Useful Links for Non-target Mass Spectrometry

Compound Databases

- ChemSpider
- PubChem
- Scifinder (login required)

Databases for MS/MS

- MassBank JP (cite Horai et al. 2010)
- MassBank EU
- Uchem MassBank (Eawag internal only!)
- METLIN (cite Smith et al. 2005)
- MetiTree (cite Rojas-Cherto et al. 2012)
- mzCloud
- NIST MS/MS (information only)

The MS and MS/MS Toolbox

- AMDIS (GC-MS)
- enviMass
- enviPat (molecular formula simulation)
- Formulator (Thermo Scientific)
- MetFrag (cite Wolf et al. 2010)
- MetFusion (MetFrag + MassBank)
- MZmine
- Proteowizard (file conversion with MS Convert)
- RMassBank
- R package "non-target"
- SIRIUS (cite Rasche et al. 2011)
- XCMS, XCMS Online and XCMS forum

MOLGEN (Structure Generation)

- MOLGEN 3.5 (structure generation, cite Benecke et al. 1997)
- MOLGEN 5.0 (newer version, structure generation)
- MOLGEN-MS (GC-MS interpretation and structure generation, cite Kerber et al. 2001, method extensions in Schymanski et al. 2008, 2012)
- MOLGEN-MS/MS (formula calculation with MS and MS/MS data, cite Meringer et al. 2011)

More Sources of Information

- Website of Tobias Kind: browse the menu for more links
- Metabolomics-Forum

Updated 22 April 2015, E. Schymanski