BIG DATA IN BIOMOLECULAR SYSTEMS

9 SEPTEMBER 2016
SCHOOL OF PHARMACY, UCL, LONDON

https://bigdatamgms.wordpress.com/

Synopsis

The aim of the conference is to discuss recent progress in managing, analysing and storing big data pertaining to biomolecular systems. The main topics of the meeting include big data and healthcare, big data and biomolecular simulations, functional genomics, biological networks, network pharmacology, functional bioinformatics and chemical data collections.

Attendees

The meeting is targeted at academic and industrial scientists dealing with all big-data aspects of biomolecular simulations and drug discovery.

Posters & Late Breaker Talk Abstracts

One talk and several poster spaces are still available – please submit a one-page abstract by 15th August 2016.
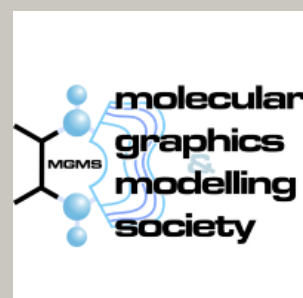
Sponsorship

This event is fully funded by donations and registration fees. Institutions interested in co-sponsoring this meeting should contact Ewa.Chudyk@evotec.com to discuss opportunities.

Registration – 15th August deadline

	Early bird	After 1st June
Non-MGMS members	£80	£130
MGMS members	£50	£100
Student non-MGMS members	£30	£80
Student MGMS members	£0	£50

Organizer

molecular graphics & modelling society

Friday, 9 September 2016
Programme

9.00 – 9.45 Registration

9.45 – 10.00 Opening

Bridging Genomics and Bioinformatics

10.00 – 10.30 **Prof. Charlotte Deane,** University of Oxford: "Understanding the difficulty behind H3 prediction and using this knowledge to develop novel prediction tools"

10.30 – 11.00 **Prof. Charlie Laughton,** University of Nottingham & The MuG consortium: "Multiscale Complex Genomics: the Big data challenge"

11.00 – 11.30 Coffee break & networking

Big Data and Molecular Simulation

11.30 – 12.00 **Dr Arvind Ramanathan**, Oak Ridge National Laboratory: "Big Data Statistical Inference Techniques for Molecular Biophysics"

12.00 – 12.30 **Athina Meletiou**, Nottingham University: "Utilising IBM's World Community Grid virtual supercomputer to model mycolic acids from *Mycobacterium tuberculosis*"

12.30 – 13.00 **Dr Christian Lemmen**, BioSolveIT GmbH: "*De novo* design in the synthetically accessible compounds universe"

13.00 – 14.00 Lunch break & poster session

Big Data and Healthcare

14.00 – 14.30 **Dr Bryn Williams-Jones**, Open PHACTS Foundation: "Open semantic data services for drug discovery"

14.30 – 15.00 **Dr Jon Fuller**, KNIME: "KNIME for (Big) Data and Tool Blending for Advanced Analytics in the Life Sciences"

15.00 – 15.30 **Prof. Nataša Pržulj**, University College London: "Data-driven Medicine"

15.30 – 16.00 Coffee break & networking

16.00 – 16.30 **Prof. Carlos P. Sosa**, University of Minnesota & Mayo Clinic: "Toward the integration of mate-pair and RNA sequencing in Biomarker Discovery"

16.30 – 17.00 **Dr Dean Plumbley**, Stratified Medical, London, *title TBC (abstract coming soon)*

17.00 – 17.30 **Dr Ed Griffen**, Medchemica Ltd: "Extracting and sharing and exploiting medicinal chemistry ADMET knowledge automatically from multiple large Pharma data"

17.30 Wine reception & networking

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