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Automated Applications of *BnP*. II. Test Results. C.M. Weeks¹, S.A. Potter¹, H. Xu¹, R. Miller^{1,2}, L. Pasupulati³ & W. Furey³, ¹Hauptman-Woodward Inst. Buffalo NY, ²Center for Comp. Res., SUNY at Buffalo, ³VA Med. Center, Pittsburgh PA & Dept. Pharmacol., U. Pittsburgh.

BnP is a protein structure-determination package that provides a common graphical user interface for the direct-methods program *SnB* and the protein-phasing suite PHASES. Thus, it provides a convenient pathway from intensity data to interpretable protein map. In automatic mode, the user needs only to specify a few parameters, and the entire phasing process is carried out by clicking a single button. On the other hand, a manual mode is available for difficult cases and allows the user to control many parameters and execute the major steps in the phasing process sequentially.

The results of *BnP* applications to a variety of test data sets containing as many as 70 heavy-atom sites will be described. In most cases, substructure solutions are obtained and recognized within minutes, sites are validated, and the proper hand is determined. Next, the (optional) application of a standard substructure/phase refinement protocol is followed by solvent flattening. A quantitative comparison of map quality with and without refinement will be presented in terms of map correlation coefficients and traceability by RESOLVE. *BnP* is available for download from <http://www.hwi.buffalo.edu/BnP/>. This work was supported by NIH grant EB002057.