

# DEPARTMENT OF CHEMISTRY



## Other software and data analysis approaches

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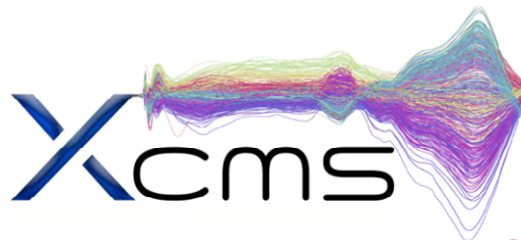
MS-SRF

Wednesday 7<sup>th</sup> December 2022

# Data processing/visualisation

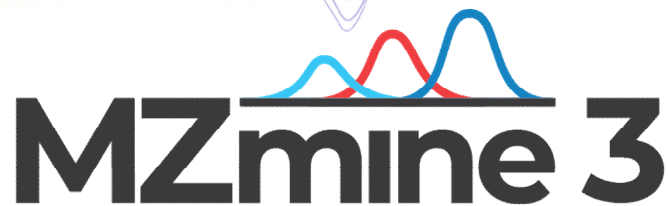
- XCMS

- <https://xcmsonline.scripps.edu>



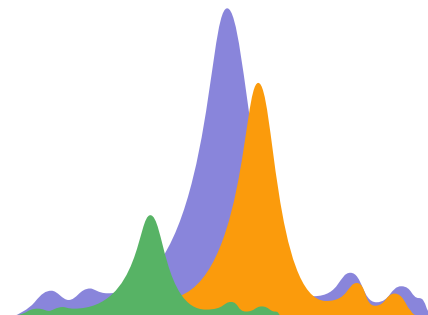
- Mzmine

- <http://mzmine.github.io/>



- EI-MAVEN

- <https://elucidata.io/el-maven/>



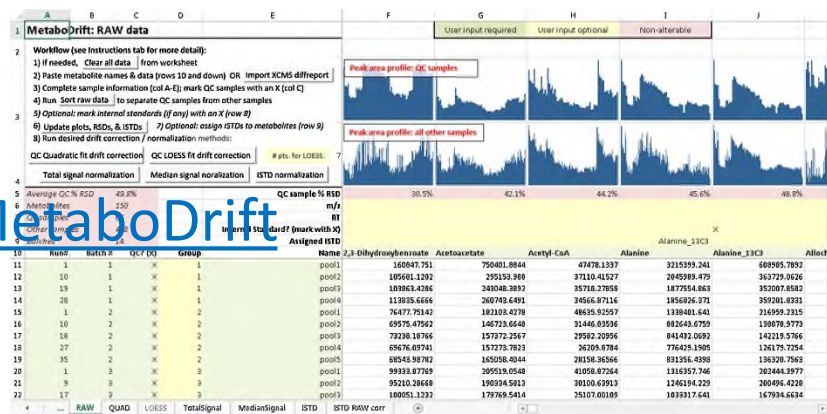
EI-MAVEN

# Conversion/peak detection/normalisation

- Vendor specific software
  - Convert to .csv or .mzXML
- ProteoWizard
  - <https://proteowizard.sourceforge.io/>

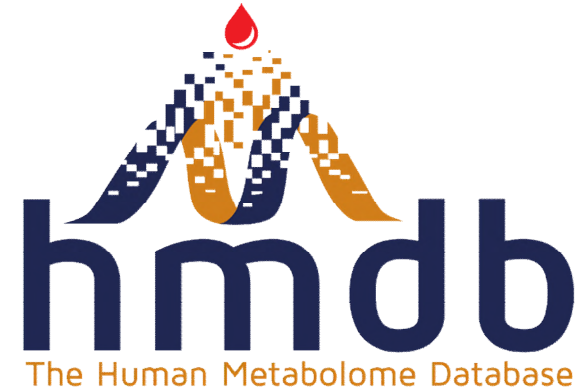


- MetaboDrift
  - <https://github.com/evanscr/MetaboDrift>



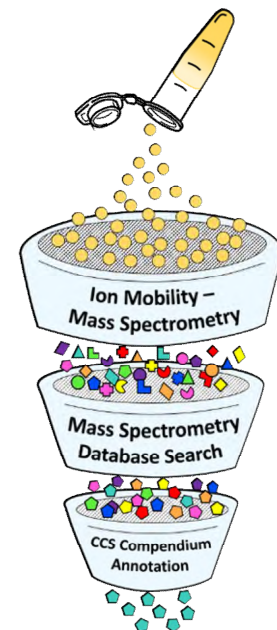
# Databases

- HMDB
  - <https://hmdb.ca/>
- BRENDA
  - <https://www.brenda-enzymes.org/>



# Compound feature identification

- Previous databases and vendor specific software
  - HMDB, METLIN, Compound Discoverer, etc.
- Metabosearch
  - <https://omics.georgetown.edu/tools/metabosearch>
- Unified CCS Compendium
  - <https://mcleanresearchgroup.shinyapps.io/CCS-Compendium/>

