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Incorporating Green Chemistry Concepts into Mobile Chemistry Applications and Their Potential Uses

Sean Ekins,*[,†,∥] Alex M. Clark,[‡,∥] and Antony J. Williams[§,∥]

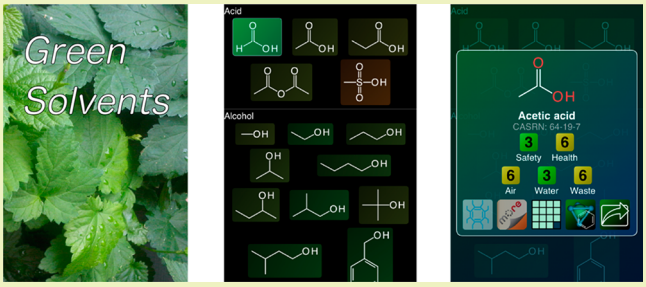
[†]Collaborations in Chemistry, 5616 Hilltop Needmore Road, Fuquay-Varina, North Carolina 27526, United States

[‡]Molecular Materials Informatics, 1900 St. Jacques #302, Montreal, Quebec, Canada H3J 2S1

[§]Royal Society of Chemistry, 904 Tamaras Circle, Wake Forest, North Carolina 27587, United States

Supporting Information

ABSTRACT: Green Chemistry related information is generally proprietary, and papers on the topic are commonly behind pay walls that limit their accessibility. Several new mobile applications (apps) have been recently released for the Apple iOS platform, which incorporate green chemistry concepts. Because of the large number of people who now own a mobile device across all demographics, this population represents a highly novel way to communicate green chemistry, which has not previously been appreciated. We have made the American Chemical Society Green Chemistry Institute (ACS GCI) Pharmaceutical Roundtable Solvent Selection Guide more accessible and have increased its visibility by creating a free mobile app for the Apple iOS platform called Green Solvents. We have also used this content for molecular similarity calculations using additional solvents to predict potential environmental and health categories, which could help in solvent selection. This approach predicted the correct waste or health class for over 60% of solvents when the Tanimoto similarity was >0.5. Additional mobile apps that incorporate green chemistry content or concepts are also described including Open Drug Discovery Teams and Yield101. Making green chemistry information freely available or at very low cost via such apps is a paradigm shift that could be exploited by content providers and scientists to expose their green chemistry ideas to a larger audience.



KEYWORDS: *Drug discovery, Green chemistry, Mobile applications, Open Drug Discovery Teams*

INTRODUCTION

One mission of the chemicals industry is to discover and develop products that are useful for global populations, without damaging the environment. Green Chemistry is "*the utilization of a set of principles that reduces or eliminates the use or generation of hazardous substances in the design, manufacture, and application of chemical products*".[1] As an example, the pharmaceutical industry has the goal of improving the health of people throughout the world and, through various green chemistry initiatives, is also committed to ensuring a healthy environment. There are many challenges associated with supporting a healthy environment as the majority of pharmaceutical molecules require multiple complex synthetic steps to produce. There is high attrition in pharmaceutical research, so many compounds will need to be made. However, only a very small fraction will make it into the clinic and far less into the marketplace. It is therefore important to design a green process as early as possible when the cost is lower and the quantities of chemicals made are relatively small compared to when they are dramatically scaled up for manufacturing. Much of the focus has been on optimizing material and energy use, preventing and minimizing waste, increasing use of renewable materials and energy, having safe processes, and eliminating or minimizing the use of hazardous chemicals.

As solvents can make up a large percentage of materials used in the manufacture of bulk active pharmaceutical ingredients, if we are to make synthetic processes "greener" it would be ideal to select greener solvents.[2] This has stimulated several companies to implement their own guides regarding the importance of solvent selection.[2] A recent consortium organized by the American Chemical Society called the Green Chemistry Institute (ACS GCI) Pharmaceutical Roundtable[3] currently involves 14 pharmaceutical companies, and has developed a solvent selection guide publicly available on their Web site.[4] The ACS GCI Pharmaceutical Roundtable Solvent Selection Guide lists the 60 solvents by chemical name and rates the solvents against safety, health, air, water, and waste categories with scores from 1 (few issues) to 10 (most concern) with additional color coding (green, yellow, and red). In our opinion, the availability of this guide is not widely known because to our knowledge it has not been extensively publicized

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Table 1. Mobile Apps Discussed in This Article

Green Solvents[10] A reference app that compiles a list of common solvents with information about their environmental impact and hazards.[37] Content can be viewed within the app and shared with other apps.

