MOBILE APPS FOR CHEMISTRY IN THE WORLD OF DRUG DISCOVERY

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Short Biographies

Antony J. Williams graduated with a Ph.D. in chemistry as an NMR spectroscopist. Dr Williams is currently VP, Strategic development for ChemSpider at the Royal Society of Chemistry. Dr. Williams has written chapters for many books and authored or >120 peer reviewed papers and book chapters on NMR, predictive ADME methods, internet-based tools, crowdsourcing and database curation. He is an active blogger and participant in the internet chemistry network.

Sean Ekins graduated from the University of Aberdeen; receiving his M.Sc., Ph.D. and D.Sc. He is Principal Consultant for Collaborations in Chemistry and Collaborations Director at Collaborative Drug Discovery Inc. He has written over 170 papers and book chapters on topics including drug metabolism, drug-drug interaction screening, computational ADME/Tox, collaborative computational technologies and neglected disease research. He has edited or co-edited 4 books.

Alex M. Clark graduated from the University of Auckland, New Zealand, with a Ph.D. in synthetic organometallic chemistry, then went on to work in computational chemistry. His chemistry background spans both the lab bench and development of software for a broad variety of 2D and 3D computer aided molecular design algorithms and user interfaces. He is the founder of Molecular Materials Informatics, Inc., which is dedicated to producing next-generation cheminformatics software for emerging platforms such as mobile devices and cloud computing environments.

J. James Jack graduated from the University of Aberdeen with a PhD in chemistry specializing in Organometallics, Vibrational Spectroscopy and Computational Chemistry. He currently works

for Accelrys Ltd. as an ELN consultant with over 10 years experience in the cheminformatics industry. He is a prolific programmer creating many chemistry applications in his spare time, including mobile apps.

Richard L. Apodaca received a Ph.D. in Chemistry from the University of Texas at Austin. He is currently founder and CEO of Metamolecular, LLC, maker of high-performance scientific data visualization components for web and mobile applications. Prior to this, he worked for 8 years as a medicinal chemist at a global pharmaceutical R&D organization. Richard has co-authored 15 peer-reviewed publications in synthetic and medicinal chemistry, and is co-inventor on 12 issued patents in the area of neuroscience.

Teaser Sentence:

Smartphones and tablet computers can now be used to perform many of the operations previously addressed by laptops or desktop computers and they represent an exciting new computing platform for drug discovery, particularly in chemistry.

Abstract:

Mobile hardware and software technology continues to evolve very rapidly and presents drug discovery scientists with new platforms for accessing data and performing data analysis. Smartphones and tablet computers can now be used to perform many of the operations previously addressed by laptops or desktop computers. Although the smaller screen sizes and requirements for touch screen manipulation can present user interface design challenges, especially with chemistry related applications, these limitations are driving innovative solutions. In this early review of the topic, we collectively present our diverse experiences as software developer, chemistry database expert and naïve user, in terms of what mobile platforms may provide to the drug discovery chemist in the way of apps in the future as this disruptive technology takes off.

Key words

Apps, Chemistry, Cheminformatics, Drug Discovery, iPad, iPhone, Android

Introduction

2011 is the International Year of Chemistry [1] and at a time when we are celebrating the impact of this science on the world we want to reflect on how new mobile computational technologies could make chemical information more accessible for drug discovery. Mobile devices in parallel with the advances in chemistry, have become more powerful and continue to influence our daily lives at an unprecedented pace, and as a result have been enhancing productivity [2]. Mobile computing has permeated into our everyday lives to such an extent that many expect to be online at any time of day, in any location. We can now use sophisticated

software applications (– “app” is the abbreviation we will use for mobile applications) in our hand that just a few years ago were restricted to desktop computers. Mobility is no longer expected to be limited to booting up a laptop computer but rather simply opening a handheld device that is always on and always connected, whether it is a smartphone or tablet device. It is likely that other classes of mobile device will soon become available. As scientists, and in particular chemists or those involved in drug discovery, we should be asking the question: When will mobile devices find their way into common use in scientific laboratories? Drug discovery is a domain of continuing change, and computational science has been embraced by the industry. It is essentially guaranteed that the possibilities provided by mobile devices will be accepted. What might this ‘mobile enabled future’ look like? What value could these mobile devices bring to drug discovery scientists? Are organizations ready to embrace mobile devices? We will address some of these questions in this article.

Shrinking device size - big vision for drug discovery

In just over 30 years, the use of computers in drug discovery has evolved from a few specialists using software to graph data and create documents, to daily data analysis in laboratories, computers on the desktop of every scientists and on most lab benches, access to in-house and public databases, and the utilization of complex computational modeling and simulation routines [3]. The turn of the century delivered an explosive expansion of websites for business applications where the user accessed software in the cloud and laptops and netbooks increasingly replaced PCs. In this decade, smartphones and tablet devices are now moving into roles once held by other forms of portable computers. The lines between laptops and tablets are blurring very quickly and with it the line between netbooks and smartphones.

In parallel we are also witnessing dramatic changes in the pharmaceutical industry including restructuring and a move toward increasing use of outsourcing for key R&D functions (commonly to offshore). This geographical dispersion of R&D activities has created a need for software to facilitate collaboration across company and national boundaries, to capture and integrate disparate data, and to process, analyze and visualize them in real time. Mobile devices represent the next chapter in the evolution of personal and business commuting and a tool the pharmaceutical industry and others involved in drug discovery could be leveraging at all stages of the drug discovery and development process (Figure 1).

