19th RSC / SCI Medicinal Chemistry Symposium  
Monday, 11th September 2017

Programme of Flash Poster Presentations  
5.40 to 6.00 pm

1st Development of disulfide-rich peptides as potential drug leads  
Claudia Cobos Caceres, AITHM, James Cook University, Australia P11

2nd Addressing the aqueous solubility challenge by matched molecular pair analysis and collaboration: finding rules to the ‘age-old’ problem  
Alexander Dossetter, MedChemica Ltd, UK P15

3rd VIdentification of low clearance indole acid AMPK activators for the treatment of diabetic nephropathy  
David Edmonds, Pfizer Inc, USA P17

4th Fragment properties and application of FBDD to disrupting the KEAP1:NRF2 interaction  
Charlotte Griffiths-Jones, Astex Pharmaceuticals, UK P23

5th Gaining selectivity within BET bromodomains - development of a chemical probe for the second bromodomain  
Robert Law, GlaxoSmithKline, UK P33

6th Investigating small molecules to inhibit germinal center kinase-like kinase (GLK/MAP4K3) to prevent PKC θ phosphorylation: potential therapy to modulate T cell dependent effector functions  
Tricia May-Dracka, Biogen, USA P39

7th Structure-based rational design of mineralocorticoid receptor antagonists: from non-selective HTS hit to the first macrocyclic nuclear hormone receptor antagonists  
Gavin O’Mahoney, AstraZeneca, Sweden P43

8th A new class of the hedgehog signalling pathway modulators  
Tanja Poljak, Fidelta, Croatia P47

9th The discovery of novel gold(I) complexes for the treatment of gram-positive and gram-negative bacterial infections  
Jonathan Powell, Domainex, UK P49

10th Medicinal chemistry in the time of machine learning: toward a golden age of ADMET predictions?  
Thomas Ryckmans, Roche Pharmaceutical Research and Early Development, Switzerland P51

11th Structure-based optimization of potent and cell active inhibitors of the pVHL-HIF-1α protein-protein interaction  
Pedro Soares, University of Dundee, UK P55

12th Towards reliably predicting solvent-dependent conformational preferences of druglike molecules: the ReSCoSS workflow  
Rainer Wilcken, Novartis Institutes for BioMedical Research, Switzerland P63

13th Discovery of novel, potent and highly selective factor Xla Inhibitors - from HTS to the identification of ONO-3520509 and ONO-9690505  
Chris Yarnold, Evotec UK Ltd, UK P65
Programme of Flash Poster Presentations
4.50 to 5.10 pm

1st  Design, synthesis and pharmacological evaluation of fluorescent ligands as tools for studying cannabinoid type 2 receptor  
Anna Cooper, University of Otago, New Zealand  
P12

2nd  What can be learnt from the testing of over 6 million compounds in antimalarial phenotypic whole parasite high throughput screens?  
James Duffy, Medicines for Malaria Venture (MMV), Switzerland  
P16

3rd  Rational drug design of topically administered caspase I inhibitors for the treatment of inflammatory acne  
Jean-François Fournier, Nestlé Skin Health, France  
P22

4th  Diarylpyrazine as a novel fast acting antimalarial chemotype  
Mercedes García, GlaxoSmithKline, Spain  
P26

5th  Conformationally constrained peptides to inhibit the α/β protein-protein interaction of CK2  
Jessica Iegre, University of Cambridge, UK  
P28

6th  Design and synthesis of potent and selective Calmodulin-dependent Kinase II (CaMKII) inhibitor GS-122  
Dmitry Koltun, Gilead Sciences, USA  
P30

7th  Characterization of the next generation PET tracer 18F-PI-2620 for the assessment of Tau pathology in Alzheimer’s disease and other tauopathies  
Heiko Kroth, AC Immune, Switzerland  
P32

8th  Covalent inhibition prevents Protac-mediated degradation of BTK  
Christopher Tinworth, GlaxoSmithKline / University of Strathclyde, UK  
P34

9th  Discovery of pyrazolo[1,5-a]pyrimidine B-cell lymphoma 6 (BCL6) binders and optimization to high affinity macrocyclic inhibitors  
William McCoull, AstraZeneca, UK  
P40

10th  Discovery of a potent, selective and non-cytotoxic series of inhibitors of Plasmodium falciparum HDACs  
Jesus M Ontoria, IRBM Science Park, Italy  
P42

11th  The NTD drug discovery booster: collaborative virtual screening to boost neglected tropical disease drug discovery  
Benjamin Perry, Drugs for Neglected Diseases initiative, Switzerland  
P58

12th  Macrolide inspired macrocycles as effective disruptors of the IL-17A/IL-17RA interaction  
Dijana Pešić, Fidelta, Croatia  
P46

13th  Development of novel peptide-based Michael Acceptors targeting Rhodesain and Falcipain-2 for the treatment of Neglected Tropical Diseases (NTDs)  
Santo Previti, University of Messina, Italy  
P48