**Human Saliva Cystic Fibrosis**

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

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**Abstract**

This study was designed as a pilot to determine if the concentrations of selected ions in salivary gland secretions were influenced by the absence of CFTR on the apical surfaces of glandular cells and ductal epithelia. To this end, five cystic fibrosis children homozygous for Phe508 were to be recruited with their heterozygous non-CF mothers. Unstimulated glandular secretions to include parotid and submandibular/sublingual saliva samples as well as whole, mixed saliva collected with masticatory stimulation were to be collected from the child and the mother and analyzed for nitrate (NO3), nitrite (NO2), bicarbonate (HCO3), thiocyanate (SCN), reduced and oxidized glutathione (GSH and GSSG) and buffering capacity (pH before and after addition of HCl to 3.75mN). For adaptation and development of the assays to a microtiter format, saliva samples were collected from non-CF control subjects initially to optimize the assays recognizing that the volumes for analyses would be small. The values obtained with these non-CF control samples were also compared to that of the homozygous and heterozygous CF subjects. As residual volume permits, these samples will be further analyzed for metabolic constituent profiles.

**Goals**

This study is designed to provide a comparative metabolomics analysis of CF vs non-CF samples by RTI.

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

Procedures: 1. Human Saliva Cystic Fibrosis Procedures.docx

1.a. GCMS Procedures Flowchart.pdf

1.b. GCMS Preparation of fatty acid methyl esters mixture.pdf

Study Design Table: 2. Human Saliva Cystic Fibrosis Study Design.xlsx

Metadata: 3. Human Saliva Cystic Fibrosis METADATA.xlsm

Raw Data: 4. Human Saliva Cystic Fibrosis Raw GCMS Data.zip

Processed Data: 5. Human Saliva Cystic Fibrosis Processed Data.xlsx

**Notes:**

Full sample preparation and instrumentation parameters are detailed in accompanying file **1. Human Saliva Cystic Fibrosis Procedures.docx.** A flowchart detailing the sample preparation steps is located in accompanying file **1.a. GCMS Procedures Flowchart.pdf.** The preparation of the fatty acid methyl esters (FAME) mixture is located in accompanying file **1.b. GCMS Preparation of fatty acid methyl esters mixture.pdf**.

Factors listed in the study design are defined in the Variable Dictionary located in the accompanying file entitled **2.Human Saliva Cystic Fibrosis Study Design.xlsx.** Available in the same file is information linking the Data File names to the Sample IDs.

Data files for each sample are generated by Leco’s ChromaTOF software and are exported in netCDF format . These files arelocated in the accompanying file entitled **4. Human Saliva Cystic Fibrosis Raw GCMS Data.zip.**

The spreadsheet in accompanying file **5. Human Saliva Cystic Fibrosis Processed Data.xlsx** has one data tab entitled BinBase Processed Data. The BinBase Processed Data shows raw output from BinBase. The height values have not been normalized.

**Reference**

O Fiehn, G. Wohlgemuth, M Scholz, T Kind, DY Lee, Y Lu, S Moon and B Nikolau: Quality control for plant metabolomics: reporting MSI-compliant studies. The Plant Journal2008; 53:691-704.