

E0030

Automated Applications of *BnP*. I. Methodology. W. Furey¹, L. Pasupulati¹, S.A. Potter², H. Xu², R. Miller^{2,3}, & C.M. Weeks², ¹VA Med. Center, Pittsburgh PA & Dept. Pharmacol., U. Pittsburgh, ²Hauptman-Woodward Inst., Buffalo NY, ³Center for Comp. Res., SUNY at Buffalo.

BnP is a protein structure determination package with a graphical user interface. The interface controls and runs processes required for the complete solution of protein crystal structures in a point-and-click manner. *BnP*'s main function is to couple the direct-methods program *SnB*, used to determine heavy atom/anomalous scatterer substructures, with the protein-phasing package PHASES, used to determine and refine protein phases. It also serves as an interface passing results to other popular packages used for map fitting and structure refinement. In addition to seamlessly interfacing the various packages, a high degree of automation is implemented such that one needs only to specify a few parameters, and the entire phasing process starting with diffraction data and resulting in interpretable electron-density maps is carried out by clicking a single button. With only a few more button clicks, one can graphically examine the statistical results and maps, or carry out skeletonization and automated chain tracing with map fitting. The overall strategies and methodology employed will be described, with emphasis on those aspects required to facilitate automation. This work was supported by NIH grant EB002057.