

Welcome to the March 2013 SMSdrug.net Newsletter a regular 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

**Establishing an Academic User Network for ChEMBL:
Seminar/Workshop Tour 8-18th April 2013**

SMSdrug.net is supporting a UK wide tour of University Chemistry departments by Dr Louisa Bellis (EBI-EMBL) to Showcase the ChEMBL database.

ChEMBL is a database of over 1 million bioactive drug-like small molecules and contains 2-D structures, calculated properties and abstracted bioactivities. It is an open-access, free resource that is currently used world-wide to aid in drug discovery. To find out more please contact ljbellis@ebi.ac.uk.



Dates of Tour:

Monday 8th April 2013	University of Edinburgh
Tuesday 9th April 2013	University of Strathclyde
Wednesday 10th April 2013	Durham University & Newcastle University
Thursday 11th April 2013	University of Bradford & University of Sheffield
Friday 12th April 2013	University of Birmingham
Monday 15th April 2013	University of Nottingham & University of Warwick
Tuesday 16th April 2013	University of Bath & Cardiff University
Wednesday 17th April 2013	University of Southampton
Thursday 18th April 2013	University of Sussex



Double grant success for Simon Mackay, University of Strathclyde

Of the 1 in 6 men diagnosed with prostate cancer, 1 in 33 will die of metastatic disease. IKK α represents a viable therapeutic target in CRPC which has been vindicated in mouse models of prostate cancer. Through access to a unique matched hormone-naïve and CRPC cohort, Professor Simon Mackay's group (University of Strathclyde) has linked these findings with clinical data to highlight the central role played by IKK α in the development of CRPC and metastasis. Targeting the single IKK α isoform would also bring the benefit of a reduced side-effect profile by avoiding IKK α inhibition. To date, there are no reported selective inhibitors of IKK α .

With funding from Cancer Research UK, the group has generated a potent IKK α selective lead series with selectivity over IKK α that is recapitulated in the cellular environment. They have just been awarded £249,000 and £111,000 from Prostate Cancer UK and MRC to continue the lead optimisation phase of combining desirable ADME properties with potency for in vivo efficacy studies to drive a further round of optimisation to progress towards a first-in-class pre-clinical candidate.

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