



# 3<sup>rd</sup> RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry

Monday-Tuesday, 28<sup>th</sup>-29<sup>th</sup> September 2020

A virtual meeting - online only

## Second Announcement and Call for Abstracts

## 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.

## Who should attend?

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

## Confirmed Speakers

*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

*Artificial neural network enhanced synthesis and retrosynthesis prediction*

Esben Jannik Bjerrum, AstraZeneca, SE

*Machine learning for free energy calculations*

Hannah Bruce McDonald, Memorial Sloan Kettering Cancer Center, US

*Data driven representations for predicting molecular properties: benchmarking and applications in generative chemistry*

Jessica Lanini, Novartis, CH

*Using machine learning for molecular dynamics simulations*

Sereina Riniker, ETH Zürich, CH

## 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** 

 **MSD**  
INVENTING FOR LIFE

## Organising Committee

Nathan Brown, BenevolentAI (Chairman)

Samantha Hughes, AstraZeneca

Garrett M Morris, University of Oxford

Chris Swain, Cambridge MedChem Consulting

Joe Sweeney, Lancaster University

## Secretariat Contact

Mrs Maggi Churchouse, RSC BMCS Secretariat

Telephone: +44 (0)1359 221004

E-mail: [maggi@maggichurchouseevents.co.uk](mailto:maggi@maggichurchouseevents.co.uk)

## Websites

[www.maggichurchouseevents.co.uk/bmcs](http://www.maggichurchouseevents.co.uk/bmcs)

[www.rsc.org/bmcs](http://www.rsc.org/bmcs) and [www.rsc.org/cicag](http://www.rsc.org/cicag)

## Call for Abstracts

Applications for oral and poster presentations are invited. Posters will be displayed during a dedicated poster session, and applicants are asked if they wish to provide a two-minute lightning oral presentation.

The abstract due date has been extended to 14th August by popular request and due to high levels of interest.

## Registration

Free-of-charge registration is open, and additional information may be found on our website.

## Twitter Hashtag

#AIChem20

