

Welcome to the October SMSdrug.net Newsletter a 6-weekly update on some of the initiatives within the Network. If you would like to highlight any news to our industrial and academic network please contact the network administrator helen.feilden@strath.ac.uk

Unity: An open access, web-based resource for precompetitive drug discovery – A grant application has been submitted to the Wellcome trust for the provision of Unity. The proposal outlines the delivery of Unity, a freely available web-based precompetitive platform that will support drug discovery efforts world-wide. Unity will integrate the 1,000 targets of the [SGC](#) and other Wellcome Trust Centres with medicinal chemists and chemical biologists globally through the 1.2 million compounds within the [EBI ChEMBL](#) database. This ambitious and visionary initiative led by [Blair Johnston](#) will represent one of the major outputs from the Network.

A public-private partnership to unlock the untargeted kinome, Stefan Knapp et al. A manuscript has been accepted for publication in Nature Chemical Biology from members of the Network which proposes a large scale public-private partnership as a new approach which offers economies of scale, minimized redundancy, and sharing of risk and cost to access new chemical probes targeting the kinome. It is hoped that this consortium will deliver chemical probes which are urgently needed to functionally annotate hitherto untargeted kinases and stimulate new drug discovery efforts to address unmet medical need.

Predictive and rational allosteric site identification – The working group will meet again on 5th December 2012 at Edinburgh University. This will follow an Allosteric Workshop taking place on 4th December organised by [Prof. Malcolm Walkinshaw](#) from the Edinburgh [Centre for Translational Chemical Biology](#). The Workshop, sponsored by the British Council, involves an extensive delegation of scientists from Turkey led by [Burak Erman](#), [Koc University](#), Istanbul and will bring together a diverse area of disciplines including Biology, Chemistry, Computer Science, Informatics, Mathematics and Medicine. Within the subsequent working group [Nick Tomkinson](#) and [Simon Mackay](#) will present a draft proposal to the grouping based on the outputs of the members over the summer.

This Newsletter highlights some of the efforts within SMSdrug.net. For more information and full details of our initiatives to bridge the gap between Chemistry and Biology please visit our [website](#), or contact the network administrator helen.feilden@strath.ac.uk

New Students at Strathclyde – Welcome to Tony, Lola, Camille, Chris, Sam and Melissa.

As part of the drug discovery efforts at Strathclyde six new students have joined the team on interdisciplinary projects. Driven by the modelling group within [Strathclyde Institute of Pharmaceutical and Biomedical Sciences](#) efforts in predictive allostery, kinases, informatics, the drug discovery portal, and ChemSpace will be supported by this new team.



Melissa, Sam, Camille & Lola

Dates for Diary:

4th Dec 2012

Allosteric workshop

5th Dec 2012

Predictive and rational allosteric site identification

10th Dec 2012

[Therapeutic strategies targeting the spliceosome](#)

RSC Chemistry Centre, London