Supplementary Information

Lipidomic response to coffee consumption

Supplementary Notes

1. Coffee Trial

The coffee trial design and primary clinical results have been reported in detail previously[1]. Habitual coffee consumers <65 years of age, residing in Finland, free of T2D, but with an elevated risk of T2D (≥13 points in the Finnish diabetes risk score) were eligible for participation. Exclusion criteria were the use of blood glucose–lowering medication or drugs that interfere with glucose metabolism, a history of chronic diseases likely to interfere with study participation, a history of alcohol or drug abuse, and pregnancy or breastfeeding. Eligible participants received 0, 3, or 5 packages with 500 g coffee/mo (Juhla Mokka, Paulig Group, Finland) prior to the first, second and third stage of the trial, respectively. The participants brewed the coffee daily at home with their own coffee machine using paper filters. They were allowed to divide their daily coffee dose as it suited them best and to keep the brewed coffee in a thermos if it was impossible to prepare it freshly before drinking. Instructions pertaining to the weight/volume of coffee to use per cup or the addition of cream, milk or sugar, were not provided. During the first month, participants refrained from drinking coffee, whereas in the second month they consumed 4 cups coffee/d (1 cup = 150 mL) and in the third month 8 cups/d. No restrictions were made on the consumption of other caffeine sources throughout the study. Participants were advised to maintain their normal physical activities and diet during the trial. Body weight remained stable throughout the trial. Of the 49 participants recruited, 47 completed the trial. Baseline characteristics of these 47 participants are shown in **Table S1**. At the end of each treatment stage, serum samples were collected after an overnight fast (including coffee) for ≥8 h and stored at -80ºC. Analysts performing the biochemical analyses were blinded to the treatment stage of each participant. The trial was conducted in accordance with the Declaration of Helsinki (1964), as amended in South Africa (1996), and approved by Joint Authority for the Hospital District of Helsinki and Uusimaa Ethics Committee, Department of Medicine, Helsinki, Finland. Written informed consent was obtained from all participants. Trial registration: http://www.isrctn.com/ISRCTN12547806 .

2. Multivariate Analysis: Coffee Drinker Classification and Predictive Lipid-Screening

Multilevel partial least squares discriminant analysis (MPLSDA)[2] was performed to examine whether coffee consumption led to systemic lipid changes and which lipids were the most differentiating biomarkers across the

stages of the coffee trial as described previously[3]. Because repeated measure multivariate methods that model three or more levels simultaneously are prone to bias[4], we performed separate MPLSDA for each treatment comparison (4 cups vs 0 cups, 8 vs 0 and 8 vs 4)[2].

Upon visual inspection of the multilevel PCA score plots for each coffee stage comparison, no clear classification was evident when modeling all lipid species (**Figure S5**). Comparing the non-coffee period (0 cups/d) to 4 cups/d and to 8 cups/d, on average 42.1 (44.8%) and 20.3 (21.6%) samples, respectively, out of 94 were misclassified. CV was not warranted.

Table S1. Baseline characteristics of coffee trial participants (N=47)[1]

Characteristic	Value
age, years	54.0 (9.0)
female, n (%)	36 (77)
body mass index, kg/m^2	29.2 (4.6)
waist circumference, cm	98.1 (10.5)
systolic blood pressure, mm Hg	141 (15)
diastolic blood pressure, mm Hg	90 (9)
current smoker, n (%)	2 (4)
habitual coffee intake, 150-ml cups/d	4.0 (1.7)
tea consumers, n (%)	17 (36)

Data are mean (SD) unless otherwise noted

Table S2: Lipid species excluded from the current analysis

Lipid Class	Lipid
CER	CER(20:1)
DAG	DAG(12:0/18:2)
DAG	DAG(14:0/14:0)
DAG	DAG(14:0/20:4)
DAG	DAG(14:0/22:6)
DAG	DAG(16:1/20:4)
DCER	DCER(14:0)
DCER	DCER(22:1)
DCER	DCER(26:1)
HCER	HCER(14:0)
LPC	LPC(18:4)
LPE	LPE(14:0)
LPE	LPE(14:1)
LPE	LPE(18:4)
LPE	LPE(20:0)
LPE	LPE(22:4)
PC	PC(12:0/16:1)
PC	PC(12:0/18:4)
PC	PC(12:0/20:4)
PC	PC(14:0/14:0)
PC	PC(14:0/20:1)
PC	PC(14:0/22:1)
PC	PC(14:0/22:2)
PC	PC(14:0/22:4)
PC	PC(14:0/22:5)
PC	PC(14:0/22:6)
PC	PC(15:0/16:1)
PC	PC(15:0/20:3)
PC	PC(15:0/20:4)
PC	PC(15:0/22:5)
PC	PC(15:0/22:6)
PC	PC(16:0/14:1)
PC	PC(16:0/18:4)
PC	PC(17:0/16:1)
PC	PC(17:0/18:3)
PC	PC(17:0/20:5)
PC	PC(17:0/22:5)
PC	PC(17:0/22:6)
PC	PC(18:0/18:4)
PC	PC(18:0/22:1)
PC	PC(18:1/22:1)
PC	PC(18:1/22:2)
PC	PC(18:1/22:4)

PC	PC(18:1/22:5)
PC	PC(18:2/22:1)
PC	PC(18:2/22:4)
PC	PC(18:2/22:5)
PC	PC(18:2/22:6)
PC	PC(20:0/16:1)
PC	PC(20:0/18:3)
PC	PC(20:0/20:3)
PE	PE(16:0/16:1)
PE	PE(16:0/18:3)
PE	PE(16:0/20:1)
PE	PE(16:0/20:2)
PE	PE(16:0/20:5)
PE	PE(16:0/22:4)
PE	PE(17:0/18:1)
PE	PE(17:0/18:2)
PE	PE(17:0/20:2)
PE	PE(17:0/20:4)
PE	PE(17:0/22:4)
PE	PE(18:0/15:0)
PE	PE(18:0/16:0)
PE	PE(18:0/16:1)
PE	PE(18:0/17:0)
PE	PE(18:1/14:1)
PE	PE(18:1/18:3)
PE	PE(18:1/20:1)
PE	PE(18:1/20:2)
PE	PE(18:1/20:3)
PE	PE(18:1/20:5)
PE	PE(18:1/22:4)
PE	PE(18:1/22:5)
PE	PE(18:1/22:6)
PE	PE(18:2/14:1)
PE	PE(18:2/18:2)
PE	PE(18:2/18:3)
PE	PE(18:2/20:4)
PE	PE(O-16:0/16:0)
PE	PE(O-16:0/20:3)
PE	PE(O-16:0/20:5)
PE	PE(O-16:0/22:4)
PE	PE(O-18:0/16:1)
PE	PE(O-18:0/18:0)
PE	PE(O-18:0/18:3)
PE	PE(O-18:0/20:5)
PE	PE(O-18:0/22:2)
PE	PE(O-18:0/22:4)

PE	PE(O-18:0/22:5)
PE	PE(O-18:0/22:6)
PE	PE(P-14:0/18:1)
PE	PE(P-16:0/16:1)
PE	PE(P-16:0/18:0)
PE	PE(P-16:0/18:3)
PE	PE(P-16:0/20:1)
PE	PE(P-16:0/20:2)
PE	PE(P-16:1/18:1)
PE	PE(P-18:0/16:1)
PE	PE(P-18:0/18:0)
PE	PE(P-18:0/18:3)
PE	PE(P-18:0/20:2)
PE	PE(P-18:0/22:4)
PE	PE(P-18:1/16:1)
PE	PE(P-18:1/18:0)
PE	PE(P-18:1/18:3)
PE	PE(P-18:1/22:4)
PE	PE(P-18:1/22:5)
PE	PE(P-18:2/18:2)
PE	PE(P-18:2/20:4)
PE	PE(P-18:2/22:6)
PI	PI(16:0/18:3)
PI	PI(16:0/22:4)
PI	PI(16:0/22:5)
PI	PI(16:0/22:6)
PI	PI(18:0/20:5)
PI	PI(18:0/22:4)
PI	PI(18:0/22:6)
PI	PI(18:1/20:3)
PI	PI(18:2/18:2)

Table S3: Lipids analyzed in the current study

Analysis	Lipid Group	Lipid Class	Trait Type	Lipid	Unit
Primary	Neutral Lipids	CE	Lipid Species	CE(12:0)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(14:0)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(14:1)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(15:0)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(16:0)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(16:1)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(17:0)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(18:0)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(18:1)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(18:2)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(18:3)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(18:4)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(20:0)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(20:1)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(20:2)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(20:3)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(20:4)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(20:5)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(22:0)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(22:1)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(22:2)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(22:4)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(22:5)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(22:6)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(24:0)	uM or %mole
Primary	Neutral Lipids	CE	Lipid Species	CE(24:1)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(12:0/16:0)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(12:0/18:0)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(12:0/18:1)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(14:0/16:0)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(14:0/16:1)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(14:0/18:1)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(14:0/18:2)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(14:0/18:3)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(14:0/20:0)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(14:1/16:0)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(14:1/18:1)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(15:0/18:1)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(15:0/18:2)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:0/16:0)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:0/16:1)	uM or %mole

Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:0/18:0)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:0/18:1)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:0/18:2)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:0/18:3)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:0/20:3)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:0/20:4)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:0/22:6)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:1/16:1)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:1/18:0)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:1/18:1)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:1/18:2)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:1/18:3)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:1/20:0)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:1/20:2)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(16:1/22:6)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:0/18:1)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:0/18:2)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:0/18:3)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:0/22:6)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:1/18:1)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:1/18:2)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:1/20:1)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:1/20:2)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:1/20:3)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:1/20:4)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:1/22:4)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:1/22:6)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:2/18:3)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:2/20:3)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:2/20:4)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:2/22:4)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(18:2/22:6)	uM or %mole
Primary	Neutral Lipids	DAG	Lipid Species	DAG(20:0/20:0)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(12:0)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(14:0)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(14:1)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(15:0)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(16:0)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(16:1)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(17:0)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(18:0)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(18:1)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(18:2)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(18:4)	uM or %mole

Primary	Neutral Lipids	FFA	Lipid Species	FFA(20:0)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(20:1)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(20:2)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(20:3)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(20:4)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(20:5)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(22:0)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(22:1)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(22:2)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(22:4)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(22:5)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(22:6)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(24:0)	uM or %mole
Primary	Neutral Lipids	FFA	Lipid Species	FFA(24:1)	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG36:0-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG38:0-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG40:0-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG40:0-FA14:0	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG42:0-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG42:0-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG42:1-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG42:1-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG42:1-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG42:1-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG42:1-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG42:2-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG42:2-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:0-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:0-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:0-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:0-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:1-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:1-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:1-FA14:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:1-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:1-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:1-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:2-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:2-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:2-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:2-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:2-FA18:1	uM or %mole

Primary	Neutral Lipids	TAG	Lipid Species	TAG44:2-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG44:3-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG45:0-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG45:0-FA15:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG45:0-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG45:1-FA15:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG45:1-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG45:1-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:0-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:0-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:0-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:0-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:1-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:1-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:1-FA14:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:1-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:1-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:1-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:1-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:2-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:2-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:2-FA14:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:2-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:2-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:2-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:2-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:3-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:3-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:3-FA14:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:3-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:3-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:3-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:3-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:3-FA18:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG46:4-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:0-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:0-FA15:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:0-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:0-FA17:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:1-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:1-FA15:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:1-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:1-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:1-FA17:0	uM or %mole

Primary	Neutral Lipids	TAG	Lipid Species	TAG47:1-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:2-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:2-FA15:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:2-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:2-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG47:2-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:0-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:0-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:0-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:1-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:1-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:1-FA14:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:1-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:1-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:1-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:1-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:2-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:2-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:2-FA14:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:2-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:2-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:2-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:2-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:2-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:3-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:3-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:3-FA14:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:3-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:3-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:3-FA18:1	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG48:3-FA18:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:4-FA12:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:4-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:4-FA14:1	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG48:4-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG48:4-FA18:1	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG48:5-FA18:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG49:0-FA15:0	uM or %mole

Primary	Neutral Lipids	TAG	Lipid Species	TAG49:0-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG49:0-FA17:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG49:0-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG49:1-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG49:1-FA15:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG49:1-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG49:1-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG49:1-FA17:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG49:1-FA18:1	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG50:0-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG50:0-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG50:0-FA18:0	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG50:1-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG50:1-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG50:1-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG50:1-FA18:1	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG50:2-FA14:1	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG50:3-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG50:3-FA18:1	uM or %mole

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Primary	Neutral Lipids	TAG	Lipid Species	TAG50:4-FA16:1	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG51:3-FA16:1	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG51:4-FA16:1	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG52:0-FA16:0	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG52:2-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG52:2-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG52:2-FA18:2	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG52:3-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG52:3-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG52:3-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG52:3-FA18:1	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG52:3-FA22:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG52:4-FA14:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG52:4-FA16:0	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG53:2-FA17:0	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG54:2-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:2-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:2-FA18:2	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG54:2-FA20:1	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG54:3-FA18:2	uM or %mole
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Primary	Neutral Lipids	TAG	Lipid Species	TAG54:3-FA20:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:3-FA20:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:4-FA16:0	uM or %mole

Primary	Neutral Lipids	TAG	Lipid Species	TAG54:4-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:4-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:4-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:4-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:4-FA18:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:4-FA20:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:4-FA20:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:4-FA20:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:4-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:4-FA22:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:4-FA22:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA18:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA20:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA20:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA20:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA22:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA22:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:5-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:6-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:6-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:6-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:6-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:6-FA18:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:6-FA20:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:6-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:6-FA20:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:6-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:6-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:7-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:7-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:7-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:7-FA18:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:7-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:7-FA20:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:7-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:7-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:8-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:8-FA18:3	uM or %mole

Primary	Neutral Lipids	TAG	Lipid Species	TAG54:8-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:8-FA20:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG54:8-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:1-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:1-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:2-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:2-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:3-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:3-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:4-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:4-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:5-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:5-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:5-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:6-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:6-FA20:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:6-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:7-FA15:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:7-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:7-FA20:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:7-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:7-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG55:8-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:10-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:1-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:1-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:2-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:2-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:2-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:2-FA20:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:2-FA20:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:3-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:3-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:3-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:3-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:3-FA20:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:3-FA20:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:3-FA20:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:4-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:4-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:4-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:4-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:4-FA20:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:4-FA20:2	uM or %mole

Primary	Neutral Lipids	TAG	Lipid Species	TAG56:4-FA20:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:4-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:4-FA22:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:5-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:5-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:5-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:5-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:5-FA20:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:5-FA20:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:5-FA20:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:5-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:5-FA22:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:5-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:6-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:6-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:6-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:6-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:6-FA18:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:6-FA20:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:6-FA20:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:6-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:6-FA20:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:6-FA22:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:6-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:6-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:7-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:7-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:7-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:7-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:7-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:7-FA18:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:7-FA20:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:7-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:7-FA20:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:7-FA22:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:7-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:7-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:8-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:8-FA16:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:8-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:8-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:8-FA18:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:8-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:8-FA20:5	uM or %mole

Primary	Neutral Lipids	TAG	Lipid Species	TAG56:8-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:8-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:9-FA18:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:9-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:9-FA20:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG56:9-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG57:2-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG57:3-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG57:8-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG57:9-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:10-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:10-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:10-FA20:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:10-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:10-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:2-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:3-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:5-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:6-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:6-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:6-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:6-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:6-FA22:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:6-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:7-FA16:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:7-FA18:0	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:7-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:7-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:7-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:7-FA22:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:7-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:7-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:8-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:8-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:8-FA20:3	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:8-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:8-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:8-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:9-FA18:1	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:9-FA18:2	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:9-FA20:4	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:9-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG58:9-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG60:10-FA22:5	uM or %mole

Primary	Neutral Lipids	TAG	Lipid Species	TAG60:10-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG60:11-FA22:5	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG60:11-FA22:6	uM or %mole
Primary	Neutral Lipids	TAG	Lipid Species	TAG60:12-FA22:6	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(14:0)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(15:0)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(16:0)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(16:1)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(17:0)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(18:0)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(18:1)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(18:2)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(18:3)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(20:0)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(20:1)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(20:2)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(20:3)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(20:4)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(20:5)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(22:1)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(22:2)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(22:4)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(22:5)	uM or %mole
Primary	Phospholipids	LPC	Lipid Species	LPC(22:6)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(15:0)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(16:0)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(16:1)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(17:0)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(18:0)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(18:1)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(18:2)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(18:3)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(20:1)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(20:2)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(20:3)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(20:4)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(20:5)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(22:5)	uM or %mole
Primary	Phospholipids	LPE	Lipid Species	LPE(22:6)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(12:0/18:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(12:0/18:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(12:0/18:3)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(14:0/16:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(14:0/18:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(14:0/18:2)	uM or %mole

Primary	Phospholipids	PC	Lipid Species	PC(14:0/18:3)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(14:0/20:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(14:0/20:3)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(14:0/20:4)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(15:0/18:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(15:0/18:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/12:0)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/14:0)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/16:0)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/16:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/18:0)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/18:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/18:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/18:3)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/20:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/20:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/20:3)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/20:4)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/22:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/22:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/22:4)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/22:5)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(16:0/22:6)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(17:0/18:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(17:0/18:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(17:0/20:3)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(17:0/20:4)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/12:0)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/14:0)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/16:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/18:0)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/18:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/18:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/18:3)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/20:0)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/20:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/20:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/20:3)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/20:4)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/22:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/22:4)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/22:5)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:0/22:6)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:1/16:1)	uM or %mole

