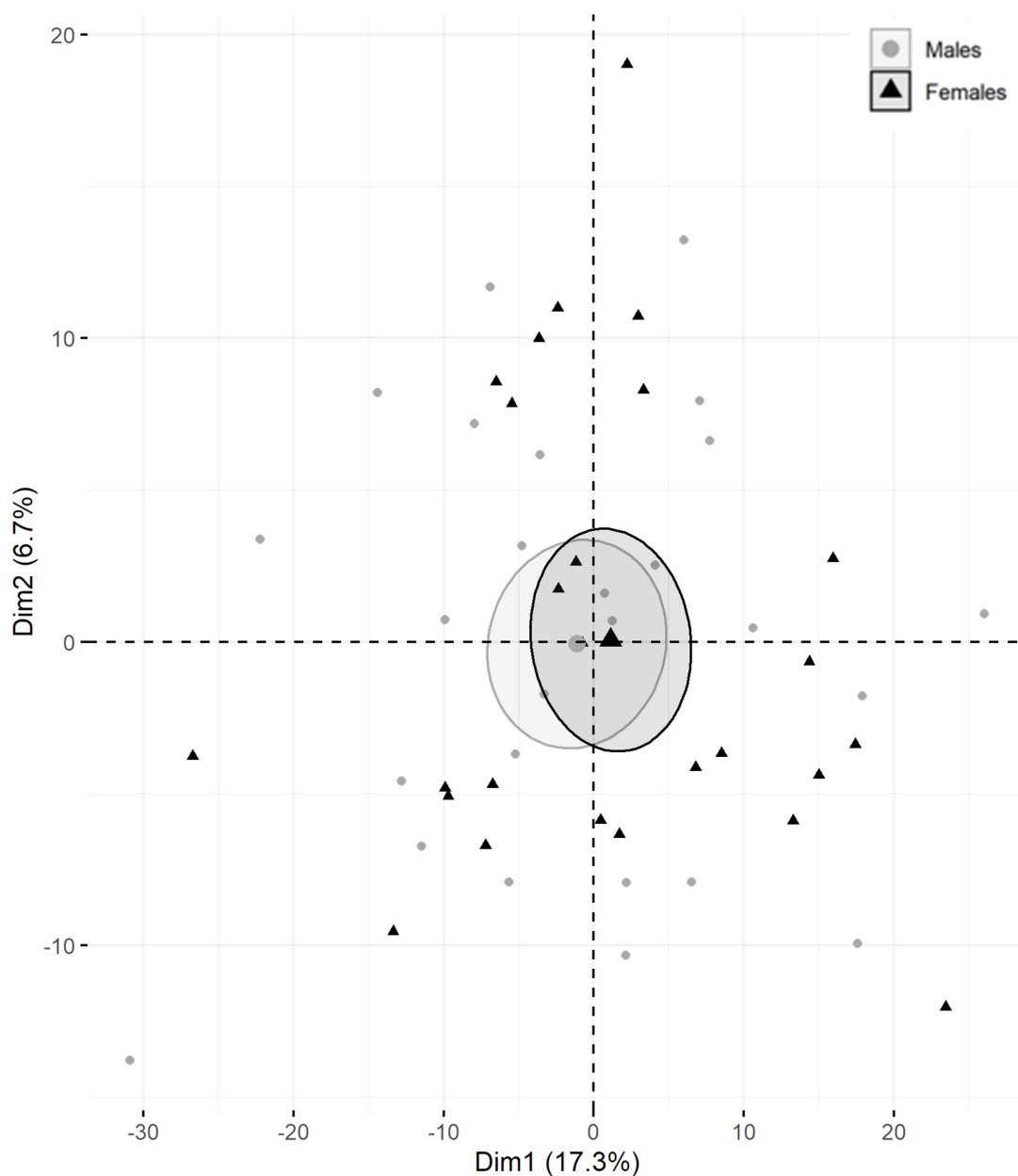
