PUBLISHED METHODS IN CRYSTALLOGRAPHY
Reference database on personal computers

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The history of protein crystallography is very rich by ideas, their developments and applications. However, the usual way of making references on review, secondary references etc. leads to cases when the ideas loose their "parents", change their original form or even disappear and are "rediscovered" a second time.

A number of existing general reference databases help, naturally, to avoid this situation. However, information of particular interest might be "buried" under the huge information of general databases, on one hand, and lacks necessary details, on another hand. A set of smaller databases which include references on papers of only some particular interest, but have also extra information on another questions, can solve this problem.

The described database contains basically the references on papers more or less related to the methods of macromolecular structure determination. The database contains about 3000 references. It has 2 levels of paper classification. The first level indicates main topics, includes the following ones :

- type of the structure under investigation
- experiment (crystallisation, data collection and analysis)
- phase problem
- phase improvement
- electron density
- atomic models
- atomic model refinement
- dynamics; thermal motion
- X-ray theory
- computational problems
- molecular graphics
- program description
- non-diffractional approaches to structure solution
- tutorials; information
- others.

The number of these topics can be extended.

At the second level, each topic can be divided in a set of subtopics with use specific details. For example, "Atomic model refinement" currently has the following subtopics:

refinement type

- free-atom refinement
- restrained refinement
- constrained refinement
- restrained/constrained refinement
- dynamics refinement
- stereochemical refinement
- energy refinement
- refinement against electron density

data used

- X-ray data refinement

- neutron data refinement
- joint X-ray/neutron refinement.

Again, any combination of subtopics is admissible. Each reference can be selected through any combination of these topics of both of levels.

The database contains references on main journals on (macromolecular) crystallography - Acta Crystallographica, Journal of Applied Crystallography, Journal of Molecular Biology, Proceeding of National Academy of Sciences, USA, Nature, Science etc., as well as references on different particular publications. There is no special deadline for the starting year of publications, e.g., for Acta Crystallographica, there are references of its first issues. The database is quite complete until 1991, and the information for 1992-1994 years is currently being added.

Normally, each reference has the following information:

- list of authors
- title
- year of publication
- type of the publication
- publishing information
- the address of the authors.
- 2-levels classification
- date of including into the database,

The reference can also have an abstract and (subjective) estimation of its methodological interest.

This database on methods of X-ray protein crystallography does not pretend to be absolutely complete. However, even in its current state it was useful enough to be used in the review by Bhat and Podjarny on the atomic mode refinement (personal communication, sent to the publisher) and in the review on density modification method by Podjarny, Rees and Urzhumtsev (sent to the publisher). It may be very helpful not only for the scientific reviews but for students to prepare their theses, also as for current scientific work. The database is under further development.

The database currently is kept in the EndNote format which makes usable both on MacIntosh and IBM PC personal computers. It is available by request from the authors (e-mail address is sacha@ ibmc.u-strasbg.fr or com@impb.serpukhov.su).

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