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The three-dimensional structural information available for macromolecules (proteins, nucleic acids and sugars) is expanding rapidly, and is becoming increasingly important to molecular biologists, cell biologists and biochemists as they develop molecular hypotheses for biological processes. It is not easy for the majority of scientists to access these structures because of the large quantity of information and a general lack of familiarity with on-line computer database systems. Therefore, bench scientists and students, most of whom do not have easy access to the sophisticated software required to visualize molecular structures, frequently remain unaware that such data even exist.

For a number of years, the Protein Data Bank (PDB) archive of the Brookhaven National Laboratory (BNL) has been available on the Internet for access via FTP (file transfer protocol

The Swiss-3DImage collection and PDB-Browser on the World-Wide Web

under TCP/IP), more recently through Gopher, and now via the World-Wide Web (WWW)[1]. These tools provided access to the individual entries of the PDB and allowed limited searches of the data bank.

Two new features have been added to the PDB and ExPASy WWW servers, which should enhance their accessibility and usability: first, a PDB-Browser has been introduced, which allows the submission of complex search queries and the downloading of selected entries via the WWW; and second, the Swiss-3DImage collection, consisting of a large number of annotated images describing the PDB entries, has been added.

The WWW PDB-Browser

The PDB-Browser (D. R. Stampf, C. E. Felder and J. L. Sussman, unpublished) accessed by the WWW allows the user to search over various PDB record

Table I. How to download Swiss-3DImages and GIF viewers

Connection	ExPASy	Brookhaven Data Bank
WWW[a] Uniform resource locator (URL)	http://expasy.hcuge.ch/pub/Graphics/	ftp://pdb.pdb.bnl.gov/images/GIF ftp://pdb.pdb.bnl.gov/images/RGB
Downloading Images Connect using FTP (TCP/IP)[b] Login as: Password to use: Set file type to binary: Change directory for	FTP expasy.hcuge.ch or connect to expasy.hcuge.ch[b] anonymous Your email address binary	ftp pdb.pdb.bnl.gov or connect to pdb.pdb.bnl.gov[b] anonymous Your email address binary
GIF format (Mac and PC): Silicon Graphics RGB format: List the directory content: Download the selected files: Disconnect:	cd /pub/Graphics/IMAGES/GIF cd /pub/Graphics/IMAGES/SGI ls get file_name quit or disconnect[b]	cd /images/GIF cd /images/RGB ls get file_name
Downloading GIF viewers		
Get the program: Macintosh[b] Silicon Graphics PC-Windows[b,c]	Connection, login and set binary file type as described above get /pub/Graphics/mac/quick-gif.hqx get /pub/Graphics/SGI/xv3 get /pub/Graphics/Windows/lview31.zip get /pub/Graphics/Windows/pkunzip.exe	

[a]The Swiss-3DImages are also referenced on the **scop** WWW server (http://www.bio.cam.ac.uk/scop).
[b]The Macintosh program Fetch and the PC-Windows program WinFtp offer user-friendly interfaces for file transfer under TCP/IP. Fetch will automatically generate an executable from the quick-gif.hqx file.
[c]lview31.zip must be uncompressed under DOS using 'pkunzip'.

types in the HEADER section of PDB entries using search strings that can be combined by boolean functions (AND, OR, NOT). The searchable fields include functional classification, compound, author, source organism, experimental technique, literature references, crystal symmetry, heterogen names and formulas. The user may then select an entry from a list of entries matching their search criteria, and download a copy of the entry to his or her computer. When an entry is transmitted to the client, it is filtered through a program that inserts links to other WWW resources (such as the Enzyme Commission Database), other PDB entries with identical fields and explanatory text, and relevant Swiss-3DImage files. The data can also be linked to local application programs such as RasMol, which gives a three-dimensional image that can be manipulated by the user*. This combination of narrowing (via the search criteria) and expansion (via links to other databases) of the search space provides the research community with versatile tools that can be extended easily to allow for new, as yet unanticipated, information resources. The WWW interface for the PDB-Browser is accessible from PC-Windows, Macintosh, most Unix-based computers and even text-based systems through WWW clients such as Mosaic and Lynx (downloading information for these tools was discussed in Ref. 1). All the software that builds the PDB-Browser page and performs the searches is freely available from the PDB, so any site that already has a complete set of PDB entries installed can also have its own copy of the Browser. Updates of the PDB now also include the latest Browser index files. This should help local servers or national centres to support their research community more effectively, by allowing faster retrieval times and thus more efficient use of the Internet. The master copy of the PDB-Browser interface remains reachable through the PDB home page at http://www.pdb.bnl.gov.

