

## W0240

**S-SAD, Se-SAD and S/Se-SIRAS using  $\text{CuK}_\alpha$  Radiation.** P. Lynne Howell<sup>1,2</sup>, Christopher T. Lemke<sup>1,2,4</sup>, G. David Smith<sup>1,3</sup>, <sup>1</sup>Structural Biology and Biochemistry, Hospital for Sick Children, 555 University Ave., Toronto, Ont. CANADA, <sup>2</sup>Dept. of Biochemistry, Univ. of Toronto, Ont., CANADA, <sup>3</sup>Hauptman-Woodward Medical Research Inst., 73 High St., Buffalo, NY, 14203, USA. <sup>4</sup>Present address: Boehringer Ingelheim (Canada) Ltd., 2100 Cunard St., Laval, Quebec, CANADA.

The structure of *E. coli* argininosuccinate synthetase (EAS) has been determined using S-SAD, Se-SAD and S/Se-SIRAS data measured with  $\text{CuK}_\alpha$  radiation. EAS contains 16 methionines and 3 cysteines in 455 amino acids. At a wavelength of 1.54 Å the native (S-Met) and derivative (Se-Met) proteins yield anomalous signals of approximately 0.86 % and 1.6 %, respectively. Highly redundant data were measured to 2.0 Å from native and derivative EAS crystals. All three structure determinations were carried out in a highly automated manner using *SnB* and SOLVE/RESOLVE. Despite the minute Bijvoet differences at 1.54 Å, the signal was sufficient to determine the heavy atom substructure and produce high quality electron density maps in all three cases. These maps were readily interpretable by the RESOLVE automated building algorithm, which modeled greater than 75% of all three structures. The strategies and protocols used to solve the structures, and lessons learned will be discussed.