Mobile Reagents[38] A mobile access point to a large collection of commercially available compounds, with associated vendor information. Searches can be done by name, by drawing structures, or by photographing structures or QR codes.

ChemSpider Mobile[39] A mobile client for the ChemSpider service that provides structure drawing capabilities. Once located, entries are viewed by launching the mobile Web browser to open the mobile-friendly result page.

Mobile Molecular DataSheet (MMDS)[40] A multifunctional chemistry app, which provides editing tools for structures, reactions, and collections with auxiliary data. Supports all of the communication techniques described in this article.

Open Drug Discovery Teams (ODDT)[31] A mobile app, that is "Flipboard-like"[24] and chemistry aware, which aggregates tweets and Google Alerts RSS feeds for select scientific topics including Malaria, Tuberculosis, Huntington's Disease, HIV/AIDS, Sanfilippo Syndrome, Green Chemistry, Drug Repurposing, Hunter Syndrome, Global Genes, H5N1 (bird flu), and Giant Axonal Neuropathy.

and its utility may be hampered because it only exists as a document in PDF format that is on the ACS GCI Web site (that also requires registration). The limitations in access and utility encouraged us to recast the content in a novel manner to greatly enhance its visibility and availability to practicing chemists. We have also used the solvent classification data for enabling predictions for solvents outside the guide.

Mobile devices such as smartphones and tablet computers have seen rapid uptake in recent years, and the associated app stores include a growing number of chemistry software apps.[5] These apps generally perform one or two functions and can be thought of as individually packaged features rather than the relatively heavyweight programs commonly used in desktop computing. However, such apps *can* use data interchange and be used in the workflow to increase the productivity of chemists.[6] Mobile apps for chemistry are a nascent area to delivering or "appifying" data and may be disruptive to many currently used paradigms for presenting information and for education.[7]

We have used the ACS GCI Pharmaceutical Roundtable Solvent Selection Guide data as a starting point to develop the first mobile app for green chemistry called Green Solvents (Table 1, Figure 1) that is currently freely available for iPhone, iPod, and iPad. The advantages of developing such software is that it makes the solvent guide available at the bench or whenever the chemist is away from a desktop computer with Internet connectivity. We will describe the development and uses of this app including its value as an educational tool for students with the goal being to foster an understanding of green chemistry through selecting a "greener solvent". This work has also stimulated the implementation of other green chemistry features in cheminformatics apps (that we will describe) and suggested additional apps that could be created in future.