Primary	Phospholipids	PC	Lipid Species	PC(18:1/18:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:1/18:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:1/18:3)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:1/20:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:1/20:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:1/20:3)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:1/20:4)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:1/22:6)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:2/16:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:2/18:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:2/18:3)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:2/20:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:2/20:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:2/20:3)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(18:2/20:4)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(20:0/14:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(20:0/18:1)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(20:0/18:2)	uM or %mole
Primary	Phospholipids	PC	Lipid Species	PC(20:0/20:4)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(16:0/16:0)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(16:0/18:1)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(16:0/18:2)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(16:0/20:3)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(16:0/20:4)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(16:0/22:5)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(16:0/22:6)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/18:0)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/18:1)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/18:2)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/18:3)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/20:1)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/20:2)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/20:3)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/20:4)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/20:5)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/22:2)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/22:4)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/22:5)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:0/22:6)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:1/16:1)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:1/18:1)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:1/18:2)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:1/20:4)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(18:1/22:0)	uM or %mole

Primary	Phospholipids	PE	Lipid Species	PE(18:2/16:1)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(O-16:0/18:1)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(O-16:0/18:2)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(O-16:0/20:4)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(O-16:0/22:5)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(O-16:0/22:6)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(O-18:0/16:0)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(O-18:0/18:1)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(O-18:0/18:2)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(O-18:0/20:3)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(O-18:0/20:4)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-16:0/16:0)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-16:0/18:1)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-16:0/18:2)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-16:0/20:3)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-16:0/20:4)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-16:0/20:5)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-16:0/22:4)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-16:0/22:5)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-16:0/22:6)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:0/16:0)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:0/18:1)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:0/18:2)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:0/20:3)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:0/20:4)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:0/20:5)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:0/22:5)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:0/22:6)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:1/16:0)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:1/18:1)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:1/18:2)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:1/20:3)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:1/20:4)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:1/20:5)	uM or %mole
Primary	Phospholipids	PE	Lipid Species	PE(P-18:1/22:6)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(16:0/16:0)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(16:0/16:1)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(16:0/18:1)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(16:0/18:2)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(16:0/20:3)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(16:0/20:4)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(18:0/16:0)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(18:0/16:1)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(18:0/18:1)	uM or %mole

Primary	Phospholipids	PI	Lipid Species	PI(18:0/18:2)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(18:0/18:3)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(18:0/20:2)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(18:0/20:3)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(18:0/20:4)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(18:0/22:5)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(18:1/16:1)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(18:1/18:1)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(18:1/18:2)	uM or %mole
Primary	Phospholipids	PI	Lipid Species	PI(18:1/20:4)	uM or %mole
Primary	Sphingolipids	CER	Lipid Species	CER(14:0)	uM or %mole
Primary	Sphingolipids	CER	Lipid Species	CER(16:0)	uM or %mole
Primary	Sphingolipids	CER	Lipid Species	CER(18:0)	uM or %mole
Primary	Sphingolipids	CER	Lipid Species	CER(18:1)	uM or %mole
Primary	Sphingolipids	CER	Lipid Species	CER(20:0)	uM or %mole
Primary	Sphingolipids	CER	Lipid Species	CER(22:0)	uM or %mole
Primary	Sphingolipids	CER	Lipid Species	CER(22:1)	uM or %mole
Primary	Sphingolipids	CER	Lipid Species	CER(24:0)	uM or %mole
Primary	Sphingolipids	CER	Lipid Species	CER(24:1)	uM or %mole
Primary	Sphingolipids	CER	Lipid Species	CER(26:0)	uM or %mole
Primary	Sphingolipids	CER	Lipid Species	CER(26:1)	uM or %mole
Primary	Sphingolipids	DCER	Lipid Species	DCER(16:0)	uM or %mole
Primary	Sphingolipids	DCER	Lipid Species	DCER(18:0)	uM or %mole
Primary	Sphingolipids	DCER	Lipid Species	DCER(20:0)	uM or %mole
Primary	Sphingolipids	DCER	Lipid Species	DCER(22:0)	uM or %mole
Primary	Sphingolipids	DCER	Lipid Species	DCER(24:0)	uM or %mole
Primary	Sphingolipids	DCER	Lipid Species	DCER(24:1)	uM or %mole
Primary	Sphingolipids	DCER	Lipid Species	DCER(26:0)	uM or %mole
Primary	Sphingolipids	HCER	Lipid Species	HCER(16:0)	uM or %mole
Primary	Sphingolipids	HCER	Lipid Species	HCER(18:0)	uM or %mole
Primary	Sphingolipids	HCER	Lipid Species	HCER(18:1)	uM or %mole
Primary	Sphingolipids	HCER	Lipid Species	HCER(20:0)	uM or %mole
Primary	Sphingolipids	HCER	Lipid Species	HCER(20:1)	uM or %mole
Primary	Sphingolipids	HCER	Lipid Species	HCER(22:0)	uM or %mole
Primary	Sphingolipids	HCER	Lipid Species	HCER(22:1)	uM or %mole
Primary	Sphingolipids	HCER	Lipid Species	HCER(24:0)	uM or %mole
Primary	Sphingolipids	HCER	Lipid Species	HCER(24:1)	uM or %mole
Primary	Sphingolipids	HCER	Lipid Species	HCER(26:0)	uM or %mole
Primary	Sphingolipids	HCER	Lipid Species	HCER(26:1)	uM or %mole
Primary	Sphingolipids	LCER	Lipid Species	LCER(14:0)	uM or %mole
Primary	Sphingolipids	LCER	Lipid Species	LCER(16:0)	uM or %mole
Primary	Sphingolipids	LCER	Lipid Species	LCER(18:0)	uM or %mole
Primary	Sphingolipids	LCER	Lipid Species	LCER(18:1)	uM or %mole
Primary	Sphingolipids	LCER	Lipid Species	LCER(20:0)	uM or %mole

Primary	Sphingolipids	LCER	Lipid Species	LCER(20:1)	uM or %mole
Primary	Sphingolipids	LCER	Lipid Species	LCER(22:0)	uM or %mole
Primary	Sphingolipids	LCER	Lipid Species	LCER(22:1)	uM or %mole
Primary	Sphingolipids	LCER	Lipid Species	LCER(24:0)	uM or %mole
Primary	Sphingolipids	LCER	Lipid Species	LCER(24:1)	uM or %mole
Primary	Sphingolipids	LCER	Lipid Species	LCER(26:0)	uM or %mole
Primary	Sphingolipids	LCER	Lipid Species	LCER(26:1)	uM or %mole
Primary	Sphingolipids	SM	Lipid Species	SM(14:0)	uM or %mole
Primary	Sphingolipids	SM	Lipid Species	SM(16:0)	uM or %mole
Primary	Sphingolipids	SM	Lipid Species	SM(18:0)	uM or %mole
Primary	Sphingolipids	SM	Lipid Species	SM(18:1)	uM or %mole
Primary	Sphingolipids	SM	Lipid Species	SM(20:0)	uM or %mole
Primary	Sphingolipids	SM	Lipid Species	SM(20:1)	uM or %mole
Primary	Sphingolipids	SM	Lipid Species	SM(22:0)	uM or %mole
Primary	Sphingolipids	SM	Lipid Species	SM(22:1)	uM or %mole
Primary	Sphingolipids	SM	Lipid Species	SM(24:0)	uM or %mole
Primary	Sphingolipids	SM	Lipid Species	SM(24:1)	uM or %mole
Primary	Sphingolipids	SM	Lipid Species	SM(26:0)	uM or %mole
Primary	Sphingolipids	SM	Lipid Species	SM(26:1)	uM or %mole
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA12:0]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA14:0]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA14:1]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA15:0]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA16:0]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA16:1]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA18:0]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA18:1]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA18:2]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA18:3]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA20:0]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA20:1]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA20:2]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA20:3]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA20:4]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA22:4]	uM
Secondary	Neutral Lipids	DAG	Fatty acid	DAG[FA22:6]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA12:0]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA14:0]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA14:1]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA15:0]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA16:0]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA16:1]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA17:0]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA18:0]	uM

Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA18:1]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA18:2]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA18:3]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA20:0]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA20:1]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA20:2]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA20:3]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA20:4]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA20:5]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA22:1]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA22:4]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA22:5]	uM
Secondary	Neutral Lipids	TAG	Fatty acid	TAG[FA22:6]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA12:0]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA14:0]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA14:1]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA15:0]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA16:0]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA16:1]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA17:0]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA18:0]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA18:1]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA18:2]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA18:3]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA20:0]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA20:1]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA20:2]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA20:3]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA20:4]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA22:1]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA22:2]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA22:4]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA22:5]	uM
Secondary	Phospholipids	PC	Fatty acid	PC[FA22:6]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA16:0]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA16:1]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA18:0]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA18:1]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA18:2]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA18:3]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA20:1]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA20:2]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA20:3]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA20:4]	uM

