Enhancement of Research Infrastructure

ISSF has supported our strategy to have innovative core facilities in key research areas and to develop computational and informatics resources that underpin our biomedical research.

Project Title - "Software Developers - PEP TRACKER - Scientific data platform containing tools for management, visualisation and analysis of quantitative information."

ISSF has supported investment into our research infrastructure, including software development posts within our Laboratory of Quantitative Proteomics, led by Professor Angus Lamond. These positions have pioneered the development of a unique new Laboratory Information Management System (LIMS), called ‘Data Manager’ (see; www.peptracker.com). This incorporates user-led design and state of the art computational technologies for handling complex, large data sets, incorporating business intelligence strategies for big data analytics. This system enables the proteomics facility to effectively and efficiently manage sample collection and user communication, thereby supporting a wide-range of research activity across the University. For example, it allows users to monitor experimental progress using the live-tracking capabilities.

The Data Manager system provides the means to conveniently and systematically capture and store detailed descriptions for metadata, raw data and interpreted results for all experiments performed in the laboratory. This information is fully searchable and available to users via a user-friendly, web based interface. The search features are powerful, fast and scalable to very large and complex datasets.

The PepTracker Data Manager software thus adds great value to all of the data collected from laboratory experiments.

First, it allows interactive data exploration and the efficient cross analysis of datasets generated under either similar, or different, conditions. This facilitates answering broad ranging questions by combining information from as many sources as possible. Second, it ensures that we have detailed, secure and easily accessible records of exactly how each data set was generated and how each experiment was performed. This adds value by helping us to optimize workflows and establish ‘best practice’ and SOPs for many types of analyses. It also means that we can recover the requisite experimental information from work carried out previously by students and researchers who have left the University, should their work need to be repeated or checked in future. This adds value by helping to ensure the reproducibility and accuracy of work carried out in the University.

A custom version of the PepTracker Data Manager LIMS software is now being deployed at the Stoller Biomarker Discovery Centre at the University of Manchester and has helped forge key links between these two leading UK proteomics facilities.

Going forward, these posts will help aid the development of further computational and bioinformatics resources that will provide novel ways of managing, visualising and analyzing ‘big data’ in the field of quantitative, mass spectrometry-based proteomics and beyond. By building a suite of inter-linked software modules, the aim is to provide the analytical tools for effective open access sharing of complex, large-scale mass spectrometry data via user-friendly, searchable online databases.