

Bioinformatics Center

- Bioinformatics Training Unit -

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Scope of Research

Evolutionary studies based on molecular biology is called "molecular evolutionary biology", which is one of the origins of the current bioinformatics. Living organisms have acquired wide variety of functions during the course of the evolution by changing the information encoded by the genomes. Inversely, reconstruction of the evolutionary history related to the functions would bring us a great insight into the acquired functions and the life. Furthermore, such evolutionary information is useful for practical fields such as drug design and proteins engineering. We develop new methodologies with evolutionary information, to extract biological knowledge from various molecular biological data including sequence and structure data of individual genes and proteins, genome data, and expression profile data. We also analyze the data of molecular biology from the evolutionary viewpoint, to obtain novel biological knowledge.

Research Activities (Year 2003)

Presentations

Study on the change of constraints associated with the topological change of membrane proteins, Toh H, Ichihara H, Daiyasu H, 3rd Japan Protein Science Society of Japan, 23 June, 2003.

Analysis of sites involved in the functional difference between cryptochrome and photolyase, Daiyasu H, Toh H, 3rd Japan Protein Science Society of Japan, 24 June, 2003

Phylogenetic tree among three domains: horizontal gene transfers and origin of Eukarya, Kuma K, 5th Society of Evolutionary Studies, Japan, 3 August, 2003.

Development of HocDB (Homology-based clustering DataBase), a sequence classification system for database searching, Ishikawa M (Mitsubishi Space Software Co. Ltd.), Sato Y (Mitsubishi Space Software Co. Ltd.), Toh H, 4th Annual meeting of the Chemo-Bioinformatics Society, 18 September, 2003.

A current wave for the study of protein function, Toh H, Bioinformatics Course of KAST education, 20 October,

2003.

Molecular phylogenetic analysis of pulmonary surfactant-associated protein C and the relatives, Osaka K (Mitsubishi Pharma. Co.), Takei T (Mitsubishi Pharma Co.), Toh H, 39th Annual meeting of Japanese Medical Society for Biological Interface, 1 November, 2003.

Bioinformatics for prediction of protein function, Toh H, Senri Life Science Sminar, 11 November, 2003.

Evolutionary analysis of membrane-associated proteins, Toh H, Workshop France-Japan on Structural Genomics, 12 November, 2003.

Prediction of protein function and drug design, Toh H, Genomic Drug Design Forum, 17 November, 2003.

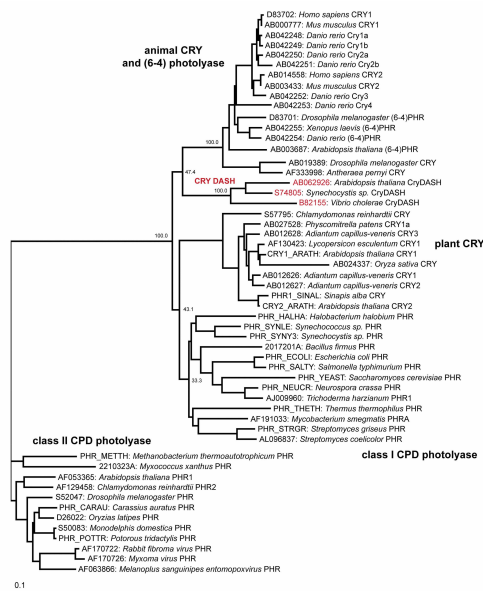
Evolutionary analysis of membrane-associated proteins, Toh H, Ichihara H, Daiyasu H, 10th Congress of the Federation of Asian and Oceanic Biochemists and Molecular Biologists, 10 December, 2003.

The evolutionary relationship between genome size and nucleotide composition, Kuma K, Hoshiyama D (Grad.

Identification of a new cryptochrome class. Structure, function, and evolution.

Cryptochrome flavoproteins, which share sequence homology with light-dependent DNA repair photolyases, function as photoreceptors in plants and circadian clock components in animals. The presence of a new cryptochrome class in bacteria and plants was suggested by a phylogenetic analysis. Coupling studies of sequencing of Arabidopsis cryptochrome gene with the X-ray crystallographic study and biochemical characterization supported the prediction by the phylogenetic study. That is, The crystallographic structure of Synechocystis DASH reveals commonalities with photolyases in DNA binding and redox-dependent function, despite distinct active-site and interaction surface features. Whole genome transcriptional profiling together with experimental confirmation of DNA binding indicated that Synechocystis cryptochrome DASH functions as a transcriptional repressor. The new class of cryptochrome was named DASH.

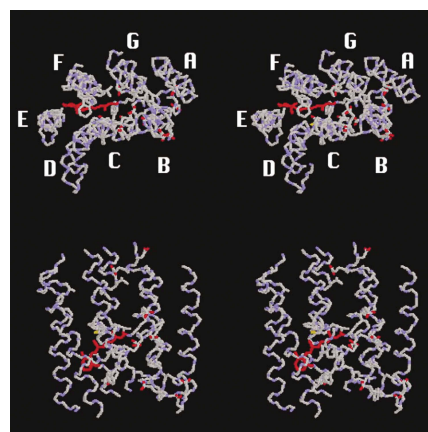
Brudler R, Hitomi K, Daiyasu H, Toh H, Kucho K, Ishiura M, Kanehisa M, Roberts VA, Todo T, Tainer JA, Getzoff ED, *Mol Cell*.11(1), 59-67 (2003).



Archaeal-type rhodopsins in Chlamydomonas: model structure and intracellular localization.

Phototaxis in the unicellular green alga, *Chlamydomonas reinhardtii*, is mediated by rhodopsin-type photoreceptor(s). Recent expressed sequence tag database from the Kazusa DNA Research Institute has provided the basis for unequivocal identification of two archaeal-type rhodopsins in it. One is located near the eyespot, wherein the photoreceptor(s) has long been thought to be enriched, along with the results of bioinformatic analyses. Secondary structure prediction showed that the second putative transmembrane helices (helix B) of these rhodopsins are rich in glutamate residues, and homology modeling suggested that some additional intra- or intermolecular interactions are necessary for opsin-like folding of the N-terminal ca. 300-aa membrane spanning domains of 712 and 737-aa polypeptides. These results complement physiological and electrophysiological experiments combined with the manipulation of their expression.

Suzuki T, Yamasaki K, Fujita S, Oda K, Iseki M, Yoshida K, Watanabe M, Daiyasu H, Toh H, Asamizu E, Tabata S, Miura K, Fukuzawa H, Nakamura S, Takahashi T, *Biochem Biophys Res Commun*, 301(3), 711-717 (2003).



Sch. of Sci., Kyoto Univ.), Katoh K (Grad. Sch. of Sci., Kyoto Univ.), 26th The Molecular Biology Society of Japan, 12 December, 2003.

Molecular phylogenetic analysis of a novel cryptochrome subfamily, DASH, Daiyasu H, Kuma K, Ishikawa T (Rad. Biol. Center., Kyoto Univ.), Todo T (Rad. Biol. Center., Kyoto Univ.), Toh H, 26th The Molecular Biology Society of Japan, 12 December, 2003.

Grants

Toh H, Development of the tools for protein structure comparison, BIRD, 1 April 2003 - 31 March 2004.

Toh H, Domain Prediction in Structural Genomics for Signal Transduction (Inagaki group), Protein 3000, 1 April 2003 - 31 March 2004.