ROYAL SOCIETY OF CHEMISTRY | CHEMICAL INFORMATION AND COMPUTER APPLICATIONS GROUP

# NEWSLETTER winter 2017-18


Above: Local cub scouts with Catalyst Education Manager, Lucinda Lewis and Graham Phillips, Deputy Lord Lieutenant of Cheshire (see 'Widnes Success' page 5)

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 Websites**:
http://www.rsc.org/CICAG
https://www.liverpool.ac.uk/~ngberry/cicag/index.htm

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

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

https://twitter.com/RSC_CICAG

QR Code

## Table of Contents



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 Chris Swain, email: swain@mac.com*

This is my first Chair's report and I'd like to start by thanking Helen Cooke for her invaluable stewardship over the last three years as CICAG Chair. Helen oversaw a number of diverse and highly successful meetings. She was also responsible for supporting a number of collaborations with external organisations. Fortunately for CICAG Helen has agreed to stay on the committee where her guidance and support will be greatly welcomed.

Another change to the committee is that Michelle Lynch has decided to stand down. Michelle, together with another ex-committee member Keith White, was responsible for the CICAG social media presence on Twitter, LinkedIn and Facebook. These news feeds are proving to be increasingly important in highlighting CICAG events and flagging items that might be of interest to members and I'd like to thank them for their contributions. This baton has now been passed to the "next generation" and we have organised group of post-docs and post-graduate students to take over the social media channels.

In addition to the social media feeds, CICAG has begun the process of creating a new CICAG website under the direction of Neil Berry; the aim being to create a more dynamic site that can also be more regularly updated.

CICAG has continued to support the Tony Kent Strix Award. The 2016 winner Maristella Agosti, Professor in Computer Science, Department of Information Engineering, University of Padua, Italy, gave her lecture at The Geological Society, Burlington House, Piccadilly, during the afternoon of Friday 20th October 2017. At the meeting the 2017 winner was announced - Maarten de Rijke of the Informatics Institute at the University of Amsterdam.

The critical role informatics plays in all areas of research has long been recognised by CICAG and back in 2015 CICAG ran a popular one day meeting "*Big Data to Chemical Information*" (http://www.rsc.org/Membership/Networking/InterestGroups/CICAG/meetings.asp). The next step is to provide tools to extract information and learning from the vast amounts of data now available and CICAG together with BMCS are organising a meeting entitled "*Artificial Intelligence in Chemistry*" (http://www.rsc.org/events/detail/30272/rsc-bmcs-rsc-cicag-artificial-intelligence-in-chemistry). I have been involved with the organisation of many meetings and I've never seen such positive feedback to a first circular; this looks like it will be another very popular event!

## CICAG Planned and Proposed Future Meetings

The table below provides a summary of CICAG's planned and proposed future scientific and educational meetings. For more information, please contact CICAG's Chair, Dr Chris Swain.

| Meeting | Date | Location | Further Information |
|---|---|---|---|
| Predicting Reaction Outcomes | 26 Mar 2018 | Bradfield Centre, Cambridge Science Park | Dial-a-Molecule meeting (see details on page 4 below) |
| Artificial Intelligence in Chemistry Meeting | 15 Jun 2018 | Burlington House, London | Registration, etc. (see details on page 4 below) |
| Spectroscopic Data to Chemical Knowledge | 2018 | AstraZeneca, Macclesfield | To be organised jointly with the Molecular Spectroscopy Interest |

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|---|---|---|---|
| | | | Group and Dial-a-Molecule Grand Challenge Network |
| Tony Kent Strix Award and Annual Lecture | 23 Nov 2018 | Geological Society, London | |
| Celebrate the Centenary of IUPAC | Spring 2019 | Burlington House, London | To be organised jointly with the Historical Chemistry Interest Group |
| Practical Computational Chemistry | Spring 2019 | University venue TBC | One-day workshop for small groups |
| Structure, Reaction and Patent Information for Small Organisations | TBD | TBD | Proposed joint meeting with RSC Consulting Group |
| Software Update for Medicinal Chemists | TBD | EBI, Hinxton, Cambridge | Proposed training workshop (Joint workshop with the SCI) |
| Big Data | TBD | TBD | Proposed joint meeting with the SCI) |

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## Dial-a-Molecule Meeting: Predicting Reaction Outcomes

*Contributed by RSC CICAG Committee member Prof Jonathan Goodman, email: jmg11@cam.ac.uk*

26th March 2018
Bradfield Centre, Cambridge Science Park
Organisers: Jonathan Goodman and Richard Whitby
Meeting partnered with RSC CICAG

This one day meeting, bringing together chemists, engineers, computer scientists, mathematicians and data scientists from both academic and commercial backgrounds, will be a symposium and discussion forum looking at prediction of chemical reaction outcomes through data analysis and acquisition. In particular we aim to identify the barriers currently preventing us from being able to predict reaction outcomes and to propose next steps.

Topics will include the invention of new reactions, data acquisition and understanding mechanisms.

Registration via: http://generic.wordpress.soton.ac.uk/dial-a-molecule/predictingreactionoutcomes/

Dial-a-Molecule is a Grand Challenge Network funded by the EPSRC between 2010 and 2015 and 2016 and 2019 to promote research aimed at a step change in our ability to deliver molecules quick and efficiently.

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## Artificial Intelligence in Chemistry Meeting

*A joint meeting, organised by RSC-BMCS & RSC-CICAG*
*15th June 2018*
*Royal Society of Chemistry, Burlington House, London*
*Twitter Hashtag: #RSC_AIChem*

*Details contributed by RSC CICAG Committee member Dr Nathan Brown FRSC, email: nathan.brown@benevolent.ai*

Artificial Intelligence is presently experiencing a renaissance in helping develop new methods and practical applications to ongoing challenges in Chemistry. We are pleased to announce that the RSC's Biological & Medicinal Chemistry Sector (BMCS) and Chemical Information & Computer Applications Group (CICAG) are organising a one-day conference to highlight current efforts in applying these new methods. The meeting

will illustrate current efforts in combining aspects of artificial intelligence and deep machine learning methods to applications in chemistry.

Important Dates:

- 31st January–closing date for oral abstract submissions
- 13th April–closing date for poster abstract submissions
- 3rd May–closing date for bursary applications
- 11th May–early bird discount deadline
- 15th June–conference

Outline Programme:
The programme will include a keynote lecture from a key opinion leader in the field, followed by a number of talks and flash poster presentations throughout the day. Confirmed speakers are:

- Dr Ola Engkvist (AstraZeneca) – Molecular de novo design through deep learning
- Dr Willem van Hoorn (Exscientia) – Scaling de novo design, from single target to disease portfolio
- Dr Nadine Schneider (Novartis) – TBC
- Dr Marwin Segler (BenevolentAI) – TBC

Who should attend?
This meeting will be of interest to scientists of any level of experience from academia and industry.

Call for Papers
Applications for oral and poster presentations are welcomed. Posters will be displayed throughout the day and applicants will be asked if they would like to provide a two-minute flash oral presentation when submitting their abstract.

Venue and Travel
Library, Royal Society of Chemistry at Burlington House, Piccadilly, London, W1J 0BA, UK
Situated in central London, the RSC is easily accessible by public transport, and close to Green Park tube station.

Exhibition Opportunities:
There will be a small, relevant trade exhibition – the charge is £500 including one full delegate.

Registration Fees
Registration is open, and fees are:

- £120 RSC member
- £145 Non-member
- £90 RSC student* member
- £100 Student* non-member

* Student is undergraduate or post-graduate.

Member is a paid-up member of the RSC. A late fee of £30 will apply to payments received from 11th May onwards.

