

Protein Data Bank Japan (PDBj) Advisory Committee (PDBj-AC) Meeting via Zoom

Meeting Minutes

Date and Time: 13 March 2024, 13:00-14:30 (JST)

In Attendance (Zoom):

Prof. Genji Kurisu, Head of PDBj, Institute for Protein Research (IPR), Osaka University

Prof. Yohei Miyanoiri, IPR, Osaka University

Prof. Kaoru Mitsuoka, Research Center for Ultra-High Voltage Electron Microscopy, Osaka University

Dr. Masaki Yamamoto, Advanced Photon Technology Division, RIKEN SPring-8 Center

Dr. Satoshi Sogabe, Principal Scientist, Axcelead Drug Discovery Partners, Inc.

Prof. Chwan-Deng Hsiao, Academia Sinica, Taiwan

Prof. Kyeong Kyu Kim, Sungkyungkwan University School of Medicine, Korea

Observers from JST Department of NBDC program:

Dr. Takashi Ito, Professor, Department of Basic Medicine, Kyushu University

Dr. Takeshi Yoshioka, Senior Staff

Dr. Toshio Ota, Senior Staff

Apology:

Prof. Daisuke Kohda, Medical Institute of Bioregulation, Kyushu University

Prof. Toshiya Senda, Institute of Material Structure Science, High Energy Accelerator Research Organization

Topics:

1. PDBj activity report for 2023
2. PDBj activity plan for 2024
3. Others

The meeting commenced at 13:00. Prof. Kurisu met with committee members online, thanked their cooperation and introduced a new advisor, Dr. Sogabe. He also appreciated attendance of observers from a funding agency, Department of NBDC of Japan Society of Science and Technology (JST). Prior to the scheduled agenda, members confirmed a meeting minutes for the previous year.

1. PDBj activity report for 2023

Prof. Kurisu reported PDBj activities implemented in 2023 including: status of the core archives, project meetings, workshops/seminars for researchers, outreach activities as well as related events of worldwide Protein Data Bank (wwPDB).

- Basic statistics of PDBj and BMRBj showed the total number of depositions, EM depositions to PDBj+PDBc, BMRB depositions with ratio by country/region, access statistics together with deposition numbers for Electron Microscopy Public Image Archive (EMPIAR), X-tal Raw Diffraction Archive (XRDa) and Biological Structure Model Archive (BSMA).
- Among project meetings, Prof. Kurisu explained the importance of wwPDB PIs meeting held on irregular basis. PIs are always flexible to discuss any issues in order for quality maintenance of databases.
- Things almost went back to normal after the COVID-19 pandemic, and PDBj joined several on-site academic meetings. All of them were so fruitful that PDBj and wwPDB could show substantial presence there.
- In commemoration of 20 years of wwPDB partnership, PDBj lead wwPDB student prize in the 61st Annual Meeting of the Biophysical Society of Japan. Three students awarded prize for their outstanding oral presentation.
- PDBj supported PDB China (PDBc) very much in data annotation. A lead annotator of PDBj assigned entries to PDBc biocurators. Ratio of annotation to the entire entries from mainland China was around 25%.
- Number of entries from mainland China was reported. Since the number was increasing dramatically, it was explained that the stable data annotation to the entries from Asia could not be achieved without PDBc.
- EMPIAR-PDBj activity was successful last year, however the the entire size of archive was too big for PDBj to keep it identical to that in EBI. Based on the discussion with EBI EMPIAR team, PDBj will focus on the entries from Asia and frequently downloaded entries. Also, based on the bilateral agreement between EBI and PDBj, PDBj has started compression of some entries to save the disk space. Entries not stored in the EMPIAR server will be stored in LTO tapes and will be provided on demand format from the tape.
- PDBj appreciated active participation of Prof. Senda as well as Prof. Hsiao in the virtual wwPDB Advisory Committee Meeting (wwPDB AC) last year hosted by EMDB on 27 October 2023 (GMT). It was announced that Kyle Morris had joined EMDB as a new team leader last year.
- A paper was published to announce the launch of Protein Data Bank China (PDBc) as an associate member of the wwPDB. It described how community members welcomed PDBc, established mechanisms for adding new wwPDB data centers and the processes developed to bring PDBc in the partnership.