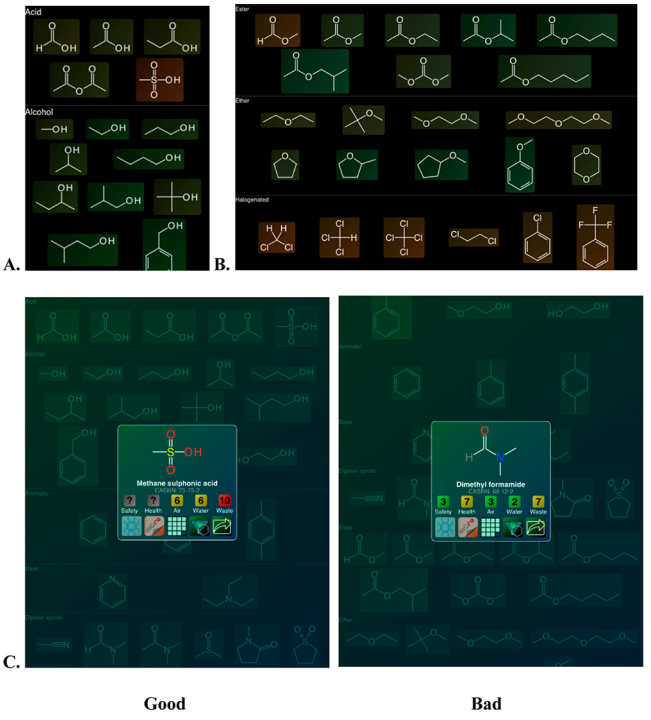


Figure 1. Entry page on the Green Solvents App for iPhone (A) and iPad (B). The content is assessed by touching a molecule, and it opens a new page (C) with molecule details that lists scores (good = 1, bad = 10) for safety, health, air, water, and waste criteria. In addition, the CAS number and links out to ChemSpider[15] and Mobile Reagents[16] databases for more details on the solvent are included. Touch anywhere else on the screen and the page closes.

EXPERIMENTAL METHODS

Solvent Selection Guide. The ACS GCI Pharmaceutical Roundtable Solvent Selection Guide[3] rates the listed solvents against five categories: safety, health, environment (air), environment (water), and environment (waste).[8] Key parameters and criteria were then chosen for each category (e.g., flammability is one of the safety criteria). The summary table assigns a score from 1 to 10 for each solvent under the respective categories, with a score of 10 being of most concern and a score of 1 suggesting few issues. This is further simplified by using color coding with scores in the range of 1−3 shown as green, 4−7 shown as yellow, and 8−10 shown as red. This allows quick comparison between various solvents.

Green Solvents App Software Development. The app was built using the Objective-C programming language, the API provided by Apple for native iOS development, and the MMDSLib library for cheminformatics functionality such as structure rendering. MMDSLib was originally developed for the Mobile Molecular DataSheet app and is used to provide key functionality for a number of other apps.[9] The solvent information was entered manually and is bundled as part of the app resources. Within a period of three days, the app was developed and submitted to iTunes for approval[10] as a free app for the iPhone, iPod, and iPad platforms. The Green Solvents app went from an idea to a downloadable app available within a week.[11−14]

Green Solvents App Software Application. The Green Solvents app uses solvent structures grouped by chemical class as the primary point of entry. These solvents are also color coded with a brown background suggesting those that are less desirable and a green background suggesting those that are more desirable. The user can scroll through all the solvents and click on a molecule of interest. This opens a box that lists the molecule name, CAS registry number, scores for each category with color coding as well as links out to the ChemSpider Web site,[15] the Mobile Reagents app[16], and the Mobile Molecular

DataSheet.[17] By clicking away from this box, it returns to the list of solvents.

Categorization of Additional Solvents. Additional solvents not in the Green Solvents App were extracted from the GSK solvent selection guide.[2] The 2D structures were downloaded as Molfiles from ChemSpider.[15,18] Their similarity to the 60 solvents used in the Green Solvents app was calculated using MDL public keys with the Tanimoto similarity (Discovery Studio 3.5 (San Diego, CA)).[19−22] The solvent(s) with the closest similarity was used to infer the likely scoring information for two of the five categories defined by the ACS GCI (health and environment (waste)). These were then compared with the available classifications published by GSK[2] to assess utility of the app for such gap-filling or decision-making exercises. It is important to note that the scoring scales as published for these two solvent selection guides are opposite, and thus the predictions were compared via the color coding (red, green, and yellow).

RESULTS

While the focus of this work is on the development of the Green Solvents app that is freely available, we have accumulated considerable data that can be used for inference of solvent classification for categories important for green chemistry. We now describe the results from this analysis. Sixty-four unique solvents that were not in the Green Solvents app were extracted from the GSK solvent selection guide[2] to create a "test set". The similarity of these 64 solvents to the solvents from the ACS GCI Pharmaceutical Roundtable Solvent Selection Guide in the Green Solvents app was assessed (Table S1, Supporting Information). The most similar solvent was used to predict potential waste and health scoring information classes (Table S2, Supporting Information). These represent two of the five categories of scoring information in the ACS GCI Pharmaceutical Roundtable Solvent Selection Guide that most closely overlap. After excluding predictions for GSK solvents with Tanimoto similarity $\leq$0.5 to those in the ACS GCI Pharmaceutical Roundtable Solvent Selection Guide, 50 solvents remained (Table S2, Supporting Information). Of these, the waste class was correctly predicted for 31 (62%) solvents and the health class was predicted for 33 (66%) solvents.

