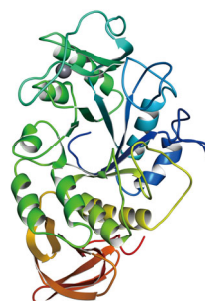
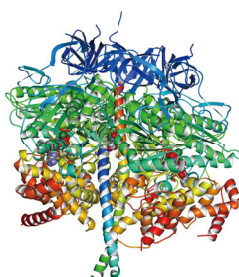
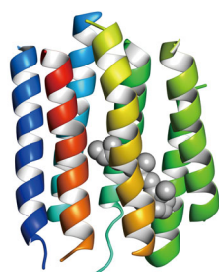
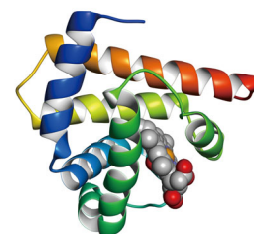
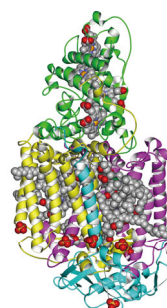
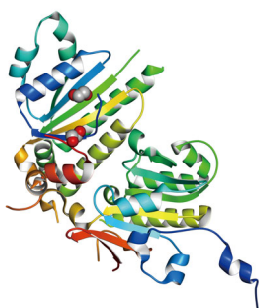
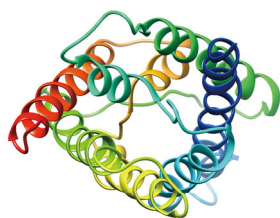
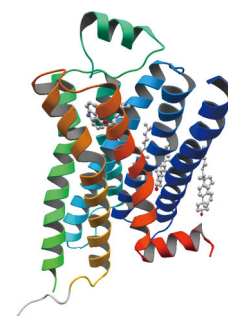
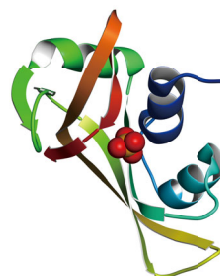
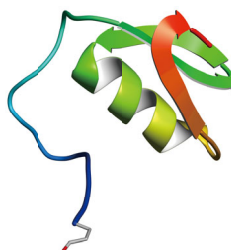
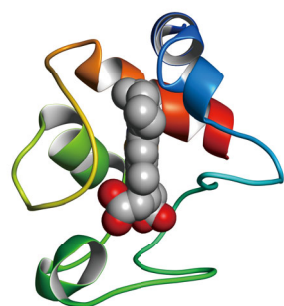
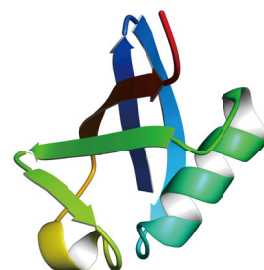
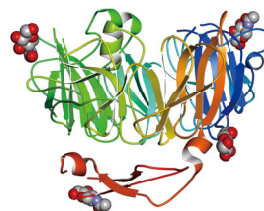
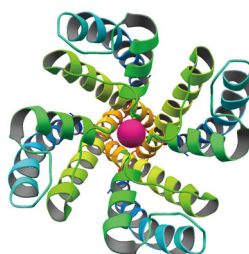
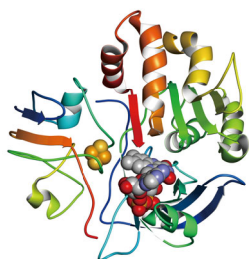
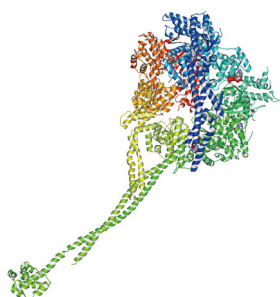
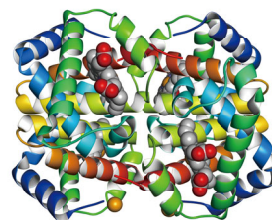


