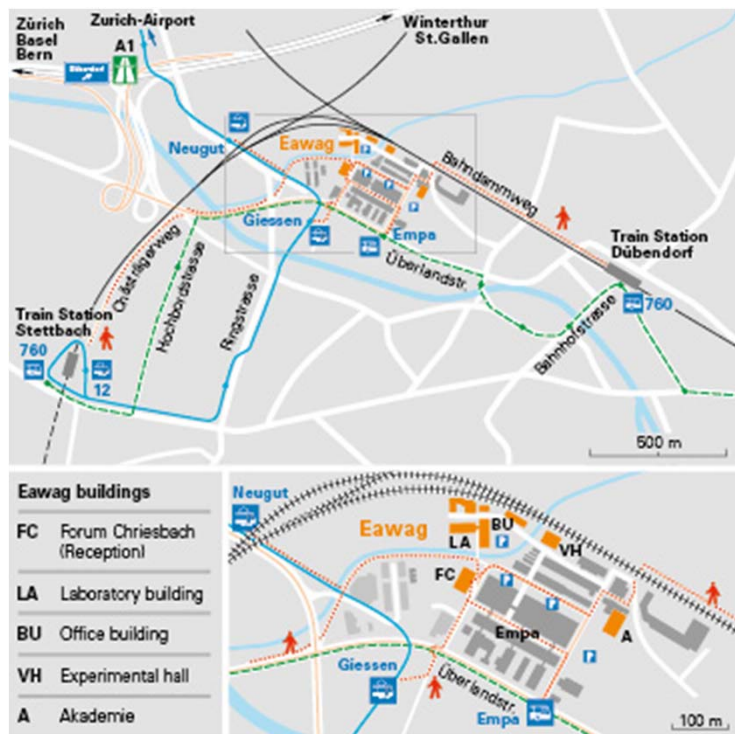


How to find Eawag:



Public transport

- From *Zurich Main Station (HB)* take the train S3, S9 or S12 to Stettbach. From there it is 20 minutes walk to Eawag (see map), or take tram No. 12 to “Giessen” or bus No. 760 to “Empa”.
- From *Zurich Oerlikon*, take the S14 train to Dübendorf and then bus No. 760 to “Empa”, or walk to Eawag, about 20 minutes (see map).
- From *Zurich-Airport*, take tram No. 12 to either stop “Neugut” or “Giessen” (about 20 minutes ride).

Car

- From the Motorway A1, take exit Dübendorf, to the right towards Dübendorf, 300 meters after the major crossing turn left into the Eawag-Empa premises. Parking tickets for visitors can be obtained at the reception if visitor bays are full.

For more details : http://www.eawag.ch/about/standorte/anreise_dd/index_EN

Contact: Emma Schymanski, Eawag: emma.schymanski@eawag.ch
Tobias Schulze, UFZ: tobias.schulze@ufz.de



eawag
aquatic research



Final Program

NORMAN MassBank Workshop 2014

Organised by

Eawag - Swiss Federal Institute of Aquatic Science and Technology
UFZ – Helmholtz Centre for Environmental Research (Germany)

On behalf of the

NORMAN Association Working Group 3 “Effect-directed
analysis for hazardous pollutant identification”

**17 September 2014 (14:00 – 18:00)
to 18 September 2014 (9:00 – 18:00)**

Eawag: Dübendorf, Switzerland

Room FC-C20 (first floor)

Attendance is free of charge.

For further information contact

Emma Schymanski, Eawag, Switzerland: emma.schymanski@eawag.ch
Tobias Schulze, UFZ, Germany: tobias.schulze@ufz.de
Steffen Neumann, IPB, Germany: sneumann@ipb-halle.de

RM|MassBank

<http://www.norman-network.net/>
<http://www.eawag.ch>



Background & Objectives

In 2011, the NORMAN Association joined the MassBank consortium and established NORMAN MassBank, www.massbank.eu/MassBank/, hosted at the UFZ and now acting as the main European MassBank server. Over 7,100 spectra of standard compounds have been added by NORMAN members to date, as well as literature and tentative/unknown spectra for the exchange of data.

