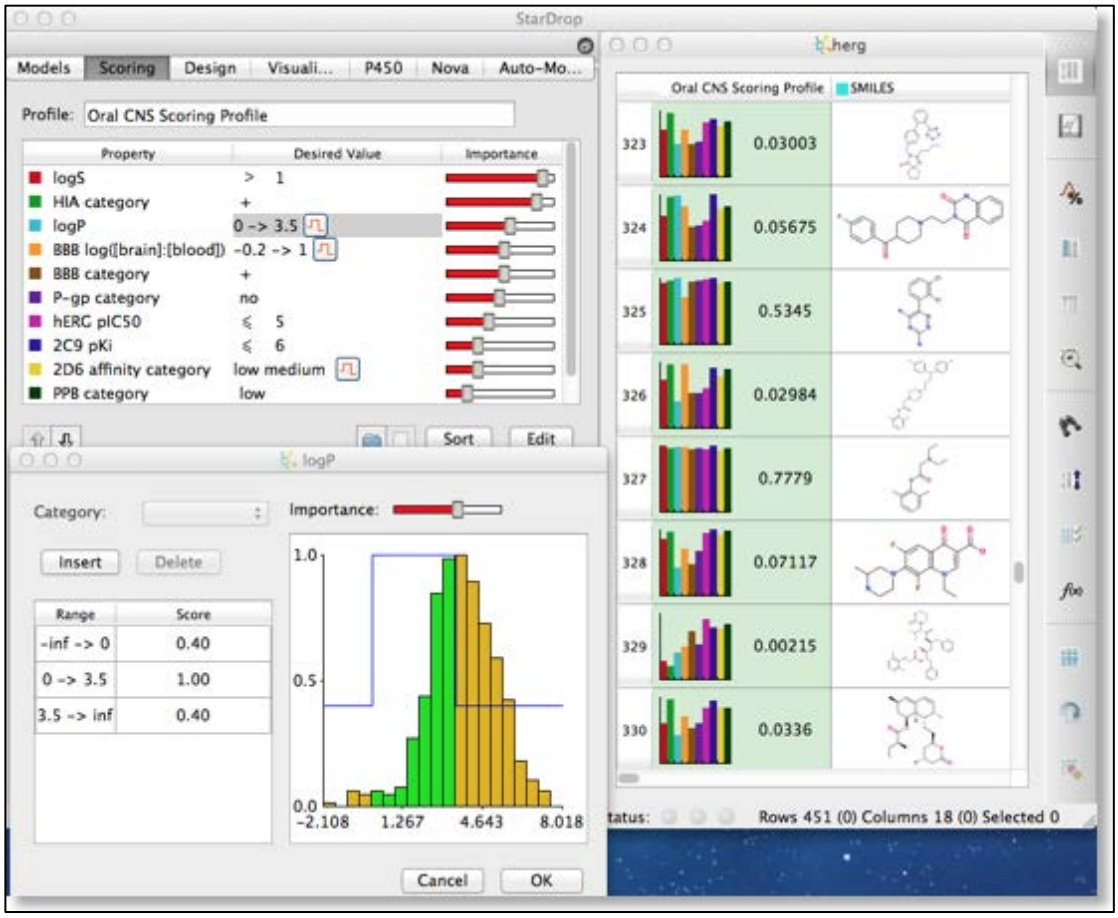
ROYAL SOCIETY OF CHEMISTRY | CHEMICAL INFORMATION AND COMPUTER APPLICATIONS GROUP

NEWSLETTER winter 2016-2017



See 'Meeting Report: Cheminformatics for Drug Design: Data, Models and Tools', page 13

CICAG aims to keep its members abreast of the latest activities, services, and developments in all aspects of chemical information, from generation through to archiving, and in the computer applications used in this rapidly changing area through meetings, newsletters and professional networking.

Chemical Information & Computer Applications Group: http://www.rsc.org/CICAG

http://www.linkedin.com/groups?gid=1989945

MyRSC http://my.rsc.org/groups/cicag

https://twitter.com/RSC_CICAG

QR Code

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Contributions to the CICAG Newsletter are welcome from all sources - please send to the Newsletter Editor:
Stuart Newbold, email: stuart@psandim.com

Chemical Information & Computer Applications Group Chair's Report

Contributed by RSC CICAG Chair Dr Helen Cooke, email: helen.cooke100@gmail.com

2016 has seen the CICAG Committee working on a diversity of activities to support our members, including scientific meetings, sponsoring a student bursary and the Tony Kent Strix Award, building our social media presence. You'll find articles about all of these within this Newsletter.

During the second half of the year, we organised two successful scientific meetings in Cambridge: *Chemistry on Mobile Devices* and *Cheminformatics for Drug Design* (the latter in collaboration with the Society of Chemical Industry). We are finding that partnering with other RSC interest groups, and external organisations (the joint meeting with the SCI being an example), can be very worthwhile, providing opportunities for developing shared interests, widening our network of potential speakers and broadening our audience for events. With this in mind, in the next couple of years we are planning events with the RSC's Molecular Spectroscopy and Historical interest groups, and also external organisations and programmes including Dial-a-Molecule and the Chemical Structure Association Trust. If you know of, or are a member of, other groups or organisations who might like to work with us on events or other activities concerned with chemical information and computer applications please get in touch – we are keen to explore new opportunities.

We are also seeking to broaden our outreach by holding some events outside London. In 2017 we will be running a meeting on 22 June in Liverpool, entitled *Chemical Structure Representation: what would Dalton do now?* More information about this is provided in a separate article in this Newsletter.

We are also aware that not everyone can travel to face-to-face meetings, so for 2017 we are also exploring the possibility of running webinars, probably one hour duration, on specific topics. The first is likely to be in partnership with the RSC Library, on the RSC's Historical Collection. Look out for further information via our social media channels and in future CICAG Newsletters.

Concerning social media, we are pleased to announce that our Social Media Editor, Michelle Lynch, will be setting up a Facebook page for CICAG and we envisage this will be an informal way for CICAG members and others who share our interests to get in touch and discuss ideas.

We are always pleased to hear from CICAG members with ideas for future activities and how we can better engage with our members. Please get in touch with your suggestions via email or social media – we look forward to hearing from you.

Undergraduate Research Bursaries - 2016 Report

Contributed by RSC CICAG Chair Dr Helen Cooke, email: helen.cooke100@gmail.com

As mentioned in the summer 2016 Newsletter, CICAG sponsored an Undergraduate Research Bursary this year which was awarded to Abigail Hanby, who is studying chemistry at the University of Oxford. Abigail's research project was at the University of Leeds, where she was working in Professor Steve Marsden's group on lead-oriented synthesis and making novel scaffolds for medical chemistry discovery based upon a new dearomatising diamination reaction. Professor Marsden has published (see *Chem. Commun.*, ***2016***, *52, 7209-7212. DOI: 10.1039/c6cc03244c*) on the development of LLAMA as a tool for analysing lead-likeness and molecular novelty and Abigail applied this to her novel scaffolds.

Abigail has summarised her experience and research outcomes:

> "During the summer I spent eight weeks working for Professor Steve Marsden at the University of Leeds. As part of the Marsden group I helped to create novel compound libraries as part of the European Lead Factory project. With the continuing decline in the rate of new drug discoveries, it is important to look at new ways to design and synthesise drugs. I was therefore extremely interested in this project. It was also fascinating to see during my time at Leeds that the line between industrial and academic research in drug discovery is becoming increasingly blurred.
>
> For this project I synthesised my own lead compounds using a novel dearomatisating diamination reaction. Once I had created a compound I was then able to use computer programs to predict the lead-likeness of the scaffold. This computer program was able to prepare a virtual library of functionalised compounds by taking the deprotected scaffolds and combining them with different capping groups that are common in medicinal chemistry. It was exciting to see that the scaffolds I had created were diverse, novel and lead-like. Overall my project was very successful.
>
> However, through this project I was also shown the reality of research, as reactions did not always 'work' the way they were expect to. Despite this I learnt a lot from this intensive practical experience and enjoyed it immensely. I particularly liked having the opportunity to carry out research at a different university to where I am studying for my undergraduate degree. It was interesting to see the similarities and differences between the universities and I enjoyed getting to know new people in a different environment. As a result of this experience I am now keen to pursue a career in research. "

In September Abigail returned to Oxford for the fourth year of her degree course. During this final year, she is working for Professor S.G. Davies. The Davies group is currently working on a wide variety of topics including development of new synthetic methodology, total synthesis, and collaborative projects in medicinal chemistry. This therefore fits in and complements the work that she has undertaken during the summer.

Undergraduate Research Bursaries – CICAG Sponsorship in 2017

Contributed by RSC CICAG Chair Dr Helen Cooke, email: helen.cooke100@gmail.com

As in previous years, a number of Undergraduate Research Bursaries, funded by the Royal Society of Chemistry, will be available to students in UK and Republic of Ireland Chemistry and related departments from June-September 2017. The purpose of the awards is to give to undergraduates with research potential in the middle years (i.e. 2/3, 2/4 or 3/4) of their degree and to encourage them to consider a career in scientific research. CICAG will again be sponsoring one student project in 2017 and applications will be welcomed in the areas of cheminformatics, chemical information, chemical data management, chemistry data analytics, chemistry IT solutions and applications. Applications for UG Bursaries 2017 open on 16 January and close on 27 February 2017.
Further information, including guidelines, the application form and deadlines, can be found at http://www.rsc.org/ScienceAndTechnology/Funding/undergraduate-bursary.asp

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RSC CICAG Social Media

Contributed by Dr Michelle Lynch, RSC CICAG Social Media Editor, email mklchems@gmail.com

CICAG runs a number of social media feeds including LinkedIn, Twitter and MyRSC. In 2017 we will add a Facebook group to this list. The current social media platforms broadly serve two important purposes - one being to publicise information specifically related to RSC CICAG's activities, e.g. meetings, events, news, publications and announcements, and the second to disseminate web links on topics relevant to our members and the wider chemical information and computer application community.

Our social media feeds are open to individuals and organisations with interests and activities that fall under RSC CICAG's remit as described above. Only RSC CICAG MyRSC is restricted to RSC members - one does not need to be a member of the RSC or RSC CICAG to follow our Twitter feed or to become a member of the Linkedin group.

Our Twitter feed had its five year anniversary in December 2016. It has grown both in numbers and in its coverage of not only traditional information science and chemical information publications, but also more aspects of computational chemistry, cheminformatics, advanced and digital manufacturing.

Taking a look at our Twitter statistics - we now have 373 followers, up from 229 in December 2015. Key topics of interest for our followers are science and technology news, biology, chemistry, biotechnology and medicine. Almost half of our followers (48%) are based in the UK, with the second most popular location being the USA (16%) and in third place India (6%).

