

# Metabolomics



The metabolome is the complement of low-molecular-weight compounds present in the cells, tissues, or biological fluids of an organism in a particular physiological state. Metabolomics involves the study of how the balance of these compounds and their related biochemical pathways alter under the different physiological states that result from development or aging, environmental exposure, disease progression or treatment, or intervention.

Metabolomics can provide valuable information to inform drug discovery and development. Applications span the development of *in vitro* and *in vivo* screening assays to the defining of markers for early detection and diagnosis of disease, disease staging, and therapeutic monitoring—providing mechanistic insights for linking exposure to disease. Because metabolites and their related pathways are largely conserved across animal species, metabolomics is an ideal tool for discovering biomarkers in animal models for translation to clinical and field investigations.

## Approach and Capabilities

RTI International has a wide range of instrumentation to facilitate broad-spectrum analysis of polar or nonpolar components and methods for targeted analysis and analysis of minerals. Our capabilities include nuclear magnetic resonance (NMR) spectroscopy, liquid chromatography mass spectrometry (LC-MS/MS; UPL-Q-TOF-MS), gas chromatography mass spectrometry (GC-MS, 2D-GC-TOF-MS), inductively coupled plasma mass spectrometry, Orbitrap, and MALDI imaging.

We have experience with analysis of cells, organ tissue (e.g., liver, uterus, testes, brain), biological fluids (e.g., urine, serum, plasma, amniotic fluid), and exhaled breath collected from human subjects or animal models.

Following signal detection, RTI scientists apply statistical and mathematical tools (SAS, Umetrics, Spotfire) and use their expertise to identify data trends that show the correlation of specific signals with the phenotypic response under investigation. Identified signals are mapped to biochemical pathways through the use of GeneGo software and expert biochemist interpretation to derive biomarkers and mechanistic insights.

## Working Closely with Our Clients

RTI's technical, research, and development services meet the highest standards of professional performance. We work closely with clients to identify their unique requirements and to clarify their expectations, cost parameters, and time constraints. RTI's business systems and processes make it easy to partner with us. We have the contractual, legal, and business structures to serve any client with projects of all sizes.

## Selected Publications and Presentations

Banerjee, R., Pathmasiri, W., Snyder, R., McRitchie, S., and Sumner, S. (2012, in press). Metabolomics of brain and reproductive organs: Characterizing the impact of gestational exposure to butylbenzyl phthalate on dams and resultant offspring. *Metabolomics*, DOI: 10.1007/s11306-011-0396-y.

Collier, D. N., Pathmasiri, W., Pratt, K. J., Crawford, Y., Henes, S., Gross-McMillan, A., Lutes, L., & Sumner, S. (2011, April 30–May 3). Obesity treatment and the biology of behavior: Metabolomic analysis of response to a behavioral intervention. Presented at the American Pediatrics Society Meeting, Denver, CO.

Pathmasiri, W., Pratt, K. J., Collier, D. N., Lutes, L. D., McRitchie, S., & Sumner, S. C. J. (2012). Integrating metabolomic signatures and psychosocial parameters in responsivity to an immersion treatment model for adolescent obesity. *Metabolomics* DOI: 10.1007/s11306-012-0404-x. .

Pathmasiri, W., Snyder, R. W., Burgess, J. P., Popp, J. A., Fennell, T. R., & Sumner, S. (2011). Metabolomics of urine and liver for the assessment of acetaminophen induced liver injury. In D. Casiano and S. C. Saru (Eds.). *Handbook of Systems Toxicology*. New York, NY: John Wiley & Sons.

Sumner, S. (2011, November 8–12). Keynote: Personalized medicine and environmental omics. Presented at the First International Conference on Environmental Omics. Gaungzhou, China.

Sumner, S. (2011, February 19). Biomarkers in personalized medicine: Applications of metabolomics to provide biomarkers for the treatment of obesity, liver injury, and reproduction and development outcomes. Presented at the American Association for the Advancement of Sciences, Washington, DC.

Szabo, D., Pathmasiri, W., Diliberto, J., Sumner, S., & Birnbaum, L. (2011). Metabolomic analysis of serum after treatment with the emerging POP flame retardant Hexabromocyclododecane (HBCD): Commercial mixture, alpha and gamma stereoisomers elicit differential effects in infantile mice. *Toxicologist* 2248, 482.

Gika, H. G., Theodoridis, G. A., Earl, M., Sumner, S., & Wilson, I. D. (2010). Does the Mass Spectrometer Define the Marker? A Comparison of global metabolite profiling data generated simultaneously via UPLC-MS on two different mass spectrometers. *Analytical Chemistry* 82(19), 8226–8234.

Sumner, S., Burgess, J., Snyder, R., & Fennell, T. (2010). A non-invasive marker of isoniazid induced liver injury. *Metabolomics* 6(2), 238–249.

Sumner, S., Snyder, R., Burgess, J., Tyl, R., & Fennell, T. (2010). Omics in the study of reproduction and development. In R. Kapp and R. Tyl (Eds.). *Reproductive Toxicology* (3rd ed.). London, UK: Informa Healthcare.

Sumner, S. C., Snyder, R., Fennell, T., Fernando, R., & Collins, B. J. (2010). Metabolomics analysis of urine from resveratrol-treated male, female, and pregnant Wistar Han rats. *Toxicologist* 131, 284.

Sumner, S., Snyder, R., Fennell, T., Taylor, G., & Lewin, A. (2010). Distribution of [<sup>14</sup>C]C60 in the pregnant and lactating rat and the effect on endogenous metabolism. *Journal of Applied Toxicology* 30(4), 354–360.

Sumner, S., Snyder, R., Burgess, J., Myers, C., Tyl, R., Sloan, C., & Fennell, T. (2009). Metabolomics in the assessment of chemical-induced reproductive and developmental outcomes using non-invasive biological fluids: Application to the study of butylbenzyl phthalate. *Journal of Applied Toxicology* 29(8), 703–714.

Weis, B. K., Balshaw, D., Barr, J. R., Brown, D., Ellisman, M., Liou, P., Omenn, G., Potter, J. D., Smith, M. T., Sohn, L., Suk, W. A., Sumner, S., Swenberg, J., Walt, D. R., Watkins, S., Thompson, C., & Wilson, S. 2005. Personalized exposure assessment: Promising approaches for human environmental health research. *Environmental Health Perspectives* 113(7), 840–848.

Xirasager, S., Gustafason, M. A., Tomer, K., Stasiewicz, S., Yost, J., Yates, J. R., Sumner, S., & Ziao, W. M. (2004). CEBS object model for systems biology data. CEBS MAGE SysBio-Om. *Bioinformatics* 20(13), 2004–2015.

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#### More Information

Susan Sumner, PhD, Senior Scientist, Discovery and Analytical Sciences  
919.541.7479, ssumner@rti.org

RTI International  
3040 Cornwallis Road, PO Box 12194  
Research Triangle Park, NC 27709-2194 USA

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