



ACS Local Section
North Jersey

Unique Strengths of NMR Metabolomics: *In vivo* Metabolism and Improved Compound Identification

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Date: Tuesday May 16th, 2023

Time: 12:00 pm ET via Microsoft Teams

Abstract

Metabolomics is an important component of systems biology research in biology and biomedicine. Two major technologies are widely used in metabolomics research, mass spectrometry and NMR spectroscopy. Both have their own strengths and weaknesses. Recently, LC-MS has gained in popularity, thanks largely to its high sensitivity and ability to detect 10s of thousands of features. In this talk, I will highlight some of the unique strengths of NMR metabolomics, most notably approaches to study metabolic dynamics in real-time in cells or microorganisms. We call this continuous *in vivo* metabolism by NMR (CIVM-NMR). I will also discuss the difficulty that the entire field faces in confident metabolite identification and will present recent approaches to better combine NMR with LC-MS and computational chemistry to improve compound identification.

Judge, M. T., Wu, Y., Tayyari, F., Hattori, A., Glushka, J., Ito, T., Arnold, J., and Edison, A. S. (2019) Continuous *in vivo* Metabolism by NMR, *Front Mol Biosci* 6, 26.

Edison, A. S.; Colonna, M.; Gouveia, G. J.; Holderman, N. R.; Judge, M. T.; Shen, X.; Zhang, S. NMR: Unique Strengths That Enhance Modern Metabolomics Research. (2021) *Anal Chem* 93 (1), 478-499.

Connection Information

This will be a virtual meeting hosted via Microsoft Teams. A direct link to the meeting is located [HERE](#).

Further information can be found on the [NMR Topical Group website](#).

Please reach out to Tom Osborn Popp (thomas.osbornpopp@rutgers.edu) or Christine Jorge (christine.jorge@bms.com) with any questions.

Presented by the NMR Topical Group – North Jersey ACS