SUPPLEMENTAL MATERIAL

Differences in Metabolomic Profiles between Black and White Women and Risk of Coronary Heart Disease: An Observational Study of Women from 4 US Cohorts

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Supplemental Methods (Study population)

Women's Health Initiative

The Women's Health Initiative (WHI) is a long-term nation-wide study funded by the National Heart, Lung, and Blood Institute (NHLBI). The WHI study focuses on strategies for preventing heart disease, breast and colorectal cancer, and osteoporosis in postmenopausal women. The original WHI study, initiated in 1994, had three parts – a clinical trial (i.e., Hormone Therapy trial; WHI-HT), an observational study (i.e., WHI-OS), and a community prevention study – and completed data collection in 2005. The WHI has continued to follow up study participants since 2005 as Extension Studies, which are annual collections of health updates and outcomes in active participants. The second Extension Study enrolled 93,500 women in 2010 and follow-up of these women continues annually.

In the WHI, participants were asked "How would you describe your racial or ethnic group? If you are of mixed blood, which group do you identify with most?" The participants could only select one of the following options:1) American Indian or Alaskan Native; 2) Asian or Pacific Islander (ancestry is Chinese, Indo-Chinese, Korean, Japanese, Pacific Islander, Vietnamese); 3) Black or African-American (not of Hispanic origin); 4) Hispanic/Latino (ancestry is Mexican, Cuban, Puerto Rican, Central American, or South American); 5) White (not of Hispanic origin); 6) Other (Specify).

Women from the present study were drawn from the WHI in a prior nested case-control study of coronary heart disease (CHD).[15] We define "Black" as self-reported "Black or African-American (not of Hispanic origin)" and "White" as self-reported "White (not of Hispanic origin)."

WHI-OS (discovery/training): The full WHI-OS enrolled 93,676 postmenopausal women ineligible or unwilling to participate in the related hormone trials, enrolled between 1994 and 1998 in the US. All participants provided written informed consent. In our published study, 472 women who developed CHD after the baseline examination (cases) were selected and were matched to 472 women who did not develop CHD on 5-year age, race/ethnicity, hysterectomy status, and 2-year enrollment groups.[15] In the present study, we included 834 women (417 incident CHD cases with a median time to event of 6.4 years and 417 matched controls; Black/White: 138/696) who had baseline metabolomics data and had no missing covariate data.

WHI-HT (validation/testing): In the WHI-HT, one of the trials randomly assigned 16,608 postmenopausal women to estrogen plus progesterone or placebo, whereas the other 10,739 women with prior hysterectomy were randomly assigned to estrogen or placebo. All women provided written informed consent. Using the same criteria mentioned above, the present study included 1,294 women (647 incident CHD cases with a median time to event of 4.0 years and 647 matched controls) from the WHI-HT, including 156 Black and 1,138 White women.

Blood samples: Plasma samples were collected using EDTA tubes in the WHI and processed immediately. All collected specimens were stored in a –70°C freezer within 2 hours of collection or stored at –20°C for up to 2 days and shipped on dry ice and stored at –70°C until processing. The majority of the WHI samples had been thawed once before our study, with 7 samples (6 cases and 1 control) having been thawed twice.

Metabolomics profiling: Plasma metabolomics profiling was performed in samples collected at the study baseline for both WHI-OS and WHI-HT. The detailed information on metabolomics profiling has been published.[15] Briefly, Metabolomic measurements were made using 4 complimentary liquid chromatography–tandem mass spectroscopy (LC-MS) methods resulting in over 6,000 metabolites, including 509 known metabolites. For each method, pooled plasma reference samples were included every 20 samples, and results were standardized using the ratio of the value of the sample to the value of the nearest pooled reference multiplied by the median of all reference values for the metabolite. The 4 LC-MS methods are:

1) **HILIC-pos**: The HILIC analyses of water-soluble metabolites in the positive ionization mode were conducted using an LC-MS system composed of a Shimadzu Nexera X2 U-HPLC (Shimadzu Corp) coupled to a Q Exactive hybrid quadrupole orbitrap mass spectrometer (Thermo Fisher Scientific).
2) **HILIC-neg**: HILIC analyses of water-soluble metabolites in the negative ionization mode were conducted by using an LC-MS system composed of an AQUITY UPLC system (Waters and a 5500 QTRAP mass spectrometer [SCIEX])
3) **C8-pos**: Positive ion mode analyses of polar and nonpolar plasma lipids were conducted by using an LC-MS system composed of a Shimadzu Nexera X2 U-HPLC (Shimadzu Corp) coupled to a Exactive Plus orbitrap mass spectrometer (Thermo Fisher Scientific).
4) **C18-neg**: Negative ion mode analyses of free fatty acids and bile acids were conducted using an LC-MS system composed of a Shimadzu Nexera X2 U-HPLC (Shimadzu Corp)

coupled to a Q Exactive hybrid quadrupole orbitrap mass spectrometer (Thermo Fisher Scientific).

Multi-Ethnic Study of Atherosclerosis

The Multi-Ethnic Study of Atherosclerosis (MESA) study is a study of the characteristics of subclinical cardiovascular disease (disease detected non-invasively before it has produced clinical signs and symptoms) and the risk factors that predict progression to clinically overt cardiovascular disease or progression of the subclinical disease. The MESA began in 2000 with 6,814 men and women aged 45 to 84 years recruited at 6 clinical centers across the US. The study participants were self-identified belonging to 4 racial/ethnic groups: Black, Hispanic, Asian, or White.

In the present study, we included 333 women (114 Black and 219 White women) from the MESA as an external replication and testing set. These women were drawn from a multi-omics pilot study in which participants were randomly selected from the full MESA study. Metabolomics profile was measured using the same methods as the WHI in plasma samples collected at the Exam 1 (between 2000 and 2002).

Jackson Heart Study

The Jackson Heart Study (JHS) is a single-site, prospective, population-based cohort study of cardiovascular disease and risk factors in Black/African-American individuals aged 21-84 years from 3 counties surrounding Jackson, Mississippi, US. Participants were recruited and examined according at baseline (between 2000 and 2004) and in subsequent follow-up visits. Clinic visits included physical examination, anthropometry, surveys of medical history and of cardiovascular risk factors, and collection of blood and urine for analysis. Ongoing surveillance methods include annual follow-up telephone interviews and medical records review for adjudication of selected events such as coronary heart disease (CHD). The JHS was approved by the institutional review bords of Jackson State University, Tougaloo College, and the University of Mississippi Medical Center in Jackson, Mississippi. Written informed consent was obtained from all study participants. The research protocol for the current replication analysis on metabolomics of incident CHD risk was approved by the institutional review board at Beth Israel Deaconess Medical Center in Boston, Massachusetts.

Women included in the present study were drawn from a recently published study on metabolomics of incident CHD, which included 2,346 participants with plasma metabolomic profiling data.[16] The replication analysis of the present study included 1,465 women from the JHS. During a median of 11.7 years, 107 incident CHD cases were documented.

Metabolomics profiling: Details of metabolomics profiling methods has been previously published.[16] To measure water-soluble metabolites in the positive ionization mode, hydrophilic interaction liquid chromatography (HILIC, Waters; Mildford, MA) was performed using a Shimadzu Nexera X2 U Exactive massHPLC (Shimadzu Corp.; Marlborough, MA) coupled to a Q spectrometer (Thermo Fisher Scientific; Waltham, MA). To measure organic acids and other intermediary metabolites in negative ionization or amide mode, chromatography was performed on an Agilent 1290 infinity LC system equipped with a Waters XBridge Amide column, coupled to an Agilent 6490 triple quadrupole mass spectrometer. Metabolite transitions were assed using a dynamic multiple reaction monitoring system. LC-MS were analyzed with Agilent Masshunter QQQ Quantitative analysis software.

LC-MS peaks were manually reviewed in a blinded manner to assess peak quality. As part of the QC protocol, isotopically labeled standards were interspersed throughout the run every 10 injections in order to monitor and correct for temporal drift in mass spectrometry performance. The nearest neighbor flanking pair of pooled plasma was used to normalize experimental samples in a metabolite-by-metabolite manner by dividing the experimental sample's peak area by the average of the two nearest neighbor flanking pairs. Metabolites that were defined as having a biological to analytical CV ratio <1 were removed from analysis. Metabolites that were determined to have poor peak quality during blinded peak review were also removed from subsequent processing. Finally, metabolites that failed QC as determined by group review were removed from subsequent processing. The median CV of the final metabolites analyzed was 4.2%, indicating that these metabolites were well-measured overall.

Nurses' Health Study

The Nurses' Health Study (NHS) is a prospective cohort study initiated in 1976 and enrolled 121,700 female registered nurses, aged 30 between 55 years, from 11 states in the US. The study participants completed a baseline questionnaire collecting information on lifestyle, medical history, and health-related questions, and with similar biennial questionnaires through follow-up.

Blood samples were collected in a sub-set of participants during 1989-1990 (n=32,826), with a questionnaire regarding blood draw information and medication use status. A high follow-up rate (>95%) was maintained among participants who provided blood samples. The study protocol was approved by the Institutional Review Boards of Mass General Brigham/Brigham and Women's Hospital, with participants' consent implied by the return of the questionnaires.

As a replication cohort, we included women from the NHS who provided blood samples and had metabolomic profiling data available.[24] Participants included in the current replication analyses were pooled from 10 prior metabolomics sub-studies – nested case-control studies (NCC) originally designed for different outcomes, including amyotrophic lateral sclerosis, breast cancer, colon cancer, glaucoma, inflammatory bowel disease, ovarian cancer, Parkinson's disease, rheumatoid arthritis, stroke, and type 2 diabetes. Women within each original NCC study were free of originally designed endpoints at the time of blood collection. Metabolomics profiling was performed using the same methods as the WHI.[24] We used a standard framework to combine metabolomic profiles from each sub-study. At the sample level, we first removed QC and drift pool samples, and then removed duplicate samples across sub-studies (if identified, only include the most recently measured one). At the metabolite level, we excluded metabolites that failed the blood processing delay pilot (i.e., metabolites were not robust with respect to the way NHS samples were collected, shipped on ice overnight, and should be excluded from all metabolomic studies[25]). We also excluded duplicate metabolites 1) within a given sub-study by keeping the best performing one (i.e., lowest CV and highest ICC) and 2) across different LC-MS methods by including ones that were measured using the preferred method according to the Broad metabolomics team. When combining the metabolomic profiling data from different sub-studies, datasets were grouped and merged by method (i.e., metabolites measured using the same LC-MS method were merged across sub-studies).

In the current replication analysis, we only included White women from the NHS who had prior measured metabolomics data and excluded women who had CVD or cancer at the time of blood collection or missing blood lipids measurements (i.e., total and high-density lipoprotein cholesterol). After QC steps, 2,506 White women were included in the replication analyses, and 136 incident CHD cases were documented during a median follow-up of 24.3 years.

Supplementary Tables

Table S1. Baseline characteristics of women from the MESA.

Mean ± SD or No. (%)	Black women (N = 114)	White women (N = 219)	*P*
Age, years	60.7 ± 9.6	61.6 ± 10.1	0.42
Body mass index, kg/m^2	31.9 ± 6.1	27.7 ± 5.6	<0.0001
Alcohol intake, Drinks/week	1.4 ± 2.5	3.0 ± 5.0	0.006
Physical activity, MET-hour/week	108.5 ± 45.6	94.3 ± 29.8	0.0007
Total cholesterol, mg/dl	195.4 ± 38.1	204.1 ± 37.6	0.05
HDL-cholesterol, mg/dl	57.5 ± 15.3	59.0 ± 14.7	0.39
LDL-cholesterol, mg/dl	119.8 ± 34.2	118.9 ± 31.2	0.81
Baseline diabetes	11 (9.7%)	9 (4.1%)	0.044
Baseline hypertension	68 (59.7%)	74 (33.8%)	<0.0001
Baseline depression (CES-D Scale)	9.4 ± 7.9	7.3 ± 6.5	0.008
Hormone therapy status			
Non-users	54 (47.4%)	82 (37.4%)	0.02
Past users	18 (15.8%)	38 (17.4%)	0.95
Current users	26 (22.8%)	79 (36.1%)	0.09
Unknown	16 (14.0%)	20 (9.1%)	0.09
Medication use			
Anti-depression	1 (0.9%)	5 (2.3%)	0.36
Lipid-lowering	17 (15.0%)	37 (16.9%)	0.67
Aspirin	35 (30.7%)	75 (34.3%)	0.51
Antihypertensive meds	61 (53.9%)	65 (29.7%)	<0.0001
Antihyperglycemic meds	10 (8.8%)	8 (3.7%)	0.05
Smoking status			
Never smokers	61 (53.5%)	99 (45.2%)	0.15
Past smokers	33 (29.0%)	92 (42.0%)	0.02
Current smokers	19 (16.7%)	28 (12.8%)	0.33
Unknown			
Education			0.03
Below high school	11 (9.7%)	10 (4.6%)	
High school diploma or GED	27 (23.7%)	50 (22.8%)	
Vocational or training school	12 (10.5%)	11 (5.0%)	
Some college or Associate Degree	35 (30.7%)	53 (24.2%)	
Baccalaureate Degree and above	28 (24.6%)	95 (43.4%)	
Income			0.0002
Less than $19,999	24 (21.1%)	23 (10.5%)	
$20,000 to $34,999	37 (32.5%)	48 (21.9%)	
$35,000 to $49,999	22 (19.3%)	43 (19.6%)	
$50,000 to $74,999	15 (13.2%)	50 (22.8%)	
$75,000 or more	12 (10.5%)	53 (24.2%)	

Abbreviations: SD, standard deviation; CHD, coronary heart disease; MET, metabolic equivalent; HDL, high-density lipoprotein; GED, General Educational Development.

Table S2. Baseline characteristics of women from the JHS and NHS.