The popularity of our tweets is always of interest to us. As of writing, we've tweeted around 200 times in total since the beginning of September. Some popular tweets from the last 3 months are shown in the table below, sorted by engagements. Twitter engagements include the number of times the audience clicks on the pictures, links or hashtags in the tweet, the RSC CICAG profile, or quotes, replies to or retweets the tweet. Twitter impressions relate to the number of times the tweet has been delivered to a user's account. A quote or retweet from a user with more followers therefore results in higher total impressions.

Recent articles with high popularity as judged by the tweet's exposure statistics relate to stories about the RSC Time4Chem initiative. Time4Chem was intended to be an opportunity for RSC members to help celebrate the RSC's 175th Anniversary by dedicating 175 minutes of their time to a chemistry related activity and to share their story. Our top recent tweet is an interview by the RSC with chemist and active Twitter user, Dr Nadine Borduas who tweets on the subject of "RealTimeChem". RealTimeChem is quite literally the study of chemistry measured in real time, often on mobile devices. Perhaps not surprising that our audience and followers show a preference for such inspiring stories about "real people" in our community; live coverage with photographs of RSC CICAG's events also stimulates a high number of Twitter engagements.

The growing importance of artificial intelligence and advanced manufacturing is reflected in our Twitter statistics, while traditional topics of big data, drug databases and libraries, chemical publishing trends and information for chemical education all still feature heavily.

We hope our Twitter followers and other social media members have enjoyed a positive experience of RSC CICAG social media in 2016 and would love to hear from you with any suggestions for topics to include for 2017.

Top 20 Most Popular Tweets Sept-Dec 2016 on the @RSC_CICAG Twitter Feed

Title of Tweet and Hashtags	Impressions	Engagements
#Where #Time4Chem meets #RealTimeChem	957	45
The Future of Artificial Intelligence and Cybernetics #AI	455	32
RSC CICAG Conference: Chemistry on Mobile Devices off to a great start! #RealTimeChem	482	27
A hands-on approach to chemistry with 3D printed molecules #3Dprinting #Chemspider #chemed	986	22
All together now: Why research papers have so many authors	779	20
#Insilico study of in vitro #GPCR assays by #QSAR modeling	260	17
Batch and flow: united at last #flowchemistry #realtimechem	922	16
Keynote Speech by Les Ebdon Director from Office for Fair Access on #diversity in Chemical Education #RSCGA16 #chemed	461	16
'Robo-chemist' optimises reactions in one day #flowchemistry #realtimechem #robotics #catalysis	1205	15
Our journals celebrate the winners of the 2016 Nobel Prize in Chemistry	639	14
Lufthansa Technik Flies with Mindbreeze InSpire #bigdata #KM	475	14
From haystack to needle: finding value with #DNA encoded library technology at GSK	732	13
York University gifted £1m for 'world-leading' chemistry research #chemed	420	11
New Approach to Computationally Designing Drugs for #GPCRs #supercomputers	383	11
The Future of #Spreadsheets: A workshop bringing together academia and industry... #bigdata	267	11
Royal Society of Chemistry President Sir John Holman giving the welcome address at RSC General Assembly 2016 in Belfast #RSCGA16	208	11
Materials #informatics: a journey towards material design and synthesis #bigdata	414	10
Prof Maristella Agosti, from the University of Padua, accepting the 2016 Tony Kent Strix Award	336	10
The death of the Job plot, transparency, open science and online tools #openaccess #supramolecular	311	10
A comprehensive analysis of #drug #repurposing #workflows published by...	594	8

Open Source Malaria Project Data

Contributed by Dr Chris Swain, email: swain@mac.com

The Open Source Malaria project (OSM) (http://opensourcemalaria.github.io/NewSite/) is trying a different approach to curing malaria. Guided by open source principles, everything is open and anyone can contribute. To date a lot of people around the world have made contributions and the project is at a very exciting stage. Whilst everyone can see the compounds that have been made and the biological data, historically it was spread over multiple web pages and it was impossible for newcomers to link molecule identifier with data. Over several months a significant effort was put into populating a spreadsheet with all the information (http://docs.google.com/spreadsheets/d/1Rvy6OiM291d1GN_cyT6eSw_C3lSuJ1jaR7AJa8hgGsc).
The plan is that all new molecules will be added to the spreadsheet and new assays will added as additional columns. Storing the structures in a text format like SMILES provides a compact and efficient way to store molecular information which does not require any special software. Whilst this provides a useful repository it is not particularly helpful for the chemists who would actually prefer to be able to search by structure and

see the structures of the molecules. In collaboration with Luc Patiny at http://www.cheminfo.org/ we have been able to provide a visualiser that pulls data directly from the spreadsheet.
In addition there is a Vortex script (http://www.macinchem.org/reviews/vortex/tut26/scripting_vortex26.php) that pulls the live data from the Google doc and populates a Vortex workspace. More recently we have created a Jupyter Notebook (http://www.macinchem.org/reviews/osm/osmipython.php) and DataWarrior (http://www.openmolecules.org/datawarrior/) has been scripted to allow automatic import of the Google doc spreadsheet.
Whilst the spreadsheet has been absolutely critical to providing access to the OSM data, it is apparent that the limitations of a spreadsheet are going to be an issue in the future and the data needs to be moved to a database. The OSM team is now looking for help building an open-source chemically intelligent database, ideally with a web interface to allow collaborators around the world access. So if you feel you can contribute feel free to get in touch via the OSM website (http://opensourcemalaria.github.io/NewSite/#).

Tony Kent Strix Award

Contributed by Dr Michelle Lynch, RSC CICAG Social Media Editor, email mklchems@gmail.com

The UK e-Information Group, Geological Society, Burlington House, London, 31st October 2016

Picture courtesy of CILIP

The Tony Kent Strix Award is presented at the Strix Annual Lecture which is organised by the UK eInformation Group (UKeiG) in conjunction with RSC CICAG, the British Computer Society Information Retrieval Specialist Group (BCS IRSG) and the UK Chapter of the International Society for Knowledge Organisation (ISKO UK), in recognition of outstanding contributions to the field of information retrieval. It has been sponsored in part by CICAG for a number of years.

The meeting began with a presentation from Doug Veal, a former CICAG chairperson who worked with Tony Kent for 13 years. He began the meeting by setting the context and mentioned that a booklet is on sale, (contact CILIP http://www.cilip.org.uk/) with the proceedings of the previous year's event. He went on to describe his experience of working with Tony Kent while the two were at the RSC and of his dynamic and spontaneous nature.

The first of the speakers was Professor Stephen Robertson who presented on the history of search. Robertson is a visiting professor at the University College London (UCL) Computer Sciences Department and Professor Emeritus of City University, London. He taught Information Science alongside Tony Kent at City University in the 1970's. Tony Kent agreed to provide the Strix software package at City University. This gave the students practical experience of a commercial product for online searching whereas previously they had been using in-house program that they set up themselves.

Robertson's presentation charted the timeline of information retrieval and described the forces that shaped the modern search engine followed by a look at how search engines use data. Early indexing systems all employed some form of standardised process (e.g. hierarchical or faceted classification) with controlled vocabulary and human assignment indexing. Mechanisation during the 1950-1960's existed mostly in the form of punch cards using Boolean principles. Towards the 1970's, computers were brought into the printing process by the large scientific abstract suppliers. Document digitisation at these companies became a key enabler of computerised searching, making it possible to carry out Boolean searches of both indexes and unstructured text. These enhanced search features expanded to be a commercial service provided by the scientific abstract and accumulator companies such as Dialog. Initially, computerised Boolean searches were performed by dedicated libraries off-line but moved to a slow dial-up online search for individuals and thereafter to a faster process enabled by packet-switch networks. Software began to be developed for online searching within organisations and internal departments. The Tony Kent Strix software is one such example.

Post introduction of the Web in the 1990's, search engines began to appear. Early versions were slow and based on pattern matching. Systems using full-text indexing of web pages and ranked results followed. The advent of web search engines resulted in considerable advances in ranking capability outside academic environments. Word matching, word frequency, use of fields, anchor text and authority were all incorporated in the web-based ranking systems. Inference of Boolean operators from natural language queries typed into search boxes proved difficult, whereas ranking proved more practical.

Lycos, Yahoo and Alta Vista all appeared in the 1990's, the last incorporating both ranking and natural language search. Alta Vista had a promising product, but eventually lost out to Google due to a number of factors, and in particular when at one stage it failed to update its index for a period of months. Brin and Page introduced Google in 1998 which successfully implemented many existing web search features and offered additional page-rank and anchor text features. This resulted in a ranking system superior to many of its competitors and is attributed to its rise to dominance in the web search arena. Robertson commented that he finds Bing to be a useful search engine to use alongside Google.

Web search engines adapt to their users by adopting analytics that monitor search terms and alter indexing and ranking to suit. One effect of this manifests itself in the way that search engines display advertisements. Natural language clues in a search query indicating a desire for a purchase may push advertisements higher in the result ranking. Methods such as machine learning algorithms and organisational learning techniques have been introduced to continuously improve the ranking and quality of the search results in order to promote repeat visits by users. Ultimately search engines have evolved, in Robertson's opinion, to a position of searching by free text association and require fewer decisions on search terms from the external user.

Award Presentation

The Tony Kent Strix Award was presented by Doug Veal to Professor Maristella Agosti, from the Department of Information Engineering of the University of Padua. Professor Agosti is highly regarded in the area of information retrieval and has been instrumental in bringing into being the information retrieval system in Italy. Many of her students have gone on to make significant contributions in the field. Her other research areas include user engagement, databases, digital cultural heritage, and data engineering.

Right: Doug Veal presents the award to Professor Maristella Agosti. Picture courtesy of CILIP

The final presentation of the day was given by the 2015 Tony Kent Strix Award winner, Emeritus Professor Peter Ingwersen from the Royal School of Library and Information Science (LIS), Copenhagen, Denmark. Professpr Ingwersen's presentation topic was Context in Interactive Information Retrieval (IR).

Context is necessary for users to obtain factual information and evidence from IR. Various pictorial models of Context in Interactive IR were presented including the Holistic Cognitive Framework (HCF) and the Laboratory Research Framework (LRF). The HCF model encompasses the raw information objects and computing contexts on the left, through to the social context on the right with various feedback loops within the various elements. The interaction between left and right (computer and human) is imperative for successful IR - searchers need to understand why they doing the search and the computer needs to be optimised to help them.