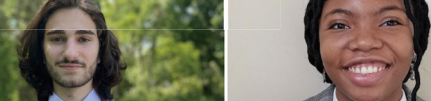
PDBj Newsletter

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PDB50 Award

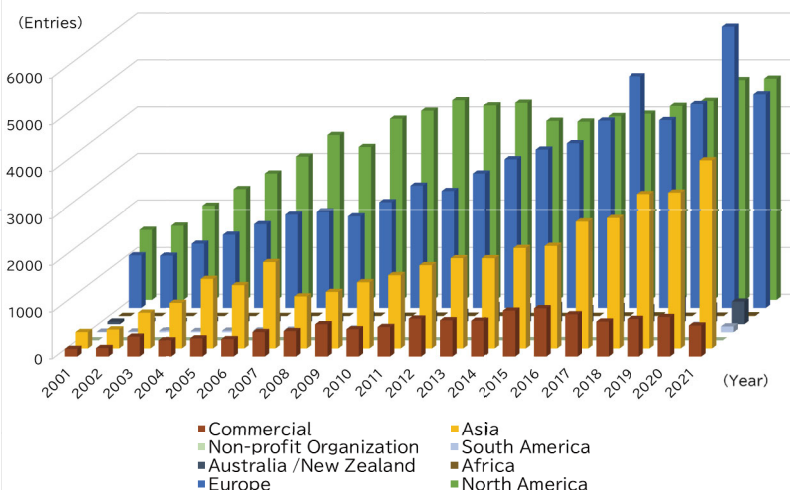
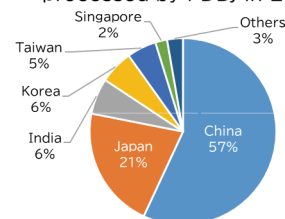


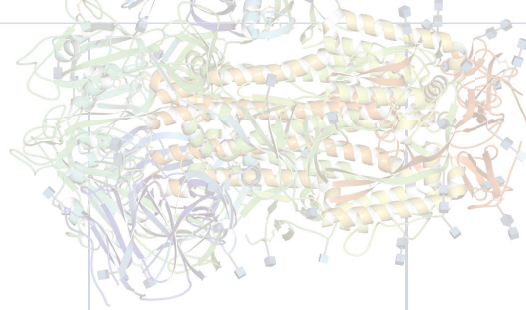
6PEY.pdb—a Novel Mutation in the Enzyme Methylenetetrahydrofolate Reductase

Best among Graduates: Daniel Sultanov; New York University; Mining for functional ribosomal variants in *Saccharomyces cerevisiae*

Best among Postdoctoral Scholars: Seda Kocaman; National Institute of Environmental Health Sciences;
Different ATP binding states of the essential AAA (ATPases associated with various cellular activities)-ATPase Rix7 facilitate substrate translocation in ribosome biogenesis

PDBj
**Data
Growth**





"PDB 50th Anniversary Symposium in Asia" and PDBj Poster Award

On Wednesday, November 24, 2021, the "PDB 50th Anniversary Symposium in Asia-Advanced Structural Biology in Asia and 50 Years of Protein Data Bank" was held online to commemorate the 50th anniversary of the PDB. The grand ceremony attended by over 300 Japanese researchers among other researchers from outside Japan was conducted successfully.

At the poster session, there were 78 presentations from 7 countries, mainly from within Asia, among which 57 presentations by students and young researchers were evaluated for the meritorious PDBj Poster Award.

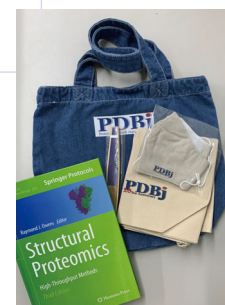
After a successful selection process, we are pleased to announce the following four winners and extend our sincere congratulations to them. All winners will receive certificates and supplementary prizes (books and PDBj novelty goods).

We would like to thank the judges of the poster awards for their cooperation. We would also like to express our gratitude to all the presenters who participated in the session.

- * "Structural Insights into the Clustering and Activation of Tie2 Receptor Mediated by Tie2 Agonistic Antibody" – Gyunghee Jo (Center for Biomolecular and Cellular Structure, Institute for Basic Science (IBS), Republic of Korea)
- * "Crystal structure of methylenetetrahydrofolate reductase from *Sphingobium* sp. SYK-6" – Hongyang Yu (Structural Biology Research Center (SBRC), Institute of Materials Structure Science, High Energy Accelerator Organization (KEK), and Department of Materials Structure Science, School of High Energy Accelerator Science, The Graduate University for Advanced Studies (SOKENDAI), Japan)
- * "Exploring the structural aspects of a novel phospholipid-binding protein" – Angshu Dutta (Department of Biosciences and Bioengineering, Indian Institute of Technology Guwahati, India)
- * "A new trend of protein crystallography: Polymorph analysis using hierarchical clustering of diffraction data" – Hiroaki Matsuura (RIKEN/SPRING-8 Center)

Poster judges :

