

Bioinformatics Research at the University of Dundee

The Barton Group

The primary emphasis of the bioinformatics research conducted by the Barton Group at Dundee is on the computational analysis and prediction of the function and three-dimensional structure of proteins from their amino acid sequence.

The Barton Group moved to the University of Dundee College of Life Sciences in 2001 and is based in the Post Genomics and Molecular Interactions Centre. The group's core research goal is to develop effective methods to predict protein structure and function from the amino acid sequence. Current research in the group includes the analysis and prediction of protein-protein interactions, the prediction of protein functional sites, protein secondary structure and protein crystallisation propensity. Research also includes the classification and analysis of large gene families such as the protein kinases and snf-2 like helicases and the development of novel computational tools to assist in these analyses. Software, databases and web servers developed by the group are widely used by the global scientific community for tasks such as predicting protein structure. The group's location in the Wellcome Trust Biocentre facilitates close integration of bioinformatics with the 75 research groups that make up the College of Life Sciences at the University of Dundee.

Protein structure prediction

The group has exceptional experience in predicting the secondary structure of proteins. Algorithms based on Artificial Neural Networks (ANNs) have been developed from the statistical analysis of proteins for which the three dimensional structure has been determined by X-ray and NMR methods. The group has raised the accuracy of protein secondary structure prediction to over 80% by exploiting information from similarities between different proteins within the same and different species. Future work will integrate information from other experimental techniques to raise the accuracy of structure predictions still further.

"The School of Life Sciences Research at Dundee offers a unique internationally competitive collaborative research environment with excellent core facilities for bioinformatics research."



Algorithm development

The Barton group has developed a wide range of software tools for the analysis of protein structure, and these tools are freely available on the group's website

www.compbio.dundee.ac.uk. Examples include the JPred secondary structure prediction server that implements the JNet neural network method and performs over 2,000 predictions per week for researchers in more than 50 different countries, and the JalView multiple alignment editor and analysis program which is in regular use by around 10,000 users worldwide.

Advancing biological research

The group also provides valuable bioinformatics resources for researchers at Dundee's world renowned College of Life Sciences. The College collaborates with the world's major pharmaceutical and biotechnology companies in the fight against diseases such as cancer, diabetes and rheumatoid arthritis and the recently completed Sir James Black Centre supports research to develop drugs for the treatment of neglected tropical diseases including malaria and African sleeping sickness. For example, the bioinformatics group has used novel methods to predict gene product function in the recently sequenced genome for *Plasmodium falciparum* by annotation with Gene Ontology (GO) terms, thus increasing their colleagues' understanding of this major cause of malaria.

By applying bioinformatics techniques to experimental data, the results can inform the rational design of subsequent experiments.

Vision for the Future

Computational approaches are becoming central to modern biology. As scientists try to understand complex biological systems, the modelling of these systems becomes more mathematical. The unique organisational structure of the College of Life Sciences at Dundee, which has no hard boundaries between specialities, ensures that bioinformatics is a resource that can be accessed by all of its research groups.

"Our bioinformatics research speeds up the process of determining protein structures, thus improving the understanding of protein functions."

The Scottish Bioinformatics Forum (SBF) was created for all developers and users of bioinformatics methods, and supports both the academic research base and commercial organisations by actively promoting training and facilitating access to bioinformatics skills. It is funded by the Scottish Executive, the Scottish Funding Council, and Scottish Enterprise.

www.sbforum.org