Bursaries:
A number of RSC-BMCS and RSC-CICAG student bursaries are available up to a value of £250, to support registration, travel and accommodation costs for PhD and post-doctoral applicants studying at European academic institutions. The closing date for bursary applications is *3rd May*.

Registration is now open via http://www.maggichurchouseevents.co.uk/bmcs/

## Widnes Successes: The Widnes Research Laboratory and the Catalyst Science Discovery Centre & Museum

*Contributed by RSC CICAG Treasurer Dr Diana Leitch MBE, FRSC email diana.leitch@googlemail.com*

Photographs – with thanks to Meryl Jameson, Marketing Manager of the Catalyst Science Discovery Centre and CICAG's Dr Diana Leitch MBE, FRSC

*Left: Prof Dominic Tildesley (representing RSC President) presents Catalyst Trustee, Dr Mike Pitts, with his FRSC badge*

On 5th October 2017 I received an email from Ian Campbell, a former ICI Research Chemist, who is a *Friend of the Catalyst Science Discovery Centre* in Widnes to say there was an interesting article in that week's Widnes Weekly News. It was entitled 'Science Honour for Lab' and said that a former ICI laboratory in Widnes where a life-saving invention was created had been named among the top 10 places in the science and discovery section of Historic England's campaign '*Irreplaceable: a History of England in 100 places*'. He wondered if I knew anything about this, as the Widnes Research Lab had been chosen by Professor Lord Robert Winston.

Indeed I did. Back at the end of June 2017 an article had appeared in the Manchester Evening News entitled '*Search on for Historic Places*', which encouraged the public to nominate famous places that would be voted for. At the end of the article it said that Historic England was looking for places in North West England in the hope of uncovering some hidden gems. The closing date for submission was early July 2017. So with two days to go I put forward a proposal for the great Widnes Research Laboratory of ICI General Chemicals Division where in the 1950s the first ever non-flammable anaesthetic Halothane (Fluothane) was invented by Dr Charles Suckling (1920-2013) CBE, FRS, BSc, PhD, DSc (Liverpool).

I heard no more until I received the email from Ian Campbell. On investigation I discovered that the 10 places chosen for their historic scientific significance were Greenwich Observatory, Bletchley Park, Jodrell Bank, Ouse Wastes in Cambridgeshire, Calder Hall/Sellafield, Brown Firth of Sheffield (stainless steel), Jenner Hut in Gloucestershire, the MRC Biophysics Unit at King's College (DNA Structure), Soho water pump (cholera)...and Widnes Research Laboratory.

What a line-up to be part of! Many other major achievements occurred at Widnes Lab (uranium analysis, the vinyl chloride process, the insecticide Gammexane, the weedkiller Methoxone, Freons and PTFE to name a few)' but Halothane revolutionised surgery and greatly improved patient safety when anaesthetics were used. It was also the first drug to be created by molecular design following on from a precise definition of the functional requirements of a new anaesthetic agent, a definition that allowed the necessary clinical response to be translated into chemistry. Dr James Raventos (1905-1982), a Catalan pharmacologist with an exemplary record as an experimentalist, based at ICI Dyestuffs Division at Blackley in north Manchester, defined the key requirement, and ICI Research Director John Ferguson (1899-1981) initiated the project. In February 1951 he met with Charles Suckling at his lab bench in Widnes and asked the question 'Do you think these two papers of mine (on narcosis) could help a search for an inhalant anaesthetic amongst compounds containing fluorine'? Suckling was able to invent such a molecular compound (CF3CHBrCl) with all the key required properties, and it was first prepared in January 1953 and patented in February 1957.

Clinical trials were carried out by Dr Michael Johnstone at Manchester Royal Infirmary and an internal ICI report from Raventos and Suckling written on 20th January 1956 said 'Fluothane was used for the first time on human beings this morning in MRI with results which so far have proved entirely satisfactory'. Professor

Robert Winston as a doctor would have known and appreciated what a change Halothane brought about for surgeons, anaesthetists and millions of patients alike for several decades after its invention. Today Fluothane is not the anaesthetic of choice in the UK but is still employed and was being used in surgery in Malawi just two weeks ago.

The building where it was invented has gone, swept away partially in the decline of the chemical industry in Widnes and finally just a few months ago to create the new road system for the Mersey Crossing Gateway Bridge, opened on 14th October 2017. Widnes Research Lab was built on Victoria Road in 1891 under the direction of Swiss chemist Dr Ferdinand Hurter when the United Alkali Company (UAC) was created. Almost certainly it was the first research laboratory built in the UK for a chemical industry company to do pure and applied research and set a milestone in the history of the chemical industry. A short distance from this building was an administrative block called the Tower Building of ICI. From 1855 it had been part of the enormous soap firm of Gossages' on Mersey Road in Widnes which was closed by Unilever in 1933. It was in this building that Sir John Brunner and Ludwig Mond met in the 1860s and where much of the early work of ICI on narcosis was done which formed an important part of the scientific basis for the discovery of halothane. Ian Campbell himself spent part of his working career in this building. When the decision was taken to celebrate the invention of halothane by positioning a Royal Society of Chemistry blue plaque on an appropriate building in 2011 it was this latter building which was chosen. The plaque was unveiled by Professor Sir Martyn Poliakoff CBE, FRS, FRSC and Professor Colin Suckling OBE, FRSC and stands proudly on the front face of that building which has, since 1987, been the Catalyst Science Discovery Centre and Museum. Inside Catalyst in its '*Birth of an Industry Museum*' are artefacts from the production of halothane and a display panel about the story of its invention.


*Above: RSC Blue plaque celebrating the discovery of Halothane at Widnes Research Laboratory/Catalyst*

*Above: Catalyst Director Jayne Edwards and staff cutting the birthday cake*

On 28th September 2017 there was a 30th Anniversary celebration of the creation of the Catalyst Science Discovery Centre and Museum on its current site and in the building so deeply involved with not just halothane but the whole development of the soap and chemical industry in Runcorn and Widnes. Industrial, academic and local people attended and heard a sterling address from Professor Dominic Tildesley, representing the current President of the Royal Society of Chemistry, on the value of everything the Catalyst does in promoting the chemical sciences and STEM to people of all ages. In the 'WOW Laboratory' a group of cubs from Widnes did a Workshop and were very pleased to show the County Commissioner for Scouts and Deputy Lord Lieutenant of Cheshire what they were learning. Catalyst's determination to continue in its essential work is summed up in its slogan '*Preserving the Past and Inspiring the Future*.' It is run entirely by a Charitable Trust and receives no public funds. Its Trustees are constantly seeking funds to maintain its work.

## 11th International Conference on Chemical Structures

The 11th International Conference on Chemical Structures will take place on 27th - 31st May 2018 at the Conference Centre in Noordwijkerhout, Holland. Papers are welcome in the areas of cheminformatics and molecular modelling, including for example structure-activity relationships, virtual screening, modelling metabolite networks, and so forth. The closing deadline for the submission of abstracts is Thursday, 1st February. Abstracts can be submitted directly via http://www.int-conf-chem-structures.org/call-for-papers.html.

Student Bursaries

CICAG will be offering a limited amount of bursary funding for the ICCS meeting, details of which are currently being finalised. In the meantime, interested parties should contact RSC CICAG Chair Dr Chris Swain for further details.

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## 6th RDKit User Group Meeting

*Contributed by RSC CICAG Committee member Nathan Brown, email: nathan.brown@benevolent.ai*

In the ten or so years since the RDKit API was released to the community, it has had a huge impact on the democratisation of Chemoinformatics. In concert with the release of open data sources, such as ChEMBL, it is now entirely feasibly to develop very complex chemical structure analysis workflows in a matter of hours and days, compared to what used to take weeks and months only 15-20 years ago. Therefore, it is important that the RDKit, with its ever-growing user base, continues with its traditional annual User Group Meeting, which was first held at the Institute of Cancer Research in London in 2012. In 2017, the RDKit UGM was held in Berlin, organised locally by Andrew Volkamer and Gerhard Wolber.