Mean ± SD or No. (%)	JHS (N = 1,465)	NHS (N = 2,506)
Incident CHD	107 (7.3%)	136 (5.4%)
Age, years	56 ± 13	59.31 ± 6.52
Body mass index, kg/m2	33 ± 8	25.92 ± 4.90
Total cholesterol, mg/dl	202 ± 41	215.89 ± 38.39
HDL-cholesterol, mg/dl	55 ± 15	56.77 ± 15.40
Alternative Healthy Eating Index-2010	-	53.67 ± 10.59
Systolic blood pressure, mmHg	126 ± 18	129.25 ± 14.52
Baseline diabetes	311 (21.2%)	204 (8.1%)
Baseline hypertension	915 (62.5%)	918 (36.6%)
Menopausal status		
Pre-menopause	158 (10.8%)	326 (13.0%)
Post-menopause	987 (67.4%)	1999 (79.8%)
Unknown	320 (21.8%)	181 (7.2%)
HT use status		
Never/past users	1107 (75.6%)	1536 (61.3%)
Current users	358 (24.4%)	970 (38.7%)
Smoking status		
Never smokers	1075 (73.4%)	1126 (44.9%)
Past smokers	247 (16.9%)	1025 (40.9%)
Current smokers	130 (8.9%)	355 (14.2%)
Unknown	13 (0.9%)	-
Medication use		
Aspirin	324 (22.1%)	1223 (48.8%)
Lipid-lowering medications	147 (10.0%)	91 (3.6%)
Antihypertensive medications	783 (53.4%)	694 (27.7%)
Antihyperglycemic medications	209 (14.3%)	93 (3.7%)
Education		
Below high school	255 (17.4%)	-
High school diploma or GED	294 (20.1%)	-
Vocational or training school	74 (5.1%)	-
Some college or Associate Degree	345 (23.5%)	-
Baccalaureate Degree and above	491 (33.5%)	-
Unknown	6 (0.4%)	-
Family income		
Poor	199 (13.6%)	-
Lower-middle	323 (22.0%)	-
Upper-middle	380 (25.9%)	-
Affluent	347 (23.7%)	-
Unknown	216 (14.7%)	-

Abbreviations: SD, standard deviation; CHD, coronary heart disease; HDL, high-density lipoprotein; GED, General Educational Development.

Table S3. Regression coefficients of metabolome-wide association analyses in WHI-OS and WHI-HT.

