PDBj
Protein Data Bank Japan

http://www.pdbj.org/

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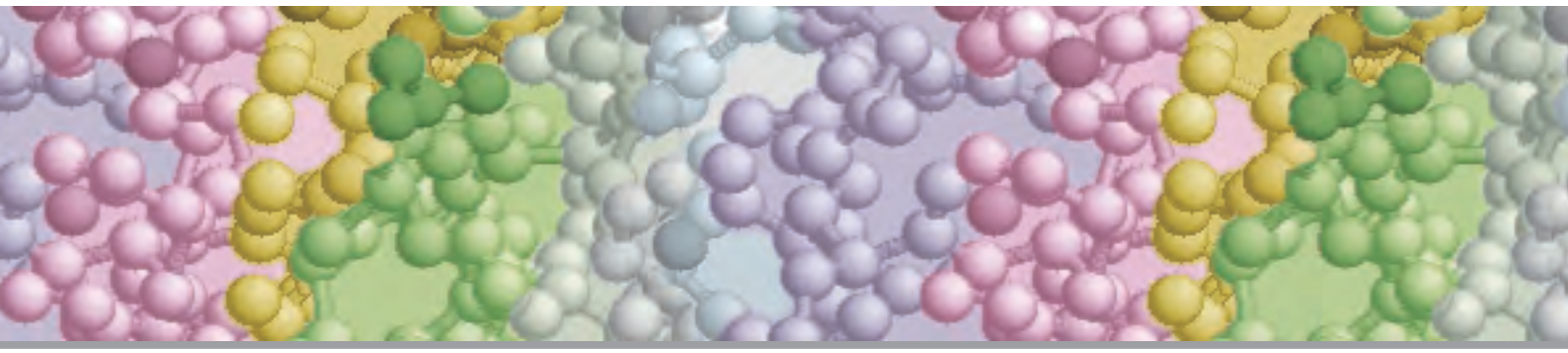


PDBj is maintained at the Protein Research Institute, Osaka University, and supported by Japan Science and Technology Agency.

Since fiscal year 2001, PDBj has been supported by JST-BIRD (Japan Science and Technology Agency-Institute for Bioinformatics Research and Development) to construct and maintain the PDB (Protein Data Bank) and BMRB (BioMagResBank) databanks, collaborating with the RCSB-PDB in the USA, PDBe in Europe, and BMRB for NMR chemical shift data, as one of the founding members of the wwPDB (worldwide PDB). In particular, PDBj mainly processes deposition from Asian and Oceania regions in the wwPDB, and provides the web pages described in Japanese, simplified Chinese, traditional Chinese, and Korean languages, in addition to English. We, PDBj, have so far processed about a quarter (16,345 entries) of all deposited structural data to the wwPDB (66,490 entries in the same period). All the available PDB data as of the middle of March 2011 is 71,800 (See Chart for Data Growth below).

On March 8th, 2011, a symposium entitled “Challenge to Knowledge Discovery” was held in Tokyo, as many JST-BIRD programs will finish at the end of this March. Professor Haruki Nakamura, Head of the PDBj, attended the symposium, and made a presentation entitled “International Development and Advancement of Protein Structure Databank (PDBj)” . He first introduced how the PDBj has accomplished its three missions: 1) To develop and manage the three-dimensional structural database for biological macromolecules with the international collaboration, keeping its qualities. 2) To develop new derived databases and tools covering experimental data by NMR and Electron Microscope, and computational models. 3) To develop services for rapid similarity search of analog data such as protein folds and molecular surfaces, in addition to text data search. Then, several examples were introduced as the Knowledge Discovery from protein structures: examples to estimate the protein functions based on the remote homolog information [Refs. 1 and 2], analysis of similarities search of specific atom dispositions around ligand binding sites and protein-protein interfaces [Refs. 3 and 4], and prediction of functional sites from similar molecular surface search [Ref. 5].