Secondary	Phospholipids	PE	Fatty acid	PE[FA20:5]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA22:0]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA22:2]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA22:4]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA22:5]	uM
Secondary	Phospholipids	PE	Fatty acid	PE[FA22:6]	uM
Secondary	Phospholipids	PI	Fatty acid	PI[FA16:0]	uM
Secondary	Phospholipids	PI	Fatty acid	PI[FA16:1]	uM
Secondary	Phospholipids	PI	Fatty acid	PI[FA18:0]	uM
Secondary	Phospholipids	PI	Fatty acid	PI[FA18:1]	uM
Secondary	Phospholipids	PI	Fatty acid	PI[FA18:2]	uM
Secondary	Phospholipids	PI	Fatty acid	PI[FA18:3]	uM
Secondary	Phospholipids	PI	Fatty acid	PI[FA20:2]	uM
Secondary	Phospholipids	PI	Fatty acid	PI[FA20:3]	uM
Secondary	Phospholipids	PI	Fatty acid	PI[FA20:4]	uM
Secondary	Phospholipids	PI	Fatty acid	PI[FA22:5]	uM
Secondary	Neutral Lipids	CE	Lipid class	CE	uM
Secondary	Neutral Lipids	TAG	Lipid class	TAG	uM
Secondary	Neutral Lipids	DAG	Lipid class	DAG	uM
Secondary	Neutral Lipids	FFA	Lipid class	FFA	uM
Secondary	Phospholipids	PC	Lipid class	PC	uM
Secondary	Phospholipids	PE	Lipid class	PE	uM
Secondary	Phospholipids	PI	Lipid class	PI	uM
Secondary	Phospholipids	LPC	Lipid class	LPC	uM
Secondary	Phospholipids	LPE	Lipid class	LPE	uM
Secondary	Sphingolipids	SM	Lipid class	SM	uM
Secondary	Sphingolipids	CER	Lipid class	CER	uM
Secondary	Sphingolipids	HCER	Lipid class	HCER	uM
Secondary	Sphingolipids	LCER	Lipid class	LCER	uM
Secondary	Sphingolipids	DCER	Lipid class	DCER	uM

Table S4: Metabolite markers of coffee response reported by Cornelis et al, 2016*

Super Pathway	Sub Pathway‡	Metabolite
Amino Acid	Creatine Metabolism	creatinine
		guanidinoacetate
	Histidine Metabolism	hydantoin-5-propionic acid
		imidazole lactate
	Leucine, Isoleucine and Valine Metabolism	isovalerylcarnitine
	Methionine, Cysteine, SAM and Taurine Metabolism	cysteine
		methionine sulfone
	Polyamine Metabolism	4-acetamidobutanoate
		N-acetylputrescine
	Tryptophan Metabolism	5-bromotryptophan
		indolelactate
		kynurenine
	Tyrosine Metabolism	2-hydroxyphenylacetate
	Urea cycle; Arginine and Proline Metabolism	homoarginine
Carbohydrate	Aminosugar Metabolism	glucuronate
	Glycolysis, Gluconeogenesis, and Pyruvate	1,5-anhydroglucitol (1,5-AG)
Cofactors & Vitamins	Nicotinate and Nicotinamide Metabolism	trigonelline (N'-methylnicotinate)
Energy	Oxidative Phosphorylation	phosphate
	TCA Cycle	citraconate/glutaconate
Lipid	Diacylglycerol	linoleoyl-linoleoyl-glycerol (18:2/18:2)[1]*
	Endocannabinoid	linoleoyl ethanolamide
		N-oleoyltaurine
		palmitoyl ethanolamide
		stearoyl ethanolamide
	Fatty Acid Metabolism (Acyl Choline)	arachidonoylcholine
		dihomo-linolenoyl-choline
		docosahexaenoylcholine
		oleoylcholine
		palmitoloelycholine
		palmitoylcholine
	Glycerolipid Metabolism	glycerol 3-phosphate
	Phospholipid Metabolism	choline
	Polyunsaturated Fatty Acid (n3 and n6)	arachidonate (20:4n6)
		docosapentaenoate (n6 DPA;
	Secondary Bile Acid Metabolism	glycocholenate sulfate*
	Sphingolipid Metabolism	palmitoyl dihydrosphingomyelin
	Steroid	4-androsten-3alpha,17alpha-diol monosulfate (3)
		4-androsten-3beta,17beta-diol monosulfate (2)
		epiandrosterone sulfate
		etiocholanolone glucuronide
		pregn steroid monosulfate*
	Sterol	3beta,7alpha-dihydroxy-5-
		campesterol
Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine	urate
	Purine Metabolism, Adenine containing	N6-carbamoylthreonyladenosine
	Purine Metabolism, Guanine containing	7-methylguanine
	Pyrimidine Metabolism, Uracil containing	2'-deoxyuridine
Peptide	Dipeptide Derivative	N-acetylcarnosine
	Fibrinogen Cleavage Peptide	DSGEGDFXAEGGGVR*
Xenobiotics	Benzoate Metabolism	3-(3-hydroxyphenyl)propionate
		3-(3-hydroxyphenyl)propionate sulfate
		3-hydroxyhippurate
		3-methyl catechol sulfate (1)
		3-phenylpropionate
		4-vinylphenol sulfate
		catechol sulfate
		hippurate

		O-methylcatechol sulfate
	Chemical	3-hydroxypyridine sulfate
		N-methylpipecolate
		succinimide
	Food Component/Plant	cinnamoylglycine
		dihydroferulic acid
		homostachydrine*
		N-(2-furoyl)glycine
		pyrraline
		quinate
	Xanthine Metabolism	1,3,7-trimethylurate
		1,3-dimethylurate
		1,7-dimethylurate
		1-methylurate
		1-methylxanthine
		3,7-dimethylurate
		3-methylxanthine
		5-acetylamino-6-amino-3-methyluracil
		7-methylxanthine
		caffeic acid sulfate
		caffeine
		paraxanthine
		theobromine
		theophylline

*Listed are 82 metabolites of known identity associated with coffee response from our previous metabolomics analysis of these coffee trial samples{Cornelis, 2018 #8582}. These metabolites were measured by UPLC-ESI-MS/MS (nontargeted) and processed as previously described{Cornelis, 2018 #8582}. Mass spectral peaks, retention times, and m/z were used to determine the relative quantities of each metabolite. Twenty-four of these 82 were also lipids but are herein referred to as 'metabolites' to distinguish them from the new lipid species data.

‡Colors correspond to color scheme used in **Figure S3**.

Table S5. Population-based lipidomic studies of habitual coffee consumption*

Ref	Study sample	Coffee measurement†	Metabolite measurement‡	Significant LIPID findings
[5]	Germany, EU§ N=284, M age: 55-79 y	FFQ 2004-2005 cups/d	Overnight fasting serum, morning draws, 2006 ESI-MS/MS (Biocrates): 363 metabolites	Coffee intake was positively associated with SM species: SM (OH,COOH) x:y — 20:2, 16:2, 18:2, 24:0, 18:1 SM (OH) x:y — 20:3, 22:1, 28:0 Coffee intake was negatively associated with long- and medium-chain acylcarnitines: C16:1, C10:1, C12:1, C14:1, C6.
[6]	UK, EU N=1003, F, twins age: 58.5±10.45 y	FFQ categories (0 to 6+ cups/d)	Overnight fasting serum Absolute-IDQ Kit p150 (Biocrates): 126 metabolites	Coffee intake was negatively associated with acylcarnitine C10:1.
[7]	Germany, EU N=2380, M/F age: 49.8± 8.9 y	FFQ 1994-1998 categories (0 to 5+ cups/d)	Serum, fasting status unknown, 1994-1998 Absolute-IDQ Kit p150 (Biocrates): 127 metabolites	Diet pattern with high intake of margarine, non-whole-grain bread, meat, and coffee and low intake of butter, pasta/rice, and tea was positively associated with LPCs: C20:4, C18:2. Diet pattern with high intake of butter, garlic, and coffee and low intake of margarine, fresh fruit, and soup was positively associated with SMs, notably OH-C16:1, OH-C14:1, OH-C24:1, OH-C22:2, OH-C22:1
[8]	Germany, EU N=2380, M/F age: 49.8± 8.9 y	FFQ 1994-1998 categories (0 to 5+ cups/d)	Serum, fasting status unknown, 1994-1998 Absolute-IDQTM Kit p150 (Biocrates): 127 metabolites	Limited species details. Acylcarnitines were inversely associated with coffee Sphingomyelins were particularly positively related to coffee. Acyl-alkyl-phosphatidylcholines were positively linked to coffee. Most lysophosphatidylcholines were positively associated with coffee. Diacylphosphatidylcholines were inversely with coffee and cake and cookies.
[9]	Germany, EU N=1610, M/F age: 35-64 y	FFQ 1994-1998 categories (0 to 5+ cups/d)	Serum, fasting status unknown, 1994-1998 Absolute-IDQTM Kit p150 (Biocrates) Hypothesis testing: 13 metabolites previously associated with type 2 diabetes Exploratory: 113 metabolites	Hypothesis testing: Coffee was inversely associated with diacylphosphatidylcholine C32:1 in M/F. Coffee was positively associated with acyl-alkyl-phosphatidylcholines C34:3, C40:6, and C42:5 in F. Exploratory: none significantly associated with coffee.
[10]	USA, AA Discovery: N=1500, M/F age: 52.9 ± 5.8 y Replication: N=477, M/F age: 52.7 ± 5.7 y	FFQ 1987-1989 categories (0 to 6+ cups/d)	8-hr + fasting serum, 1987-1989 GC/LC-MS (Metabolon): 356 metabolites	No known lipids
[11]	USA, EU N=502, M/F (cancer cases and matched controls) age: 64 ± 5 y	FFQ 1993-2001 cups/d	Serum, fasting status unknown GC/LC-MS (Metabolon): 412 “knowns” and 231 “unknowns” detected	No known lipids
[12]	USA, EU N=253, M/F (cancer cases, matched controls) Age: 57 ± 9 y	FFQ Total coffee Regular coffee Decaf coffee g/d +55 other diet traits	12-h overnight non-fasting urine sample Nonfasting serum GC/LC-MS (Metabolon): 824 in urine, 648 in serum	No known lipids
[13]	USA, Mix N=1369, nonsmoking PM F Age=68.3± 5.7 y	FFQ 1999-2000 Total coffee Regular coffee Decaf coffee +90 diet traits	Nonfasting serum (1998-2001) GC/LC-MS (Metabolon): 1186 metabolites	Total coffee: No known lipids Regular coffee: No known lipids Decaf: No known lipids
[14]	Brazil,	2 24-h recalls FFQ	Fasting-plasma FIA-MS/MS and HPLC-MS/MS:	Coffee decreased LPC a C16:1, C18:1, C20:4 Coffee increased LPC a C16:0/C16:1, C18:0/18:1 (ratios)

