

Targeted Metabolomics Method Development Across Liquid Chromatography Domains

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The purpose of this study is the development of targeted metabolomics methods for biomarker discovery in cattle and swine gut health. Livestock biomatrices like rumen fluid, serum, urine, and feces vary greatly in composition, yet have been much less studied than human samples [1]. In order to comprehensively search such a metabolomic space for quantitative biomarkers of health and disease, multiple chromatographic domains are likely to be required even within the boundary of liquid chromatography coupled mass spectrometry (LCMS) [2]. To that end, analytical reference standards that are part of the metabolic pathways of mammalian hosts and gut fermenters have been collected. These range from polar analytes like sugars, amines, and short chain fatty acids to highly apolar fatty acids, as well as intermediate compounds like prostaglandins, acyl amines, and bile acids. Here we present the systematic approach being used to build an in-house library of tandem mass spectrometric (MS/MS) transitions and their use to survey the retention of these metabolites with multiple mobile and stationary phases.

[1] Goldansaz SA, et al. (2017) Livestock metabolomics and the livestock metabolome: A systematic review. *PLoS One* 12(5):e0177675.

[2] Boudah S, et al. (2014) Annotation of the human serum metabolome by coupling three liquid chromatography methods to high-resolution mass spectrometry. *J Chromatogr B Analyt Technol Biomed Life Sci* 966:34–47.