The Apple iOS (on iPhones and iPads specifically) and the Google Android operating system have invigorated the computer market. For the consumer however the transition has been rather seamless as the internet browser is a generic interface to access a website via a URL, at which point they are accessing the same database via a desktop, laptop, tablet or hand-held phone. Mobility, very simply defined, is a new found capability to access people, data, and software regardless of physical location.

While the apps presently available on phones are generally rather simple their complexity is likely to escalate to the point where sophisticated business tools are apps on mobile devices. It is not really just an issue of compute power, as because this power is sitting remotely in the “cloud” with the mobile device as an interface. How apps fit into the changing laboratory environment will evolve over time. For example, they may start by serving as wireless access points to laboratory hardware, but then shift to more varied roles including collaboration tools, laboratory notebook, idea generation devices, prediction devices, and data mining tools.

The perfect storm: data availability, collaboration and mobility

The increasing pace of investment by governments to facilitate access to publicly funded scientific research and associated data (e.g. NIH, NSF, etc.), the agreement of the life sciences companies to collaboratively enable access to pre-competitive data (e.g GSK [4-6]), and the driving business need for pharmaceutical companies to improve their R&D efficiency and return on investments, is resulting in unprecedented access to data, information and knowledge via queries against online resources. The increasing prevalence of public domain databases and query engines/web services supporting the life sciences includes the PubChem database [7], the European Bioinformatics Institute-European Molecular Biology Laboratory databases (ChEMBL, ChEBI etc) [8], DrugBank [9,10], the Human Metabolome Database [11,12] and ChemSpider [13,14] has created an audience of drug discovery scientists to access data and capabilities that were previously only available to organizations behind firewalls and via expensive licensing. The expectation of immediate access to these online resources and tools on demand is now the *modus operandi*. In parallel, crowdsourced data deposition and curation [6] are gaining in importance and the increasing connectivity of mobile devices suggests that they will soon become part of the array of tools to facilitate scientific collaboration.

This “perfect storm” of available computing power in smaller devices, the adoption of internet standards to allow seamless browser access, the portability of code to support multiple platforms and the growing availability of both public domain and commercial databases supporting the life sciences can enable scientists in new ways. To date there has been little discussion of the role that such mobile devices could have apart from those focused on the “library in your pocket” enabled by publishers on mobile devices [15,16]. Later we will discuss how such technological innovations are already benefiting drug discovery and how this might expand and morph in the future, especially in the area of collaboration.

Apps for mobile devices

We are seeing the development of an app ecosystem. In general there are tools for creation (e.g. molecule drawing), look up (molecule searching), portals to other software (e.g. more sophisticated databases or informatics hosted on the web), educational (how to guides etc), recreational and gaming (flashcard tests, games, puzzles) and scientific content (mainly publishers). Supplemental Table 1 represents only a partial list of some of the apps that have evolved around chemistry. Until recently there has been no definitive source or reference of scientific apps. Later we will describe a Wiki that two of the authors (SE and AJW) have put online to host information regarding scientific mobile apps and although in its infancy, the content will grow through community adoption and crowdsourcing.

General Overview of Chemistry Apps

A recent review by one of us (AJW) outlined the new world of “Mobile Chemistry” and “Generation App”, [17] a generation of users who expect “an app for that” on their smart phone. Developers have responded to the new market opportunity with new applications that can be downloaded at no charge or purchased for a tiny fraction of the cost of desktop software. This has benefited not only the professional but also students by bringing “Smart phones into the classroom” [18].

Applications are already available for chemists to practice their chemistry skills, to access detailed tables of chemistry and drug-related data, to sketch small molecules and to view large biomolecules (refer to Supplemental Table 1). Simple smartphone apps can deliver facts and figures while chemical calculator apps provide utilities to allow bench chemists to calculate

molarities or the dilutions of stock solutions. Many chemical data tables associated with either the elements or chemical compounds are available and it is likely that we will see many of the standard data collections become available on mobile devices in the future (e.g. the Merck Index [19] and US Pharmacopeia [20]). In the authors view however, similar content may already be sourced directly from any of the numerous mobile interfaces for Wikipedia content and this may be a credible challenger in future. Detailed articles regarding most marketed drugs are freely available at Wikipedia, and continually expand without a need for “publishing” new editions every few years.

There are many examples of periodic table apps [21,22]. Mild EleMints [23] is a free example with links to Wikipedia pages and YouTube videos. Our chosen “gold standard” for an electronic form of the periodic table is the eBook “The Elements” as discussed below.

Structure Drawing

While ChemMobi [24], ChemSpider Mobile [25] and any of the multiple PubChem searching mobile interfaces (e.g [26]) offer text based searching of online databases, the development of touch-based interfaces to sketch chemical structures is already a maturing technology and a series of structure drawing apps are already available. The recently introduced MolPrime [27], a free app, demonstrates a straightforward workflow: draw a chemical structure, check its properties, then search a number of databases. MolPrime was developed based on the Mobile Molecular DataSheet [28] (see Figure 2) that is a foundation platform from which other apps have been developed (*vide infra*). ChemJuice [29] from IDBS is a simple molecule sketching tool which contains a facility to save molecules in a gallery, the ability to email molecules as .mol files and links to a periodic table. The recently introduced partner product for

the iPad, ChemJuice Grande extends the ChemJuice app to the iPad offering additional functionality that is more appropriate to the larger form factor [30]. The limitations of the on-screen keyboard relative to a touchpad and or mouse/keyboard combination has been adequately overcome using the touch gestures and this is likely to improve even further overtime as users become more used to touch-based systems.