N=169 (survey 2008-2009), M/F Age: 50.7 ±18.9	Non (0 ml/d), low (≤100 ml/d and high (>100 ml/d) coffee consumers Regular filtered coffee (no one consumed instant, espresso or other brewing methods, no decaf) + polyphenol intake	Absolute-IDQ p180 Kit (Biocrates) Only 14 LPC species used in analysis

*Studies examined predominately regular or total (regular and decaffeinated) coffee. Presented studies are those employing targeted or untargeted analysis of lipid classes captured by the current study.

†Includes method of dietary assessment, year of collection, and type of data collected (if reported).

‡Includes fasting status at time of specimen collection, year of blood/urine collection, and platform used for metabolomic profiling (if reported).

§Population ancestry: EU European, AA African American; Sex: M male, F female

Shown are studies applying metabolomic platforms with *potential* for lipid detection.

Annotation for PCs: “aa” indicates that both moieties at the sn-1 and sn-2 position are fatty acids and bound to the glycerol backbone via ester bonds. “ae” denotes that one of the moieties, either in the sn-1 or at sn-2 position is a fatty alcohol and bound via an ether bond. Total number of carbon atoms and double bonds present in both lipid fatty acid chains are denoted as “C x:y”, where x is the total carbon number of both chains and y is the total number of double bonds.

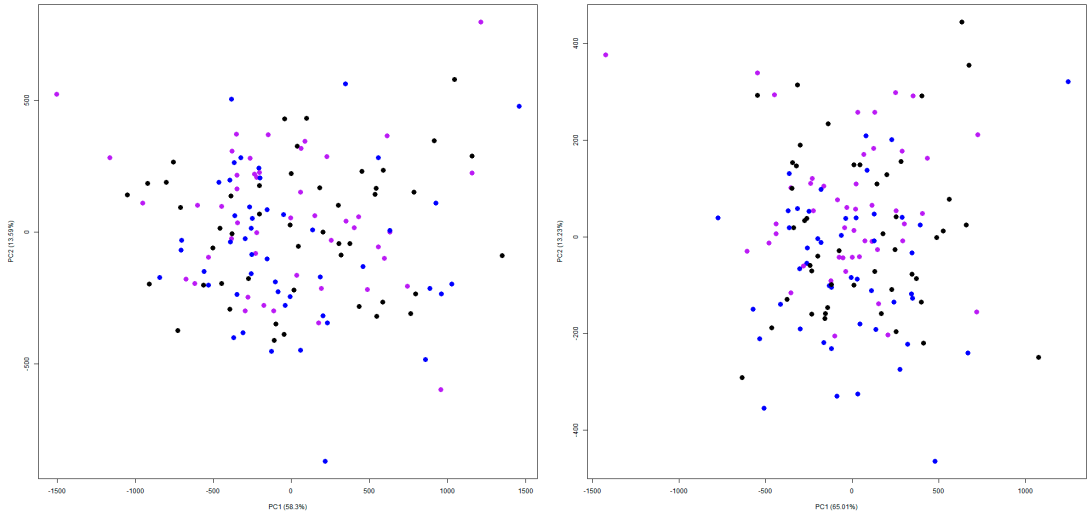
Annotation for SMs: Total number of carbon atoms, the number of double bonds or the presence of hydroxyl group (OH) are indicated only for the fatty acid in the amide bond under assumption that the backbone is formed by sphingosine (d18:1). Total number of carbon atoms and double bonds present in fatty acid chain is denoted as “C x:y”, where x is the carbon number and y is the number for double bonds

Table S6. Circulating lysophosphatidylcholines and coffee-implicated disease or conditions*

LPC	Increased Risk / Positive Association	Decreased Risk / Negative Association	Null Results
LPC(15:0)		Obesity/BMI [15,16] CRP [16] HCC [17] CVD [18] T2D & related traits [19]	Breat Ca [20] Prostate Ca [20] CRC [20] T2D & related traits [21,22] CVD[23,24] Obesity/BMI [22]
LPC(17:0)	HCC [25]	HCC [17] Obesity/BMI [26] T2D & related traits [27-29]	T2D & related traits [19,21,22] CVD [23,24] Obesity/BMI [22,30]
LPC(18:1)	AD/Cognition[31,32] Aging[31] LDL[33] HDL [33] Lung Ca [34] Obesity/BMI[35] Weight loss[36] Ovarian Ca[37]	Obesity/BMI [15,16,26,30,33,38-40] MS [41] Lung Ca [42] Weight loss [16] CRP [16,38] HCC [17] Chronic renal failure [43] Ovarian Ca [44] CVD [45] CRC [46] T2D & related traits [19,27,47]	Obesity/BMI [22,39,48] T2D & related traits [21,27,28,48] HTN/BP [48] Breast Ca [20] Prostate Ca [20] CRC [20] CVD [23] [24] Mortality [49] Ovarian Ca [50]
LPC(20:2)		T2D & related traits [19]	LDL [33] HDL [33] Obesity/BMI [33,40] CVD [23]
LPC(20:3)	Lung Ca [34] Obesity/BMI [35] Ovarian Ca [37]	Huntington's [51] Weight loss <100 [16] HCC 200 [17] CVD [18]	Breat Ca [20] Prostate Ca [20] CRC [20] CVD [23,24] Obesity/BMI [30,39] T2D & related traits [27,28]
LPC(20:4)	HDL [52] Lung Ca [34] Obesity/BMI [35] Weight loss [36] Ovarian Ca [37]	CVD [52] HTN/BP [52] Obesity/BMI [15,16,30,52] CRP [16] HCC [17]	LDL [33,35] TG [35] HDL [33] [35] Obesity/BMI [22,33,39] Breat Ca [20] Prostate Ca [20] T2D & related traits [19,21,22,27,28] Ovarian Ca [44,50] CVD [23,24] Mortality [49] CRC [20,46]
LPC(22:1)	T2D & related traits [22]		Obesity/BMI [22] T2D & related traits [19,21]
LPC(22:2)			
Total (LPC)	AD/Cognition [31] Aging [31] Lung Ca [34] Depression [53] Ovarian Ca [44]	Obesity/BMI [15,16] Weight loss/RYGB [16,54] CRP [16] Lung function [55] T2D & related traits [21] CVD [45] CRC [46]	AD/Cognition [56] Obesity/BMI [48] T2D & related traits [48] HTN/BP[48] CVD [24] Ovarian Ca [50]

*Shown are results from a non-comprehensive literature search for human clinical or observational studies relating circulating lysophosphatidylcholine with coffee-implicated disease or conditions [57].

