**Metabolomics and Childhood Obesity: A Pilot and Feasibility Study With Multiple Phenotypic Anchors**

Metabolomic Analysis: NIH Eastern Regional Comprehensive Metabolomics Resource Core (RTI RCMRC)

PI, RTI RCMRC Core Collaboration: David N. Collier, MD, PhD

IRB Number(s):

**Abstract:**

“Metabolomics” is a powerful new analytical approach for measuring and evaluating all small and intermediate sized metabolites in a variety of tissues or samples in conditions of health and disease. The purpose of this research is to determine if “metabolomics” can be used to address several important unanswered questions about obesity in children. First we will use metabolomics to identify patterns of metabolites in blood that are unique to obese children. We will then determine if these patterns are predictive of excessive weight gain and/or poor weight loss response in non-obese and obese children enrolled in an exercise program. This knowledge will help us understand why some children are destined to become obese and/or are poorly responsive to treatment. This will help identify children who might need more aggressive, expensive or personally tailored obesity treatments. Second we plan to use metabolomics to identify metabolic signals specifically associated with the early initiation of atherosclerosis (and hence increased risk for cardiovascular disease [CVD]) in obese children. We expect that this knowledge will ultimately lead to better early risk assessment and opportunities for risk reduction in both obese and non-obese children than allowed by current clinical practices. Finally the knowledge gained from this research could be applied in the future to prospectively assess – and therefore proactively manage ~ a broad range of risk factors in large numbers of young children in a rational and cost effective manner.

**Sample Description:**

Aliquots of each de-identified plasma sample were shipped to the NIH RTI-RCMRC on dry ice and immediately stored at -80 °C after being logged in for metabolomics analysis. A total of 219 study samples were thawed on ice for sample preparation. 200 uL of plasma sample were thawed and transferred to labeled tubes on ice where they were mixed with 50 uL Saline master mix (5mM Formate). Analytical quality control (QC) phenotypic pooled samples were generated by transferring a 25 µL of each sample of each respective phenotypical experimental sample into different 1.5 mL tubes. Whole study (total) pools were generated by transferring 200 uL of plasma from each Pool sample into a 2.0 mL tube. The tubes were vortexed for 4 min on a multi-tube vortexer and centrifuged at 16,000 rcf for 4 min. A 200 µl aliquot of the supernatant was transferred into pre-labeled 3mm NMR tubes for data acquisition on a 700 MHz spectrometer.

The data obtained for the NMR metabolomics analysis can be found in the accompanying files:

Procedures: 1. Childhood Obesity Metabolomics Procedures.docx

Study Design Tables: 2. Childhood Obesity Metabolomics Study Design Table.xls

Metadata: 3. Childhood Obesity Metabolomics METADATA.xlsm

Processed Data: 4. Childhood Obesity Metabolomics Normalized Binned Data.xlsx

Raw Data: 5. Childhood Obesity Metabolomics NMR Raw Data.zip

**Notes:**

Full sample preparation and analysis procedures are available in the accompanying document entitled **1. Childhood Obesity Metabolomics NMR Procedures**.

Descriptions of abbreviations for factors are available in the Variable Dictionary in the accompanying file no. **2. Childhood Obesity Metabolomics NMR Study Design Table.xls**.

The phenotypic and normalized data are available in the accompanying files: **4. Childhood Obesity Metabolomics NMR Normalized Binned Data.xlsx** for normalized binned NMR data. Sample ID and factors can be found in the first 5 columns and other columns in the spreadsheet contain sample metadata and the normalized binned data. If the statistical program does not allow variable names to begin with a number then add a prefix to the column names, for example, bin\_8.98 instead of 8.98.

The Sample ID serves as the unique identifier (Graphical ID) of the individual samples and is used as the NMR folder name in the raw NMR data file **5. Childhood Obesity Metabolomics NMR Raw Data.zip**.