Icahn School of Medicine at Mount Sinai

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Date 9/10/2018
From CHEAR Data Center
Subject 2017-1762 – Study data for Smoking Metabolites
To Dr. Mahabee-Gittens

The smoking metabolites in saliva data (N=244) analyzed by the Minnesota Lab Hub for CHEAR project #2017-1762 are now finalized and available on the CHEAR Data Submission and Review Portal (DSRP). One biomarker was submitted for this panel, free cotinine (COT), as per Lab Analysis Plan. No data submitted for 6 samples due to insufficient volume for either the initial analysis or a required repeat analysis of sample.

The Limit of Quantitation (LOQ) values were reported and used to identify the valid values for each sample. In cases where the measured value was below LOQ (comment code 199), the value of the LOQ was reported. The following approaches can be considered for handling these values that are below the LOQ:

- Investigators may substitute a surrogate value for all values <=LOQ, which is often LOQ/sqrt2, first recommended by Hornung and used by CDC *(note that CDC utilizes LOD for determining valid values)*.
- Investigators can consider using a multiple imputation method (see Lubin). In general, a surrogate value is not used in models with continuous variables unless >60% of the observations are detectable, as described in Lubin.

16 samples total were run as statistical field samples, also referred to in this report as CHEAR QC pools, 8 urine pool A and 8 urine pool B, with 2 samples of each pool run for each of the 4 batches. Additionally, the PI included 12 duplicate samples, unevenly distributed amongst the batches.

These laboratory results have been reviewed and approved by the CHEAR Lab Hub to assure that they conform to acceptable quality standards. Summary tables of the study sample data and relevant quality control data are appended at the end of this document.

Signed,

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Statistical Analyst

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REPORT OF LAB RESULTS

1 - Summary Table of Sample Data:

Geometric mean and geometric mean standard deviation calculated for subjects with detectable levels (NC- not calculated when detection frequency was less than 70%). The LOQ was utilized to determine detectable values.

Lab Report for CHEAR Project 2017-1762 (PI: Mahabee-Gittens) : Cotinine
Matrix : saliva

Analyte	Number of Samples Analyzed	Number of Samples >LOQ	Percent Detect	LOQ	Geometric Mean	Geometric Mean STD	Min	10th Percentile	25th Percentile	Median	75th Percentile	90th Percentile	Max	Reported Units
COT	244	237	97%	0.1	4.43	4.24	<LOQ	0.5	1.5	4.6	10.9	22.6	382	ng/mL

2 - Summary Table of CHEAR QC Pools:

Two samples each of CHEAR QC urine pool A and B were run per batch. Means and CVs were calculated per pool per batch and overall. Values reported in ng/ml. Note that results near the LOQ are subject to greater uncertainty (see table 1 for analyte specific LOQs).

		Batch														
		1			2			3			4			Overall		
Analyte	Pool	N	Mean sample value	%CV	N	Mean sample value	%CV	N	Mean sample value	%CV	N	Mean sample value	%CV	N	Mean sample value	%CV
COT	A	2	52.2	4	2	50.3	2	2	51.5	2	2	51.7	2	8	51.4	2
	B	2	151	2	2	157	3	2	159	2	2	162	1	8	157	3

3 - QC Data (Duplicates):

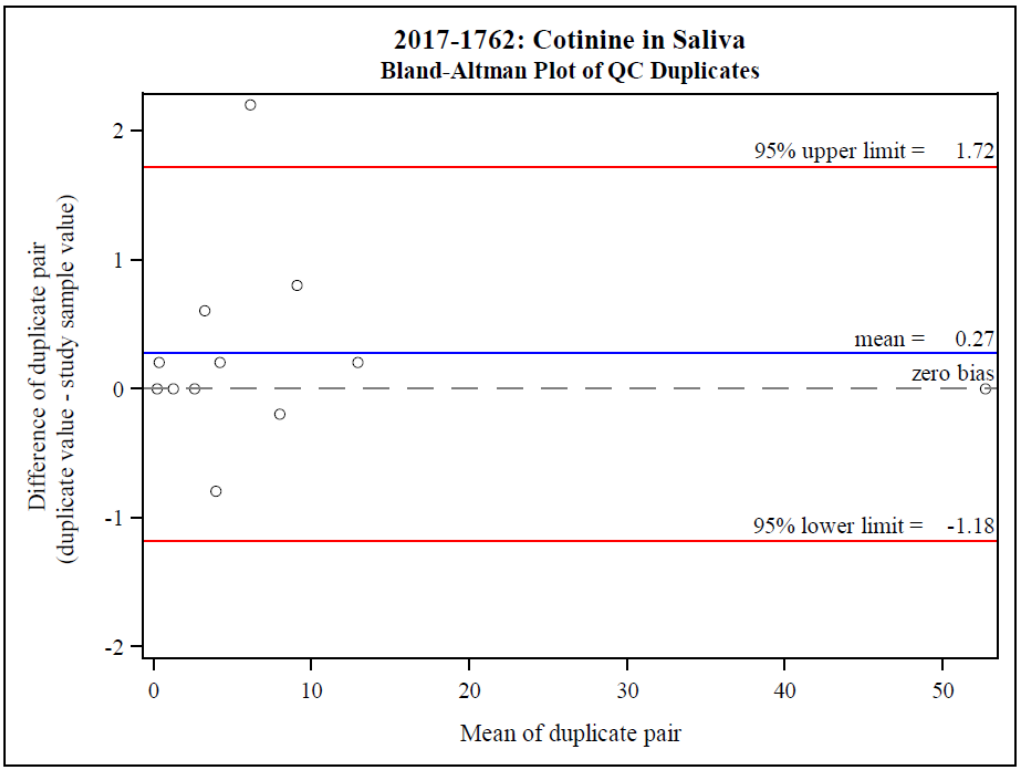
A) ***QC Duplicates Summary Table****- The Relative Percent Difference (RPD)* and % Recovery** were calculated for each valid duplicate pair (N) per analyte. Inclusion criteria requires analyte measures be greater than the LOQ for both samples. The mean values of the valid duplicate pairs reported as ng/ml. Note that results near the LOQ are subject to greater uncertainty (see table 1 for analyte specific LOQs).*

Analyte	N valid duplicate pairs	% valid duplicate pairs	Average of valid duplicate pair means	RPD Mean	RPD Median	RPD P75	RPD P90	RPD Max	% Recovery Mean
COT	12	100	8.7	13	4	20	36	67	113

$$*RPD = \frac{|study\ sample\ result - duplicate\ result|}{(study\ sample\ result + duplicate\ result)/2} *100$$

$$**\%\ Recovery = \frac{duplicate\ \ result}{study\ sample\ result} *100$$

B) ***Bland-Altman Plot of QC Duplicates****- The difference of the 12 valid duplicate pair measurements for cotinine plotted against the mean value of the pair in the chart below with reference lines indicating mean difference and 95% upper and lower limits. Inclusion criteria requires analyte measures be greater than the LOQ for both samples. All values reported as ng/ml. Note that results near the LOQ are subject to greater uncertainty (see table 1 for analyte specific LOQs).*



Reference:

1. Hornung, R. W., & Reed, L. D. (1990). Estimation of average concentration in the presence of nondetectable values. Applied occupational and environmental hygiene, 5(1), 46-51.
2. Lubin, J. H., Colt, J. S., Camann, D., Davis, S., Cerhan, J. R., Severson, R. K. Hartge, P. (2004). Epidemiologic evaluation of measurement data in the presence of detection limits. Environmental health perspectives, 112(17), 1691.