2. PDBj activity plan for 2024

- Prof. Kurisu reported PDBj activity plan for 2024: scheduled activities including regular team meetings, the attendance plan to the local society meetings and/or outreach activities. As a representative regional data center in Asia, PDBj is planning to organize a luncheon seminar at the ICMRBS 2024 in Seoul, Korea, in August. One of the speakers would be Prof. Miyanoiri, who is a member of BMRBj.

- One of the important activities of PDBj this year would be to host the wwPDB Advisory Committee Meeting together with OneDep Summit Meeting in mid-October in Japan with the venue at the Institute of Protein Research (IPR), Osaka University.
- Most updated information for the funding situation are reported as follows: 1) MEXT Japan approved the activity plan of joint usage/research to be performed by IPR. Prof. Nei-Li Chan, National Taiwan University has been officially appointed to join our AC in replacement of Prof. Chwan-Deng Hsiao from Taiwan, who is retiring from his institute shortly. 2) Main grant from JST-NBDC is supporting the development of a portal site integrated with the genome databases, especially with jMorp in Tohoku University. 3) Our second important research fund, a grant from AMED is supporting the database of Integrated/Hybrid method named PDB-Dev that includes the Neutron crystallography/XL-MS/SAXS/SANS etc. PDBj is providing the GPU server machine for cryo-EM users by the financial support from AMED.
- PDBj will keep biocuration activity at the branch lab located at the IPR Foundation.
- PDBj will continuously support PDBc.
- Once again, PDBj would like to appreciate Dr. Hsiao's contribution to this committee meeting. Especially on the issue of regional assignment of entries from Taiwan and Hong-Kong, his insights and community network helped very much.

3. Comments and questions from the advisors

- At the end of agenda, Prof. Kurisu was requesting all attendees for any questions and comments.
- Prof. Kyeong-Kyu Kim concerned about the predict structures, especially by AlphaFold.
 - ✧ Prof. Kurisu replied in two points; as a Data-in activity the wwPDB started curating the AlphaFold DB information already but did not collaborate with Deep Mind. As the Data-out activity, PDBc team has a collaboration with DeepMind, but PDBj has not. PDBj has a plan to provide the predicted structure information carefully distinguishing it from the experimental data.
- Dr. Satoshi Sogabe asked about the security policy about the integrated use of genome data from Tohoku University, which include human genome data from cohort study and also about the data deposition from big pharma companies.
 - ✧ Prof. Kurisu answered that PDBj will only take the open data from jMorp and welcome big data from pharma companies. Actually, Prof. Nakamura developed semi-automatic refinement system for researchers from pharma companies.
- Dr. Masaki Yamamoto asked the archiving policy of XRDa and EMPIAR-PDBj, because the size of the entries in these archives must be really big and a threat to the machine operation.
 - ✧ Prof. Kurisu replied that PDBj will focus on the new type of experimental data, e.g. recorded by newly developed detector etc. He also answered that current limit of PDBj's disk is 3PB honestly. If PDBj may accept more data from the community, some of them must be stored in LTO tapes or blue ray disks.
- Prof. Kaoru Mitsuoka asked the change of Cryo-EM depositions near future.
 - ✧ Prof. Kurisu replied that wwPDB will develop more new function of deposition and validation, but the resource is limited.
- Prof. Takashi Ito, as a program supervisor of JST NBDC project, acknowledge the contributions from advisors and announced a mid-term evaluation to PDBj in Oct 2024, and also expressed his strong wish to a success of collaboration between PDBj and jMorp.

Attended members approved all the discussions and the advisory meeting concluded at 14:30.