



VMOL Seminar Series

Seminar Description:

This bi-weekly seminar series is targeted to give a general introduction to contemporary mass spectrometry and in particular how to analyze biomolecules. We will cover fundamental hardware principles on how a mass spectrometer works and application focused data analysis approaches. The seminar is meant to be very interactive and will have a large hands-on component for the data analysis tools.

The goal is to start from zero and bring everybody to a level of executing independently different mass spec data analysis tasks within a few sessions.

As the seminar will be very user focused, the content will only be set for the first lectures and will then evolve based on the participants interest. The idea is hereby that we will have guest lectures from experts in the field (e.g. mass spec software developers) as well as participants of the seminar who want to highlight their own data acquisition and data analysis approaches. That said, the seminar shall serve as a dynamic platform to teach and exchange ideas and concepts in mass spectrometry. The focus is now on advanced mass spectrometry-based metabolomics methods and multi-omics data integration.

Current Organizers:

Allegra Aron, Daniel Petras, and Ming Wang

Time:

The seminar will be held bi-weekly:

Every other Tuesday at 8:00 - 9:00 AM PST (17:00-18:00 CET)

Place:

The seminar will be held remotely through Zoom. The zoom link will be sent via email (you need to sign up through the link below).

Recording:

All seminar sessions will be recorded and uploaded to youtube here:

www.youtube.com/@functionalmetabolomics

Participants:

The seminar will be open to everybody. If you have friends/colleagues who you think could be interested in this, feel free to forward the information. For better exchange of information and announcements, we encourage you to **sign up with your email and some background information here: [LINK](#)**

VMOL Program 25/26:

[illegible]

Past Seminars and Recordings:

#	Topic	Youtube Link
1	Intro and Mass Spec Fundamentals (Ionization) Notes: Papers mentioned during the discussion: Single cell metabolomics: https://www.nature.com/articles/s41592-021-01333-x https://www.nature.com/articles/s41592-021-01198-0 Single cell proteomics: https://www.nature.com/articles/d41586-021-02530-6 https://www.biorxiv.org/content/10.1101/2020.12.22.423933v2 Human skin molecular mapping: https://www.pnas.org/content/112/17/E2120	https://youtu.be/6kFXWPD30o0
2	Mass Spec Fundamentals (Analyser Types)	https://youtu.be/h2B8era0YDw
3	HPLC-MS and Tandem Mass Spectrometry Link for Hands-On part: https://tinyurl.com/HPLC-MS-2020	https://youtu.be/SS2LXVplM4M
4	Data Acquisition and Data Sharing (Hands-On)	https://youtu.be/VZq5k3JT76o
5	Molecular Networking (Hands-On) Links for hands-on part: gnps.ucsd.edu MSV000088759 https://www.unimod.org/modifications_... https://gnps.ucsd.edu/ProteoSAFe/stat...	https://youtu.be/s5y1XNKENbk
6	Feature Detection	https://youtu.be/K889Zuepz8g
7	MZmine3 (Hands-On) Slides: https://docs.google.com/presentation/d/1Frmv-kj7sm-Mmbcx_6z7FGhV78_ejXrjC_k0rd1k9Sq/edit?usp=sharing Batch file: https://drive.google.com/file/d/1ViKvNg527DhJvZVFkPLQ3kEyK_Z1DOUT/view?usp=sharing Output files (for GNPS and SIRIUS): https://drive.google.com/drive/folders/1cQMgGjPbt8JD59QCM1gzeqK87qGCJ_7C?usp=sharing	https://youtu.be/hk7WeXibReg
8	Feature-based Molecular Networking (Hands-On)	https://youtu.be/3txu84K-ST4

	Link for example FBMN job: https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=24bc5ea2e6cc43fa8f09c50eb1bd54cd	
9	SIRIUS (Hands-On) Windows: https://github.com/boecker-lab/sirius/releases/download/v5.4.1-SNAPSHOT/sirius-5.4.1-SNAPSHOT-win64.msi Mac: https://github.com/boecker-lab/sirius/releases/download/v5.4.1-SNAPSHOT/sirius-5.4.1-SNAPSHOT-osx64.pkg and a test-data: https://drive.google.com/drive/folders/1cQMgGiPbt8JD59QCM1qzegK87qGCJ_7C?usp=sharing	https://youtu.be/VN_c0P8drzM
10	pyOpenMS (Hands-On) https://github.com/axelwalter/pyopenms-workshop	https://youtu.be/XWDFZXYp1qM
11	GNPS Dashboard, MASST and MassQL (Hands-On) https://tinyurl.com/3mx42ytr	https://youtu.be/J33e-azt6Nk
12	Metabolomics with Flow Injection Analysis	https://youtu.be/MrrKYGT5GGk
13	Molecular Network Visualization in Cytoscape Cytoscape download: https://cytoscape.org/download.html Example data: https://drive.google.com/drive/folders/1tmocp63dSJBqccNPqgmivPHmvHHCzrY?usp=sharing	https://youtu.be/KDVYRzYSQDg
14	Excel magic, table juggling and multivariate Statistics in R Test Data: https://github.com/Functional-Metabolomics-Lab/CMFI_Seminar_Multivariate_Statistics/tree/main/Test_Data Jupyter Notebook (colab): https://github.com/Functional-Metabolomics-Lab/CMFI_Seminar_Multivariate_Statistics	https://youtu.be/CqTHrJQkoic
15	Basics of Protein Mass Spectrometry	https://youtu.be/3lTP8Z_XMZk
16	Proteomics Data Acquisition Methods Orbi DDA Simulator: http://humos.bmb.sdu.dk/ Test Questions: https://edupad.ch/p/vEqp1IYbUK	https://youtu.be/9mJz1uhtgEQ
17	Quantitative Proteomics and Phosphoproteomics	https://youtu.be/sA1zh9UHKsl
18	Machine Learning for Mass Spectrometry Slides: https://docs.google.com/presentation/d/1idqp0VIO3B_KgdnJm1dMWmNDzIEzZ4C8CB7A0gWEOHo/edit?usp=share_link	https://youtu.be/4CufnU8XsGA
19	Proteomform Identification with Top-Down MS	https://youtu.be/s_NDgiQzRYc
20	Top-Down Proteomics: Spectral Deconvolution	https://youtu.be/A3sTrIN52l8