Metabolite name	Method	Category	HMDB ID	WHI-OS														WHI-HT													
				Model 1		Model 2		Model 3		Model 4		Model 5		Model 6		Model 7		Model 1		Model 2		Model 3		Model 4		Model 5		Model 6		Model 7	
				Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR
C30:0 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07011*	-0.47	8.7E-07	-0.32	2.9E-04	-0.47	7.8E-07	-0.49	8.3E-07	-0.47	2.4E-06	-0.48	1.1E-06	-0.25	1.6E-01	-0.59	4.8E-11	-0.32	8.6E-05	-0.60	4.1E-11	-0.58	1.0E-09	-0.58	1.0E-09	-0.60	1.0E-10	-0.60	n/a
C32:0 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07098*	-0.60	3.5E-09	-0.40	1.5E-05	-0.61	2.6E-09	-0.61	1.3E-08	-0.59	2.4E-08	-0.63	1.9E-09	-0.39	4.4E-02	-0.59	7.8E-12	-0.31	4.1E-05	-0.60	3.7E-12	-0.58	2.5E-10	-0.58	1.7E-10	-0.61	6.4E-12	-0.59	2.0E-12
C32:1 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07099*	-0.87	7.8E-18	-0.65	1.5E-13	-0.88	4.6E-18	-0.89	3.3E-17	-0.87	9.3E-17	-0.90	6.1E-18	-0.71	6.0E-05	-0.86	1.0E-22	-0.55	5.5E-14	-0.87	8.3E-23	-0.85	4.7E-20	-0.85	3.7E-20	-0.88	1.6E-22	-0.87	1.8E-23
C32:2 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07128*	-0.76	3.4E-15	-0.54	2.8E-11	-0.76	2.8E-15	-0.78	4.0E-15	-0.77	1.9E-14	-0.78	2.2E-15	-0.59	2.7E-04	-0.89	5.8E-22	-0.56	4.6E-13	-0.89	9.4E-22	-0.87	2.3E-19	-0.87	2.2E-19	-0.90	1.4E-21	-0.90	1.7E-22
C34:0 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07100*	-0.59	1.4E-07	-0.43	5.3E-05	-0.60	1.2E-07	-0.62	1.2E-07	-0.61	1.7E-07	-0.60	1.8E-07	-0.36	9.9E-02	-0.43	1.6E-07	-0.24	2.2E-03	-0.44	6.7E-08	-0.42	9.0E-07	-0.42	7.6E-07	-0.45	7.2E-08	-0.43	n/a
C34:1 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07102*	-0.65	3.2E-11	-0.42	5.6E-07	-0.66	2.2E-11	-0.67	7.1E-11	-0.66	1.3E-10	-0.69	8.3E-12	-0.50	4.8E-03	-0.66	3.6E-14	-0.33	2.8E-06	-0.68	1.3E-14	-0.67	3.2E-13	-0.66	4.5E-13	-0.69	1.3E-14	-0.67	6.5E-15
C34:2 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07103*	-0.83	1.0E-16	-0.58	2.4E-12	-0.83	8.8E-17	-0.84	6.9E-16	-0.83	1.6E-15	-0.86	6.2E-17	-0.66	9.7E-05	-0.86	1.3E-22	-0.50	1.3E-13	-0.85	2.8E-22	-0.87	8.1E-21	-0.86	9.0E-21	-0.89	5.0E-23	-0.87	2.1E-23
C34:3 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07132*	-0.95	3.9E-21	-0.71	1.9E-17	-0.95	5.7E-21	-0.96	3.6E-20	-0.95	9.5E-20	-0.97	7.8E-21	-0.76	7.4E-06	-0.97	2.2E-27	-0.62	2.5E-18	-0.96	2.8E-26	-0.97	1.5E-24	-0.97	1.2E-24	-0.99	3.7E-27	-0.98	7.2E-28
C36:1 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07216*	-0.50	1.9E-07	-0.28	8.8E-04	-0.51	1.3E-07	-0.53	1.4E-07	-0.52	1.9E-07	-0.55	2.8E-08	-0.36	4.9E-02	-0.56	7.4E-10	-0.24	1.6E-03	-0.58	1.5E-10	-0.58	1.3E-09	-0.56	4.4E-09	-0.59	2.0E-10	-0.57	1.6E-10
C36:2 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07218*	-0.85	2.8E-17	-0.58	2.5E-12	-0.85	1.5E-17	-0.88	5.5E-17	-0.87	9.3E-17	-0.90	1.8E-18	-0.73	1.7E-05	-0.82	6.3E-20	-0.49	2.0E-11	-0.84	1.9E-20	-0.87	1.3E-19	-0.84	7.3E-19	-0.86	1.4E-20	-0.83	1.1E-20
C36:3 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07219*	-0.79	8.9E-15	-0.52	1.1E-09	-0.79	6.6E-15	-0.81	2.5E-14	-0.79	8.0E-14	-0.83	1.7E-15	-0.63	1.1E-04	-0.78	4.7E-18	-0.45	1.2E-09	-0.78	6.6E-18	-0.83	7.0E-18	-0.79	1.0E-16	-0.81	3.4E-18	-0.79	1.2E-18
C36:4 DAG-A	C8-pos	Glycerolipids - Diacylglycerols	HMDB07248*	-0.59	4.2E-09	-0.36	5.3E-05	-0.59	4.3E-09	-0.61	2.9E-09	-0.60	1.0E-08	-0.62	2.1E-09	-0.42	1.3E-02	-0.61	2.7E-11	-0.31	1.2E-04	-0.60	7.7E-11	-0.65	2.9E-11	-0.61	3.7E-10	-0.63	2.9E-11	-0.62	1.3E-11
C36:4 DAG-B	C8-pos	Glycerolipids - Diacylglycerols	HMDB07248*	-0.33	1.1E-03	-0.14	1.5E-01	-0.33	1.3E-03	-0.36	7.5E-04	-0.35	9.8E-04	-0.34	9.5E-04	-0.06	7.8E-01	-0.43	1.2E-06	-0.12	n/a	-0.42	2.8E-06	-0.41	1.2E-05	-0.42	4.8E-06	-0.46	3.9E-07	-0.43	n/a
C38:3 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07168*	-0.72	2.1E-13	-0.50	1.2E-08	-0.72	2.4E-13	-0.74	3.9E-13	-0.74	4.0E-13	-0.76	4.9E-14	-0.57	1.8E-04	-0.68	6.3E-14	-0.37	1.3E-06	-0.67	3.1E-13	-0.69	1.2E-12	-0.68	1.0E-12	-0.72	1.2E-14	-0.69	2.1E-14
C42:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42061*	-0.48	5.3E-07	-0.34	2.6E-04	-0.49	2.8E-07	-0.50	6.2E-07	-0.48	1.2E-06	-0.51	2.5E-07	-0.23	2.0E-01	-0.54	4.5E-08	-0.34	3.2E-04	-0.56	1.5E-08	-0.52	5.5E-07	-0.50	1.5E-06	-0.53	1.1E-07	-0.54	n/a
C43:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42062*	-0.31	6.2E-04	-0.20	2.2E-02	-0.32	3.0E-04	-0.33	3.8E-04	-0.31	7.4E-04	-0.32	4.9E-04	-0.11	5.0E-01	-0.49	1.4E-06	-0.32	1.3E-03	-0.51	6.8E-07	-0.47	1.7E-05	-0.46	1.9E-05	-0.48	4.1E-06	-0.49	n/a
C43:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42098*	-0.59	1.6E-09	-0.45	2.6E-06	-0.60	6.7E-10	-0.60	3.8E-09	-0.58	6.6E-09	-0.62	5.4E-10	-0.33	8.0E-02	-0.48	1.2E-07	-0.29	7.8E-04	-0.51	3.3E-08	-0.48	8.4E-07	-0.47	1.2E-06	-0.47	4.4E-07	-0.49	n/a
C44:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42063*	-0.51	2.5E-07	-0.36	1.6E-04	-0.52	1.3E-07	-0.53	3.2E-07	-0.51	6.7E-07	-0.53	1.4E-07	-0.31	1.0E-01	-0.54	9.1E-09	-0.34	1.5E-04	-0.56	3.3E-09	-0.52	2.0E-07	-0.51	2.4E-07	-0.55	1.7E-08	-0.55	n/a
C44:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42301*	-0.73	1.2E-12	-0.56	1.1E-08	-0.74	5.7E-13	-0.76	1.1E-12	-0.74	2.6E-12	-0.77	4.8E-13	-0.52	5.3E-03	-0.65	1.2E-12	-0.44	2.8E-07	-0.67	2.7E-13	-0.63	8.1E-11	-0.61	1.9E-10	-0.65	4.1E-12	-0.66	3.3E-13
C44:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB47770*	-0.72	2.7E-12	-0.53	3.5E-08	-0.73	1.4E-12	-0.74	2.4E-12	-0.73	6.3E-12	-0.76	6.5E-13	-0.47	9.9E-03	-0.64	6.3E-12	-0.41	1.4E-06	-0.66	1.5E-12	-0.62	3.0E-10	-0.59	9.8E-10	-0.64	1.9E-11	-0.65	1.4E-12
C45:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42093*	-0.21	2.9E-02	-0.16	1.1E-01	-0.23	1.5E-02	-0.24	1.8E-02	-0.22	2.9E-02	-0.22	2.7E-02	-0.05	8.0E-01	-0.40	5.5E-05	-0.25	n/a	-0.42	2.0E-05	-0.38	2.7E-04	-0.38	2.3E-04	-0.38	1.9E-04	-0.40	n/a
C45:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42099*	-0.76	1.2E-13	-0.61	8.2E-10	-0.78	3.0E-14	-0.79	1.4E-13	-0.77	3.0E-13	-0.79	8.9E-14	-0.56	1.9E-03	-0.63	8.2E-12	-0.43	6.0E-07	-0.65	1.7E-12	-0.62	3.1E-10	-0.61	3.6E-10	-0.62	5.4E-11	-0.64	2.3E-12
C45:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB43170*	-0.81	7.2E-15	-0.64	1.6E-10	-0.83	2.3E-15	-0.84	1.3E-14	-0.82	3.0E-14	-0.85	3.5E-15	-0.59	8.3E-04	-0.63	4.9E-12	-0.42	4.9E-07	-0.64	1.7E-12	-0.61	2.5E-10	-0.60	2.6E-10	-0.62	3.4E-11	-0.64	1.0E-12
C45:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	n/a	-0.50	1.1E-07	-0.32	2.9E-04	-0.50	6.5E-08	-0.47	1.4E-06	-0.46	1.9E-06	-0.53	3.6E-08	-0.26	1.4E-01	-0.50	1.1E-07	-0.30	6.3E-04	-0.51	5.2E-08	-0.45	5.2E-06	-0.45	3.6E-06	-0.50	1.9E-07	-0.51	n/a
C46:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10411*	-0.46	4.6E-06	-0.34	7.1E-04	-0.47	3.3E-06	-0.47	7.4E-06	-0.46	1.1E-05	-0.48	3.1E-06	-0.32	1.0E-01	-0.52	1.0E-08	-0.34	1.1E-04	-0.54	3.5E-09	-0.49	3.5E-07	-0.49	2.3E-07	-0.53	1.6E-08	-0.53	n/a
C46:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10412*	-0.76	2.0E-13	-0.58	2.0E-09	-0.77	9.0E-14	-0.78	2.1E-13	-0.77	5.7E-13	-0.79	1.3E-13	-0.57	1.8E-03	-0.69	1.5E-14	-0.47	1.1E-08	-0.71	2.8E-15	-0.67	2.0E-12	-0.65	2.7E-12	-0.70	2.8E-14	-0.70	3.7E-15
C46:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10419*	-0.86	1.4E-16	-0.66	5.5E-12	-0.87	6.2E-17	-0.89	1.6E-16	-0.87	5.2E-16	-0.89	6.1E-17	-0.65	3.1E-04	-0.77	2.2E-17	-0.53	9.6E-11	-0.79	5.7E-18	-0.75	5.0E-15	-0.73	1.4E-14	-0.78	5.8E-17	-0.78	6.2E-18
C46:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42541*	-0.82	3.4E-15	-0.60	2.1E-10	-0.82	2.0E-15	-0.85	3.3E-15	-0.83	1.2E-14	-0.86	8.1E-16	-0.58	1.1E-03	-0.73	1.2E-15	-0.48	3.4E-09	-0.74	4.8E-16	-0.72	1.0E-13	-0.69	4.5E-13	-0.74	2.3E-15	-0.74	3.4E-16
C46:4 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42781*	-0.69	6.9E-12	-0.49	1.8E-07	-0.70	4.9E-12	-0.72	7.9E-12	-0.70	2.4E-11	-0.74	1.3E-12	-0.44	1.6E-02	-0.60	1.9E-10	-0.37	1.8E-05	-0.61	7.9E-11	-0.58	5.1E-09	-0.55	1.8E-08	-0.60	3.5E-10	-0.61	5.2E-11
C47:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42100*	-0.75	2.0E-13	-0.61	8.0E-10	-0.77	3.3E-14	-0.77	2.3E-13	-0.76	4.0E-13	-0.78	1.2E-13	-0.59	1.5E-03	-0.75	4.5E-16	-0.55	2.7E-10	-0.78	2.9E-17	-0.73	7.1E-14	-0.73	3.9E-14	-0.73	1.0E-14	-0.76	1.1E-16
C47:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB48435*	-0.92	6.4E-19	-0.73	4.2E-14	-0.94	1.3E-19	-0.94	1.1E-18	-0.94	1.7E-18	-0.95	4.2E-19	-0.74	3.8E-05	-0.85	1.7E-20	-0.62	6.8E-14	-0.87	1.9E-21	-0.82	1.5E-17	-0.82	8.6E-18	-0.84	3.0E-19	-0.86	3.5E-21
C48:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05356*	-0.40	9.2E-05	-0.27	6.8E-03	-0.40	8.1E-05	-0.40	2.2E-04	-0.39	2.5E-04	-0.42	7.1E-05	-0.25	2.1E-01	-0.43	9.4E-07	-0.25	3.4E-03	-0.45	4.2E-07	-0.40	2.0E-05	-0.41	1.1E-05	-0.44	8.8E-07	-0.44	n/a
C48:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05359*	-0.74	2.9E-13	-0.58	1.2E-09	-0.75	1.7E-13	-0.76	5.1E-13	-0.75	1.2E-12	-0.77	2.0E-13	-0.61	7.7E-04	-0.75	2.4E-17	-0.51	2.7E-10	-0.77	6.0E-18	-0.73	6.2E-15	-0.72	4.6E-15	-0.76	5.0E-17	-0.76	4.7E-18
C48:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05376*	-0.91	1.7E-18	-0.71	1.2E-13	-0.92	7.9E-19	-0.94	2.4E-18	-0.92	1.0E-17	-0.94	1.4E-18	-0.76	3.2E-05	-0.86	2.7E-22	-0.61	7.5E-15	-0.87	7.3E-23	-0.84	1.8E-19	-0.83	2.2E-19	-0.87	4.9E-22	-0.87	6.4E-23
C48:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05432*	-1.02	7.5E-23	-0.79	1.1E-17	-1.03	4.4E-23	-1.06	1.0E-22	-1.04	4.8E-22	-1.06	4.0E-23	-0.83	2.6E-06	-0.92	1.2E-24	-0.65	3.9E-17	-0.93	6.7E-25	-0.91	1.1E-21	-0.89	3.1E-21	-0.93	2.0E-24	-0.92	4.3E-25
C48:4 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42631*	-0.90	6.2E-18	-0.66	1.0E-12	-0.90	4.6E-18	-0.93	4.7E-18	-0.91	2.1E-17	-0.94	1.4E-18	-0.67	1.4E-04	-0.81	1.1E-18	-0.55	8.0E-12	-0.81	1.0E-18	-0.79	2.5E-16	-0.76	1.3E-15	-0.82	1.2E-18	-0.81	4.7E-19
C48:5 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42841*	-0.72	2.1E-12	-0.50	1.1E-07	-0.72	2.0E-12	-0.75	2.2E-12	-0.73	6.2E-12	-0.76	4.6E-13	-0.46	1.3E-02	-0.63	1.3E-11	-0.41	1.5E-06	-0.64	1.2E-11	-0.60	1.1E-09	-0.58	2.9E-09	-0.64	2.0E-11	-0.64	6.0E-12
C49:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB11705*	-0.63	2.8E-10	-0.51	2.1E-07	-0.65	6.8E-11	-0.65	3.1E-10	-0.65	3.3E-10	-0.65	2.4E-10	-0.52	4.4E-03	-0.75	1.1E-15	-0.55	5.4E-10	-0.78	7.0E-17	-0.71	4.5E-13	-0.72	1.3E-13	-0.73	2.0E-14	-0.76	3.3E-16
C49:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB11706*	-0.98	1.1E-21	-0.82	3.1E-17	-1.00	8.7E-23	-1.00	2.4E-21	-0.99	2.9E-21	-1.00	9.9E-22	-0.85	2.2E-06	-0.99	2.8E-27	-0.77	9.7E-20	-1.02	9.2E-29	-0.97	7.9E-24	-0.97	3.5E-24	-0.97	1.6E-25	-0.99	1.1E-27