An interesting theme of the presentation was the need for information science, computer science and social science aspects of IR. These disciplines are quite separate but individual optimisation and effective interaction is required between them for holistic IR. Separation of social and computing elements of IR makes for poor design and a compromise of the successful IR process. Neither party can explain the design or see its effects for the other. More advanced 'probabilistic models' allow for relevance feedback from the user to the computer. Professor Ingwersen went on to describe research that has been carried out to improve IR including poly-representation and cognitive overlap.

The next Tony Kent Strix Lecture will take place at Burlington House on Friday 20th October 2017 and the award will be presented by this year's winner - Professor Maristella Agosti.

Dalton Anniversary Celebration Events, Manchester

Dr John Hudson, Chair of the RSC Historical Group, has contributed an article for the RSC Website News and Events section about the Dalton celebration events in Manchester on 26th October 2016, which marked the 250th anniversary of Dalton's birth.

Chair of the RSC Historical Group, Dr John Hudson, with Steve Howe impersonating John Dalton Picture: courtesy of Dr Diana Leitch, FRSC, MBE, CICAG Treasurer

Dalton is, of course, best remembered for his work on atomic theory, and it was Dalton who produced the first table of atomic weights, setting chemistry along its modern path, but Dalton's life had many other facets, as a Quaker, teacher, and scientist whose passion was stirred by his early interest in meteorology. This October's celebrations were organised by Dr Diana Leitch, current President of the Manchester Literary and Philosophical Society, who is the Treasurer of CICAG and also a member of the RSC Historical Group. Dalton was himself President of the Lit. and Phil. for 28 years. Among the many guests present was Steve Howe who, soberly dressed in period Quaker costume, impersonated John Dalton.

Read the full article here: http://www.rsc.org/news-events/articles/2016/dec/john-dalton-anniversary-celebration/.

RSC General Assembly, Europa Hotel Belfast 18-19th November 2016

Contributed by Dr Michelle Lynch, RSC CICAG Social Media Editor, email mklchems@gmail.com

The RSC's General Assembly (GA) is the main annual event for representatives of the RSC membership and governance committees. It also incorporates the RSC Prizes and Awards ceremony. This important event facilitates information exchange and news on RSC initiatives amongst stakeholders and bolsters collaboration between representatives involved in the RSC's publishing and education functions, member divisions and special interest groups.

This year's event consisted of the RSC President Sir John Holman's welcome address, keynote speaker Professor Les Ebdon from the Office for Fair Access (OFFA), followed by a half day of discussion sessions covering the Membership Survey, Governance Review and Future of the Chemistry Profession. The Prize and Awards Ceremony and dinner took place on the evening of day one at the Titanic Museum, Belfast. A morning of member network sessions were held dedicated to Interest Groups and Local Sections took place on day two.

Welcome Address, Sir John Holman, RSC President

The GA was opened with an address from RSC President, Sir John Holman, who spoke about education and the factors involved in motivating students to go on to study chemistry through further and higher education. There are many factors to consider, in particular a positive interaction between student and teacher. Sir John highlighted the recommendations of the Sainsbury review of technical education which outlined the need for appropriate technical education pathways which are inclusive, encourage diversity in the industry, and are effective in bridging the current skills gap in the UK. Apprenticeships are a key route and should not, he said, be considered a second rate option compared to a University degree.

On garnering public support and student interest in chemistry, Sir John spoke about framing of chemistry in relation to other everyday industries sectors as well as the ability and willingness of scientists to communicate their subject areas in an accessible manner. In summing up Sir John emphasised the need for RSC governance activities to result in a "professional body fit for the future".

RSC President Sir John Holman delivers his welcome address to the General Assembly; © Royal Society of Chemistry/MPP

Keynote Speech

Professor Les Ebdon, Director from the Office for Fair Access (OFFA), gave a very interesting keynote speech covering the need for diversity in chemical education. OFFA's remit is "to promote and safeguard fair access to higher education for people from lower income backgrounds and other under-represented groups". OFFA's activities cover all full and part time undergraduate courses as well as teacher training courses in England.

Professor Ebdon spoke about the current difficulties in getting a representative proportion of female students as well as students from poorer socio-economic groups to study chemistry. Strategies proposed for improving diversity include "tailored, evidenced based spending", collaboration and a "student lifecycle" approach which engages the "whole institution". The sharing of responsibility was put forward with educational bodies, government departments, professional institutes, employers, unions, charities, families and student support functions all taking a role in improving diversity.

The RSC has played a key role through its campaigning and outreach initiatives such as "Chemistry for All" (Chem4All). Chem4all is an initiative being undertaken with several UK universities, local secondary schools and the Institute of Education. It is a five-year project that runs between 2014-2019 following secondary level students through years 8-12 of their education, and aims to overcome barriers to chemical education, widen participation in chemistry, and raise pupil awareness of their career options

Key Points from Workshops

Discussion Sessions

Membership Survey

The RSC membership survey was carried out to understand members' perceptions of the RSC's performance as well as their satisfaction and engagement rates. The information has been fed back into the RSC's strategy and communication processes. The results of the RSC membership survey were presented and discussed in this session. The survey shows some very positive attitudes from members - with nine out of ten respondents giving an overall positive rating, and one third rating the RSC as excellent. The majority of members state that they are proud to be a member of the RSC. Networking is seen as a clear benefit to members. Engagement with the RSC through Local Sections or Interest Groups is currently very low (10%). Fewer than 40% would be interested in volunteering but there is a clear desire for more access to information and local initiatives and activities which could improve this figure.

Governance Review

The RSC's governance activities cover RSC organisational structure and working processes. The governance review was carried out to discuss and debate their effectiveness, and to develop strategies on how the RSC can stay on track with the goal outlined by President Sir John Holman to be a "professional body fit for the future". One outcome of the Governance Review in 2017 will be include new meetings for Local Sections and Interest Groups in which awards and prizes will be made at different times, rather than at one General Assembly event.

Future of the Chemistry Profession

This session was based around The RSC's Future of the Chemical Sciences (FCS) initiative that was launched in early 2015 to look at how the chemical sciences might evolve over the next 10-20 years. The initiative involved a structured Scenario Planning exercise and a report was subsequently published with the findings. Some results of the study were presented during the discussion session, and possible future scenarios in the chemical industry in 2030 were put forward to the teams and debated. Examples of the scenarios included: the prospect of chemistry research being driven more by the free market and looking to solve immediate real world problems rather than basic research funded by government. Another scenario looked at the possibility of chemistry becoming subsumed into other subjects, with students more attracted to biology and physics due to the perception of these subjects as having "celebrity status" and growing in importance in society while chemistry declines. Each table put forward views on tackling the scenarios provided.

Interest Groups and Local Sections

Discussions were held around increasing participation of younger RSC members both in general and within local sections and interest groups. Some suggestions put forward included:

- lowering membership fees for younger members
- providing them with free access to the online RSC journals
- hosting short webinars for school age members that can easily be fitted into the school timetable
- encouraging participation in local RSC groups
- providing information on bursaries and travel funding for undergraduates e.g. to RSC events and conferences
- specific prizes and awards for younger members as an incentive to take on committee roles

Closer interaction between Interest Groups and the possibility of a "Best Practice" developed collaboratively was a key theme put forward in this session.

The method of communication used by Interest Groups and Local Sections was debated. The process by which emails are sent out to group members by a central RSC department was regarded as slow and cumbersome, but there was a mixed attitude toward use of social media for announcements and communications. It was agreed that email was the one platform likely to be universal to all members.

Prizes and Awards Ceremony

The RSC has a portfolio of over 80 prizes and awards covering all areas of the chemical sciences including research, business, industry and education. These awards recognise achievements and excellence by individuals, teams and organisations in advancing the chemical sciences. The ceremony for the 2016 Prizes and Awards took place at a dinner in the Titanic Museum, Belfast.

Titanic Museum, Belfast; © Royal Society of Chemistry/MPP

This year, CICAG's Dr Diana Leitch was awarded the RSC Award for Service, which recognises outstanding non-academic service to the chemistry community. Diana has contributed over 30 year's work and commitment to the areas of chemistry and chemical information, including as a respected academic librarian, information scientist, and 10 years as a CICAG Committee Member. Diana has been a Fellow of the RSC since 2005 and in 2014 was awarded an MBE for services to chemistry. She has played an instrumental role in developing science in the north west of England via her activities with the Catalyst Science Discovery Centre in Widnes. She was recently elected as President of the Manchester Literary and Philosophical Society (a role previously held by John Dalton for 28 years) and is she is also a member of the RSC Historical Group. Congratulations to Dr Diana Leitch on behalf of all of CICAG.

CICAG's Dr Diana Leitch is presented with the RSC Award for Service (Left to Right: Sir John Holman, Dr Diana Leitch, Dr Robert Parker); © Royal Society of Chemistry/MPP

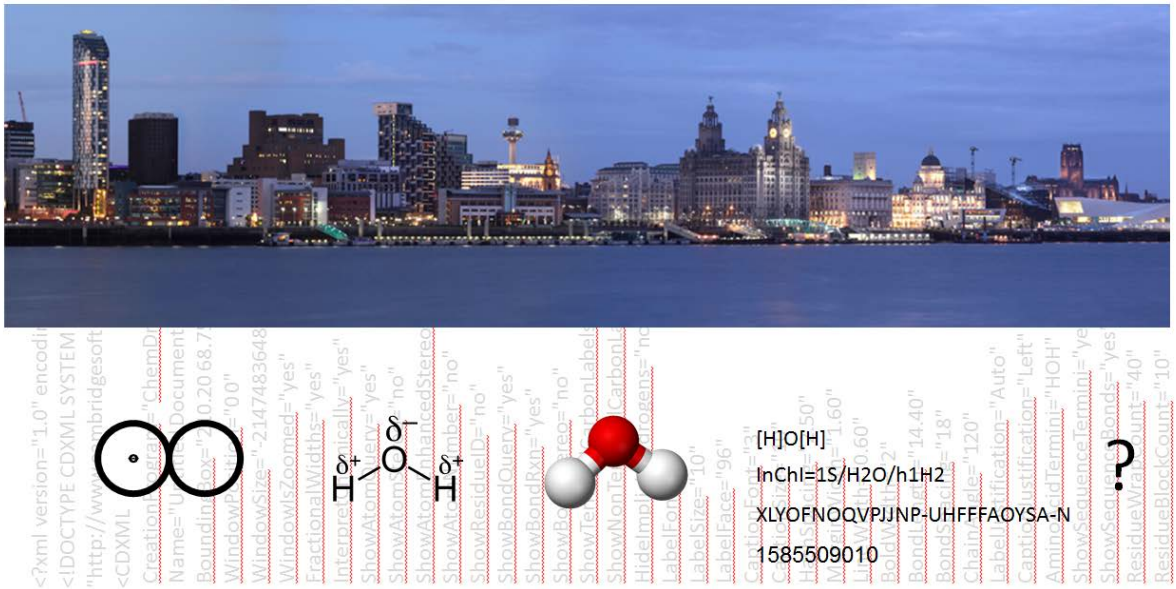
CICAG Planned and Proposed Future Meetings

The table overleaf provides a summary of CICAG's planned and proposed future scientific and educational meetings. For more information, please contact CICAG's Chair, Dr Helen Cooke (helen.cooke100@gmail.com).

