

Ph.D. Dissertation Defense

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Friday, March 22 at 1:30 pm in room 1111 Biotech Center

"Integrated Tools for Global Lipidomic Analysis"

The application of mass spectrometry (MS) for biomolecule identification and quantitation has been driven, in part, by significant advances in chromatographic separation, MS data acquisition, and informatics tools. These breakthroughs now allow for the system-wide characterization of proteins and metabolites in biologically relevant systems. However, only recently have these advances been applied to the global analysis of lipids. Lipids play vital biochemical roles as structural components, energy stores, and signaling molecules making them high-value targets for research on metabolic diseases. Unfortunately, these species contain remarkable structural heterogeneity which complicates the direct application of many existing MS techniques to lipidomic analysis. In this presentation, I will detail the development of (1) novel software tools to generate, curate, and utilize *in silico* lipid spectral libraries for high-confidence lipid identification; and (2) a new approach for the simulation of lipidomic LC-MS/MS data acquisition to rapidly optimize lipid method parameters for comprehensive lipidomic analysis. Overall, these software tools aim to streamline the implementation of advanced lipidomic data analysis for large experimental cohorts and empower the generation of biochemically-informative discovery lipidomic datasets.

	902.685 m/z (-)	MS/MS Scans	Lipid ID
	— Sample 1		PC 16:0_24:1
	Sample 2 Sample 3 MS/MS	2	PC 16:0_24:1
		3	PC 18:1_22:0
		4	PC 18:1_22:0
		5	PC 16:1_24:0
12.4 12.6 12.8 1 Retention Time (Minut	3.0 13.2 es)	6	PC 16:1_24:0