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Rapid and Automated Substructure Determination. Hongliang Xu, Charles M. Weeks, Herbert A. Hauptman, Hauptman-Woodward Medical Research Inst. & Dept. of Structural Biology, SUNY at Buffalo, 700 Ellicott St., Buffalo, NY 14203.

Direct methods of phase determination have played important role in determining heavy-atom substructure from difference amplitudes of native-derivative crystal pairs or anomalous scattering crystals. The minimal principle based *Shake-and-Bake* procedure is one of the most successful direct methods for heavy-atom substructure determination. The computer program *SnB*, which implements *Shake-and-Bake* procedure and is part of the protein structure determination package *BnP*, has recently been optimized for rapid and automated substructure determination. Specifically, *SnB* has drastically increased cost effectiveness *via* the implementation of (1) newly developed statistical minimal function, (2) optimal FFT grid size, (3) dynamic figure-of-merits for automatic solution detection and false solution rejection, and (4) effective strategies for difficult structures. With these recent improvements, the 160 Se substructure of KPHMT, originally solved by *SnB* after 8 CPU days on an SGI Origin 2000 server, now can be determined within 2 CPU days on an SGI R10000 machine.

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