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

Meeting Minutes

Date and Time: 28 February 2020, 15:00 (JST)

Venue: 4th Floor Seminar Room, Institute for Protein Research (IPR), Osaka University, Osaka

In Attendance (Zoom):

<Tokyo>

Dr. Midori Kamimura (Teijin Pharma Ltd.)

Prof. Kei Yura (Graduate School of Humanities and Science, Ochanomizu University)

<Osaka>

Prof. Genji Kurisu (Head of PDBj, IPR, Osaka University)

<Fukuoka>

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

<Seoul>

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

<Taipei>

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

Apology:

Prof. Toshimichi Fujiwara (IPR, Osaka University)

Prof. Tsuyoshi Inoue (Graduate School of Pharmaceutical Science, Osaka University)

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

Observers:

<Tokyo>

Dr. Toshiyuki Shingo (National Bioscience Database Center, Japan Science and Technology Agency (JST-NBDC)), one of funding agencies

<Osaka>

Prof. Takayuki Kato (IPR, Osaka University)

Topics:

- 1. PDBj activity report for 2019
- 2. PDBj activity plan for 2020
- 3. Others

The meeting commenced at 15:00. Prior to the discussion, Prof. Kurisu met with committee members through Zoom online video conference system and introduced new members and observers. At the same time, he briefly explained the situation about cancellation of face-to-face meeting due to spread of coronavirus (SARS-COV-2). It was followed by confirmation of previous meeting minute's draft (2019) by attendees. No further comments have been provided.

- 1. PDBj activity report for 2019 (By Prof. Kurisu)
- Prof. Kurisu reported PDBj activities in 2019 with following items: project meeting activities including meetings for researchers or depositors, outreach activities, PDB/EMDB 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.
- It was emphasized that wwPDB activities require close communication and collaboration between 4 local data centers based in UK, US and Japan for quality maintenance of the database. PDBj staff members participate not only regular online meetings but also to face-to-face seminars/workshops to discuss tasks and challenges.
- wwPDB single-particle EM data-management workshop was held at the European Bioinformatics Institute (EMBL-EBI) in January 2020 with participation of external experts. New policies on data management and validation have been fruitfully discussed. Output from the workshop is scheduled to be published on academic papers.
- Current situation of PDBj data-in activity was reported with statics in the Asian countries. It is obvious that roughly half of depositions are coming from China.
- ➤ In Asian region, almost 2/3 of the EM deposition were coming from China as well. World-wide perspective shows nearly half of the EM depositions are submitted from North American countries.
- New policy on BMRB deposition was reported.
- Current situation of PDBj data-out services was reported. The number is gradually increasing. In 2019, number of accesses were highest in June. PDBj is not sure of the reasons, but estimates it as a start of paper preparation.
- Deposition to EMPIAR database was reported. Currently, it is difficult to process raw data in PDBj. All the data submitted from Japanese researchers were forwarded to UK, which sometimes takes 4-5 days. Hopefully, PDBj handles all of those data locally in the future.
- ➤ One of the important PDBj events in 2019 was reported. PDBj hosted the wwPDB Advisory Committee Meeting on 18 October 2019 at IPR, successfully.
- ➤ Prof. Hsiao raised a question on the quality management of EM deposition. Prof. Kurisu explained the current status.
- > Dr. Kamimura pointed out how to synchronize data between UK and Japan. Prof. Kurisu explained the updated status.
- 2. PDBj activity plan for 2020 (By Prof. Kurisu)
- Prof. Kurisu reported activity plan of PDBj with the items listed as below.
- ▶ PDB China will launch in 2020. At the wwPDB advisory meeting, Prof. Wenqing Xu, one of the leadership team members of PDB China, introduced its outline: office location, key personnel, budget plan, proposed activities, and so on.
- PDBj and PDB China have started discussion on on-site training of staff members of PDB China. In specific terms, Prof. Kurisu together with technical staff of PDBj will visit PDB China offices in 2020 (with a condition that COVID-19 concerns are totally disappeared) to see facility and network status. Then a few annotation staff of PDB China will be invited to Osaka as a guest annotator of PDBj to carry out one-month (approximately) on-the-job training. Upon return to Shanghai, they will be provided on-line advice for data registration from Osaka. By the end of 2020, it is expected that PDB China annotation