Database Access

While the web browsers on mobile devices can access online databases for browsing there is also an increasing shift to lightweight apps dedicated to the platform. For ChemSpider [31], an online database containing information for over 26 million chemical compounds has recently added browser-based access, optimized for mobile devices [25] (see Figure 3). The capability was also extended to support the ChemSpider SyntheticPages [32] database of community crowdsourced chemical syntheses (see Figure 4). On the other hand, ChemMobi [32] is an iPhone/iPad based app and provides combined access to over 30 million chemicals from both the Accelrys DiscoveryGate and ChemSpider databases. The app allows for searching by chemical names or other identifiers and retrieves the chemical structures, calculated properties, safety data and commercial availability from over 860 suppliers (an Android version of ChemMobi is currently under development and future versions on iPhone/Android are anticipated to offer the ability to perform complex property calculations using Accelrys Pipeline Pilot via web services).

Mobile Reagents [33], from Eidogen-Sertanty, is an example of such an application: it provides lookup tools for a repository of structure data with vendor information and simple properties, as well as some properties that are calculated on the server side, including AlogP,

PSA, blood brain barrier penetration, aqueous solubility and human intestinal absorption. Structure searches are facilitated by an embedded structure editor derived from the Mobile Molecular DataSheet ([33], vide infra). The app also supports substructure and similarity searching capabilities and allows for the modification of structures to allow customized searches. MolPrime [33], described above, is a simplified workflow app that allows chemical structures to be drawn and then used for various purposes, such as evaluating simple calculated properties, copying to the clipboard as an image, communication via email, transfer to other apps via interprocess communication, or searching against the ChemSpider database.

Chemical Reactions

While chemical compounds and their associated properties are certainly of interest to chemists, chemical reactions, their balancing, search and associated details are similarly of interest to chemists. A number of reaction apps have already been released. Reaction101 [34] and Yield101 [35], the result of a collaboration between Molecular Materials Informatics and Eidogen-Sertanty, provide reaction editing capabilities, which makes them tools for content creation as well as content consumption. Reaction101 is an education-friendly app which provides tools for drawing reaction components and balancing reactions with correct stoichiometry. It also provides access to a collection of named reactions to which can be used as templates, and is integrated with the Mobile Reagents service, which allows searches to be carried out from within the app. Yield101 is a companion app that adds automatic calculation of and interconversion between mass, molar mass, volume, density, concentration and yield, with the help of stoichiometry and molecular weight, which is derived from the component structures.

An app called Green Solvents (see supplementary info) was recently developed of us (AMC) that lists solvents selected by a consortium organized by the ACS Green Chemistry Institute (GCI), with many pharmaceutical partners. This app lists solvents and scores (bad = 10) for safety, health, air, water and waste criteria. The App also motivated the addition of other green chemistry features into Yield 101 discussed above. The hope is that chemists around the world can learn about the environmental impact of the solvents they use to influence their selection and have a positive effect on the environment.

Named Reactions [36] allows searching of reactions by name and tag. The user can read reaction descriptions for historical context and follow links to related reactions. The user can learn what substitution patterns and which functional groups are tolerated by each reaction and can view each reaction mechanism in detail. ReactionFlash™ [37], associated with the Reaxys database from Elsevier is another app for providing access to named reactions and also includes a game mode (see Figure 5).

Biological Data

The overlap between biology and chemistry apps is likely great and their potential for integration into drug discovery has not been addressed. There are few data warehouse type apps yet apart from iKinase [38] which is a database of kinase inhibitor structures, biological data and references or patents and is searchable across all of this content. There are also a small number of kinase inhibitors listed with P450 inhibitor data for CYP2C9 and CYP3A4.

GenomePad [39] offers customizable searches across desired biological species, and maps from a genome assembly or specific chromosomal positions. GenomePad allows you to query any and all genomes present at the UCSC site [40].

The app-based visualization of biomolecules is possible with using Molecules [41] and provides 3D renderings available from the RCSB Protein Data Bank [42]. Mobile browser-based access to other public domain databases is likely to expand in the near future.

Publishers, Publications and their Management

Perhaps the area where apps are most advanced is in the area of publications. Scientists are a community committed to staying updated to advances in their field and commonly utilize a series of alert services to ensure that they stay informed. An increasing number of chemistry publishers are providing smart phone access to news stories and feeds of their latest publications (the latter usually for a fee). The abstracts are immediately viewable and the full text articles can be saved locally. The American Chemical Society iPhone app [43] searches over 850,000 research articles and book chapters by author, keyword, title, abstract, digital object identifier or bibliographic citation. PLoS, one of the community's primary Open Access publishers, has recently released an iPad app to allow users to peruse its content for PLoS Medicine [44]. The Nature Publishing Group has recently released an iPad-optimized app [45] and the Journal of Biological Chemistry [46] provides app-based access to their content. These are just a few of the many journals or publishers that have gone mobile. Distributed content from the publishers is not limited to access to papers but also they make podcasts available.

While not a chemistry app, the management of publications in the cloud (e.g. with apps such as Papers [47], (see Figure 6) and Mendeley [48]) is providing a rich set of intuitive tools that would be useful to chemists and drug discovery scientists alike. Seamless integration and access to a user's personal library of publications via desktop applications, browser-based access and apps on the iPhone and iPad enables easy management of a personal library of publications.

