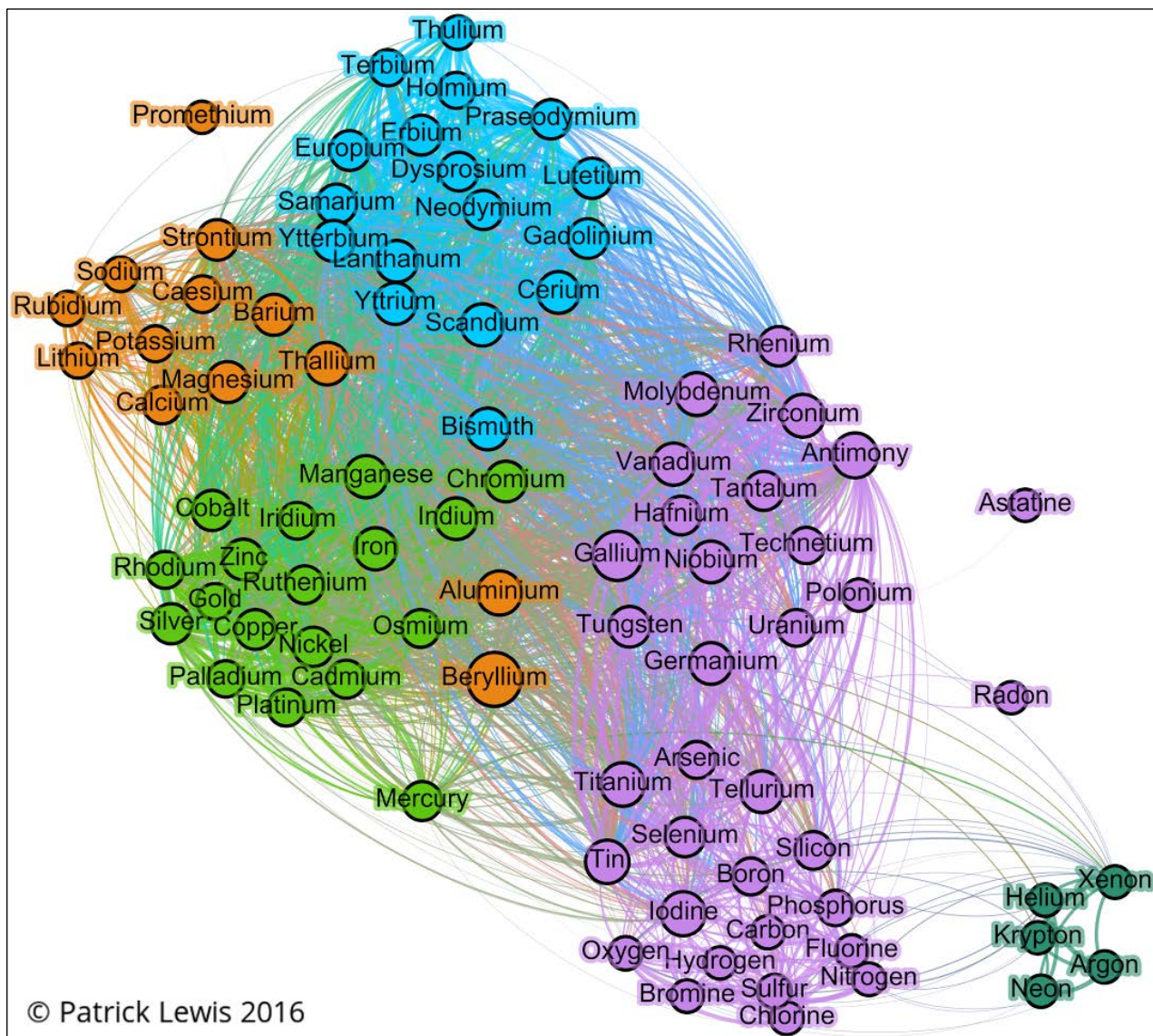




ROYAL SOCIETY  
OF CHEMISTRY

CHEMICAL INFORMATION  
AND COMPUTER  
APPLICATIONS  
GROUP

## NEWSLETTER Summer 2016



Network graph showing inferred relationships between selected chemical elements detected in semantic analysis of 650,000 chemistry-related article titles and abstracts. Close spatial relationships indicate semantic similarities between nodes in the model and hence implied chemical similarity. Colours are assigned by detecting communities of closely connected nodes. Edges are drawn between nodes above a heuristic threshold of similarity. Thicker edges indicate stronger similarity. Node size indicates the degree of connectedness of the node.

For more information contact Patrick Lewis [p1375@cam.ac.uk](mailto:p1375@cam.ac.uk)

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>

**LinkedIn**  <http://www.linkedin.com/groups?gid=1989945>

**MyRSC** <http://my.rsc.org/groups/cicag>

 [https://twitter.com/RSC\\_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](mailto:stuart@psandim.com)

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## Chemical Information & Computer Applications Group Chair's Report

Contributed by RSC CICAG Chair Dr Helen Cooke, email: [helen.cooke100@gmail.com](mailto:helen.cooke100@gmail.com)

### CICAG's Role and Scope

CICAG's scope is broader than it used to be (CICAG was previously the Chemical Information Group), and as I was reflecting on this, I decided to jot down my thoughts about our Committee's cumulative areas of expertise and experience, as noted, in no particular order, in the table below (though I am sure there are some I missed).