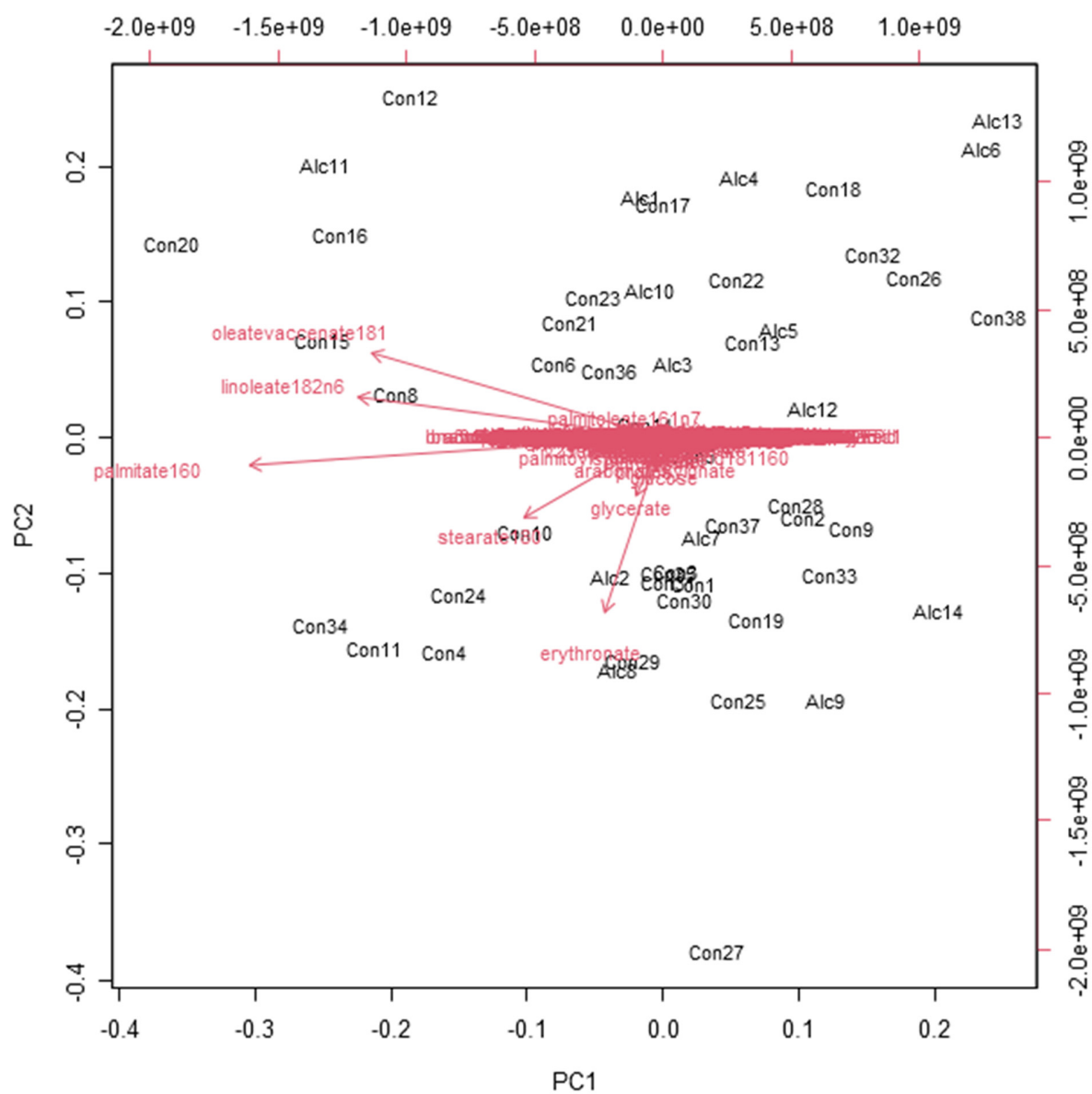