Meeting	Date	Location	Further Information
Chemical Structure Representation: What Would Dalton Do Now?	22 June 2017	University of Liverpool	See the meeting web page Jointly sponsored by CICAG and the CSA Trust
RSC Historical Collection	2017	Webinars	In partnership with the RSC Library and Historical Chemistry Interest Group
Chemistry on Mobile Devices 2	2018	Burlington House, London	An update of the successful Chemistry on Mobile Devices meeting held in Cambridge in 2016
Spectroscopic Data to Chemical Knowledge	2018	AstraZeneca, Macclesfield	To be organised jointly with the Molecular Spectroscopy Interest Group and Dial-a-Molecule Grand Challenge Network
Faraday Discussion on Big Data and Chemical Information	2018/19	Sheffield or Leeds (approved Faraday Discussion venues)	Faraday Discussions
Celebrate the Centenary of IUPAC	Spring 2019	Burlington House, London	To be organised jointly with the Historical Chemistry Interest Group
Structure, Reaction and Patent Information for Small Organisations	TBD	TBD	Proposed meeting topic
Text mining	TBD	TBD	Proposed meeting topic

Forthcoming CICAG Scientific Meeting: Chemical Structure Representation: *What Would Dalton Do Now*?

Contributed by RSC CICAG Chair Dr Helen Cooke, email: helen.cooke100@gmail.com



The CICAG Committee is pleased to announce that we are organising the above meeting, which will be held on **Thursday 22nd June 2017** at the **University of Liverpool**.

Structure representation, including the electronic storage of structures and reactions to enable effective information searching, retrieval and display, has become more challenging as the number, diversity and complexity of structures which can be elucidated has increased over time. This meeting will explore current and future challenges and possible solutions to overcome them. In addition, subject matter experts will anticipate how developments in these areas will bring opportunities and benefits to research and innovation in the future.

Use of structure representation standards and metadata to exploit new opportunities and examine how chemists and data scientists can work together to ensure capture of information from the outset, e.g. when structures are first published in the literature or proprietary databases, will also be examined.

The key themes of the meeting will be:

- Challenging structures and the limits of molecular representation, e.g. extended structures, disordered structures, nano and meta materials, biologicals, polymers
- Association of data and metadata with structures and reactions
- Future opportunities for searching, managing and displaying chemical structure information and associated data

Tours of the new Central Teaching Hub at the University of Liverpool will also be available.

Who should attend?

- Research students (bursaries available) who use chemical structures
- Cheminformaticians
- Researchers working at the chemical/biology interface
- Chemical information and data managers in industry and academia

- Those working with complex structural information
- Providers of chemical data and information management software
- Chemical information publishers

This meeting will be sponsored by the Chemical Structure Association Trust. To find out more, please visit the RSC's Events database - this page will be updated as further details are confirmed.

CIIPM Training Events in 2017

Contributed by Stuart Newbold, email: stuart@psandim.com

At the 1st Cambridge Information & Intellectual Property Meeting (CIIPM), which took place at Homerton College, Cambridge, on 13 July 2016, feedback encouraged us to not only repeat the summer meeting, but also showed strong support for IP and patent information related training events. To this effect we are planning our first four half-day training sessions. These will run on 22 and 23 March 2017. The four training events must be booked separately, with discounts available for multiple bookings. The training event topics are:

1 IP Matters

- Provides an introduction to the basics of IP and the types of protection available, how to build an IP portfolio, and how to search and retrieve the various forms of published IP.

2 IP and Commercialisation

- Introduces the business and management processes needed to successfully get your technology to market including partnering, licencing, and IP portfolio management.

3 Commercial Patent Search & Analysis

- Shows how to search and analyse patent data to answer business questions and will look at competitive intelligence, technology and market landscaping.

4 Freedom to Operate Search & Analysis

- Covers different aspects of search and analysis of patent documents needed to prepare for freedom to operate. A practical approach is taken suitable for adaptation for all budgets.

Jane List and Stuart Newbold of CIIPM will be trainers on the day. Also present at the events will be IP legal experts from J A Kemp and the UK Intellectual Property Office, plus representatives from Minesoft who will provide access to patent information products for practical sessions. To find out more about the courses and registration please contact jane@extractinfo.info or stuart@psandim.com or visit http://www.psandim.com/.

Forthcoming Scientific Meeting: - 11th International Conference on the History of Chemistry

This meeting will take place from 29 August-2nd September 2017 in Trondheim, Norway

Abstracts (maximum 200 words) are now requested for the subject:
Chemists and the IUPAC: Taking Responsibility and Taking Actions
Since its foundation in 1919, many famous chemists have contributed to the International Union for Pure and Applied Chemistry (IUPAC), with the drive to improve standardisation of methods, nomenclature, units and standards, among other things. Without a doubt, progress was made, despite power struggles, uncompleted projects and unproductive commissions.

The session aims at shedding light on the activity of chemists invested with responsibilities in the IUPAC, whose actions are often overlooked in national biographical dictionaries. This session falls into the broader project on the centennial of the IUPAC, in 2019. Each paper will focus on the responsibilities and actions of individual chemists, alone or combined in a small national or disciplinary group, inside IUPAC. The case study can however expand on roles in other international organisations (IRC, ICSU, SDN or UNESCO to name but a few). A first survey is provided by the books of R. Fennell (1994) and S. S. Brown (2001). By focusing on individual actions, the aim is to get a better sense of articulation between the local and the international, and how this articulation was constructed through the work and actions of chemists dispersed across the world.

Abstracts and a short CV can be sent to Danielle Fauque (danielle.fauque@u-psud.fr) and Brigitte Van Tiggelen (vantiggelen@memosciences.be).

The Working Party (WP) on History of Chemistry (EUCHEMS)

The meeting will also mark the fortieth anniversary of the creation of the Working Party (WP) on History of Chemistry of the European Association for Chemical and Molecular Sciences (EuCheMS). The WP business meeting will take place during the conference, and social events such as excursions, receptions, and a banquet will also enable celebration of the 40th anniversary to take place.

Specific presentations concerning the history of chemistry include:

- Hasok Chang (University of Cambridge): "What history tells us about the nature of chemistry"
- Maria Rentetzi (National Technical University of Athens): "Revising the concept of safety culture in nuclear settings"
- Anders Lundgren (Uppsala Universitet): "Science in chemical industry – what did it do?"

Noordwijkerhout Meeting 2017 - Postponed

Due to logistical issues, the board of the Noordwijkerhout Foundation have made a decision that the initially-planned 2017 International Conference on Chemical Structures will instead take place in 2018. More details will follow in CICAG's Summer Newsletter.

Reaxys and ScienceDirect at the RSC Library

As of 1 January 2017, access to Reaxys and ScienceDirect at the RSC Library has, regrettably, been discontinued. The decision to dispense with Reaxys is attributed to both increasing costs of the service combined with the relatively low usage amongst RSC members, making it difficult to justify continued provision. In addition, the Library's agreement with Elsevier has been limited to non-commercial use (research / private study), which no longer fits the potential user profile. At the same time, the Library has announced that they have cancelled the four journal subscriptions currently received through ScienceDirect as, again, the cost of maintaining these journals can no longer be justified when compared to usage. On a positive note, the RSC is in negotiation with Elsevier to have access to the ScienceDirect journal archive and eBook collections. More information should be available to members soon.

Royal Society of Library: www.rsc.org/library
Virtual Library: www.rsc.org/virtuallibrary
Search the Library Catalogue: www.rsc.org/opac

InfoChem News

Contributions from Dr Stephanie North and Dr Valentina Eigner-Pitto, email: ve@infochem.de

Dr Stephanie North has now relinquished her UK customer relationship role with InfoChem, handing over responsibility to Valentina Eigner-Pitto. Stephanie comments for CICAG "I am sure Valentina will do a wonderful job. It will be business as usual for InfoChem, who will continue to develop new and exciting products. Valentina received her degree in chemistry from the Universita' degli Studi di Genova (Italy) and her Ph.D. title in polymer chemistry from the Technical University in Dresden (Leibnitz Institute for Polymer Research). She has been responsible in marketing at InfoChem GmbH since 2004 covering the areas of corporate design, conferences and exhibitions, company and product presentation. Since 2014 she is also in charge for acquisitions and account management of the reaction prediction software tools ICSYNTH and ICFRP."

PATENTSCOPE structure search capability now live

Back in April, InfoChem announced the implementation of structure search capability for chemical compounds in PATENTSCOPE; this has now been successfully launched at the end of 2016. Users of the service offered by the WIPO (World Intellectual Property Organization) can now search 7.5 million unique chemical structures automatically indexed from USPTO patents and 7 million abstracted from the PCT corpus. Indexation of EPO patents is in progress. The results of the project were presented at the ICIC Conference in Heidelberg in the autumn (http://www.slideshare.net/Haxel/the-addition-of-chemical-search-capabilities-to-patentscope-turning-a-fulltext-search-system-into-a-chemistry-database).

About InfoChem

InfoChem is a software company for cheminformatics focusing on the development of software tools to handle, store and retrieve chemical structures and reactions. The company's main activities involve the production of synthesis planning and reaction prediction solutions and the automatic extraction of scientific information from text and images.

CAS / SciFinder / STN News

Contributed by Dr Anne Jones, CAS Applications Specialist UK & Ireland, email: annejones@acsi.info.

SciFinder® Future Leaders Programme 2017

Applications are being accepted for the 2017 SciFinder Future Leaders program, organized by CAS, a division of the American Chemical Society. The program will be held August 14–19 in Columbus, Ohio.
The program provides Ph.D. students and postdoctoral researchers from around the world with opportunities to collaborate with CAS scientists, innovators, and business leaders to expand their professional network and build connections. At the conclusion of the program in Columbus, participants will attend the fall ACS national meeting in Washington, D.C., from August 20–24.

The deadline to apply for the 2017 program is February 12th.

NCI™ Global

NCI Global is a single source for the information organizations need to meet global regulatory requirements. Built by CAS, curator of CAS REGISTRY℠ and the only authoritative source for CAS Registry Number® identifiers, NCI Global offers flexible search capabilities and up-to-date coverage of nearly 150 regulatory inventories and lists to provide information on more than 347,000 regulated substances.

