http://wwpdb.org

PDBj: Protein Data Bank Japan
Institute for Protein Research
Osaka University, 3-2 Yamadaoka Suita
Osaka, 565-0871, Japan
URL: http://pdbj.org
EMAIL: harukin@protein.osaka-u.ac.jp
Tel & Fax: 81-(0)6-6879-4310

Joint NMR VTF and NEF Workshop

Hosted by PDBj at the Institute for Protein Research (IPR) Osaka University, Japan

Organizers: John L. Markley (BMRB), Haruki Nakamura and Toshimichi Fujiwara (PDBj)

August 26-27, 2016

Sponsored by

JEOL Ltd., **Bruker BioSpin K.K.** **SI Science Co.,Ltd.**

Attendees

Name	Group(s)
A Bax	NMR VTF
RA Byrd	NMR VTF
P Güntert	NMR VTF, NEF
T Herrmann	NMR VTF, NEF
GT Montelione	NMR VTF, NEF
M Nilges	NMR VTF, NEF
T Polenova	NMR VTF
C Schwieters	NMR VTF, NEF
N Sgourakis	NEF
GW Vuister	NMR VTF, NEF
S Velankar	PDBe
A Gutmanas	PDBe
SK Burley	RCSB-PDB
J Westbrook	RCSB-PDB
K Baskaran	BMRB
P Romero	BMRB
N Kobayashi	PDBj-BMRB
JL Markley	Host, BMRB
H Nakamura	Host, PDBj
T Fujiwara	Host, PDBj-BMRB

Agenda

Friday, August 26

13:15 pm Bus will transport attendees at ICMRBS-2016 from the Conference site in Kyoto to IPR, Osaka University (Lunch will be served on bus)
Others will take taxi to IPR, Osaka University

3:30 pm Session 1

6:00 pm Transportation to hotel
7:00 pm Dinner at "China Table" (Chinese restaurant)
9:00 pm Return to hotel

Saturday, August 27

7:00 am Breakfast at hotel
8:00 am Transportation from hotel to IPR, Osaka University

8:30 am Session 2
10:30 am Coffee break

11:00 am Session 3
1:00 pm Lunch

2:00 pm Session 4
4:00 pm Coffee break

4:30 pm Session 5
6:30 pm Adjourn and Transportation to hotel

7:30 pm Dinner at "Ume-no-Hana" (Japanese restaurant)
9:30 pm Return to hotel

Sunday, August 28, 2016

Departure

Content of sessions

Session 1:

- Goals for the workshop (John Markley and Haruki Nakamura)
- Review of progress on NMR structure validation: PDB NMR validation report (Aleks Gutmanas)
- Review of progress on NEF design, implementation, and interconversion with archival format (Geerten Vuister and Pedro Romero)
- Approaches to the validation of structural restraints against structure (Guy Montelione)

Session 2:

- Issues with the current NEF format from the standpoint of software developers (software developers)
- Issues involved in the interconversion of NEF and NMR-STAR/PDBx (Kumaran Baskaran)
- NEF data dictionary (development and promulgation)
- Expansion of the NMR-STAR data dictionary required for NEF interconversion

Session 3:

- Next steps to be taken for expansion of the PDB validation report
    - Validation of chemical shift assignments against NOE peak lists
    - NOE-based distance restraints
    - Angular restraints derived from chemical shifts
    - RDC-based restraints
    - PRE-based restraints

Session 4:

- Continued discussion of expanded restraint validation
    - Restraints from: H-bonds, pseudo contact shifts, dipolar recoupling, spin-diffusion
    - SAXS-WAXS restraints
    - Coupled with modeling methods (CS-ROSETTA)
    - Additional hybrid methods

Session 5:

- Setting a deadline for the implementation of NEF as an option for deposition of structural restraints
    - Steps required to meet the deadline
        - Clear agreement on the scope of NEF
        - NEF data dictionary available at a publicly accessible site (wwPDB?)
        - Agreed upon plan for future expansion of NEF to accommodate new types of restraints
        - Testing and validation of NEF created by software programs for a variety of structures (single chain, multiple chains, protein, nucleic acid, etc.) for interoperation with NMR-STAR/PDBx
- Goals and deadlines for implementation of new validation approaches
    - Implementation of existing software as part of the PDB deposition system
    - New software needed
    - Development of a stand-alone validation system for users prior to deposition