

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

Meeting Minutes

Date and Time: 17 March 2021 11:00 AM(JST)

Venue: Conference Room, Institute for Protein Research (IPR), Osaka University, Osaka

In Attendance (Zoom):

<Osaka>

Prof. Genji Kurisu (Head of PDBj, 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))

<Shizuoka>

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

<Seoul>

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

<Taipei>

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

Apology:

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

Observers:

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

Prof. Takashi Ito, Program Organizer of Database Integration Coordination Program (DICP), and
Faculty of Medical Sciences, Kyushu University

Dr. Tetsu Kawaguchi, Manager

Dr. Takahiro Ide, Researcher

Dr. Toshio Ota, Senior Staff

Topics:

1. PDBj activity report for 2020
2. PDBj activity plan for 2021
3. Others

The meeting commenced at 11:00. Prior to the discussion, Prof. Kurisu met with committee members through Zoom online video conference system and introduced respective participant and observer. It was followed by

confirmation of previous meeting minute's draft (2020) by attendees. No further comments have been made.

1. PDBj activity report for 2020 (By Prof. Kurisu)

- Prof. Kurisu reported PDBj activities in 2020 with following items: PDBj's activities including workshops/seminars for researchers or depositors, outreach activities, PDB/EMDB/BMRB depositions to PDBj by country/region, Global PDB/EM deposition to world-wide PDB (wwPDB) by country/region, Global BMRB monthly statistics, BMRB depositions to PDBj-BMRB by country/region, PDBj access statistics and EMPIAR depositions from EMPIR-PDBj as well as access statistics.
- Among those activities and seminars affected by the spread of Covid-19, it was a good step forward to host an on-site luncheon seminar at the academic meeting outside of Japan (Asian venue: Symposium on the Federation of the Korean Societies of Biomolecular Sciences) in January 2020. Further opportunities are proactively considered.
- Annotation process was also affected by COVID-19. Due to prompt reaction to facilitate necessary equipment, however, annotation staff members were able to smoothly start work-from-home. Consequently, no delay and/or confusion in data-in activity was observed.
- In the capacity of PDBj advisory committee, data-in/data-out numbers indicated in this meeting are processed in and extracted exclusively for PDBj. Currently, wwPDB core members are discussing to establish a joint policy to officially report combined numbers on wwPDB.org to the authorities concerned. Identical global data are weekly released from 4 sites in UK, US and Japan, simultaneously.
- Our new activity was introduced, as a collaborative study with EBI in UK, to start a brokering site of EMPIAR, which archives raw images of Cryo-EM and helps Japanese depositors to deposit their big data. It is very important to take care of quality management of regional 3DEM data.
- It was reported that mirroring the data from EMPIAR in UK to EMPIAR-PDBj was continuing for 24/7. Although size of the stored data is terribly huge, it is processed slowly but steadily. Broker service for local depositor was also introduced: authors to mail HDD to PDBj and PDBj to upload the data to UK using Aspera through internet. With this service, 8 local depositors were provided assistance.
- It is reported that new organization of wwPDB was discussed and new MOU charter (effective as of 1 January 2021) is almost finalized. With this new charter, we will officially welcome PDB China located in Shanghai.
- wwPDB DOI resolution is also reported. In many cases, link destination from major journals is usually RCSB PDB and little consideration is given to other sites. It is encouraged that more requests are sent to various journals to establish the common wwPDB DOI landing page with links to regional PDB sites so that users can access and utilize closest regional PDB sites. Cooperation in Taiwan or Korea in this regard would be highly appreciated.
- Update on structure versioning is regarded as one of the important projects. Not only entries via OneDep, but versioning of entries via old deposition system are acceptable. After Covid-19 pandemic, more depositors use this coordination, which, we believe largely contributes to further improvement of the databases.
- When looking at 4 local sites, original plan of BMRB leadership transition was cancelled. Two offices of BMRB in Wisconsin and Connecticut were integrated, and the office in UConn Health became a new and single data center under supervisory of Prof. Jeffrey C. Hoch as a sole principal investigator. Fortunately, BMRB activity at PDBj was not affected by this unexpected transition.
- It was reported that new validation report of 3DEM was launched in January 2021 based on the outcome

of the wwPDB single-particle EM data-management workshop in January 2020 where Prof. Kurisu, Prof. Mitsuoka, Prof. Danev as well as other PDBj supporters in Asia had participated in. This new 3DEM validation report includes map-only validation and map/model validation, which is an important first step for us to keep the data of high quality. Related to this map/model validation, Prof. Kurisu reported the discussion about the models built based on the low/middle resolution 3DEM map in the wwPDB AC meeting last year, 2020.