A free two-week trial is available to organizations so they can see for themselves how a single, reliable resource for global regulatory information streamlines compliance reporting. For more information about NCI Global, please contact CAS, or to request a trial now, click here.

MethodsNow™ launched!

MethodsNow, a CAS solution, is a single source to search and compare the latest published scientific methods. MethodsNow was released in 2016 and comprises an Analytical Chemistry (www.MethodsNow.com) and Synthetic Chemistry component (latter available via SciFinder only). The features include:

- Easy access to millions of disclosed procedures
- Comparison of methods side-by-side
- Displays experimental details in easy-to-read table format
- Materials, instrumentation, conditions and more
- Synthetic preparations from top journal articles and patents
- Features content curated by CAS scientists for superior discoverability and CAS Method Numbers, a new unique CAS identifier, for quick reference

Read *Identifying the Perfect Method* from the December 19, 2016 edition of C&EN, highlighting how MethodsNow can be used as a shortcut in the search for analytical methods.

STN News

Embase™ Reload on Classic STN® Expands Content and Improves Precision Search Capabilities

On November 13, 2016, Embase was reloaded on classic STN. The reload featured expanded content via the incorporation of Embase Alert data into Embase and indexing enhancements for more precise searching and easier review of search results.

Key features of this reload:

- **Embase will now include data from its companion file, Embase Alert (file EMBAL)** such as article-in-press records and bibliographic citations which do not include indexing. This new data complements traditional Embase content, records with complete value-added classification and indexing. The new Embase will offer streamlined searching and more comprehensive results.
- **Triple-linking of indexing terms** provides a powerful tool for increasing search precision. This feature was previously available only on embase.com, so its inclusion in Embase on STN makes for a more competitive offering. It is now possible to link, combinations of drug, disease and device terms, in a single search statement, with the relationship between the terms defined by a controlled subheading term. Triple links allows customers to find specific information, such as a drug and its specific side effect with a single search term, e.g., atorvastatin(P)side effect(P)muscle necrosis/CT.
- A **new Controlled Terms (/CT) segment called Device Descriptors** provides all medical devices indexing in a separate section of the CT field, making it easier to find and review indexing terms specific to medical devices. Two new subheadings have been introduced for triple-linking in the Device Descriptors segment: *adverse device effect* and *device comparison*.

- The addition of **PubMed Identifiers (PMID) to the DN field** makes it easy to identify any Embase record that is also in MEDLINE®.
- **Less duplication** - MEDLINE Unique records which duplicated Embase-indexed content have been removed from Embase, making review of search results more efficient.

CAS Training in the UK 2017

In addition to the e-learning materials, CAS continues to offer instructor-led training for STN, SciFinder, NCI Global, ChemZent™, PatentPak™ and MethodsNow in the UK. CAS conducts 'in-house' or WebEx training sessions on all aspects of searching CAS solutions. Also, if you wish to know more about any of the CAS solutions or would like further information or help, then please contact annejones@acsi.info.

CICAG Meeting Report: - Chemistry on Mobile Devices

Contributed by Dr Chris Swain, email: swain@mac.com and Dr Jonathan Gooodman, email: jmg11@cam.ac.uk

Chemistry on Mobile Devices: Create, Compute, Collaborate took place on 7 September 2016, at the Centre for Molecular Informatics, University of Cambridge, Cambridge CB2 1EW, and was organised by RSC CICAG.

Mobile devices are now ubiquitous. There are now estimated to be over two billion SMART phones and tablets in use globally, each with the computing power to handle most of a chemist's needs. The aim of the meeting was to look at the many ways that mobile devices could become the chemist's essential companion. Themes and questions discussed included:

- From searching and consuming content, to performing computational calculations and providing interactive visualizations.
- From electronic notebooks to devices accessing cloud based resources.
- What are the advantages of and the security concerns of an always-connected mobile device?
- What are the challenges of a touch interface?

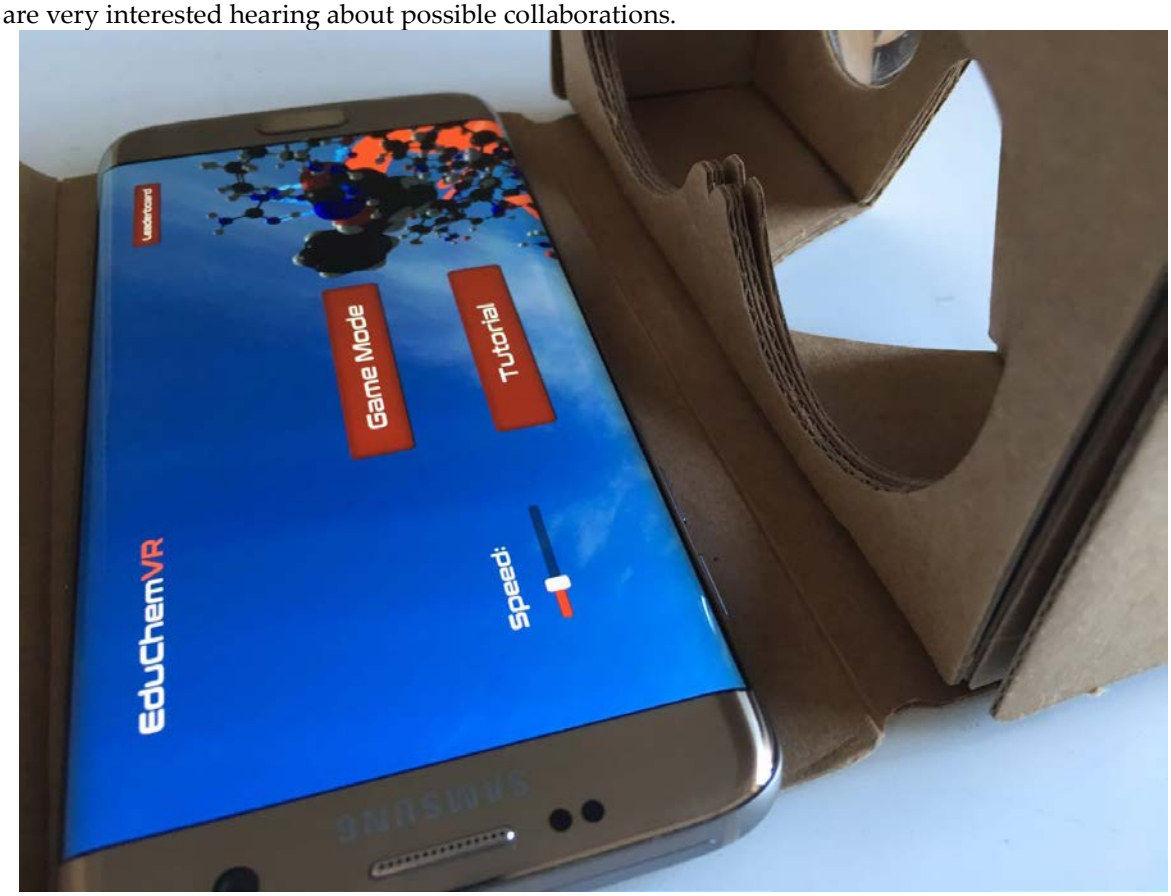
As befitting a meeting on mobile devices we had presentations given from laptops, iPads and even an iPhone, and all seemed to work perfectly.

Dr Michelle Lynch (Senior Consultant, IHS Markit/CICAG Committee) opened the meeting with an overview of mobile chemistry. Mobile chemistry usage in academia is heterogeneous with many components chosen by the researcher, or local to one institution. Electronic laboratory notebooks are becoming well established in both academia and industry, and the use of mobile devices to record experiments, in particular photographs, was common. Data input is not ideal and the ability to share and collaborate appears to be solved by using features like Dropbox, which has security concerns. The 'Internet of Things' is likely to have impact on the way devices communicate and will require open APIs and standard ways to provide security; mobile devices could be at forefront of these technologies.

The RSC has an ongoing project looking at the way that chemists interact with the products and services provided by the RSC. James Stevens, (Product Manager, Journals and Books, RSC), and Paul-Jervis Heath, (Founding Principal, Modern Human) gave a joint presentation entitled "Lab on the bus: Designing for academic modes of reading". This exercise included video recording or observing chemists at work in an effort to better understand the way that chemists search and consume content across multiple devices. Whilst the PDF has become the standard way of distributing content, it is clear that it does not provide the ideal format for viewing on different screen sizes. Whilst the RSC website provides an increasing amount of functionality this also serves to take the focus away from the content on devices with restricted screen real estate and has a significant impact on page load times. The RSC are now making efforts to reformat content to be better viewed on different devices.

Professor Nick Greeves, (Department of Chemistry, University of Liverpool), gave an interesting talk on mobile devices in chemistry education in particular thinking about the way students consume and retain information. Clearly electronic devices provide vastly superior means for searching, but once found, sometimes the students then prefer to read the content in hard copy format. Lectures can be provided as video recordings and notes/handouts as electronic files. However, the ability to annotate on mobile devices was somewhat limited, in particular to accurately draw chemical structures, curly arrows, etc. The iPad Pro and pencil seem to provide sufficient performance to overcome these issues, but at a substantial price. Mobile phones also provide a means of impromptu polling/voting during lectures to increase engagement. Airplay could be a useful way of sharing content in small meeting or tutorials, but there is a need to control what is displayed rather than the current "free for all".

