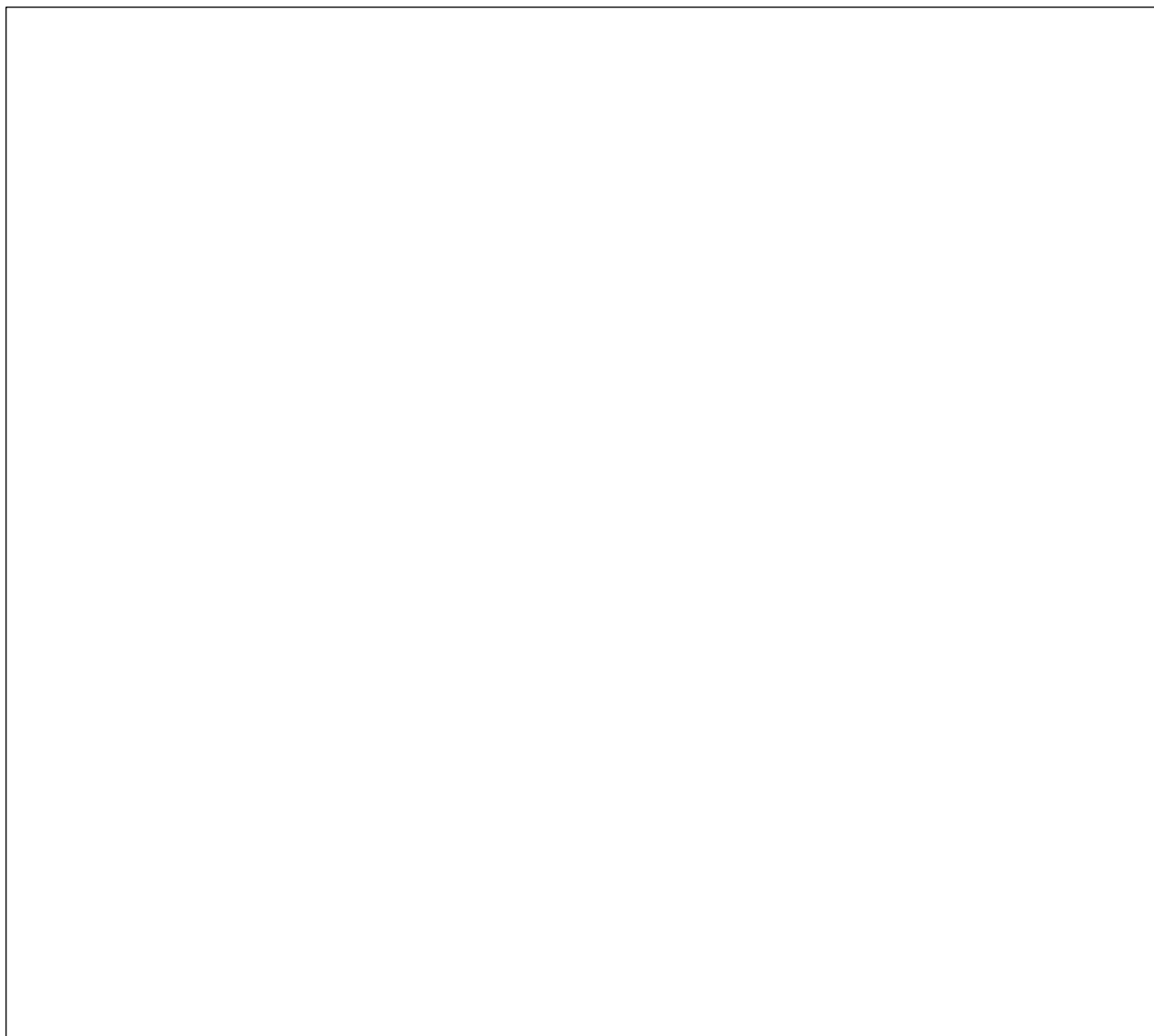


NEWSLETTER Summer 2016



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, 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 pl375@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>

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.

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!

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

- x 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

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 α_4 integrin function, both of which progressed to clinical trials. Alex was named as an author and inventor on 17 scientific articles and patents.

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”.

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 RSC's Accreditation Manager is T

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 can lead to relativistic effects.

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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CAS / SciFinder / STN News

CAS News

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

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- x Full-text patent PDFs from 31 major patent offices - over 8 million patents so far, with more being added every day.
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CAS Training in the UK 2016

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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

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) is currently asking for papers for submission, with a deadline of November 30.
