# RSC-BMCS / RSC-CICAG
# Artificial Intelligence in Chemistry

Friday, 15th June 2018

Royal Society of Chemistry at Burlington House, London, UK

Second announcement and call for posters

ROYAL SOCIETY OF CHEMISTRY | BIOLOGICAL AND MEDICINAL CHEMISTRY SECTOR

ROYAL SOCIETY OF CHEMISTRY | CHEMICAL INFORMATION AND COMPUTER APPLICATIONS GROUP

## Synopsis

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.

## Who should attend?

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

## Programme

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| 09.00 | Registration, refreshments, and exhibition |
| 10.00 | *Presentation title to be confirmed* |
| | Marwin Segler, Benevolent AI, UK |
| 10.30 | *Chemical topic modelling - an unsupervised approach to organize and explore chemical information* |
| | Nadine Schneider, Novartis, Switzerland |
| 11.00 | Refreshments, exhibition and posters |
| 11.30 | <u>Keynote</u>: *What I learned about machine learning - revisited* |
| | Bob Sheridan, Merck, USA |
| 12.30 | Lunch, posters and exhibition |
| 14.00 | *Molecular* de novo *design through deep learning* |
| | Ola Engkvist, AstraZeneca, Sweden |
| 14.30 | *Scaling* de novo *design, from single target to disease portfolio* |
| | Wilhem van Hoorn, Exscientia, UK |
| 15.00 | Refreshments, posters and exhibition |
| 15.30 | *Investigating clusters in solvent data using K-means* |
| | Ella Gale, University of Bristol, UK |
| 16.00 | *Deep learning and chemical data* |
| | Colin Batchelor, Royal Society of Chemistry, UK |
| 16.30 | *Automation, analytics and AI* |
| | Darren Green, Molecular Design UK, RD Platform Technology & Science, GlaxoSmithKline, UK |
| 17.00 | Close |

### Twitter Hashtag
#RSC_AIChem

### Call for Posters

Applications for poster presentation are welcomed. Posters will be displayed throughout the day and applicants will be asked if they would like to provide a two-minute flash oral presentation when submitting their abstract. The closing date is 13th April.

## Registration Fees and Bursaries

Registration is open and fees may be found on the event website. 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 3rd May.

## Exhibition and Sponsorship Opportunities

There will be a small, relevant trade exhibition – the charge is £500 including one full delegate. We are grateful to KNIME for their sponsorship, and additional sponsors are sought to support the low registration fees.

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## Venue and Travel

Library, Royal Society of Chemistry at Burlington House, Piccadilly, London, W1J 0BA, UK. Situated in central London, the RSC is easily accessible by public transport, and close to Green Park tube station.

## Organising Committee

Nathan Brown, BenevolentAI (chairman)
Phil Jones, University of Dundee
Chris Swain, Cambridge MedChem Consulting

## Secretariat Contact

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## Websites

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