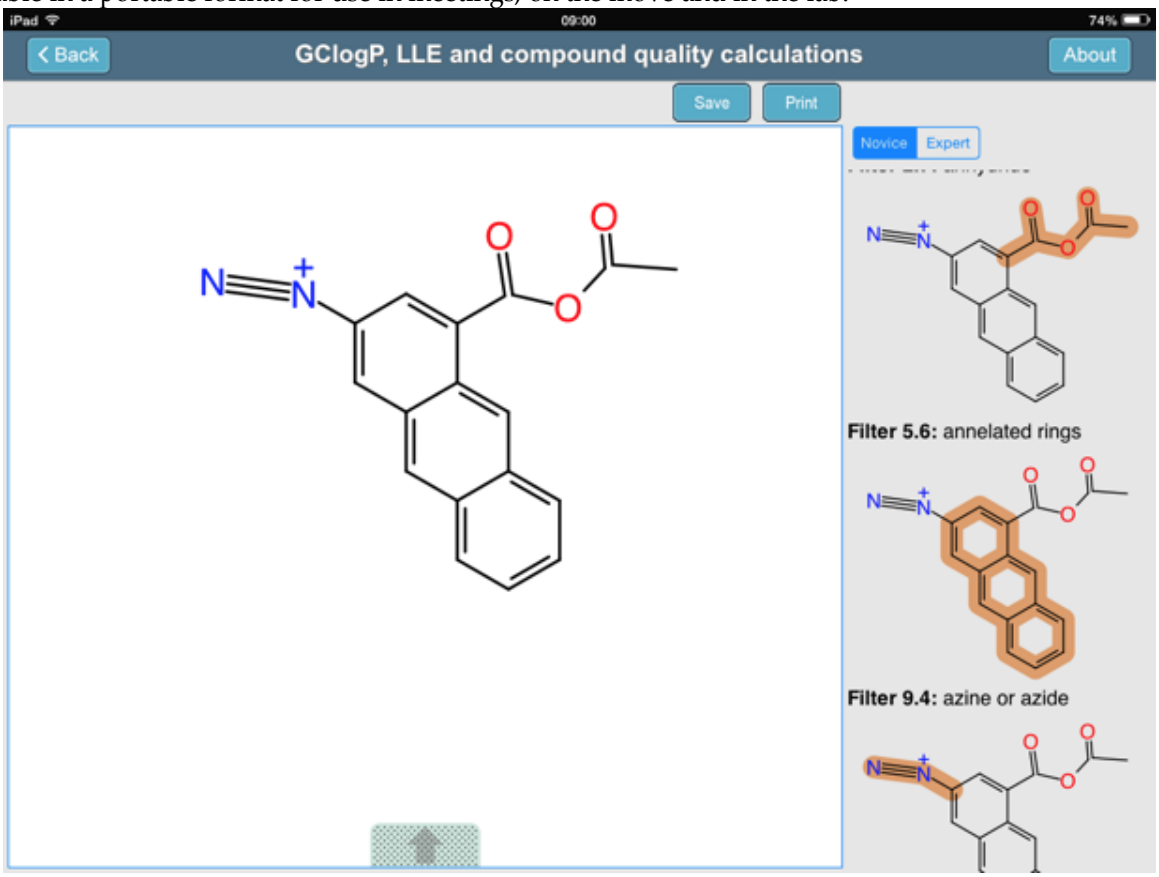
In an exciting development EduChem VR co-founders Dr Jonas Boström, CEO and Magnus Norrby, CTO, chose this meeting to announce the founding of a new company EduChem VR (http://www.educhem-vr.com) and gave a talk entitled "Virtual reality smartphone apps making chemistry look and feel cool". This project aims to enhance the learning experience for school chemistry lessons by providing virtual reality viewing of molecules using inexpensive Google Cardboard viewers (https://store.google.com/product/google_cardboard) that work with any modern smartphone. They already have apps for viewing small molecules, bonding in the different states of water, and biomolecules from PDB, and are very interested hearing about possible collaborations.



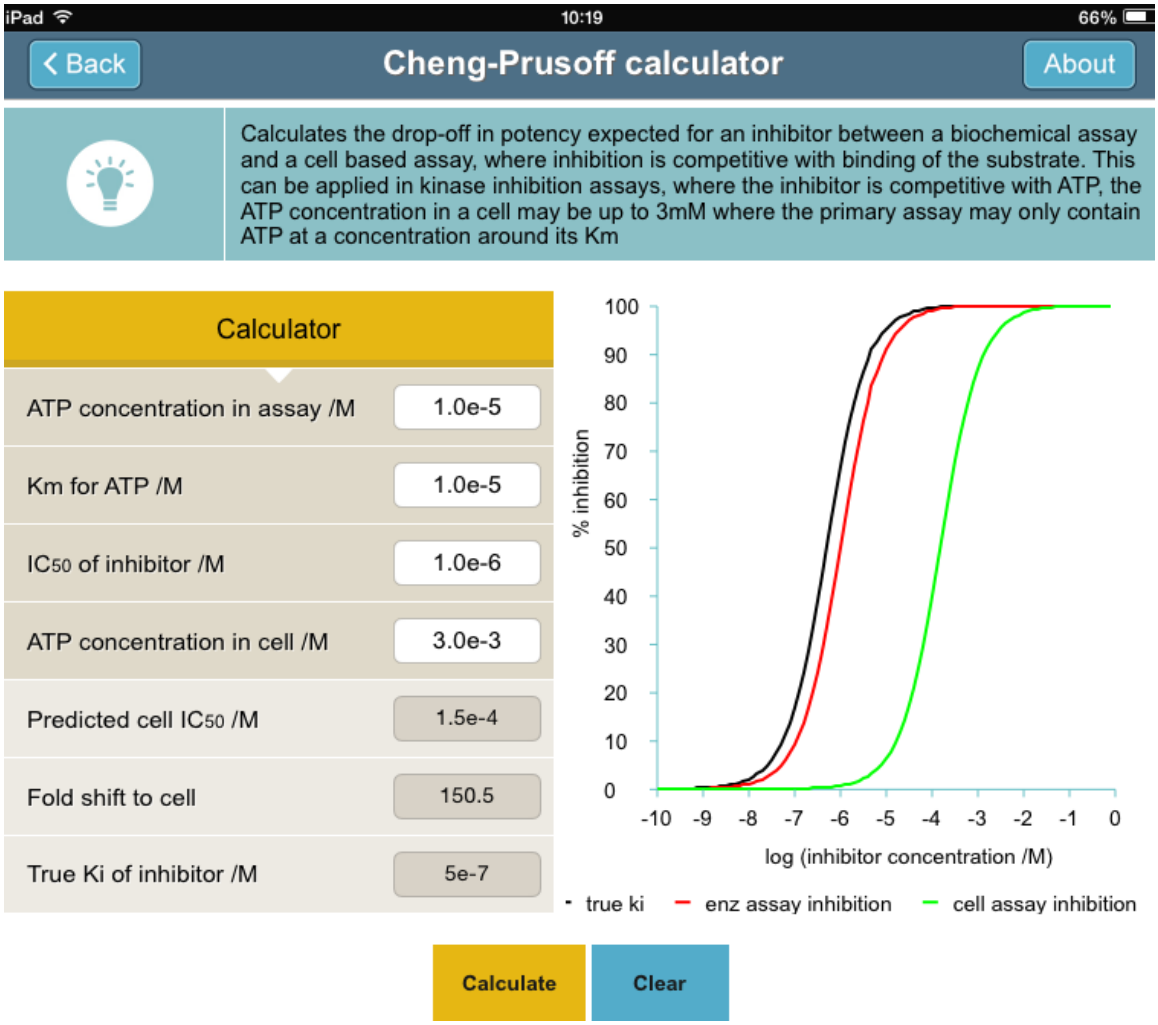
They brought a couple of viewers to the meeting and gave a very popular series of demos during the lunch session.

The flash poster session was intended to offer the opportunity for developers to give a brief introduction to new apps, and we were treated to two very interesting freehand chemical drawing applications. Historically, chemical drawing packages have relied on a series of menu items or templates to build chemical structures. Whilst now well established, they don't really emulate freehand drawing of chemical structures using pen on paper. Paul Wallace (Perkin Elmer) and Eufrozina Hoffmann (ChemAxon) gave impromptu demos of freehand chemical drawing apps.

The history behind the 'Handbook of Medicinal Chemistry and Medicinal Chemistry Toolkit app - tablet delivery by design was described by Dr Andy Davis (Projects Director, RIA Innovative Medicines, AstraZeneca). The project started as an extension to the very popular Medicinal Chemistry training course organized by the RSC, initially as an e-book with links to external resources. This then evolved into a stand-alone iPad app (https://itunes.apple.com/gb/app/medicinal-chemistry-toolkit/id910073742). The Medicinal Chemistry Toolkit app is a suite of resources to support the day to day work of a medicinal chemist.
Based on the experiences of medicinal chemistry experts, these otherwise difficult-to-access tools are now available in a portable format for use in meetings, on the move and in the lab.

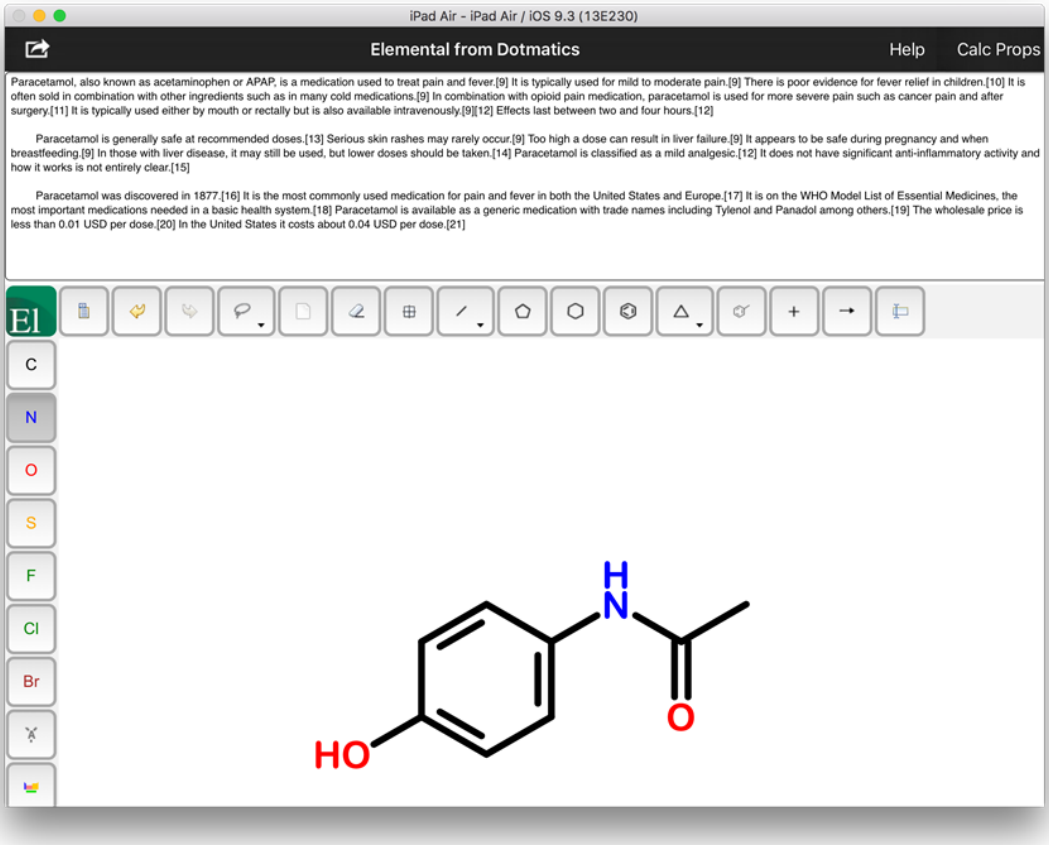


It is important to note that the calculations are done locally on the iPad and not via a web service. This is important for confidentiality when dealing with proprietary compounds. Properties are calculated as you sketch in the molecule so you can actually see the contributions of functional groups as you add them.
The Cheng-Prusoff equation, which relates IC50 values to affinities, is probably the most important equation for medicinal chemists involved in the design of inhibitors to understand.