The UGM began, as is now traditional, with Greg Landrum – the developer of RDKit – giving his '*State of the Toolkit*' address of recent improvements and innovations. Highlights from updates here were the validations of the Experimental-Torsion Distance Geometry with basic Knowledge (ETKDG) method for conformer generation. This has now been demonstrated independently to be the preferred algorithm for conformer generation. Greg also summarised those that are using to use the toolkit, including many from both small and big pharma, biotechs and start-ups, software and service providers, and academia. This is evidenced by the active contributors on the mailing list in addition to the 40 plus attendees at the last three UGMs, which was the capacity limit for these venues.

The UGM this year can be roughly divided into three themes: three-dimensional chemical structures; emerging methods from artificial intelligence; and improvements to matched molecular pair analysis. A highlight in 3D structures was from Guillaume Godin (Firmenich) on 3D descriptor developments and benchmarking in RDKit. In terms of AI approaches, Alpha Lee's talk on Random Matrix Theory for virtual screening was a fascinating new way of looking at this challenge, while Nadine Schneider's talk on automated chemical topic modelling using text-mining approaches will help structure chemistry data in a more intuitive way.

The afternoon of the first day began with Daniel Reker (MIT) discussing active learning in drug discovery and how this can improve the navigation of the chemistry space of relevance. Nadine Schneider (Novartis) presented on Chemical Topic Modelling, which was recently published in J. Chem. Inf. Model., using text-mining to assign chemistries to chemical topics to help structure data from the ChEMBL database.

Christian Kramer (Roche) and Andrew Dalke (Dalke Scientific) presented a two-hander on Matched Molecular Pairs (MMP) analysis. MMPs, defined simply, are two chemical structures that differ in only one position. With additional metadata on the structures, such as biological activity or physicochemical properties, it is then possible to calculate a difference or delta of that value, presumably caused by the

structural variation defined by the MMP. This rule derived from the MMP may then make it possible to be able to apply these data in a form of transfer learning: *i.e.* replace group A with B and you will (typically) improve solubility. While Dalke presented on an improved implementation of MMPs, called MMPDB, Kramer demonstrated their application to large ADMET datasets, and the quality of the results and concomitant speed-ups with the new Dalke implementation.

As is expected from a community-driven open source project like RDKit, the output from the User Group Meeting is also freely available online, here: https://github.com/rdkit/UGM_2017/. These resources include a selection of Jupyter notebooks to test run some of the new features presented at the UGM, as well as presentations, lightning talks, and posters.

The RDKit UGMs have always been free to attend and heavily rely on the local organisers to provide conference facilities and all the typical daily issues associated with running a conference. The organisers are to be congratulated on the smooth running of yet another great UGM and also organising the social events at some local hostelries. If you are interested in attending the next UGM, sign up to the mailing list for more information. Once announced, be quick, it 'sells out' quickly!

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## Vikki Vowles

*Contributed by CAS Applications Specialist in the UK & Ireland, Dr Anne Jones, email annejones@acs-i.org.*

It is will great sadness to report that on 31st August 2017, we lost our friend and colleague Vikki Vowles. Vikki's passing was sudden and unexpected and an enormous shock to everyone at CAS as well as all her customers that knew her well.

Vikki worked at CAS for eight years as a regional marketing manager and covered territories throughout the UK. She loved her work and threw all her energies and efforts into making sure CAS customers received the bespoke attention they needed. Her work efforts were recognised several times at the CAS annual Global Sales meeting and Vikki was the recipient of several awards over the years. Prior to joining CAS, Vikki held positions at Unilever and GSK.

In the last two years, Vikki had taken up running and had progressed so far that in May last year, she ran her first half marathon and was also appointed course leader for a "Couch to 5K" program at her local running club. Vikki's ambition and drive in her both work and personal life were infectious and we will dearly miss her kindness, friendship and humour.

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## Undergraduate Research Bursaries – CICAG Sponsorship in 2018

*Contributed by RSC CICAG Committee Member Neil Berry, email: ngberry@liverpool.ac.uk*

A number of Undergraduate Research Bursaries, funded by the Royal Society of Chemistry will be available to students in UK and the Republic of Ireland Chemistry and related departments from June-September 2018. 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. Applications relevant to the interests of the CICAG will be welcomed in the areas of cheminformatics, chemical information, chemical data management, chemistry data analytics, chemistry IT solutions and applications. The deadline for applications is 26th February 2018.

Further information, including guidelines and the application form can be found at:
http://www.rsc.org/ScienceAndTechnology/Funding/undergraduate-bursary.asp

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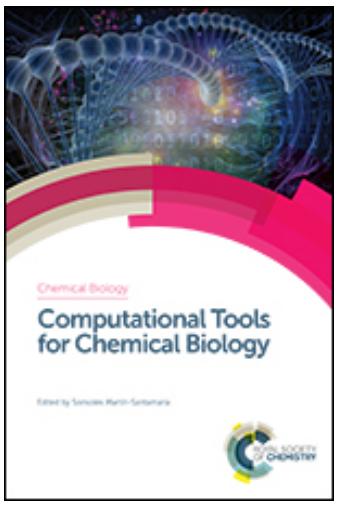
## Chemical Information / Cheminformatics and Related Books

*Contributed by RSC CICAG Newsletter Editor Stuart Newbold, email: stuart@psandim.com*

New book in the Chemical Biology Series published**:**

**Computational Tools for Chemical Biology**

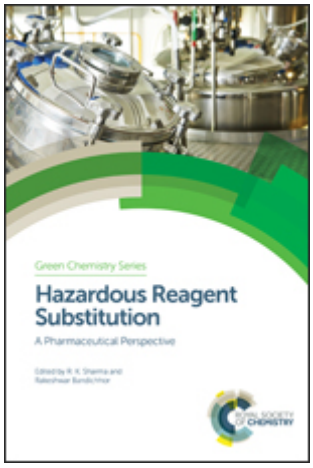



RSC Publishing
Editor: Sonsoles Martín-Santamaría
http://pubs.rsc.org/en/content/ebook/9781788010139?utm_campaign=ebookdoi-9781788010139&utm_source=toc-alert

The field of computational chemical biology involves utilising the latest techniques to visualise and manipulate processes within living cells. The rapid development of efficient computational tools has allowed researchers to tackle biological problems and to predict, analyse and monitor, at an atomic level, molecular recognition processes. This book, with contributions from internationally renowned experts as well as new leaders in the field, offers a fresh perspective on how computational tools can aid the chemical biology research community.

New book in Green Chemistry Series published**:**

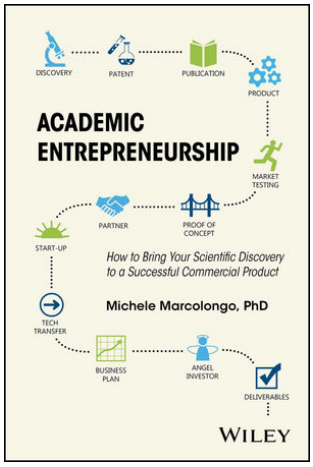
**Hazardous Reagent Substitution**




In recent years, a significant amount of progress has been made using green chemistry in the synthesis of synthetically useful compounds and molecules by replacing hazardous chemicals with greener alternatives. Presenting examples of drugs and their synthesis via green chemistry routes, this book shows how the pharmaceutical industry has adopted green chemistry. Chapters focus on drug design, engineering, process development, calculations to account for waste and the challenges related to use of non-hazardous reagents.

