

E0075

Structure Solution for SF-1 by Combined SAD Phasing from the Sulfur Anomalous Signal with Molecular Replacement. K. Madauss*, C. Yang, D. Juzumiene, S. Williams*, and J. D. Ferrara, Rigaku/MSD, Inc., 9009 New Trails Drive, The Woodlands, TX 77381, *GlaxoSmithKline Inc., 5 Moore Drive, RTP, NC 27709.

Anomalous scattering with soft X-ray radiation opens new possibilities in phasing for macromolecular crystallography. In cases, where sulfur SAD phasing is not sufficient for *ab initio* building, it could be used in conjunction with existing information to solve structures.

The experimental phase information obtained from anomalous sulfur scattering was combined with molecular replacement to solve the structure of the ligand binding domain of the orphan nuclear receptor SF1. The SF1 crystals obtained were in the space group $P2_1$, with seven molecules per asymmetric unit and 16 sulfur atoms per molecule. Crystals diffracted to 2.7 Å on the in-house chromium source, and 360 degrees of data were used to produce the final data set. Sulfur atoms were identified using AUTOSHARP, and SHARP was used to calculate and improve the phases. The final maps showed the molecular outlines, but were not amenable to tracing. Real space correlation using FFEAR with a homologous search model identified the position and orientation of one of the subunits, which was then fixed and used in conventional molecular replacement to find 5 of the remaining 6 subunits.