# Untargeted Metabolome Analysis of Alcohol-Exposed Pregnancies Reveals Metabolite Differences that Are Associated with Infant Birth Outcomes

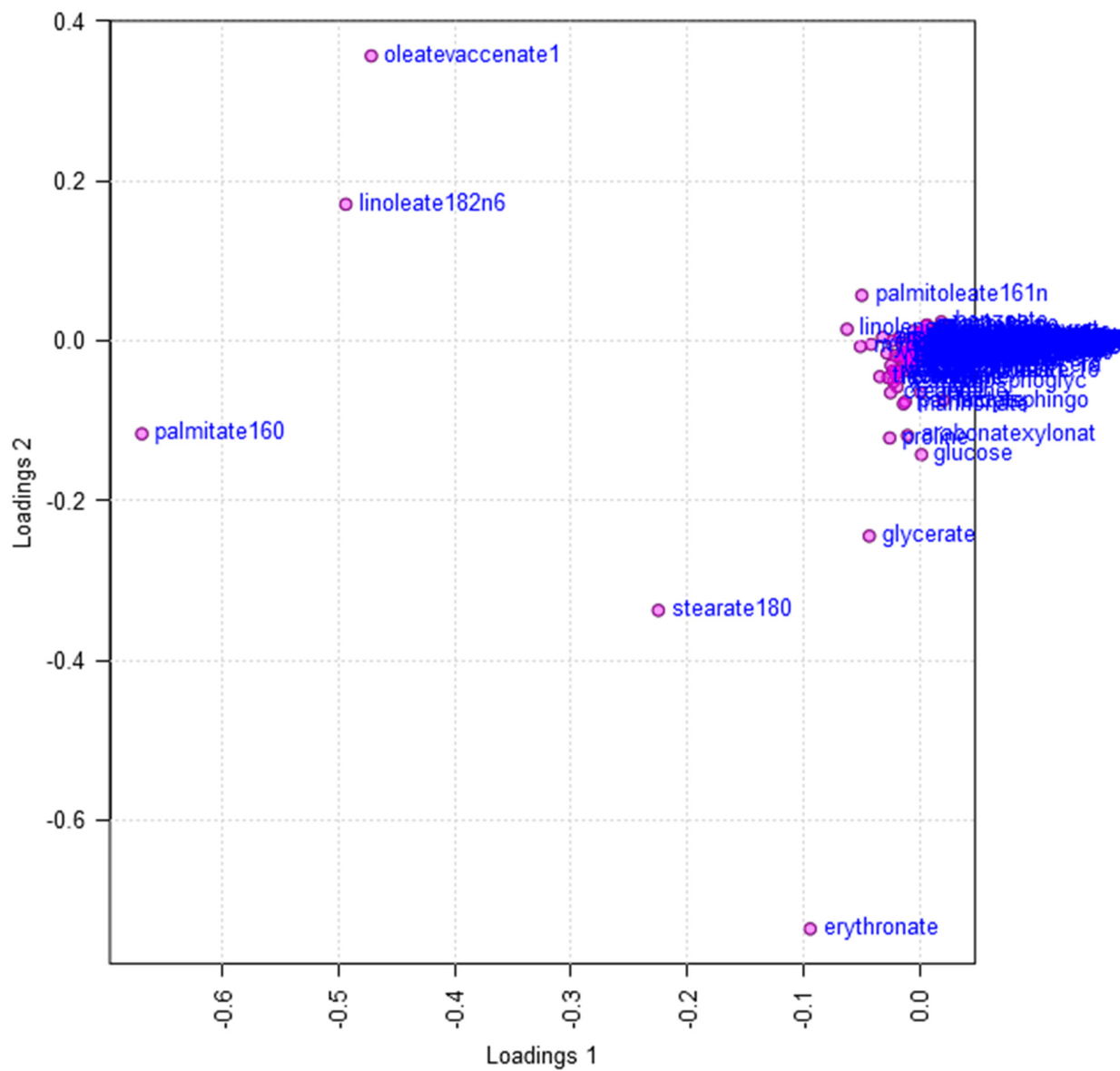