21	Native Mass Spectrometry Deconvolution with UniDec	https://youtu.be/vBwqB-YoGNI
22	DIA and High-Throughput Proteomics	https://youtu.be/my-gbrY8hWc
23	Metaproteomics Ocean Protein Portal: https://proteinportal.whoj.edu Hands-On worksheet: https://tinyurl.com/3fptn6fn	https://youtu.be/miRV9zECuM4
24	Metabolomics Intro, Recap and Outlook	https://youtu.be/F7mua0auveE
25	Statistical Analysis of Feature-based Molecular Networks	https://youtu.be/_OwAXaGfCgY
26	DIA-based Metabolomics	https://youtu.be/M7_A5w6CkHs
27	Ion-Mobility Applications in Metabolomics	https://youtu.be/T_vQ8wA-HNg
28	Spatial Lipodomics / MALDI-MS2	https://youtu.be/DrPm6uPU1a4
29	MassQL	https://youtu.be/Uzeen3a04Z0
30	Reversed Metabolomics	https://youtu.be/iQMIO1ivjAk
31	Native Metabolomics - Metals	https://youtu.be/5a2gBwCmvel
32	Native Metabolomics - Proteins	https://youtu.be/SB7N2J_R8Bo
33	MS/MS Enrichment (MicrobeMASST)	https://youtu.be/i4z5_rtCzHM
34	Functional Metabolomics	https://youtu.be/kG52K4u6Pd0
35	GNPS2 Series (basics)	https://youtu.be/wa3BeVzstLU
36	GNPS2 Series (FBMN)	https://youtu.be/q_1xfz31fqo
37	GNPS2 Series (Modifinder)	https://youtu.be/qplarmeddVY
38	GNPS2 Series (Transitive Alignments)	https://youtu.be/qplarmeddVY
39	GNPS2 Series (CMMC, Network Enrichment Analysis)	https://youtu.be/f3DzbL7WVjQ
40	GNPS2 Series (LLM Chatbots for MS)	https://youtu.be/_MCNrX66f0k
41	GNPS2 Series (Chem Walker)	https://youtu.be/rIB5g1TUJk8
42	GNPS2 Series (High-Throughput ModiFinder)	https://youtu.be/7neRtPhY1qM
43	GNPS2 em Português (MN Clássico)	https://youtu.be/l0A7usYNTJw
43	GNPS2 em Português (FBMN)	https://youtu.be/g2eiHGZuLaQ
44	GNPS2 em Português (FBMN-STATS)	https://youtu.be/ZAvmXlramlY
45	GNPS2 em Português (MASST)	https://youtu.be/OpFV2OMPD0A

46	GNPS2 en Español (MN Classico)	https://youtu.be/vRw-_ey_2rk
47	GNPS2 en Español (FBMN)	https://youtu.be/9yHTLwWr_kk
48	GNPS2 en Español (FBMN-STATS)	https://youtu.be/YuWoI5CKh8A
49	GNPS2 en Español (Modifinder)	https://youtu.be/7WIQoPuN1hw
50	mzmine Series: Non-target LC-MS ² Feature Detection, Statistical Analysis, Molecular Networking, Compound Annotation	https://youtu.be/UnqVtZngzl0
51	mzmine Series: Multimodal data processing using mzwizard: LC-MS2, GC/EI-MS, MALDI-Imaging, and lipid annotation	https://youtu.be/cGA5WIKcMpM
52	mzmine Series: LC-MS and LC-IMS-MS: PFAS, contaminants, and pesticides	https://youtu.be/Xp-G1HSozgM
53	mzmine Series: Automatic library generation: LC-MS2, MSn trees	https://youtu.be/SmEpFYV4_bY
54	IDBac (MALDI)	https://youtu.be/82eK6LTjj4w
55	Microbiome Multiomics with Qiime2	https://youtu.be/yYJ8p3GVF9U
56	JGI Secondary Metabolism Collaboratory Data Portal	https://youtu.be/dE5hVb5SxX8
57	Microbe-Metabolite Interactions	https://youtu.be/tp0Y6KKawg0
58	Metabolome-Microbiome Correlations (CorrOmics)	https://youtu.be/5i6_d8VE8DU
59	Pangenomics and Community Metabolism with Anvi'o	https://youtu.be/9lCotgBrH8o
60	BGC-Atlas	https://youtu.be/ij5GTQd8bpkw
61	Multiple Spectral Alignments	https://youtu.be/HCXPJ_lpdrrs
62	Metabolic Network Analysis in anvi'o	https://youtu.be/zqTsL8lM5o4