CONCLUSIONS

It has recently been suggested[26] that the pharmaceutical industry has perhaps adopted green chemistry as enthusiastically as it has because it has the most to gain; their manufacturing plants generate 25 to greater than 100 times more waste than product. Solvent selection is key in determining the sustainability of future commercial production as solvents can make up greater than 50% of materials used in the manufacture of bulk active pharmaceutical ingredients.[4] This shift to greener solvents is further illustrated by Pfizer's synthesis of sildenafil citrate (Viagra) in which all the chlorinated solvents were replaced with less toxic alternatives, along with steps to recover and reuse them.[27] Some have also indicated that logP drift (the undesirable preferential success of higher logP compounds in a synthesis array) may be minimized or reversed in chemical reactions performed in aqueous media[28] that are likelier greener. Green solvents however are not always more efficient than the widely used chlorinated solvents, and this may be a counteracting consideration.

In developing mobile apps for chemistry, we have assumed many chemists now have a smartphone and/or tablet computer. Our research aims to deliver cheminformatics solutions via mobile apps as they are easier to use when in the lab or in locations without a desktop computer. While the e-lab notebook is generally used in the office, in contrast a mobile phone will be in the chemist's pocket at all times, and apps can be used anywhere, anytime and are generally intuitive. It should be noted however that even e-lab notebooks are also being increasingly appified. While early chemistry apps provided minimal features like simple sketching[23] or molecule properties, newer chemistry apps are becoming increasingly sophisticated.[5,6] While for the Green Solvents app the iPhone-size limitations are minimal, the presentation on the iPad is more dramatic (Figure 1). These apps are likely excellent adjuncts for e-lab notebooks but are certainly advantageous in their mobility. It is feasible that future mobile apps for chemistry will include fully functioning lab notebooks,[5] and these may be connected with apps like Green Solvents to enable collaborative workflows.[6]

We have briefly described elsewhere how the Green Solvents app development was initiated via collaborations using social media.[11−14] It is widely understood that chemists both read and interpret chemical structures readily, and hence we chose the depiction of solvent 2D structures rather than names as the primary visual display in the app. While this takes up more display area than a molecule name, the presentation of data in large tables may be overwhelming (as would occur if the table was printed out and used for reference) and result in errors by the reader. Therefore, we have abstracted and highlighted data for just the solvent in question once a structure is selected. We have also provided links out of the app to gather more information on the solvents from additional Web sites. We have distributed the Green Solvents app as a free product as a way to disseminate information on green chemistry, and specifically we make use of the precompetitive efforts from the ACS GCI Pharmaceutical Roundtable to reach a much larger audience. This app, like most free apps, has a small banner advertisement that does not detract from the content of the app or its usability on a mobile device. Importantly, this app was not funded by the ACS or any other organization and is therefore independent. This allows us considerable flexibility in app design and content as well as future updates.

We have leveraged a cheminformatics app platform as the underlying technology to enable rapid app development for Green Solvents. This app conveys the solvent information in a manner easily and clearly discerned by chemists. The mobility, size, and flexibility of such mobile devices suggests them as obvious adjuncts to e-lab notebooks in that they can be used in the laboratory or in the field. Experiences derived from this first mobile app for green chemistry also suggests that other green chemistry content could be readily converted into apps to further increase the audience and to educate them in the benefits of green chemistry concepts and recommendations.

Creating the Green Solvents app also motivated the addition of the process mass intensity (PMI) calculation,[29] which is another green chemistry feature, into the Yield101 app[30] (Figure 2). A third recently developed mobile app connected to green chemistry is the Open Drug Discovery Teams (ODDT) app[31,32] (Figure 3). ODDT is a free mobile app intended as a research topic aggregator of science data collected from various sources on the Internet such as Twitter and Google Alerts. It exists to facilitate interdisciplinary teamwork and to deliver

