Registration and Bursaries

Registration is open, and fees include attendance at the Monday conference dinner:

£330 RSC member
£393 Non-member
£180 RSC student* member
£230 Student* non-member

* Student is undergraduate or post-graduate.

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 15th July.

Accommodation

Bedrooms have been held at Fitzwilliam College on Sunday and Monday nights on a bed and breakfast basis. The charges are £62-£69 per night, and bookings may be made via the registration process.

Venue and Travel

Fitzwilliam College, Storey's Way, Cambridge CB3 0DG. Situated a short walk from Cambridge city centre, travel information may be found on our website.

Call for Posters

Applications for poster presentations are welcomed. Posters will be displayed throughout the event and applicants are asked if they wish to provide a two-minute flash oral presentation when submitting their abstracts. Closing date is 5th July.

Exhibition and Sponsorship Opportunities

There will be a relevant trade exhibition – the charge is £1,250 including one full delegate place. Sponsors are sought to support the low registration fees for students.

charles river AstraZeneca

Twitter Hashtag
#AIChem19

Organising Committee

Nathan Brown, BenevolentAI (chairman)
Samantha Hughes, AstraZeneca
Phil Jones, BioAscent
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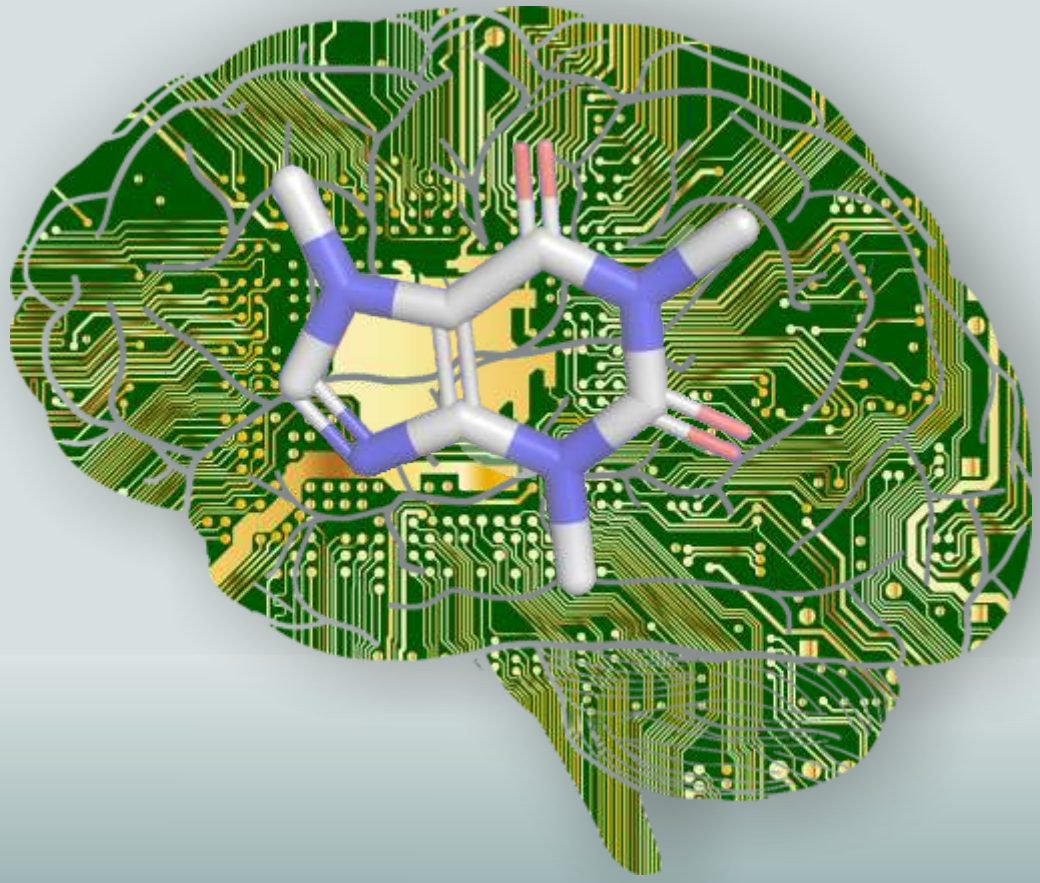