RSC Publishing
Editors: Rakesh Kumar Sharma, Rakeshwar Bandichhor
http://pubs.rsc.org/en/content/ebook/9781782623847?utm_campaign=ebookdoi-9781782623847&utm_source=toc-alert

**Academic Entrepreneurship: How to Bring Your Scientific Discovery to a Successful Commercial Product**




This new book includes interviews by faculty in the disciplines of materials science, pharmaceuticals, medical devices, information technology, energy, and mechanical devices – offering tips and discussing potential pitfalls to be avoided in the road to successful commercialisation.

Wiley Publishing
Michele Marcolongo
ISBN: 978-1-118-85908-7
http://www.wiley.com/WileyCDA/WileyTitle/productCd-1118859081.html (US)
http://onlinelibrary.wiley.com/book/10.1002/9781118859070 (UK)

## Tony Kent Strix Award and Annual Lecture 2017

*Contributed by RSC CICAG Member Alan Tonge, email a.tonge99@outlook.com*

The third Tony Kent Strix Annual Lecture, 20 October 2017

The meeting was held at the Geographical Society, Burlington House, and was introduced by Doug Veal, chairman of the Strix Awards Committee.

There were two presentations, the first by Alan Gilchrist and the second by Maristella Agosti, winner of the 2016 Strix Award.

Alan Gilchrist

*Reflections: Some thoughts on the past, present and future of Information Retrieval*

The possibilities for informational retrieval have advanced enormously in the past 50 years, moving from the use of hand-held punched cards to the search and storage of huge amounts of captured data in on-line databases.

However, this use of interactive on-line interrogation of databases has led to a situation where the end-user - typically a researcher in a library or institution - now often talks directly with the database through a GUI, rather than through an information scientist, a process known as 'disintermediation'. Furthermore, data can now be abstracted or curated automatically by machines (e.g. algorithms using natural language processing or machine learning) leading to an increased potential for errors or omissions - i.e. the potential creation of false information.

These two factors highlight the continuing need for intelligent information management.

Professor Maristella Agosti - Information Management Systems Research Group, Padua University

*Behind the Scenes of Research and Innovation*

Prof. Agosti's work has concentrated on the ways in which information retrieval can contribute to advances in research. In this lecture she presented examples of several projects undertaken at Padua - the conversion of a traditional card-based library catalogue to a searchable public on-line database, annotated document searching and a large-scale information retrieval system for experimental data.

For further details and links to video presentations:
http://www.iskouk.org/content/third-tony-kent-strix-annual-lecture

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## ACS Meeting Report: Status and Future of the IUPAC InChI: Context and Use Cases

*Contributed by RSC CICAG Secretary Prof Jeremy Frey, email: J.G.Frey@soton.ac.uk*
*and RSC CICAG Committee member Prof Jonathan Goodman, email: jmg11@cam.ac.uk*

August 16 – 18, 2017
National Center for Biotechnology Information
NLM, NIH, Bethesda MD, USA

The use of International Chemical Identifier (InChI) continues to grow especially in linking chemical information within the chemical database and publishing communities. The InChI Trust sponsored a lively meeting which looked at the development of several InChI projects that are extending the range of applicability of the InChI, for example to reactions, partial stereochemistry, labels, as well as detailed discussions on how to handle tautomeric issues. A detailed discussion and many of the presentations are available at http://www.inchi-trust.org/status-future-iupac-inchi-context-use-cases-august-16-18-2017/.

This meeting built on discussions at the EBI in March 2017 (Expanding IUPAC Standards for Chemical Information – industry applications & stakeholder perspectives). In addition to presentations on examples of use cases from a wide variety of companies and publishers, working groups reported on the status of projects to apply InChI to new areas. A development of the InChI can now be applied to reactions (RInChI) and software for this is available on the InChI Trust website (http://www.inchi-trust.org). The challenges for structural representation posed by mixtures, tautomers, organometallics, polymers, and large molecules are all being investigated. Proposals for the use of InChI in QR codes to label reagents are developing quickly. The uses and possible applications for InChI are expanding rapidly.

A key message from the meeting was that InChI is successful because people are choosing to use it. This sets a daunting challenge for the many extensions and developments of InChI that the working groups are addressing: which will have such impact that people will decide to use them spontaneously? The take up of InChI and its relatives may soon become even more pervasive.

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## CIIPM Annual Meeting and Training Classes 2018

*Contributed by RSC CICAG Committee member by Stuart Newbold, email: stuart@psandim.com*


The 3rd Cambridge Information & Intellectual Property Meeting (CIIPM) will take place on Wednesday, 11th July 2018, at Homerton College, Cambridge. The theme for this year's event is '*Innovation, Valuation, and Licensing*'. Once again there will be an exhibition to go alongside the conference, and some patent information vendors may be providing training classes in the morning prior to the afternoon meeting. A full programme and registration will soon be available at https://www.extractinfo.info/ciipm/2018-annual-meeting/.

CIIPM ½ day training classes have now commenced and the next two classes take place on Wednesday, 14th March 2018. The morning class is '*IP and Commercialisation*' – a class which was also held in October 2017, and which gives a basic understanding of how to develop, commercialise and manage IP. Topics include using NDAs, building an IP strategy, preparing an IP policy, and IP matters relating to employees, contracts and confidentiality agreements. The training will consider IP management, and provide a framework for establishing a robust practice in house. The afternoon class is '*Freedom to Operate Search & Analysis*', and this covers the different aspects of searching, retrieval, and analysis of patent documents needed to ensure

freedom to operate on developed technology. Attendees will gain an understanding of how to construct and perform business focussed patent searches and how to analyse the results for reporting.

Two further training classes take place on Wednesday, 18th October, 2018. '*Commercial Patent Search and Analysis*', involves the use of various landscaping and analytics techniques, and provides an overview of search and analysis methods for business decision making. '*IP Matters*' follows in the afternoon, and provides an introduction for people who would like to understand more about Intellectual Property, with a review of the types of protection available, a look at how to understand other people's patents, basic patent and trademark searching, and how to ascertain the legal status of third party IP.

To find out more about the meeting, the training courses and registration please contact jane@extractinfo.info or stuart@psandim.com or visit https://www.extractinfo.info/ciipm/training-ciipm/.

