



# **Population-Based Studies Using Untargeted Metabolomics and Personalized Reference Libraries**

Capturing chemical complexity with untargeted metabolomics in largescale studies with thousands of samples

Metabolomics provides insight into health and disease as it is an assessment of biochemical phenotypes present in a biological sample. Metabolomics studies can be applied to precision medicine - an approach to tailor disease treatment and prevention plans to specific subgroups within a population. Applying untargeted metabolomics in population-based studies with thousands of samples can improve precision medicine and complement other assays. However, conventional approaches to unbiased global metabolomics is not amenable to to large sample sizes. A feature of Panome Bio<sup>™</sup>'s Next-Generation Metabolomics<sup>™</sup> platform is Personalized Reference Libraries. This library is tailored to your samples so the most relevant metabolites are captured while sorting through the noise. Next-generation methods coupled with machine learning removes technical variation from metabolite profiles and normalizes data for batch effects when samples are run months apart. Panome Bio provides a global and unbiased view of the metabolome through a suite of complementary LC/MS assays coupled with our Next-Generation Metabolomics capabilities, comprehensive workflow and personalized data analysis reports to make your large-scale studies possible.





Metabolites (>3,000)

#### HIGHLIGHTS

#### Next-Generation Metabolomics™

Through an untargeted analysis and robust computational methods we provide an unbiased and global view of metabolism. We then use next generation methods to decrease the complexity of datasets, allowing more impactful experimental designs than previously possible, including multi-omic integration, longitudinal analysis, large cohorts <1k, and more.

#### **Comprehensive Workflow**

Starting from sample preparation, to experimental design and data analysis, we handle all aspects of your metabolomics screen.

#### Personalized Data Analysis Report

Metabolomics data is complex, personalized data analysis reports provide a straightforward interpretation of your results. We work with you to define an analysis plan that will meet your needs.

Our Next-Generation Metabolomics workflow makes large-scale studies possible. In this study, 2000 patient plasma samples were subjected to an untargeted metabolomics assay. After data analysis, metabolic profiles were shown to reflect geographic location, as seen in the PCA plot. The heatmap shows over 3000 metabolites profiled across the 4 population subgroups.



Samples for large-scale studies may be collected over months or years, our next-generation batch-correction algorithms have been optimized to reduce technical variation. After quality control via batch correction, the final report provides processed metabolic profiles with statistical analysis.



Missing values create noise in datasets and must be removed for data processing. Our next-generation workflow allows targeted analysis on an untargeted scale. With our methods, missing values were found to be <0.03% of all measurements. Using traditional global peak extraction methods, >9% of all peaks in the data set were missing values. Further, our targeted extraction of metabolite levels leads to much more precise measurements with CVs less than 10% for most metabolites.

Learn more: Ethan Stancliffe, Michaela Schwaiger-Haber, Miriam Sindelar, Matthew J. Murphy, Mette Soerensen, and Gary J. Patti Analytical Chemistry **2022** *94* (50), 17370-17378

## Panome Bio<sup>™</sup> - Biomarker Discovery with Next-Generation Metabolomics<sup>™</sup>



Panome Bio can help you profile and discover biomarkers with Next-Generation Metabolomics while saving you time and resources. Our next-generation methods make complex experiments possible. Our technology provides you with a global and unbiased view of metabolism with quantitative accuracy while our computational methods provide a clear view of your complex metabolomics data. Contact us to be your partner in research!

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