

Lafire: a Software for Automatic Protein Structure Refinement

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Refining an initial protein model to its final structure is usually composed of rounds of refinement performed by programs such as CNS and REFMAC, and manual model modification that includes linking and extending fragments, and fitting the ill matched residues of model by using the computer graphics program such as O. The manual model modification requires expertise of crystallography to recognize structural conformation based on electron density, and it is a time consuming process.

For the purpose of reducing the time and manual intervention of refinement, we developed a software named LAFIRE (Local-correlation-coefficient-based Automatic Fitting for Refinement) to automate the whole refinement process. Four function modules are designed: building the missing parts in the current model, fitting the model to the electron density map, monitor program and an interface for combining the first two modules and the refinement programs CNS and REFMAC5.

The LAFIRE is already in the state that builds the whole model from fragments by iterative approach, and performs structural refinement process without manual intervention in a few hours or days. LAFIRE is also available on http://altair.sci.hokudai.ac.jp/g6/Research/Lafire_English.html. The overview of LAFIRE, methods of building and fitting in LAFIRE, and refinement applications will be give in this presentation.

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