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Keywords: phase refinement; methods development; automatic structure solution

FA1-MS12-O4

APLx–Automated Protein-Ligand Crystallography Workflow. Romeu Pieritz[a], Leonard Leonard[a], Sean McSweeney[a]. [a]*European Synchrotron Radiation Facility, Grenoble, France.*
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Fragment-based approaches is a new paradigm for small-molecule drug discovery. The methodology is complementary to high-throughput screening experiments performed on modern X-ray facilities. The APLx project aims to develop an automated system to be used during the MX experiment for online data analysis. The system is designed to control and analyse the workflow to promote structure determination and screening inhibitors from a library of synthetic compounds. The first prototype executes in parallel for different data sets molecular replacement, structure refinement and ranks the structures obtained based on the "Rfree" index. The prototype is used to analysis the data during the MX experiment and can help the scientist to decide what it is the best data set for further studies. The automated workflow is used on the ESRF Macromolecular crystallography beamlines and results presented show the overall performance of the system. When completed the systematic use of this parallel workflow during the MX experiment will decrease the overall time to obtain a valid molecular structure including bound ligands. This research is funded by the SOUTH Consortium - 6th Framework Programme of the European Commission (LSH-2005-2.1.1-4).

Keywords: computational analysis of crystallographic data; automation; protein ligands

FA1-MS12-O5

Proteopedia: Scientific Wiki Bridging 3D Structure-Function. Joel L Sussman[a,b], Eran Hodis[c], Israel Silman[a,d], John Moult[f], Eric Martz[g], Jaime Prilusky[a,e]. [a]*The Israel Structural Proteomics Center.* [b]*Depts of Struct Biol.* [c]*Comp Sci & Applied Math,* [d]*Neurobiol.* [e]*Bioinformatics Unit, Weizmann Inst, Rehovot, Israel.* [f]*Center for Adv Res in Biotech, U MD Biotech Inst, Rockville, MD.* [g]*Dept of Microbiol, U MA, Amherst, MA.*
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Rather than relying on printed text to provide the understanding of biomacromolecular structures, a collaborative website called *Proteopedia* provides a new resource by linking written information and 3D structural information [1]. *Proteopedia* displays protein structures and other biomacromolecules interactively. These 3D interactive images can be rotated and zoomed, and are surrounded by text with hyperlinks that change the appearance of the 3D structure to reflect the concept explained in the text. This makes the complex structural information readily accessible and comprehensible, even to non-structural biologists. Using *Proteopedia*, anyone can easily create descriptions of biomacromolecules linked to their 3D structures, *e.g.*:
(a) Proton Channels:
http://proteopedia.org/wiki/index.php/Proton_Channels
(b) HIV-1 protease:
http://proteopedia.org/wiki/index.php/HIV-1_protease (c) *Beta*-adrenergic receptor:
http://www.proteopedia.org/wiki/index.php/A_Physical_Model_of_the_β2-Adrenergic_Receptor
Aside from content added by the hundreds of registered users of *Proteopedia*, pages on each of the more than 56,000 entries in the PDB have been automatically created, and are primed for expansion by users. Members of the scientific community are invited to request a user account to edit existing pages and to create new ones. An account can be obtained from the homepage at http://www.proteopedia.org

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Keywords: molecular computer graphics; journal publication; computer-aided education