Chemical Tools in Systems Biology III,

17 December 2018

Royal Society of Chemistry, London

The emphasis of this one-day symposium was to explore and promote the synergies that chemical and biological sciences can deliver in the procurement of a deeper understanding of the complexity of biological systems.

The symposium featured seven invited speakers and four short Oral Presentations by Early Career Scientists who had been chosen from those who had submitted a Poster Abstract. The total attendance was 49.

The delegates clearly enjoyed the symposium, since most of the lectures were followed by lively question and answer sessions. The 14 posters prompted good interactive discussions at the coffee, lunch and tea breaks. The CBID Programme Manager, Dr Wendy Niu was present and she said she had thoroughly enjoyed the symposium.

Two Poster Prizes of £50 were presented by representatives of our sponsors, Dr Wendy Niu, CBID and Marcus Köster, Boehringer Ingelheim to:

- Floriane Martins, PhD student, University of Nottingham
- Dr Andreia de Almeida, Post-Doctoral Fellow, Cardiff University

A full Programme and a List of Poster Presentations are appended to this report.

We would like to thank: (i) the staff of the Royal Society of Chemistry for their hospitality and professional support; and (ii) the RSC's Chemistry Biology Interface Division for a Scientific Meetings Grant and Boehringer Ingelheim for generous sponsorship.

Conference Committee

Dr Klaus Rumpel (Chair), Boehringer Ingelheim, Vienna, Austria and Biotechnology Group
Dr Colin Bedford Chemistry Department, UCL and Biotechnology Group January 2019

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Chemical Tools in Systems Biology III
17 December 2018, Burlington House, London
Programme

09:30 **Coffee & Registration**

09:55 **Session I** Chair: Klaus Rumpel

10:00 **Susanne Müller-Knapp** Goethe Universität Frankfurt, Germany
The impact of Open Science Chemical Probes

10:40 **Alessio Ciulli** University of Dundee, UK
Targeted protein degradation with small molecules: How PROTACs work

11:20 **Ed Tate** Imperial College London, UK
Protein lipidation: From biological systems to drug discovery

12:00 **Vicki Linthwaite** University of Durham, UK
Protein carbamylation: The discovery of a carbon dioxide control system

12:15 **Markus Köster** Boehringer Ingelheim, Germany
opnMe.com – Access well-characterised Boehringer Ingelheim tool compounds for your own research

12:20 **Lunch & Posters**

Session II Chair: Colin Bedford

13:30 **Frederike Müskens** University of Glasgow, UK
Synthesis/evaluation of a diazirine photoaffinity probe for ligand-based receptor capture targeting on GPCRs
13:45 **Richard Doveston** University of Leicester, UK
Stabilising protein-protein interactions: A challenge for ligand discovery

14:00 **Bernhard Küster** Technische Universität München, Germany
Target landscape and signaling networks of kinase inhibitor drugs

14:40 **Julio Saez-Rodriguez** Universität Heidelberg, Germany
Network models to dissect the effect of genetic and chemical perturbations in cancer

15:20 **Coffee**

15:40 **NicoleTrainor** University of Dundee, UK
Proteomic investigation of BAF/PBAF subunit degradation induced by SMARCA2/4 PROTACs

15:55 **Sila Ultanir** The Francis Crick Institute, London, UK

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Chemical genetic methods for kinase substrate identification

16:35 **Dimitrios Anastasiou** The Francis Crick Institute, London, UK Unravelling metabolic vulnerabilities of cancer cells by revisiting a drug's mode of action

17:15 **Closing Remarks** Klaus Rumpel

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Poster Titles

In silico design of an artificial metalloenzyme from an alcohol dehydrogenase

Floriane Martins, Anca Pordea, Rachel L. Gomes, Christof M. Jäger
Bioprocess, Environmental and Chemical Technologies group
University of Nottingham, University Park, NG72RD Nottingham.

Proteomic investigation of BAF/PBAF subunit degradation induced by SMARCA2/4 PROTACs

Nicole Trainor, William Farnaby, Manfred Koegl, Claire Whitworth, Nicola Wiechens, Meng-Ying Wu, Tom Owen-Hughes and Alessio Ciulli
University of Dundee, Dow Street, Dundee, DD1 5EH, Scotland, UK

Eye on chip as an advanced in vitro eye drug evaluation model

Jeong Hun Kim[1,2], Minhwan Chung[3], Somin Lee[3], Byung Joo Lee[2], Kyungmin Son[3], Jin Hyoung Kim[2], Noo Li Jeon[3]

[1]Department of Ophthalmology, Seoul National University College of Medicine, Seoul, Korea;

[2]FARB Laboratory, Clinical Research Institute, Seoul National University Hospital, Seoul, Korea

[3]Mechanical Engineering, Seoul National University, Seoul, Korea

Intravitreal injection of retinoblastoma cells into vitreous cavity of zebrafish for screening of anticancer drugs

