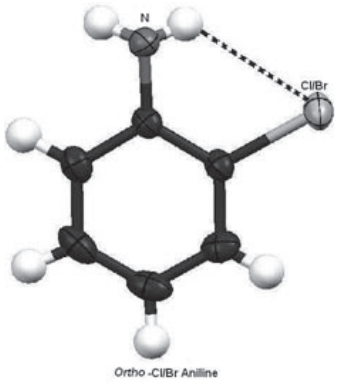
lattices and establishes that indeed fluorine has a directing influence in molecular assembly. In order to evaluate the propensity of interactions in halogens in general *ortho* chloro and *ortho* bromo anilines were crystallized from their respective liquids via *in situ* cryocrystallization method. The crystal structures are isostructural belonging to a trigonal system, space group $P\,3_1$. The crystal packing is due to intramolecular N-H…Cl or Br and intermolecular N-H...N hydrogen bonds. However, in the case of *ortho* bromo aninline short Br...Br contacts (3.64 Å) are observed suggesting that this interaction is a consequence of the size of Br atom.



Ortho -Cl/Br Aniline

1. Deepak Chopra and T. N. Guru Row,*Journal of the Indian Institute of Science*, 2007,**87**, 167

Keywords: cryocrystallography, *in-situ* structure determination, intermolecualr interactions

P01.15.77

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Relation of DLS distribution of protein samples with thermal stability

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With the rise of ultimate methods such as X-ray crystallography and NMR, the number of proteins, of which complete quaternary structure was confirmed, has rapidly increased. To be analyzed by X-ray spectroscopy, protein purification is very important to evaluate the detail of its structure. Sample separation is often used by gel permeation chromatography and it's been checked by poly acrylamide electrophoresis, such as SDS-PAGE, however it is required for crystallography to be purified as a level of quaternary structure of proteins. So we often use the system of dynamic light scattering (DLS). It is expected that protein quality is accepted by result of the DLS distribution below 20% for crystallography, but it's not always. Various kinds of proteins have various kinds of strutures and stiffness for thermal stability, and DLS distribution depends on the aspect ratio of particle or stiffness of the surface. In this study, we discuss relation of DLS distribution of proteins with thermal stability and other factors.

Keywords: dynamic light scattering, polydispersity, protein stability

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Microseed matrix screening: A modified version

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The crystallization of purified proteins has remained one of the bottlenecks for the determination of protein structures by X-ray diffraction methods. The crystallization process can be considered composed of two sequential processes. The first is an initial nucleation step and the second subsequent growth of crystal nuclei to well ordered crystals. A method that influences the first step of this process "Microseed Martix Screening" has recently been published. The method is further development of the work by Ireton and Stoddard [2] aims at influencing the nucleation event in crystallization screens. We report the implementation of and experience of with this method in our laboratory. The seed-bead method is used for preparation of the seed stocks. The protein, reservoir solution and seed stock are pipetted simultaneously using a three-bore dispensing tip mounted on the Oryx 8 robot (Douglas Instruments), setting up screening crystallization experiments with seed stock solution added. The authors of [1] used the method with 5 test proteins and observed that the number of crystals hits increase from 1-9 to 21-63. We have also observed an increased number of crystal hits, but that include both protein crystals ad nonobvious salt crystals. Salts crystals can lead the crystallization experiments astray and consume valuabe time and sample. We have therefore modified the method to inlude two control experiments: 1) Crystallization experiments with the Izit Dye for positive indentification of protin crystals and 2) Crystallization experiments with protein buffer for positive identification of salt crystals.

1. Allan D'Arcy, Frederic Villard and May March Acta Cryst. (2007) D63, p550-554
2. G.A., Ireton and Barry L. Stoddard Acta Cryst (2004) D60, 601-605.

Keywords: crystallization strategies, microseeding, protein crystallization

P01.12.79

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An open and flexible robotic system designed towards autonomous protein crystal harvesting

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Process automation with robotic mounting equipment has become an essential element of modern crystallography facilities, resulting in efficient utilization of valuable X-ray resources. However, serious rate-limiting manual operations persist in the crystal harvesting process. Based on experience gained during development of an operator-assisting universal micromanipulation robot (UMR) prototype, we discuss progress and challenges ahead for the design of a fully autonomous, integrated system capable of reliable harvesting of protein microcrystals. Harvesting of micron-sized objects requires a sophisticated mechanical system, and autonomy means that a capable real-time machine vision system embedded in powerful control software must be developed. The vision system and the mechanical system interact in a complex way, and the demands on the optical system pose additional and formidable design challenges. Real time image processing interfaced with mechanical control and

feedback are at the cutting edge of technology, and the conceptual design of autonomous systems represents a research frontier in mechatronics. We expect that the current operator-assisting UMR will evolve into a system endowed with progressively increasing autonomy capable of significantly increasing reliability of protein micro-crystal harvesting and reproducibility of cryo-cooling. In addition, advanced micro-manipulation robotics will open the field to new science and emerging crystallization technologies of far reaching impact. Major improvements in operational precision have given the UMR the capability of manipulating crystals significantly smaller than 10 microns thus facilitating nano-crystallization, harvesting from micro-fluidics, nano-diffraction techniques and novel seeding strategies.