Expertise	Background
Scientific publishing	Physical chemistry
Information science	Medicinal chemistry
Librarianship	History of chemistry
Molecular modelling	Organic chemistry
Cheminformatics	Inorganic chemistry
High throughput screening	Computational chemistry
Software development	
Drug design	Employment area
Big data	Consultancy
Chemical nomenclature	Pharmaceutical industry
Data and metadata standards	Chemical industry
Structure representation	Publishing
Patent searching	Higher education

I suspect that the Committee's interests probably mirror those of CICAG's membership as a whole, and in turn demonstrate the importance of the work CICAG members do in our diverse roles and employment sectors. The CICAG Committee would love to hear from you if you have a story to tell about how chemical information and computer applications feature in your work or help others that you support – perhaps something we could report on in a future CICAG Newsletter article.

Building on this, nowadays it would be hard to find a chemist who doesn't use chemical information and computer applications on a daily basis, so I feel that the work we do in our Interest Group should be of value to the majority of RSC members (not only those who are members of CICAG). If you have suggestions as to how CICAG can support the broader RSC membership, e.g. by organising scientific meetings, webinars, training sessions, blogs, again we would be very pleased to hear from you.

### Committee Membership Changes

There have been several changes to the Committee membership since publication of our last Newsletter.

Dr Alan Tonge decided to step down as CICAG Secretary, having served his three-year term. We are very grateful for Alan's many contributions which have helped the Committee to run smoothly throughout his period in office. Alan will remain a non-officer member of the Committee. I'm pleased to report that Professor Jeremy Frey has agreed to take over the role.

Dr Keith White has decided to step down from the Committee, which he joined in 2008. Soon afterwards, he became Vice-Chair, quickly followed by Chair, a role he fulfilled until 2014. From 2014-2016 Keith was

CICAG's Social Media Editor, looking after our Twitter, LinkedIn and MyRSC accounts, as well as other publicity. The Committee thanks Keith for his hard work and leadership, including his active participation in organising scientific and educational events. On a personal note, Keith was a great help to me when I took over from him as Chair. Michelle Lynch has kindly taken over Keith's Social Media Editor role.

For some time we have felt that organising scientific and educational meetings would be more efficient if we had a dedicated Events Manager, to provide support to other CICAG meeting organisers and to ensure smooth running of events. Following a recruitment exercise earlier in 2016, Dr Gillian Bell accepted this role. Gillian is now the first point of contact for enquiries about CICAG events. Welcome to the Committee, Gillian!

## Annual Report

CICAG's 2015 Annual report is available via the CICAG web site  
[http://www.rsc.org/images/cicag\\_annual\\_report\\_2015\\_tcm18-245531.pdf](http://www.rsc.org/images/cicag_annual_report_2015_tcm18-245531.pdf).

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## CICAG Thank You to Dr Keith White

CICAG Committee wishes to express our gratitude to Dr Keith White, who served on the CICAG committee from 2008 - 2016. We are particularly grateful for Keith's service as a highly efficient Chair of the Committee from 2008 - 2014, which Keith then followed as our first Social Media Editor by formalising the social media input he had brought to CICAG, and helping CICAG develop our profile on various platforms. Thank you Keith!

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## CICAG Meetings for 2016-17

CICAG has two scientific meetings agreed for 2016, plus a number of 2017 events which are now taking shape:

### 1. Chemistry on Mobile Devices: Create, Compute, Collaborate

- 7 September 2016 10:00-16:30, Unilever Lecture Theatre, Cambridge, United Kingdom

Mobile devices are now ubiquitous: there are 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 meeting will explore the many ways that mobile devices could become the chemist's essential companion, from consuming content to performing computational calculations, from electronic notebooks to devices accessing cloud-based resources, and much more.

This meeting will examine:

- The range of capabilities available to chemists via mobile devices compared to laptop/desktop computers
- Advantages and disadvantages (e.g. security concerns) of an always-connected mobile device
- Challenges of a touch interface
- The role of mobile devices in education
- Gaps in capabilities and content coverage
- Innovations for the future



There will be a range of demonstrations of commercially available products. In addition, attendees are encouraged to bring their mobile devices to share and discuss applications they are developing or researching with other participants.