At the end of March 2011, JST-BIRD will be closed, and the National Bioscience Database Center (NBDC) will start as a new organization in JST from April 2011. In collaboration with the NBDC, PDBj is going to continue to develop and maintain the PDB and BMRB databases as one of the missions of the Institute for Protein Research, Osaka University, which has been approved as a Joint Usage/Research Center by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) Japan. All the PDBj members would like to thank you for your continuing support and further encouragement to our activities.

【References】

[1] D. M. Standley, H. Toh, H. Nakamura, Functional annotation by sequence-weighted structure alignments: Statistical analysis and case studies from the Protein 3000 structural genomics project in Japan. *PROTEINS* 72, 1333-1351 (2008)

[2] K. Matsushita, O. Takeuchi, D. M. Standley, Y. Kumagai, T. Kawagoe, T. Miyake, T. Sato, H. Kato, T. Tsujimura, H. Nakamura, S. Akira, The CCCH-type zinc finger protein, Zc3h12a, is a ribonuclease essential for controlling immune responses by regulating mRNA decay. *Nature* 458, 1185-1190 (2009)

[3] A. R. Kinjo, H. Nakamura, Comprehensive structural classification of ligand binding motifs in proteins. *Structure* 17, 234-246 (2009)

[4] A. R. Kinjo, H. Nakamura, Geometric similarities of protein-protein interfaces at atomic resolution are only observed within homologous families: An exhaustive structural classification study. *J. Mol. Biol.* 399, 526-540 (2010)

[5] K. Kinoshita, Y. Murakami, H. Nakamura, eF-seek: Prediction of the functional sites of proteins by searching for similar electrostatic potential and molecular surface shape. *Nucl. Acids Res.* 35, W398-W402 (2007)

News

The 2010 Annual Meeting of the Crystallographic Society of Japan (2010CrSJ)

The 2010 Annual Meeting of the Crystallographic Society of Japan was held from December 3rd to 5th, 2010 at Convention Center, Osaka University. We introduced our activities and services at a booth and Luncheon-seminar. We had many feedbacks from participants for our services.

BMB2010: the 33rd Annual Meeting of MBSJ & the 83rd Annual Meeting of JBS

BMB2010: the 33rd Annual Meeting of MBSJ & the 83rd Annual Meeting of JBS was held from December 7th to 10th, 2010 at Kobe PortIsland. We exhibited a booth and demonstrated our services.

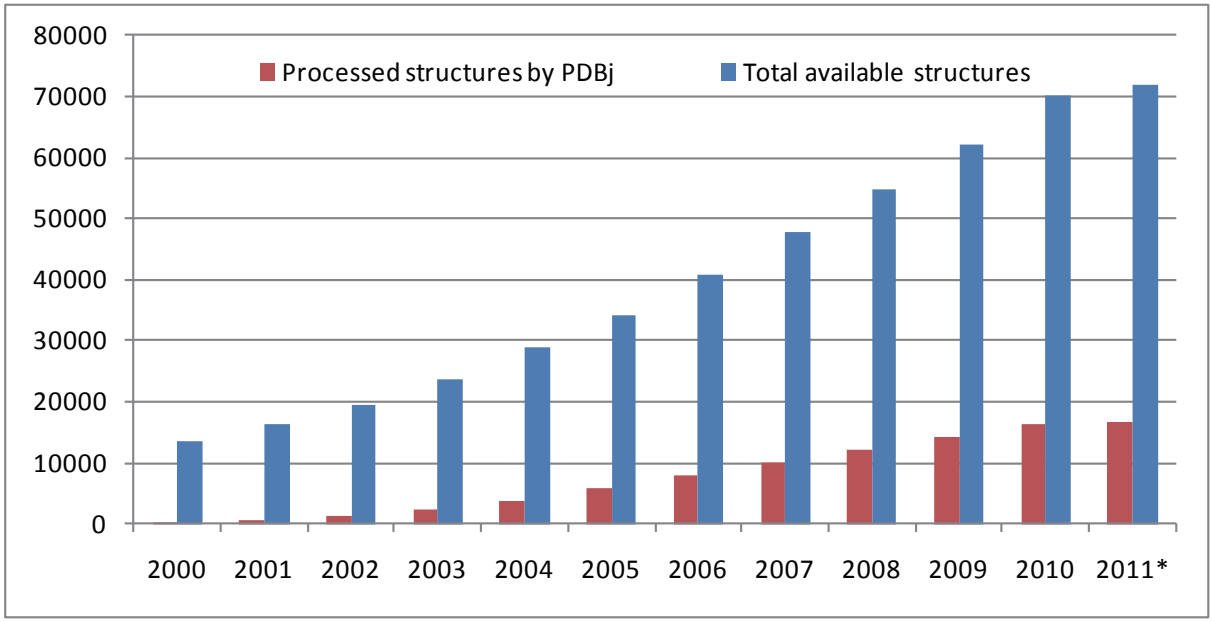
DDBJing & PDBj workshop in Nagahama Institute