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## InfoChem News

*Contribution from Dr Valentina Eigner-Pitto, email: ve@infochem.de*

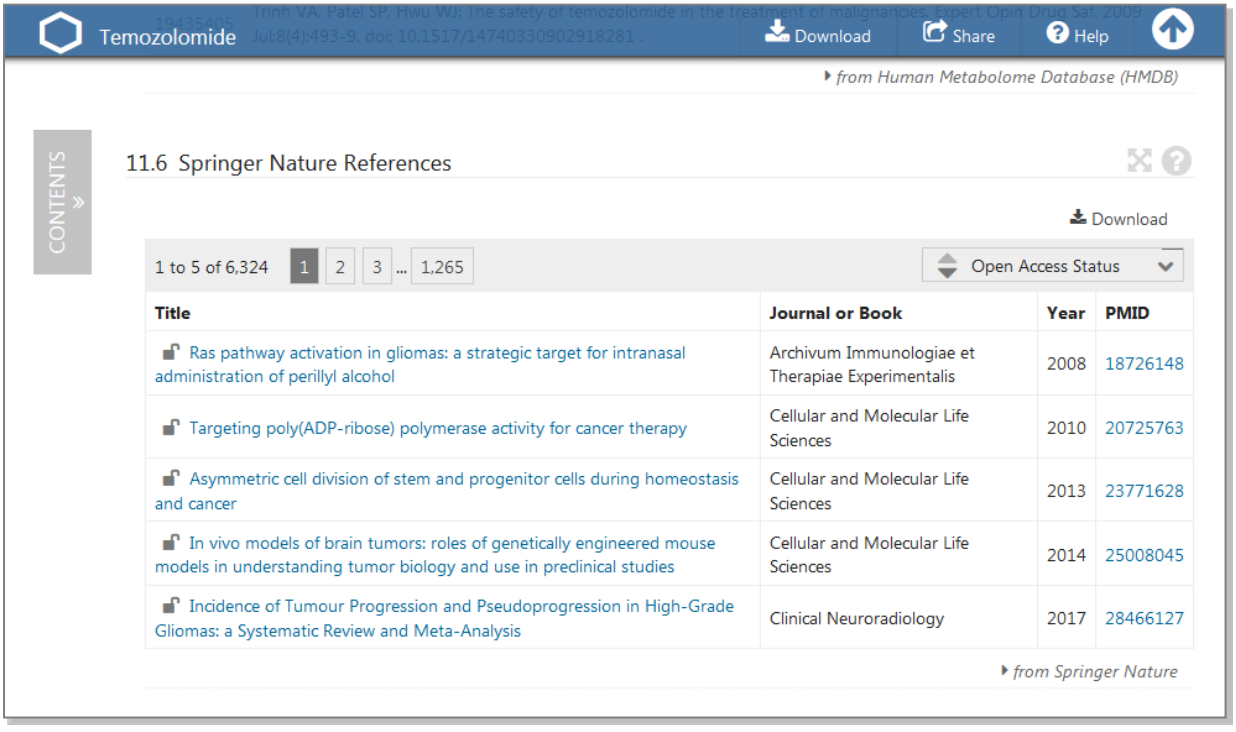
SPRINGER NATURE

InfoChem

InfoChem / Springer Nature deposits more than 600,000 chemical compounds on PubChem

InfoChem has deposited on behalf of Springer Nature more than six hundred thousand chemical compounds on PubChem, all of them offering more than 26 million links back into the primary literature, eBooks or Major Reference Works located on SpringerLink, BioMed Central or nature.com. Of these, 1.6 million links point to open or free access documents.

Documents from all chemistry and life sciences-related disciplines were automatically annotated using InfoChem's chemical named entity recognition technology.
In the PubChem Compound Summary users now will find a widget listing the Springer Nature Documents



containing that compound. The relevance of the compounds in these articles was determined using a smart algorithm which allows sorting the documents hit list by compound relevance.

Over 40 percent of the compounds are novel to PubChem and therefor provide a powerful new source of chemical content for researchers worldwide.

This initiative will enhance the discoverability and accessibility of scientific information in an easy and intuitive way, and enable access to a wider range of users. This is in line with how Springer Nature sees the rise of open research, including open data, as being one of the major forces reshaping the way that researchers collaborate to advance the pace and quality of discovery.

For more information please also contact us via info@infochem.de, +49892030432410.

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## CAS / SciFinder / STN News

*Contributed by CAS Applications Specialist in the UK & Ireland, Dr Anne Jones, email annejones@acs-i.org.*

**Welcome to the New CAS Website!**

In December 2017, CAS introduced the initial version of a new CAS website at www.cas.org. The refreshed look and new content provide visitors new and interesting ways to learn about CAS.

All of the content previously found at cas.org continues to be available at support.cas.org, and is accessible from the new home page. We have taken measures to provide a seamless experience with bookmark redirects. Should any of your bookmarks be impacted, simply reset your quick links. We will continue to build out the new site in the coming months, with the intent to fully transition to a single site in 2018.

**What is SciFindern?**

In the last edition of CICAG, we covered the introduction of SciFindern as a new member of the SciFinder family. The question has arisen as to why we have introduced this new tool.
Research shows that users of today's information tools spend far too much time trying to find relevant, actionable results. SciFinder$^n$, the newest product in the SciFinder® family, accelerates that process with a frictionless interface to the unmatched CAS content collection using the most advanced chemistry relevance engine in the industry.

SciFinder$^n$ allows scientists to do better research in less time. SciFinder$^n$ accelerates research by providing actionable results such as step-by-step synthetic methods and hard to find chemistry in patents.

- **Access** a comprehensive collection of content covering chemistry and related sciences from around the globe
- **Pinpoint** the most valuable information with chemical search relevance that helps you know where to start
- **Accelerate** your research with a streamlined, frictionless interface
- **Save time** with direct access to patent documents and step-wise synthetic procedures and methods
- **Empower** your entire organization with unlimited access to the world's most trusted and comprehensive chemistry information

If you have any questions or want to know more about SciFindern, then feel free to contact me or CAS directly.

## Other Chemical Information Related News

*With a special thanks to RSC CICAG Member Dr Keith White*

[*All hyperlinks correct & working as of 1 February 2018*]

**EuCheMS Chemistry Congress 2018**

This meeting will take place from 26 30 August 2018 at ACC Liverpool, UK. Confirmed meeting topics include:

- Practical Approaches for Laboratory Education
- Pattern Recognition for Chemometrics and Metabolomics
- ABCs of Analytics
- Methods of Computational Chemistry: challenges, demand and new developments
- Towards a more diverse and inclusive chemistry community
- Celebrating 20 years of society collaboration in physical chemistry and chemical physics
- Carbohydrates – tools for synthesis and analysis

More details and registration:
https://www.euchems2018.org/?utm_content=euchemancill&utm_source=house-list&utm_medium=email&utm_campaign=mkt-dir-cm03717

**Exploring the History of Cheminformatics (Webinar)**

There are always new tools in cheminformatics. Dr Wendy Warr looks at advances in the field that changed chemistry, and considers what the future of cheminformatics may hold.
Link to the Webinar is available from:
http://axial.acs.org/2017/12/20/history-cheminformatics/?utm_source=Newsletter&utm_medium=Email1217&utm_campaign=Axial
*Source: ACS Axial*

**millionshort.com: This Search Engine Start-up that helps you find what Google is Missing**

Million Short - What haven't you found?
"In creating a differentiated search, we aim to provide alternative methods for organizing, accessing, and discovering the vast web of information on the Internet."
https://millionshort.com/
https://www.forbes.com/sites/julianmitchell/2017/12/31/this-search-engine-startup-helps-you-find-what-google-is-missing/
*Source: Forbes Magazine*

**Protecting Artificial Intelligence IP: Patents, Trade Secrets, or Copyrights?**

https://www.lexology.com/library/detail.aspx?g=6d984fd2-d529-40f2-b87b-5acd9ad06af3
*Source: Lexology*

**PSE Releases Major gPROMS FormulatedProducts Update**

Process Systems Enterprise (PSE), the Advanced Process Modelling company, has recently released version 1.1 of its gPROMS FormulatedProducts® modelling platform for the integrated digital design of robust formulated products and their manufacturing processes.
https://www.businesswire.com/news/home/20180115005279/en/PSE-Releases-Major-gPROMS-FormulatedProducts-Update
*Source: Business Wire*

**Organic Chemistry App Game: Science Does Not Have to Be Scary**

http://www.chemistryviews.org/details/education/10739078/Organic_Chemistry_App_Science_Does_Not_Have_to_Be_Scary.html

*Source: ChemistryViews*

**ChemistryOpen Appoints New Editor-in-Chief**
ChemPubSoc Europe and Wiley-VCH have named Dr Kate Lawrence as Editor-in-Chief of ChemistryOpen, succeeding Dr Karen Hindson and Dr Haymo Ross. ChemistryOpen is a fully open access, society-owned chemistry journal, co-owned and supported by ChemPubSoc Europe, a consortium of 16 European chemical societies, and Wiley-VCH.
http://www.chemistryviews.org/details/ezine/10582105/ChemistryOpen_Appoints_New_Editor-in-Chief.html
*Source: ChemViews Magazine*