The meeting will be suitable for:

- Chemists who currently use mobile devices and are seeking to expand and optimise their usage
- Chemists looking to get started with the use of mobile devices for teaching and research in academia or industry
- Anyone interested in learning about the range of chemistry tools available for use on mobile devices

Confirmed speakers and draft topics are:

- Michelle Lynch, IHS: *Overview of mobile chemistry*
- Andy Davies, AstraZeneca: *RSC Medicinal Chemistry Toolkit*
- James Stevens, Royal Society of Chemistry: *Mobile publishing*
- Nick Greeves, University of Liverpool: *Mobile devices in chemistry education*
- Daniel Fitzpatrick, University of Cambridge: *Controlling reactions in Tokyo from Cambridge using the cloud*
- Dan Ormsby, Dotmatics: *Challenges of developing electronic lab notebooks for mobile devices and substructure searching on iPad*

See: <http://www.rsc.org/events/detail/22602/chemistry-on-mobile-devices-create-compute-collaborate>

## 2. Chemoinformatics for Drug Design, 12 October 2016, Cambridge, United Kingdom

This will be a joint meeting with the Society of Chemical Industry. More details including speakers, topics and booking information can be found at <http://www.rsc.org/events/detail/22949/cheminformatics-for-drug-design-data-models-and-tools>.

### Future CICAG Meetings

Contributed by RSC CICAG Chair Dr Helen Cooke, email: [helen.cooke100@gmail.com](mailto:helen.cooke100@gmail.com)

Although we have not run any scientific or educational events in the first half of 2016, our Committee is working on two scientific meetings for later in 2016 and developing a programme of events for the next few years.

Meeting	Date	Location	Partnering organisation	Further information
Chemistry on Mobile Devices: Create, Compute, Collaborate	Wed 7 Sept 2016	Cambridge Centre for Chemoinformatics at the Chemistry Dept, Univ. of Cambridge		<a href="http://www.rsc.org/events/detail/22602/chemistry-on-mobile-devices-create-compute-collaborate">http://www.rsc.org/events/detail/22602/chemistry-on-mobile-devices-create-compute-collaborate</a>
Cheminformatics for Drug Design: Data, Models and Tools	Wed 12 October 2016	Imperial War Museum, Duxford, Cambridge	SCI	<a href="https://www.soci.org/Events/Display-Event?EventCode=F-CHEM481">https://www.soci.org/Events/Display-Event?EventCode=F-CHEM481</a>
Chemical structure representation: what would Dalton do now?	Tues 4- Wed 5 April 2017	University of Liverpool and Catalyst Science Discovery Centre	CSA Trust	Contact CICAG Chair, Helen Cooke, for more information.

Faraday Discussion on Big Data	2017/18	Sheffield or Leeds	
Working Title: Spectroscopic data to chemical knowledge	2017/18	AstraZeneca, Macclesfield	RSC Molecular Spectroscopy Interest Group
Celebrate the centenary of IUPAC	Spring 2019	Burlington House	RSC Historical Interest Group
RSC Document Digitization project	TBD	Webinars	

As further information becomes available, it will be announced on CICAG's Forthcoming Events page: <http://www.rsc.org/events?MemberNetwork=16&PageTitle=16>.

### RSC Undergraduate Research Bursaries

Contributed by RSC CICAG Chair Dr Helen Cooke, email: [helen.cooke100@gmail.com](mailto:helen.cooke100@gmail.com)

As mentioned in CICAG's Winter 2015 Newsletter, a number of Undergraduate Research Bursaries, funded by the Royal Society of Chemistry, are available each year to students in UK and ROI Chemistry and related departments to fund research projects which this year run from June-September 2016. The purpose of the awards is to give experience of research 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 agreed to sponsor one student project. We are pleased to report that the recipient will be Abigail Hanby, who is studying at the University of Oxford. Abigail's research project will be at the University of Leeds. The topic of her research will be Development of Novel Lead-like Scaffolds for Drug Discovery.

### The 7<sup>th</sup> Capps Green Zomaya Award for Medicinal and Computational Chemistry

#### *Background*

Nigel Capps, Rich Green and Alex Zomaya died in a tragic air crash in 2001. They each had distinguished careers as medicinal chemists in the pharmaceutical industry and between them they contributed to the development of new drugs to treat cardiovascular and infectious diseases, cancer, asthma and arthritis. Their network of colleagues and contacts spanned the scientific communities of both the industrial and academic sectors. Following their deaths, a group of colleagues and friends decided to set up a lasting memorial to their lives. The four companies with whom the chemists were most closely associated, GSK, Celltech, Vernalis and NicOx, generously contributed to an Award Fund under the auspices of the Royal Society of Chemistry (RSC). In 2006, a Charitable Trust was created to administer the Award. In 2013 the Award was incorporated into the Biological and Medicinal Chemical Sector (BMCS) of the RSC and is now run in tandem with the Malcolm Campbell Award.

The biennial Award acknowledges outstanding contributions made by young scientists (up to the age of 40) to the fields of medicinal or computational chemistry. Winners of the Award receive a Royal Society of Chemistry Certificate, a commemorative medal and a cheque for £2000. They are also invited to give a Memorial Lecture at the East of England Medicinal Chemistry Symposium at the University of Hertfordshire.

## *Biographies*

### **Nigel Kenneth Capps (1960 – 2001)**

Nigel gained his BSc in chemistry from Imperial College and his PhD on novel synthetic approaches to bicyclic lactam structures under the direction of Professor Doug Young at the University of Sussex. After completing a post-doctoral fellowship with Professor Tony Barrett at Northwestern University, Illinois he joined Glaxo UK in 1986 and worked on 5HT-related drugs for migraine. He was appointed a Group Leader at Celltech in 1991, working on novel immunomodulators targeting signal transduction in T-cells. In 1994, he joined the Business Development group at Celltech for three years before moving to Cerebrus, which merged with Vanguard to form Vernalis plc in 1999. In 2000 he became Head of Business Development at the French Biotech Company, NicOx.