DDBJing & PDBj workshop in Nagahama was held from January 17th and 18th, 2011 at Nagahama Institute of Bio-Science and Technology, Shiga prefecture. We thank participants for attending our workshop despite heavy snow. The documents used at the workshop can be downloaded from the PDBj web site (http://www.pdbj. org/pdbj_prev_workshop.html).

Snapshots of the workshops. From left to right: the 2010 CrSJ in Osaka, BMB20010 in Nagoya University and DDBJing & PDBj workshop in Nagahama.

Data Growth

The statistics is also available at the wwPDB page (http://www.wwpdb.org/stats.html).



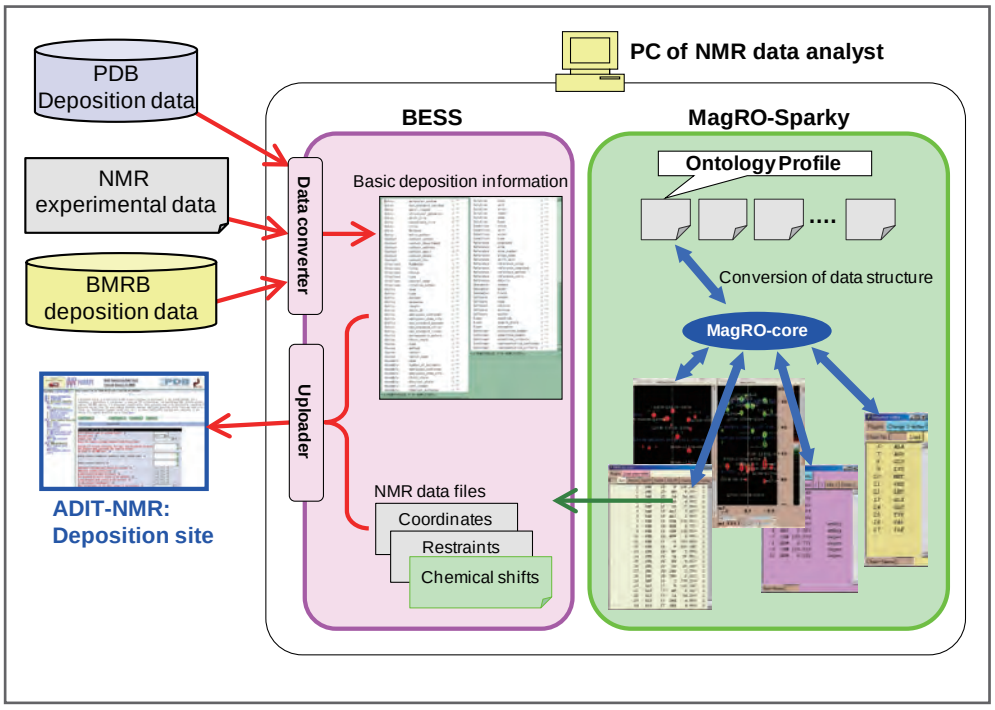
* Last updated : March 16, 2011

Services

Activities of the PDBj-BMRB group

The PDBj-BMRB group has so far constructed and maintained the NMR experimental database by processing deposited NMR data in collaboration with the BMRB group headed by Professor John L Markley at University of Wisconsin-Madison, USA. Since 2005, the PDBj-BMRB group has processed 12 % (760 entries) of the total BMRB data (6,424 entries). Since December 2010, NMR chemical shifts have become mandatory for deposition of atomic coordinates of biomolecular structures determined by NMR to PDB. Thus, the PDBj and PDBj-BMRB groups have been working on processing both atomic coordinates and chemical shifts data in an integrated and systematic manner.

