RUNNING VIRTUAL REACTIONS: A REACTION PREDICTOR APP FOR TEACHING ORGANIC CHEMISTRY

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BACKGROUND

Students are often daunted by the process of learning the functional groups (FGs) and functional group interconversions (FGIs) in undergraduate organic chemistry courses.[1-3] Problems arise when students attempt to rote learn, rather than understand and predict reactions.[4] Owing to the portability and increasing proliferation of mobile platforms (i.e., smartphones and tablet devices), a unique opportunity exists for teaching organic chemistry, via active-learning methods, which increase the meaningfulness and retention of course material. In particular, the use of reaction prediction applications has the potential to encourage students to use problem-based, self-directed and collaborative learning methods. While reaction prediction programs have been developed for desktop computers, research in the field has stagnated, and there are no predictors available for mobile platforms.[5]

AIMS

To develop a reaction predictor app with mobile and desktop support. The app will let students sketch any chemical structure, then add single or multiple reagents to the structure, to predict the reaction product(s). The purpose of the app is to increase student understanding and retention of FGIs without using rote-learning techniques. We're also interested to see if students use the app as a game, that is, for enjoyment, particularly when challenging other students in the 'head-to-head' mode.

DESIGN AND METHODS

We will code the predictor using JavaScript. Rules for FGIs will be defined using SMIRKS notation (a derivative of SMILES used for reaction transforms). All reagents in a specified reaction will be compared against the rule database, and the likely products displayed to the user as images.
Feedback analytics tools will let the app automatically sample data from all users: our focus will be on app usage duration and frequency. Touch/click and multiplayer analytics will be provided using heat maps, and real-time activity streaming.
In-app feedback screens will collect student self-evaluation, and enjoyment/satisfaction trends.
Traditional survey methods will be used to collect data that the app gathered insufficiently. Finally, student results (within application problem sets, and within subject assessments) will be compared with student self-reported data, and their duration and frequency of application use.

ANTICIPATED RESULTS

The reaction predictor will be built as a hybrid web-app, working on iOS, Android and Internet-connected desktops. Users can input structures (to be used as reagents or target molecules) by sketching them, or by taking photos of structures using their device's inbuilt camera. Problem sets will be included, wherein users are required to virtually synthesise a target molecule, from a starting material, in a specified number of steps. A multi-user mode will allow students to collaborate in building target molecules, or to compete for the same purpose (by time, or by number-of-steps). We will be using a large first year and smaller second-year cohort organic chemistry subject at the University of Wollongong as the sample frame, and beta testing. All students should report improved understanding of FGIs within each problem set, and overall in the subject, which should be reflected in the assessment of learning outcomes.

ANTICIPATED CONCLUSION

A reaction prediction application was successfully developed for multiple platforms, and improved understanding of FGIs, making it ready for wider testing and distribution among undergraduate students and other institutions.

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