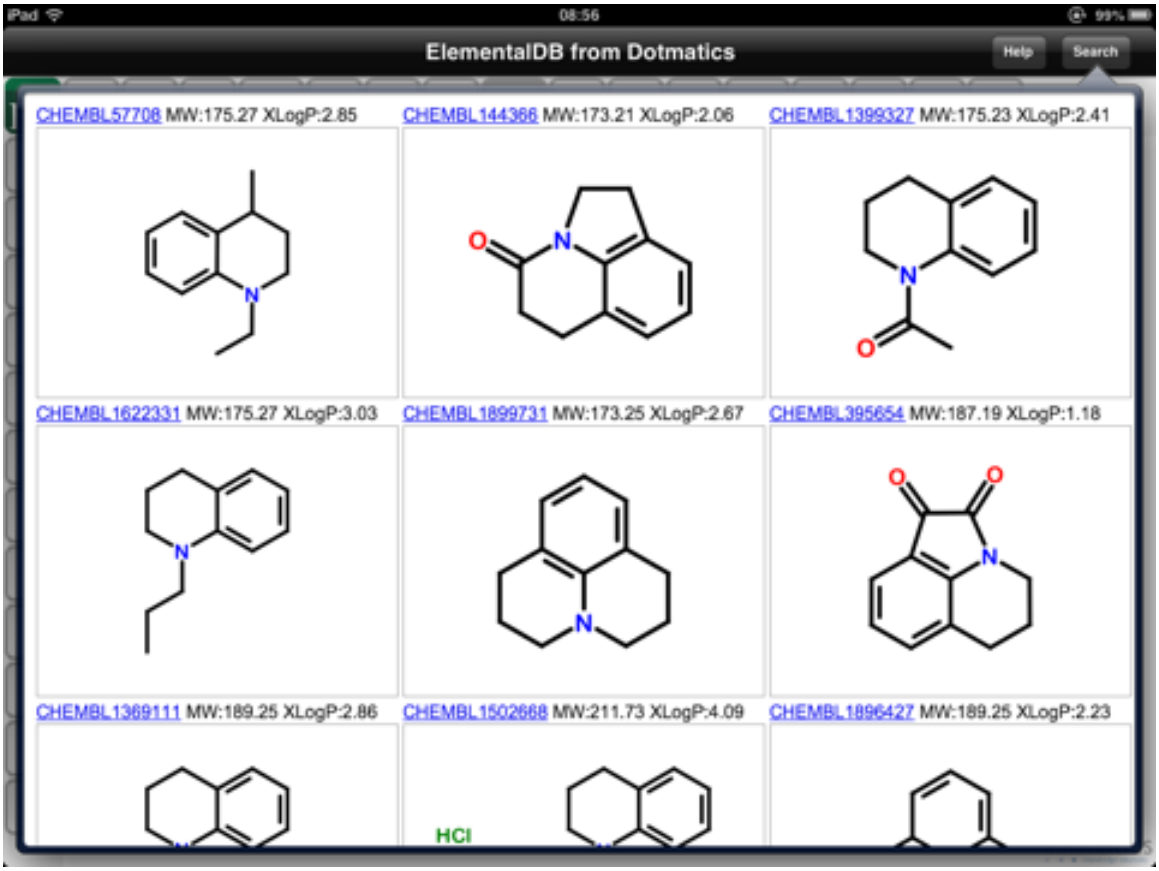


As an example, for kinase inhibitors the Ki will vary depending on the concentration of the substrate ATP. It is therefore vitally important to understand the likely range in ATP concentration in the target locations, and to be aware that accumulation of the substrate (ATP) will have an impact on inhibition. This can be part of the reason why shifts in activity are observed when moving from a biochemical assay to a cell-based assay. Andy then asked for feedback on possible future directions. People have asked for it to be ported to other platforms, the ability to add extra functionality, user defined filters, other ADME models., all of which are possible but it was not clear how this might be funded or supported in the future.

Dr Dan Ormsby (Principal Application Scientist, Dotmatics Limited) gave a talk originally entitled "Challenges of developing electronic lab notebooks for mobile devices and substructure searching on iPad" but which was updated to include new developments on connecting laboratory instruments and devices into an electronic lab notebook environment. Elemental (https://itunes.apple.com/app/elemental/id518655328) is a chemical drawing package that is available on multiple platforms and was designed to provide the same user experience on both desktop and mobile devices. Whilst the chemical intelligence is all written in C for portability, the interface uses javascript to provide a consistent user interface.



Elemental has been downloaded many 100,000's of times and accounts for 15% of the links to the company website, underlining the role of small mobile apps as advertising aids. As an extension ElementalDB (https://itunes.apple.com/us/app/elementaldb/id627422287) provides a demonstration of an iPad application that does a substructure search of a 1,500,000 structure database in less than a second. The sdf records have been compressed to reduce size and put into a sqlite database. They then use the classing of path-based fingerprints for the structure-based searching, and calculate some physicochemical properties.



If you click on the CHEMBL id a link is opened in the browser displaying the ChEMBL report card. There was some discussion about users being able to import their own structure files; if the technology is there, Dotmatics will consider making it available.

The DotSDMS product enables integration via attaching legacy devices (and new devices) to a central repository of experimental files, so the machines work automatically, recording their data to a central place. It works like Dropbox where a client task bar icon is displayed to show it is monitoring a folder for new files; however you don't have the security concerns of uploading to the internet. As new files appear they are checked,to see if they actually changed (md5sum style), and if changes are seen it is uploaded to SDMS. Versions are stored if the same file changes (some instruments always write to the same filename it seems). The client code is in straight python so works on Linux/Raspberry Pi/ ODROID (http://www.hardkernel.com/main/) like hardware so Linux collection machines of an instrument can also post updates to a SDMS. For a legacy machine there are a couple of options. One is a Moxa box. This attaches to the rs232 connection and when the user presses the button on the device (to record pH or MW) the output that would have gone to a simple printer goes instead over ethernet to a PC running the SDMS client and listening on a (virtual) COM port (up to 256 per PC). When the device does a beep it mean the COM port message was sent and also means the virtual printout is now uploaded to the SDMS server (each button press gets its own entry). In the SDMS client you can now navigate to the machine ID and see the readout with its timestamp. Information such as who pressed the button simply isn't available. It is a simple device that only really knows the button was pressed and what the MW or pH was reported to be. Holding your phone/iPad in your hand at this moment helps as you can immediately see the MW/pH on your device or more likely a pair of readings to calculate a diff to know what the weight was before and after (for example) tipping out/in some reagent. Another option is rs232 to an ODROID/Raspberry Pi like system where it is the COM port (rs232 to USB) and it uploads to SDMS directly.

Daniel Fitzpatrick (PhD Researcher, Ley Group, University of Cambridge and designer of ChemInventory: https://www.cheminventory.net) gave a very interesting talk entitled "Around the World Synthesis: Controlling Reactions in Cambridge through Tokyo". Robotic synthesis is an increasingly popular area of

research and monitoring these reactions from multiple devices is a very useful extension. Using his phone, Daniel showed us data being gathered from instruments in the laboratory, whilst the lecture proceeded.

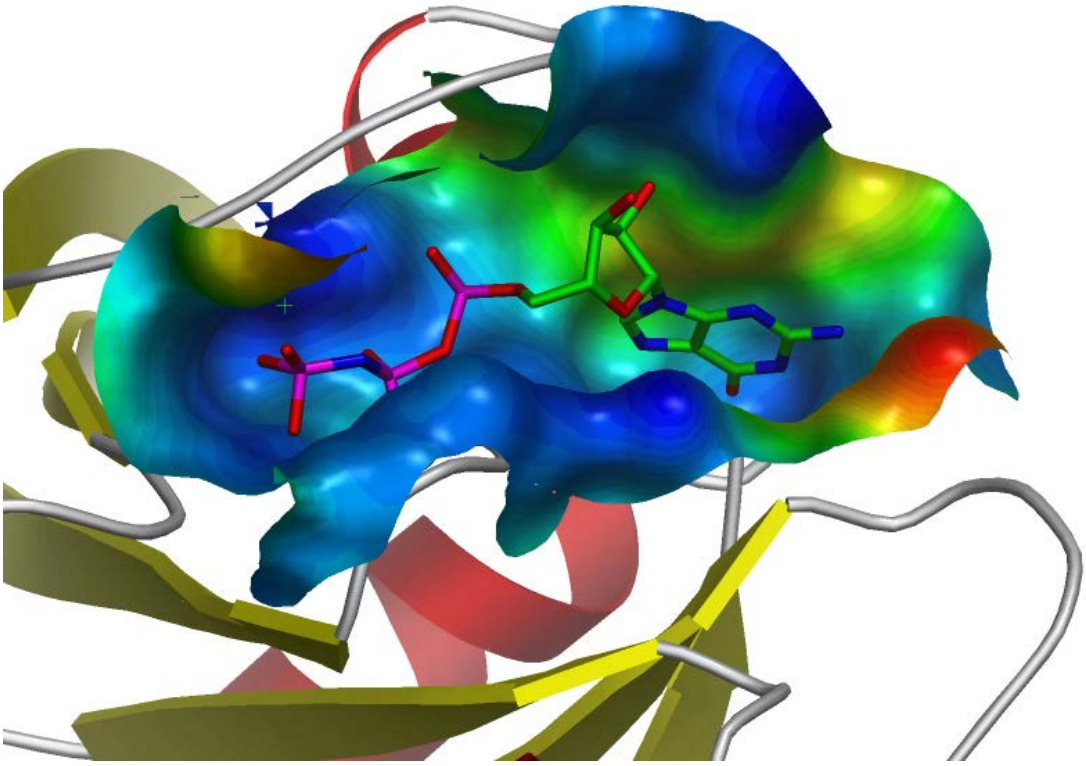
Setting aside time for demos over the lunch break was a great idea, and Jonas Bostrom provided exciting hands on experience of chemistry virtual reality. In the discussions I had with people I heard about one new product idea generated at the meeting, one person who had a coding problem solved, two collaborations that were initiated, and a discussion about making an existing product open source.