The Swiss-3DImage collection

The Swiss-3DImage collection was started with the idea that a few images, showing a molecular structure in easily

*RasMol (R. Sayle, Glaxo Research & Development) is available for PC-Windows, Macintosh and most common types of Unix workstations, and may be obtained anonymously via FTP from ftp.dcs.ed.ac.uk, where it is located in the directory /pub/rasmol.
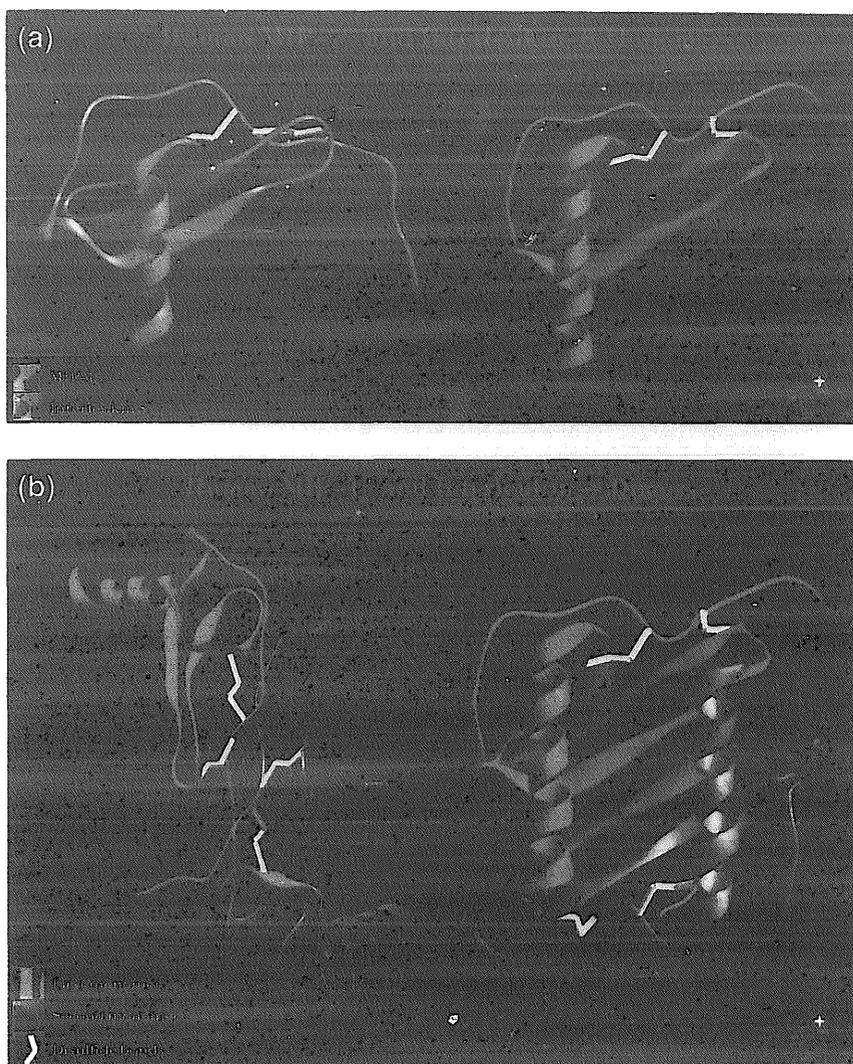

Figure 1
Sample Swiss-3DImages showing how CC and CXC chemokines differ in their three-dimensional structures. Although the monomer structure of Interleukin-8 [PDB entries 1IL8 (Ref. 3), 3IL8 (Ref. 4)] and MIP-1β [PDB entry 1HUM (Ref. 5)] are very similar (a), they dimerize in a different orientation (b).

viewable orientations and annotated in a simple way, would provide nonexpert users with the essential structural information about any particular protein (see Fig. 1) The goal of the Swiss-3DImage collection is gradually to provide a small number of images for all known three-dimensional structures contained in the PDB. This should enable scientists and students to familiarize themselves both with the proteins that they are working on and new proteins. The images show key features such as disulphide bonds, bound metal ions and residues involved in ligand binding or enzyme activity. For details on how to submit contributions to the Swiss-3DImage collection, see Box 1.

