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Research Seminar

When: August 27, 2020

Time: 2:30 PM

Location: Microsoft TEAMS

Mass Spectrometry Based Metabolomics and Lipidomics

Abstract

Strategies for metabolomics and lipidomics study can be divided into untargeted and targeted approaches. The untargeted metabolomics/lipidomics detects as many metabolites/lipids as possible, while the targeted metabolomics/lipidomics focuses on analyzing a number of known metabolites/lipids. In the research seminar, I will present my work on 4 aspects:

1) *Integrating multiple MS based platforms for untargeted metabolomics*^{1,2}

We extracted polar metabolites from biological samples, then analyzed them by multiple MS based platforms, including GC×GC-MS with MSTFA derivatization, GC×GC-MS with MTBSTFA derivatization, 2DLC-MS/MS in negative ionization mode, and 2DLC-MS/MS in positive ionization mode. Data collected from multiple platforms were merged for further analysis.

2) *Targeted metabolomic study of short-chain fatty acids (SCFAs) using GC-MS*³

We developed a GC-MS method for simultaneous analysis of eight straight-chain and branched-chain SCFAs. We used DB-225ms column hyphenated with DB-5ms column in tandem to achieve the best separation of SCFAs. This method showed good recovery and sensitivity to quantify the SCFAs in biological samples.

3) *Targeted lipidomic study of long-chain fatty acids (LCFAs) and oxylipins using LC-MS/MS*⁴

We developed a high-throughput LC-MS method for simultaneous analysis of 51 bioactive LCFAs and oxylipins. LCFAs and oxylipins were extracted via solid-phase extraction, then analyzed using a targeted metabolomics approach by reversed-phase chromatography-mass spectrometry.

4) *Developing comprehensive two dimensional LC-MS for untargeted lipidomics*

We are developing a comprehensive two dimensional LC-MS for lipid profiling. Lipids extracted from biological samples were separated into several portions by HILIC, each portion were then further separated by RPC.

References:

1. Yuan, F.; Harder, J.; Ma, J.; Yin, X.; Zhang, X.; Kosiewicz, M. M., *Journal of Proteome Research* 2020, 19 (2), 667-676.
2. Yuan, F.; Kim, S.; Yin, X.; Zhang, X.; Kato, I., *Metabolites* 2020, accepted.
3. He, L.; Prodhan, M. A. I.; Yuan, F.; Yin, X.; Lorkiewicz, P. K.; Wei, X.; Feng, W.; McClain, C.; Zhang, X., *Journal of Chromatography B* 2018, 1092, 359-367.
4. Warner, D. R.; Warner, J. B.; Hardesty, J. E.; Song, Y. L.; King, T. N.; Kang, J. X.; Chen, C.-Y.; Xie, S.; Yuan, F.; Prodhan, M. A. I.; Ma, X.; Zhang, X.; Rouchka, E. C.; Maddipati, K. R.; Whitlock, J.; Li, E. C.; Wang, G. P.; McClain, C. J.; Kirpich, I. A., *Journal of Lipid Research* 2019, 60 (12), 2034-2049.