## Supplemental Material



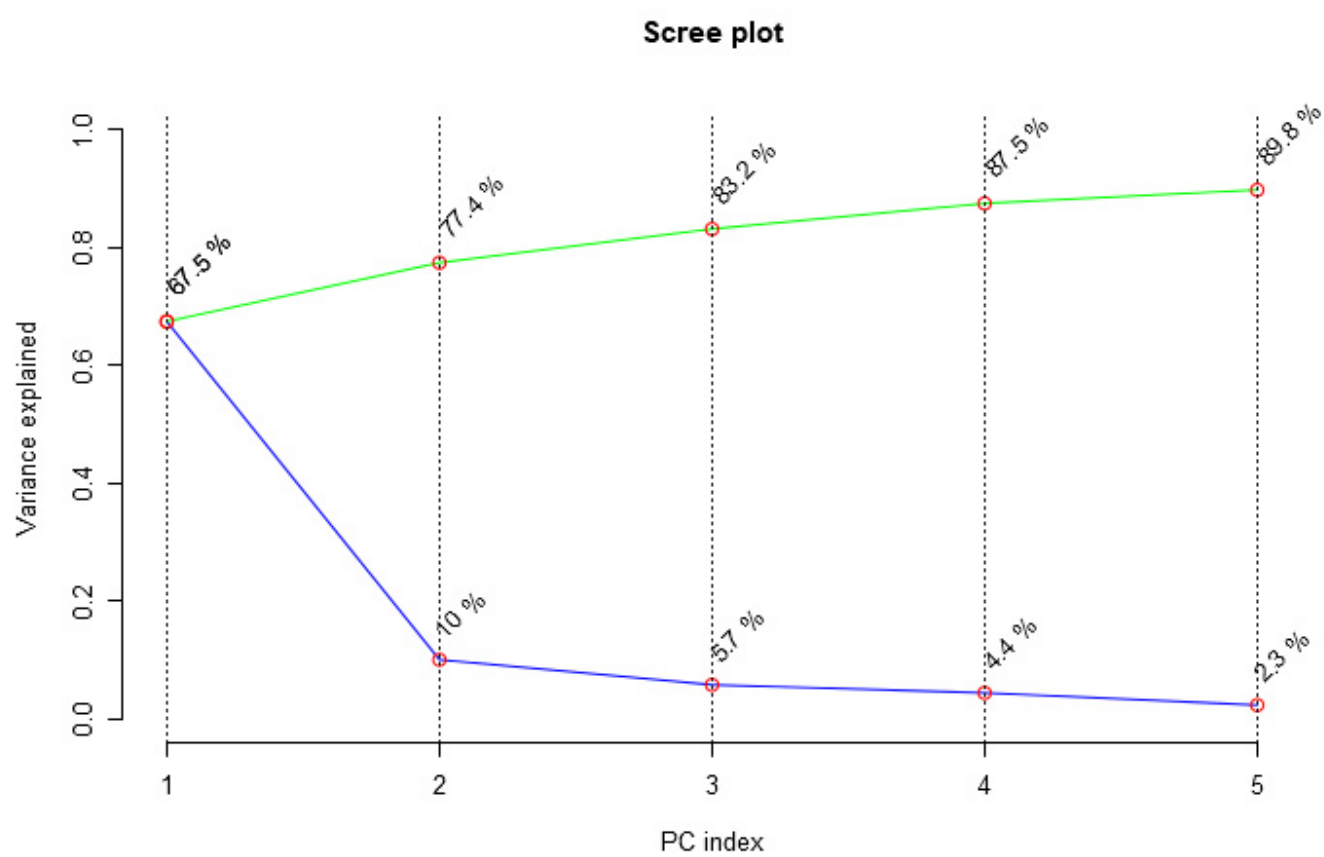
**Figure S1.** Principal Component Analysis (PCA) of 782 Metabolites by Infant Sex ( $n=52$ ). Gray circles denote male offspring. Black triangles denote female offspring.



