EXPLOITING PROTEIN STRUCTURE IN THE POST GENOME ERA

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The theme of this presentation is to describe computational studies that use information about protein structure to provide enhanced interpretation of biological data. First, a database that describes structural and functional annotation of the proteins in recently sequenced genomes will be reported (1). 40% of the human proteome can be assigned to domains of known structure. Comparative analysis of domain frequencies between different species provides insight into protein evolution. Second, the application of protein structure prediction by fold recognition will be reported (2). Despite the advances of sequence-based methods, fold recognition can identify additional probable remote homologies with its consequential suggestion of protein structure and function. The added value of expert intervention into contemporary algorithms will be assessed. Finally, recent studies to understand the evolution of metabolic networks using structural information to identify remote homologies will be reported (3). Programs available for use by the community are available at www.sbg.bio.ic.ac.uk.

References:

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The availability of synchrotron radiation has very significantly influenced the field of structural crystallography in the last few years. In particular, the macromolecular crystallography benefited enormously from the routine use of very bright radiation sources at the new, third generation synchrotrons. For example, the recent initiative of structural genomics is in large part dependent on the good access to the intense and tunable synchrotron beam lines. The use of the synchrotron radiation is very much appreciated by all involved researchers, but in practice working at the synchrotron has also the darker side. The newest synchrotron beam lines are very bright, which means that the activity at the station is usually very hectic, involving many sleepless nights. In spite of a high degree of automatization, it is not easy to avoid mistakes in such conditions, and several anecdotic stories may illustrate this point. The enormous beam intensity makes it possible to collect meaningful data from very small and weakly diffracting crystals, but it can also quickly destroy the crystalline order in biological samples even if they are frozen, leading to the loss of diffraction. However, the few small bad and ugly synchrotron faces should not obscure the big good and positive face smiling at the synchrotron radiation users

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