Metabolomics data analysis with GNPS and METASPACE

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Abstract
This course aims to explain how to use the METASPACE and GNPS platforms for large scale data analysis in mass spectrometry (MS) based metabolomics experiments. METASPACE couples advanced bioinformatics with high performance cloud computing to provide MS based annotations of Imaging MS and LC-MS datasets [1]. GNPS is an open-access knowledgebase for public sharing, processing, curation and annotation of tandem mass spectrometry (MS/MS) datasets, combining molecular networking with a community driven spectral library [2,3]. GNPS enables large scale metabolite identification through spectrum library matching and propagation of these annotations in spectral networks. Both platforms leverage the community as a resource, making cross referencing of samples and studies possible to enable researchers to perform analyses that would be impossible in a single lab.
For each platform, we will present some principles of modern data science, explain the bioinformatics for metabolite annotation as well as give a hands-on step-by-step tutorial on retrieving and annotating data, browsing annotations, and exploring the wealth of public data submitted by others. By the end of the course you should expect to understand the principles of false-discovery-rate controlled molecular annotation [4,5], be able to submit your data to our services, as well as to browse and export the metabolite annotations.

For the hands-on tutorials you need to bring your own laptop.
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References
1. http://metaspace2020.eu/
2. https://gnps.ucsd.edu/
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4. Palmer, A., et al., FDR-controlled metabolite annotation for high-resolution imaging mass spectrometry. Nature methods, 2017. 14(1): p. 57-60.
5. Scheubert, K., et al., Significance estimation for large scale metabolomics annotations by spectral matching. Nature Communications, 2017. 8(1): p. 1494.