

## Chemistry on Mobile Devices: Create, Compute, Collaborate

### Abstracts

#### **Overview of mobile chemistry**

Dr Michelle Lynch, *Senior Consultant, IHS Markit*

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This presentation will provide an overview of the current state-of-play of mobile devices and applications available to chemists. In addition, the mobile chemistry roadmap will be presented setting out a timeline covering:

- The introduction, growth, development and future of mobile chemistry;
- How each element along the “mobile chemistry value chain”, including enabling software, data collection and storage, data retrieval, cybersecurity, data analytics and visualization tools, is expected to evolve and where obstacles are anticipated;
- Which mobile solutions are gaining the most traction and how this varies in different environments;
- How chemical researchers, educators, healthcare providers and industrialists can extract the best value, optimise productivity and profitability while minimising risks from their chosen mobile solutions.

#### **Lab on the bus: Designing for academic modes of reading**

James Stevens, *Product Manager, Journals and Books, RSC*, & Paul-Jervis Heath, *Founding Principal, Modern Human*

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Academics broadly engage in two different kinds of reading, each with a distinct goal. They utilise four tactics to keep up with the latest developments in their field. In this talk, Paul-Jervis Heath, from design practice Modern Human, will examine insights into academic reading behaviour generated from their design research and discuss how these have been applied to the redesign of the Royal Society of Chemistry’s publishing platform. He will talk through the human-centred design process followed whilst revealing insights about academic reading behaviour. He will be joined by James Stevens, product manager for journals and books at the Royal Society of Chemistry, who will explain how together they applied a rapid and iterative research, design, development and testing process to create a better online publishing research experience for their readers and authors.

#### **Mobile devices in chemistry education**

Professor Nick Greeves, *Department of Chemistry, University of Liverpool*

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Smart phones and tablets are becoming an increasingly common sight on university campuses. This talk will illustrate some of the ways that they can be beneficial for learning chemistry and some of the areas in which the hardware and software that students are likely to afford comes up

short. Bring your own device (BYOD) has proved problematic in higher education: is there a solution?

### **EduChem VR – virtual reality smartphone apps making chemistry look and feel cool**

Dr Jonas Boström, *CEO & Co-founder*, & Magnus Norrby, *CTO & Co-founder*, *EduChem VR*

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We introduce a new cool way to learn chemistry and biology using smartphones. To engage students and facilitate learning, virtual reality (VR) experiences are provided. VR's potential in education is great – an immersive (VR) experience can improve the understanding of abstract concepts, such as atoms and molecules, and it has also been shown that when you are able to put a person in a place, they are more likely to remember it. By developing Google cardboard smartphone apps, we can essentially reach everyone everywhere.

The virtual reality apps can of course also be used in a pharmaceutical setting, letting drug designers step into their favourite protein-ligand complex and help them in the creative process of generating new design ideas, challenge the traditional ways of thinking and ultimately lead to new solutions and medications to patients. Our vision is to deliver affordable software solutions to increase learning in the area of life science.

### **The Handbook of Medicinal Chemistry and Medicinal Chemistry Toolkit app - tablet delivery by design**

Dr Andy Davis, *Projects Director*, *RIA Innovative Medicines*, *AstraZeneca*

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The talk will describe the motivation, vision and realisation for the Handbook of Medicinal Chemistry and its companion app, and examples of the use of the Medicinal Chemistry Toolkit within projects. The benefits and difficulties of managing a complex piece of scientific software on a mobile platform will also be discussed

### **Challenges of developing electronic lab notebooks for mobile devices and substructure searching on iPad**

Dr Dan Ormsby, *Principal Application Scientist*, *Dotmatics Limited*

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Dotmatics mainly delivers web-based software solutions to scientists, most of whom are in biotech/pharma, where mobile devices are becoming more common. To support these devices, Dotmatics has invested in making web apps and native apps for Android and iOS. The development and delivery of these apps will be discussed during this talk, with particular focus on low UI latency ELN deployments and high-performance substructure searching.

### **Around the World Synthesis: Controlling Reactions in Cambridge through Tokyo**

Daniel Fitzpatrick, *PhD Researcher*, *Ley Group*, *University of Cambridge*

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Daniel will be giving an overview of the cloud-based reaction monitoring and control system he has developed during his PhD research programme. This system, accessible from anywhere on any device (including tablets and smartphones), is based on servers in Tokyo, Japan, and can be used to automate reactions being conducted in any laboratory in the world. Daniel will describe how the system has been used for multi-step reaction sequences, and will demonstrate it live by controlling a reactor system in a Cambridge laboratory in real-time.

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### Speaker Biographies

#### **Dr Michelle Lynch, *Senior Consultant, IHS Markit***

Michelle is a Senior Consultant in IHS Markit Chemicals Consulting based in London. She has 18 years' experience in the chemical industry including catalyst development, market research, intellectual property (IP) analysis, information science and consulting. She has written several multi-client reports on chemical process technology and economics and carried out a variety of consulting assignments for clients including technology benchmarking, value chain analysis, commercial due diligence, and acquisition screening.

