maps, and only four residues were incorrectly identified; three of these residues were subsequently found to be seriously disordered while the fourth suffered from high thermal motion. The structure has been refined to a residual of 0.160 for 512 protein atoms, 112 water molecules, and 418 protein hydrogen atoms. A mean phase error of 19.1° was calculated for the difference between the *SnB* phases and the final refined phases. It is estimated that given the sequence, 88% of the backbone atoms and 30% of the side chain atoms could have been extracted from the initial *SnB* phase set. Research supported by NIH grant GM-46733 and NSF grant IRI9412415.

MS02.06.08 THE AB INITIO SOLUTION OF THE HALORHODOPSIN AND OMP F PORIN MEMBRANE PROTEINS AT 6Å FROM ELECTRON DIFFRACTION PROJECTION DATA USING THE MAXIMUM ENTROPY-LIKELIHOOD METHOD IN THE MICE COMPUTER PROGRAM. C.J.Gilmore, W.N.Nicholson Department of Chemistry, University of Glasgow, Glasgow G12 8QQ, Scotland U.K. and D.L.Dorset, Electron Diffraction Department, Hauptman-Woodward Institute, 73 High Street, Buffalo, New York 14203, U.S.A.

Using the combination of maximum entropy and likelihood (Bricogne (1984) Acta Cryst. A40, 410-445) in the MICE computer program (Gilmore, Bricogne & Bannister (1990) Acta Cryst. A46, 297-308), an ab initio phase determination was carried out at low resolution (6Å) for two dissimilar membrane proteins, the Omp F porin from the outer membrane of E. coli (which is largely beta-sheet) and halorhodopsin (which is largely alpha-helix). Surprisingly for a structure of this complexity and at this resolution, accurate phase information was found for the most likely solutions which enabled potential maps to be calculated that contained most of the essential structural details at 10Å resolution of these macromolecules in projection without the need for any image derived phases. The mean phase errors for the porin structure were less than 10°, whilst those from halorhodopsin were less than 20°. The calculations were remarkably easy using the MICE program more or less in default mode. A comparison with the use of the Sayre equation and phase annealing as an *ab initio* phasing procedure is made. (Dorset (1995). Proc. Natl. Acad. Sci. USA 92, 10074-10078, Dorset, Kopp, Fryer & Tivol (1995) Ultramicroscopy **57**, 59-89.) Both methods have their strengths and weaknesses which will be discussed.

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PS02.06.09 APPLICATION OF THE SAS TANGENT FORMULA TO MULTIPLE SITE PROBLEMS: A FEASIBILITY STUDY. Chun-Shi Chang, Charles M. Weeks, Debashis Ghosh, Herbert A. Hauptman, Hauptman-Woodward MRI, 73 High Street, Buffalo, New York 14203-1196, USA

The SAS tangent formula [Hauptman, *Acta Cryst.* A, in press] provides the basis for an *ab initio* multisolution (or multitrial) phasing procedure which utilizes invariant values estimated from SAS data [Hauptman (1982) *Acta Cryst.* **A38**, 632-641]. This procedure has been tested by application to 2Å single-wavelength, error-free data for a fabricated 10 Se analog of cucumber basic protein [Guss *et al.* (1988) *Science*, **241**, 806-811]. Se isotropic thermal parameters in the range 6.7-25.5Å^2 were based on the average side-chain values in the real structure, and Se anomalous scattering factors (f', f'') of (-7. 623, 5.083) at 0.9789Å were used.

Trial sets of random phases were refined iteratively until the corresponding values of the SAS maximal function converged, and solutions were identified on the basis of mean phase error. Nonsolutions consisting of part of the protein structure having the correct hand combined with enantiomorphic positions of the anomalous scatterers occurred frequently and had SAS maximal function values similar to solutions. In addition, under some circumstances trials yielding no locations for anomalous scatterers had even higher maximal function values. In either case, solutions could be detected automatically by picking the top 10 peaks on a Bijvoet difference Fourier and then computing protein phases based on these positions and comparing them to the corresponding original set of SAS tangent phases. Solutions had the smallest mean phase differences and, in this way, the proper absolute configuration could be selected. The SAS tangent solutions compared favorably to maps phased by the 10 Se placed at their true positions and given precisely correct thermal parameters. This research was supported by GM-46733 (NIH).

PS02.06.10 LOW RESOLUTION AB INITIO ENVELOPES OF YEAST RNA POLYMERASE II. David, P. R., Bushnell, D. A., Leuther, K. K., Subbiah, S., Bellamy, H. and Kornberg, R. D, Structural Biology Dept. Stanford University Medical Center MS 5400 Stanford, CA, 94305-5400 USA

Low resolution ab initio envelopes for yeast RNA polymerase II, an enzyme complex of 550,000MW, have been computed, using the condensing protocol methods. These envelopes show the packing within the unit cell and a strong similarity to the existing envelopes from two dimensional electron microscopy. The special methods used to obtain the lowest resolution reflections for such a large protein and assymmetric unit will be discussed. Despite the large size of the protein, envelopes can be calculated easily in a matter of minutes.

PS02.06.11 DIRECT-METHOD STRUCTURE DETERMINATION OF THE NATIVE AZURIN II PROTEIN USING ONE-WAVELENGTH ANOMALOUS SCATTERING DATA. Q. Hao, Department of Applied Physics, De Montfort University, Leicester LE1 9BH, England; Zheng Xiao-feng & Fan Hai-fu, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China; F. E. Dodd & S. S. Hasnain, CCLRC Daresbury Laboratory, Warrington WA4 4AD, England.

The one-wavelength anomalous scattering (OAS) X-ray diffraction data of azurin II, a copper-containing protein from *Alcaligenes xylosoxidans* were collected at the Photon Factory at a "routine" wavelength of 0.97Å. The structure had been originally solved by the molecular replacement method (Dodd, Hasnain, Abraham, Eady & Smith (1995) *Acta Cryst.*, **D51**, 1052-1064). As a technique of *ab initio* structure determination, the direct method (Fan, Hao, Gu, Qian & Zheng (1990). *Acta Cryst.* **A46**, 935-939) was attempted to break the phase ambiguity intrinsic to one-wavelength anomalous scattering data. The phases were then improved using the solvent-flattening method. The final electron-density map clearly shows most Cα positions and many side chains and it is traceable without prior knowledge of the structure. It is concluded that the direct method is capable of phasing anomalous scattering data collected at one wavelength from moderate sized native proteins (Mw ~ 20kDa) which contain copper or atoms with a similar scattering power.