There are even apps that link to PubMed [49] such as “PubMed on Tap” [50] that optimize the capabilities of PubMed for the smartphone, e.g. abstracts fit to the screen page, rather than having to zoom in on a webpage.

eBooks

The explosion of e-readers such as the Kindle [51], Nook [52] or other similar devices has very quickly resulted in publishers clamoring to produce consumable ebook formats. The combination of the increasing popularity of ebooks and the willingness of people to read material on smartphones and tablets may make them even more popular for the delivery of instructional material. Publishers are already providing chemistry “texts” in this format. ebooks are, however, not just texts but are already being released as rich, multimedia experiences. Touchpress [53] appears to be leading the charge to demonstrate what can be delivered as a different experience as ebooks transform into apps. A recent example related to chemistry is “The Elements: A Visual Exploration” [54], (see Figure 7). This example offers access to videos, 3D images and stunning photography as demonstrated in the online multimedia demonstration [55]. While initially only available for the iPad the Elements was recently made available for the iPhone. Even though the investment to deliver such texts and instructional material is significant, software tools will make their delivery easier with time and viewing on mobile phones may become as commonplace as dedicated e-readers. Chemistry and drug discovery sorely needs authors that can make the subject matter accessible to a general reader and mobile devices may be the media to enable this.

Other Uses of Mobile Platforms

Apps as advertising vehicles

The chemistry marketplace is small in terms of potential app sales when compared with the much larger consumer market for games and entertainment applications. With the additional expectation of “Free” for many users, generating sufficiently high returns on investment can be difficult and alternative means by which to monetize apps are required. Many of the free or ‘lite versions’ of apps therefore use banner advertising as a revenue generating device. This may impede already limited screen real estate. However, business models involving the development of free or low-cost applications that serve as marketing tools for service-based industries related to chemistry and drug discovery may become viable. (e.g. chemicals, reagents, equipment and CRO testing facilities).

Augmented Reality

In recent years libraries and museums have initiated developments in augmented reality, the combination of digital information with images from the real world. There are two types of augmented reality commonly used on smartphones, markerless and marked [18]. Markerless augmented reality adds digital information to the image on a cell phone camera based on the Global Positioning System (GPS) location while marked augmented reality uses a reference point such as a two-dimensional barcode to connect a cell phone to information. Marked augmented reality is especially useful in a laboratory environment since it provides an easy way to connect information directly to a physical object or to place a web link on a sheet of paper or a book. Barcode-labeled smart objects could be very useful in a laboratory; a barcode on an instrument could connect the user to up-to-date operating instructions or even a video showing the correct use. Since instructions would be available via a web page and could be updated whenever necessary. A chemist could scan a bottle of a chemical and a series of database lookups could retrieve and display availability in the organization (room and contact details),

availability from external vendors (including pricing and availability), associated analytical data (spectral reference data), physicochemical properties, safety data, assay data from both internal and public domain databases and so on.

Optical Structure Recognition

Imagine being able to take a photo of a sketch of a molecule from a whiteboard, sheet of paper or a printout and use it as a query for a database search on a mobile device. This is not all that difficult to imagine in context and technologies already exist to perform optical structure recognition (OSR), namely CLiDE (Simbiosys Inc.) [56], OSRA [57] and ChemReader [58]. Recently, the Mobile Reagents app introduced the ability to perform optical structure recognition on iOS devices [59]. While OSR is imperfect in its conversion procedures, whichever software package is used, the ability to further edit the converted structure using a structure drawing package on the mobile device makes this technology viable.

A vision of how drug discovery can use mobile devices

Mobile devices and associated apps represent the flexibility of doing work anywhere, for example from seeing raw data, using compute intensive technologies on the cloud, mining public and private data, text mining and data visualization. It is not too distant a vision to imagine employees carrying around a smartphone or tablet computer, accessing their e-lab notebook, using internally created apps that calculate chemical properties specific to proprietary targets, mining the internal databases of structures and data while in parallel putting it in context with external data.

Mobile Devices, Collaboration and Games

In recent years we have seen a communal shift to greater collaboration across organizations, geographies and even political views and in particular a shift in thinking about collaboration for drug discovery facilitated by software [6,60-63]. Wikipedia has become the most popular central portal to a good proportion of written human knowledge and increasingly this includes information related to drugs and drug discovery. There is no going back from the social network that has developed on platforms such as Facebook, Twitter and a myriad of blogging and wiki'ing environments. Wikinomics [64] now drives entire businesses and mainstream cultural activities.

While the protection of intellectual property will need to continue to enable a business entity to retain intellectual property rights and build profits to sustain itself, there is a collective understanding now, even across the life sciences, that for too long pre-competitive data, experimental approaches and even software tools have been overly guarded. The era of pre-competitive collaboration is upon us. For example, the recently funded Innovative Medicines Initiative (IMI) funded Open PHACTS project [65] brings together over 20 organizations to focus on the production of a Linked Data Cache integrating data and concepts from a multitude of both public and private databases relevant to drug discovery. The project will agree on and adhere to standards that will enable and encourage other organizations to build applications (possibly mobile) and capabilities around the resulting triple store, facilitating a semantic web for the Life Sciences. One important aspect of this project, and many others, will be the call to action for the community to participate in crowdsourcing the data, both in terms of deposition and curation. One of the authors (AJW) is a member of the OpenPHACTS project leadership team

and can report that the application of mobile technologies for the purpose of data validation and annotation will be an important part of the project.

Any molecule-related database can be expanded, curated and annotated to increase the coverage, clean up the data and enhance the knowledge contained within. We have issued numerous calls to action regarding the need to develop a public ADME database [66], to encourage action regarding the quality of data in public databases and to participate in curation and validation. Many online data resources can already be enhanced using the standard web browser to login and curate and annotate the data. Examples include Wikipedia and ChemSpider. The “Million Minds Approach” suggested by Mons [67] would bring to bear the skills of scientists to map concepts in biomedical space, in particular small molecules, genes and diseases. Using continuous text-mining approaches to harvest concepts from the literature together with triggered alerts and notifications to a scientist of activities in their area of interest would allow that scientist to participate in tagging and concept mapping. Simple interfaces on mobile devices would make such activities very simple to execute but have not been developed as yet. It could be envisaged that such activities would not only be available to map relationships across public domain data but also intersect with similar activities inside an organization.

