

**Protein Data Bank Japan (PDBj) Advisory Committee (PDBj-AC)
through Zoom online video conferencing system**

Meeting Minutes

Date and Time: 10 March 2022, 10:30AM(JST)

In Attendance (Zoom):

<Osaka>

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

Prof. Toshimichi Fujiwara (IPR, Osaka University)

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

<Fukuoka>

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

<Tsukuba>

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

<Hyogo>

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

<Seoul>

Prof. Bong-Jin Lee (College of Pharmacy, Seoul National University)

<Taipei>

Prof. Chwan-Deng Hsiao (Academia Sinica, Taiwan)

Apology:

Dr. Junichi Saito (Institute for Small Molecule Drug Discovery, Kyowa Hakko Kirin Co. Ltd.)

Observers:

<Tokyo, from National Bioscience Database Center (NBDC)>

Dr. Takashi Ito

Professor, Faculty of Medical Sciences, Kyushu University

Research Supervisor, Database Integration Coordination Program (DICP),

Ms. Mari Iwashima, Director

Mr. Tetsu Kawaguchi, Manager

Dr. Takahiro Ide, Researcher

Dr. Toshio Ota, Senior Staff

Ms. Izumi Kinoshita, Staff

Ms. Yukiko Okamoto, Staff

Topics:

1. PDBj activity report for 2021
2. PDBj activity plan for 2022
3. Others

The meeting commenced at 10:30. Prior to the discussion, Prof. Kurisu met with committee members and thanked their cooperation. He also appreciated attendance of observers from a funding agency, National Bioscience Data Base Center (NBDC) of Japan Society of Science and Technology (JST).

1. PDBj activity report for 2021

Prof. Kurisu reported PDBj activities implemented in 2021 including: project meetings, workshops/seminars for researchers or depositors, outreach activities as well as related events of worldwide Protein Data Bank (wwPDB). All of them were organized online due to Covid-19.

- Among them, he picked out two important anniversary meetings. One was PDB50: a special symposium celebrating the 50th anniversary of the Protein Data Bank in May 2021 organized by wwPDB. The other was PDB anniversary symposium in Asia in November 2021 organized by PDBj with active participation of more than 300 local and international scientists from Asia.
- As a part of anniversary activities, two special issues of academic journals edited/contributed by PDBj members were introduced. One of them is a special issue of the Journal of Biochemistry whose cover image is the molecule of month by David S. Goodsell.
- PDBj basic statistics are shown. They included: total number of depositions to PDBj, EM depositions, BMRB depositions with ratio by country/region, access statistics together with deposition numbers for Electron Microscopy Public Image Archive (EMPIAR), X-ray Diffraction Archive (XRDa) and Biological Structure Model Archive (BSMA). It is summarized that: number of depositions (from Asia and Middle East) are still increasing, fluctuated seasonally, and high in winter. Roughly fifty percent of them are coming from mainland China. Number of EM depositions were rapidly increasing, implying the growing number of Cryo-EM machines in Asia.
- Prof. Kurisu appreciated active participation of Prof. Senda as well as Kohda in the online wwPDB Advisory Committee Meeting (wwPDB AC), hosted by EMDB on 19 October 2021 (GMT). Prof. Jennifer L. Martin (Australia) nominated by PDBj was elected from Asia/Pacific region as the next chairperson of wwPDB AC.
- Among various topics, hot issue discussed was the data ecosystem, including raw image archives and AI-based predicted structure model archives. We will discuss further how to interact with these new archives.
- Question from the AC members;
 - ✧ Prof. Senda asked why PDB only depositions were allowed in the statistics. Prof. Kurisu answered that they must be related to the previously deposited EM maps in EMDB. All PDB depositions are now deposited with experimental data and accompanied by validation report updated recently.
 - ✧ Prof. Senda asked how to welcome PDB China to the wwPDB. Prof. Kurisu replied a corresponding part of wwPDB Charter describing that PDB China would be an associate member first with some limited activities. After evaluation of their performance by the existing wwPDB core members, they will be a core member. Procedure is step-by-step.
 - ✧ Prof. Hsiao asked the possibility and rule of depositing the AlphaFold-based/assisted structures to PDB. Prof. Kurisu answered that purely computational models are unable to be deposited to PDB, however the models calculated by the integrated/hybrid methods can be deposited to PDB-Dev which will be merged to PDB in future.
 - ✧ Prof. Yamamoto asked the regional differences in the ratio of MX and 3DEM and in the average resolution and molecular size of entries. Prof. Kurisu indicated a big increase of 3DEM but showed his personal view of potential differences between Asia and Europe/America because he did not have

specific numbers. A trend in Asia will usually follow those in Europe/America with a few years delay. Prof. Mitsuoka commented that the resolution may not be so different.

- ✧ Prof. Senda asked whether the method-based number of entries by country/region was publicly available or not. Prof. Kurisu answered that that number is not public but may be provided if needed.

2. PDBj activity plan for 2022 (Prof. Kurisu)

- Prof. Kurisu reported activity plan of PDBj in 2022. Scheduled activities including in-house regular meetings, society meetings and/or outreach activities were introduced. Some of them are still supposed to be on-line.
- New PDBj representatives for the 2022 wwPDB Advisory Committee Meeting organized by RCSB, were appointed. Prof. Senda and Prof. Hsiao accepted the offer. Currently, on-site meeting is scheduled in the US. However, on-line participation is possible depending on the travel guideline of representative's country.
- Funding to PDBj will be updated: 1) MEXT approved the activity of joint usage/research performed by the Institute for Protein Research, 2) a grant-renewal application for JST-NBDC for April 2022- March 2027 is under review. Our new application is focusing on the several sub-projects facilitating the data-driven activities suitable for AI-based research using the linked data of PDB, 3) a grant-renewal application for AMED for April 2022-March 2027 was submitted as a member of big structural biology consortium.
- New branch lab of PDBj was introduced. It will be located at the Protein Research Foundation close to Osaka University.
- New Data Ecosystem plan under the wwPDB brand was introduced. PDBj will participate in the raw image archive of MX.
- Start-up plan for PDBc has been approved by the wwPDB AC. Current timeline states that Chinese biocurators would be invited to Japan for on-site training hopefully in April. Important trainings such as on ethics and equipment set-up will be taken place one by one with careful consideration.

3. Others

At the end of discussion, Prof. Kurisu was requesting all attendees for any questions and comments.

- Prof. Senda raised a question on the long-term plan for sustainable operation of PDBj in terms of human resources. Prof. Kurisu explained the current employment status of PDBj staff members together with possible plan to hire new young biocurators from April 2022.
- Prof. Senda asked the status of deposition by sub-tomograph averaging. Prof. Kurisu answered that it was potentially important, but its number was not so big.
- Prof. Yamamoto asked the divided numbers of PDBj's budget by each funder. Prof. Kurisu showed the rough numbers and percentiles.
- Prof. Senda also gave an important question on budget for PDBj for long-term basis. Prof. Yamamoto added a concern a stable budget after the next 5 years when competitive grants end. Prof. Kurisu greatly appreciated JST's continuous support for more than 20 years to make it stable. At the same time, he promised constant communication with the university stressing PDBj's unique contribution not only for academic but also for commercial users.
- As the final topic of the meeting, it was announced that the term as a PDBj-AC members for Dr. Bong-Jin Lee would end at the end of March 2022 because of his retirement from the university within 2022. Prof.

Kyeong Kyu Kim of Sungkyunkwan University School of Medicine, Republic of Korea is nominated as a successor. PDBj obtained his internal consent.

All the discussions were approved by attended members and the advisory meeting was concluded.