### **Richard Howard Green (1947 – 2001)**

Rich was awarded his BSc in chemistry from the University of Sheffield in 1969, and his PhD on acid catalysed rearrangements of cyclo-octyl and anisyl systems from the University of Leicester in 1973. He joined Glaxo as a medicinal chemist in 1973 where he worked on a number of projects including cephalosporin, prostaglandins and Beta-3-adrenoceptor agonists. Rich identified several novel synthetic routes in pursuit of these targets, which greatly aided the generation of structure activity (SAR) relationships. He developed a particular interest in natural product chemistry and was the author of several outstanding reviews in the area. In 1997, he became a full-time computational chemist at Glaxo with interests in intelligent compound selection. He achieved success in identifying several lead series for G-protein-coupled receptor targets. He also had interests in utilisation of protein crystal structure for compound selection, pharmacophore compound design and the creation of virtual and real libraries. He brought these skills to Celltech in 2000, where he was appointed as a Principal Scientist in computational chemistry. He had a significant impact in enabling Celltech's structure based drug design approaches in the short time before his death in 2001. Throughout his career, Rich was an excellent teacher and mentor to his younger colleagues.

### **Alexander Ishu Zomaya (1946 – 2001)**

After his schooling in Baghdad, Alex came to England in 1962 to continue his education. He obtained his BSc in chemistry at the London South Bank University before joining Beechams in 1970 where he stayed, working as a medicinal chemist, for 23 years. His work focussed mainly on antibiotic research and he made major contributions to therapies based on the chemistry of erythromycin and clavulanic acid; programmes which ultimately led to the discovery of augmentin. In 1993 he joined Celltech where he worked on novel anti-inflammatory therapeutics. He contributed to the discovery of CDP840, an inhibitor of phosphodiesterase type 4 and CDP323, an antagonist of  $\alpha 4$  integrin function, both of which progressed to clinical trials. Alex was named as an author and inventor on 17 scientific articles and patents.

### **The 2016 7th Capps Green Zomaya Award was jointly awarded to:**

**Alison Woolford** in recognition of her work at Astex Pharmaceuticals on the application of fragment-based drug discovery (FBDD) to identify new anti-cancer drugs and progress them to clinical evaluation. In particular, the development of novel inhibitors of apoptosis proteins (IAPs) for the treatment of advanced solid tumours and lymphomas.

and

**Alessio Ciulli** in recognition of his work at the University of Dundee on protein-protein interactions involved in cancer. In particular the discovery of first-in-class molecules which disrupt the binding of the ubiquitin-related complex VHL-E3 to the transcription factor HIF1 $\alpha$ ; also for his contribution to the engineering of highly selective BET (Bromodomain and Extra Terminal motif) inhibitors using the 'bump and hole' approach. Both of these targets are widely believed to have important implications for the development of new immunosuppressive and anti-cancer medicines.



*Above, Dr Alison Woolford with the 2016 Award, which she said "was possible only because of all the hard work put in by many colleagues at Astex".*

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## Chemical Information / Cheminformatics and related Books

1. [Practical Tips for Facilitating Research](#), Moira J Bent, Facet Publishing, Mar 2016



Moira Bent writes: Over a year ago, I asked for ideas and contributions for a book I was writing exploring the different ways in which library staff can engage with researchers. I was delighted with the responses I received from folks and I've been able to incorporate many of them into this book, which I'm pleased to say has finally been completed and published. The book comprises ideas and examples from librarians from around the world on many different aspects of how we can contribute to the research process – my job has



been to organise them into a logical structure. I'd like to thank everyone for their contributions and encouragement – the whole thing took far longer than I'd originally anticipated!

Full details can be found from the link above, whilst a few brief details are included below.

Grounded in current theory and informed by practitioners from around the world, this practical book offers a wide range of ideas and methods to assist library and information professionals in developing and managing their role in the research environment.

Part of the *Practical Tips for Library and Information Professionals* series, the book is organised into eight sections:

- Landscapes and models
- Structures and strategies
- Places and spaces
- Library staff roles
- Collections
- Specific interventions in the research process or lifecycle
- Teaching approaches
- Information literacy skills workshops and programmes.

Author: Moira Bent, Faculty Liaison Librarian & National Teaching Fellow, Robinson Library, Newcastle University, NE2 4HQ; Copyright: Moira J Bent, 2016

Print ISBN 978-1-78330-017-4 (paperback), 978-1-78330-109-6 (hardback);

PDF <http://www.booksonix.co.uk/facetpublishing/9781783300174.pdf>

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## How 'Information Literate' do Chemists Need to be?

