

# Automated Synthesis Forum

Strathclyde University, 18<sup>th</sup> - 19<sup>th</sup> November 2019

## Monday, 18<sup>th</sup> November

9:00 Registration and refreshments

9:30 Introduction and Safety announcements

9:40 **Plenary: *CHEMIFY: A Universal System for Validating the Synthetic Chemical Literature***

**Professor Lee Cronin**, University of Glasgow, UK

10:30 Break and equipment exhibition

### **Session 1: Electrochemistry and Photochemistry**

Session chairs: **David Pearce**, Syngenta, UK and **Tobias Moechel**, Sygnature Discovery, UK

11:00 ***Electrochemistry in Flow using custom 3D printed electrochemical cells***

**Dr Kevin Lam**, University of Greenwich, UK and

**Dr Steve Hilton**, University College London, UK

11:30 ***Electrochemical Oxidation as an Alternative to Chemical Oxidation***

**Dr Alastair Lennox**, University of Bristol

11:50 ***Development of a multifunctional electrochemical flow platform for high-throughput synthesis and optimisation of catalysts***

**Dr Christiane Schotten**, University of Leeds

12:15 ***Synthesis in fragment-based drug discovery (FBDD) with enabling technologies***

**Dr Rachel Grainger**, Astex, UK

12:45 Lunch and equipment exhibition

2:00 **Plenary: *Automated processes to assist with mechanistic understanding in "simple" and "complicated" Pd-catalysed cross-couplings***

**Professor Ian Fairlamb**, University of York, UK

2.50 Break and equipment exhibition

### **Session 2: Synthesis and Post-Synthesis Process Improvements**

Session chairs: **Jenny Kingston**, AstraZeneca, UK and **Alexander Marziale**, Novartis, Switzerland

3:20 **AstraZeneca iLab: Accelerating Drug Discovery through automation**

- ***Automated Synthesis in the DMTA workflow***

**Dr Javier Mazuela**, AstraZeneca, Sweden

- ***Analysis and purification within the iLab***

**Dr Pernilla Korsgren**, AstraZeneca, Sweden

- ***Miniaturised HT synthesis for PicoSAR***

**Dr Victoria Helan**, AstraZeneca, Sweden

4:20 ***Software-driven automated parallel chemistry purification processes***

**Dr Marcus Koppitz**, Bayer, Germany

- 4:50 **Dial-a-Molecule – user perspective**  
**Dr Francesca Dennis**, University of Sheffield, UK
- 5:30 **Meet at Arta Restaurant (62 Albion Street) for conference reception (dinner at 7.15)**

## Tuesday, 19<sup>th</sup> November

- 9:00 **Plenary: Escaping Flatland Using Flow Chemistry: Ready for Automation**  
**Dr Jesus Alcazar**, Janssen, Spain

- 9:50 **Break and equipment exhibition**

### **Session 1: Flow Chemistry**

Session chairs: **Cara Brocklehurst**, Novartis, Switzerland and **Andrew Ledgard**, Lilly, UK

- 10:20 **Overcoming the challenges of flow chemistry: A look back over 10 years of experience**  
**Dr Hansjoerg Lehmann**, Novartis, Switzerland

- 10:50 **Automated Flow Systems for Medicinal Chemistry Applications**  
**Prof Antimo Gioiello**, University of Perugia, Italy

- 11:10 **Automated Library Synthesis in Flow using Photoredox Catalysis**  
**Dr Gianvito Vilé**, Idorsia Pharmaceuticals Ltd

- 11:50 **fReactor integrated flow chemistry equipment**  
**Professor Nikil Kapur and Professor John Blacker**, University of Leeds, UK

- 12:15 **Lunch and equipment exhibition**

### **Session 2: Machine Learning and AI**

Session chairs: **Gemma Turner**, Concept Life Sciences, UK and **Jason Tierney**, Top Tier Consultancy, UK

- 1:15 **DigitalGlassware: Contextualising Chemical Outcomes for Faster Discovery**  
**Dr Robbie Warringham**, Deepmatter, UK

- 1:35 **Synthia (formerly Chematica) Retrosynthesis Software: Validation at the Bench**  
**Dr Sarah Trice**, Merck KGaA, USA

- 1:50 **Break and equipment exhibition**

### **Session 3: New Technologies**

Session chairs: **Melanie Bayford**, Domainex, UK and **Steve Brough**, Key Organics, UK

- 2:20 **T.I.M.E. for Next Gen Drug Discovery: Nanna Therapeutics Droplet Based Drug Discovery Platform**  
**Dr Martin Fisher**, Nanna Therapeutics, UK

- 2:40 **Towards high fidelity, parallel gene synthesis utilising flow cell methodologies**  
**Mr Mathew Jennison**, Evonetix, UK

- 3:05 **Electron Diffraction: Crystallographic Approach and Application to Organic Molecules**  
**Dr. Gustavo Santiso-Quñones**, Eldico Scientific, Switzerland

- 3:35 **Synple Chem User perspective**  
**Dr Claudio Bomio**, Novartis, Switzerland

- 3:35 – 3:40 **Closing remarks**