JAMES RENNIE BEQUEST

REPORT ON EXPEDITION/PROJECT/CONFERENCE

Expedition/Project/Conference Title: the 4th European Conference on Computational Biology ....

Travel Dates: September 28 – October 1, 2005 .....

Location: Madrid, Spain .....

Group Member(s): Xueping Quan.....

Aims: To learn about the latest advances and development in the field of computational biology research, to gain information and ideas that may influence my own work, and to make contacts and talk to people and get feedback about my work.....

OUTCOME (not less than 300 words):-

The European Conference on Computational Biology (ECCB) is one of the major international conference series in Bioinformatics, together with its partner conference ISMB and RECOMB. It starts in 2002, and is hosted annually in a different country or region. Every year, five hundreds to seven hundreds scientists from all over Europe and overseas were brought together to present the latest advances and development in this field, exchange their ideas and information. Integrated and well structured, the conference's research activities focus on the following areas of bioinformatics:

- Databases
- Protein Structure and Function
- Genes and Genomes
- Microarrays
- Phylogeneticcs
- SNPs
- System Biology
- Algorithms
- Text Mining

Each above area was scheduled into one session, with leading keynote at the beginning, followed by participating researchers and guest speakers. Over the four days of the conference there were more than 60 talks, lasting from 10 to 45 minutes each, 345 posters displayed, two workshops, four tutorials, 13 demonstrations, and one student symposium.

The conference has proved to be very useful to me for many reasons. Perhaps most importantly, I had a chance to present my Ph.D work on the student symposium in the form of fifteen minutes presentation and on the poster session. I received some very useful comments that will certainly help me to write up my thesis. My Ph.D project works towards a better understanding of the sequence-structure relationship that determines the specificity of protein-protein interaction, developing computational methodology combining multiple components from several existing methods to predict specific transient protein-protein interactions. To predict which specific CDK homologue interacts with which cyclin homologue in *Arabidopsis thaliana*, a comparative modelling strategy was applied to model the 3-D structures of these proteins. All-by-all docking of

the model structures using the program ZDOCK, combined with additional selection criteria, yielded 19 most likely interacting CDK-cyclin pairs.

The session “Protein Structure and Function”, the area I specialised in, offered a wide range of talks, including protein structure alignment algorithm, protein structure change prediction, protein classification, the prediction of protein function based on protein structure. Perhaps one of the most exciting talks is the systematic construction of dictionary of super-secondary structure that can be used as “protein parts”trait locus mapping in natural to describe fold-sized strucutes, which was illustrated by Zhiping Wen’s talk (Boston University, USA).

Another session that is privately interesting is the “Algorithms” session, which specially focused on developing new algorithm. A new algorithm for learning Bayesian network models of gene networks from seed gene expression data was proposed by Peňa JM et al. (LinkŐping University, Sweden). This new algorithm differs from other Bayesian network models as it provides a window of radius R (a positive integer from user) around seed gene S to look at the Bayesian network model of a gene network without exclusion any gene in advance. Other new algorithms include a new complete NMR branch-contract-and-bound search algorithm for backbone resonance assignment, a new RNA secondary structure alignment algorithm, and a image refinement algorithm, all gave me some ideas of different area of bioinformatics and inspiration about the improvement of my own work.

During the poster sessions I was particularly pleased to read the poster of Diego Miranda-Saavedra from the Bioinformatics Group in Dundee University and chat with him about our work. Both his and my works focus on prediction of protein-protein interaction specificity. But his prediction methodology was mainly based on protein sequence analysis, and mine mainly based on protein structural and surface property analysis. Our discussion gave both of us some inspiration about our future work.

Because ECCB is such a large conference, near one thousand Bioinformaticians coming from all over the world were gathered together, I not only had the chance to listen to the fantastic talks given by some big names, but also were able to talk to many young researchers in similar field, exchanging our ideas and views, broadening our knowledge. In conclusion, it is a great chance for young scientist to broaden their knowledge in this field, develop their own views, and get some feedback and advice about their own work. All these are essential for the development of young Bioinformaticians and I am glad I joined it.