The RSC plays a role in ensuring professional skills are embedded into many key activities we undertake. Professional skills such as literacy are extremely important for practicing chemists. These types of skills are developed over time and underpin the theoretical knowledge imparted by undergraduate degree courses and beyond. As such there is a key requirement for professional skills within the Royal Society of Chemistry's degree accreditation framework "Programmes must develop the professional skills for those intending to practice chemical science as a profession." All accredited degree programmes must have learning outcomes that demonstrate this aspect. As the professional body for the chemical sciences the RSC played a role in helping to develop the QAA Chemistry Benchmark Statement which gives a clear outline for provider expectations at a university level.

Following on from an education perspective, professional recognition with the Royal Society of Chemistry in the form of Chartered Chemist (CChem) status will display an individual's commitment to developing professional skills over a period of time. Specifically Section C of the CChem attributes considers literacy skills directly:

- C. Communicate effectively and demonstrate influence in your role
  - C.1 Demonstrate good communication skills by writing clear, concise and orderly documents and/or giving clear oral presentations.
  - C.2 Discuss work convincingly and objectively with colleagues, customers and others, responding appropriately to alternative views.
  - C.3 Exert effective influence.

CChems have an obligation to continuing professional development to stay relevant in the field.

The RSC's Accreditation Manager is Toby Underwood, MChem CSci CChem MRSC. Toby can be contacted at Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF; Tel: +44 (0) 1223 432458

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## Promoting Science to Young People and their Families

Contributed by Dr Diana Leitch, MBE, email: [diana.leitch@googlemail.com](mailto:diana.leitch@googlemail.com)

CICAG and the RSC Historical Group have jointly and generously funded two *mini-interactives* created by 'Ian Russell Interactives' for use by staff at the Catalyst Science Discovery Centre and Museum in Widnes at external events. Over the last few weeks they have taken them to the Big Bang Show in Liverpool, the Science Open events at the Daresbury Innovation Centre and the World Museum in Liverpool where they have been used to demonstrate scientific principles to thousands of visitors including school pupils and families. The children loved them and Catalyst used the occasions to distribute leaflets about their Education Programme for schools and also their intensive Holiday Workshop programme running from 25th July to the beginning of September 2016 at Catalyst itself.

The two interactives were a Cartesian-Diver 'Pressure' and a Bubble Box 'Bubble Colours' which can be seen in the photos taken by Diana who attended both the Daresbury event and the World Museum event. Two of the young people who attend Saturday Science Club at Catalyst came along to help with the demonstrations.



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## CICAG's Dr Diana Leitch Receives 2016 RSC Award for Service

With thanks to RSC News August 2016 Issue p.4.

The RSC's Chemistry Award for Service recognises outstanding non-academic service to the chemistry community, and with over 30 year's work and commitment to the areas of chemistry and chemical information, Diana is a worthy recipient. As well as making a significant contribution to chemical information through 10 years as a CICAG Committee Member, as we can see above on page 10, Diana has been a passionate advocate for science in the north west through her involvement with the Catalyst Science Discovery Centre in Widnes and has provided significant support to Catalyst with the help of RSC involvement and funding, including joint initiatives with CICAG.

Currently a highly-respected information consultant and following a distinguished career as an academic librarian, in 2005 Diana was elected a Fellow of the RSC. In 2014 Diana was also awarded an MBE for services to chemistry. The next award ceremony is now set for the 2016 General Assembly in Belfast this November, when the 2016 RSC Award for Service will be presented. Congratulations to Dr Diana Leitch on behalf of all CICAG.

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## New Elements get a Name: The 7th Row is now Complete

Contributed by RSC CICAG Secretary Prof. Jeremy Frey, email: [J.G.Frey@soton.ac.uk](mailto:J.G.Frey@soton.ac.uk)

As soon as Mendeleev had demonstrated the power of the periodic table to explain the relationships and trends in the behaviour of the elements the hunt was on to fill the missing slots. For the most part the need was to isolate the new elements from minerals (or in the case of Helium identified first from solar spectra). Once Moseley had identified the concept of atomic number from x-ray spectra, the table all fell into place and it was clear where there might still be gaps and where it was complete. Those who established their existence and properties named the new elements; in some cases it took time to establish that some 'elements' were not!

With most of the table complete and extended to include the f-shell lanthanides, the radioactive elements up to Uranium suggested the table was incomplete. The transuranic elements, with atomic number greater than 92, needed to be "created" in nuclear reactions. Post WWII studies of nuclear reactions mainly at LBL enabled quantities of the increasingly unstable elements to be isolated. A different process involving collisions of a high energy atomic beam with a heavy atom target were used to form the new elements by fusion. Despite the very low yields, and the microscopic (or indeed nanoscopic) quantities of the elements generated, their physical and in some cases even chemical properties could be measured. The periodic table as we now usually see it with the row of actinides below the lanthanides is credited to Seaborg who was responsible for generating at least 9 of these elements.

The extreme difficulties of these experiments led to an internationally agreed process to approve the discovery and assign priority and thus the right to name the element. A joint committee of IUPAC and IUPAP looks to see the initial evidence and that it has then been repeated by others, ideally on two occasions.