This workshop is a dual purpose event. The first afternoon is a general information and discussion session about NORMAN MassBank, where attendees will be updated on the activities over the last two years and have the opportunity to discuss the future plans and potential contributions to NORMAN MassBank. Participants of all backgrounds and interests are welcome to attend. On the second day, those wishing to contribute data to NORMAN MassBank will have the opportunity to bring their own data, create and upload MassBank records of their own substances, with support provided by the team developing RMassBank.

Date and Venue

The workshop will take place on 17-18 September 2014 in Room FC-C20, Forum Chriesbach, Eawag, Dübendorf, Switzerland (see reverse). The room will be signposted. Eawag computers will be available on the 18th. WiFi will be available.

Lunch break and dinner

Participation in the workshop is free, including refreshments during the break on the first day. The remaining breaks and meals are not included. Please indicate special wishes for the meal at Sonnentag on the 17th (a list will be provided).

Preparation for the Workshop

Where possible, please pre-install the following:

- Java update <http://www.java.com/en/download/manual.jsp> (Version 7 Update 67)
- R <http://cran.r-project.org/>
- RStudio <http://www.rstudio.com/products/rstudio/download/>
- NIST Demo <http://chemdata.nist.gov/mass-spc/ms-search/>

If you intend to convert raw data into mzML files:

- Proteowizard <http://proteowizard.sourceforge.net/downloads.shtml>

For participants planning to bring their own data and contribute MassBank records, please send us a brief description of your data and what you wish to do prior to the workshop. This will help us greatly in anticipating how we can best help you.

For the exchange of large data files, we have set up a FTP site.

Windows Explorer: <ftp://massbank@ftp.eawag.ch/> or Host: <ftp.eawag.ch>;

User: massbank Password: MassBankEawag2014 (the first "a" is "@")

Please save your data in a well-named, unique directory under "RawData".



Final Program

Wednesday 17 September

Update on NORMAN MassBank Activities - Open to all

- 14:00 Welcome (J. Hollender, Eawag)
- 14:05 MassBank: The Japanese Perspective (M. Arita, NIG, Japan)
- 14:30 NORMAN MassBank: Current State and Future Activities (T. Schulze, UFZ)
- 14:50 RMassBank: Automatic Recalibration and Processing of Tandem HR-MS Spectra for MassBank (M. Stravs, Eawag)
- 15:10 Expanding RMassBank with XCMS/MetShot (S. Neumann, IPB)
- 15:30 **Coffee break**
- 16:00 Enhancing Spectral Exchange: Tentative and Unknown Spectra, NIST and Crowdsourcing Trends (E. Schymanski, Eawag)
- 16:20 NORMAN Data Storage: Data Requirements and Examples (T. Schulze, UFZ)
- 16:40 Applying Metabolomics Methods to Environmental Data (S. Neumann, IPB)
- 17:00 **Discussion and prioritisation of plans for NORMAN MassBank (all)**
- 18:00 Preparatory meeting for contributors participating on Thursday.
- 19:00 **Common dinner**, location to be announced at the workshop

Thursday 18 September

Contribute your own spectra to NORMAN MassBank - Open to contributors

- 9:00 Welcome: Plan for the Day (E. Schymanski, Eawag)
- 9:10 MassBank: Interactive Demonstration (E. Schymanski, Eawag)
- 9:30 Introduction to MetFrag and MetFusion (S. Neumann, IPB)
- 9:50 Metabolights Online Demonstration (S. Neumann, IPB)
- 10:10 **Coffee break**
- 10:30 RMassBank Demo on Orbitrap Data (E. Schymanski, Eawag)
- 11:00 RMassBank Demo on XCMS/MetShot (S. Neumann, IPB)
- 11:30 Questions/Discussion/Help/Free time
- 12:00 **Lunch**
- 13:00 Free time: hosts help participants to get to know MassBank & RMassBank
- 19:00 **Common dinner**, Restaurant Sonnentag (15 min walk)

NORMAN Association

NORMAN, a network of reference laboratories and research centres, is an independent and competent platform in the monitoring of emerging environmental contaminants. NORMAN facilitates an exchange of information, debate and research collaboration at the global level, with the European Union's in-house science service. See <http://www.norman-network.net/>.