



**Member Networks Annual Report Form**  
*Reporting events held in 2017 and those planned for 2018*

In line with the rules for member networks and to enable us to better support our networks and their activities all member networks (Local Sections, Interest Groups and Analytical Division Regions) are asked to complete this form and return it to [networks@rsc.org](mailto:networks@rsc.org) or by post to; Networks Team, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF.

**Deadlines**

Deadline for receipt of Financial Accounts by RSC Finance Team: **9<sup>th</sup> February 2018**

Deadline for receipt of Annual Report by Networks Team: **26<sup>th</sup> February 2018**

If there is any reason that your committee will **not** be able to meet either or both of these deadlines please inform [networks@rsc.org](mailto:networks@rsc.org) as soon as possible.

This report will be uploaded to your web page to share with the members of your network. Staff will also share a digest of all member networks activities taken solely from these annual reports with appropriate staff and governance boards and committees including Division Councils with similar interests.

<b>Committee</b>	CICAG – Chemical Information and Computer Applications Group
<b>Completed by</b>	Jeremy Frey
<b>Date</b>	12 Feb 2018

Please list below the dates of all of your planned committee meetings and, if held, AGM.

**Annual General Meeting (if being held)**

<b>Date:</b>	Interest Group Rules require the attendance of at least 20 non-committee group members in order for an AGM to be quorate. We would propose to add a 2018 AGM to a future Members' Meeting if at least 20 members have registered.
<b>Venue:</b>	N/A

**Proposed Committee Meetings Dates**

<b>Date</b>	<b>Venue</b>
<b>31 Jan 2018</b> <b>16 May 2018</b> <b>5 Sept 2018</b>	<b>All Burlington House,</b>

## 2017 Events

Please append electronic copies of any meeting reports, newsletters or relevant materials to this report.

Please report below on activities undertaken in the past year. If you have more detailed information about any particularly successful events, or advice to share please use a separate sheet. For more events continue as necessary.

<b>Event Name</b>	<b>Chemical Structure Representation: What Would Dalton Do Now?</b>
<b>Event Type (key)</b>	Scientific Conference
<b>Comments</b>	<p>The meeting was held in the University of Liverpool on 22 June 2017 and covered structure representation, including the electronic storage of structures and reactions to enable effective information searching, retrieval and display, has become more challenging as the number, diversity and complexity of structures which can be elucidated has increased over time. This meeting explored current and future challenges and possible solutions to overcome them. We were pleased to be able to have equal number of male and female speakers at this event.</p> <p><a href="http://www.rsc.org/events/detail/23638/chemical-structure-representation-what-would-dalton-do-now">http://www.rsc.org/events/detail/23638/chemical-structure-representation-what-would-dalton-do-now</a></p>

<b>Event Name</b>	<b>The third Tony Kent Strix Annual Lecture, 20 October 2017</b>
<b>Event Type (key)</b>	Award lecture
<b>Comments</b>	<p>The meeting was held at the Geological Society, Burlington House with the award speaker Prof. Maristella Agosti, on</p> <p><b>Behind the Scenes of Research and Innovation</b></p> <p>We often excel in producing scientific achievements, but at times turning those achievements into innovation and technology transfer can be a tall order. Furthermore, even though we may document our findings well in scientific publications and reports, we are far less accomplished and proficient in documenting and explaining how the complex process of transforming scientific results into innovation has been performed and proven successful. In general, most of the knowledge of this transfer process remains only with those taking part in it, while certain aspects such as the time and context when the transfer took place may be rich in lessons to be learnt and provide opportunities for future teaching in diverse fields. This talk addresses the complex process of transforming research outcomes into innovation using some relevant examples in the fields of information</p>

	retrieval and digital libraries.
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<b>Event Name</b>	<b>From Spectral Data To Chemical Knowledge</b>
<b>Event Type (key)</b>	Scientific Conference
<b>Comments</b>	<p>Joint meeting with the Molecular Spectroscopy group held at the University of Bath. 7 Nov 2017</p> <p>This was a cross disciplinary meeting which focussed on the spectroscopic analysis of chemical processes, application of this data to advance chemical knowledge and the role of computers and automation. The meeting will included topics on how to handle and manipulate multiple data streams acquired concurrently, direct comparison of reaction profiles form different techniques, archiving and data security, the use of self-optimising reactors and scientific data management</p> <p><a href="https://sites.google.com/site/rscmolecularspectroscopygroup/calendar/from-spectral-data-to-chemical-knowledge">https://sites.google.com/site/rscmolecularspectroscopygroup/calendar/from-spectral-data-to-chemical-knowledge</a></p>



## **Awards and Bursaries**

Please list any awards or bursaries presented by your committee in the past 12 months and indicate any which will be open for nomination/application in the next calendar year.

Please ensure that all members of your network are notified of any awards or bursaries for general application.

### **Undergraduate Research Bursary**

CICAG in discussion with the RSC's Undergraduate Research Bursaries team and, following the success of 2016, continued to support a Bursary in 2017 (and will for 2018), in one or more of the following areas: cheminformatics, chemical information, chemical data management, chemistry data analytics, applications of computational chemistry. Neil Berry was the CICAG member of the judging panel. The student supported this year was Grzegorz Winter, currently studying at Newcastle University in the School of Chemistry with the project Supervisor: Dr Daniel Cole (Newcastle University in the School of Chemistry) and project title: Re-writing the functional form of classical force fields for molecular simulations

### **Bursaries for Student Attendance at Scientific Meetings**

It is our intention to fund up to five student bursaries to enable attendance at scientific or educational meetings organized by CICAG.

### **Sponsorship of the Tony Kent Strix Award**

We will continue with our sponsorship of this event in 2017 and plan to do so for 2018 and are discussing combining this with other activities to give it a higher profile (see details below).