Keywords: robotic crystal harvesting, cryotechniques, automation

P01.15.80

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Facilitating low volume protein crystallography set-ups using the mosquito® liquid handler

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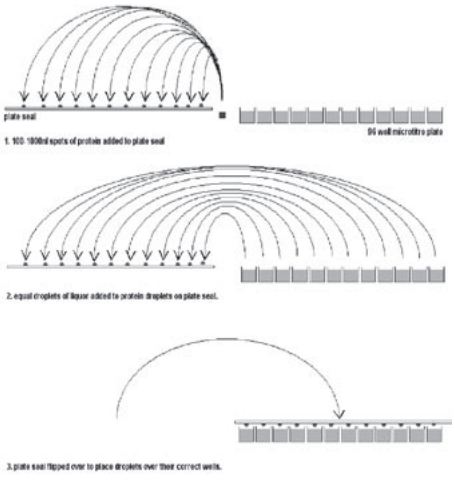
A prerequisite for efficient high throughput protein crystallisation screening is the accurate pipetting and positioning of the low volume drops used in hanging and sitting drop setups. Screening the many different conditions under which a protein crystal may form lends itself to automation, since it requires hundreds of similar experiments to be set up to find the few 'hits'. Automated solutions exist for low volume pipetting, however, the variable viscosities of protein and reservoir/screen solutions present significant challenges for many liquid handling systems. Another challenge is that of drop positioning. The mosquito® (TTP LabTech) offers fast positive displacement pipetting for accurate and reproducible aspiration and dispensing throughout the 50 nL - 1.2 μL range, producing CVs of < 8% at 50 nL irrespective of viscosity. This, plus its columnar arrangement of pipettes, allows it to automate hanging drop as well as sitting drop set-ups. Mosquito's micropipettes are also disposable, thus guaranteeing zero cross-contamination where required.



Keywords: protein crystallization, robots, laboratory automation

P01.02.81

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A simplified unified approach for animations and movies using SBEVSL

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RasMol, Jmol, and PyMol, and many other molecular graphics programs are used to produce animations and movies. Each program takes a different approach making it necessary to use different commands and scripts when moving among programs, thereby making the development of lectures and tutorials more complex than necessary. The Structural Biology Extensible Visualization Scripting Language (SBEVSL) project is developing a common scripting language to access the common features of several molecular graphics packages. For some uses, the scripting language can be used as a black box, much the way we use Postscript for text documents, but, where feasible, SBEVSL is designed to be comprehensible to scientists by using simple menu-click-like commands and reasonable defaults. RasMol, PyMol and Jmol are being given "native" SBEVSL support and external translators will allow the approach to be applied to other packages, such as CCP4mg. For movies and animations the very useful but somewhat cryptic Jmol "moveto" command will be provided, but the SBEVSL version will be based on simple selection and recording of benchmark images using commands based on the PyMOL mset command combined with both time window and frame range based morphing. This work is part of the combined efforts of the SBEVSL groups at Dowling College and Rochester Institute of Technology. The people at Dowling are: Isaac Awuah Asiamah, Darina Boycheva, Georgi Darakev, Nikolay Darakev, John Jemilawon, Nan Jia, Petko Kamburov, Greg McQuillan, Daniel O'Brien, Georgi Todorov, Herbert J. Bernstein. The people at RIT are: Scott E. Mottarella, Brett Hanson, Charles Westin, Corey Wischmeyer, Paul A. Craig.
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Keywords: animation, graphics, script

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Remote data collection and rapid scheduling at the Molecular Biology Consortium beamline ALS 4.2.2

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The Molecular Biology Consortium consists of academic institutions throughout the USA and Taiwan. The cost of making regular synchrotron trips to the Advanced Light Source in Berkeley is not trivial and Beamline 4.2.2 initially addressed this issue with the addition of Service Crystallography. Since February of 2007 the MBC has also offered full remote collection capabilities and this has significantly improved access to the beamline. A Rigaku ACTOR sample mounting system is at the heart of remote operations and has been integrated into the Blu-Ice collection interface. Onsite computers installed with NX server software allow users to connect remotely via free client software. Sample mounting, exchanges,