

Summary of the NORMAN MassBank Workshop at Eawag, Sept. 17-18, 2014

Wednesday 17th September: Update on NORMAN MassBank

Over 70 interested listeners heard updates on the following (presentations available for download from the NORMAN Website):

- MassBank: A Japanese Perspective (Maranori Arita, NIG, Japan)
- NORMAN MassBank: Current State and Future Activities (Tobias Schulze, UFZ)
- RMassBank: Automatic Recalibration and Processing of Tandem HR-MS Spectra for MassBank (Michael Stravs, Eawag)
- Expanding RMassBank with XCMS/MetShot (Steffen Neumann, IPB)
- Enhancing Spectral Exchange: Tentative and Unknown Spectra, NIST and Crowdsourcing Trends (Emma Schymanski, Eawag)
- NORMAN Data Storage: Data Requirements and Examples (Tobias Schulze, UFZ).
- Live Metabolights Demo (Steffen Neumann, IPB).
- Discussion (summary below).

Discussion Points/Future Activities on Wed 17th Sept.

- NORMAN MassBank Web interface upgrade
 - Download MassBank data in different ways (see below)
 - Updatable news and activities
- More functionality to MassBank (development team)
 - MONA (MassBank of North America) will complement massbank.jp and massbank.eu soon, led by Oliver Fiehn.
- More spectra into MassBank
 - Offer training courses (suggestion: once a year)
 - Encourage people to add more spectra (e.g. missing targets from NT Trial)
 - Consider a NORMAN curator in the future (not 2015)
 - Encourage vendor support (Bruker converter, Agilent in discussion, ABSciex present)
 - Pursue active cross-linking of MassBank
 - Encourage people to use MassBank for Supporting Information
- Raw data storage is of interest to many, but independent of MassBank
- Curation of MassBank data to ensure quality
 - Some efforts towards this with MONA (MassBank of North America)
- Improve access to MassBank records
 - E.g. SVN versus downloadable zip versus NIST format
 - Offer alternatives on massbank.eu website
- Establish MassBank groups
 - MassBank user group – mailing list and/or forum?
 - Repositories: <https://github.com/MassBank/>

NORMAN MassBank Hands-on day: Thurs 18th Sept.

35 keen attendees were present on Thursday for a hands-on day of MassBank, RMassBank, RMassBankGUI and MetFrag/MetFusion. After introductory talks from Emma Schymanski (MassBank Interactive Demonstration, RMassBank Demo on Orbitrap data) and Steffen Neumann (Introduction to MetFrag/MetFusion and RMassBank GUI demonstration), participants worked on their own data in a really productive atmosphere. Two bottles of wine were up for grabs for the first participants who could provide MassBank records of their own data that could be uploaded to MassBank.

Participants were assisted by (alphabetical order): Erik Müller, Steffen Neumann, Christoph Ruttkies, Tobias Schulze, Emma Schymanski, Michael Stravs. Many thanks to them all for their efforts!

By the end of the day, six participant (groups) successfully uploaded MassBank records generated with their own data – see photo! Congratulations to Lee from Duke University who used RMassBank to convert his records and claimed the first bottle. Nikos, Pablo and Anna (University of Athens), claimed the second bottle using a Bruker conversion. Ronald and Martijn from Rijkswaterstaat and Thomas from Agilent were very, very close behind (within minutes), both using RMassBank. Christoph from INUA with more challenging DIA data managed his upload just before having to leave for the airport and the day was rounded out by Michael Stravs, who converted a MetaboLights dataset into records for MassBank. The workshop provided valuable feedback also to the developing team and will be used to further improve functionality to upload more spectra to MassBank.



Figure 1: Participants and volunteers hard at work during the NORMAN MassBank workshop. Inset: The resulting workshop database. Photo: R. Schaffner, Eawag.