**Smoking Status**

Metabolomic Analysis: Untargeted Analytical Resource Core – NMR (RTI)

PI, RTI RCMRC Core Collaboration: NIH

IRB Number(s):

**Abstract:**

**Sample Description:**

Pooled urine samples from smokers (NIST SRM 3672) and non-smokers (NIST SRM 3673) were provided by NIH.

Samples were shipped to the RTI CHEAR on dry ice and immediately stored at -80 °C after being logged in for analysis.

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

Procedures: 1. CHEAR Smoking Status NMR Procedures.docx

Study Design Tables: 2. CHEAR Smoking Status NMR Study Design Table.xls

Metadata: 3. CHEAR Smoking Status METADATA.xlsm

Processed Data: 4. CHEAR Smoking Status NMR Normalized Binned Data.xlsx

Concentration Data: 5. CHEAR Smoking Status NMR Concentration Data.xlsx

Raw Data: 6. CHEAR Smoking Status NMR Data.zip

**Notes:**

Full sample preparation and analysis procedures are available in the accompanying document entitled **1. CHEAR Smoking Status NMR Procedures.**

Descriptions of abbreviations for factors are available in the Variable Dictionary in the accompanying file no. **2. CHEAR Smoking Status NMR Study Design Table.xls**.

The phenotypic and normalized data are available in the accompanying files: **4. CHEAR Smoking Status 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.

Identifiable metabolites were semi-quantified with Chenomx and available in the attached file: **5. CHEAR Smoking Status NMR Concentration Data.xlsx.** Metabolites were fit relative to the internal standard, d6-DSS. Sample ID and factors can be found in the first X columns.

The Sample ID serves as the unique identifier (DRCC ID) of the individual samples and is used as the NMR folder name in the raw NMR data file **6. CHEAR Smoking Status NMR Raw Data.zip**.