Takao Arimori (Osaka Univ.), Toshimichi Fujiwara (Osaka Univ.), Shuya Fukai (Kyoto Univ.), Hiroshi Hashimoto (Univ. of Shizuoka), Kosuke Hashimoto (Osaka Univ.), Kunio Hirata (RIKEN/SPRING-8 Center), Takayuki Kato (Osaka Univ.), Takeshi Kawabata (Protein Research Foundation), Akihiro Kawamoto (Osaka Univ.), Jun-ichi Kishikawa (Osaka Univ.), Chojiro Kojima (Yokohama National Univ.), Hiroyasu Koteishi (Osaka Univ.), Genji Kurisu (Osaka Univ.), Yoh Matsuki (Osaka Univ.), Yohei Miyanoiri (Osaka Univ.), Kenji Mizuguchi (Osaka Univ.), Chioko Nagao (Osaka Univ.), Atsushi Nakagawa (Osaka Univ.), Nobutaka Numoto (Tokyo Medical and Dental Univ.), Takuji Oyama



(Yamanashi Univ.), Toshihiko Sugiki (Osaka Univ.), Masakazu Sugishima (Kurume Univ.), Junichi Takagi (Osaka Univ.), Hiroko Takazaki (Osaka Univ.), Hideaki Tanaka (Osaka Univ.), Sachiko Toma-Fukai (NAIST), Eiki Yamashita (Osaka Univ.)

* Ordered alphabetically based on the last name

We would like to express our sincere gratitude to the Protein Research Foundation for their generous support to this Symposium. The symposium was also conducted as a satellite event of the 59th Annual Meeting of the Biophysical Society of Japan and as an International Protein Research Seminar of the Institute for Protein Research, Osaka University. We would like to thank everyone for their support, contribution, and cooperation.

PDBj Topics

Deposition of Half-maps for Certain EM Entries Now Mandatory

As previously announced, deposition of half-maps for single-particle, single-particle-based helical, and sub-tomogram averaging reconstructions to the EM Data Bank (EMDB) has become mandatory with effect from February 25, 2022.

<https://pdbj.org/news/Mandatory-deposition-half-maps2> (February 25, 2022)

Distributing PDBx/mmCIF-Formatted Assembly Files

The structure files of biological assemblies have been provided in the PDB format, and we will start presenting them in the PDBx/mmCIF format from May 3, 2022. The chain IDs were not altered nor distinguished from the individual model ID chain when the chains were duplicated. However, unique chain IDs are assigned for every chain in biological assemblies in the new format.

https://pdbj.org/news/Assembly_files_mmCIF_format (February 2, 2022)

PDBj Publications

Protein Science

In commemoration of the 20th anniversary of PDBj activities, this paper introduces the history and recent activities of PDBj.

Protein Data Bank Japan: Celebrating our 20th anniversary during a global pandemic as the Asian hub of three dimensional macromolecular structural data, Gert-Jan Bekker, Masashi Yokochi, Hirofumi Suzuki, Yasuyo Ikegawa, Takeshi Iwata, Takahiro Kudou, Kei Yura, Toshimichi Fujiwara, Takeshi Kawabata, Genji Kurisu, Protein Science 31(1) 173-186 2022 doi:10.1002/pro.4211

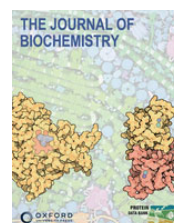
Journal of Biochemistry

The PDB 50th anniversary issue was released by the *Journal of Biochemistry* (JB).

<https://academic.oup.com/jb/issue/171/1>

Furthermore, the Protein Data Bank 50th Anniversary Virtual Issue "Featured structural articles from The Journal of Biochemistry" is also available [@https://academic.oup.com/jb/pages/protein-data-bank-50th-anniversary](https://academic.oup.com/jb/pages/protein-data-bank-50th-anniversary)

In this issue, we celebrate the 50th anniversary of PDB by highlighting the top 10 articles in terms of citation numbers and 5 articles with the highest resolution published in JB since 1971, along with two papers on the 1st NMR structure and one database article.



The "Togo no Hi" symposium 2021

At the "Togo no Hi Symposium 2021," an event held online on October 5, 2021, which was organized by the National Institute of Science and Technology Development (NIST), PDBj and BMRBj made online poster presentations to introduce our activities, and we discussed issues pertaining to data integration in life science.

SciDataCon

At "SciDataCon 2021: The Global Open Science Cloud Initiative," a conference held online on October 27, 2021, the XRDa, our new archive of raw X-ray diffraction images was introduced as a case study, which was authorized by the Committee on Data, International Science Council. Further development and utilization of XRDa were encouraged.

IPR retreat

We introduced PDBj/BMRBj's Data-in activities and Molmil, a web-based, lightweight molecular viewer, at the 19th IPR Retreat, held online on November 15, 2021.