### **Other information/comments:**

The LinkedIn (360 members) and Twitter (537 followers) social media accounts are now well established, and we have a limited Facebook presence, which is now under review. After surveying members, we have decided to update the social media presence, this will be under the oversight of Dr. Frank Longford EPSRC Doctoral Prize Research Fellow at Southampton University.

### **Newsletters**

CICAG publishes two Newsletters per annum, which are available at <http://www.rsc.org/Membership/Networking/InterestGroups/CICAG/Newsletters.asp>

### **Committee and Group Membership Changes**

In 2017, Stephanie North stepped down from the committee, Michelle Lynch has resigned from the committee and Alan Tonge has indicated that he plans to resign once we have recruited new committee members. Helen Cooke stepped down as chair and has been replaced by Chris Swain. The secretarial role has been undertaken by Jeremy Frey and

the plan is for this responsibility to be transferred to Gillian Bell in late 2018. We plan to undertake a recruitment campaign in 2018 with the objective of recruiting at least two new members to the committee.

### **Future Activities**

When planning any activities please remember to ensure that all events are logged on our events database and ensure that all contracts are sent to our Legal Team with enough time for amendments and, where necessary, approval by the Board.

Please outline any activities already in planning for the next calendar year.

<b>Event Name</b>	<b>Computer aided Reaction Outcomes</b>
<b>Comments</b>	Bradfield Centre, Cambridge, 26 March 2018, in collaboration with Dial a Molecule. 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

<b>Event Name</b>	<b>Artificial Intelligence in Chemistry</b>
<b>Comments</b>	Burlington House Friday, 15th June 2018 CICAG in partnership with BMCS. Artificial Intelligence is presently experiencing a renaissance in development of new methods and practical applications to ongoing challenges in Chemistry. We are pleased to announce that the Biological & Medicinal Chemistry Sector (BMCS) and Chemical Information & Computer Applications Group (CICAG) of the Royal Society of Chemistry are organising a one-day conference entitled Artificial Intelligence in Chemistry to present the current efforts in applying these new methods. We will combine aspects of artificial intelligence and deep machine learning methods to applications in chemistry.

<b>Event Name</b>	<b>Spectroscopic Data to Chemical Knowledge</b>
<b>Comments</b>	To be organised jointly with the Molecular Spectroscopy Interest Group and Dial a molecule Grand Challenge Network probably at AstraZeneca but this is still under discussion

<b>Event Name</b>	<b>Tony Kent Strix Award and Annual Lecture</b>
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<b>Comments</b>	23 The Strix award and lecture are given in memory of Dr. Tony Kent. In the 1960s and 70s, Tony became an increasingly important and influential member of the RSC staff, ending up as the Society's first Director of Information. It is proposed that the future annual lecture meeting be held in the RSC, rather than, as hitherto, in the Geological Society.
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<b>Event Name</b>	<b>CICAG Annual Meeting</b>
<b>Comments</b>	We have had some preliminary discussions regarding instigating a CICAG annual meeting, this would probably be a multiday meeting with the aim that it would be a regular event in the calendar. We feel that this would serve to increase the profile of CICAG and an opportunity to showcase the diverse areas of research that come under the CICAG umbrella. We will explore options in 2018 and hope to have a concrete proposal by the end of the year.

<b>Event Name</b>	<b>Catalyst Centre Careers week</b>
<b>Comments</b>	CICAG members will be supporting Chemistry at Work Week in June 2018 at the Catalyst Science Discovery Centre, the exact nature of the support is in under discussion.

<b>Event Name</b>	<b>Undergraduate Research Bursary</b>
<b>Comments</b>	As in previous years we will support an undergraduate research bursary in conjunction with the RSC scheme in an area relevant to the interest group's activities.

## Committee

This information will be used to update our membership database and your web page. Please ensure that any changes to the committee are sent to [networks@rsc.org](mailto:networks@rsc.org) as soon as possible.

Position	Name	Dates on committee (20xx – 20xx)
Chair	Dr Chris Swain	2015 to date
Secretary	Prof. Jeremy Frey	2016 to date
Treasurer	Dr Diana Leitch	2009 to date
Ordinary Members	Dr. Alan Tonge Ms. Gillian Bell Prof Jonathan Goodman Mr Stuart Newbold Dr Helen Cooke Dr Nathan Brown Dr Neil Berry Dr Peter Bladon  *Alan Tonge plans to retire when a suitable replacement has been recruited.	2008 -2018* 2012 to date 2015 to date 2010 to date 2014 to date 2015 to date 2015 to date 2015 to date
Chemists' Community Fund Representative (if relevant)		
Co-opted members and their affiliation	Mrs. Yvonne Pope CAS	2009 to date

## Diversity & Inclusion

Our trustees are aiming to embed diversity and inclusion in all of our activities and networks. Our [online network handbook](#) contains more information to support our networks in achieving this.

Please comment on how your group is showing that it has embraced Diversity and Inclusion within its practices.

- Yvonne Pope has taken on the diversity and inclusion role
- To broaden our outreach, we held events outside of London and will be continuing to do so in 2018.
- We always take account of dietary requirements at events and committee meetings.
- We ensure that event venues have wheelchair access, and lifts if events are not held on the ground floor.
- We will be undertaking a recruitment campaign in 2018 and will aim to broaden the diversity of the committee.
- We have actively encouraged diversity of speakers at meetings, recognising the need for more role models.
- Chris Swain organised a session at the Cambridge MedChem meeting on neglected and tropical diseases. This was broadcast as a live webinar, and the recording has been made publically available to allow greater engagement in this important therapeutic area.
- Exploring how CICAG can aid the educational work at the Catalyst Science Discovery Centre in Widnes, including interactions with young people and families in some of the most deprived areas in the UK