It is possible that gaming approaches could be applied to chemistry or drug discovery applications such as the Fold-It game [68] for human intervention in optimizing protein folding would become more popular if they were also delivered through an interface optimized for mobile devices. The Spectral Game [69] has utilized ChemDoodle HTML5 compliant components [70] to deliver spectral gaming via smart phones and on the iPad. This game is used to teach NMR spectroscopy by serving up NMR spectra and suggested structures via a public application programming interface from ChemSpider. The user has to match the appropriate

structure to the spectrum. The game becomes increasingly more complex varying from two potential structures per spectrum to five potential structures per spectrum with a time limit. Already played by tens of thousands of students and scientists around the world via simple web browser access its availability on the iPad will potentially encourage a new group of users to participate and provide comments regarding each of the spectra to expose incorrect data. This form of unintended collaboration was very much intended when designing the game!

Mobile devices offer a window into how scientists will operate in the future (research as a game with subsequent rewards both ‘real’ or ‘virtual’) equipped with such devices, these will further enhance the provision of collaborative software to biomedical scientists, an existing limitation being how much information you can show on a current mobile device screen. This is an area currently existing collaborative drug discovery platforms need to address which are optimized to the PC or laptop (e.g. CDD [71], HEOS [72] etc), The science of biomedical R&D may change in the years ahead and will more likely involve more crowdsourcing, pre-competitive collaborations and aggregation of data from diverse sources. We see opportunities for app vendors, publishers and companies to create more useful apps for collaborative drug discovery that impacts how we do research and development.

IT Organizations and Mobile Devices

One of the growing challenges for corporate IT organizations (and this is not limited to those with chemistry apps) is ensuring security as the loss of a single mobile device could can endanger proprietary information for an organization, not only because of what might be stored locally on the device but more so the login information to internal resources that could be stored. Fortunately the iPhone and iPad devices already allow remote wiping of the device [73]. With

the built in camera and high resolution displays already available we can envision iris or facial recognition software being required for login on these devices very shortly. Even fingerprint reading is not out of the question. While the challenges are not insurmountable the costs for an organization to deal with many of these challenges may be the primary hurdle. For example, while Windows 7 is already a tried and tested operating system in the public sector, many companies remain committed to Windows XP as the hurdles to updating an operating system (OS) to support all internally developed applications and platforms integrated to the OS is enormous. Such corporate rollouts across an international organization can cost many tens of millions of dollars, with a minority of the costs dedicated to the purchase of operating system licenses. Such challenges are very real in regards to a company not being able to use modern, convenient and enabling technologies and, ultimately, an organizational IT infrastructure could become very fragile if they lag too far behind.

Additional Challenges

What are the challenges ahead for mobile devices? One of the biggest chemistry related challenges is ergonomic data input tools, particularly on the smaller screen sizes of smartphones. Quite possibly the biggest challenge for developers of mobile chemistry software is the need to provide a chemical structure editor. While modern devices are far more powerful than the desktop computers that were originally used to run structure editors such as ISIS/Draw and ChemDraw, the tiny screens and absence of an accurate pointing device renders the traditional mouse driven user interface paradigms impractical. The toolbar/click/drag approach to drawing molecular entities is all but useless on any phone-sized device, and does not perform well on touchscreen tablets. Since many chemistry software applications require the sketching of a

chemical diagram as part of their workflow, it is necessary to re-imagine ways to provide a drawing interface that is well suited to the user interface constraints of a mobile device.

Some innovative solutions have been proposed such as a chemical structure editor based on fundamental drawing capabilities developed by Molecular Materials Informatics [74]. This editor, specifically tailored to the limited screen sizes of smartphones, uses an innovative set of context-specific menu options and intelligent chemical reasoning to guide structure drawing. This tool appears in the Mobile Molecular DataSheet and Mobile Reagents [33] apps, discussed earlier, among others.

Another challenge is financial, who pays for app development which is essentially another content delivery device? This is akin to having multiple platforms for music, we already have the web as an interface and now we need software so that small devices can view chemistry content. Naturally the providers are footing the bill for app development in an attempt to reach a new market, the early adopters. There may be a space here for entrepreneurs to find gaps such as what is missing from the app ecosystem and how can we source content cheaply or freely to wrap in an app? This clearly suggests there needs to be venture capitalists or some funding mechanism for scientific app development, similar to small short term grants like SBIR or STTR [75] to foster this innovation in the USA and perhaps give some of our recently redundant chemists a new challenge.

Software Development for Mobile Platforms

A high level of sustained innovation in the mobile device space has resulted in a number of approaches to developing mobile apps. We have identified three development styles in common use today: (1) native apps created with the device's Software Development Kit (SDK);

(2) HTML apps designed to be run within the device's web browser; and (3) hybrid apps that run natively, but which are primarily created using browser technologies. (See Supplemental Text for more details).

Viewing and manipulating scientific datasets on mobile devices will require access to custom software libraries. This is especially true for chemists who have become accustomed to viewing and interacting with their graphical data in real-time. For native app development there is only one commercially supported developer toolkit in chemistry, MMDSLib [76] but, at the time of writing, this is not available to the general public. For HTML and hybrid mobile app development, however, three tools are now available:

- ChemWriter by Metamolecular [77] is a JavaScript library that enables the display and editing of chemical structures. Written in JavaScript, ChemWriter runs unmodified on both older desktop browsers including Internet Explorer 6, as well as mobile browsers including Safari on iPad.
- ChemDoodle Web Components by iChemLabs is a suite of chemistry tools for both structure display and editing, as well as spectral visualization [70]. Recently, a mobile application based on ChemDoodle was released on both the Apple and Android App Stores [78].
- JSDraw by Chemene is a chemical structure editor and viewer written in JavaScript [79]. In partnership with Eidogen-Sertanty, JSDraw has been incorporated into the iOS application iKinase [38].