- Prof. Hsiao gave a question if there are any database equivalent to EMPIAR in US. Prof. Kurisu replied NO and explained that he did not hear that RCSB was interested in a plan to archive raw image data of 3DEM. Prof. Mitsuoka raised a concern that EMPIAR-PDBj would reach an unmanageable situation in the near future due to a huge data size. Prof. Senda showed an expectation to find any clue to solve this issue, which is believed to be helpful for the community.
2. PDBj activity plan for 2021 (Prof. Kurisu)
- Prof. Kurisu reported activity plan of PDBj with the items listed as below.
 - In 2021, it is predicted that business meeting, workshop, and/or most of the society meeting as well as wwPDB advisory committee meeting would be organized through on-line or hybrid due to the negative influence of COVID-19.
 - wwPDB advisory committee meeting 2021 requires to nominate 2 PDBj delegates. Prof. Kurisu newly sought Prof. Senda's cooperation, in addition to Prof. Kohda who is currently serving this role.
 - Training plan for data-in/data-out activities for the staff members of PDB China and PDB India are now carefully planned for a successful start. It is delayed due to COVID-19 confusion. Data-in training for PDB Chain biocurators will be started using simple X-ray entries. It should be confirmed that new regional biocurators can process the variety of deposited data with identical quality to other existing data centers. It is expected for them to take some time to fulfill our requested biocuration quality.
 - wwPDB will take a same scenario when PDBj started local data processing 20 years ago. PDBj will help out all the steps. At the same time, PDBj realizes that we have the strong firewall (Grate firewall): OneDep system needs online communication with other servers for unreleased CCD assignment etc. We need careful consideration to various items, in addition unique internet system in China. In wwPDB Advisory Committee Meeting last year, delegates were discussing possible struggles and hardships coming from this issue.
 - Prof. Kurisu solicited a comment from Prof. Hsiao regarding Taiwanese and Hong Kong researchers' deposition through mainland China. He proposed to provide them options to choose sites through mainland China or through Japan. Prof. Kurisu appreciated Prof. Hsiao's acceptance of his proposed option and promised further discussion at wwPDB PI meetings or other equivalent opportunities
 - New archive of X-ray diffraction images (XRDa) started in 2020 was introduced. Prof. Kurisu explained the background of why PDBj started this new activity. There is no X-ray diffraction raw image archive in Asia. Active utilization of this archive is requested.
 - PDB50 memorial symposium in May 2021 hosted by wwPDB Foundation was also introduced. With all the PDB core members' presence, valuable presentations are listed. PDBj will cordially invite all the advisors to this meeting. Although it will be held at midnight in Asia, your participation would be appreciated.
 - In Asia, another PDB50 memorial symposium is scheduled as an on-line satellite meeting attached to the

59th Annual Meeting of the Biophysical Society of Japan on 24 November 2021. Prof. Kurisu was requesting international advisors to cooperate with PDBj in nominating key speakers.

- Prof. Lee pointed out at the end of report if number of depositions to PDBj was affected by COVID-19. Prof. Kurisu mentioned ‘partly’ since most of synchrotron facilities were closed and experimental research need to halt.

3. Others

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

- Prof. Hsiao started with a question about course of action on the improvement of EM validation report. Prof. Kurisu explained the current status of map itself and map/model validation. In the past, only simple structure chemistry was checked. PDBj realizes the current system is not sufficient. In the near future, wwPDB validation report will surely be further strengthened by provided half maps or other related maps.
- Prof. Hsiao gave an advice for the possibility of PDBj’s co-hosting a seminar at the biological society meetings in Taiwan.
- Prof. Senda explained the purpose of community letter submitted to wwPDB, to disclose depositor’s details under ‘To be published’ status. Prof. Kurisu forwarded information that it was being discussed and waiting for wwPDB Advisory Committee’s reaction.
- Dr. Saito mentioned, based on his personal opinion and not reflecting his company’s, difficulty in providing a lot of structural data stored in pharmaceutical companies to wwPDB in view of their in-house policy. Prof. Kurisu explained that wwPDB had so-called ‘group deposition’ system, which is currently only available at RCSB. Should the need arise, PDBj is willing to install the system.

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