**Multifunctional Materials – a new multidisciplinary journal from IOP Publishing**
This is a new a new, high-impact journal uniquely designed to serve an emerging field that now connects the materials science, physics, chemistry, bioscience and engineering communities, as well as industry. Broad areas of specific interest include:

- The design and manufacture of programmed materials for multifunctionality, morphing and adaptivity;
- "Meta-materials" designed and created through current chemistry or synthetic biology;
- Multifunctional materials designed with capabilities of intelligent systems, such as sensing and self-diagnosis;
- Characterization methods for functions, multiscale modelling and computational materials engineering;
- Novel applications of functional multi-materials.

http://ioppublishing.org/news/introducing-multifunctional-materials-a-new-multidisciplinary-journal-from-iop-publishing/
*Source: IOP Publishing*

**CiteScoreT shines a spotlight on high-quality journals neglected by other metrics**
CiteScore metrics were launched in December 2016 in response to academia's call for metrics that provide a broader, more transparent view of an academic journal's citation impact. CiteScore metrics are part of a basket of metrics available on Scopus (including journal, author, institutional, and article-level metrics), supporting a holistic view of research performance.
https://www.elsevier.com/about/press-releases/science-and-technology/citescore-shines-a-spotlight-on-high-quality-journals-neglected-by-other-metrics
*Source: Elsevier*

**More researchers to now benefit from Plum Analytics Metrics**
PlumX Metrics from Plum Analytics are now integrated into several of Elsevier's research products, and its journal and society partner sites - Scopus, Pure, Elsevier.com and Elsevier's Journal Branded Solutions all now incorporate PlumX Metrics, with ScienceDirect to be added soon.
https://www.elsevier.com/about/press-releases/science-and-technology/more-researchers-to-now-benefit-from-plum-analytics-metrics
*Source: Elsevier*

**ACS Publications Enhances Article Email Alerts**
http://axial.acs.org/2017/06/27/article-email-alerts/
Three new features have been introduced:

- Responsive Design - the enhanced e-Alerts are both desktop and mobile friendly
- TOC Images - both TOC and Articles ASAP e-Alerts feature TOC images for each research article listed in each message
- Social Sharing - recipients can share articles on social media directly from the e-Alert

*Source: ACS*

**Ingenta to enhance access to publisher content through new agreement with Chan Zuckerberg Initiative's Meta discovery engine - Ingenta**
http://www.ingenta.com/news-article/ingenta-enhance-access-publisher-content-new-agreement-chan-zuckerberg-initiatives-meta-discovery-engine/
*Source: Ingenta*

**SSRN Launches ChemRN - A New Network Dedicated to Chemistry**
http://www.prnewswire.com/news-releases/ssrn-launches-chemrn---a-new-network-dedicated-to-chemistry-639005473.html
*Source: PR Newswire*

**Wiley Content Sharing launches across Wiley Online Library**
https://www.readcube.com/press/wileyexpand
John Wiley and Sons has formally launched *Wiley Content Sharing* across its research portfolio. The launch follows a successful trial in 2017. *Wiley Content Sharing* facilitates collaboration by allowing authors and subscribers to share free-to-read full-text articles with non-subscribers. This new functionality is available to all journals on Wiley Online Library. In addition, *Wiley Content Sharing* provides the public with greater access to research when following links from selected media outlets globally. *Wiley Content Sharing* will be available to more than 1,700 journals from across Wiley's portfolio.
*Source: readcube*

**Elsevier acquires bepress, a leading service provider used by academic institutions to showcase their research**
https://www.elsevier.com/about/press-releases/corporate/elsevier-acquires-bepress,-a-leading-service-provider-used-by-academic-institutions-to-showcase-their-research
*Source: Elsevier*

**JSTOR Expands in the Sciences with Scientific American**
JSTOR, the digital library of academic journals, books, and primary sources, has concluded an agreement with Springer Nature to include *Scientific American*
https://www.ithaka.org/news/jstor-expands-sciences-scientific-american
*Source: ITHAKA*

**German Universities continue to challenge Elsevier**
The rejection comes after nearly a year of negotiations. The German side, represented by a consortium founded in 2014 called Project DEAL, includes the German Research Foundation (DFG), the Fraunhofer–Gesellschaft, the German National Academy of Sciences Leopoldina, the Helmholtz and the Leibniz associations, and the Max Planck Society. Backed by these research giants plus dozens of universities, Project DEAL is demanding a nationwide contract from Elsevier that includes fair pricing, open access in Germany to all papers authored by researchers at German institutions, and permanent full-text access to all electronic journals published by Elsevier.
https://www.chemistryworld.com/news/german-universities-take-on-elsevier-/3007807.article
*Source: Chemistry World*

**ChemRxivT Beta open for submissions and powered by Figshare**
https://www.acs.org/content/acs/en/pressroom/newsreleases/2017/august/chemrxiv-beta-open-for-submissions-and-powered-by-figshare.html
*Source: American Chemical Society*

**Copyright Clearance Center RightFind™ Delivers Improved Workflow for Ease-of-Use**
http://www.copyright.com/copyright-clearance-center-rightfind-delivers-improved-workflow-ease-use/
*Source: Copyright Clearance Center*

**Amplifying intelligent drug design**
https://www.chemistryworld.com/news/amplifying-intelligent-drug-design/3007667.article
Source: Chemistry World

**ACS Publications introduces ACS Direct Correct to improve the author experience**
ACS Direct Correct allows for proof corrections and comments to be entered directly into the copy-edited manuscript file. This online process will make it significantly easier and more efficient for individuals and groups of authors to make and communicate any corrections prior to the rapid publication of their research paper.
https://www.acs.org/content/acs/en/pressroom/newsreleases/2017/august/acs-publications-introducing-acs-direct-correct-to-improve-the-author-experience.html
*Source: American Chemical Society*

**Creativity in action – the information professional is poised to exploit the fourth industrial revolution**
The business information survey 2017
http://journals.sagepub.com/doi/pdf/10.1177/0266382117722440
*Source: Business Information Review*

**Preprint servers making waves in chemistry community**
https://www.chemistryworld.com/news/preprint-servers-making-waves-in-chemistry-community/3007888.article
*Source: Chemistry World*

**A 3D periodic table?**
https://www.chemistryworld.com/opinion/a-3d-periodic-table/3007821.article
*Source: Chemistry World*

**American Chemical Society Moves to Block Access to Sci-Hub**
https://www.insidehighered.com/quicktakes/2017/09/06/american-chemical-society-moves-block-access-sci-hub
*Source: Inside Higher Ed*

**Chemists retract 15-year-old paper and publish a revised version**
http://cen.acs.org/articles/95/i36/Chemists-retract-15-year-old-paper-and-publish-a-revised-version.html
*Source: Chemical & Engineering News*

**Twitter discussion of academic articles - not worth counting?**
When it comes to metrics, an analysis of tweets suggests that 77% of tweets referencing academic articles are mechanical in nature.
http://www.infotoday.eu/Articles/News/InfoToday-Europe-Blog/Twitter-discussion-of-academic-articles-not-worth-counting-120347.aspx
*Source: Informatioin Today*

**CAS to Preserve ChemZent product with Portico**
CASS is preserving its ChemZentTM solution through Portico's d-collection service, ensuring that it will be secure and available to ChemZent customers in the future. ChemZent provides academic, commercial and government organizations with access to the first and only English-searchable version of Chemisches Zentralblatt, the oldest journal of chemistry abstracts, covering the literature from 1830-1969.
http://www.portico.org/digital-preservation/news-events/news/cas-to-preserve-chemzent-product-with-portico
*Source: Portico*