Several years ago IUPAC assigned working symbols and names to refer to the elements that would complete the 7th row of the periodic table, the funny Uu names, that have puzzled many a chemistry student. Steadily the main labs in the USA, Russia and Germany produced the remaining elements. The announcement of the final four elements comes with the right to suggest a name and symbol and includes a relatively new player from Japan.

Traditionally the names of the place the discovery, the minerals, and significant scientific figures have been used. The suggestions go out for a period for international approval as there can be many potential conflicts

with symbols previously used for other elements in different languages. The final approval will be given by an IUPAC general assembly meeting.

There is considerable interest in the transuranic elements. There have long been predictions of islands of stability where particular combinations of protons and neutron numbers would lead to more stable nuclei and there are suggestions that even higher atomic numbers could be stable but I suspect these would need a very different approach to generate them.

The chemistry is another important aspect of the very high atomic number elements. Will their oxidation states follow the expected pattern of the groups they lie in? This is not a trivial question to answer experimentally (due to the very few atoms generated) nor theoretically as the quantum calculations of atoms with so many electrons is hard due to both the number of electrons and the fact that the high nuclear charge means that many of the electrons would be travelling at relativistic speeds (if we consider them in a type of classical orbit) and so relativistic quantum mechanical calculations are needed. Recent calculations suggest that the relativistic effects have a significant impact on the chemical properties and they diverge from the 'periodic pattern'. Perhaps time will yield sufficient atoms to be able to engage in a full discovery of the chemical properties. Meanwhile the 7th period is now filled, with the proposed names - nihonium (with the symbol Nh), moscovium (Mc), tennessine (Ts), and oganesson (Og), out for public review.

- *Nihonium* references the Japanese name for Japan. The atom was discovered at the RIKEN Nishina Center for Accelerator Science
- *Moscovium* was named after the Moscow region, the location of the Joint Institute for Nuclear Research in Dubna
- *Tennessine* recognises the US state of Tennessee and the local contributions made to the discovery by the Oak Ridge National Laboratory and Vanderbilt University
- *Oganesson* honours the nuclear physicist Yuri Oganessian, who has played a leading role in the search for new elements including the one that will now bear his name

Meanwhile I am sure that we will soon hear of new speculative approaches on creating the first element of the 8th period (if indeed the periodicity continues).

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## The 1st Cambridge Information & Intellectual Property Meeting (CIIPM)

Contributed by Stuart Newbold and Jane List

On Wednesday 13<sup>th</sup> July Extract Information and Patent Search & Information Management successfully hosted an IP meeting with a difference bringing together forty people with an interest in intellectual property, information and successful commercialisation of technology for an afternoon of learning, knowledge sharing and discussion. With eight presentations, and six exhibitors there was a lot to fit in. Not many of us made it outside with our prosecco at the end of the afternoon due to the fascinating conversations happening inside. Buoyed by our success we are already thinking about the 2017 meeting, and hope to see more people next year.

Our headline speaker, Jaideep Prabhu, from Judge business school got us off to a thought provoking start looking at frugal innovation which is well established in India, and how this method of using existing techniques to bring about nonetheless ground breaking changes to improve people's lives can also have a place in western industry to improve creativity, engagement and productivity. Following on we toured the innovation lifecycle, looking at IP practicalities and using information to make wise commercial decisions for early stage businesses. Rachel Hodge from HMRC gave a very useful update on the Patent Box scheme, and how it can bring benefits for those who licence and productise directly their patented technologies. Pauline Stasiak from MRCT gave insights into working collaboratively. An overview of search techniques to establish freedom to operate was ably presented by Stuart Newbold. There was much interest also in our exhibitors from Aistemos to the IPO, with J A Kemp and Birketts representing the legal sector.

Our final speaker Nigel Swycher from Aistemos was also very well received with his demonstration of Cipher, the IP analytics for business tool, which his company is creating. Interest in understanding IP outside of the legal and IP departments is increasingly important, as investment decisions are made on the basis of IP assets within a company. It's in everyone's interest if the business community can get to grips with patents, and the information as technical, legal, and commercial knowledge that is held within. Peter Evans from the UK IPO economics unit, working on big data analysis, also presented some of the misconceptions, and things to be wary of when interpreting patent data.

Extract Information and PSIM are now planning to organise follow on training courses and workshops, which we hope to also host at Cambridge's Homerton Conference Centre in 2017 under the CIIPM initiative. Look out for the 2nd Cambridge Information and Intellectual Property Meeting will take place in July 2017.

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## **Tony Kent Strix Award and Annual Lecture 2016**

### **The 2016 Tony Kent Strix Award**

The call for nominations for the prestigious Tony Kent Strix Award has been published, given in recognition of outstanding practical innovations or achievements in the field of information retrieval in its widest sense. The nomination could highlight achievements in an application or service, or an overall appreciation of past works from which significant advances have emanated. Nominations should reach UKeIG no later than Friday, 26<sup>th</sup> August.

Full details of where to send nominations and of the information which should be included in the nomination are given in the full call, which call can be found at:

<http://www.cilip.org.uk/uk-einformation-group/awards-bursaries/tony-kent-strix-award/2016-call-tony-kent-strix-nominations>

Further details of the award and a list of previous winners is also available at

<http://www.cilip.org.uk/uk-einformation-group/awards-and-bursaries/tony-kent-strix-award>

The Tony Kent Strix Award is sponsored by the Royal Society of Chemistry Chemical Information & Computer Applications Group.