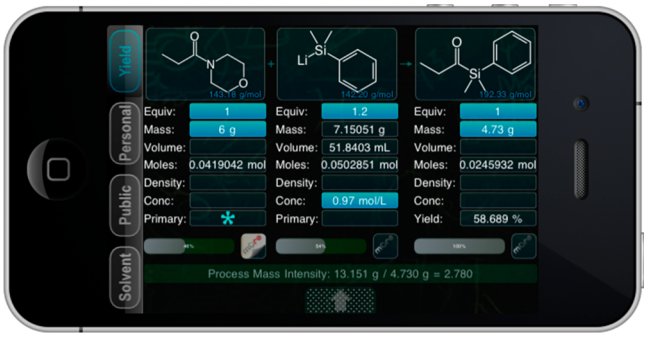
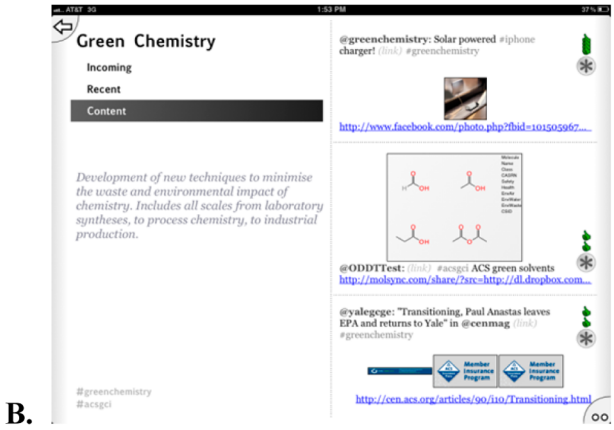


Figure 2. Illustration of how the green chemistry concept Process Mass Intensity (PMI) is incorporated into the Yield101 app on an iPhone.

access to information that is highly relevant and focused on the topic areas of interest. Research topics include areas of chemistry and adjacent molecule-oriented biomedical sciences, with an emphasis on those that are most amenable to open research at present. We have focused on green chemistry as a topic within this app due to its potential importance for scientists involved in drug discovery for rare and neglected diseases in particular. There is high attrition in drug discovery, so many compounds will need to be made. However, only a very small fraction will make it into the clinic and far less into the marketplace. It is therefore important to design a green process as early as possible when the cost is lower and the quantities of chemicals made are relatively small compared to when they are dramatically scaled up for manufacturing. We feel these global neglected and rare disease researchers would benefit greatly from being informed about green chemistry principles early on and that this has not been considered by any of the major organizations driving green chemistry educational initiatives. The ODDT app has also been used to visualize the ACS GCI Pharmaceutical Roundtable Solvent Selection Guide in a different format as it was tweeted out as a table of structures and classifications to reach an even wider audience for those following the hashtag #greenchemistry. This list of solvents is now freely accessible by anyone using ODDT and can be readily exported and used for other purposes. To date, we are the first researchers that have created and used mobile apps to communicate green chemistry concepts, and this could revolutionize how we educate scientists in the future via simple intuitive mobile apps.

Our aim is that chemists around the world can readily learn about the environmental impact of the solvents they use while they are in the lab using their iPhone or iPad, and thereby use the information to influence their solvent selection. Since the release of the Green Solvents app in June 2011, it has been downloaded more than 4700 times. While we have used the Apple iOS operating system, other mobile operating systems, specifically Android,[33] can be used to further increase its adoption to an even wider global audience.

Apps for science continue to expand in number, diversity, and capabilities. They may be categorized into scientific discipline and further subcategorized on the basis of applications within a branch of science. As a service to the community, we have established a wiki site[34] hosting a growing list of scientific apps for all available mobile platforms. This is a valuable resource that will continue to expand in content and may be useful for creation of future science-focused app stores by us or others. A new mobile app recently developed for the