**Elsevier signs up to TOP guidelines & develops new data-sharing guidelines for journals**

Transparency, open sharing, and reproducibility are core values of science, but not always part of daily practice. Journals, funders, and societies can increase reproducibility of research by adopting the TOP Guidelines and helping them evolve to meet the needs of researchers and publishers while pursuing the most transparent practices.
https://www.elsevier.com/connect/editors-update/supporting-data-openness,-transparency-and-sharing
*Source: Elsevier*

**IBM Has Used Its Quantum Computer to Simulate a Molecule**
A team of researchers at IBM have successfully used their quantum computer, IBM Q, to precisely simulate the molecular structure of beryllium hydride (BeH2).
https://www.technologyreview.com/the-download/608866/ibm-has-used-its-quantum-computer-to-simulate-a-molecule-heres-why-thats-big/
*Source: MIT technology Review*

**Authorship for sale: Some journals willing to add authors to papers they didn't write**
http://retractionwatch.com/2017/09/13/authorship-sale-journals-willing-add-authors-papers-didnt-write/
*Source: Retraction Watch at Retraction Watch*

**Pay up or retract? Drug survey spurs conflict**
Over the past decade, public health specialist Donald Morisky of the University of California, Los Angeles, has moved aggressively to enforce his copyright on a questionnaire he developed that examines how likely it is that a patient will adhere to a recommended drug regimen. Together with a colleague, he has demanded payments of as much as tens of thousands of dollars each from hundreds of researchers who have used Morisky's scale, and threatened to force the retraction of papers if the alleged infringers don't pay. Morisky is well within his legal rights to seek the payments. But observers say Morisky's vigorous enforcement and the size of his demands stand out. At least two teams have withdrawn papers rather than pay.
http://science.sciencemag.org/content/357/6356/1085
*Source: Science*

**Merck to co-lead Big Data alliance**
http://www.pharmatimes.com/news/merck_to_co-lead_big_data_alliance_1204960
*Source: PharmaTimes*

**Elsevier Launches ScienceDirect Topics to Help Researchers Quickly**
Elsevier has announced the launch of ScienceDirect Topics; a free layer of content which provides a quick snapshot of definitions, terms and excerpts on scientific topics, built on Elsevier's highly trusted book content.
https://www.prnewswire.com/news-releases/elsevier-launches-sciencedirect-topics-to-help-researchers-quickly-build-their-knowledge-and-save-valuable-time-searching-644170623.html
*Source: Cision PR Newswire*

**Ingenta and The British Library collaborate to digitise and distribute archive content**
http://www.ingenta.com/news-article/ingenta-british-library-collaborate-digitise-distribute-archive-content/
*Source: Ingenta*

**ResearchGate under pressure to restrict article sharing**
https://www.chemistryworld.com/news/researchgate-under-pressure-to-restrict-article-sharing/3008044.article
*Source: Chemistry World*

**Wikipedia shapes language in science papers**
http://www.nature.com/news/wikipedia-shapes-language-in-science-papers-1.22656?WT.ec_id=NEWSDAILY-20170926

*Source: Nature News & Comment*

**ACS expands its applied materials journals portfolio**
ACS Applied Energy Materials and ACS Applied Nano Materials have been added to the Society's portfolio. These two new journals, and others planned to follow, are positioned within the editorial purview of the Society's highly successful journal, ACS Applied Materials & Interfaces.
https://www.acs.org/content/acs/en/pressroom/newsreleases/2017/september/acs-expands-its-applied-materials-journals-portfolio.html
*Source: American Chemical Society*

**Taking labour out of the laboratory**
Free software makes automation easy.
https://www.chemistryworld.com/news/taking-labour-out-of-the-laboratory/3008065.article
*Source: Chemistry World*

**Saying Goodbye to a QSAR Pioneer**
Dr. Toshio Fujita.
http://axial.acs.org/2017/09/18/saying-goodbye-qsar-pioneer/
*Source: ACS Axial*

**ProQuest Dissertations Now Discoverable in Google Scholar**
ProQuest and Google are expanding their collaboration by indexing almost half a million full text dissertations from the ProQuest Dissertations & Theses Global™ database (PQDT). Google Scholar users can now seamlessly discover and access this set of full text dissertations in their libraries' subscription collections.
http://www.proquest.com/about/news/2017/ProQuest-Dissertations-Now-Discoverable-in-Google-Scholar.html
*Source: ProQuest*

**Publishers threaten to remove millions of papers from ResearchGate**
https://www.nature.com/news/publishers-threaten-to-remove-millions-of-papers-from-researchgate-1.22793
*Source: Nature*

**De Gruyter presents Science Discoveries**
Science Discoveries, an international science news site focused on research advancements in medicine, health, environment and technology. The website features selected research published in De Gruyter journals.
https://www.degruyter.com/dg/newsitem/233/
*Source: De Gruyter*

**Publishers take academic networking site to court**
http://science.sciencemag.org/content/358/6360/161
*Source: Science*

**Universities and Science Minister calls on universities to do more to commercialise UK research and innovation**
https://www.gov.uk/government/news/universities-and-science-minister-calls-on-universities-to-do-more-to-commercialise-uk-research-and-innovation
*Source: GOV.UK*

**Male scientists share more — but only with other men**
https://www.nature.com/news/male-scientists-share-more-but-only-with-other-men-1.22820
*Source: Nature News & Comment*

**Bentham Science Journals indexed in The Emerging Sources Citation Index (ESCI)**
https://www.eurekalert.org/pub_releases/2017-10/bsp-bsj101317.php
*Source: EurekAlert! Science News*

**BASF starts up supercomputer located at the company's headquarters in Ludwigshafen, Germany**
With a computing power of 1.75 petaflops (1 petaflop equals one quadrillion floating point operations per second), the computer, called "Quriosity", offers around ten times the overall computing power previously available. Tasks such as simulations of industrial catalysts, crop protection products, and materials, are among the first computational tasks being run.
http://www.chemistryviews.org/details/news/10671176/Start_of_Supercomputer.html
*Source: ChemistryViews*

**Future Medicinal Chemistry and the International Chemical Biology Society announce their official partnership**
https://www.future-science-group.com/future-medicinal-chemistry-and-the-international-chemical-biology-society-announce-their-official-partnership/
*Source: FSG*

**Elsevier Announces Winners of the 2017 Reaxys PhD Prize**
Joshua Barham from the Murphy group, University of Strathclyde

- Presentation title: Contra-Thermodynamic Hydrogen Atom Transfer: The Selective N-CH3 Functionalisation of Trialkylamines
- Moritz Malischewski from the Seppelt group, Freie University of Berlin
- Presentation title: Organometallic Chemistry in Superacids
- Changchun Yuan from the Liu group, Sichuan University
- Presentation title: Total Syntheses of Bolivianine, Sarcandrolide J and Shizukaol D: Inspired but not Limited by Nature

https://www.prnewswire.com/news-releases/elsevier-announces-winners-of-the-2017-reaxys-phd-prize-653063873.html
*Source: Cision PR Newswire*

**Finding the needle in a haystack**
The publishing industry is facing a monumental challenge: how do we ensure research is read?
https://www.researchinformation.info/news/analysis-opinion/finding-needle-haystack
*Source: Research Information*

**AAAS launches SciLine, new service for journalists to enhance science coverage**
https://www.eurekalert.org/pub_releases/2017-10/aaft-als102517.php
*Source: EurekAlert! Science News*