NMR analyses for biological macromolecules can provide rich information with high space and time resolution, related to such as interactions with ligands and dynamic structural changes, which should contribute to reveal their functions. In order to construct a valuable NMR experimental database, which covers those many different kinds of NMR parameters, highly structured data would be strongly desired to relevantly describe the different states of experimental materials, applied protocols, and the observed data. In 2009, the PDBj-BMRB group developed a program BESS, which simplifies the complicated processes of deposition and annotation works for the NMR chemical shift data, and successfully completed more than 300 entries in a year from RIKEN with a few annotators. Recently, the group has developed a new core program MagRO which reconstructs and converts the complicated NMR data into the other file format using ontology engineering technology. MagRO has been implemented as a plug-in module of Sparky, the standard software for NMR data analysis (Fig. 2). In addition, the group has developed a new program fit_robot which automatically searches and extracts the converged regions from structural ensembles determined by NMR experiments. The group has also developed MagMol, which displays the regions of tertiary structure and highlights the regions with inconsistency with experimental NMR data. Those programs are expected not only to reduce the deposition burden for the NMR researcher and annotator, but also to enhance the quality of the NMR data in database. Those programs are available from the PDBj-BMRB web site upon request.



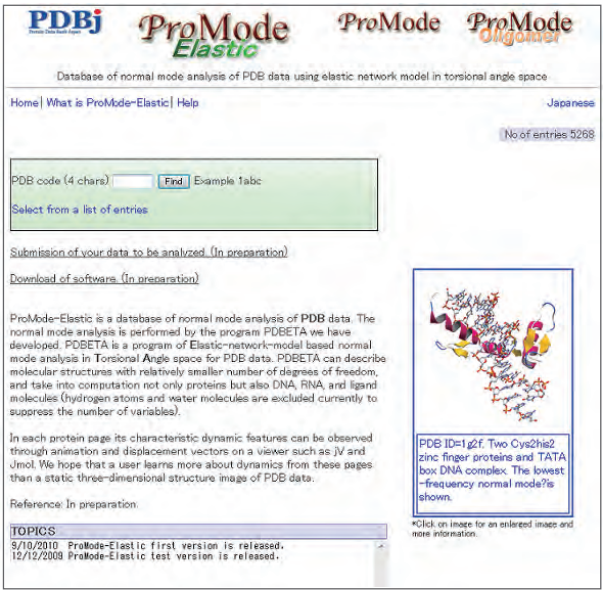
Tools developed by PDBj-BMRB: MagRO-Sparky for NMR data analysis and BESS for BMRB data deposition.

Development and releasing of a new database for protein dynamics: ProMode-Elastic

Protein structures are essentially dynamic. It is well known that their structures often change upon forming complexes with ligands, depending on the environments with solvent molecules or membranes. These dynamic properties are crucial for their functions, and current drug developers also pay attention to them. Namely, the structures deposited in the PDB are only the snapshots of those dynamic structures.

In order to extract dynamic features from the "static" PDB structures, Dr. Hiroshi Wako et al. in PDBj made efforts to develop a precise method of normal mode analysis (NMA), and their results are available from the PDBj site as "ProMode" [6]. However, this original ProMode employs an orthodox molecular mechanics algorithm, rigorously minimizing the force field potential using the hessian matrix with dihedral angles as the independent variables. Consequently, it requires a long computational time and huge memory size for large protein complex structures, and the database is able to cover only a part of the PDB entries.

