

completely included in the dimerization surface.

Furthermore, we carried out a variety of physicochemical measurements (ITC, DLS and the analytical ultracentrifugation) to elucidate the functional aspects of the multimerization property of Rch1. As a result, we found out a valid correlation between the multimerization state of Rch1 and its NLS recognition property, where the IBB domain of Rch1 plays a role to control the multimerization. More detailed scenario about the NLS recognition mechanism of the Rch1 will be presented in the poster session.

[1] N. Okazaki, K. Hasegawa, G. Ueno, H. Murakami, T. Kumasaka, M. Yamamoto. *J Synchrotron Radiat.* **2008** *15*, 288-291.

Keywords: importin- α

MS23.P01

Acta Cryst. (2011) **A67**, C352

Recent practices on sulfur SAD phasing using soft X-rays

Zhi-Jie Liu, National Laboratory of Biomacromolecules, Institute of Biophysics, Chinese Academy of Sciences, Beijing, (China). E-mail: zjliu@ibp.ac.cn

A single crystal X-ray diffraction data set contains critical three-dimensional structural information about the molecules which make up the crystal. This information is the major direct experimental source for the subsequent elucidation of spatial structures of the crystallized molecules.

In recent years, single wavelength anomalous diffraction (SAD) phasing has become the major method used in macromolecular structure determination. Sulfur atoms are natively present in most protein molecules and their anomalous scattering signal when measured with soft X-rays makes them an ideal phasing probe. With the advances in methodology and diffraction data collection hardware, sulfur SAD phasing has contributed to many *de novo* crystal structure determinations. We have been actively trying this phasing method in routine crystal structure determinations. Several new structures have been determined by the S-SAD method with the data collected using either home lab Cr X-rays or synchrotron X-rays (Photon Factory beamlines 1A and 17A). Details of the data collection, data processing and phasing process will be presented.

Keywords: S-SAD, soft X-rays

MS23.P02

Acta Cryst. (2011) **A67**, C352

Multivariate methods for density modification of SAD phased maps

Pavol Skubak, Willem-Jan Waterreus, Navraj S. Pannu. *Department of Biostructural Chemistry, Leiden University, Leiden (The Netherlands)*. E-mail: p.skubak@chem.leidenuniv.nl

Recently, we have derived and implemented a multivariate likelihood distribution for phase combination of density modified phases with initial SAD experimental phases [1] and a technique to reduce bias in the phase combination process [2].

Preliminary results suggest that the power of these methods can be further improved by incorporation of structure factors from a partially built model into the SAD multivariate function.

The new function is used for simultaneous refinement and density modification which is iterated with automated model building.

Many structures can be built automatically by the Crank software suite [3] that previously failed thanks to the combination of these new methods.

[1] P. Skubak, W.-J. Waterreus, N.S. Pannu. *Acta Cryst.* **2010**, *D66*, 783-738.
[2] P. Skubak, N.S. Pannu. *Acta Cryst.* **2011**, *D67*, 345-354. [3] N.S. Pannu, W.J. Waterreus, P. Skubak, I. Sikharulidze, J.P. Abrahams, R.A.G. de Graaff. *Acta Cryst.* **2011**, *D67*, 331-337.

Keywords: density modification, model building, refinement

MS23.P03

Acta Cryst. (2011) **A67**, C352

Phasing in the Home Laboratory

Joseph D. Ferrara, Pierre Le Magueres, Michael Murray, James W. Pflugrath, Cheng Yang. *Rigaku Americas Corp. 9009 New Trails Drive, The Woodlands, TX, 77381 (USA)*. E-mail: joseph.ferrara@rigaku.com

Many examples of S-SAD and Se-SAD phasing have been reported with diffraction data collected away from absorption edges with copper radiation (1.54 Å) as well as at the K absorption edge of selenium with synchrotron radiation (0.979 Å). Chromium radiation (2.29 Å) has been available for in-house data collection for a few years now. As a result, a number of successful SAD experiments using Cr radiation have been performed by several groups [1], [2]. Furthermore, unpublished results from the PDB [3] indicate a higher utilization than the publication record shows. However, Cr radiation has not been fully utilized despite being ideally suited for measuring anomalous signals from weak anomalous scatterers such as sulfur, selenium, calcium, and other atoms commonly found in protein crystals.

We explore why softer X-rays generated by a Cr anode may be better than a synchrotron source. Beam stability, radiation damage, and mechanical issues are less of a problem with in-house experiments. The human psychology of travel and use of an unfamiliar experimental station may also be avoided with an in-house system. This is a cost effective method of single crystal X-ray diffraction data collection and structure determination that is especially useful when time is of the essence and synchrotron time is unavailable due to shutdowns and maintenance. In the end the tortoise may win the race.

With the addition of Cr radiation to the crystallographer's toolkit, in-house X-ray sources can routinely provide at least two wavelength options. This report also discusses the results of phasing by combining diffraction data from both Cu and Cr-collected data sets, as well as data sets collected with only Cu radiation.

[1] L. Chen, L.R. Chen, X.E. Zhou, Y. Wang, M.A. Khsai, A.T. Clark, S.P. Edmondson, Z.J. Liu, J.P. Rose, B.-C. Wang, E.J. Meehan, J.W. Shriver, *J. Molecular Biology* **2004**, *34*, 73-91. [2] N. Watanabe, Y. Kitago, I. Tanaka, J. Wang, Y. Gu, C. Zheng, H. Fan, *Acta Crystallographica* **2005**, *D61*, 1533-1540. [3] F.C. Bernstein, T.F. Koetzle, G.J.B. Williams, E.F. Meyer Jr., M.D. Brice, J.R. Rodgers, O. Kennard, T. Shimanouchi, M. Tasumi, *J. Molecular Biology* **1977**, *112*, 535-542.

Keywords: sulfur, SAD, phasing

MS23.P04

Acta Cryst. (2011) **A67**, C352-C353

Structural studies of serine acetyltransferase 1 from *Entamoeba histolytica*