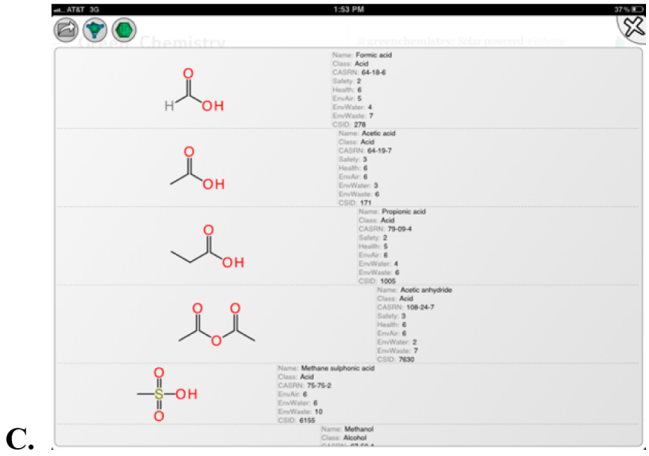


Figure 3. (A) How the Open Drug Discovery Teams app incorporates green chemistry as a topic. (B) How content is automatically captured from tweets with the hashtags #greenchemistry and #acsgci. (C) Green solvents app molecule contents were tweeted from the MolSync[25] app and are available in the app as stored content along with properties.

Android operating system called Lab Solvents[35] extends the Green Solvents app by including solvents from the 110 molecule GSK solvent selection guide.[2]

We have previously used a two-dimensional method using MDL keys and Tanimoto similarity[20−22] to predict cross-reactivity with immunoassays for drugs of abuse and therapeutic monitoring. We now extend this approach further to suggest the use for solvents. We have used the solvents in the GSK solvent selection guide that are not in the ACS GCI

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Pharmaceutical Roundtable Solvent Selection Guide as a prediction set for molecular similarity calculations to categorize them for two classifications relevant to green chemistry. We found that 62−66% of the classification predictions for solvents were correct when using the Tanimoto similarity to suggest the closest solvent. It is likely that increasing the similarity coefficient threshold could also improve the success rate further as would having consistent scoring systems between the GSK and ACS GCI Pharmaceutical Roundtable Solvent Selection Guides. Perhaps more importantly, it should also be considered that using other molecular descriptors or physicochemical properties besides the MDL Keys (e.g., other fingerprint descriptors, predicted hydrophobicity, etc.) would impact the similarity results such that other solvents could be returned and therefore differing classifications produced. For example, we have previously compared MDL fingerprints and long-range functional class fingerprint description 6 used with the Tanimoto Coefficient for the same sets of compounds for cross-reactivity with immunoassays for drugs of abuse and therapeutic monitoring and illustrated differences in the resulting values.[21] However, from previous studies, MDL Keys seem a useful starting point for such analyses.[19,21,22,36] Analysis of different approaches for inference of solvent categorization classification as well as similarity metrics (Tanimoto versus Euclidean versus Manhattan coefficients) are worthy of further exploration that is outside the scope of this present study. The value of such similarity predictions is that they could be used to assist and accelerate categorization of solvents and produce updated solvent selection guides. Such a similarity calculation could be readily implemented in the Green Solvents or other apps.

The use of the Green Solvents, Yield101, and ODDT apps are likely the first of many future green chemistry apps to be created by us or others. Later apps may provide educational value by describing the 12 principles of green chemistry,[1] presenting the latest news on this topic (as in ODDT), providing calculators for green chemistry metrics, or using crowdsourcing for enhancing collaboration in the field.[8] Mobile apps represent the latest paradigm in scientific communication, and a pursuit of green chemistry should exploit these new capabilities. Green chemistry apps can promote the topic effectively, which is also highly desirable.

■ ASSOCIATED CONTENT

Supporting Information

Table S1 (Excel) and Table S2 (PDF). This material is available free of charge via the Internet at http://pubs.acs.org.

■ AUTHOR INFORMATION

Corresponding Author

*E-mail: ekinssean@yahoo.com.

Author Contributions

‖These authors contributed equally.

Notes

The authors declare the following competing financial interest(s): Antony J. Williams is employed by the Royal Society of Chemistry which produces ChemSpider and ChemSpider Synthetic Pages mobile apps discussed in this article. Alex M. Clark is the owner of Molecular Materials Informatics, Inc., which has produced the apps described in this article.

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■ ABBREVIATIONS

ACS GCI, American Chemical Society Green Chemistry Institute
API, Application programming interface
GSK, GlaxoSmithKline
MMDS, Mobile molecular datasheet
ODDT, Open Drug Discovery Teams

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