C49:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42103*	-1.10	2.3E-27	-0.88	4.4E-22	-1.12	3.9E-28	-1.12	8.5E-27	-1.12	1.1E-26	-1.13	1.9E-27	-0.94	1.2E-08	-1.06	1.8E-31	-0.80	2.0E-24	-1.08	3.0E-32	-1.05	7.9E-28	-1.04	8.2E-28	-1.06	4.6E-30	-1.07	4.9E-32
C50:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05357*	-0.39	1.2E-04	-0.22	2.5E-02	-0.40	1.0E-04	-0.41	1.3E-04	-0.40	1.3E-04	-0.42	5.5E-05	-0.25	2.3E-01	-0.41	5.6E-06	-0.18	3.1E-02	-0.43	2.0E-06	-0.39	3.8E-05	-0.38	4.6E-05	-0.42	3.8E-06	-0.41	n/a
C50:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB44109*	-0.61	1.1E-09	-0.43	2.6E-06	-0.62	6.7E-10	-0.63	1.7E-09	-0.62	2.7E-09	-0.63	6.6E-10	-0.47	9.1E-03	-0.62	5.2E-13	-0.35	3.7E-06	-0.64	1.1E-13	-0.62	7.7E-12	-0.61	9.4E-12	-0.64	3.2E-13	-0.63	1.3E-13
C50:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05377*	-0.85	6.8E-17	-0.67	4.4E-13	-0.86	5.1E-17	-0.87	2.4E-16	-0.86	4.1E-16	-0.87	6.6E-17	-0.72	5.4E-05	-0.84	8.5E-23	-0.56	3.5E-14	-0.85	4.6E-23	-0.84	1.5E-20	-0.84	7.8E-21	-0.88	1.5E-23	-0.85	1.8E-23
C50:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05433*	-1.10	1.1E-26	-0.86	5.4E-22	-1.11	6.2E-27	-1.13	1.0E-25	-1.11	3.8E-25	-1.14	7.3E-27	-0.94	3.3E-08	-1.05	1.1E-32	-0.75	7.7E-25	-1.05	1.1E-32	-1.07	1.5E-30	-1.05	5.4E-30	-1.07	1.3E-32	-1.05	4.6E-33
C50:4 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05435*	-1.01	1.7E-22	-0.74	4.2E-17	-1.01	1.7E-22	-1.04	3.0E-22	-1.03	9.8E-22	-1.05	6.3E-23	-0.83	2.6E-06	-0.94	5.0E-26	-0.65	2.5E-18	-0.94	1.2E-25	-0.95	9.9E-24	-0.93	6.5E-23	-0.97	3.1E-26	-0.95	2.7E-26
C50:5 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10471*	-0.85	3.3E-16	-0.60	8.3E-11	-0.85	4.5E-16	-0.88	4.4E-16	-0.86	1.1E-15	-0.89	6.2E-17	-0.65	4.0E-04	-0.78	6.8E-18	-0.52	4.6E-11	-0.77	2.4E-17	-0.77	1.7E-15	-0.75	4.0E-15	-0.80	5.1E-18	-0.78	3.9E-18
C50:6 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10497*	-0.64	7.8E-10	-0.42	1.6E-05	-0.63	1.1E-09	-0.66	1.2E-09	-0.65	1.7E-09	-0.68	1.8E-10	-0.40	4.2E-02	-0.53	9.4E-09	-0.32	1.5E-04	-0.52	2.2E-08	-0.49	4.5E-07	-0.48	6.1E-07	-0.54	1.1E-08	-0.53	6.0E-09
C51:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB31106*	-0.41	3.4E-05	-0.24	1.1E-02	-0.42	1.8E-05	-0.43	2.8E-05	-0.43	2.6E-05	-0.44	1.5E-05	-0.26	1.7E-01	-0.50	1.9E-07	-0.25	4.2E-03	-0.52	5.7E-08	-0.48	1.9E-06	-0.47	3.1E-06	-0.51	2.3E-07	-0.50	n/a
C51:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42104*	-0.58	1.7E-08	-0.40	4.9E-05	-0.60	4.3E-09	-0.60	1.8E-08	-0.60	1.4E-08	-0.61	8.5E-09	-0.47	1.2E-02	-0.60	2.4E-11	-0.36	8.8E-06	-0.63	2.2E-12	-0.58	7.5E-10	-0.57	8.3E-10	-0.60	9.3E-11	-0.61	6.2E-12
C51:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB49721*	-0.86	8.8E-17	-0.67	2.9E-12	-0.88	8.6E-18	-0.88	1.6E-16	-0.89	8.0E-17	-0.89	4.7E-17	-0.80	7.6E-06	-0.83	3.1E-20	-0.60	3.2E-13	-0.86	1.4E-21	-0.83	4.7E-18	-0.83	1.7E-18	-0.82	6.1E-19	-0.84	1.0E-20
C51:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	n/a	-0.97	6.9E-23	-0.78	1.2E-18	-0.99	5.2E-24	-1.00	4.8E-23	-1.00	5.0E-23	-1.01	2.1E-23	-0.88	1.0E-08	-1.02	1.8E-29	-0.73	1.9E-20	-1.04	3.7E-30	-1.06	5.9E-28	-1.03	3.5E-27	-1.01	6.6E-28	-1.03	6.8E-30
C52:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05367*	-0.46	3.8E-06	-0.24	9.0E-03	-0.47	2.5E-06	-0.49	3.2E-06	-0.48	3.6E-06	-0.51	8.7E-07	-0.35	7.3E-02	-0.46	2.8E-07	-0.18	2.0E-02	-0.48	5.4E-08	-0.47	4.9E-07	-0.45	1.4E-06	-0.48	1.2E-07	-0.46	n/a
C52:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05369*	-0.72	1.7E-13	-0.48	6.2E-09	-0.73	7.2E-14	-0.75	1.6E-13	-0.74	2.7E-13	-0.75	4.9E-14	-0.64	1.1E-04	-0.78	6.3E-18	-0.46	1.1E-09	-0.80	1.9E-18	-0.82	7.0E-18	-0.80	2.3E-17	-0.81	2.4E-18	-0.79	1.1E-18
C52:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05384*	-0.64	1.5E-11	-0.40	1.3E-06	-0.65	8.3E-12	-0.67	1.3E-11	-0.66	3.5E-11	-0.67	6.7E-12	-0.60	1.0E-04	-0.81	5.3E-18	-0.49	7.7E-10	-0.82	3.9E-18	-0.87	2.6E-18	-0.84	1.5E-17	-0.83	4.7E-18	-0.82	1.1E-18
C52:4 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05363*	-0.73	3.1E-13	-0.51	1.1E-08	-0.73	2.4E-13	-0.75	3.5E-13	-0.73	1.2E-12	-0.76	1.3E-13	-0.61	1.7E-04	-0.74	1.1E-15	-0.45	4.1E-08	-0.74	2.2E-15	-0.81	3.1E-16	-0.75	1.5E-14	-0.77	4.9E-16	-0.75	6.7E-16
C52:6 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05436*	-0.72	2.4E-12	-0.47	3.3E-07	-0.72	4.6E-12	-0.75	3.8E-12	-0.74	4.9E-12	-0.76	5.8E-13	-0.55	3.5E-03	-0.66	3.5E-13	-0.43	2.0E-07	-0.64	3.1E-12	-0.64	3.5E-11	-0.63	3.8E-11	-0.68	2.3E-13	-0.66	2.2E-13
C52:7 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10517*	-0.53	3.1E-07	-0.32	1.1E-03	-0.52	6.6E-07	-0.54	5.8E-07	-0.54	4.8E-07	-0.56	1.2E-07	-0.35	8.0E-02	-0.45	6.5E-07	-0.28	1.2E-03	-0.42	3.8E-06	-0.41	2.6E-05	-0.41	1.7E-05	-0.46	7.7E-07	-0.45	n/a
C54:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05395*	-0.37	1.8E-04	-0.16	7.8E-02	-0.38	1.1E-04	-0.42	4.1E-05	-0.41	5.2E-05	-0.43	2.3E-05	-0.24	2.2E-01	-0.38	2.8E-05	-0.11	n/a	-0.42	3.6E-06	-0.42	1.6E-05	-0.38	8.5E-05	-0.40	1.6E-05	-0.39	n/a
C54:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05403*	-0.56	1.1E-08	-0.31	2.4E-04	-0.57	6.0E-09	-0.60	3.3E-09	-0.60	4.4E-09	-0.63	4.5E-10	-0.45	9.1E-03	-0.53	4.1E-09	-0.22	3.2E-03	-0.56	4.1E-10	-0.60	5.2E-10	-0.55	5.2E-09	-0.57	8.9E-10	-0.54	9.7E-10
C54:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05405*	-0.72	1.1E-12	-0.48	8.3E-08	-0.73	7.4E-13	-0.77	2.7E-13	-0.76	5.0E-13	-0.78	4.9E-14	-0.69	1.7E-05	-0.69	5.2E-14	-0.41	5.3E-07	-0.71	1.3E-14	-0.78	2.0E-15	-0.73	5.3E-14	-0.73	7.9E-15	-0.71	1.1E-14
C54:4 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05370*	-0.60	6.0E-09	-0.43	1.4E-05	-0.60	6.0E-09	-0.65	1.6E-09	-0.63	4.3E-09	-0.65	1.3E-09	-0.56	6.8E-04	-0.53	9.1E-09	-0.32	2.7E-04	-0.53	1.3E-08	-0.61	4.3E-10	-0.56	8.9E-09	-0.56	2.5E-09	-0.53	4.4E-09
C54:6 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05391*	-0.41	5.9E-05	-0.24	1.6E-02	-0.40	8.2E-05	-0.42	7.0E-05	-0.41	1.3E-04	-0.44	2.4E-05	-0.30	1.3E-01	-0.40	2.9E-05	-0.22	1.6E-02	-0.38	8.2E-05	-0.44	1.6E-05	-0.40	7.4E-05	-0.42	2.0E-05	-0.40	n/a
C54:7 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05447*	-0.36	7.1E-04	-0.15	1.5E-01	-0.34	1.4E-03	-0.36	1.2E-03	-0.37	9.2E-04	-0.40	2.7E-04	-0.20	3.8E-01	-0.23	1.1E-02	-0.07	n/a	-0.19	3.4E-02	-0.18	6.4E-02	-0.21	3.0E-02	-0.24	1.1E-02	-0.23	n/a
C54:8 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10518*	-0.33	1.9E-03	-0.14	1.7E-01	-0.30	3.8E-03	-0.32	3.2E-03	-0.34	2.0E-03	-0.35	1.2E-03	-0.19	3.9E-01	-0.24	9.7E-03	-0.10	n/a	-0.20	3.5E-02	-0.19	6.1E-02	-0.20	3.9E-02	-0.24	1.1E-02	-0.24	n/a
C55:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB50319*	-0.66	1.2E-11	-0.44	5.6E-07	-0.67	4.0E-12	-0.66	4.5E-11	-0.67	2.3E-11	-0.71	7.4E-13	-0.55	8.3E-04	-0.65	4.1E-12	-0.37	3.2E-06	-0.68	4.3E-13	-0.67	2.4E-11	-0.65	3.6E-11	-0.66	5.4E-12	-0.66	6.5E-13
C55:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	n/a	-0.85	1.4E-16	-0.66	1.2E-11	-0.86	2.8E-17	-0.86	5.3E-16	-0.86	2.5E-16	-0.90	5.5E-18	-0.83	9.6E-08	-0.67	3.2E-13	-0.48	4.3E-08	-0.69	1.2E-13	-0.73	1.7E-13	-0.71	2.1E-13	-0.68	6.3E-13	-0.68	7.7E-14
C56:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05404*	-0.53	2.5E-07	-0.32	8.2E-04	-0.53	2.5E-07	-0.55	3.0E-07	-0.55	1.9E-07	-0.60	1.3E-08	-0.47	9.8E-03	-0.53	1.5E-08	-0.29	6.7E-04	-0.56	1.7E-09	-0.53	6.4E-08	-0.51	1.2E-07	-0.55	6.4E-09	-0.54	3.1E-09
C56:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05410*	-0.70	2.7E-12	-0.49	8.9E-08	-0.69	3.6E-12	-0.73	1.6E-12	-0.73	1.2E-12	-0.76	8.6E-14	-0.64	8.4E-05	-0.67	3.2E-13	-0.39	1.2E-06	-0.68	2.3E-13	-0.72	2.8E-13	-0.70	6.5E-13	-0.71	3.6E-14	-0.68	5.1E-14
C56:5 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05406*	-0.56	5.9E-08	-0.42	2.6E-05	-0.56	7.8E-08	-0.62	8.7E-09	-0.61	1.1E-08	-0.58	4.9E-08	-0.41	2.7E-02	-0.43	3.1E-06	-0.22	1.1E-02	-0.41	1.2E-05	-0.46	2.2E-06	-0.46	2.2E-06	-0.47	7.0E-07	-0.43	2.6E-06
C56:8 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05392*	0.26	1.2E-02	0.37	3.6E-04	0.29	5.0E-03	0.29	6.6E-03	0.26	1.5E-02	0.26	1.5E-02	0.32	1.4E-01	0.33	2.4E-04	0.41	6.9E-06	0.39	2.0E-05	0.37	1.4E-04	0.33	5.8E-04	0.34	2.2E-04	0.33	n/a
C58:10 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05476*	0.58	7.6E-09	0.60	3.8E-09	0.61	9.4E-10	0.60	3.8E-09	0.57	2.7E-08	0.59	8.1E-09	0.66	5.8E-04	0.65	2.1E-13	0.60	2.1E-11	0.70	1.6E-15	0.72	1.9E-14	0.66	1.4E-12	0.66	3.4E-13	0.65	8.9E-14
C58:11 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10531*	0.41	6.0E-05	0.45	1.1E-05	0.44	1.2E-05	0.44	1.9E-05	0.41	9.1E-05	0.42	5.5E-05	0.49	1.2E-02	0.45	4.0E-07	0.41	3.9E-06	0.50	1.3E-08	0.54	1.1E-08	0.48	4.2E-07	0.47	3.4E-07	0.46	2.1E-07
C58:8 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05413*	0.52	8.8E-09	0.49	1.8E-07	0.55	1.1E-09	0.54	5.3E-09	0.51	5.4E-08	0.53	1.3E-08	0.44	1.5E-02	0.70	1.8E-14	0.64	7.4E-12	0.75	1.4E-16	0.78	8.4E-16	0.69	6.5E-13	0.71	1.7E-14	0.70	8.4E-15
C58:9 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05463*	0.52	1.1E-07	0.51	4.6E-07	0.55	1.3E-08	0.55	4.2E-08	0.52	3.4E-07	0.53	1.3E-07	0.52	8.1E-03	0.65	1.8E-13	0.58	6.8E-11	0.70	1.2E-15	0.72	1.2E-14	0.66	1.8E-12	0.66	2.2E-13	0.65	8.1E-14
C60:12 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05478*	0.58	9.4E-10	0.57	3.5E-09	0.60	7.3E-11	0.63	5.2E-11	0.59	1.0E-09	0.59	9.3E-10	0.58	1.2E-03	0.77	2.8E-18	0.71	1.7E-15	0.82	9.8E-21	0.85	1.5E-19	0.78	6.4E-17	0.80	1.2E-18	0.77	1.3E-18
C16:1 LPC plasmalogen	C8-pos	Glycerophospholipids - Lysophosphatidylcholine plasmalogens	n/a	0.50	4.1E-07	0.54	5.5E-08	0.50	4.2E-07	0.54	2.8E-07	0.52	4.7E-07	0.50	8.1E-07	0.38	4.1E-02	0.41	6.1E-06	0.33	3.2E-04	0.43	2.3E-06	0.39	4.8E-05	0.36	1.0E-04	0.38	4.3E-05	0.41	2.9E-06
C18:0 LPC plasmalogen	C8-pos	Glycerophospholipids - Lysophosphatidylcholine plasmalogens	HMDB11149*	0.40	5.9E-05	0.48	1.3E-06	0.38	1.3E-04	0.39	2.0E-04	0.40	1.2E-04	0.38	2.1E-04	0.28	1.2E-01	0.27	3.4E-03	0.27	3.2E-03	0.25	7.8E-03	0.18	6.8E-02	0.22	2.4E-02	0.24	1.1E-02	0.27	n/a
C14:0 LPC	HILIC-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10379	-0.88	1.8E-17	-0.75	2.9E-13	-0.88	1.6E-17	-0.91	1.8E-17	-0.91	1.4E-17	-0.89	7.6E-17	-0.72	3.2E-05	-0.78	6.3E-18	-0.71	2.2E-15	-0.79	9.1E-18	-0.74	8.2E-15	-0.75	3.2E-15	-0.78	9.0E-17	-0.80	1.5E-18
C14:0 LPC-A	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10379*	-0.82	4.8E-16	-0.69	6.5E-12	-0.83	3.0E-16	-0.83	1.7E-15	-0.83	2.4E-15	-0.82	2.1E-15	-0.69	8.8E-05	-0.86	1.7E-20	-0.79	2.0E-18	-0.86	1.3E-20	-0.83	9.3E-18	-0.83	5.9E-18	-0.84	4.8E-19	-0.86	5.3E-21

