

PHENIX: New methods for automated structure solution, model-building, ligand-fitting and refinement

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PHENIX is a collaborative project aimed at developing a comprehensive software package for automation of the macromolecular structure determination process. PHENIX algorithms currently available include a complete refinement package (phenix.refine), maximum-likelihood based molecular replacement and phasing (Phaser), heavy-atom substructure searches (HYSS), fully automated iterative model-building, density modification and refinement (using phenix.refine, Resolve and Textal), analysis of experimental data (phenix.xtriage) and ligand-fitting (ELBOW, Resolve). The PHENIX Wizards allow automation of major steps in the structure determination process. The Wizards carry out decision-making, provide suggestions for the user, and form a flexible environment for investigating alternative strategies for structure determination.

New algorithms available in PHENIX include a Iterative-build OMIT procedure for prevention of model bias and ligand identification in electron density maps. The PHENIX AutoBuild Wizard can carry out iterative model-building, density modification and refinement to improve the quality of models at resolutions as low as 3 Å. Electron density maps calculated using an atomic model can be affected by model bias introduced during refinement of the model. We have developed a Iterative-build OMIT procedure that prevents model bias in iterative procedures for model-building and refinement while producing a high-quality electron-density map. The PHENIX LigandFit automated ligand-fitting Wizard can fit flexible ligands into an electron density map. The Wizard can identify unknown ligands by comparing a set of potential ligands to the map and finding the one that fits the density most closely.

PHENIX is available at <http://www.phenix-online.org>.