Supplemental Information

Gas Chromatography-Mass Spectrometry and Single Nucleotide Polymorphism-Genotype-By-Sequencing reveal the chemotypes of *C. canephora* genotypes Nigeria

Supplementary Table 1: **The eight classes of metabolites identified in the Nigerian *C. canephora* coffee genotypes**. Metabolite classes include amines, amino acids, fatty acid, organic/inorganic compounds, polyphenol, sugar derivatives, sugar and vitamins. Metabolites in bold have the highest concentration within each of the classes. Metabolites in the top rows within a class are most abundant, and those in the bottom row are least abundant.

Amines			
Putrescine	Tyramine	Urea	Uric acid
Uridine	Guanosine	Pseudo uridine	Maleimide
Hydroxylamine			

Amino acids			
Aspartic acid	Glutamic acid	Proline	Tryptophan
Phenylalanine	Homoserine	Cysteine	Trans-4-hydroxyproline
Citrulline	Tyrosine	Isoleucine	Beta-alanine
Alanine	Glycine	Methionine	Valine
Leucine	Beta-glutamic acid	N-acetyl-D-galactosamine	Serine
Histidine	Threonine	Cyanoalanine	Asparagine
Lysine	Glutamine	Oxoproline	

Fatty acid			
Stearic acid	Glycerol	Palmitic acid	Linoleic acid
Pelargonic acid	Lactic acid	Oleic acid	Cis-gondoic acid
Arachidic acid	Lauric acid	Isohexonic acid	Stigmasterol
Capric acid	Hexadecylglycerol	Nonadecanoic acid	Lignoceric acid
1-monoolein	1-monopalmitin		

Organic/inorganic compounds			
Citric acid	Malic acid	Fumaric acid	Maleic acid
2-hydroxyglutaric	Alpha-ketoglutarate	Lithocholic acid	Allantoic acid
5-hydroxy-3-indole	Isocitric acid	Aconitic acid	2-deoxytetronic acid

D-erthro-sphingos	Adipic acid	Succinic acid	Shikimic acid
Phosphate	Pipecolinic acid	Alpha-aminoadipic	4-aminobutyric acid
Benzoic acid	3,4-dihydroxyhydrocinnamic acid NIST	3-hydroxybenzoic acid	Digalacturonic acid
Itaconic acid	Propane-1,3-diol	Vanillic acid	Glucosaminic acid
Citramalic acid	3,4-dihydroxybenzoate	Tartaric acid	4-hydroxybenzoate
Oxalic acid			

Phenolic acids/Alkaloids

Caffeine	Chlorogenic acid	Quinic acid	3,4-dihydroxy-cinnamic acid
Gluconic acid	Ferulic acid	Gluconic acid lactone	Beta-sitosterol
Tocopherol beta NIST	Isochlorogenic acid	Tyrosol	Nornicotine

Sugar derivatives

Galactinol	5-methoxytryptamine	Saccharic acid	Glycerol-3-galactoside
6-deoxyglucitol	Mannitol	1-methylgalactose	Butane-2,3-diol NIST
Lactobionic acid	3,6-andro-D-galactose	Glucose-1-phosphate	1,2-andro-myo-inositol
Ribonic acid	Catechinflavan-3-ol	Methanolphosphate	5-hydroxynorvaline NIST
Conduritol-beta-epoxide	2-monoolein	1-monostearin	Galactitol
Galactonic acid	Maltitol	Hexitol	Hydroquinoaromatic
Arbutin	Lactitol	4',5-dihydroxy-7-glucosyloxyflavanone	Threonic acid
Glycolic acid	6-deoxyglucose	2-monostearin NIST	Butyrolactam NIST
Glycerol-alpha-phosphate	Lyxitol	Arabitol	UDP-glucuronic acid
Isothreonic acid	Glyceric acid	Erythritol	Mucic acid

Sugars

Sucrose	Fructose	Glucose	Galactose
Sophorose	Threitol	Palatinitol	Sorbitol
Pentitol	Inulotriose	Melezitose	Tagatose
Raffinose	N-acetyl-D-mannosamine	Beta-gentiobiose	Fucose
Xylose	Trisaccharide	Mannose	

Vitamins		
Myo-inositol	Nicotinic acid (Vit B3) or Niacin	Inositol-4-monophosphate
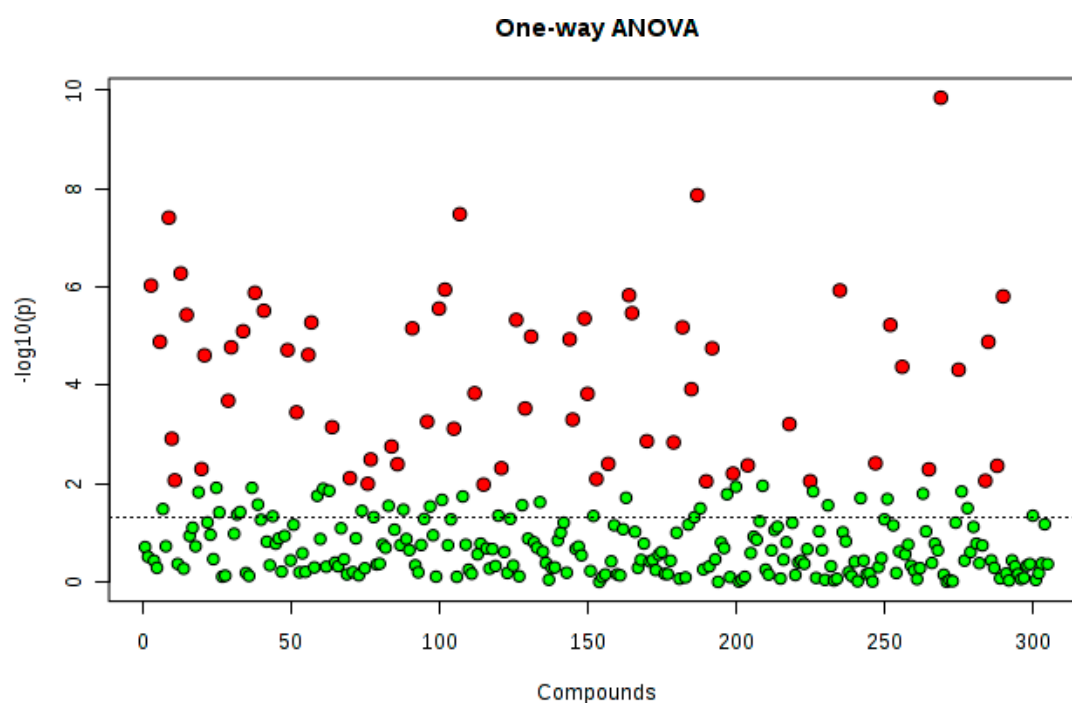
One-way ANOVA

Figure S1. **Metabolites detected by One-Way Analysis of variation that significantly varied across genotypes.** With the statistical significant level cut-off at 2 (p=0.01), there were 66 metabolites (red circles) that met this criteria.

Supplementary Table 2: Fatty acids with high Pearson's Coefficient correlative scores (r^2>0.80; p<0.05)

	Glycerol	Linoleic acid	Arachidic acid	Stearic acid	Palmitic acid
Glycerol	1	0.89409	0.83245	0.80049	0.88363
Linoleic acid	0.89409	1	0.86853	0.88823	0.91323
Arachidic acid	0.83245	0.86853	1	0.82577	0.85591
Stearic acid	0.80049	0.88823	0.82577	1	0.89874
Palmitic acid	0.88363	0.91323	0.85591	0.89874	1