Meeting Report

The Smart Laboratory: Towards a national ELN

28-29 July 2011

Chilworth Manor, Southampton, UK

The Smart Laboratory: Towards a national ELN thematic meeting organized by the Lab of the Future theme of the **Dial-a-Molecule** Grand Challenge, took place on the 28th–29th July 2011 in the beautiful Edwardian manor house of Chilworth Manor. It was tackling the often repeated observation that we must capture information on all reactions carried out, not just the most successful, if we are to progress to **'Dial-a-Molecule'**. A big step would be the implementation of an ELN system in academia, which formed the main theme of the meeting. The meeting included showcases from ELN developers, current users of ELN sharing their experience and views on existing systems as well as small group discussions on topics such as a 'wish list' of capabilities of an ELN, how could a national roll-out of ELN's be funded and implemented, how to collect more data with less effort, and store it in a more usable form and more.

The meeting was opened by Prof. Whitby who presented the aims of the **Dial-a-Molecule** Grand Challenge and the objectives of this meeting. The introduction was followed up by the excellent plenary lecture by Dr. Richard Bolton (GSK) who introduced the Pistoia Alliance and their working groups to the attendees underlying the importance of data sharing. There then followed the first of the many talks sharing the experience of current users on ELN presented by Dr. Robin Attrill (GSK) who presented the benefits that ELN brought to the activities of a large pharmaceutical company such as GSK.
These talks were followed by presentations from ELN developers who were supporting the meeting: IDBS, Accelrys, Perkin Elmer (CambridgeSoft) and ACD/Labs. Each of them presented their latest developments on this rapidly evolving market as well as insights into their future plans, providing an excellent introduction for the discussion planned in the afternoon.

The afternoon session was opened by a presentation from open-source ELN developers represented at this meeting by Dr. Simon Coles and Prof. Jeremy Frey (University of Southampton) who presented their plans for The Smart Research Framework: LabTrove, blog3 and LabBroker. The session broke out into small group discussions with each of the ELN developer present at the meeting to answer crucial questions such as: Why has uptake of ELNs in academia been poor?, What features would make adoption compelling?, What other features would we like? and Any problems that would limit adoption?.
The session was closed by Dr. Martin Sweet (EPSRC) who introduced the audience to the new research data policy adopted by EPSRC, introduced on 1 May 2011 with full compliance expected by 1 May 2015.

DAY 1 was concluded by a session of informal discussions around demonstrations stations provided by each of ELN developers which provided an ideal opportunity for delegates to find out and try the products on offer.

DAY 2 was kicked-off by Prof. Whitby who gave a brief review of the discussion from DAY 1. The introduction was followed by an excellent plenary talk from Dr. Brian Brooks (University of Cambridge) on the intelligent fume cupboard project from the research group of Dr. Murray-Rust. The project aimed to find improved ways that computers can help chemists in the lab and explores technologies such as speech recognition, video, infra-red and ultrasonic sensors, touch screens, laser keyboards, etc.
The talk was an excellent starting point for the following small group discussions on equipment and techniques that can help us to get more useful information into an ELN with less effort.
Dr. Dovey (JISC) presented means through which JISC can help universities to modernize and improve their digital infrastructure ensuring that UK remains world-class in research, teaching and learning.
The morning session was concluded by two excellent presentations delivered by Dr. Tim Dickens (University of Cambridge) and Mr. John Leonard (AstraZeneca) giving valuable insights from users that have already adopted

the use of ELNs. They made a compelling case for the adoption of an ELN and, as Dr. Dickens eloquently said: *The question now is not if we should adopt it but rather when and how*.

The afternoon session was entirely dedicated to small group discussions focussed on four main topics: how can an ELN system be financed, what is the best strategy to deploy an ELN system, what disciplines outside of synthetic chemistry should be involved at this stage, and defining a common format for data exchange.

The major outputs from the meeting were to establish a group to lead the development of an open standard for electronic storage of experimental procedures and data, and to work with developers to pilot the use of electronic lab notebooks at selected universities. If you are interested in either initiative please let us know by email at dialamol@soton.ac.uk or contact Prof. Richard Whitby at rjw1@soton.ac.uk .