Metabolite name	Method	Category	HMDB ID	WHI-OS														WHI-HT													
				Model 1		Model 2		Model 3		Model 4		Model 5		Model 6		Model 7		Model 1		Model 2		Model 3		Model 4		Model 5		Model 6		Model 7	
				Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR
C14:0 LPC-B	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10379*	-0.69	1.2E-13	-0.58	4.7E-10	-0.70	6.8E-14	-0.70	4.1E-13	-0.70	4.4E-13	-0.69	7.2E-13	-0.56	3.2E-04	-0.62	1.6E-10	-0.57	3.5E-09	-0.63	9.3E-11	-0.59	9.3E-09	-0.60	4.0E-09	-0.61	1.0E-09	-0.63	5.8E-11
C15:0 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10381	-0.63	2.1E-10	-0.52	1.9E-07	-0.64	8.7E-11	-0.64	3.5E-10	-0.65	2.2E-10	-0.64	4.0E-10	-0.58	8.3E-04	-0.85	2.2E-21	-0.82	5.9E-20	-0.86	1.7E-21	-0.85	1.5E-19	-0.85	1.0E-19	-0.82	3.6E-19	-0.86	4.9E-22
C16:0 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10382	-0.35	1.6E-03	-0.17	1.4E-01	-0.35	1.9E-03	-0.34	3.7E-03	-0.34	3.7E-03	-0.36	1.9E-03	-0.35	9.9E-02	-0.40	6.4E-06	-0.35	n/a	-0.38	1.7E-05	-0.42	6.1E-06	-0.42	5.6E-06	-0.42	3.7E-06	-0.41	n/a
C16:1 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10383	-0.83	1.3E-15	-0.73	2.2E-12	-0.82	2.3E-15	-0.83	1.6E-14	-0.83	1.6E-14	-0.83	6.6E-15	-0.78	1.7E-05	-0.96	4.5E-27	-0.96	1.4E-26	-0.95	4.1E-26	-0.98	1.1E-25	-0.98	1.3E-25	-1.00	6.6E-28	-0.96	1.8E-27
C18:1 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB02815	-0.22	3.4E-02	-0.16	1.6E-01	-0.23	3.4E-02	-0.23	4.2E-02	-0.23	4.2E-02	-0.25	2.1E-02	-0.24	2.4E-01	-0.32	2.4E-04	-0.40	n/a	-0.33	2.0E-04	-0.38	3.6E-05	-0.35	1.1E-04	-0.35	8.7E-05	-0.32	n/a
C18:2 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10386*	-0.22	4.0E-02	-0.20	7.6E-02	-0.23	3.9E-02	-0.22	5.4E-02	-0.21	6.0E-02	-0.24	2.9E-02	-0.21	3.0E-01	-0.28	9.3E-04	-0.41	n/a	-0.29	7.5E-04	-0.34	n/a	-0.29	n/a	-0.28	1.4E-03	-0.28	n/a
C18:3 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10387*	-0.35	6.2E-04	-0.30	4.0E-03	-0.34	9.9E-04	-0.36	9.1E-04	-0.36	9.2E-04	-0.37	5.2E-04	-0.24	2.0E-01	-0.53	6.7E-09	-0.60	1.1E-10	-0.51	2.2E-08	-0.53	7.2E-08	-0.53	3.4E-08	-0.55	3.9E-09	-0.53	n/a
C20:3 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10393*	-0.42	8.3E-05	-0.33	2.3E-03	-0.42	1.1E-04	-0.46	3.4E-05	-0.47	2.5E-05	-0.44	6.5E-05	-0.38	3.9E-02	-0.49	1.1E-07	-0.51	4.6E-08	-0.48	2.4E-07	-0.50	3.9E-07	-0.50	4.0E-07	-0.52	3.4E-08	-0.49	9.4E-08
C20:4 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10395	0.42	5.5E-05	0.48	4.3E-06	0.42	6.0E-05	0.43	1.1E-04	0.42	1.2E-04	0.42	8.1E-05	0.49	5.3E-03	0.21	2.2E-02	0.11	2.1E-01	0.21	1.9E-02	0.20	3.7E-02	0.18	5.4E-02	0.18	5.1E-02	0.21	1.9E-02
C22:6 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10404*	0.33	8.2E-04	0.36	3.2E-04	0.35	2.8E-04	0.36	3.8E-04	0.33	1.1E-03	0.32	1.4E-03	0.24	2.1E-01	0.47	1.9E-07	0.41	6.9E-06	0.52	1.2E-08	0.51	8.1E-08	0.47	1.1E-06	0.47	3.4E-07	0.47	n/a
C16:0 LPE	C8-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11503	-0.49	1.1E-06	-0.41	5.5E-05	-0.48	1.7E-06	-0.46	1.2E-05	-0.46	1.3E-05	-0.49	2.7E-06	-0.44	9.9E-03	-0.51	3.3E-08	-0.50	1.1E-07	-0.49	1.7E-07	-0.51	1.2E-07	-0.53	5.3E-08	-0.55	8.6E-09	-0.52	1.2E-08
C18:0 LPE	C8-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11130*	-0.32	3.0E-03	-0.19	8.6E-02	-0.32	2.9E-03	-0.33	3.6E-03	-0.32	4.7E-03	-0.33	2.3E-03	-0.20	3.5E-01	-0.40	1.9E-05	-0.37	n/a	-0.40	3.1E-05	-0.46	4.1E-06	-0.43	1.1E-05	-0.45	3.7E-06	-0.41	n/a
C18:1 LPE	C8-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11506	-0.43	3.3E-05	-0.36	6.7E-04	-0.44	2.5E-05	-0.44	4.0E-05	-0.43	5.7E-05	-0.47	1.0E-05	-0.27	1.9E-01	-0.53	3.2E-08	-0.55	1.7E-08	-0.55	1.2E-08	-0.60	3.4E-09	-0.56	2.7E-08	-0.57	7.9E-09	-0.54	n/a
C18:2 LPE	C8-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11507*	-0.79	3.5E-14	-0.72	1.0E-11	-0.80	1.6E-14	-0.82	2.8E-14	-0.80	1.1E-13	-0.82	1.9E-14	-0.66	2.6E-04	-0.89	8.7E-23	-0.90	8.1E-23	-0.91	2.4E-23	-0.97	4.4E-24	-0.90	2.5E-21	-0.91	2.7E-22	-0.90	5.6E-23
C20:1 LPE	C8-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11512*	-0.48	4.1E-07	-0.43	8.5E-06	-0.48	3.6E-07	-0.47	2.8E-06	-0.49	9.2E-07	-0.49	4.0E-07	-0.53	8.0E-04	-0.49	2.2E-07	-0.55	9.7E-09	-0.49	2.7E-07	-0.49	9.5E-07	-0.52	1.9E-07	-0.49	3.4E-07	-0.49	1.1E-07
C20:4 LPE	HILIC-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11517	-0.38	4.8E-04	-0.30	6.2E-03	-0.39	3.5E-04	-0.41	2.6E-04	-0.41	3.3E-04	-0.40	2.9E-04	-0.23	2.9E-01	-0.40	1.3E-05	-0.45	1.7E-06	-0.41	1.2E-05	-0.43	1.3E-05	-0.40	3.5E-05	-0.45	1.5E-06	-0.40	n/a
C20:4 LPE-A	C8-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11517	-0.26	1.7E-02	-0.19	9.6E-02	-0.28	1.1E-02	-0.29	1.2E-02	-0.28	1.7E-02	-0.28	1.5E-02	-0.15	4.9E-01	-0.47	2.8E-07	-0.52	n/a	-0.48	2.0E-07	-0.53	7.8E-08	-0.50	3.0E-07	-0.52	3.8E-08	-0.48	n/a
C32:1 PC plasmalogen-A	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB13404*	-0.49	5.5E-07	-0.52	5.0E-08	-0.49	6.6E-07	-0.43	3.1E-05	-0.45	1.2E-05	-0.54	7.7E-08	-0.53	5.6E-03	-0.50	5.3E-08	-0.63	2.1E-12	-0.49	1.3E-07	-0.54	2.2E-08	-0.54	1.3E-08	-0.50	1.1E-07	-0.49	4.8E-08
C32:1 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB13404*	0.33	1.2E-03	0.32	9.2E-04	0.33	1.4E-03	0.40	1.3E-04	0.38	2.7E-04	0.30	3.8E-03	0.29	1.5E-01	0.40	1.3E-05	0.24	5.4E-03	0.42	7.7E-06	0.37	1.3E-04	0.33	5.0E-04	0.41	1.6E-05	0.40	n/a
C34:1 PC plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11208*	-0.29	8.1E-03	-0.27	7.0E-03	-0.29	6.9E-03	-0.26	2.2E-02	-0.26	2.0E-02	-0.36	1.0E-03	-0.39	7.0E-02	-0.22	1.6E-02	-0.35	5.0E-05	-0.23	1.4E-02	-0.32	1.1E-03	-0.28	3.1E-03	-0.24	1.0E-02	-0.22	n/a
C34:2 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11210*	0.22	2.6E-02	0.17	4.8E-02	0.22	2.7E-02	0.27	8.6E-03	0.26	1.4E-02	0.19	7.6E-02	0.11	6.1E-01	0.37	2.6E-05	0.14	6.3E-02	0.37	2.6E-05	0.34	2.2E-04	0.32	4.8E-04	0.34	n/a	0.38	n/a
C34:3 PC plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11211*	0.31	1.9E-03	0.28	1.3E-03	0.31	2.4E-03	0.38	2.2E-04	0.35	8.1E-04	0.30	4.7E-03	0.22	2.7E-01	0.49	1.3E-07	0.27	8.3E-04	0.48	2.7E-07	0.48	6.5E-07	0.48	4.9E-07	0.48	3.7E-07	0.50	n/a
C34:4 PC plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11212*	-0.37	5.4E-05	-0.46	2.7E-07	-0.37	5.8E-05	-0.31	1.1E-03	-0.33	5.2E-04	-0.42	8.8E-06	-0.41	3.5E-02	-0.39	1.1E-04	-0.50	9.5E-07	-0.37	2.4E-04	-0.44	3.3E-05	-0.44	3.4E-05	-0.38	2.3E-04	-0.38	1.0E-04
C36:2 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11243*	0.50	1.0E-06	0.41	3.6E-06	0.48	2.5E-06	0.53	5.6E-07	0.52	8.3E-07	0.47	6.7E-06	0.33	8.2E-02	0.59	7.7E-12	0.36	1.3E-06	0.56	7.3E-11	0.54	1.8E-09	0.54	1.1E-09	0.57	9.9E-11	0.59	n/a
C36:3 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11244*	0.35	7.0E-04	0.31	8.0E-04	0.33	1.4E-03	0.39	2.4E-04	0.37	6.1E-04	0.32	2.7E-03	0.18	3.6E-01	0.47	2.5E-07	0.25	1.4E-03	0.45	9.3E-07	0.41	1.0E-05	0.43	4.8E-06	0.46	8.4E-07	0.47	n/a
C36:4 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11310*	0.27	1.2E-02	0.34	8.7E-04	0.25	1.8E-02	0.33	3.5E-03	0.30	8.5E-03	0.22	4.5E-02	0.26	2.4E-01	0.33	4.9E-04	0.22	1.0E-02	0.31	1.3E-03	0.34	7.5E-04	0.32	1.2E-03	0.33	8.0E-04	0.35	n/a
C36:5 PC plasmalogen-A	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11221*	0.24	1.7E-02	0.28	5.0E-03	0.26	1.1E-02	0.34	1.0E-03	0.29	6.7E-03	0.22	4.1E-02	0.14	4.9E-01	0.24	1.1E-02	0.14	1.2E-01	0.25	8.3E-03	0.31	1.8E-03	0.25	1.1E-02	0.24	1.1E-02	0.25	n/a
C36:5 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11220*	0.58	1.6E-08	0.61	5.9E-10	0.57	2.8E-08	0.65	1.2E-09	0.61	1.4E-08	0.56	1.4E-07	0.54	5.9E-03	0.69	2.0E-13	0.53	6.3E-10	0.68	6.7E-13	0.73	1.7E-13	0.68	3.0E-12	0.68	1.2E-12	0.70	8.2E-14
C38:4 PC plasmalogen-A	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11252*	-0.24	3.1E-02	-0.13	2.3E-01	-0.26	1.9E-02	-0.26	2.4E-02	-0.26	2.2E-02	-0.31	5.2E-03	-0.25	2.4E-01	-0.25	7.0E-03	-0.29	n/a	-0.28	2.7E-03	-0.30	2.4E-03	-0.27	6.3E-03	-0.27	5.2E-03	-0.24	n/a
C38:4 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11252*	0.34	1.7E-03	0.41	5.5E-05	0.30	4.5E-03	0.31	6.1E-03	0.32	5.9E-03	0.27	1.5E-02	0.30	1.5E-01	0.38	4.2E-05	0.30	5.6E-04	0.32	5.0E-04	0.33	8.5E-04	0.36	2.5E-04	0.38	8.0E-05	0.39	n/a
C38:6 PC plasmalogen-A	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11319*	0.58	3.2E-08	0.64	7.3E-10	0.59	1.8E-08	0.64	2.0E-09	0.60	3.0E-08	0.54	6.3E-07	0.43	3.7E-02	0.69	3.8E-14	0.62	8.5E-13	0.70	1.5E-14	0.73	1.8E-14	0.68	6.5E-13	0.71	3.4E-14	0.70	1.3E-14
C38:6 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11319*	0.45	1.3E-05	0.47	1.3E-06	0.44	2.3E-05	0.50	3.8E-06	0.47	1.5E-05	0.43	6.7E-05	0.35	7.4E-02	0.52	4.5E-08	0.33	7.2E-05	0.50	1.2E-07	0.49	7.8E-07	0.48	1.1E-06	0.51	1.3E-07	0.52	n/a
C38:7 PC plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11229*	0.62	1.9E-10	0.63	3.9E-11	0.63	6.8E-11	0.70	2.8E-12	0.65	1.1E-10	0.60	1.7E-09	0.47	8.5E-03	0.91	1.4E-23	0.78	5.3E-20	0.94	1.1E-24	0.99	4.7E-25	0.91	1.0E-21	0.93	2.2E-23	0.91	1.2E-23
C40:11 PC plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	n/a	-0.78	5.8E-14	-0.74	2.7E-12	-0.81	2.1E-15	-0.78	2.3E-13	-0.78	2.6E-13	-0.78	1.6E-13	-0.65	3.1E-04	-0.82	2.3E-19	-0.83	1.6E-19	-0.86	7.1E-21	-0.82	1.5E-17	-0.81	1.1E-17	-0.78	8.0E-17	-0.84	4.2E-20
C40:7 PC plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11294*	0.49	1.5E-06	0.53	6.8E-08	0.48	2.9E-06	0.50	3.4E-06	0.48	7.2E-06	0.44	3.6E-05	0.33	1.0E-01	0.66	2.6E-12	0.53	8.8E-10	0.65	6.8E-12	0.65	6.5E-11	0.63	8.8E-11	0.67	4.9E-12	0.67	n/a
C28:0 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07866*	-0.70	5.5E-14	-0.64	1.3E-11	-0.71	2.4E-14	-0.71	1.4E-13	-0.70	3.0E-13	-0.71	9.3E-14	-0.52	8.3E-04	-0.60	7.4E-10	-0.57	2.1E-09	-0.61	3.7E-10	-0.58	1.9E-08	-0.58	1.3E-08	-0.59	2.8E-09	-0.61	3.0E-10
C30:0 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07869*	-0.79	1.3E-15	-0.70	2.2E-12	-0.80	1.1E-15	-0.78	2.8E-14	-0.78	2.9E-14	-0.81	1.8E-15	-0.66	5.4E-05	-0.68	1.1E-14	-0.67	1.9E-15	-0.68	1.1E-14	-0.65	3.9E-12	-0.66	8.5E-13	-0.68	4.4E-14	-0.69	1.8E-15
C30:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07870*	-0.98	4.2E-24	-0.92	6.7E-21	-0.99	3.4E-24	-0.99	7.7E-23	-0.98	1.9E-22	-0.99	2.1E-23	-0.84	3.1E-07	-0.91	1.1E-24	-0.89	1.6E-24	-0.92	8.6E-25	-0.88	6.6E-21	-0.90	1.4E-21	-0.92	6.4E-24	-0.92	2.3E-25
C31:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07936*	-1.06	1.2E-28	-1.01	1.4E-25	-1.07	5.4E-29	-1.06	1.1E-26	-1.07	1.1E-26	-1.08	1.1E-27	-0.94	4.0E-09	-1.09	2.1E-33	-1.06	1.4E-33	-1.09	2.8E-33	-1.06	1.1E-28	-1.08	5.4E-30	-1.09	5.4E-32	-1.10	6.0E-34
C32:0 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07871*	-0.46	5.3E-06	-0.33	7.7E-04	-0.46	6.5E-06	-0.41	1.1E-04	-0.42	7.5E-05	-0.51	1.1E-06	-0.36	5.0E-02	-0.37	3.3E-05	-0.40	9.5E-07	-0.36	7.0E-05	-0.38	6.3E-05	-0.40	2.5E-05	-0.41	9.7E-06	-0.38	n/a