- staff are able to go through entire annotation process by herself/himself. For the initial 1-2 years, under careful guidance of PDBj, annotators of PDB China will learn how to process deposited data: from simple data in all formats, gradually.
- In regard to start of PDB China data-in service, one critical concern was reported how to categorize deposition from Taiwan and Hong Kong (or Macau). Prof. Kurisu was requesting Prof. Hsiao to seek advice and insight from local community in this matter.
- Prof. Yura requested clarification of the specific location of PDB China. Prof. Kurisu explained that PDB China is located at National Facility for Protein Science in Shanghai (NFPS) and supported by NFPS and Shanghai Tech University, both of which are next each other.
- Prof. Kato made a comment that Great Firewall in China could be a challenging task for data processing. Prof. Kurisu totally agreed it. He is hoping that it will not turn to be an obstacle. OneDep curators are working on annotation by simultaneously operating multiple databases as well as processing systems with frequent update, which is requesting them to have not only substantial data transfer but also remote access from wwPDB partner sites. Even in some in-service offices, confusion has been observed and they cannot install up-to-date version of the systems. Prof. Kurisu emphasized that staff members of PDB China Datain should fully understand this entire picture of annotation.
- Prof. Kurisu went back to introduction of other scheduled PDBj activities in 2020. With great contribution of participants, it was reported that OneDep Developer Summit would be held through Zoom in April in spite of big time difference in UK, US and Japan. The wwPDB PI team believed that it would be mandatory to have this meeting regularly, hopefully twice a year.
- ➤ PDBj organized a luncheon seminar in FKSBS in Gwangju, Republic of Korea, on 10 January 2020. It was the first one held outside Japan. In this regard, Prof. Kurisu expressed appreciation for cooperation, great assistance and hospitality tendered by Prof. Lee, his lab members as well as his students.
- When we look at the long-term schedule, wwPDB will celebrate 50th anniversary in 2021. It was reported that Memorial symposium would be held on 5 May 2021 in Indianapolis, US. It was also reported that PDBj would organize a memorial workshop, for the researchers based in Asia, as a part of AsCA 2021 in Malaysia. Prof. Kurisu was seeking Profs. Hsiao and Lee's cooperation and collaboration in this matter to invite key researchers from Asian countries.
- > Current status of PDB/EMDB core archive was reported.

Others

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

- Prof. Lee gave a question about relation between PDBj and BMRB mirror site in Italy. Prof. Kurisu explained that only a copy of BMRB data-out service was located in Italy and no actual data processing was made.
- > Dr. Kamimura solicited Prof. Kurisu's comment on the long-term plan for EMPIAR. He explained that PDBj was currently focusing on single particle structure analysis. Now that number of structural data in high resolution using subtomogram averaging is increasing, he explained that PDBj has started discussion how to deal with these data.
- Prof. Hsiao pointed out that it was a good opportunity to organize a luncheon seminar in the academic conference outside Japan. He recommended further opportunity such as biophysical society meeting in Taiwan.

Last but not least, Prof. Kurisu reported termination of term for Dr. Kamimura, Prof. Inoue and Prof. Yura. He showed appreciation of their great contribution and cooperation to this advisory committee. As new members for the next term, he introduced Prof. Kaoru Mitsuoka, Research Center for Ultra-High Voltage Electron Microscopy, Osaka University and Dr. Junichi Saito, Deputy Director, Institute for Small Molecule Drug Discovery, Kyowa Hakko Kirin Co. Ltd. He also reported that Prof. Kohda as well as Dr. Yamamoto would serve a member of wwPDB Advisory Committee as a delegate from PDBj AC.

All the reports were approved by attended members and the advisory meeting was concluded at 16:40.