

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 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 on 13th December 2016. MCID 13 >>BDC6.687TJ 0 Tc 0 Tw 4.699

			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

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

Important Dates:

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

x

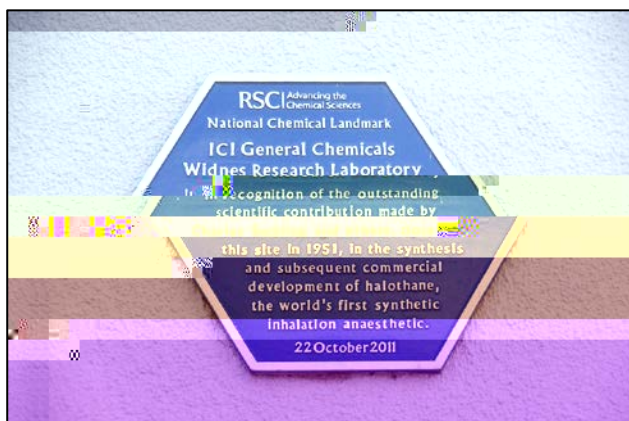
Widnes Successes: The Widnes Research Laboratory and Catalyst Science Discovery Centre & Museum

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

Photographs – with thanks to MerCCp AyETw

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

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 hostelrys. 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!

Vikki Vowles

Contributed by CAS Applications Specialist in the UK & Ireland, Dr Anne Jones, email annejones@act.org.



It is with 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.

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

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

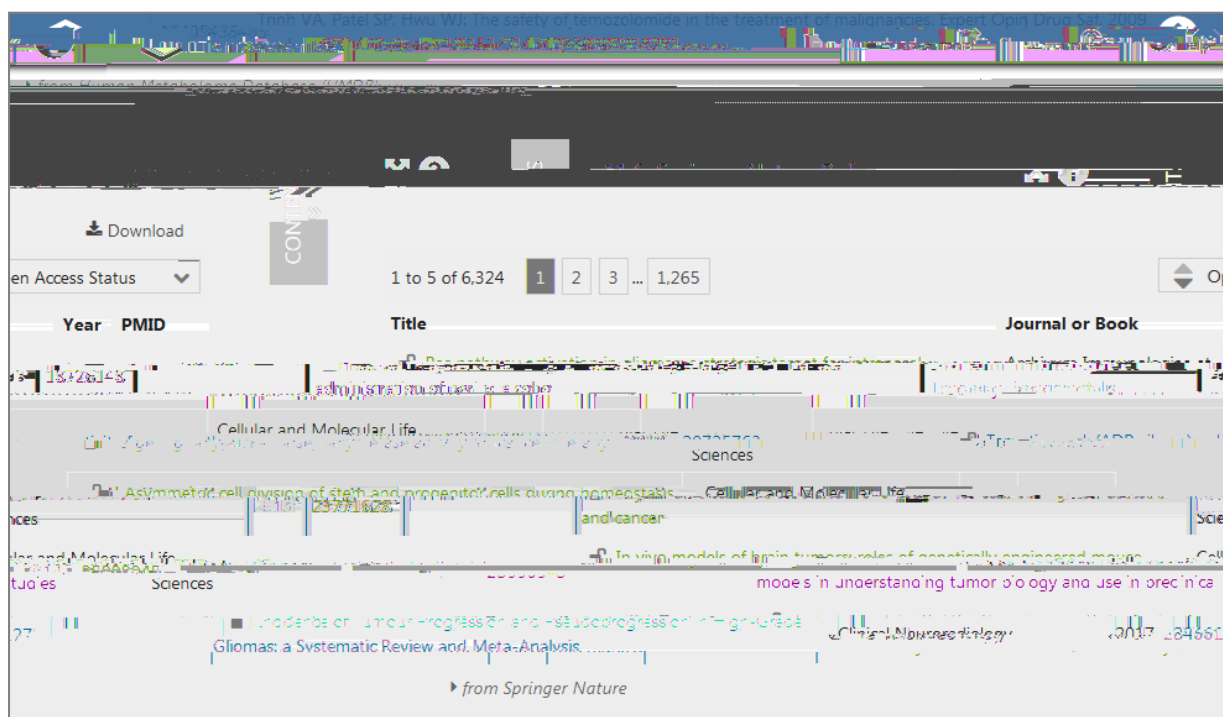
freedom to operate on developed technology. Attendees will gain an understanding of how to construct and perform business focussed patent searches and how to analyse the results for reporting.

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 decisionmaking. '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_ciiipm/.

InfoChem News

Contribution from Dr Valentina EignerPitto, email: ve@infochem.de



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 therefore 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.

CAS/ SciFinder / STNNews

Contributed by CAS Applications Specialist in the UK & Ireland Dr Anne Jones, email annejones@cas.org.

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 book1 nDC /TT01

Other Chemical Information Related News

With a special thanks to RSC CICAG Member Dr Keith White

[All hyperlinks corrected & 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:

- x Practical Approaches for Laboratory Education
- x Pattern Recognition for Chemometrics and Metabolomics
- x ABCs of Analytics
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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, societyowned chemistry journal, co-owned and supported by ChemPubSoc Europe, a consortium of 16 European chemical societies, and Wiley-VCH.

http://www.chemistryviews.org/details/ezone/10582105/ChemistryOpen_Appoints_New_Editor_in_Chief.html

Source: ChemViews Magazine

Multifunctional Materials – a new multidisciplinary journal from IO

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-accesspublisher -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/ssrnlaunches-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/elsevieracquires-bepress,a->

Tran

SourceNature 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.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

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

EPSRC announces opening of call for £492 million investment in Centres for Doctoral Training

<https://www.epsrc.ac.uk/newsevents/news/cdts2018call/>

Source: EPSRC

China declared world's largest producer of scientific articles

<https://www.nature.com/articles/d41586-018-009274>