### **The 2016 Tony Kent Strix Annual Lecture**

The 2016 Tony Kent Strix Annual Lecture, the second in the series, will take place on Monday, 31<sup>st</sup> October, at The Geological Society, Burlington House, Piccadilly, London, from 2.00 p.m. The lecture will be given by the 2015 Tony Kent Strix award winner, Peter Ingwersen, Professor Emeritus at The Royal School of Library and Information Science, University of Copenhagen. There will be a supporting lecture. Further details and application forms will be available later.

Please note that, as last year, this lecture will be sponsored by Google, and will be free of charge. Tea and biscuits are provided.



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## National Chemical Database Service News

[National Chemical Database Service](#) (NCDS) has seen a number of recent enhancements:

DETERM been updated to correspond to the all-new DETERM website – users are invited to try it out now, thereby accessing 8.9 million data sets relating to 44,200 pure compounds and 139,400 mixtures. DETERM remains an invaluable resource for researchers in chemistry and related fields. The new update features a much-improved search system and user interface, making it easier to search the DETERM database of thermophysical properties.

The Available Chemicals Directory search interface has been improved allowing users to get the most out of this resource. Various search options including substructure searching of ACD allows retrieval of available chemicals complete with pricing and supplier information for 3.2 million unique compounds from over 800 suppliers.

Meanwhile a new NCDS introductory video has been produced showcasing content and how to use the various resources. The video can be seen here on [YouTube](#).

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## 175 Minutes for Chemistry

As CICAG members will know, 2016 marks the 175th anniversary of the RSC. As part of the celebrations, the RSC is asking members to dedicate 175 minutes of their time to chemistry, and to then let the RSC know what they have done. Have any readers contributed a “175”? If so please let CICAG know, and we will endeavour to include whatever contribution you have come up with in the newsletter. Contact the editor on [stuart@psandim.com](mailto:stuart@psandim.com).

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## InfoChem News

*Contributed by Stephanie North, InfoChem GmbH*

InfoChem GmbH ([www.infochem.de](http://www.infochem.de)), is pleased to announce that they have been designated by the World Intellectual Property Organization (WIPO) in Geneva to implement the project "Addition of chemical search capabilities to the WIPO PATENTSCOPE search system".

The goal of the project is to identify, tag and index chemical entities such as IUPAC Names, trade and brand names and trivial names in the PATENTSCOPE full-text documents using InfoChem's highly acknowledged named entity recognition technology ICANNOTATOR.

Additionally, structure search capabilities for chemical compounds will be added to the PATENTSCOPE search user interface.

The cooperation is planned for at least three years, during which time various enhancements to the PATENTSCOPE search system will be implemented with the aim of improving the discoverability of the PATENTSCOPE patent full-text collections.

For more information email [info@infochem.de](mailto:info@infochem.de) or tel. +49 (0) 89583002.

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## CAS / SciFinder / STN News

*Contributed by Dr Anne Jones, CAS Applications Specialist UK & Ireland*

### CAS News

#### **New CAS solution now MethodsNow™ launched!**

MethodsNow, a CAS solution, is your single source to search and compare the latest published scientific methods. MethodsNow:

- Saves time with easy access to hundreds of thousands of disclosed procedures
- Lets you quickly compare methods side-by-side
- Displays experimental details in easy-to-read table format
- Includes materials, instrumentation, conditions and more
- Covers 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

Access the CAS collection of analytical methods at [www.MethodsNow.com](http://www.MethodsNow.com) and synthetic methods exclusively through SciFinder®.

#### **ChemZent™, the first English-searchable version of Chemisches Zentralblatt is now available in SciFinder**

ChemZent, a new solution available in SciFinder, provides access to the first and only searchable, English-language version of Chemisches Zentralblatt. ChemZent features:

- Integration with SciFinder allows for the exploration, discovery and isolation of historic chemistry information using familiar SciFinder features
- English-language searching is a first for Chemisches Zentralblatt
- Indexing of relevant concepts and substances provides additional access/entry points to ChemZent abstracts
- Abstract markers pinpoint the location of the abstract within original German PDF
- CAS controlled vocabulary promotes discoverability
- Original German and English translated abstracts available for print and export

### STN News

#### **Launch of PatentPak™ in STN® Promises Improved Efficiency for IP Search Professionals**

Effective from January 2016, PatentPak, a time-saving solution for IP professionals, is available for subscription by classic STN customers under any pricing plan. Subscribing customers will be able to use PatentPak in STN in both the STN Express® 8.6 and STN on the Web<sup>SM</sup> platforms.

Also available now, free downloads of STN Express 8.6 will be available to STN login ID holder. STN Express users must upgrade to STN Express 8.6 in order to use PatentPak.

In May 2016, PatentPak won an industry impact award from CODiE for Best Science & Technology Information Solution!