C32:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07873*	-1.00	1.1E-23	-0.92	3.6E-20	-1.00	1.5E-23	-0.99	7.1E-22	-1.00	6.7E-22	-1.01	8.2E-23	-0.92	9.6E-08	-0.92	2.2E-27	-0.88	8.4E-27	-0.91	7.1E-27	-0.90	2.7E-24	-0.92	3.3E-25	-0.94	1.3E-27	-0.92	5.1E-28
C32:2 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07874*	-1.14	1.2E-28	-1.01	1.9E-24	-1.15	5.4E-29	-1.15	8.5E-27	-1.13	1.3E-26	-1.15	1.1E-27	-0.98	1.0E-08	-1.05	2.6E-35	-1.03	8.1E-40	-1.06	7.9E-36	-1.05	1.4E-31	-1.03	3.9E-31	-1.04	3.8E-33	-1.06	5.3E-36
C34:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07972*	-0.69	8.2E-12	-0.56	1.4E-08	-0.69	8.4E-12	-0.67	2.9E-10	-0.68	1.2E-10	-0.71	6.2E-12	-0.65	2.3E-04	-0.53	4.3E-09	-0.50	1.8E-09	-0.53	4.0E-09	-0.55	4.0E-09	-0.56	2.5E-09	-0.55	1.7E-09	-0.54	1.3E-09
C34:2 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07973*	-0.86	1.1E-17	-0.72	2.7E-14	-0.87	4.6E-18	-0.83	1.1E-15	-0.82	2.7E-15	-0.90	2.4E-18	-0.82	4.6E-06	-0.73	4.3E-16	-0.73	8.1E-20	-0.75	9.5E-17	-0.79	5.0E-17	-0.75	1.3E-15	-0.74	2.1E-15	-0.75	3.3E-17
C34:3 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08006*	-1.12	2.3E-27	-0.97	1.0E-23	-1.11	3.4E-27	-1.11	4.0E-25	-1.10	3.9E-25	-1.15	1.9E-27	-0.99	2.6E-08	-1.00	1.2E-32	-1.01	3.2E-40	-1.01	2.0E-32	-1.03	1.6E-30	-1.00	1.0E-29	-1.02	2.7E-32	-1.01	1.0E-32
C34:4 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07883*	-0.66	1.5E-11	-0.55	6.2E-09	-0.66	1.4E-11	-0.67	3.7E-11	-0.67	3.2E-11	-0.67	2.1E-11	-0.49	3.5E-03	-0.82	4.0E-20	-0.84	5.3E-23	-0.82	7.5E-20	-0.81	1.2E-17	-0.79	4.0E-17	-0.83	7.0E-20	-0.82	2.9E-20
C34:5 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07885*	-0.41	2.2E-05	-0.32	8.0E-04	-0.40	3.7E-05	-0.39	9.4E-05	-0.41	4.5E-05	-0.42	2.3E-05	-0.37	2.3E-02	-0.44	1.2E-06	-0.48	5.0E-08	-0.43	3.1E-06	-0.38	9.6E-05	-0.41	2.4E-05	-0.42	6.2E-06	-0.44	8.4E-07
C36:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08038*	-0.43	5.5E-05	-0.29	5.4E-03	-0.44	4.2E-05	-0.47	2.1E-05	-0.48	1.2E-05	-0.49	5.8E-06	-0.41	3.2E-02	-0.33	5.7E-04	-0.30	6.0E-04	-0.34	3.4E-04	-0.38	1.9E-04	-0.36	3.1E-04	-0.36	2.3E-04	-0.33	4.3E-04
C36:2 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08039*	-0.67	1.1E-10	-0.51	1.1E-07	-0.68	2.9E-11	-0.71	2.9E-11	-0.70	8.3E-11	-0.73	3.0E-12	-0.66	7.3E-05	-0.56	4.5E-09	-0.56	4.3E-11	-0.59	5.5E-10	-0.66	4.1E-11	-0.59	2.9E-09	-0.56	7.7E-09	-0.56	2.4E-09
C36:3 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08105*	-0.84	9.4E-16	-0.70	2.4E-12	-0.85	7.1E-16	-0.84	7.7E-15	-0.84	9.6E-15	-0.91	2.6E-17	-0.77	1.8E-05	-0.82	3.4E-20	-0.82	1.1E-24	-0.84	6.5E-21	-0.86	3.3E-20	-0.82	7.7E-19	-0.86	5.7E-21	-0.82	3.5E-20
C36:4 PC-A	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07983*	-0.75	6.6E-12	-0.66	1.0E-09	-0.75	9.2E-12	-0.73	1.2E-10	-0.72	1.6E-10	-0.79	1.9E-12	-0.67	4.3E-04	-0.27	2.3E-03	-0.32	9.9E-05	-0.28	1.8E-03	-0.26	5.0E-03	-0.26	4.7E-03	-0.30	1.0E-03	-0.27	1.7E-03
C36:5 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07890*	-0.28	7.8E-03	-0.17	1.0E-01	-0.26	1.4E-02	-0.23	3.3E-02	-0.27	1.5E-02	-0.29	8.1E-03	-0.24	2.3E-01	-0.35	4.0E-05	-0.39	n/a	-0.32	1.7E-04	-0.29	1.4E-03	-0.33	2.4E-04	-0.36	4.7E-05	-0.35	n/a
C37:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07952*	-0.39	1.4E-04	-0.27	7.9E-03	-0.41	9.1E-05	-0.41	1.5E-04	-0.43	6.6E-05	-0.44	2.6E-05	-0.40	2.0E-02	-0.26	5.4E-03	-0.28	1.1E-03	-0.27	3.7E-03	-0.29	3.7E-03	-0.30	2.4E-03	-0.27	5.4E-03	-0.27	3.2E-03
C38:2 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08270*	-0.39	1.9E-04	-0.24	2.1E-02	-0.39	2.4E-04	-0.44	4.1E-05	-0.45	3.0E-05	-0.47	1.2E-05	-0.38	3.7E-02	-0.24	1.2E-02	-0.20	2.1E-02	-0.22	2.1E-02	-0.27	6.9E-03	-0.26	1.0E-02	-0.26	6.7E-03	-0.24	1.1E-02
C38:3 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08047*	-0.50	2.5E-06	-0.30	3.5E-03	-0.49	2.8E-06	-0.56	1.6E-07	-0.57	1.4E-07	-0.55	2.3E-07	-0.43	2.1E-02	-0.48	3.0E-07	-0.36	2.6E-05	-0.48	3.7E-07	-0.49	8.4E-07	-0.48	1.2E-06	-0.52	6.3E-08	-0.47	3.0E-07
C40:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08026*	-0.21	3.6E-02	-0.13	1.9E-01	-0.20	4.3E-02	-0.21	4.2E-02	-0.21	4.4E-02	-0.26	1.1E-02	-0.27	1.1E-01	-0.21	2.7E-02	-0.28	n/a	-0.21	2.9E-02	-0.24	1.8E-02	-0.19	5.4E-02	-0.24	1.5E-02	-0.22	n/a
C40:6 PC-A	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08057*	-0.41	1.3E-04	-0.21	4.1E-02	-0.41	1.3E-04	-0.49	7.4E-06	-0.49	7.4E-06	-0.46	1.9E-05	-0.34	8.8E-02	-0.38	4.2E-05	-0.28	1.4E-03	-0.38	5.0E-05	-0.39	8.8E-05	-0.38	1.0E-04	-0.42	1.2E-05	-0.38	n/a
C40:6 PC-B	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08057*	0.29	3.8E-03	0.41	2.3E-05	0.31	2.0E-03	0.28	5.9E-03	0.26	1.1E-02	0.25	1.5E-02	0.25	1.8E-01	0.58	2.5E-10	0.61	6.3E-12	0.62	1.6E-11	0.62	2.1E-10	0.58	2.4E-09	0.57	2.0E-09	0.58	n/a
C34:2 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB08952*	0.30	4.7E-03	0.34	1.2E-03	0.29	6.5E-03	0.33	2.9E-03	0.31	5.4E-03	0.24	2.7E-02	0.25	2.8E-01	0.45	3.4E-06	0.32	5.2E-04	0.44	7.9E-06	0.44	1.7E-05	0.43	2.8E-05	0.46	4.4E-06	0.46	n/a
C34:3 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB11343*	0.23	3.2E-02	0.25	2.0E-02	0.22	4.5E-02	0.22	4.9E-02	0.20	8.0E-02	0.20	6.9E-02	0.15	4.6E-01	0.33	5.1E-04	0.22	1.8E-02	0.30	1.7E-03	0.34	7.0E-04	0.35	n/a	0.37	n/a	0.34	n/a
C36:2 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB09082*	0.31	3.6E-03	0.34	8.8E-04	0.28	7.2E-03	0.31	4.1E-03	0.30	6.7E-03	0.24	2.7E-02	0.25	2.5E-01	0.44	4.0E-06	0.33	3.0E-04	0.40	2.7E-05	0.40	9.2E-05	0.40	7.1E-05	0.43	1.5E-05	0.44	n/a
C36:5 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB11410*	0.75	3.0E-12	0.80	5.4E-13	0.75	4.0E-12	0.77	5.8E-12	0.75	2.4E-11	0.74	3.3E-11	0.79	5.4E-05	0.82	1.0E-19	0.74	1.0E-16	0.82	1.8E-19	0.87	5.4E-20	0.83	2.3E-18	0.85	9.7E-20	0.84	1.3E-20
C38:5 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB11386*	0.64	1.4E-09	0.68	1.5E-10	0.62	3.3E-09	0.64	3.9E-09	0.63	1.2E-08	0.60	2.4E-08	0.64	2.9E-04	0.75	9.4E-16	0.64	6.0E-13	0.73	4.5E-15	0.75	1.4E-14	0.73	1.0E-13	0.76	2.4E-15	0.76	1.7E-16
C38:6 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB11387*	0.70	1.7E-11	0.74	1.9E-12	0.69	3.5E-11	0.72	2.0E-11	0.69	2.2E-10	0.68	3.1E-10	0.65	5.8E-04	0.77	1.6E-16	0.62	6.7E-13	0.75	6.4E-16	0.79	4.6E-16	0.77	2.7E-15	0.79	8.0E-17	0.79	1.5E-17
C38:7 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB11420*	0.66	2.2E-11	0.70	1.0E-12	0.67	1.0E-11	0.72	1.0E-12	0.68	2.3E-11	0.63	4.5E-10	0.59	1.3E-03	0.99	1.8E-27	0.89	2.7E-25	1.00	4.4E-28	1.07	1.3E-28	1.01	1.6E-26	1.03	1.8E-28	0.99	7.2E-28
C40:7 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB11394*	0.77	2.4E-14	0.80	1.4E-15	0.76	3.4E-14	0.78	2.8E-14	0.76	2.8E-13	0.72	2.3E-12	0.61	7.2E-04	1.06	6.4E-30	0.94	3.3E-27	1.06	1.7E-29	1.10	1.1E-28	1.06	3.5E-27	1.09	2.3E-30	1.06	2.5E-30
C42:11 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	n/a	-0.61	9.8E-09	-0.63	7.2E-09	-0.62	5.0E-09	-0.65	3.9E-09	-0.63	1.8E-08	-0.63	8.6E-09	-0.74	3.3E-05	-0.66	2.7E-13	-0.63	6.2E-12	-0.68	7.8E-14	-0.76	1.8E-15	-0.69	3.9E-13	-0.65	1.9E-12	-0.67	5.6E-14
C44:13 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	n/a	0.75	1.9E-12	0.73	2.5E-11	0.74	2.9E-12	0.74	3.2E-11	0.73	5.4E-11	0.77	1.4E-12	0.77	7.9E-05	0.48	1.6E-08	0.44	5.6E-07	0.49	1.3E-08	0.52	6.3E-09	0.47	1.3E-07	0.44	3.5E-07	0.48	1.5E-08
C34:2 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB08928*	-0.74	1.6E-13	-0.66	9.8E-11	-0.75	1.4E-13	-0.73	2.8E-12	-0.72	3.7E-12	-0.76	2.6E-13	-0.52	2.4E-03	-0.61	6.5E-12	-0.43	3.8E-07	-0.61	8.7E-12	-0.62	6.1E-11	-0.59	1.8E-10	-0.63	4.9E-12	-0.61	2.5E-12
C36:0 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB08991*	-0.62	2.2E-09	-0.51	4.6E-07	-0.65	4.3E-10	-0.61	1.6E-08	-0.63	6.2E-09	-0.66	9.4E-10	-0.58	8.3E-04	-0.51	3.2E-08	-0.54	3.8E-10	-0.53	8.7E-09	-0.49	6.1E-07	-0.50	2.0E-07	-0.49	1.7E-07	-0.52	8.7E-09
C36:1 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB08993*	-0.42	1.9E-05	-0.30	2.7E-03	-0.43	1.9E-05	-0.42	5.3E-05	-0.42	4.4E-05	-0.47	3.7E-06	-0.21	2.7E-01	-0.36	9.4E-05	-0.18	3.6E-02	-0.37	7.5E-05	-0.42	2.1E-05	-0.40	4.1E-05	-0.39	4.5E-05	-0.37	n/a
C36:2 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB08994*	-0.87	6.4E-18	-0.74	1.2E-13	-0.88	4.6E-18	-0.86	2.1E-16	-0.86	2.4E-16	-0.90	4.0E-18	-0.66	1.2E-04	-0.70	8.5E-15	-0.52	1.0E-09	-0.71	5.4E-15	-0.75	4.9E-15	-0.71	5.4E-14	-0.72	9.9E-15	-0.70	3.0E-15
C36:3 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB09060*	-0.83	3.5E-16	-0.74	6.3E-13	-0.83	2.7E-16	-0.82	8.2E-15	-0.81	1.3E-14	-0.88	4.5E-17	-0.65	1.6E-04	-0.66	1.8E-13	-0.56	3.6E-10	-0.68	7.8E-14	-0.71	6.1E-14	-0.67	1.4E-12	-0.69	7.2E-14	-0.66	9.0E-14
C38:2 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB08942*	-0.72	4.3E-12	-0.62	2.1E-10	-0.75	5.6E-13	-0.72	2.0E-11	-0.73	1.7E-11	-0.77	6.4E-13	-0.74	4.9E-05	-0.60	3.7E-11	-0.67	7.7E-16	-0.63	3.2E-12	-0.64	2.8E-11	-0.60	2.5E-10	-0.57	6.2E-10	-0.60	1.5E-11
C38:5 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB09069*	-0.36	4.5E-04	-0.28	7.7E-03	-0.37	3.6E-04	-0.33	2.1E-03	-0.33	1.8E-03	-0.40	1.5E-04	-0.20	3.0E-01	-0.29	1.3E-03	-0.28	2.0E-03	-0.30	1.2E-03	-0.31	1.4E-03	-0.30	2.0E-03	-0.32	5.0E-04	-0.28	n/a
C40:6 PS	C8-pos	Glycerophospholipids - phosphatidylserine	HMDB10167*	-0.84	8.9E-17	-0.77	5.2E-14	-0.86	2.8E-17	-0.84	1.5E-15	-0.86	4.1E-16	-0.86	8.1E-17	-0.76	1.1E-05	-0.95	1.5E-25	-0.92	2.5E-24	-0.97	4.9E-26	-0.94	1.2E-22	-0.96	6.0E-24	-0.94	7.0E-24	-0.96	5.2E-26
4-cholesten-3-one	C8-pos	Sterol lipids - Cholesterol and derivatives	HMDB00921	-0.73	1.1E-15	-0.50	6.9E-10	-0.72	1.4E-15	-0.74	6.5E-15	-0.75	3.3E-15	-0.76	1.5E-16	-0.71	2.6E-05	-0.91	2.5E-20	-0.75	2.6E-18	-0.91	5.3E-20	-0.98	5.8E-21	-0.98	2.2E-21	-0.95	3.9E-21	-0.93	2.4E-21
C14:0 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06725	-0.50	1.9E-07	-0.44	6.4E-06	-0.51	1.2E-07	-0.51	1.9E-07	-0.51	2.2E-07	-0.49	7.8E-07	-0.57	7.2E-04	-0.56	1.7E-09	-0.59	2.4E-10	-0.57	1.1E-09	-0.53	1.3E-07	-0.54	3.7E-08	-0.54	1.9E-08	-0.57	8.9E-10
C16:0 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB00885	0.60	1.3E-10	0.62	2.4E-12	0.60	1.4E-10	0.59	1.6E-09	0.59	2.0E-09	0.62	1.6E-10	0.40	2.5E-02	0.73	3.9E-14	0.52	1.2E-08	0.76	4.5E-15	0.74	2.3E-13	0.71	9.0E-13	0.78	3.3E-15	0.74	1.1E-14
C16:1 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB00658*	-0.68	2.0E-12	-0.65	2.5E-11	-0.67	3.2E-12	-0.67	5.8E-12	-0.68	1.3E-11	-0.67	1.7E-11	-0.79	2.2E-06	-0.58	1.0E-10	-0.65	4.6E-13	-0.57	3.9E-10	-0.54	8.0E-09	-0.60	4.1E-10	-0.58	4.5E-10	-0.59	6.1E-11

