HT Structure Determination at SER-CAT: Five Structures in 23 Hours

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Researchers at the University of Georgia (UGA) have developed an optimizing, high throughput structure determination pipeline (SCA2Structure) capable of providing fitted or partially refined structures in a matter of hours from anomalous scattering (MAD or SAD) data [1]. This powerful structure determination engine coupled with the excellent data collection facilities provided by the SER-CAT, beamlines at the Advanced Photon Source (www.ser-cat.org) provides the basis for high-throughput structure determination.

Using prescreened crystals and data collected at SER-CAT, UGA researchers were able to determine five SAS structures on-site during a recent 24-hour run. Data were processed at SER-CAT and input to the SCA2Structure pipeline running on a Linux cluster at UGA via the web. The average total time for data collection and structure determination was 191 minutes. The structures solved represented an average mix of structural genomics targets with molecular weights ranging from 12 - 25 kDa. Details of the experiments will be presented. Work supported in part with funds from the NIH (GM62407), The Georgia Research Alliance and The University of Georgia Research Foundation.

[1] Liu, et al., *Acta Cryst*., 2005, D**61,** *in press*.

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