Recently, Wako et al. have overcome this problem, by developing a new computational program for NMA with an elastic network model using dihedral angles as the independent variables. The new database is now open as ProMode-Elastic [7]. In this algorithm, since each PDB structure is assumed to be the minimum energy structure, no calculation for energy minimization is required. Therefore, the computational time is much shorter than before, and it is now possible to perform the NMA analyses for any systems provided in PDB. The advantage of this method is that dihedral angles are used as the independent variables, much reducing the number of the independent variables, so that our model has all the atoms in contrast to other ordinary elastic network models which usually include only Cα atoms. In addition, it is also possible to include small ligand molecules, DNA, RNA, and sugars. We have already performed exhaustive NMA computations for most of the PDB entries, and they will soon appear on our ProMode-Elastic web site. Moreover, another "on-demand" service will also start to perform the NMA calculations for the structures uploaded by the user.



The ProMode-Elastic frontpage.

【Reference】

[6] H. Wako, M. Kato, S. Endo, ProMode: a database of normal mode analyses on protein molecules with a full-atom model. Bioinformatics 20, 2035-2043 (2004), http://promode.socs.waseda.ac.jp/
[7] http://promode.socs.waseda.ac.jp/promode_elastic/

Stop by our booth at APPA!

The 3rd APPA (Asia Pacific Protein Association) Conference in conjunction with the 3rd Symposium of the Chinese Protein Society will be held from May from 5th to 9th, 2011 at Shanghai University, Shanghai, China.

PDBj will have our booth at the conference. Please stop by our booth to ask your questions about the PDBj and the wwPDB, and give us your feedback.

Staff

Head
Nakamura, Haruki, Prof. (IPR, Osaka Univ.)

Group for PDB Database Curation
Nakagawa, Atsushi, Prof. (IPR, Osaka Univ.)
Matsuura, Takanori, Dr. (IPR, Osaka Univ.)
Igarashi, Reiko (JST-BIRD)
Kengaku, yumiko (JST-BIRD)
Matsuura, Kanna (JST-BIRD)
Chen, Minyu (IPR, Osaka Univ.)

Group for Development of new tools and services
Kinjo, Akira, Dr. (IPR, Osaka Univ.)
Iwasaki, Kenji, Dr. (IPR, Osaka Univ.)
Suzuki, Hirofumi, Dr. (IPR, Osaka Univ.)
Yamashita, Reiko (JST-BIRD)
Kamada, Chisa (JST-BIRD)
Shimizu, Yukiko (JST-BIRD)
Kudou, Takahiro (IPR, Osaka Univ.)
Ikegawa, Yasuyo (IPR, Osaka Univ.)

Group for NMR Database
Fujiwara, Toshimichi, Prof. (IPR, Osaka Univ.)
Akutsu, Hideo, Prof. (IPR, Osaka Univ.)
Kobayashi, Naohiro, Dr. (IPR, Osaka Univ.)
Nakatani, Eiichi（JST-BIRD)
Harano, Yoko (IPR, Osaka Univ.)

Collaboratory Researchers
Toh, Hiroyuki, Deputy Director (CBRC-AIST)
Wako, Hiroshi, Prof. (Waseda Univ.)
Ito, Nobutoshi, Prof. (Tokyo Medical and Dental Univ.)
Kinoshita, Kengo, Prof. (Tohoku Univ.)
Standley, Daron, Dr. (iFReC, Osaka Univ.)
Katoh, Kazutaka, Dr. (CBRC-AIST)
Tsuchiya, Yuko, Dr. (Ochanomizu Univ.)

Contacting

PDBj
Research Center for Structural and Functional Proteomics,
Institute for Protein Research (IPR), Osaka University
3-2 Yamadaoka, Suita, Osaka 565-0871, Japan
TEL (PDBj office): +81-(0)6-6879-4311
TEL (PDBj deposition office): +81-(0)6-6879-8634
FAX: +81-(0)6-6879-8636
URL: http://www.pdbj.org/