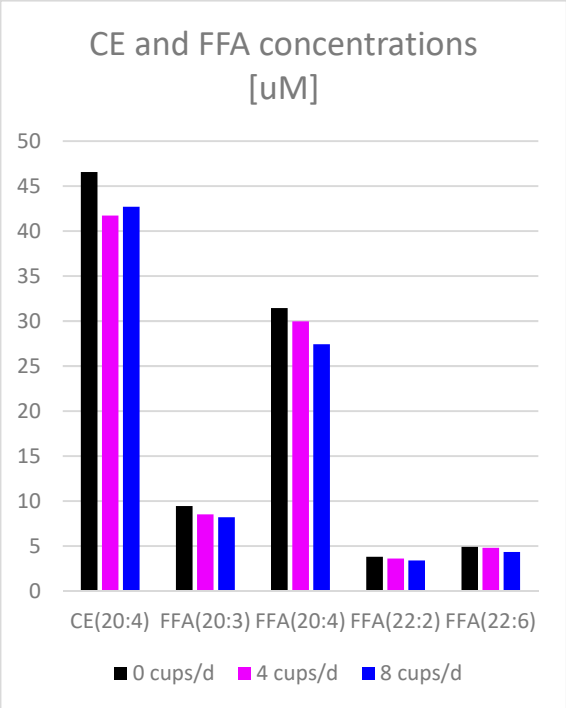
Figure S1.



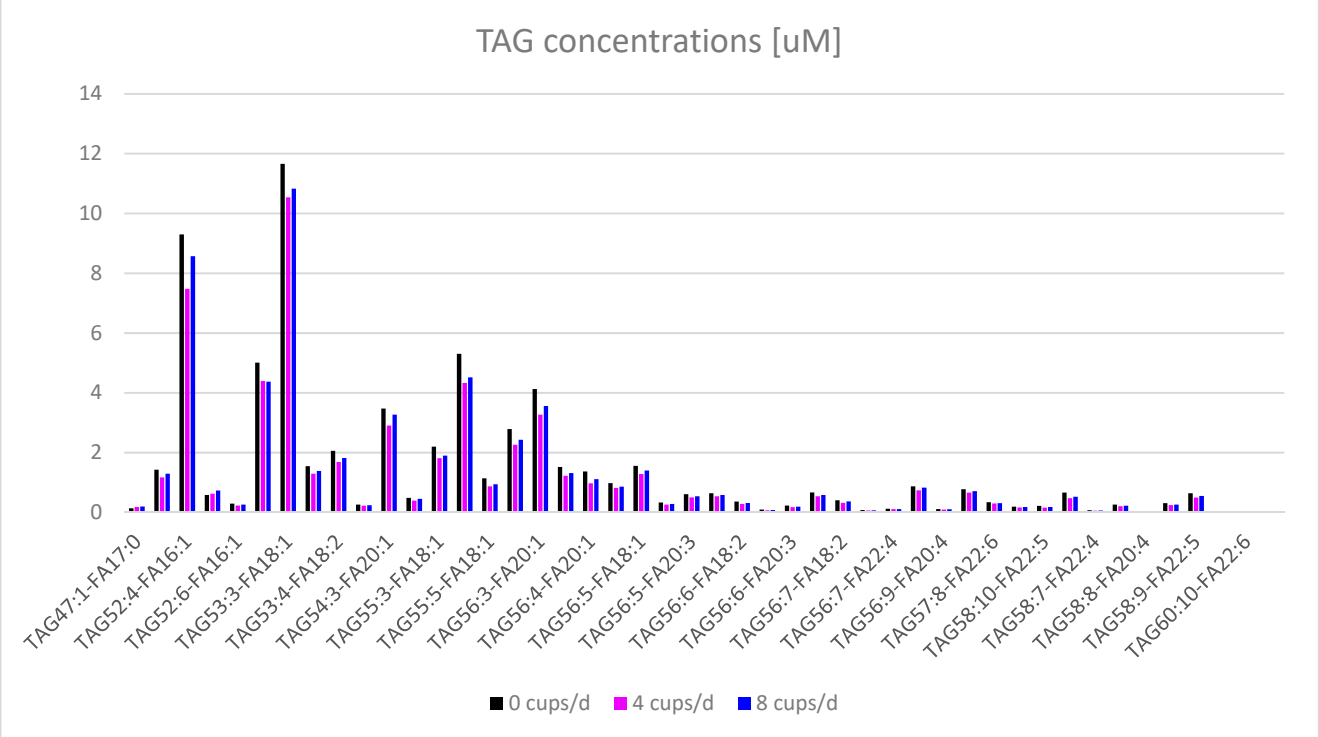
Results from PCA (A) and multilevel PCA (B) analysis. Score plot of the first and second PC. Black, purple and blue points represent samples measured after the 0 cups/d, 4 cups/d and 8 cups/d trial periods, respectively.

