

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

Meeting Minutes

Date and Time: 6 March 2023, 10:00-11:30AM (JST)

In Attendance (Zoom):

<Osaka>

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

<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

<Suwon, Korea>

Prof. Kyeong Kyu Kim, Sungkyunkwan University School of Medicine

<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)>

Prof. Takashi Ito, Faculty of Medical Sciences, Kyushu University

Ms. Mari Iwashima

Mr. Tetsu Kawaguchi

Mr. Mutsumi Idani

Dr. Toshio Ota

Topics:

1. PDBj activity report for 2022
2. PDBj activity plan for 2023
3. Others

The meeting commenced at 10:30. Prof. Kurisu met with committee members, introduced a new advisor Prof. Kyeong Kyu Kim from Korea, and thanked their cooperation. He also appreciated attendance of observers from a funding agency, Department of NBDC of Japan Society of Science and Technology (JST).

1. PDBj activity report for 2022

Prof. Kurisu reported PDBj activities implemented in 2022 including: project meetings, workshops/seminars for researchers or depositors, outreach activities as well as related events of worldwide Protein Data Bank (wwPDB).

- As a remarkable topic of 2022, Prof. Kurisu announced the start of remote data processing by PDBc biocurators in September 2022, after having fruitful on-site training provided to two Chinese biocurators, Drs. Ma and Zhang, by PDBj. During training period, other RCSB PDB and PDBe helped to process overflowed entries from Asia. PDBc biocurators started to process the simple X-ray or Cryo-EM entries first. PDBj has taken care of all NMR entries or complicated entries of supramolecular complexes by Cryo EM, which were provided from mainland China.
- Basic statistics of PDBj and BMRBj were shown: 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-ray Diffraction Archive (XRDa) and Biological Structure Model Archive (BSMA).
- Biocuration at the branch office of PDBj in the Protein Research Foundation started successfully, supported by JST-NBDC.
- Prof. Kurisu appreciated participation of Prof. Senda as well as Hsiao in the online wwPDB Advisory Committee Meeting (wwPDB AC) hosted by RCSB-PDB on 14 October 2022 (US EDT). Official start of PDBc as an associate member (not core members) was announced. They will join a core member with full recognition of the present core members. PDBj will serve as a mentor.
- Total access to PDBj servers including www, ftp and rsync were shown. Data-out activities were increasing as well.
- Outreach activities by PDBj were shown. In AsCA2022 meeting in Jeju, Korea, PDBj prize was awarded to Dr. Hyunmin Kim from Seoul National University, Korea.
- Questions from the AC members:
 - ✧ Prof. Senda was seeking clarification how to share processing activities of Asian entries between PDBj and PDBc. Prof. Kurisu explained the current situation that only simpler depositions were assigned to PDBc, which is 6% of the entire Asian entries. PDBj is still responsible for the entire Asian entries including the entries processed by PDBc. In the future, when PDBc biocuration is fully worked and can cover all entries from Mainland China, he added that Oceanian entries that is currently processed by RCSB, would be transferred back to PDBj.
 - ✧ Prof. Senda sent a 2nd question about the status of EMPIAR database at PDBj (EMPIAR@PDBj). Prof. Kurisu strongly encouraged raw data depositions to PDBj for brokering the data to EBI for their curation. All EMPIAR entries were once downloaded from EBI and then PDBj selected the LTO tape-archiving entries to save the disk space. Current disk space for EMPIAR at PDBj was 2.5 PB.
 - ✧ Prof. Yamamoto asked how to access to data that were archived in the LTO tapes. Prof. Kurisu answered two options: 1) ask PDBj to restore the data to EMPIAR@PDBj, 2) download from EMPIAR@EBI through globus.

- ✧ Prof. Yamamoto asked whether PDBj can accept any kind of raw images including Cryo-EM and XRD. Prof. Kurisu replied that PDBj focused on the raw images that were linked to the PDB/EMDB entries, which means PDBj want to exclude the images of cells and include the diffraction images from Neutron or MicroED. Images from SFX experiments would be also acceptable but depend on the disk space prepared by PDBj.

2. PDBj activity plan for 2023

- Prof. Kurisu reported PDBj activity plan for 2023: scheduled activities including regular team meetings, the attendance to society meetings and/or outreach activities were introduced. Many of them will be back to in-person style.
- Important ones are listed as follows: participation in the IUCr 2023 exhibition booth as a member of wwPDB and organizing a luncheon seminar in Taiwan Biophysical Society Meeting as a part of Asian regional activities.
- Preparation of PDB-Dev page in Japanese was announced.
- Prof. Senda and Prof. Hsiao will delegate PDBj once again to wwPDB Advisory meeting on-line, which will be hosted by EMDB in October 2023.
- Continuous support from PDBj to PDBc would be required under the concrete timeline and regular evaluation recommended by wwPDB Advisory Committee, in the aim of full launch of PDBc within 2-3 years, presumably.
- Updated information for the funding to PDBj follows: 1) MEXT Japan approved the activity of joint usage/research performed by the Institute for Protein Research; 2) main grant from JST-NBDC for 5 years from April 2022 was successfully renewed; and 3) second important research fund for 5 years from April 2022 as well, from AMED was successfully merged into that from a big structural biology consortium headed by one of our advisor, Prof. Yamamoto.
- Questions from the AC members:
 - ✧ Prof. Senda asked the ratio of Small molecules/Macromolecules by MicroED. Prof. Kurisu answered that more data of small molecule structures were solved by MicroED but less of macromolecules. The structural data of small molecules were deposited to CSD of CCDC. Prof. Kurisu noted that R-factors of small molecule structures solved by MicroED were usually high because of the dynamical effect. Therefore, the raw images of MicroED would be more important than the case of other methods. Prof. Kurisu is a chair of National Affiliated Data Center of CCDD in Japan, that is a different activity from wwPDB.
 - ✧ Prof. Hsia asked that PDBj was able to accept all Asian entries not only from Japan or not. Prof. Kurisu replied YES.

3. Others

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

- Prof. Kurisu greatly appreciated cooperation and community support from East Asia representing Taiwan and Korea in this committee.
- As the final topic of the meeting, replacement of an advisor from private company was announced. Dr.

Satoshi Sogabe, Principal Scientist, Axcelead Drug Discovery Partners, Inc. will succeed Dr. Saito from Kyowa Hakko Kirin for this committee from the next term starting from 1 April 2023. PDBj has obtained his internal consent.

- Prof. Kurisu acknowledged Prof. David Hsiao for his kind invitation to the Biophysical Society of Taiwan meeting.

- Questions from the AC members:
 - ✧ Prof. Kurisu highlighted that smooth start of PDBc was critical in the PDB activity in Eas Asian region. He continued to ask a friendly support from the community in Asia.

Attended members approved all the discussions and the advisory meeting was concluded.