R&D field: Life science

Prediction of Protein Structure

- Program name: SimFold
- Developer
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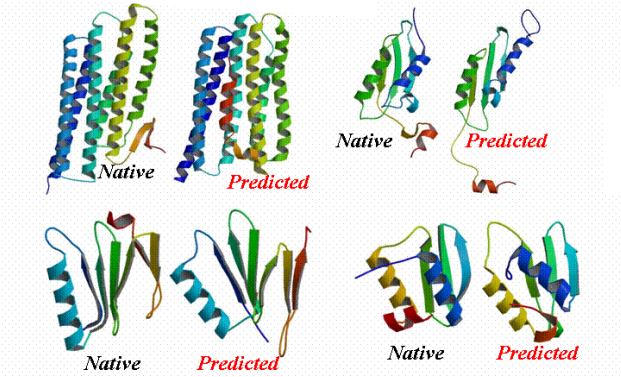
- Abstract
  - Prediction of protein three-dimensional structure via pseudo-folding simulation based on amino-acid sequence of unknown structure.
- Algorithm
  - SimFold (an energy function of knowledge base).
  - Fragment-assembly Monte-Carlo method.
  - Extended ensemble method.
  - FORTRAN77.
- Current computation size
  - Up to 120 amino-acid residues for coarse-grained models.
  - 4 billion accumulated Monte-Carlo steps.
  - Memory 1 GB and disk 1GB.
- Future computation size in 2010
  - 300 amino-acid residues or less for coarse-grained models.
  - 120 amino-acid residues or less for atomic models.

Prediction of protein structure with SimFold. Left and right figures are experiment and simulation results, respectively. The method works very well for alpha and small proteins.



- Expected results
  - SimFold can determine unknown three-dimensional structure of proteins via pseudo-folding simulation based on structure information such as Protein 3000 Project.
  - Precise protein modeling is one of the core bioinformatics technologies in structure-based drug-design research. Establishment of these technologies will realize high-throughput screening of lead compounds.
- Reference
  - Yoshimi Fujitsuka, George Chikenji, and Shoji Takada, SimFold energy function for de novo protein structure prediction: Consensus with Rosetta, Proteins:Structure, Function, and Bioinformatics, 62:381-398, 2006.