

W0227

High-Throughput Structure Determination: Exploring Different Software Paths. Joseph S. Brunzelle, W.F. Anderson, Northwestern Univ., Chicago, IL, USA.

The demands on high-throughput crystallography are continually growing and the number of software packages and version releases are growing too. Through the utilization of the Automated Crystallographic System, AcrS[1] a series of 40 different protein targets were systematically tested. The targets varied in diffraction resolution limits, space groups, the identity and number of anomalously scattering atoms, and the number of wavelengths. The following programs: CNS[2], SOLVE[3]/RESOLVE[4], AutoSHARP[5], HYSS[6], SHELXD[7], and ARP/warp[8] were tested with each of the 40 different proteins. The results from each experiment were warehoused in a relational database to allow quick data analysis and displayed via web-interface and downloadable CIF formatted files. The results clearly show program strengths and how to best combine different programs.

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3. Terwilliger & Berendzen. (1999). *Acta Cryst.* D55, 849-61.
4. Terwilliger (2001). *Acta Cryst.* D57, 1755-62.
5. delaFortelle & Bricogne, (1997) *METHOD ENZYMOL.* 472-494
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7. Schneider & Sheldrick. (2002). *Acta Cryst* D58, 1772-1779.
8. Perrakis *et al.* (1997). *Acta Cryst.* D53, 448-455.