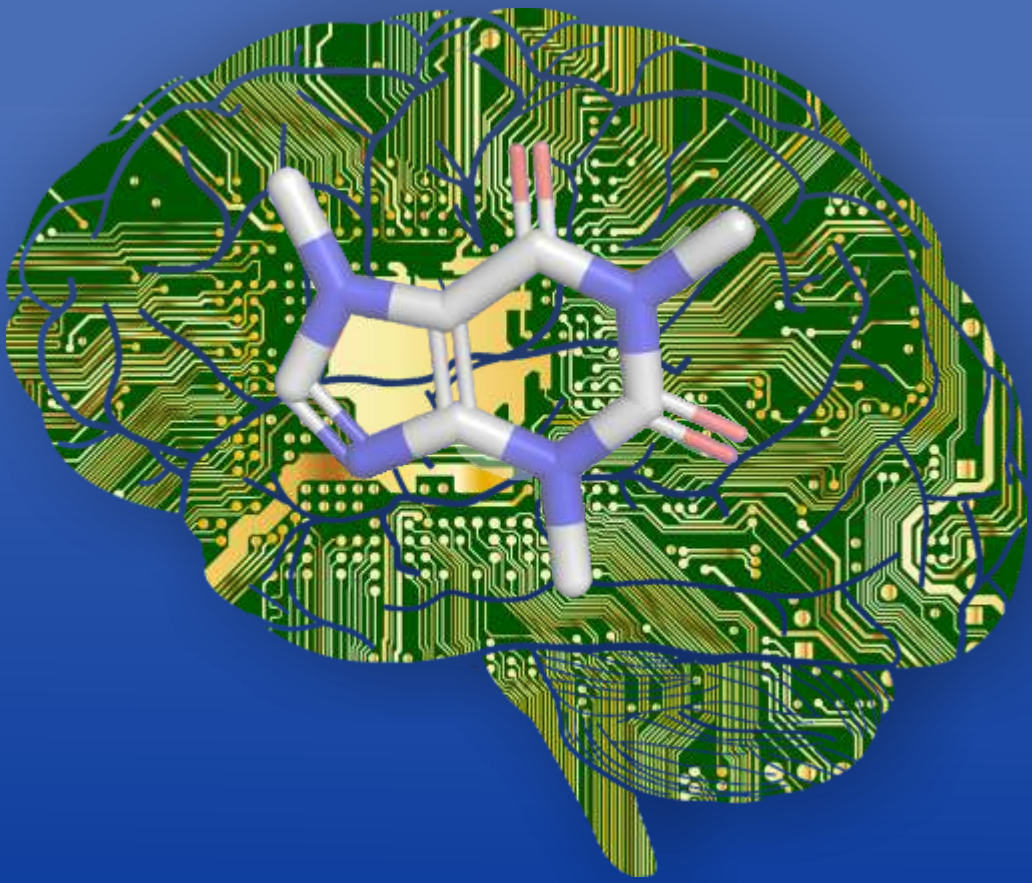

3rd RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry

Monday-Tuesday, 28th-29th September 2020

A virtual meeting - online only

Third Announcement

RSC INTEREST GROUP
CHEMICAL INFORMATION
AND COMPUTER APPLICATIONS

RSC INTEREST GROUP
BIOLOGICAL AND MEDICINAL
CHEMISTRY SECTOR

Synopsis

Artificial Intelligence is presently experiencing a renaissance in development of new methods and practical applications to ongoing challenges in Chemistry. Following the successes of two "Artificial Intelligence in Chemistry" meetings in 2018 and 2019, 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 combine aspects of artificial intelligence and deep machine learning methods to applications in chemistry.

Confirmed Speakers

Machine learning for efficient design of industrial formulations
Keynote: **Gareth Conduit**, Intellegens, UK

Teaching neural network to attach and detach electrons from molecules
Keynote: **Olexandr Isayev**, Carnegie Mellon, US

DNA-encoded small molecules libraries meet machine learning
Keynote: **Patrick Riley**, Google, US

Using machine learning for molecular dynamics simulations
Keynote: **Sereina Riniker**, ETH Zürich, CH

Artificial neural network enhanced synthesis and retrosynthesis prediction - **Esben Jannik Bjerrum**, AstraZeneca, SE

Barking up the right tree: de novo design via searching over molecule synthesis DAGs - **John Bradshaw**, University of Cambridge, UK

Novel chemical structure input method for machine learning to capture 3D information like chirality and rotational symmetry - **Ella Gale**, University of Bristol, UK

Bayer's in silico ADMET platform: how the combination of artificial and human intelligence can make a difference in drug discovery - **Andreas Göller**, Bayer AG, DE

Free energy calculations for drug discovery with hybrid ML/MM potentials - **Hannah Bruce McDonald**, MSD, UK

Data driven representations for predicting molecular properties: benchmarking and applications in generative chemistry - **Jessica Lanini**, Novartis, CH

The data is the filter is in the data: meaningful machine learning models and machine-learned pharmacophores from fragment screening campaigns - **Carl Poelking**, Astex Pharmaceuticals, UK

Unassisted noise-reduction of chemical reactions data sets - **Alessandra Toniato**, IBM Research - Zurich, CH

Who should attend?

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

Exhibitor and Sponsorship Opportunities

Please refer to our website for details of exhibitor sponsor opportunities. Sponsors are sought to support the administrative costs for this meeting.

AstraZeneca

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Twitter Hashtag

#AIChem20

Organising Committee

Nathan Brown, BenevolentAI (Chairman)
Samantha Hughes, AstraZeneca
Garrett M Morris, University of Oxford
Chris Swain, Cambridge MedChem Consulting
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