**Figure S2.** Principal Component Analysis (PCA) Biplot

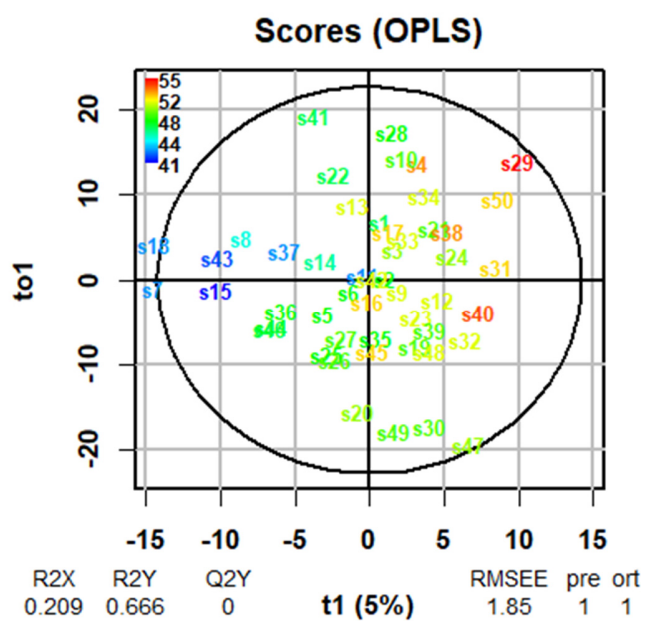


**Figure S3.** Principal Component Analysis (PCA) Loading Plot

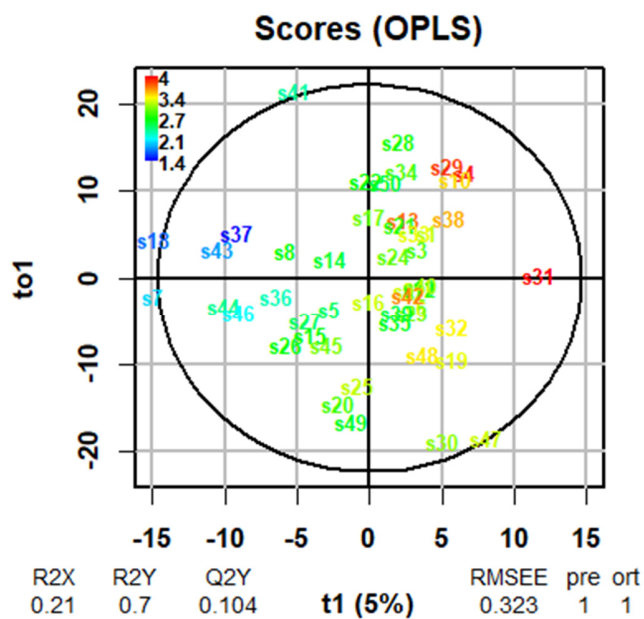


**Figure S4.** Principal Component Analysis (PCA) Scree Plot

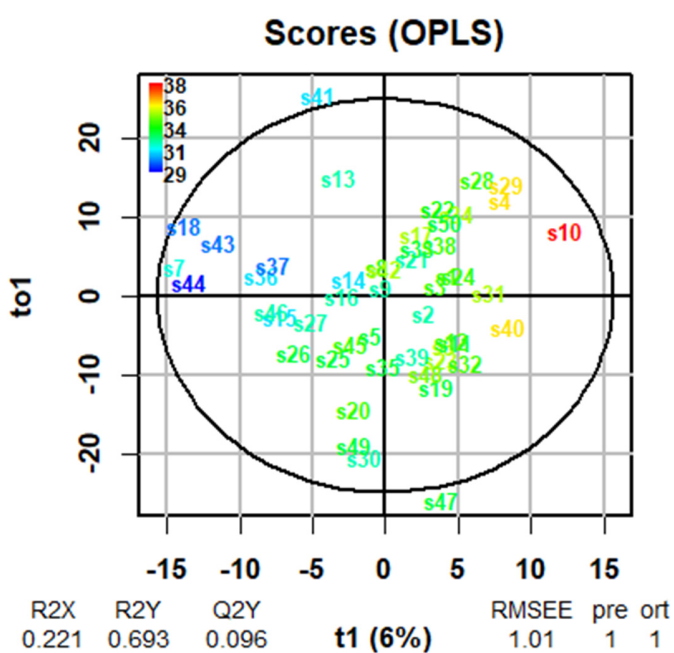
a) Infant Birth Length



b) Infant Birth Weight



c) Infant Birth Head Circumference



**Figure S5.** oPLS-DA Plots: a) infant birth length; b) infant birth weight; c) infant birth head circumference (OFC)

Table S1. Top 30 Metabolites Loading on PC1

Metabolite	PC1 Loading
palmitate (16:0)	-0.66919
linoleate (18:2n6)	-0.49372
oleate/vaccenate (18:1)	-0.47183
stearate (18:0)	-0.22477
erythronate	-0.094114
linolenate [alpha or gamma; (18:3n3 or 6)]	-0.062449
myristate (14:0)	-0.05094
palmitoleate (16:1n7)	-0.049739
glycerate	-0.043289
13-HODE + 9-HODE	-0.041659
threonate	-0.034225
arachidonate (20:4n6)	-0.031866
1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	-0.028133
isoleucine	-0.027176
proline	-0.025723
creatine	-0.024977
leucine	-0.02468
5-oxoproline	-0.022927
laurate (12:0)	-0.022821
2,3-diphosphoglycerate	-0.022443
1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	-0.020905
valine	-0.020764
lactate	0.020177
X-21796	-0.019337
creatinine	-0.019283
benzoate	0.018692
1-palmitoyl-GPC (16:0)	-0.017483
choline	-0.017385
margarate (17:0)	-0.016828
phosphate	-0.015233

Table S2. Top 30 Metabolites Loading on PC2

Metabolite	PC2 Loading
erythronate	-0.73632
oleate/vaccenate (18:1)	0.3564
stearate (18:0)	-0.33767
glycerate	-0.24458
glucose	-0.14277
proline	-0.12188
arabonate/xylonate	-0.11883
palmitate (16:0)	-0.11669
mannonate	-0.079249
palmitoyl sphingomyelin (d18:1/16:0)	-0.076379
lactate	-0.074887
betaine	-0.0654
creatine	-0.065166
X-21796	-0.057841
2,3-diphosphoglycerate	-0.051236
isoleucine	-0.046392
creatinine	-0.046322
threonate	-0.045161
valine	-0.039162
1-palmitoyl-GPC (16:0)	-0.039058
p-cresol sulfate	-0.038733
adenosine 5'-monophosphate (AMP)	-0.038565
5-oxoproline	-0.037776
caproate (6:0)	-0.033666
3-phosphoglycerate	-0.032251
leucine	-0.0309
carnitine	-0.026464
phosphate	-0.023961
arachidate (20:0)	-0.023829
alanine	-0.022703