While newer mobile devices are equipped with a state of the art, standards compliant web browser, the performance difference between a native app and one built using JavaScript/HTML/CSS is significant, and allows native apps to provide a distinctly more fluid

user experience. However, due to the rapid pace of hardware and browser innovation, the importance of this gap is quickly narrowing, and the advantage of supporting all mobile devices with a single codebase makes for a compelling incentive.

Mobile Devices and Laboratory Informatics

Of all the characteristics differentiating mobile devices from laptops and desktops, we believe two ergonomic factors in particular have the greatest potential to drive rapid adoption in drug discovery: touch interface and form factor. The touch interface represents the first significant mainstream change in human-computer interaction since the popularization of the graphical user interface and mouse in the 1980s [80]. Tightly coupled to the touch interface is a flat, rectangular, often keyboard-less form factor offering a more comfortable working environment than laptops in many poses: standing; sitting without a desk; reclining; and walking. It therefore seems reasonable to expect mobile devices to make the most immediate headway in those drug discovery activities requiring extended maintenance of one or more of these poses.

We see two main ergonomics-based entry points for mobile devices in drug discovery in the near future: (1) front-ends for laboratory instruments; and (2) interfaces to electronic laboratory notebooks (ELNs). Isolated examples of the former have begun to appear. For example, Shimadzu recently announced updates enabling the control of some HPLC instruments using an iPad [81].

In addition to ergonomics, the continued miniaturization of scientific instruments may also play an important role in the adoption of mobile devices in drug discovery. Two examples include picoSpin, a 45-megahertz tabletop NMR spectrometer [82], and the Vernier Mini GC [83]. As the number and types of environments suitable for these miniature instruments

continues to expand, the ergonomic and portability features of tablet computers and smartphones are likely to fill an increasingly important niche as controllers and data viewers. The same factors are already showing promise in medical diagnostic devices, where smartphones can enable new ways to data capture and analyze data [84].

With Pharma investing large sums of money in traditionally desktop bound ELN implementations, how can that investment be protected and exploited in the world of mobile apps? One obvious solution is to make use of readily available remote desktop type software. This would allow users, for instance working in a lab, to interact fully with their traditional desktop. A good example might be a user working with an automated balance where data is pulled from the balance directly to the ELN, but the user needs to be able to weigh out a sample and interact with the balance from inside the ELN. By providing access from a mobile device the user gets the best of both worlds – a desktop that they really can “carry” but also access to their familiar ELN system.

Naïve user perspective

One of us (SE) prior to writing this article had not used a smartphone or tablet computer before. A naïve user perspective presents us with new ways to see apps compared to that of the long term user. For example, looking at the apps for the iPhone it became apparent that one can go from searching for a drug that one might read about in an article to finding it with ChemMobi. Then suppliers can be found, along with some simple molecular properties etc. But still we are left with what can the user do with this information next? How does one save the structure or send it to email? Some options are not always intuitive and the help functions on apps are not developed or available. With Mobile Reagents one can search known structures, then find

vendors and email the results to yourself. The user can then find some relevant ADME calculations. What if they wanted more? Where are the tools for custom descriptor calculations? How does the user run small libraries of compounds? All the chemistry apps are very limited in functionality and in sum they represent just one of two key features (search, draw, retrieve pre-calculated properties). Could several apps be linked together, to form a pipeline of a whole process? Could I draw a structure with one tool, calculate properties with another, run similarity against the tens of millions compounds in the various database apps, aggregate results and present as a simple scrolling table, perhaps another App would enable graphical visualization of properties? The tools would have to be smart enough to enable this connectivity. Alternatives include web-based tools like ChemSpider using the internet connection but, to date, there is no comprehensive chemistry solution in the form of an app. Many of these are questions other naïve users will ask and it is important that user testing of apps by developers captures this feedback to ensure users have the most productive and intuitive experience possible.

Conclusions

Scientists with mobile devices can currently access a virtual information commons that is equivalent to the holdings of a major research library. There is every indication that prices for both devices and connectivity will decrease and there will be an ever increasing number of chemistry applications (both free and licensed) that enhance the usefulness of the devices.

While it is unlikely (but not unthinkable) that e-readers will be distributed across life science organizations to distribute reading materials, it *is* likely that tablet devices, such as the iPad, will become increasingly popular inside corporations, and our experience from attendance at conferences tells us that a good percentage of attendees already have them. There are many

apps useful to business users, but fewer so far for chemists and other scientists, involved in drug discovery.

Where do we go from here? In our opinion it is likely that there will be widespread adoption of mobile devices and apps inside pharmaceutical companies and academia, both for data storage, data sharing, and both internal and external collaboration. In parallel, we will need to see a greatly increased number and variety of apps that cover as many stages of the drug discovery process (as shown in Figure 1). In addition, data content could become focused in small slices in the same way iKinase is focused on one target class, similar types of databases could be created around other targets of high interest in the industry. Mobile devices represent an opportunity for cheminformatics companies [85] and academic groups to put their technologies into the hands of a much larger user base to augment the computational and informatics capabilities of individual scientists.