Figure S2

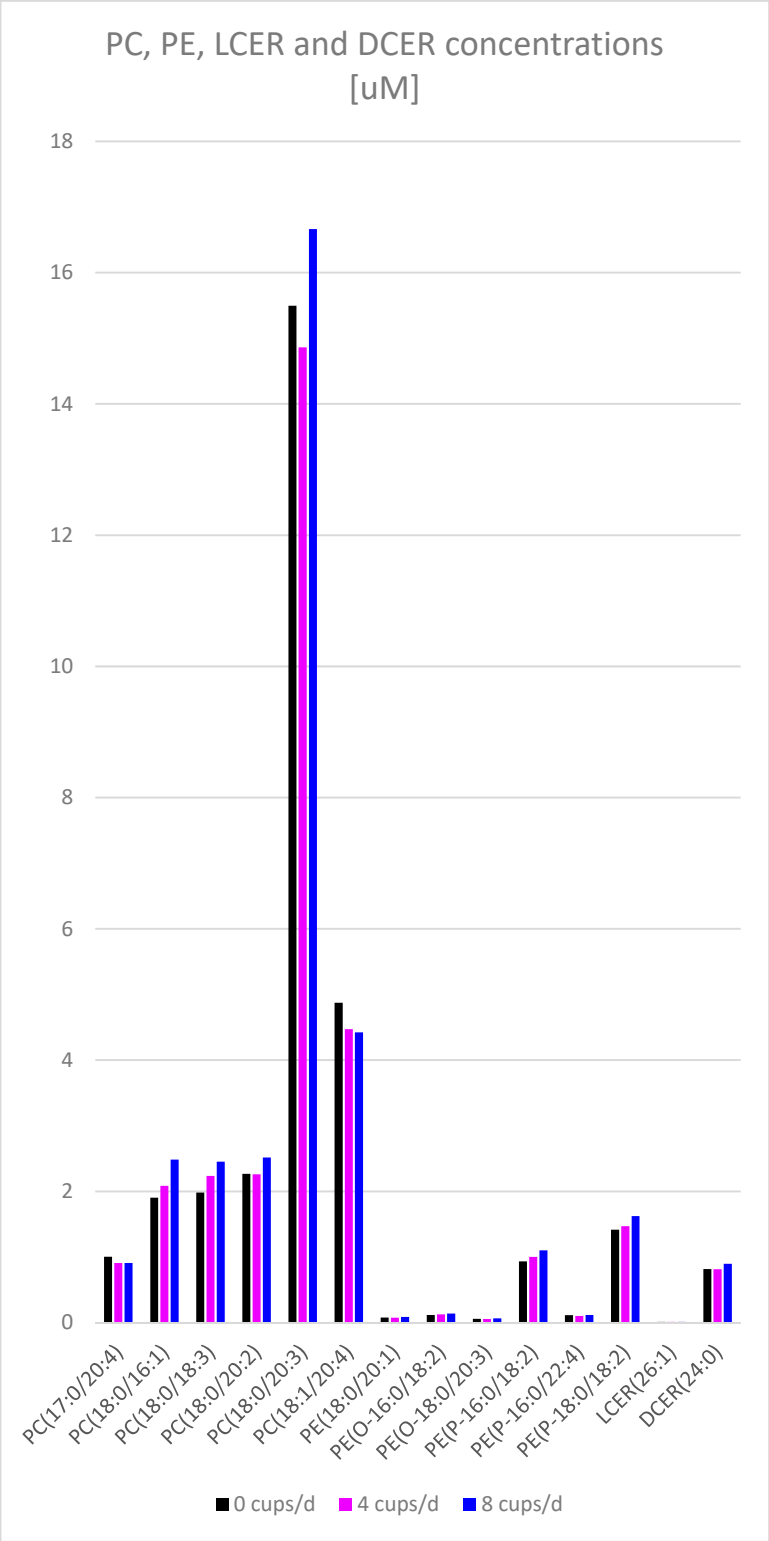
A



B



C

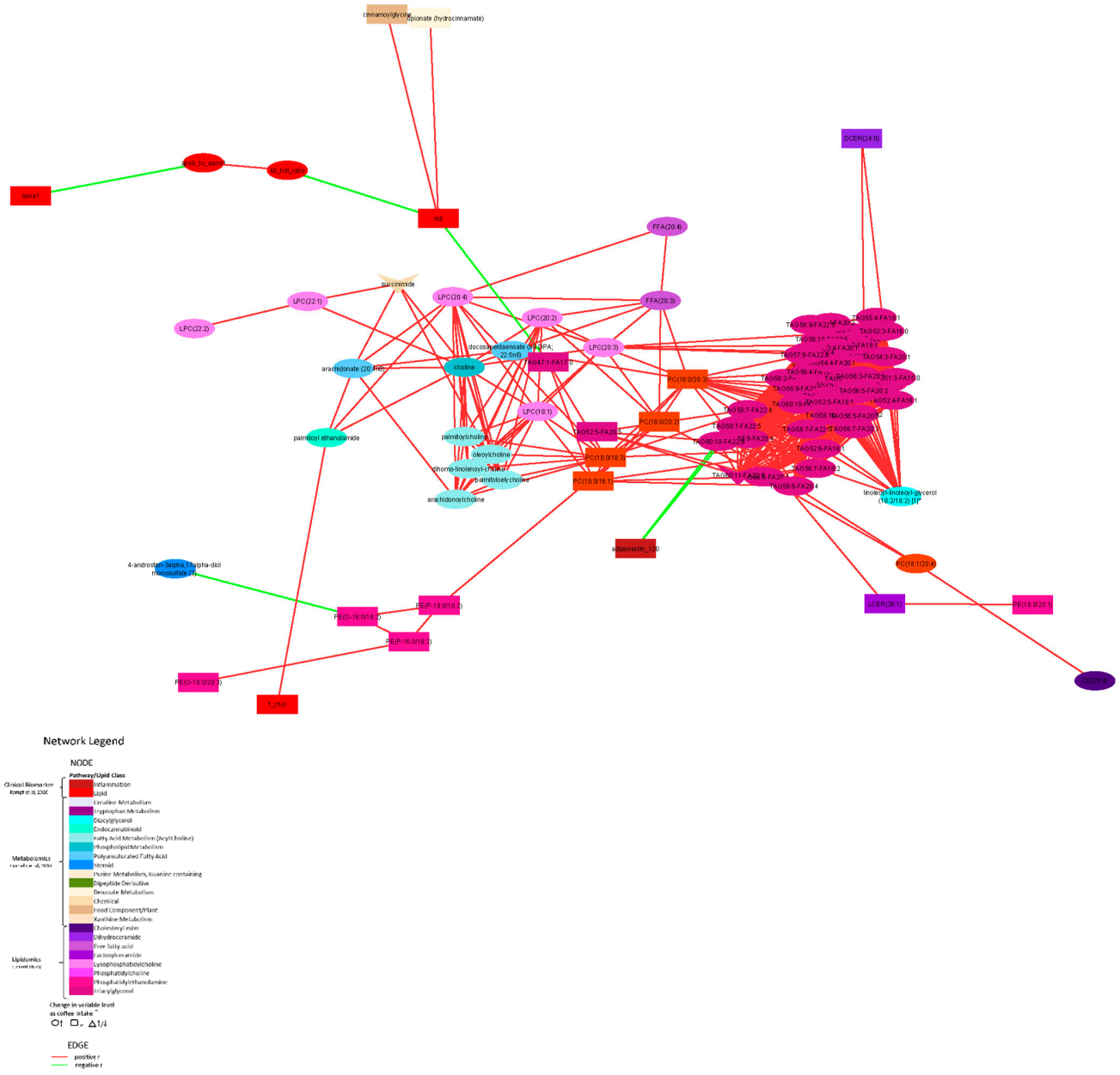


Serum concentrations [uM] of lipid species nominally associated with changes in response to coffee intake ($P<0.05$, FDR>0.05). Data for TAG54:3-FA18:1 not displayed (0 cups/d: 104.9 uM, 4 cups/d: 86.4 uM, 8 cups/d: 94.3 uM).

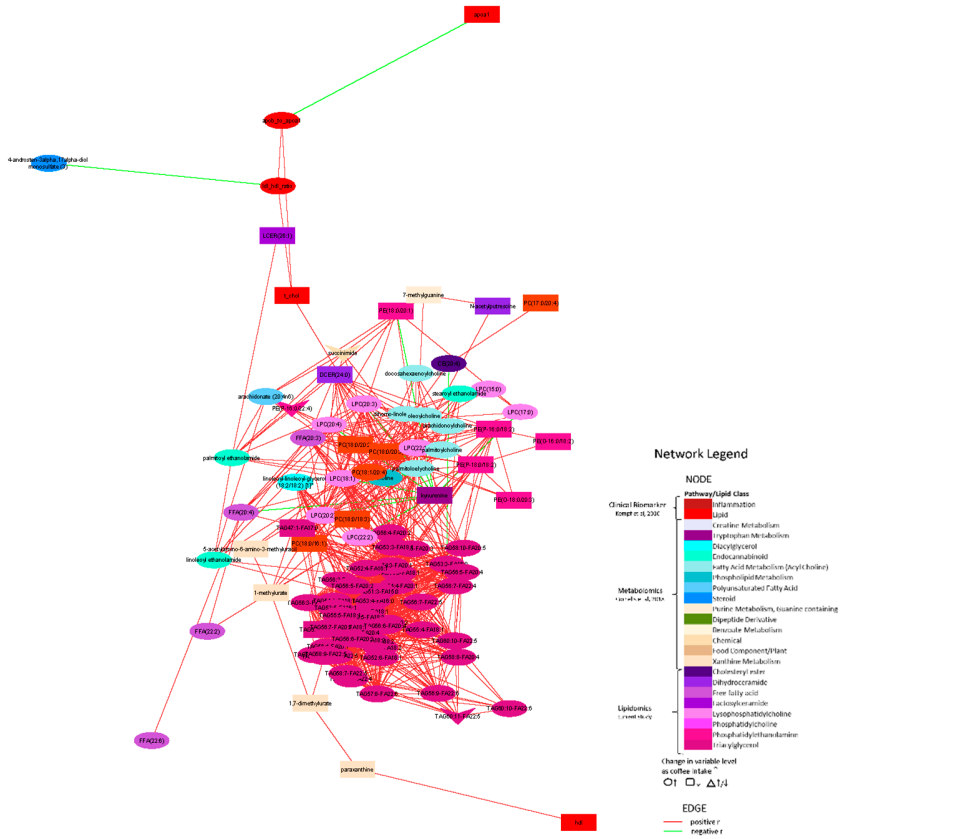
Figure S3.

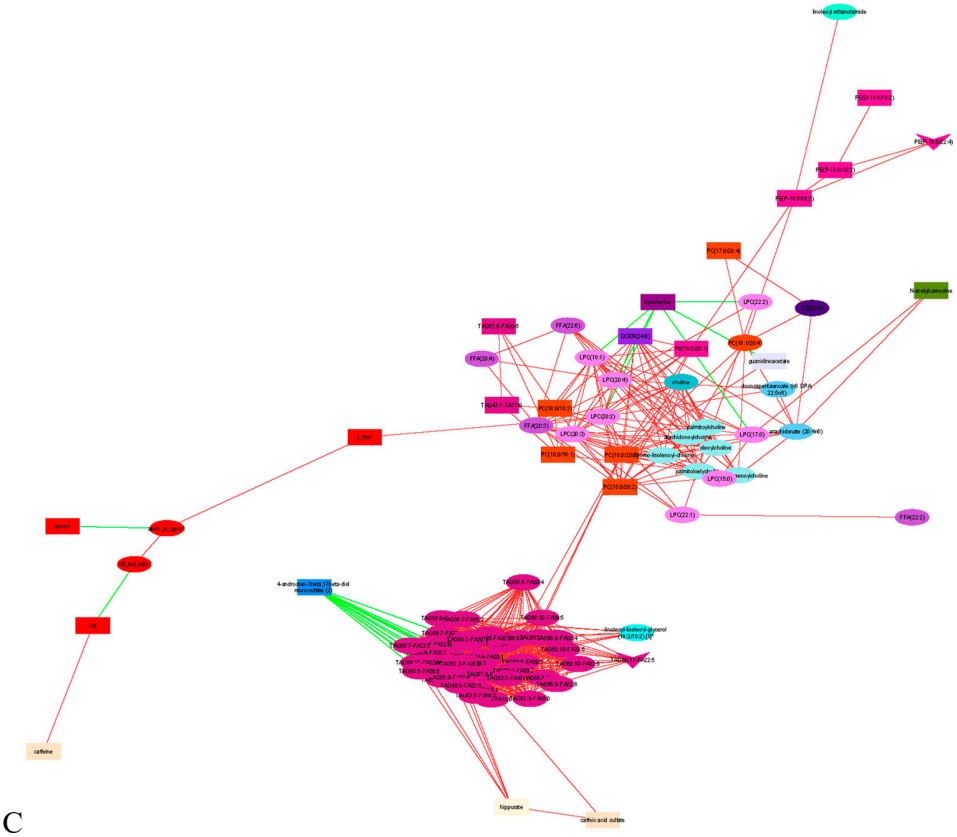
Pearson correlations (r) of changes in variable (lipid/metabolite/biomarker) levels after A) 4 cups/d compared to 0 cups/d B) 8 cups/d compared to 0 cups/d and C) 8 cups/d compared to 4 cups/d. Edges correspond to r and are shown if > |0.50| (corresponding to a nominal $P<3.5\times10^{-4}$). Distances between nodes reflect strength of correlations. Metabolites that did no correlate with lipid species or clinical markers but correlated with other metabolites have been trimmed from the network since these were previously reported in Cornelis et al 2018.

