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PROTEIN CRYSTALLOGRAPHY AS TAUGHT IN ACA SUMMER COURSE IN CRYSTALLOGRAPHY

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Since 1992 the American Crystallographic Association (ACA) has sponsored a summer course in crystallography. Initially conceived as a 10 day course in basic crystallography and small molecule structure determination, the course has evolved over the past decade to include lectures and workshops in macromolecular crystallography. The summer course in its present form is an intensive 12-day course with lectures in mornings and evenings, and hands-on laboratory sessions and workshops in afternoons. The first seven days of the Course are devoted to fundamental crystallography as applied to small molecule structure determination. This gives the students both crystallographic knowledge and hands-on experience in all aspects of a structure determination from area detector data collection through structure validation.

The last five days of the course are focused on the application of crystallography to macromolecular structure analysis. The macromolecular lectures build on the basics learned earlier in the course while the laboratory sessions are replaced by workshops covering selected aspects of crystal growth, data collection, phasing, model building and refinement given by experts in the field.

The Course has been very successful over the past decade with an average attendance of 50+ students each of the last five years and a total of 407 students in the last ten years. Details of the design, logistics and macromolecular content of this successful summer course will be described in detail.

Keywords: TEACHING, MACROMOLECULAR CRYSTALLOGRAPHY, ACA SUMMER COURSE

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TEACHING AND LEARNING PROTEIN CRYSTALLOGRAPHY OVER THE INTERNET

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The Internet, IT and the increased need for lifelong learning are changing the education system. We have been in the vanguard of this by delivering complete courses over the Internet since 1993. For the past five years we have successfully run the Advanced Certificate in Protein Crystallography on the Web. This one-year course gives a qualification approximately equivalent to half a UK master's degree.

The course materials have been mainly developed in-house. They include a) traditional book-like text and figures, b) multimedia materials consisting of text, images, image maps, 'movies', c) programs like RasMol to manipulate molecules in three dimensions, and Fourier to do simple transformations. The most difficult physico-mathematical concepts of protein crystallography are taught visually, e.g. symmetry concepts with the aid of point-and-click space group diagrams using the 3 commonly occurring space groups $P2_1$, $P2_12_12_1$ and $C2$. Programs have been written to provide a security-enhanced web interface to allow the students to run the AMORE computer program at Birkbeck for a molecular replacement project.

Course material is mounted on the Internet in sections, to ensure optimum pacing. The course employs a variety of means of student/tutor communication: e-mail lists, individual e-mail support, MUD, and electronic course work. Formal assessment consists of two components. The two projects have to be submitted as web pages. An examination by unseen paper, which the student takes in person at a temporarily established local centre, enforces academic standards.

Keywords: PROTEIN CRYSTALLOGRAPHY, TEACHING, INTERNET

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USING THE WEB AS A CRYSTALLOGRAPHIC TEACHING RESOURCE

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The Web is rapidly developing into a tremendous teaching resource, with its possibilities for linking a wide range of sites providing information in text, graphics and animations, and for providing interactive computing. We have made a simple start at building a resource for the teaching of protein crystallography (**http://www-structmed.cimr.cam.ac.uk/course.html**).

Our initial goal is something like a hyperlinked textbook, with a few simple animations. I will describe our experiences in building and using this site for local teaching, and point out some of the highlights in other sites that provide an interactive experience of crystallographic concepts.

Keywords: WORLD WIDE WEB, TEACHING

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StarDDL: TOWARDS THE UNIFICATION OF Star DICTIONARIES

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Data dictionaries play vital role in the reliable exchange of electronic data by providing precise, machine-parseable definitions of data items. Two main dictionary languages are in use, DDL1 [1] for the core and powder CIF dictionaries, and DDL2 [2], which has stronger relational attributes, for the macromolecular and symmetry CIF dictionaries. The similarities between DDL1 and DDL2 means that STAR compliant software are often applicable to both languages. Nevertheless, there are a number of significant differences and a common language for all Star dictionaries is clearly a desirable future objective. The development of a relational expression language, dREL [3] capable of expressing complex relationships between data items in the methods of a dictionary has involved the development of new DDL attributes, referred to as StarDDL. StarDDL is a compact semantically-rich dictionary language with a simple organisational framework in which inheritance between related data categories is used to reduce definition complexity and redundancy. StarDDL supports a wide range of data types, including Measurement which enables standard uncertainty values to be handled consistently within the definition of a value, and to be derived automatically from methods expressions written in dREL. StarDDL will facilitate all existing DDL1 and DDL2 definitions and is a candidate for the future unification of Star dictionaries.

References

[1] Hall, S.R. & Cook, A.P.F 1995 J. Chem. Inf. Comp. Sci. 35, 819-825.
[2] Westbrook, J.D. & Hall, S.R. 1995 **ndbserver.Rutgers.edu/mmcif/ddl/**
[3] Spadaccini, N. Hall, S.R. and Castleden, I.R. 2000 J. Chem. Inf. Comp. Sci. 40, 1289-1301.

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