Metabolite name	Method	Category	HMDB ID	WHI-OS														WHI-HT													
				Model 1		Model 2		Model 3		Model 4		Model 5		Model 6		Model 7		Model 1		Model 2		Model 3		Model 4		Model 5		Model 6		Model 7	
				Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR
C18:0 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB10368	0.21	4.4E-02	0.50	1.1E-09	0.18	8.2E-02	0.14	2.2E-01	0.14	2.1E-01	0.16	1.5E-01	0.20	3.5E-01	0.28	2.2E-03	0.38	3.8E-07	0.26	n/a	0.26	n/a	0.28	n/a	0.30	n/a	0.29	n/a
C18:1 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB00918	0.48	2.5E-07	0.45	5.7E-08	0.48	2.9E-07	0.48	8.0E-07	0.47	1.2E-06	0.50	2.3E-07	0.27	1.4E-01	0.61	7.3E-11	0.33	7.9E-05	0.63	2.8E-11	0.62	6.3E-10	0.59	2.4E-09	0.65	1.4E-11	0.62	n/a
C18:2 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB00610*	0.54	1.3E-08	0.46	1.8E-07	0.53	1.9E-08	0.52	1.5E-07	0.53	1.4E-07	0.55	2.0E-08	0.29	9.9E-02	0.54	9.4E-09	0.24	3.7E-03	0.54	9.9E-09	0.51	2.2E-07	0.51	1.6E-07	0.59	7.6E-10	0.54	n/a
C20:1 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB05193	0.23	2.5E-02	0.37	1.3E-04	0.24	2.1E-02	0.25	2.1E-02	0.24	2.9E-02	0.22	4.7E-02	-0.01	9.6E-01	0.63	4.4E-12	0.53	1.3E-10	0.65	6.3E-13	0.60	2.5E-10	0.61	7.8E-11	0.60	8.7E-11	0.63	n/a
C20:2 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06734	0.50	1.6E-07	0.48	7.0E-08	0.51	1.1E-07	0.51	4.0E-07	0.51	3.9E-07	0.51	1.8E-07	0.32	7.2E-02	0.79	1.8E-18	0.54	2.5E-11	0.82	1.4E-19	0.78	2.7E-16	0.79	3.3E-17	0.81	2.2E-18	0.80	n/a
C20:3 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06736*	0.49	1.9E-06	0.48	6.9E-07	0.49	1.7E-06	0.45	2.9E-05	0.44	4.4E-05	0.49	4.0E-06	0.30	1.4E-01	0.53	2.0E-08	0.30	6.2E-04	0.54	1.3E-08	0.60	2.3E-09	0.56	2.1E-08	0.56	9.5E-09	0.54	n/a
C20:4 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06726	1.07	6.9E-28	1.02	6.5E-29	1.06	1.3E-27	1.05	4.0E-25	1.04	4.1E-25	1.07	7.3E-27	0.93	1.2E-07	1.12	2.1E-33	0.85	7.7E-25	1.12	2.8E-33	1.14	1.9E-31	1.10	4.4E-30	1.14	5.7E-33	1.13	6.0E-34
C20:5 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06731	0.47	5.0E-06	0.53	7.3E-08	0.49	1.6E-06	0.51	1.2E-06	0.48	8.2E-06	0.49	4.3E-06	0.31	1.1E-01	0.40	4.6E-06	0.23	4.0E-03	0.43	8.8E-07	0.47	3.6E-07	0.41	8.7E-06	0.42	3.4E-06	0.40	n/a
C22:4 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06729*	0.84	1.4E-20	0.76	2.7E-19	0.84	1.6E-20	0.82	2.2E-18	0.83	1.3E-18	0.87	8.2E-21	0.80	3.4E-07	1.07	1.7E-30	0.78	2.4E-21	1.10	9.9E-32	1.10	1.1E-28	1.09	6.7E-29	1.08	1.1E-29	1.09	1.4E-31
C22:5 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB10375*	0.93	4.9E-19	0.91	2.7E-19	0.93	6.8E-19	0.89	2.4E-16	0.89	2.4E-16	0.95	7.4E-19	0.79	4.1E-05	0.94	4.5E-27	0.74	1.6E-19	0.95	9.9E-28	1.00	8.4E-28	0.96	4.2E-26	0.95	1.7E-26	0.95	6.0E-28
C22:6 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06733	0.96	1.5E-23	0.93	5.8E-23	0.98	3.4E-24	1.00	1.7E-23	0.97	1.1E-22	0.96	2.4E-22	0.74	1.7E-05	1.24	4.9E-44	1.06	4.1E-36	1.27	5.4E-46	1.30	1.6E-43	1.24	1.0E-40	1.28	6.6E-45	1.24	4.6E-44
C16:0 Ceramide (d18:1)	C8-pos	Sphingolipids - Ceramides	HMDB04949	-0.26	1.2E-02	-0.03	7.6E-01	-0.27	9.2E-03	-0.27	1.2E-02	-0.28	8.6E-03	-0.30	4.3E-03	-0.46	8.9E-03	-0.27	5.0E-03	-0.14	n/a	-0.29	3.1E-03	-0.33	1.3E-03	-0.29	4.2E-03	-0.32	1.5E-03	-0.27	5.1E-03
C22:0 Ceramide (d18:1)	C8-pos	Sphingolipids - Ceramides	HMDB04952	-0.28	6.7E-03	-0.01	9.0E-01	-0.29	4.4E-03	-0.33	1.9E-03	-0.33	1.9E-03	-0.33	1.4E-03	-0.26	1.6E-01	-0.38	8.1E-05	-0.21	n/a	-0.42	1.1E-05	-0.45	9.9E-06	-0.37	1.8E-04	-0.40	3.8E-05	-0.38	n/a
C23:0 Ceramide (d18:1)	C8-pos	Sphingolipids - Ceramides	HMDB00950	-0.36	3.4E-04	-0.10	3.0E-01	-0.38	1.4E-04	-0.40	1.1E-04	-0.40	9.1E-05	-0.41	6.9E-05	-0.31	9.9E-02	-0.50	1.8E-07	-0.35	n/a	-0.54	1.7E-08	-0.54	7.8E-08	-0.49	9.2E-07	-0.49	4.9E-07	-0.50	n/a
C24:0 Ceramide (d18:1)	C8-pos	Sphingolipids - Ceramides	HMDB04956	-0.21	4.9E-02	0.06	5.6E-01	-0.22	4.3E-02	-0.26	2.1E-02	-0.26	2.0E-02	-0.26	1.9E-02	-0.24	2.4E-01	-0.21	2.6E-02	-0.09	n/a	-0.24	1.1E-02	-0.30	3.2E-03	-0.22	2.6E-02	-0.23	1.9E-02	-0.21	n/a
C24:1 Ceramide (d18:1)	C8-pos	Sphingolipids - Ceramides	HMDB04953	-0.31	4.1E-03	-0.11	3.3E-01	-0.31	3.8E-03	-0.26	2.3E-02	-0.28	1.4E-02	-0.36	9.5E-04	-0.37	5.2E-02	-0.31	1.0E-03	-0.16	n/a	-0.29	2.1E-03	-0.31	2.2E-03	-0.33	8.4E-04	-0.35	2.4E-04	-0.31	n/a
sphinganine	HILIC-pos	Sphingolipids - Sphingolipids	HMDB00269	0.33	6.9E-05	0.35	5.5E-05	0.34	6.0E-05	0.34	1.1E-04	0.34	1.3E-04	0.33	1.5E-04	0.37	8.9E-03	0.24	2.5E-02	0.26	1.6E-02	0.24	2.7E-02	0.21	6.9E-02	0.21	5.5E-02	0.21	5.1E-02	0.25	1.5E-02
sphingosine-1-phosphate	C18-neg	Sphingolipids - Sphingolipids	HMDB00277	0.22	4.9E-02	0.23	4.3E-02	0.22	4.7E-02	0.23	5.3E-02	0.23	5.3E-02	0.21	6.9E-02	0.17	4.5E-01	0.20	3.2E-02	0.16	9.3E-02	0.20	3.5E-02	0.15	n/a	0.16	n/a	0.20	n/a	0.18	n/a
C14:0 SM	C8-pos	Sphingolipids - Sphingomyelins	HMDB12097	-0.53	2.8E-07	-0.37	9.2E-05	-0.54	1.2E-07	-0.55	4.1E-07	-0.55	3.0E-07	-0.53	5.1E-07	-0.51	3.8E-03	-0.47	3.8E-07	-0.52	2.3E-11	-0.50	9.2E-08	-0.49	8.0E-07	-0.48	8.5E-07	-0.45	2.2E-06	-0.47	2.7E-07
C18:0 SM	C8-pos	Sphingolipids - Sphingomyelins	HMDB01348	0.30	4.8E-03	0.48	1.0E-07	0.28	7.2E-03	0.29	9.2E-03	0.29	9.0E-03	0.26	1.5E-02	0.14	4.9E-01	0.21	2.9E-02	0.21	9.8E-03	0.18	6.6E-02	0.18	7.4E-02	0.20	4.0E-02	0.21	3.2E-02	0.22	n/a
C18:1 SM	C8-pos	Sphingolipids - Sphingomyelins	HMDB12101	0.34	1.1E-03	0.49	1.6E-07	0.33	1.7E-03	0.35	1.4E-03	0.35	1.3E-03	0.30	5.0E-03	0.23	2.4E-01	0.28	2.3E-03	0.24	2.9E-03	0.25	5.7E-03	0.21	2.8E-02	0.24	1.0E-02	0.27	3.5E-03	0.29	n/a
C24:1 SM	C8-pos	Sphingolipids - Sphingomyelins	HMDB12107	0.31	6.5E-03	0.44	1.3E-05	0.32	5.1E-03	0.35	2.8E-03	0.33	4.7E-03	0.28	1.7E-02	0.13	5.9E-01	0.42	2.4E-06	0.35	8.8E-06	0.45	5.3E-07	0.41	1.4E-05	0.38	3.4E-05	0.41	8.1E-06	0.42	n/a
2-hydroxyhexadecanoate	C18-neg	Fatty acids	HMDB31057	-0.30	6.4E-03	-0.30	9.3E-03	-0.30	7.1E-03	-0.26	2.9E-02	-0.26	2.6E-02	-0.31	6.5E-03	-0.40	5.2E-02	-0.28	1.9E-03	-0.28	2.7E-03	-0.25	5.5E-03	-0.31	1.4E-03	-0.31	1.0E-03	-0.30	1.6E-03	-0.32	n/a
8,11,14-eicosatrienoic acid	C18-neg	Fatty acids	HMDB02925	-0.29	5.5E-03	-0.28	7.9E-03	-0.28	7.4E-03	-0.26	1.5E-02	-0.27	1.2E-02	-0.27	1.2E-02	-0.31	1.3E-01	-0.30	7.0E-04	-0.26	4.3E-03	-0.26	2.7E-03	-0.28	3.0E-03	-0.30	1.0E-03	-0.31	4.9E-04	-0.33	n/a
eicosanedioate	C18-neg	Fatty acids	n/a	0.33	1.4E-03	0.31	3.8E-03	0.32	2.0E-03	0.37	6.5E-04	0.38	5.5E-04	0.25	1.9E-02	0.44	1.6E-02	0.34	3.8E-04	0.29	2.5E-03	0.31	1.2E-03	0.28	4.8E-03	0.31	1.9E-03	0.34	4.2E-04	0.31	9.8E-04
gamma-linolenic acid	C18-neg	Fatty acids	HMDB03073	-0.37	8.5E-04	-0.39	6.0E-04	-0.35	1.5E-03	-0.35	3.2E-03	-0.35	3.3E-03	-0.35	2.6E-03	-0.27	2.4E-01	-0.38	3.2E-05	-0.40	2.2E-05	-0.35	1.3E-04	-0.38	1.0E-04	-0.38	7.7E-05	-0.41	1.1E-05	-0.41	n/a
hexadecanedioate	C18-neg	Fatty acids	HMDB00672	-0.61	6.2E-09	-0.63	4.4E-09	-0.61	4.3E-09	-0.59	7.2E-08	-0.57	1.5E-07	-0.62	7.9E-09	-0.67	3.8E-04	-0.59	4.3E-11	-0.60	4.1E-11	-0.60	2.9E-11	-0.65	6.0E-12	-0.64	5.3E-12	-0.62	1.3E-11	-0.62	1.3E-12
hydroxymyristate	C18-neg	Fatty acids	HMDB02261	-0.67	4.1E-10	-0.68	6.0E-10	-0.67	4.1E-10	-0.65	7.2E-09	-0.66	6.0E-09	-0.69	5.0E-10	-0.76	1.0E-04	-0.69	7.1E-14	-0.72	2.8E-14	-0.68	2.6E-13	-0.71	2.7E-13	-0.71	1.4E-13	-0.69	2.0E-13	-0.72	2.3E-15
myristic acid	C18-neg	Fatty acids	HMDB00806	-0.21	3.4E-02	-0.23	2.2E-02	-0.21	2.9E-02	-0.19	6.7E-02	-0.19	6.8E-02	-0.20	4.2E-02	-0.11	5.1E-01	-0.21	1.4E-02	-0.23	1.0E-02	-0.23	9.0E-03	-0.21	n/a	-0.21	n/a	-0.21	1.7E-02	-0.24	n/a
oleate	C18-neg	Fatty acids	HMDB00207	-0.30	3.1E-03	-0.33	1.2E-03	-0.30	3.4E-03	-0.28	9.6E-03	-0.27	1.0E-02	-0.29	4.9E-03	-0.18	3.9E-01	-0.29	3.2E-03	-0.32	1.4E-03	-0.29	3.7E-03	-0.33	1.3E-03	-0.32	2.0E-03	-0.31	2.2E-03	-0.33	n/a