CICAG Meeting Report: - Cheminformatics for Drug Design: Data, Models and Tools

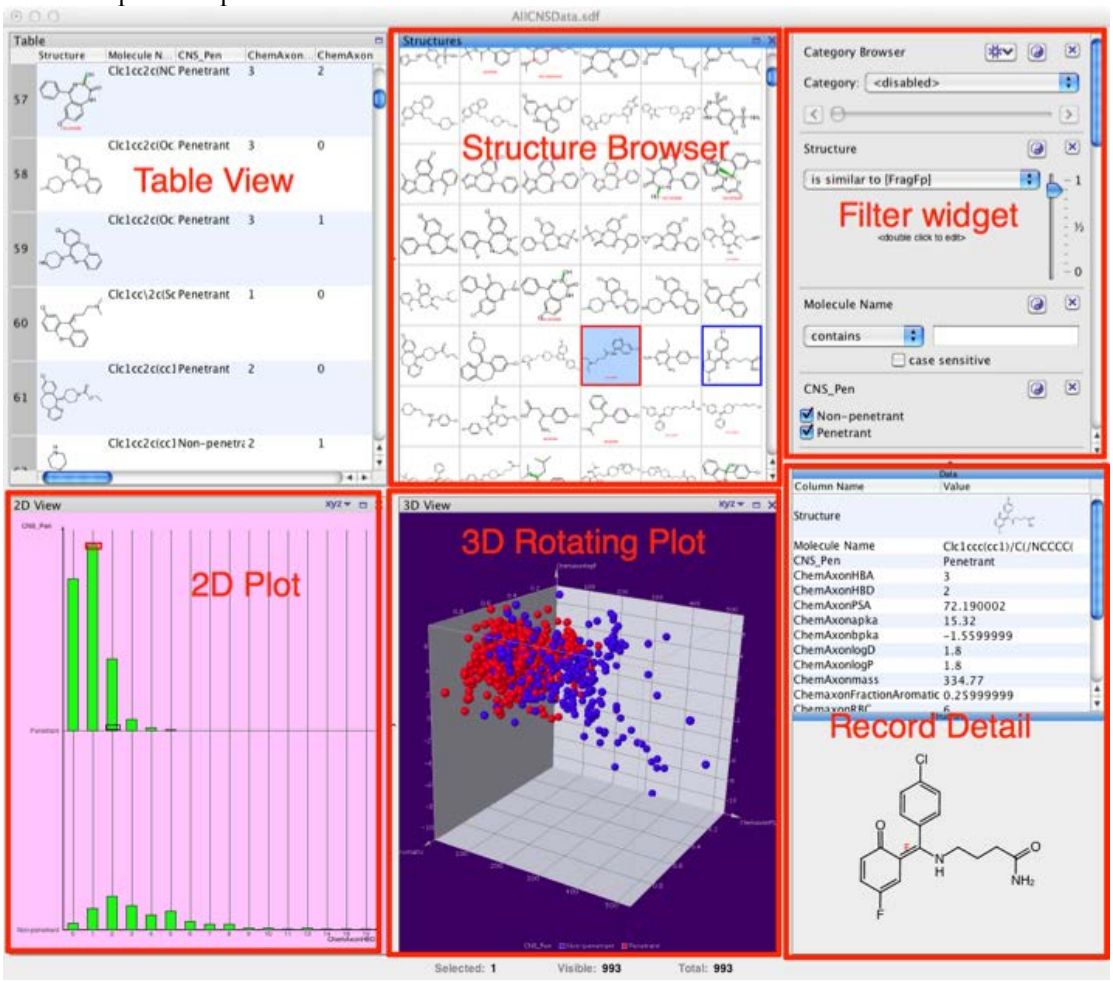
Contributed by Dr Chris Swain, email: swain@mac.com

Cheminformatics for Drug Design: Data, Models and Tools took place on 9 November 2016 at the Imperial War Museum, Duxford, Cambridgeshire.

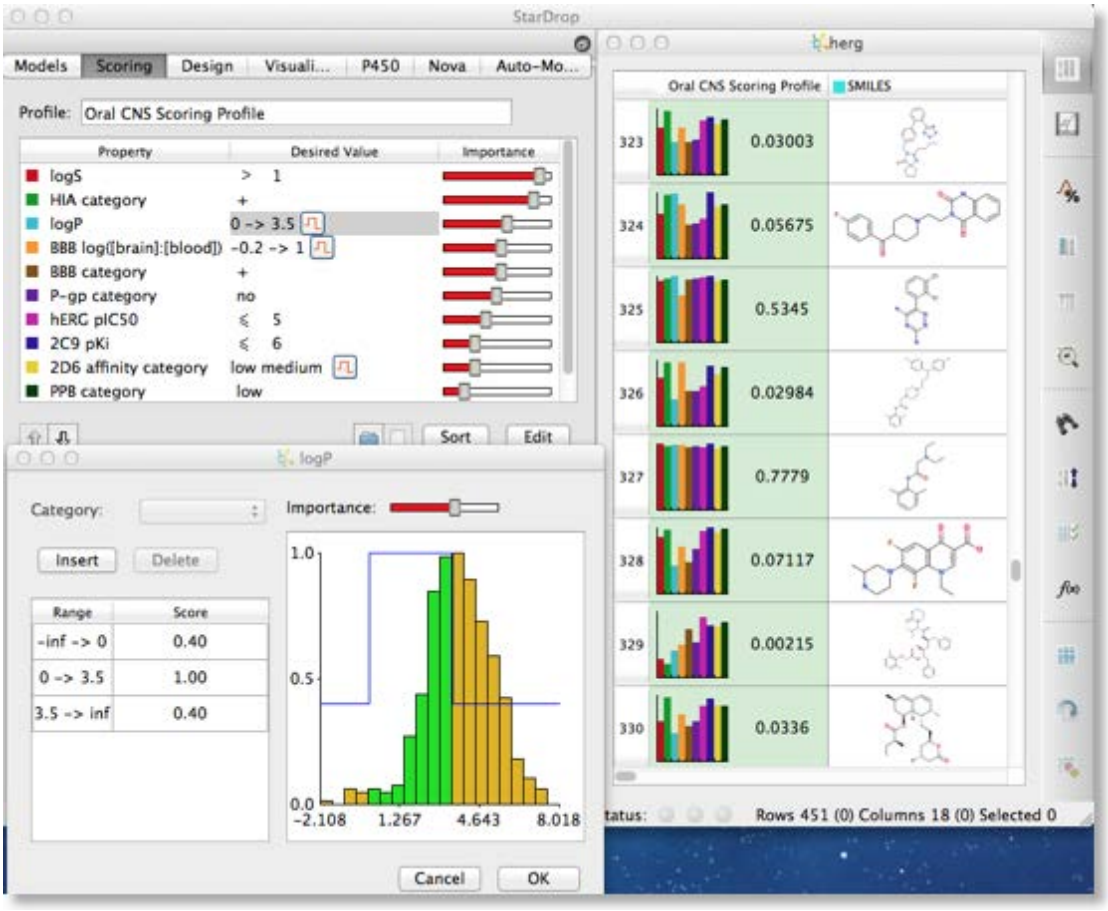
Paul Mortenson (Astex) described the informatics platform that Astex have built to support their drug discovery group. Astex did a detailed analysis of their needs and decided that at the time no commercial vendor was suitable. In particular they wanted an ease of use and responsiveness that they felt required a bespoke design. They designed the system to be entirely within a web-browser since this meant there was no need to install anything specific on the desktop, tablet or smart phone. Responsiveness was an important consideration, and having all the servers locally was critical. Users were familiar and comfortable with a web environment. Since Astex is focused on structure-based design as well as the usual tables and spreadsheets, they needed a 3D molecule viewer - for this they used OpenAstexViewer (http://openastexviewer.net/web/) M.J.Hartshorn, JCAMD, 16, 871 (2002). This provides high quality display of both small molecules and proteins; it can also provide shaded molecular surfaces, with transparency and property mapping and protein schematics, and can be controlled using javascript.



Isabelle Giraud (Actelion) then described DataWarrior (http://www.openmolecules.org) a freely available open source cross platform data analysis tool that understands chemistry, it provides an efficient way to search, sort and analyse structure-activity data. DataWarrior was developed at Actelion and it is highly integrated into their drug discovery platform. In 2014 it was decided to release DataWarrior without the integration layer as a stand-alone tool to the public. Actelion made the decision to open source DataWarrior in an effort to help development.



Matt Segall (Optibrium) gave a very interesting presentation dealing with the critical issue of decision making when the data/information is uncertain. He also made the important point that with most experimental data or calculated properties it is as important to understand the confidence in the score as the score itself. He then gave a demonstration of the desktop tool StarDrop (http://www.optibrium.com/stardrop/) that can be used for multi-parameter optimization (MPO) in which the relative importance of each parameter can be fine-tuned to give an overall score.



Julian Blagg (The Institute for Cancer Research) gave a great talk describing the informatics platform at the ICR. After many years with data held in multiple spreadsheets, presentations and reports, they decided they needed a platform that would allow them to share data seamlessly with both internal and external scientists. After careful review of the options they decided to go forward with the Dotmatics platform (http://www.dotmatics.com). Julian described the initial set-up that that allowed users to browse biological data and link to chemical structures. This has now been expanded to include electronic notebooks and also the capture of high content screening data. The emphasis has been ease of use and unobtrusive capture of information. An added benefit has been the ability to share project specific data easily with external collaborators.

Subsequently CRUK has decided to roll this out across all the research labs. Julian highlighted that CRUK is a particularly enlightened research funding agency, recognizing that sharing and long-term storage and retrieval of data is a mission critical activity.

Vivienne Allen (Charles River Laboratories) gave an interesting talk on the tools used in screening library design, in particular in the design of soft-focus libraries. These are small libraries designed to target a specific protein class (e.g. GPCR, kinase, epigenetic). They use a combination of cheminformatic tools to explore literature sources (e.g. ChEMBL) and fragment known ligands to identify interesting substituents. These are combined with novel scaffolds and the subsequent virtual libraries evaluated using docking to prioritize targets.

Jerome Hert (Roche) gave a talk on the impact of computer aided drug discovery (CADD) at Roche. The process was defined as a series of design, synthesis, testing and analysis steps, and there are opportunities for CADD to contribute to all of these. The presentation used examples from different projects in illustration.

Al Dossetter (Medchemica) talked about how Medchemica have used ADME/T data from a consortium of

pharma companies and applied a matched molecular pairs analysis (MMPA) to define a set of rules for favourable transformations (http://dx.doi.org/10.1016/j.drudis.2013.03.003). They can apply these rules to novel targets to suggest new compounds that would be worth making in an unbiased manner. Their analysis showed that whilst the data from an individual company provided a very limited set of useful rules, combining data from multiple sources resulted in a greater than additive number of rules.

David Leahy (Discovery Bus Ltd.) gave a thought-provoking final talk in which he argued the large pharma companies should be investing in artificial intelligence (AI) to replace medicinal chemists in drug design. There was an unresolved discussion about the patentability of molecules suggested by AI.
