A New Direction for the Computational Biology Research Center

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The Computational Biology Research Center (CBRC) was established by National Institute of Advanced Industrial Science and Technology (AIST) in 2001. It was reorganized in April 2007. CBRC developed unique technologies in bioinformatics and produced many software tools and databases for public use (http://www.cbrc.jp) as well as academic papers. The qualities of their technologies have been shown, for example, in *Aspergilli* genome analyses (three papers in Nature 438) and in CASP6 & CASP7 (protein structure prediction contests).

Since April 2007, they put more emphasis on developing more practical technologies by integrating their achievements in bioinformatics. By comprehensive analyses of the biological information from a viewpoint of engineering, they aim to develop useful technologies for supporting drug discoveries.

The director, Dr Kiyoshi Asai, leads the research activities of CBRC in three research areas, genome informatics, molecular informatics and cellular informatics, and educational activities for the trainees from private companies and universities with Dr Tamotsu Noguchi (the deputy director) and Dr Makiko Suwa (the principal research scientist). CBRC has approximately 20 research scientists, 10 postdocs, whose backgrounds are physics, mathematics, computer science, chemistry, biology, etc. There are 25 technical staff and 10 SEs supporting the research activities in CBRC. There are 15 scientists, who frequently work at CBRC as invited researchers and collaborators, including Professor Osamu Gotoh (Kyoto University), Professor Hiroyuki Tou (Kyushu University), Professor Yutaka Akiyama (Tokyo Institute of Technology) and Professor Yasubumi Sakakibara (Keio University.). There are also more than 30 trainees and students who come from private companies and universities including University of Tokyo, Waseda University and Keio University.
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**Genome Informatics**
The RNA informatics team (Leader: Dr. Taishin Kin) is developing new technologies for RNA sequence analysis based on both sequence similarities and the secondary structures, finding functional RNA genes and their functions, and building the functional RNA database. Dr. Koji Tsuda, Dr. Hisanori Kiryu, Dr. Michiko Yamana and Dr. Kengo Sato are the members of the team. The sequence analysis team (Leader: Dr. Paul Horton) aims to discover the regulatory mechanism hidden in biological sequences by motif discovery algorithms, analysis of genome regulatory regions, and prediction of protein structures and localizations from amino acid sequences. Dr. Kentaro Tomii, Dr. Martin Frith, Dr. Larisa Kiseleva are the members of the team.

**Molecular Informatics**
The molecular modeling and drug design team (Leader: Dr. Takatsugu Hirokawa) conducts practical research on the development and application of accurate drug discovery support technologies based on protein structures and molecular design. Dr. Chie Motono and Dr. Tomoshi Kameda are the members. The molecular function team (Leader: Dr. Kazuhiko Fukui) is developing technologies for the analyses of protein structures and their complexes with other proteins or with other biological molecules, using large-scale computation. Dr. Michael Gromiha, Dr. Masakazu Sekijima, Dr. Koki Tsukamoto, Dr. Yuichiro Hourai, Dr. Kana Shimizu and Dr. Wataru Nemoto are the members of the team.

**Cellular Informatics**
The cell function design team (Leader: Dr. Wataru Fujibuchi) is working on the analyses of the relations between the cell types and the gene expression data and on the metabolism based on the functions of enzymes. Dr. Nozomi Nagano and Dr. Yoshifumi Okada are the members of the team. The biological network team (Leader: Dr. Katsuhisa Horimoto) develops technologies for biological network analysis, for the support of drug discovery and the prediction of adverse drug reactions. Dr. Daisuke Tominaga, Dr. Kenichiro Fukuda, Dr. Sachiyu Aburatani and Dr. Koji Nakagawa are the members of the team.

A unique feature of CBRC is their facilities for large-scale computations. They have Blue Protein (Blue Gene/L with 8192 CPUs) and Magi Cluster (1040 CPUs) and are heavy users of AIST Super Cluster (over 3000 CPUs). Those facilities enable the study of heavy computation in molecular dynamics, large scale analyses of the genomes and gene expression data. They also seek to achieve seamless integration of their information infrastructure, including internally developed and maintained software applications and databases, with corresponding external resources.

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