Annual Meeting of the Molecular Biology Society of Japan

In the forum "How to use the databases and tools in life science" of 44th Annual Meeting of Molecular Biology Society of Japan held on December 2, 2021, we announced the improvement of the PDB/RDF archive initially written in an RDF graph data model which served for the extensive research in conjunction with PDB metadata and information stored in other databases. The PDB/RDF archive has been enhanced by integrating SIFT data, which can be linked with databases, such as UniProt and PDB, that assess consistency between experimental data and structure models.

Cooperation in the creation of computer graphics for the TV program "NHK Special"

The three-dimensional structural model of spike protein, a highly glycosylated and large type 1 protein created by Invitee Associate Professor Takeshi Kawabata was used in the NHK Special "Omicron strain: The Sixth Wave" which was broadcast on January 25, 2022, at 10:00 p.m. The PDBj also cooperated in the creation of the CG of the coronavirus used in the NHK specials aired in 2020 and 2021.



Chem-Bio Informatics Society (CBI) Annual Meeting

A sponsored session was held online on October 26, 2021, in collaboration with Cambridge Crystallographic Data Centre (CCDC) at the 2021 Congress of the Society for Computational Biochemistry and Information (CBI).

During the session, the activities of PDBj in the pandemic and for quality improvement and validation of structural data and a case study of structural refinement were presented by BUSTER using CSD, which was used by wwPDB for data validation.

Annual Meeting of the Japanese Biochemical Society

At the Annual Meeting of the Japanese Biochemical Society held online from November 3 to 5, 2021, the review of the PDB entries was reported in the *Journal of Biochemistry* published by the society since 1925. The title of the poster presentation was "50 years of Protein Data Bank in the Journal of Biochemistry." A statistical analysis of all 317 structural reports in J. Biochem. has already been carried out using the relational database system at PDBj and reviewed according to the yearly distribution, resolution, quality of structure, type of target protein, number of citations, and comparison against other major journals.

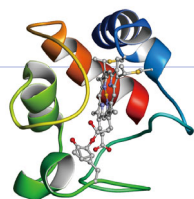
Integrated Database Workshop: AJACS

Invited Associate Professor Takeshi Kawabata gave a lecture on how to read PDB data, how to use Molmil, a molecular viewer, and HOMCOS, a homology modeling service, at the online course "Using Protein Databases" (AJACS Online 10) held by the National Bioscience Database Center (NBDC) on Thursday, January 20, 2022.

The movie of the lecture is available at the following URL (in Japanese).

<https://youtu.be/Iapa-dAwmpU>





The first protein structure determined in Asia

The first protein structure deposited in the PDB from Asia was the structure of bonito cytochrome c, solved by Prof. Masao Kakudo's group (PDB ID: 1cyc). Based on this information, in my previous talks I referred to the structure of bonito heart cytochrome c as the 1st protein structure solved in Asia. However it came out that there was another structure independently solved but wasn't deposited to

PDB. A colleague kindly told me that Prof. D. C. Hodgkin, a Nobel laureate reported in the IUCr congress held in Kyoto in 1972 that there was another structure of insulin independently solved in China, which surprised many crystallographers in the world. I have checked the abstract of the IUCr congress, 1972 held in Kyoto and found that the 5th talk was given by Prof. Kakudo on the cytochrome c structure at 2.3 Å resolution, the 4th talk was by Prof. Hodgkin on the insulin structure at 1.9 Å, and the 3rd talk was by Prof. N.

Sakabe on the isomorphous phasing of rhombohedral insulin crystal at 3.1 Å. This episode clearly shows that there were two protein structures available in Asia at that time. Since I cannot read Chinese though I can understand its characters, I asked our librarian to download a copy of the article in the journal Scientia Sinica from 1972, written in Chinese with the title "2.5 埃分辨率胰岛素晶体结构的研究 (the English translation is 2.5 Å structure analysis of insulin crystal)" and checked the main text mentioning 4.0 Å structure in 1970 and 2.5 Å in 1971. Regarding the bonito heart cytochrome c structure, I have studied the original articles in the Journal of Crystallographic Society of Japan written in Japanese and in the Journal of Biochemistry in English published by the Japanese Biochemical Society from 1925 and found that the structure of the bonito cytochrome c at 6.0 Å was presented in the International Biochemical Society meeting held in Switzerland in 1970, whose abstract cover was the e-density map of bonito cyt c. The 4.0 Å structure was published in J. Biochem. in 1971, while the 2.3 Å structure was presented in IUCr1972, as mentioned above. I would like to correct my previous statements about the first protein structure in Asia and expressing my sincere respect for the significant pioneering works in China and Japan, I will not try to determine which structure was solved first in Asia, but will say instead that "there were the first two structures in Asia solved at the same period."



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