The 7th International Workshop on Advanced Genomics

第7回 国際ゲノム会議
「見えてきた新たなる地平」

Abstracts

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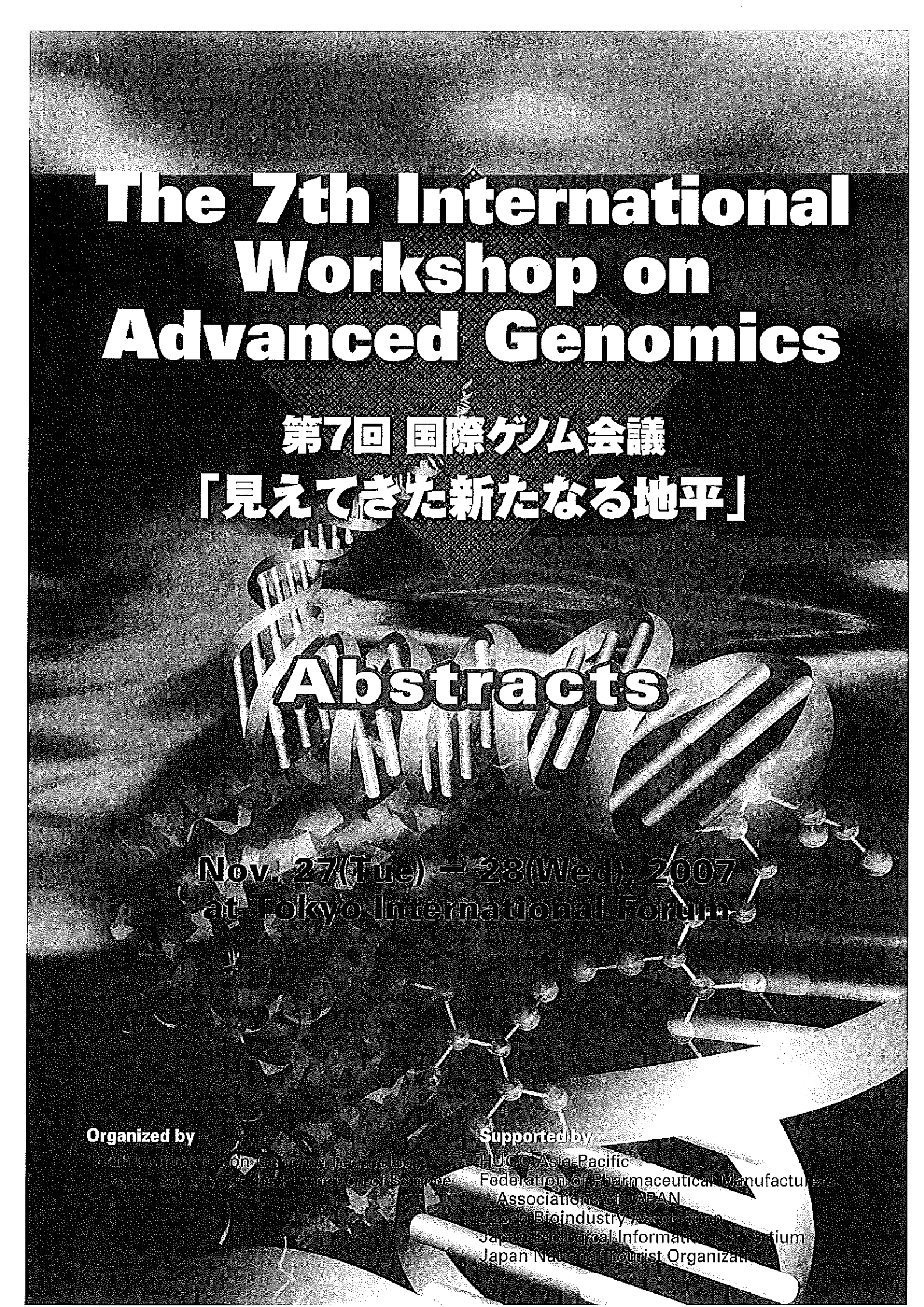

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Automated homology modeling using multiple reference proteins: FAMS-multi

Kazuhiko Kanou

Kazuhiko Kanou, Mitsuo Iwadate, Genki Terashi, Mayuko Takeda-Shitaka, Daisuke Takaya, Hiroko Sakai and Hideaki Umeyama

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We had developed an automated method of the protein structure prediction called FAMS (Full Automatic Modeling System). FAMS adopt homology modeling method, and can construct high accuracy model when appropriate reference protein was detected. For predicting more accurate model (especially loop structure and side-chain torsion angles), we developed new version of FAMS, called FAMS-multi, which use multiple reference proteins.
For the purpose of assessment of this modeling method, we participated in CASP7 (7th Critical Assessment of Techniques for Protein Structure Prediction) experiment. CASP is a world-wide experiment for protein structure prediction held every two years since 1994. All procedure of our 'fams-multi' had been performed full automatically. Models which were predicted by other automatic predictors were used to generate the better alignments, and we rebuilt models by FAMS-multi program. Results of CASP7 experiment are available on following URL.
http://predictioncenter.org/casp7/

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fams_ace : Model selection from server results using original threading(3D1D) program and consensus

Mitsuo Iwadate

Mitsuo Iwadate, Kazuhiko Kanou, Genki Terashi, Daisuke Takaya, Kazuhiro Ohta, Akio Hosoi, Mayuko Takeda-Shitaka and Hideaki Umeyama

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"fams_ace" is meta-selector team using all the server models. Concept of the meta-selector that appears with CASP5 2002, has freed many predictors from suffering hardship work. Then we have registered as the manual team, "fams_ace" in CASP7. This team downloaded all the server answers in the CASP7 sight and chose an appropriate model from the submitted model. Again, "fams_ace" has registered in the manual team, but in fact it is a meta-selector or a meta server.

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CIRCLE: Model quality assessment program using the 3D1D scoring functions.

Genki Terashi

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We have developed CIRCLE server focused on scoring function which evaluates predicted 3D protein model quality. The scheme of CIRCLE is based on searching for the best models from many models, using the side-chain packing and accuracy of secondary structure without alignment score, biological information and consensus scoring function such as 3d-jury. A new scoring function refined by CASP6 decoy set was applied to select the models. During CASP7, the CIRCLE performed well in the selecting the best model from candidate 3D models. In the poster, we introduce the methodology of CIRCLE, the detail scheme, scoring function, and discuss the successes and failures of this approach during CASP7.

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Protein Structure Prediction using SKE-CHIMERA in CASP7

Hiroko SAKAI

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In CASP7, we improved SKE-CHIMERA, a system for protein structure prediction, through which a lot of data we prepare can be analyzed, and homology modeling is easily carried out with human intervention. One of the major improvements is the development of a model evaluation method called CIRCLE.
In the case of side chain refinement targets, model structures constructed by FAMS were refined by energy minimization and molecular dynamics simulation.
Our new program FAMS Complex is a fully automated homology modeling system protein complex structures. It requires only sequences and alignments of the target protein as input and constructs all molecules simultaneously and automatically.
We evaluated the main-chain structures by the GDT_TSs and side-chain conformations by comparing the side-chain $\chi 1$ with those in the native structures. Side-chain conformations were considered correct if $\chi 1$ were within 40° of the experimental structure values.