#### **James Stevens, *Product Manager, Journals and Books, RSC***

James Stevens is the product development manager for the journals and books platform at the Royal Society of Chemistry. In partnership with the business and the agile team, he manages the development and commercial aspects of the journals and books product line ([pubs.rsc.org](http://pubs.rsc.org)), creating superior customer satisfaction while simultaneously providing long-term value. His role ensures a range of digital services are developed that deliver in line with a clear and effective strategy, while also optimising them to realise their business goals and to maximise return on investment.

James previously project managed the delivery of the new Royal Society of Chemistry corporate site identity and led the work to engage authors and readers in China through a dual language website.

#### **Paul-Jervis Heath, *Founding Principal, Modern Human***

Paul-Jervis Heath is a designer and innovation consultant. He is the founding principal of Modern Human, a design practice and innovation consultancy that helps clients to imagine what's next. He leads design projects and builds capability for design thinking within organisations.

Over a 15-year career, he has introduced human-centred design methods to many organisations and led diverse design projects, such as in-car information systems, smart home appliances, concepts for retail stores of the future and countless other multichannel services and digital products.

**Professor Nick Greeves, *Department of Chemistry, University of Liverpool***

Nick is a Cambridge graduate, obtaining his PhD there in 1986 for work on the stereoselective Horner-Wittig reaction with Stuart Warren. He then held a Harkness Fellowship at the University of Wisconsin-Madison and at Stanford University, California, with Barry Trost and a Research Fellowship at Cambridge University before joining Liverpool in 1989, where he was promoted to Professor in 2015. He was selected for a HEA National Teaching Fellowship in 2009 and SFHEA in 2014. Nick is married with two children and lives in Formby. His interests include Macs, music (iPhone), photography (iPhone), and social media. He is saving up for the next version of Apple Watch.

**Dr Jonas Boström, *CEO & Co-founder*, & Magnus Norrby, *CTO & Co-founder*, *EduChem VR***

EduChem VR was founded during the summer of 2016 in Göteborg, Sweden by Jonas Boström and Magnus Norrby. Magnus Norrby is computer scientist and professional java programmer and Jonas Boström is a computational medicinal chemist at AstraZeneca, Sweden. Magnus and Jonas have a track record of working efficiently and collaboratively while delivering powerful and user-friendly software tools to enhance drug discovery within AstraZeneca. A notable example is the first easily accessible virtual reality (VR) molecular visualiser – “Molecular Rift” – used by the King of Sweden during a recent state visit.

**Dr Andy Davis, *Projects Director, RIA Innovative Medicines, AstraZeneca***

Andy gained his first degree in chemistry from Imperial College of Science and Technology, University of London, in 1982 and his PhD at University of Huddersfield with Professor MI Page, studying kinetics and mechanisms of rearrangements of penicillins. He joined Fisons in 1988 as a physical organic chemist, and subsequently became Associate Director of Physical Chemistry at AstraZeneca R&D Charnwood. Through his work on the application of physical chemistry to drug design, he was honoured to be appointed an AstraZeneca Senior Principal Scientist. He has also been awarded two AstraZeneca global Scientific and Technical Achievement Awards for work on a global ADMET prediction program called C-Lab, and contributions to the development of a high throughput hERG assay. In 2008 he became chair of the Charnwood Local Projects Forum, and member of the Respiratory and Inflammatory research area Portfolio Team. In 2011 he moved to Sweden, and a new challenge as a project leader in the Respiratory Inflammation and Autoimmunity Innovative Medicines Unit at AstraZeneca R&D Gothenburg. Through this time, he has maintained his involvement in QSAR method development. He has been a tutor and lecturer on the Royal Society of Chemistry Medicinal Chemistry Summer School since 1990, and scientific course organiser since 2005. He has published many highly-cited articles in leading peer-reviewed journals, covering his key interests of compound quality, the energetics of drug-receptor interactions, QSAR methods and the co-operative application of physical organic and computational chemistry to drug discovery. Most recently, with Prof Simon Ward from University Sussex, he has edited the Royal Society of Chemistry Handbook of Medicinal Chemistry – Principles and Practice, together with its companion suite of applications for iPad, The RSC Medicinal Chemistry Toolkit.

**Dr Dan Ormsby, *Principal Application Scientist, Dotmatics Limited***

Dr Dan Ormsby joined Dotmatics Ltd in 2008. He spends around 50% of his time traveling the globe to work with customers in dozens of countries. He is responsible for many of the small-molecule algorithms implemented at Dotmatics for property calculation, matched-pair analysis chemical clustering, fast sub-/super-/similarity-searching chemistry features and has brought these algorithms to Windows, Mac, Linux, Android, iOS and Raspberry Pi.

**Daniel Fitzpatrick, *PhD Researcher, Ley Group, University of Cambridge***

Following his completion of a Bachelor of Engineering (Hons) in Chemical and Materials Engineering, in 2013 Daniel joined the research group of Prof Steven Ley at the University of Cambridge to embark on a PhD programme. His research interests lie at the intersection of synthetic chemistry, chemical engineering and modern advances in information technology. More specifically, he has developed a cloud-based reaction monitoring, control and self-optimisation platform that enables chemists to automate their reactions in any location throughout the world, using the internet. This system has also been employed to facilitate the full integration between batch and flow processes, breaking through what has been a historical hindrance to synthetic work.