Despite the impressive array of capabilities represented in this article, mobile technologies are only in their infancy. Even the commonplace term “iPad” was only introduced in April 2010 [86]. Already scientists are viewing spectra, viewing proteins and navigating genomes on this device. Evidenced by their investments, publishers see smartphones and tablets as critical delivery vehicles for scientific content and online databases are already searchable in ways that only a few years ago were possible only on powerful desktop computers. Mobile technologies are the latest iteration in a world of improved accessibility in which we are online all the time. Drug discovery scientists, such as chemists, are sure to benefit as they become more connected to their data and collaborators by going mobile. Writing this article motivated two of us to set up a Wiki (at <http://www.SciMobileApps.com>) as a dynamic listing of mobile apps for science, as the field is so young we envisage rapid growth around drug discovery apps [87]. This

is also indicative of how scientists will continue to garner value from the increasingly popular mobile platforms in all of their formats.

Acknowledgements

We thank Steven M. Muskal and Maurizio Bronzetti, from Eidogen-Sertanty, for providing copies of the iKinase and Mobile Reagents apps for testing.

Conflicts of interest

Antony J Williams is employed by The Royal Society of Chemistry which produces ChemSpider and ChemSpider Synthetic Pages mobile apps and is one of the hosts of the SciMobileApps wiki discussed in this article. Sean Ekins consults for Collaborative Drug Discovery, Inc. and is the co-host of the SciMobileApps wiki. Alex Clark is the owner of Mobile Molecular Informatics and the developer of the Mobile Molecular DataSheet, Reaction101, Yield101 and MolPrime apps discussed in this article. Richard Apodaca is the owner of Metamolecular, the developer of the software product ChemWriter discussed in this article.

Supporting Information Available

Supplemental material is available online

ABBREVIATIONS

ADME, absorption, distribution, metabolism and excretion; apps, applications; CDD, Collaborative Drug Discovery; CROs, clinical research organizations; GSK, GlaxoSmithKline; HEOS, hit explorer operating system; HTML, hypertext markup language;

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Figure Legends

Figure 1: The schematic shows the linear process of drug discovery and development alongside areas where we think mobile computing tools could be implemented.

Figure 2. Screenshots of the various screens associated with the Mobile Molecular Datasheet.

Figure 3: An example of how a website can be adjusted for mobile applications on smart phones using the Royal Society of Chemistry's ChemSpider as an example.

Figure 4: Screenshots from the Royal Society of Chemistry's ChemSpider SyntheticPages.

Figure 5: Screenshots of Elsevier's Reaxys ReactionFlash^{TM} app.

Figure 6: Screenshots of the iPhone Papers app.

Figure 7: A screenshot of the data page of the element Hafnium taken from Touchpress's "The Elements – A Visual Exploration". Note the integration to the Wolfram Alpha computational engine.

Figure 1

Figure 2

Figure 3

ChemSpider - Home

cs.m.chemspider.com/ Google

Mobile version | [Full version](#)

ChemSpider
Building community for chemists

Systematic Name, Synonym, Trade Name, Registry Number, SMILES or InChI

Search

RSC | Advancing the Chemical Sciences

ChemSpider

Properties | [Predicted](#) | [Identifiers](#) | [RSC](#) | [Google](#)

Chemical structure of 1-methyl-2-phenyl-4-chloro-1H-benzotriazole.

Property	Value
ChemSpider ID	2034
Empirical Formula	C ₁₇ H ₁₃ ClN ₄
Molecular Weight	308.7649
Nominal Mass	308 Da

Chemical structure of 1-methyl-2-phenyl-4-chloro-1H-benzotriazole.

Property	Value
ACD/LogP	2.499
ACD/LogD (pH5.5)	2.5
ACD/BCF (pH5.5)	46.67
ACD/KOC (pH5.5)	544.74
ACD/LogD (pH7.4)	2.5
ACD/BCF (pH7.4)	46.71
ACD/KOC (pH7.4)	545.23
# of Rule of 5 Violations	0
#H bond acceptors	4
#H bond donors	0
#Freely Rotating Bonds	1
Polar Surface Area	43.07

Figure 4

Mobile version Full version Back to Search Nucleophilic substitution at benzyl halide with azide; (azidomethyl)benzene SyntheticPage 408 DOI: 10.1039/SP408 Submitted May 06, 2010, published May 06, 2010 Suzanne Elizabeth Howson (s.e.howson@warwick.ac.uk) A contribution from Scott group, Warwick University Chemicals Used Benzyl bromide	Procedure Benzyl bromide (2.0 ml, 16.84 mmol, 1.0 eq.) was dissolved in DMSO (40 ml). Sodium azide (1.64 g, 25.26 mmol, 1.5 eq.) was added as a solid and the reaction mixture was stirred overnight at ambient temperature. Water (75 ml) was added <i>slowly</i> (exothermic) before extracting the product into diethyl ether (3 × 150 ml). The combined diethyl ether layers were washed with brine (2 × 150 ml), dried over sodium sulfate and the solvent removed to leave a clear oil which was sufficiently pure for use in further reactions (see uploaded NMR spectra) and gave a reasonable combustion analysis. Yield = 1.63 g, 12.24 mmol, 73%. Author's Comments Organic azides are energy-rich molecules and there is a risk of explosion. You should perform a risk assessment. See also Kolb, H.C., Finn, M.G., Sharpless, K.B. Angew. Chem. Int. Ed., 2001, 40, 2004-2021. Data ¹H NMR (400 MHz, 298 K, CDCl₃) 7.42-7.32 (5H, m, Ph), 4.35 (2H, s, CH₂).

Figure 5

Figure 6

Figure 7

Supplementary Table 1: A list of chemistry specific apps – A current listing is available at www.scimobileapps.com

ACS Mobile: Provides up-to-the-minute access to recent peer-reviewed research publications across the Society's research journals, including the Journal of the American Chemical Society.