A



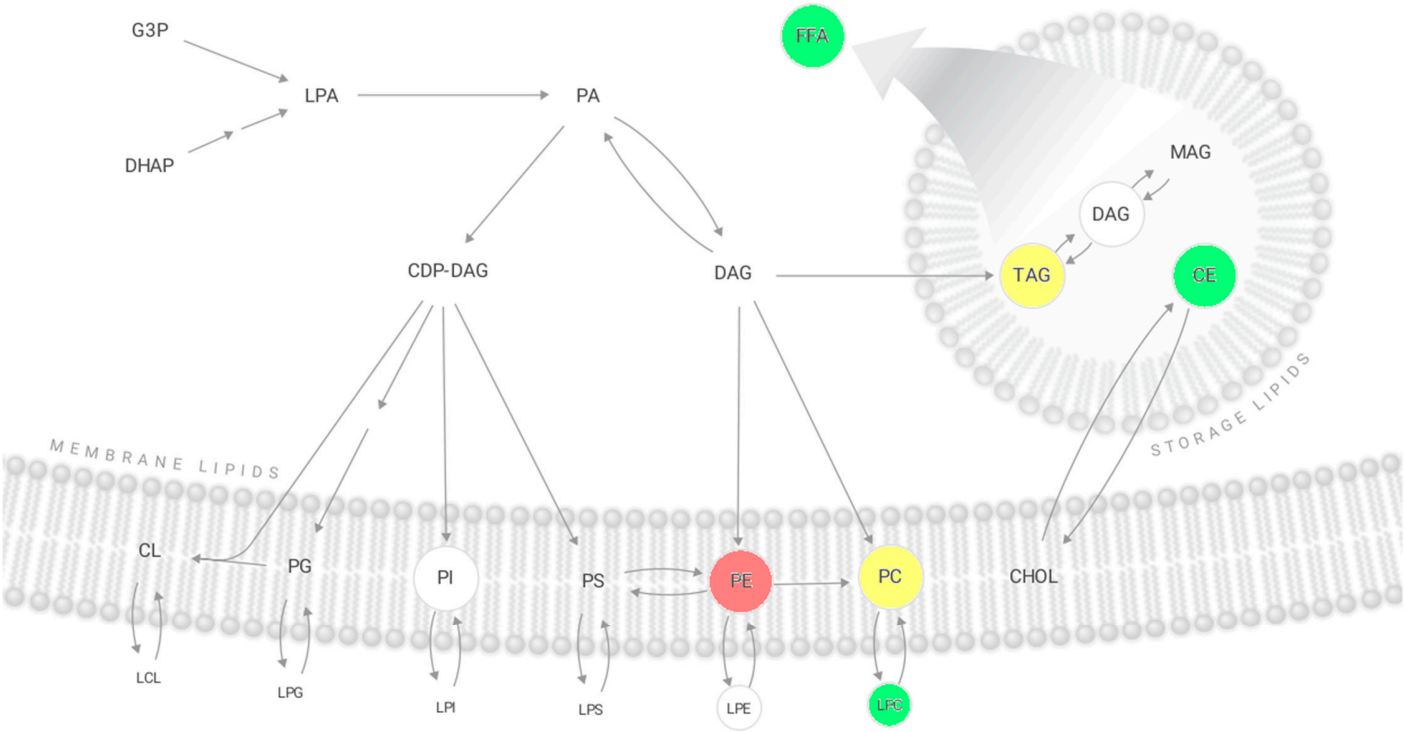
B


Network Legend
NODE
Clinical Biomarker
Metabolomics
Lipidomics
Pathway/Lipid Class
Inflammation
Lipid
Creatine Metabolism
Tryptophan Metabolism
Diacylglycerol
Endocannabinoid
Fatty Acid Metabolism (Acylcholine)
Phospholipid Metabolism
Polyunsaturated Fatty Acid
Steroid
Purine Metabolism, (guanine containing
Dipeptide Derivative
Benzoate Metabolism
Chemical
Food Component/Plant
Xanthine Metabolism
Cholesteryl ester
Dihydroceramide
Free fatty acid
Lactosylceramide
Lysophosphatidylcholine
Phosphatidylcholine
Phosphatidylethanolamine
Triacylglycerol
Change in variable level as coffee intake
EDGE
positive r
negative r



C

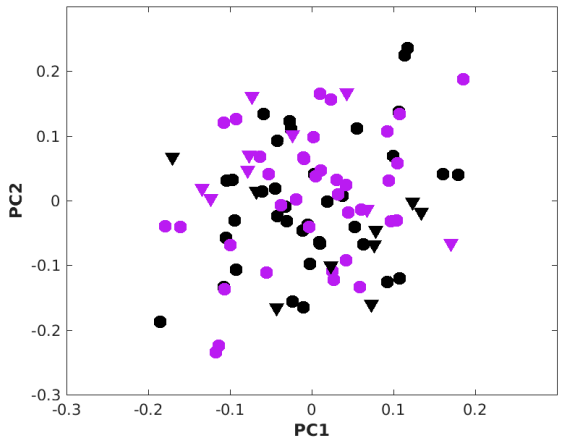
Figure S4.



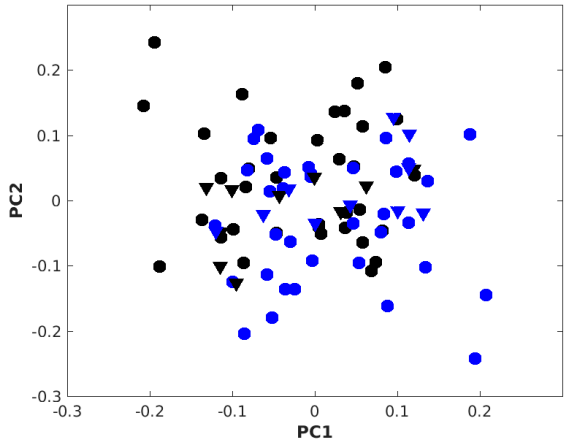
Lipid pathway including neutral and phospholipid lipid classes measured (circle nodes) in the current study. Lipid classes with lipid species that increased and decreased in response to coffee intake are colored red and green, respectively. Lipid classes with lipid species that increased or decreased are colored yellow. See Table 1 for details. CDP-DAG, CDP-diacylglycerol; CE, cholesteryl ester; CHOL, cholesterol; CL, cardiolipin; DAG, diacylglycerol; DHAP, dihydroxyacetone phosphate; FFA, free fatty acid; G3P, glycerol-3-phosphate; PA, phosphatic acid; PC, phosphatidylcholine; PE, phosphatidylethanolamine; PG, phosphatidylglycerol; PI, phosphatidylinositol; LCL, lysocardiolipin; LPA, lysophosphatidic acid; LPC, lysophosphatidylcholine; LPE, lysophosphatidylethanolamine; LPG, lysophosphatidylglycerol; LPI, lysophosphatidylinositol; LPS, lysophosphatidylserine; MAG, monoacylglycerol; TAG, triacylglycerol. Figure extracted from Metabolon's Surveyor software.

Figure S5.

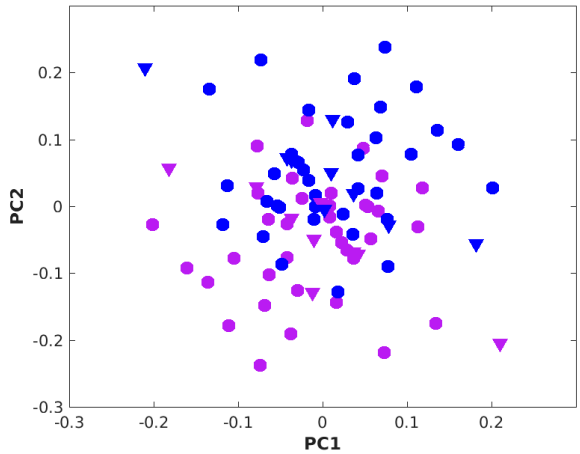
A



B



C



Multilevel PCA (A-C). Black, purple and blue PCA points represent samples measured after the 0 cups/d, 4 cups/d and 8 cups/d trial periods, respectively. Circle and triangle PCA shapes represent male and female

samples, respectively. MPLSDA score plots present overoptimistic representation of classification and thus are not presented as previously advocated [58].

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