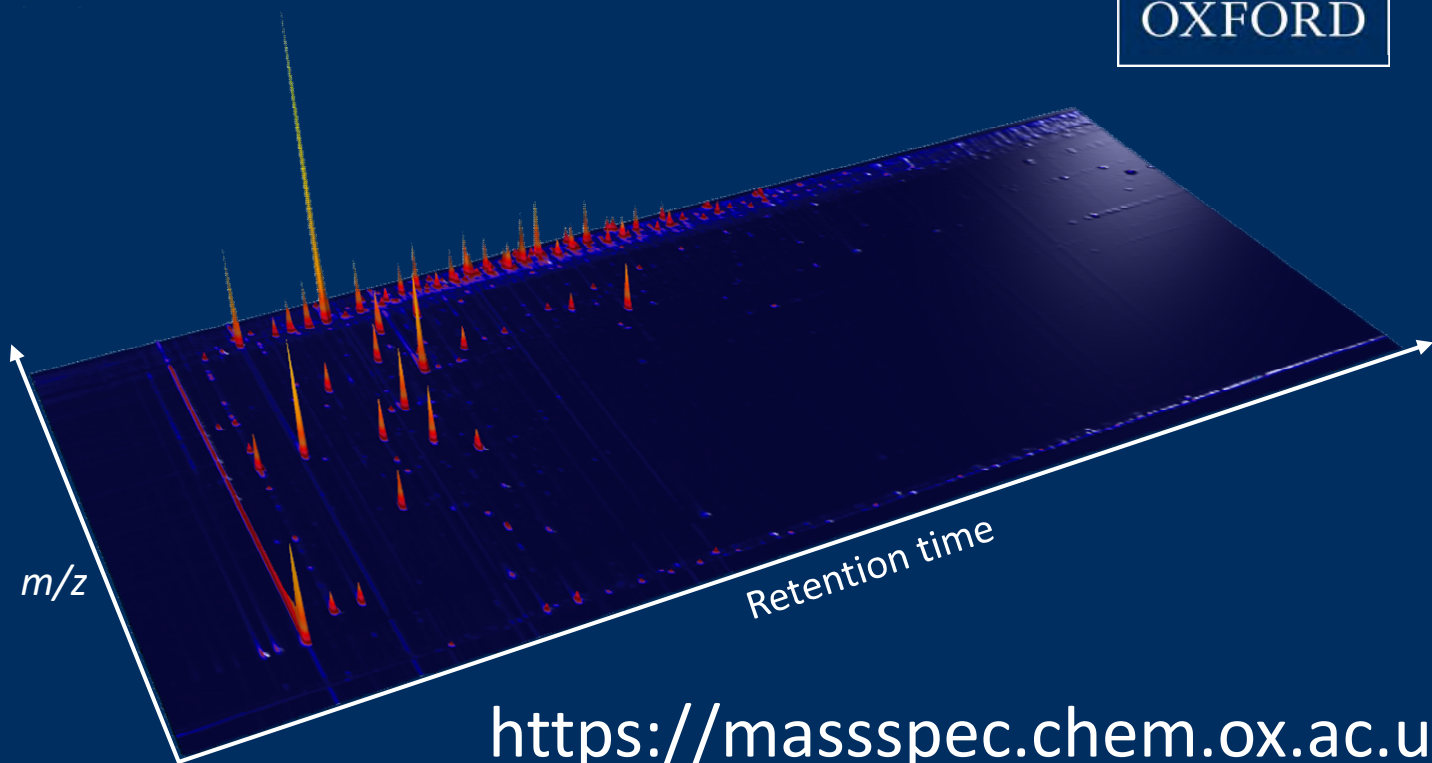


# Online data repositories

- ORA
  - <https://ora.ox.ac.uk/>
- Metabolights
  - <https://www.ebi.ac.uk/metabolights/>
- Metabolomics Workbench
  - <https://www.metabolomicsworkbench.org/>



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<https://masspec.chem.ox.ac.uk>