Box 1. Contributing to the Swiss-3DImage collection

We welcome contributions to the Swiss-3DImage collection by anyone who wishes to make them available to the world scientific community. In addition, we can answer specific requests and generate images that might not yet be available in the collection. Such questions and requests should be addressed to Manuel Peitsch by email (mcp13936@ggr.co.uk). Image files in GIF, JPEG, TARGA, Silicon Graphics RGB or BMP format can be sent in binary format using mail software such as Eudora. Alternatively, send either BinHexed or uuencoded files using VMS-Mail or SMTP-Mail. Submitted images should be accompanied by a short descriptive note including the author's name and full affiliation, since this information will be made available on the servers. All images available in the Swiss-3DImage collection are made freely available to the public.

All displayed features are generated with the program *RIBBONS*[2] and its utilities. In each case, the backbone of the protein chain is displayed as a ribbon, whereas metal ions, ligands and important sidechains are shown as spheres or cylinders. The detailed annotations were made using the *IRIX Showcase* (Silicon Graphics). Furthermore, at least one stereo pair image is generated for each structure. The Swiss-3DImage collection currently contains more than 400 images (as of November 1994) in both GIF87 and Silicon Graphics RGB format, which can be downloaded from the ExPASy[1] molecular biology and PDB WWW servers and via the PDB-Browser. The Browser greatly facilitates rapid location of the structures that the user is interested in, so anyone with an Internet connection can easily locate, download and view high-quality molecular images using public domain software such as Lview (PC-Windows) and Quick-GIF (Macintosh), and a variety of other GIF viewers for PC-Windows, Macintosh and Silicon graphics; these can also be downloaded from ExPASy via anonymous FTP to expasy.hcuge.ch, directory /pub/Graphics. Table I gives details on how to download the images and the GIF viewers.

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Some interesting and useful home pages accessible using the WWW

Uniform resource locator (URL)	Description
http://expasy.hcuge.ch/	ExPASy molecular biology server
http://www.nih.gov/	National Institutes of Health
http://expasy.hcuge.ch/sprot/sprot-top.html/	SWISS-PROT protein sequence database
http://www.nih.gov/molbio/	Molecular biology databases specifically related to DNA and protein sequence
gopher://vm1.hqadmin.doe.gov/1/	Department of Energy gopher
http://gdbwww.gdb.org/	Genome database
http://kaktus.kemi.aau.dk/	The O Protein crystallographic package
http://dapsas1.weizmann.ac.il/	Biological Computing Division at The Weizmann Institute of Science
http://ndbserver.rutgers.edu/	Nucleic acid database project at Rutgers University
http://www.prosci.ucl.edu/	Protein Science Web Server
http://cui_www.unige.ch/meta-index.html/	Search engines for WWW
http://www.mit.edu:8001/people/mkgray/compre3.html/	Comprehensive list of HTTP sites
http://www.bio.cam.ac.uk/scop/	Structural classification of proteins
http://www.pst-elba.it/Proteins	Proteins database service
gopher://pdb.pdb.bnl.gov/11/Software/PDBShell/	PDB-Shell: a browser for PC-Windows
http://bnlstb.bio.bnl.gov:8000/	Structural Biology at the Brookhaven National Laboratory
http://www.tc.cornell.edu/~richard/AChE.html/	Acetylcholinesterase: Nature's vacuum cleaner
http://gopher.montpellier.inra.fr:70/1/cholinesterase	Acetylcholinesterase
http://www.public.iastate.edu/~pedro/research_tools.html/	Pedro's biological research tools
http://csdvx2.ccdc.cam.ac.uk/	Cambridge Crystallographic Data Centre
http://www.sander.embl-heidelberg.de/dssp/	The DSSP program and database
gopher://pdb.pdb.bnl.gov/11/Software/Procheck/	Procheck information

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