are of a recognized format, which includes the industry standard MDL RXN and RDfiles (*17*). The ability to share reaction data allows both of these apps to participate in the realm of cheminformatics, as they can both create and consume content.

Reaction images can be copied to the clipboard in bitmap form, which allows them to be pasted into other apps on the device, e.g. Keynote (*18*). As previously mentioned, *Yield101* can be used to generate a PDF file of the reaction/quantity scheme, which can be viewed, printed or sent by email.

Conclusion

Both apps have features that are useful for professional chemists, but they have particular value in a learning environment. Interactive reaction balancing calculations and automatic calculation of related physical quantities provides feedback and encourages learning by trial and error. Determination of process mass intensity (PMI) for reaction schemes encourages students to consider the environmental implications of each chemical reaction. The ability to create presentation quality graphics and communicate data encourages students to collaborate and share, and also provides an entrypoint into the wealth of digitized chemistry data that is available on the Internet.

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