MS44-05 **xtalPiMS: A tool for managing your crystallization experiments.** Edward John Daniel, Rikkert W. Wierenga[a] Jonathan M. Diprose, Ian M. Berry, Robert M. Esnouf, David I. Stuart,[b] Gael Seroul, J. Marquez, [c] D. deVries, A. Perrakis, [d] L. Launer, M. Walsh, [e] S. L. Griffiths, K. Wilson, [f] A. Pajon, [g] B. Lin, C. Morris,[h] *[a]University of Oulu, Finland, [b]Oxford Protein Production Facility, University of Oxford, UK, [c] EMBL Grenoble, France, [d] Netherlands Cancer Institute, The Netherlands, [e] European Synchrotron Radiation Facility, Grenoble, France, [f] York Structural Biology Laboratory, University of York, UK, [g] European Bioinformatics Institute, Hinxton, UK, [h] STFC Daresbury Laboratory, UK*
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xtalPiMS is a tool for managing crystallization experiments, and in particular the large numbers of images that can be produced by automated imaging systems. xtalPiMS is built on top of the Protein Information Management System (PiMS), a laboratory information management system for protein production. xtalPiMS groups images taken from particular plates at particular times into "inspections". It adds specialized and intuitive interfaces to PiMS for finding plates and inspections, and a viewer that allows scientists to rapidly scan through the set of images in an inspection. Each image can be scored from a drop-down menu or using keyboard shortcuts. xtalPiMS is optimized for 96-well plates but is capable of handling plates of different sizes and also multiple crystallization trials per well. xtalPiMS is installed in the Oxford Protein Production Facility (OPPF) and the University of Oulu, where it has been integrated with automated imaging systems from Formulatrix. xtalPiMS manages >65,000,000 crystal trial images from > 25,000 trial plates in the OPPF. xtalPiMS underpins the OPPF's new facilities in the Research Complex at Harwell, adjacent to Diamond. Like PiMS, xtalPiMS is a web-based application that runs on widely-available open source software. xtalPiMS is accessed using a web browser, typically requiring no additional software to be installed on the client. xtalPiMS is available under the same terms as PiMS. To try xtalPiMS, visit http://pimstrak1.dl.ac.uk:8080/xtal/loginhome.jsp (user name "demo", password "demo").

Keywords: software; imaging; computer programs

MS45-01 **New structural insights into the sodium pump.** Linda Reinhard,[a] Maria Nyblom,[ab] Jonas Lindholt,[a] Janne Petersen,[c] Pontus Gourdon,[a] Bente Vilsen,[c] Poul Nissen,[a] *[a]Department of Molecular Biology and Genetics, Aarhus University, Denmark, [b]Novo Nordisk A/S, Maalov, Denmark.[c] Department of Biomedicine, Aarhus University, Denmark.*
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The sodium pump is a P-type ATPase of enormous physiological significance. Over the last years, in our group three crystal structures of the sodium pump in different functional states have been determined [1, 2; Nyblom*et al.*, to be published]. However, during the structure solution procedure the "typical problems" in membrane protein crystallography have to be faced and solved, including severe anisotropy of the data, phasing and model building at low resolution. A selection of examples from our laboratory will be given, including optimization of diffraction properties through re-lipidation using the HiLiDe method [3] or expanded low-resolution molecular replacement and phasing approaches [4]. As one example, the structure solution procedure and structural details of the sodium pump in the sodium bound E1 state at a resolution of 4.3 Ĺ will be presented [Nyblom *et al.,* to be published].

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