#### **Key Features**

- Full-text patent PDFs from 31 major patent offices - over 8 million patents so far, with more being added every day.
- Patent family coverage in multiple languages, including English, German, Chinese, Japanese, French, Korean and Russian.
- Direct navigation to indexed substances within the patent via page number hyperlinks.
- Exportable patent PDFs with or without summary tables and CAS analyst markup for sharing and printing.
- Conveniently share these benefits with others via links in STN Express-generated tables and reports, as well as transcripts, even if they don't use STN.

Sample CAplus record with PatentPak

## CAS Training in the UK 2016

### CAS Training in the UK 2016

In addition to e-learning materials, CAS continues to offer instructor-led training for both STN® and SciFinder® in the UK.

We conduct 'in-house' WebEx training sessions on all aspects of STN or SciFinder searching. If you wish to know more about any CAS products, or would like further information or help with STN or SciFinder, then please contact [annejones@acsi.info](mailto:annejones@acsi.info).

## ChEMBL News – 'ChEMBL 21'

ChEMBL 21 was released on 1st February 2016.

ChEMBL (<https://www.ebi.ac.uk/chembl/>) is an online database of bioactive drug-like small molecules, it contains 2-D structures, calculated properties (e.g. logP, Molecular Weight, Lipinski Parameters, etc.) and bioactivities (e.g. binding constants, pharmacology and ADMET data) that has been abstracted from the primary literature. This together with detailed biological target information make ChEMBL and absolutely essential resource for all those interested in the biological activities of small molecules. The latest update now contains

- 1,929,473 compound records
- 1,592,191 compounds (of which 1,583,897 have mol files)
- 13,968,617 activities
- 1,212,831 assays
- 11,019 targets
- 62,502 source documents

In addition it now contains information for several thousand compounds that are in clinical development or are FDA approved drugs, including target information and disease identifiers.

ChEMBL also acts as an archive for an increasing number of primary screening and medicinal chemistry programs involved with neglected tropical diseases (<https://www.ebi.ac.uk/chemblntd>), these are an invaluable resource for identifying novel starting points, but also act as a useful resource to check if hits identified elsewhere have already been evaluated. An example is the Malaria subset (<https://www.ebi.ac.uk/chembl/malaria/>), a searchable resource for publicly available compounds, targets, assays and data for malaria research.

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## Other News Items and Events

### 1. Thomson-Reuters Sale

A recent big breaking news items was the proposed acquisition of Thomson-Reuters's Intellectual Property & Science Business to two private equity firms, Onex and Baring Asia for \$3.55 billion. Toronto, New York, and London based Onex was founded in 1984 and now includes over 85 operating businesses and has a total value of approximately \$61 billion. Baring Asia, based in Hong Kong, is an even more recent fund having been formed in 1997. It has investments businesses totaling about \$10 billion. Most of the Thomson-Reuters IP and Science business portfolio will be familiar - with products such as Thomson Innovation, Web of Science, Thomson CompuMark, the pipeline databases Cortellis and Integrity all being popular in industry. Thomson-Reuters say the company has 4,100 people across more than 75 offices in over 40 countries. The acquisition is subject to various regulatory approvals, particularly in the US.

### 2. ORCID - The Unique Author Identifier

### 3. Nano, a new product from Springer Nature

Nano provides highly indexed and structured information related to nanomaterials & devices derived from high impact journals and patents. It combines the key features of a database and an A&I discovery tool supported by intelligent functionality.

Nano is available at [nano.nature.com](http://nano.nature.com) and consists of over 200,000 curated profiles on nanomaterials and devices, not available anywhere else with links to the original source. The resource covers a number of the top and high impact factor journals and patents in the field. Top peer-reviewed journals include:

- Nature, Springer Nature
- Advanced Materials, Wiley
- ACS Nano, ACS Publications
- Nano Letters, ACS Publications
- Biomaterials, Elsevier
- Nature Nanotechnology, Springer Nature
- Nanoscale, RSC Publishing
- Nanotoxicology, Taylor & Francis
- Small, Wiley

For more information, email [libraryrelations@springernature.com](mailto:libraryrelations@springernature.com)

### 4. World Library and Information Congress

- The 82<sup>nd</sup> IFLA General Conference and Assembly takes place from 13<sup>th</sup> to 19<sup>th</sup> August, in Columbus, Ohio

The International Federation of Library Associations and Institutions (IFLA) is the leading international body representing the interests of library and information services and their users.

### 5. 21st European Symposium on Quantitative Structure-Activity Relationship (21st EuroQSAR)

- "Where Molecular Simulations Meet Drug Discovery", 4<sup>th</sup> - 8<sup>th</sup> September, in Verona

### 6. International Conference on Trends for Scientific Information Professionals. ICIC 2016

- ICIC takes place on 17<sup>th</sup>-18<sup>th</sup> October, in Heidelberg, Germany, and is organized by Christoph Haxel.

CICAG notes that the related 2017 II-SDV International Information Conference on Search, Data Mining and Visualization will go ahead again in Nice, despite the horrific events in recent days. Christoph ([c@haxel.com](mailto:c@haxel.com)) is currently asking for papers for submission, with a deadline of November 30.

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