2nd RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry

Monday-Tuesday, 2nd-3rd September 2019

Fitzwilliam College, Cambridge, UK

Third announcement and call for posters

ROYAL SOCIETY OF CHEMISTRY | BIOLOGICAL AND MEDICINAL CHEMISTRY SECTOR

ROYAL SOCIETY OF CHEMISTRY | CHEMICAL INFORMATION AND COMPUTER APPLICATIONS GROUP

Artificial Intelligence in Chemistry

Synopsis

Artificial Intelligence is presently experiencing a renaissance in development of new methods and practical applications to ongoing challenges in Chemistry. Following the success of the inaugural "Artificial Intelligence in Chemistry" meeting in 2018, 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 once again organising a conference to present the current efforts in applying these new methods. The meeting will be held over two days and will combine aspects of artificial intelligence and deep machine learning methods to applications in chemistry.

Who should attend

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

Programme

Monday, 2nd September

08.30 Registration, refreshments
09.30 *Deep learning applied to ligand-based de novo design: a real-life lead optimization case study*
Quentin Perron, IKTOS, France
10.00 *Molecular transformer for chemical reaction prediction and uncertainty estimation*
Alpha Lee, University of Cambridge, UK
10.30 Flash poster presentations
11.00 Refreshments, exhibition and posters
11.30 *Are learned molecular representations ready for prime time?*
Keynote: Regina Barzilay, Massachusetts Institute of Technology, USA
12.30 Lunch, exhibition and posters
14.00 *Artificial intelligence for predicting molecular Electrostatic Potentials (ESPs): a step towards developing ESP-guided knowledge-based scoring functions*
Prakash Rathi, Astex Pharmaceuticals, UK
14.30 *A. Turing test for molecular generators*
Jacob Bush, GlaxoSmithKline, UK
15.00 *Drug discovery disrupted - quantum physics meets machine learning*
Noor Shaker, GTN, UK
15.30 Refreshments, exhibition and posters
16.00 *Application of deep learning in chemistry: where are we in drug design?*
Christian Tyrchan, AstraZeneca, Sweden
16.30 *Is your machine learning telling you anything you didn't already know?*
Keynote: Anthony Nicholls, OpenEye Scientific Software, USA
17.30 Close
18.45 Drinks reception
19.15 Conference dinner

#AIChem19

Artificial Intelligence in Chemistry

Programme (continued)

Tuesday, 3rd September

08.30 Refreshments
09.00 *Deep generative models for 3D compound design from fragment screens*
Fergus Imrie, University of Oxford, UK
09.30 *DeeplyTough: learning to structurally compare protein binding sites*
Joshua Meyers, BenevolentAI, UK
10.00 *Discovery of nanoporous materials for energy applications*
Maciej Haranczyk, IMDEA Materials Institute, Spain
10.30 Refreshments, exhibition and posters
11.00 *Centaur ChemistTM in 3D: AI powered design of small molecules accelerated by structure-based constraints*
Anthony Bradley, Exscientia, UK
11.30 *Deep learning for drug discovery*
Keynote: David Koes, University of Pittsburgh, USA
12.30 Networking lunch, exhibition and posters
14.00 *De-novo molecular design with generative models and reinforcement learning*
Olexandr Isayev, University of North Carolina at Chapel Hill, USA
14.30 *Dreaming functional molecules with generative ML models*
Christoph Kreisbeck, Kebotix, USA
15.00 Refreshments, exhibition and posters
15.30 *The ANI family of deep learned potentials: development, application to general computational chemistry problems, and future prospects*
Keynote: Adrian Roitberg, University of Florida, USA
16.30 Close

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