Buffers: A tool for designing buffer solutions for pH control. Buffers is useful both as a handy reference of available buffering agents and as an accurate, portable buffer calculator for chemical, biochemical and biological research.

ChemDoodle Web Components: While not specifically an iPhone/iPad app these web components allow chemical depiction on all platforms

ChemMobi: A tool for Chemists, Biochemists and anyone else interested in chemical structures, chemical sourcing, chemical properties and safety information. ChemMobi uses Symyx, ChemSpider and DiscoveryGate web services to access online chemical information.

Dilutions: Contains several calculators that help perform serial dilutions, molar and percentage calculations as well as make SDS-Page gels.

Green Solvents: Shows commonly used solvent structures and their scores for safety, health, air, water and waste criteria.

iKinase: Search for Kinase targets by standardized names, identify top-active molecules for each target, and drill-down into more detail.

iKinasePro: Provides access to the most recent release of the Eidogen-Sertanty's Kinase Knowledgebase (KKB), but you can also survey this large database with substructure-, similarity-, and super-similarity searches.

iProtein: Provides access to the world's largest repository of protein structures and models - Eidogen-Sertanty's Target Informatics Platform (TIP) that enables researchers with the ability to interrogate the druggable genome from a structural perspective.

IR Spec Check: Designed for organic chemists and students to quickly analyze absorbance peaks from an infrared spectroscopy graph. IR Spec Check recognizes over 75 absorbance frequencies and matches frequencies with possible R-groups.

Mobile Molecular Datasheet: Provides ways to view, edit and organise chemical structures, reactions and auxiliary data in the form of datasheets, and offers numerous methods for communicating chemical data. Allows publication quality diagrams to be drawn quickly on a phone- or tablet-sized form factor.

Mobile Reagents: Provides access to over 5 million molecules and 11 million product variations offered by more than 50 suppliers. The database of reagents can be searched by exact or partial name and formula, or by finger-drawing a complete or partial structure, or by using the camera to take a photograph of a chemical structure and having it automatically converted into a structure search query.

Molecules: An application for viewing three-dimensional renderings of molecules and manipulating them using your fingers.

MolWeight: A simple tool for scientists and students that allows calculation of the molecular weight and other key properties of peptides and oligonucleotides from their sequence. In addition, a calculator is provided for determining the molecular weight of any substance from its chemical formula.

Name Reactions Lite: This is the free version of Named Reactions Pro, which contains over 250 organic

NIOSH Chemical Hazards: In addition to the complete contents of the pocket guide it includes the following enhanced functionality: - Searchable Index of Chemical Names, Synonyms and Trade Names - Searchable index of CAS Numbers - Searchable index of RTECS Numbers.

Reaction101: A chemical reaction editor with features for reaction balancing. A list of common named reactions is available for use as starting templates. Individual reaction components can be easily searched by name, formula, structure or structure similarity methods.

Yield101: The companion app for Reaction101, which adds quantity information to reactions. Enter any data that is available, e.g. mass, molar mass, volume, density, concentration or yield. The app will use molecular weight (calculated from structures) and stoichiometry to derive any of the missing quantities, saving laborious calculations and manual checking.

Supplemental information: Software development

Native apps enable close integration with both the hardware and software of a mobile device. Benefits of this approach include consistent look and feel with other native apps, and access to specific hardware capabilities. Choosing to develop a native app requires selection of a hardware platform, and in most cases a software platform as well. The three most important mobile software platforms at this time are iOS from Apple, Google Android, and Blackberry OS. (Microsoft reportedly plans to release its own Tablet OS in 2012. (<http://www.businessweek.com/news/2011-03-04/microsoft-said-to-plan-windows-release-for-tablets-in-2012.html>) iOS devices are currently only produced by Apple, Inc. and Blackberry OS devices are only produced by Research In Motion, Inc. Android devices, in contrast, are sold by a wide array of hardware manufacturers. Whereas the single-vendor approach exemplified by Apple and Research In Motion helps ensure the consistent user experience, the more open approach taken by Google offers vendor-independence.

HTML apps offer an attractive complement to native apps, due to the ubiquity of modern web browsers on mobile devices and the increasingly competitive mobile hardware and operating system landscape (<http://www.gartner.com/it/page.jsp?id=1622614>, http://www.wired.com/magazine/2011/04/mf_android/). Most mobile web browsers now support HTML5, the next major revision of the HTML standard that offers many features ideal for creating mobile applications. Some of these features include: dynamic, evented vector graphics manipulation through Scalable Vector Graphics (SVG); dynamic raster image creation through the canvas tag; embedded video and audio via the new “video” and “audio” tags, respectively; geolocation; the ability to create standalone client applications through the “cache manifest”; and convenient storage and retrieval of large amounts of arbitrary data via “local storage”

[<http://diveintohtml5.org/>]. Although these capabilities can go far to reduce the differences between native and HTML apps, in some cases the better performance and user interface integration available in native apps will be a deciding factor.

For teams seeking both tight mobile platform integration and flexibility to deploy on a number of different devices, hybrid apps offer an alternative worth considering. Hybrid mobile apps blend software written using web browser technologies (HTML, CSS, and JavaScript) with native code enabling tight integration with the host platform. The main advantage of this approach is much easier deployment across a range of mobile platforms. Two popular development frameworks in this space are Titanium Mobile from Appcelerator Inc (<http://www.appcelerator.com/products/titanium-mobile-application-development/>) and PhoneGap from Nitobi Software (<http://www.phonegap.com/>).