Jin Hyoung Kim[1], Dong Hyun Jo[1], Dain Son[2], Seung Hyeok Seok[2], Jeong Hun Kim[1,2]

[1]FARB Laboratory, Clinical Research Institute, Seoul National University Hospital, Seoul, Korea

[2]Department of Microbiology, Seoul National University College of Medicine, Seoul, Korea;

[3]Department of Ophthalmology, Seoul National University College of Medicine, Seoul, Korea

Capture compound® mass spectrometry: Characterisation of target binding and applications in drug discovery

G. Hardman,[1] S. Almond,[1] E. Bush,[1] A. Cridland,[1] S. Dowler,[1] N. Jennings,[1] D. Kenny,[1] I. Linney,[1] N. Macabuag,[1] D. Mitchell,[1] P. Mitchell,[1] J. Huck,[2] E. De Lemos,[2] L. Nelles[3]

[1]Charles River Laboratories, Chesterford Research Park, Saffron Walden, UK

[2]Galapagos SASU, 102 Avenue Gaston Roussel, 93230 Romainville, France

[3]Galapagos NV, Generaal De Whittelaan L11 A3, 2800 Mechelen, Belgium

Protein carbamylation: The discovery of a carbon dioxide control system

Victoria L. Linthwaite, David R.W. Hodgson, Martin J. Cann,
Durham University, South Road, Durham, DH1 3LE 7

Tetrazine-triggered activation of anti-inflammatory drugs

Sarah Davies[a], Luxi Qiao[a], Bruno Oliveira[a], Goncalo Bernardes[a,b]

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b Instituto de Medicina Molecular, Faculdade de Medicina, Universidade de Lisboa, Av Prof Egas Moniz, 1649-028, Lisboa, Portugal

Stabilising protein-protein Interactions: A challenge for ligand discovery

Richard G. Doveston,[*1] Alisha Mohindra,[1] Marta Falcicchio,[1] Sara Chothia,[1] Megan Coulson,[1] Derryn Grant,[1] Ave Kuusk,[2,3] Sebastian Andrei,[2] Christian Ottmann[2], Helen Boyd[3]*

[1]Leicester Institute for Structural and Chemical Biology and Department of Chemistry, University of Leicester, University Road, Leicester, UK, LE1 7RH

[2] Laboratory of Chemical Biology, Department of Biomedical Engineering and Institute for Complex Molecular Systems, Eindhoven University of Technology, The Netherlands

[3]Discovery Sciences, AstraZeneca Research and Development, Gothenburg, Sweden

Design and synthesis of novel PRK2 tools to probe cancer

Fiona Scott[a], Simon E. Ward[a,b], Lewis E. Pennicott[a], Tristan D. Reuillon[a], Kay E. Osborn[a], Ben Wahab[a,b], Hitesh Patel[a], Mihaela-Paula Ficu[a], Jessica A. Downs[c], Jon M. Elkins[d], Angela M. Fala[d]

Sussex Drug Discovery Centre, University of Sussex, Sussex House, Falmer, Brighton, BN1 9QJ, UK 10

Semi-synthetic approaches for studying post-translational modifications

Kirti Sharma and Marina Rubini*

School of Chemistry, University College Dublin, Belfield, Dublin, Ireland

Design, synthesis and evaluation of a diazirine photoaffinity probe for ligand-based receptor capture targeting on GPCRs.

Frederike Müskens[1,2], Richard Ward[2], Helmus van de Langemheen[1], Rob Liskamp[1], Graeme Milligan[2]

[1]School of Chemistry, College of Science and Engineering

[2]Centre for Translational Pharmacology, Institute of Molecular, Cell and Systems Biology, College of Medical, Veterinary and Life Sciences, University of Glasgow, Glasgow G12 8QQ, UK

Gold compounds as Possible Aquaporin-Targeted Therapeutics

Andreia de Almeida[1] and Angela Casini[2]

[1]Tumour Microenvironment Group, Division of Cancer and genetics, School of Medicine, Cardiff University, Tenovus Building, Cardiff CF14 4XN UK

[2]School of Chemistry, Cardiff University, Main Building, Park place, Cardiff CF10 3A, UK

Identifying and utilising a new antileishmanial drug target

Rebecca Charlton[a,b], Christopher Brown[a], John G. M. Mina[a], Bartira Rossi Bergmann[b],

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Patrick G. Steel[a] *and Paul W. Denny*[a]

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[b]Instituto de Biofísica Carlos Chagas Filho, Universidade Federal do Rio de Janeiro, Ilha do Fundão, CEP 21949-900 Rio de Janeiro, RJ, Brazil

Hinokiflavone and analogues: tools for understanding the spliceosome

Lewis J. King (a), Helmi Kreinin (a), Andrea Pawellek (b), Angus I. Lamond (b), Richard C. Hartley (a)

(a)WestCHEM School of Chemistry, University of Glasgow, Glasgow, G12 8QQ, UK

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