**Former GSK boss to lead new UK accelerated drug access scheme**
http://www.reuters.com/article/us-britain-pharmaceuticals/former-gsk-boss-to-lead-new-uk-accelerated-drug-access-scheme-idUSKBN1D3007
*Source: Reuters*

**Outcry as latest global publisher bows to China censors**
https://www.ft.com/content/2d195ffc-be2e-11e7-b8a3-38a6e068f464
*Source: Financial Times*

**Springer Nature blocks access to certain articles in China**
Springer Nature said it had pulled access to a small number of articles in China to comply with regulations, adding that it viewed the move as regrettable but necessary.

https://www.reuters.com/article/us-china-censorship/springer-nature-blocks-access-to-certain-articles-in-china-idUSKBN1D14EB
*Source: Reuters*

**Energy researcher sues the US National Academy of Sciences for millions of dollars**
http://www.nature.com/news/energy-researcher-sues-the-us-national-academy-of-sciences-for-millions-of-dollars-1.22944
*Source: Nature News & Comment*

**Computer system finds 'recipes' for producing materials**
System could pore through millions of research papers to extract 'recipes' for producing materials.
https://www.sciencedaily.com/releases/2017/11/171106132021.htm
*Source: ScienceDaily*

**Speeding Up DFT Calculations with Machine Learning**
Density functional theory calculations help chemists to predict and understand the properties and reactivities of compounds. Machine-created functionals could allow DFT calculations to be performed much faster.
http://www.chemistryviews.org/details/ezine/10661444/Speeding_Up_DFT_Calculations_with_Machine_Learning.html
*Source: ChemViews Magazine*

**Open access academic books downloaded, discussed and cited far more than traditional books**
http://group.springernature.com/gp/group/media/press-releases/07-11-17/15195750
*Source: Springer Nature*

**Latest legal defeat unlikely to scuttle Sci-Hub**
https://www.chemistryworld.com/news/latest-legal-defeat-unlikely-to-scuttle-sci-hub/3008248.article
*Source: Chemistry World*

**The catalogue that made metrics, and changed science**
https://www.nature.com/news/the-catalogue-that-made-metrics-and-changed-science-1.22961
*Source: Nature News & Comment*

**How To: Sign Up for the Academic Knowledge API - Microsoft Research**
https://www.microsoft.com/en-us/research/project/academic/articles/sign-academic-knowledge-api/
*Source: Microsoft Academic*

**Need a paper? Get a plug-in**
A collection of web-browser plug-ins is making the scholarly literature more discoverable.
http://www.nature.com/articles/d41586-017-05922-9
*Source: Nature*

**ResearchGate bows to pressure from publishers on copyrighted material**
https://www.chemistryworld.com/news/researchgate-bows-to-pressure-from-publishers-on-copyrighted-material/3008288.article
*Source: Chemistry World*

**University of Oxford acquires Atos' latest supercomputer for Deep Learning program**
https://atos.net/en-gb/2017/press-release-en-gb_2017_11_16/university-oxford-acquires-atos-latest-supercomputer-deep-learning-program
*Source: ATOS*

**UK Universities get JADE supercomputer, to be supplied as-a-service**
Academics from eight universities and IT researchers will have access to the system.
http://www.datacenterdynamics.com/content-tracks/servers-storage/uk-universities-get-jade-supercomputer-to-be-supplied-as-a-service/99314.fullarticle
*Source: Datacenter Dynamics*

**Computer program finds new uses for old drugs**
https://www.eurekalert.org/pub_releases/2017-11/cwru-cpf111617.php
*Source: EurekAlert! Science News*

**Online software spots genetic errors in cancer papers**
http://www.nature.com/news/online-software-spots-genetic-errors-in-cancer-papers-1.23003
*Source: Nature News & Comment*

An artificial future
**Elsevier's Jabe Wilson predicts radical changes in the ways AI will be used in scholarly communications.**
https://www.researchinformation.info/interview/artificial-future-0
*Source: Research Information*

**sciNote adds AI capabilities**
sciNote, a free open source electronic lab notebook (ELN), has announced that it has incorporated artificial intelligence capabilities into its electronic lab notebook.
https://www.scientific-computing.com/news/scinote-adds-ai-capabilities
*Source: Scientific Computing World*

**Science Partner Journals**
The American Association for the Advancement of Science (AAAS), the nonprofit publisher of the Science family of journals, is today launching Science Partner Journals, http://www.sciencepartnerjournals.org/, a program that will feature high-quality, online-only open access publications produced in collaboration with international research institutions, foundations, funders and societies.
http://www.sciencepartnerjournals.org/
*Source: AAAS*

**Springer Nature continues to advance sharing**
http://group.springernature.com/gp/group/media/press-releases/springer-nature-continues-to-advance-sharing/15256962
*Source: Research Publisher*

**FTC Halts the Deceptive Practices of Academic Journal Publishers**
https://www.ftc.gov/news-events/press-releases/2017/11/ftc-halts-deceptive-practices-academic-journal-publishers
*Source: Federal Trade Commission*

**Digital Science Report Reveals Potential Behind Blockchain Technology for Scholarly Communication and Research**
New report considers the developments and varying perspectives of blockchain technology and its possible impact on the academic arena.
https://www.digital-science.com/press-releases/digital-science-report-reveals-potential-behind-blockchain-technology-scholarly-communication-research/
*Source: Digital Science*

**The CompTox Chemistry Dashboard: a community data resource for environmental chemistry**
https://jcheminf.springeropen.com/articles/10.1186/s13321-017-0247-6

*Source: Journal of Cheminformatics*

**Involving Students in Library Acquisitions**
At Goldsmiths College, part of the University of London, a scheme to involve students in the library acquisitions process is now in its third year and has garnered enthusiastic feedback and enhanced the library's acquisitions process.
http://www.infotoday.eu/Articles/Editorial/Featured-Articles/Involving-students-in-library-acquisitions--122056.aspx
*Source: Information Today*

**Digital in R&D: The $100 billion opportunity**
Digital promises to transform R&D productivity over the next decade. What will it take to realize this potential?
https://www.mckinsey.com/industries/pharmaceuticals-and-medical-products/our-insights/digital-in-r-and-d-the-100-billion-opportunity
*Source: McKinsey*

**New Journal: ACS Reagent Chemicals**
The Must-Have Reference Guide for Analytical, Industrial, and Research Labs.
http://pubs.acs.org/series/reagents
*Source: ACS Publications*

**Robust Chemistry: The Importance of Data and Methods Sharing**
http://www.chemistryviews.org/details/ezine/10725831/Robust_Chemistry_The_Importance_of_Data_and_Methods_Sharing.html
*Source: ChemViews Magazine*

**AI translates chemistry to predict reaction outcomes**
https://www.chemistryworld.com/news/ai-translates-chemistry-to-predict-reaction-outcomes/3008397.article
*Source: Chemistry World*

**Artificially creating articles**
https://www.researchinformation.info/news/artificially-creating-articles
*Source: Research Information*

**One billion metadata facts now on Springer Nature SciGraph**
http://www.springernature.com/gp/group/media/press-releases/one-billion-metadata-facts-now-on-springer-nature-scigraph/15313528
*Source: Springer-Nature*

**Digital Science Launches Dimensions: a Next-generation Research and Discovery Platform Linking 124 Million Documents, Providing free Search and Citation Data across 86 Million articles**
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*Source: Digital Science*

**Elsevier and University of Oxford Embark on 5-year Collaboration to Support Early Career**
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**EPSRC announces opening of call for £492 million investment in Centres for Doctoral Training**
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**Wiley Partners with Association of Health Care Journalists (AHCJ) to Provide Member Access to Health Science Research**
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*Source: Nature Index*

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