palmitoleic acid	C18-neg	Fatty acids	HMDB03229	-0.84	2.6E-15	-0.91	4.8E-17	-0.84	3.2E-15	-0.83	9.2E-14	-0.83	1.3E-13	-0.81	1.1E-13	-0.77	6.5E-05	-0.74	2.1E-17	-0.79	3.2E-19	-0.73	6.5E-17	-0.76	1.5E-16	-0.77	2.8E-17	-0.77	8.2E-18	-0.77	6.5E-19
sebacate	C18-neg	Fatty acids	HMDB00792	-0.29	2.9E-03	-0.31	1.7E-03	-0.31	1.9E-03	-0.28	6.1E-03	-0.27	9.0E-03	-0.32	1.7E-03	-0.39	3.9E-02	-0.37	1.4E-04	-0.36	3.2E-04	-0.41	3.7E-05	-0.39	1.9E-04	-0.36	4.8E-04	-0.40	6.0E-05	-0.41	2.5E-05
C12:1 carnitine	HILIC-pos	Acylcarnitines	HMDB13326	-0.50	1.5E-06	-0.54	4.1E-07	-0.52	6.6E-07	-0.49	7.5E-06	-0.48	1.0E-05	-0.49	4.4E-06	-0.34	7.3E-02	-0.31	7.6E-04	-0.34	3.0E-04	-0.33	3.5E-04	-0.30	2.1E-03	-0.29	2.7E-03	-0.33	5.3E-04	-0.32	n/a
C14 carnitine	HILIC-pos	Acylcarnitines	HMDB05066	-0.35	6.9E-04	-0.35	9.2E-04	-0.38	2.5E-04	-0.35	1.5E-03	-0.34	1.9E-03	-0.36	8.0E-04	-0.14	5.5E-01	-0.27	3.5E-03	-0.29	1.5E-03	-0.30	9.6E-04	-0.26	7.8E-03	-0.24	1.3E-02	-0.27	3.5E-03	-0.26	n/a
C14:1 carnitine	HILIC-pos	Acylcarnitines	HMDB02014	-0.32	2.4E-03	-0.36	6.4E-04	-0.33	1.6E-03	-0.30	6.2E-03	-0.30	6.5E-03	-0.31	4.3E-03	-0.21	3.4E-01	-0.19	3.7E-02	-0.25	7.0E-03	-0.21	2.5E-02	-0.21	3.7E-02	-0.19	5.1E-02	-0.21	2.5E-02	-0.19	n/a
C18 carnitine	HILIC-pos	Acylcarnitines	HMDB00848	0.35	1.5E-03	0.40	4.4E-04	0.33	3.0E-03	0.33	4.5E-03	0.34	3.5E-03	0.33	3.5E-03	0.32	1.4E-01	0.32	4.3E-05	0.31	1.3E-04	0.28	3.2E-04	0.29	4.4E-04	0.33	6.4E-05	0.33	4.4E-05	0.33	n/a
C5:1 carnitine	HILIC-pos	Acylcarnitines	HMDB02366	-0.24	1.1E-02	-0.23	1.7E-02	-0.23	1.5E-02	-0.17	8.0E-02	-0.23	1.9E-02	-0.23	1.7E-02	-0.33	5.3E-02	-0.32	1.6E-03	-0.32	2.5E-03	-0.32	2.1E-03	-0.20	n/a	-0.28	1.0E-02	-0.31	3.5E-03	-0.32	n/a
2-aminooctanoate	HILIC-pos	Amino Acids	HMDB00991	-0.32	3.6E-03	-0.36	1.2E-03	-0.33	2.8E-03	-0.33	4.8E-03	-0.31	8.6E-03	-0.38	6.8E-04	-0.29	1.6E-01	-0.28	2.2E-03	-0.33	4.9E-04	-0.32	5.6E-04	-0.27	5.8E-03	-0.25	1.0E-02	-0.26	5.9E-03	-0.31	n/a
4-acetamidobutanoate	HILIC-pos	Amino Acids	HMDB03681	-0.50	5.3E-07	-0.51	2.7E-07	-0.50	5.2E-07	-0.49	1.7E-06	-0.49	1.5E-06	-0.52	2.7E-07	-0.38	6.2E-02	-0.27	2.8E-03	-0.30	1.4E-03	-0.28	2.0E-03	-0.30	1.7E-03	-0.30	1.7E-03	-0.30	1.4E-03	-0.27	n/a
5-acetylamino-6-amino-3-methyluracil	HILIC-pos	Amino Acids	HMDB04400	-0.65	2.6E-10	-0.66	4.3E-10	-0.68	2.7E-11	-0.65	1.6E-09	-0.62	6.6E-09	-0.69	7.6E-11	-0.70	1.7E-04	-0.55	8.7E-10	-0.53	3.9E-09	-0.57	1.3E-10	-0.57	1.6E-09	-0.57	9.0E-10	-0.53	5.2E-09	-0.54	7.8E-10
ADMA	HILIC-pos	Amino Acids	HMDB01539	-0.51	4.1E-07	-0.53	3.0E-07	-0.51	4.0E-07	-0.51	9.4E-07	-0.51	8.8E-07	-0.56	5.4E-08	-0.39	3.5E-02	-0.55	1.4E-08	-0.51	2.1E-07	-0.56	5.9E-09	-0.57	3.2E-08	-0.54	8.4E-08	-0.56	1.1E-08	-0.55	5.7E-09
alanine	HILIC-pos	Amino Acids	HMDB00161	-0.47	1.9E-05	-0.36	9.2E-04	-0.46	2.2E-05	-0.48	3.3E-05	-0.47	4.4E-05	-0.51	4.8E-06	-0.34	1.1E-01	-0.43	2.4E-06	-0.31	8.7E-04	-0.45	1.0E-06	-0.45	3.7E-06	-0.44	5.4E-06	-0.42	7.4E-06	-0.46	n/a
arginine	HILIC-pos	Amino Acids	HMDB00517	0.28	5.1E-03	0.24	2.1E-02	0.27	6.3E-03	0.31	3.1E-03	0.31	2.4E-03	0.26	1.3E-02	0.28	1.4E-01	0.28	4.0E-03	0.25	1.1E-02	0.27	5.8E-03	0.31	3.0E-03	0.32	1.8E-03	0.27	7.0E-03	0.31	n/a
citrulline	HILIC-pos	Amino Acids	HMDB00904	-0.37	3.9E-04	-0.41	8.9E-05	-0.36	5.3E-04	-0.37	7.8E-04	-0.37	6.2E-04	-0.39	2.8E-04	-0.28	1.8E-01	-0.24	7.9E-03	-0.34	3.6E-04	-0.26	5.0E-03	-0.27	6.5E-03	-0.23	1.6E-02	-0.25	9.2E-03	-0.23	n/a
creatinine	HILIC-pos	Amino Acids	HMDB00562	0.29	5.7E-03	0.24	2.4E-02	0.28	7.3E-03	0.29	7.3E-03	0.29	7.8E-03	0.28	9.4E-03	0.22	3.0E-01	0.29	2.5E-03	0.32	1.3E-03	0.28	3.5E-03	0.29	4.0E-03	0.29	3.2E-03	0.28	4.0E-03	0.30	n/a
homoarginine	HILIC-pos	Amino Acids	HMDB00670	0.61	1.5E-09	0.57	3.1E-08	0.61	1.8E-09	0.64	1.6E-09	0.62	4.2E-09	0.60	9.7E-09	0.63	3.4E-04	0.63	2.2E-13	0.67	4.6E-14	0.65	5.9E-14	0.65	1.0E-12	0.65	7.7E-13	0.67	4.0E-14	0.65	5.1E-14
hydroxyproline	HILIC-pos	Amino Acids	HMDB00725	0.32	7.0E-03	0.29	1.6E-02	0.31	8.3E-03	0.33	6.6E-03	0.30	1.7E-02	0.29	1.8E-02	0.15	5.1E-01	0.59	1.4E-11	0.51	6.8E-09	0.57	7.3E-11	0.60	1.1E-10	0.59	1.4E-10	0.58	7.3E-11	0.58	n/a
kynurenine	HILIC-neg	Amino Acids	HMDB00684	-0.59	3.8E-09	-0.54	9.9E-08	-0.60	2.0E-09	-0.58	3.7E-08	-0.58	3.7E-08	-0.58	2.3E-08	-0.68	2.6E-04	-0.42	2.1E-06	-0.34	1.7E-04	-0.44	7.2E-07	-0.40	2.3E-05	-0.39	2.8E-05	-0.41	5.9E-06	-0.42	1.5E-06
lysine	HILIC-pos	Amino Acids	HMDB00182	-0.34	1.8E-03	-0.35	1.7E-03	-0.33	2.3E-03	-0.29	1.1E-02	-0.32	5.3E-03	-0.37	9.2E-04	-0.27	2.1E-01	-0.42	5.9E-06	-0.38	6.6E-05	-0.40	1.3E-05	-0.33	6.7E-04	-0.38	1.1E-04	-0.40	2.4E-05	-0.40	n/a
N-acetylornithine	HILIC-pos	Amino Acids	HMDB03357	-0.72	3.6E-11	-0.71	2.5E-10	-0.70	1.1E-10	-0.72	2.3E-10	-0.73	8.2E-11	-0.75	1.6E-11	-0.86	1.6E-05	-0.71	1.6E-15	-0.71	4.2E-15	-0.68	1.5E-14	-0.60	2.1E-10	-0.61	5.9E-11	-0.69	3.0E-14	-0.71	1.1E-15
N-alpha-acetylarginine	HILIC-pos	Amino Acids	HMDB04620	0.60	1.5E-08	0.59	4.1E-08	0.61	6.5E-09	0.64	3.9E-09	0.60	3.7E-08	0.60	2.6E-08	0.62	4.3E-04	0.75	8.7E-16	0.72	4.9E-14	0.75	9.5E-16	0.72	3.5E-13	0.73	8.9E-14	0.74	1.3E-14	0.78	2.3E-17
N6,N6-dimethyllysine	HILIC-pos	Amino Acids	HMDB13287	-1.06	1.5E-24	-1.06	1.9E-23	-1.05	3.4E-24	-1.09	3.4E-24	-1.09	4.1E-24	-1.06	2.1E-23	-0.96	3.4E-07	-0.95	6.1E-25	-0.96	1.6E-24	-0.97	2.8E-25	-0.94	1.3E-21	-0.94	4.1E-22	-0.97	1.2E-24	-0.96	1.9E-25
ornithine	HILIC-pos	Amino Acids	HMDB00214	-0.36	6.2E-04	-0.37	6.4E-04	-0.35	8.8E-04	-0.32	4.0E-03	-0.34	2.4E-03	-0.39	3.6E-04	-0.33	7.4E-02	-0.62	2.2E-11	-0.63	5.0E-11	-0.63	2.0E-11	-0.64	8.6E-11	-0.62	1.7E-10	-0.62	6.1E-11	-0.62	n/a
pantothenate	HILIC-neg	Amino Acids	HMDB00210	-0.25	1.9E-02	-0.22	4.1E-02	-0.23	3.2E-02	-0.25	2.4E-02	-0.25	2.1E-02	-0.28	1.1E-02	-0.26	2.4E-01	-0.44	3.0E-06	-0.41	1.5E-05	-0.41	1.2E-05	-0.36	2.3E-04	-0.39	7.5E-05	-0.44	5.1E-06	-0.44	n/a
phenylalanine	HILIC-pos	Amino Acids	HMDB00159	-0.25	2.6E-02	-0.19	9.2E-02	-0.24	2.9E-02	-0.25	3.2E-02	-0.27	1.7E-02	-0.28	1.5E-02	-0.11	6.2E-01	-0.26	4.3E-03	-0.19	n/a	-0.26	5.1E-03	-0.25	9.6E-03	-0.28	3.6E-03	-0.26	4.7E-03	-0.27	n/a
proline	HILIC-pos	Amino Acids	HMDB00162	-0.35	1.4E-03	-0.28	1.1E-02	-0.35	1.3E-03	-0.39	6.4E-04	-0.38	9.3E-04	-0.41	2.2E-04	-0.19	3.9E-01	-0.30	1.2E-03	-0.21	2.1E-02	-0.33	4.0E-04	-0.34	4.9E-04	-0.29	2.5E-03	-0.27	3.5E-03	-0.31	n/a
serine	HILIC-pos	Amino Acids	HMDB00187	0.29	3.9E-03	0.25	1.7E-02	0.29	3.8E-03	0.30	4.3E-03	0.30	5.4E-03	0.28	7.9E-03	0.22	2.8E-01	0.31	1.0E-03	0.23	1.5E-02	0.30	1.7E-03	0.26	1.0E-02	0.27	6.0E-03	0.33	8.1E-04	0.32	n/a
taurine	HILIC-pos	Amino Acids	HMDB00251	0.31	6.8E-03	0.31	6.8E-03	0.31	6.5E-03	0.33	6.0E-03	0.33	6.0E-03	0.28	1.7E-02	0.39	5.5E-02	0.26	4.5E-03	0.21	2.7E-02	0.27	4.0E-03	0.26	8.8E-03	0.26	7.9E-03	0.27	5.2E-03	0.29	n/a
bilirubin	HILIC-pos	Bile acids and Bilirubins	HMDB00054	-0.36	1.8E-04	-0.38	9.2E-05	-0.35	2.1E-04	-0.34	7.8E-04	-0.33	8.5E-04	-0.33	6.9E-04	-0.39	2.1E-02	-0.40	2.5E-05	-0.46	2.6E-06	-0.39	4.7E-05	-0.38	1.8E-04	-0.39	1.0E-04	-0.37	1.4E-04	-0.39	3.4E-05
biliverdin	HILIC-pos	Bile acids and Bilirubins	HMDB01008	-0.39	1.8E-04	-0.43	4.8E-05	-0.39	1.6E-04	-0.35	1.5E-03	-0.34	1.9E-03	-0.38	3.9E-04	-0.51	3.5E-03	-0.35	1.8E-04	-0.39	5.0E-05	-0.34	3.0E-04	-0.34	7.5E-04	-0.34	4.8E-04	-0.32	9.7E-04	-0.35	1.5E-04
glycochenodeoxycholate	C18-neg	Bile acids and Bilirubins	HMDB00637	-0.29	1.0E-02	-0.30	9.5E-03	-0.28	1.3E-02	-0.28	1.6E-02	-0.27	2.0E-02	-0.30	1.1E-02	-0.18	4.3E-01	-0.32	5.2E-04	-0.33	5.1E-04	-0.33	3.8E-04	-0.37	1.7E-04	-0.35	3.5E-04	-0.39	3.4E-05	-0.32	n/a
glycodeoxycholate	C18-neg	Bile acids and Bilirubins	HMDB00631	-0.24	2.8E-02	-0.25	2.6E-02	-0.24	2.9E-02	-0.23	4.1E-02	-0.22	4.7E-02	-0.23	3.9E-02	-0.24	2.9E-01	-0.26	6.1E-03	-0.26	7.3E-03	-0.28	2.7E-03	-0.29	3.9E-03	-0.26	7.9E-03	-0.30	2.0E-03	-0.26	n/a
glycodeoxycholate/glycochenodeoxycholate	HILIC-pos	Bile acids and Bilirubins	n/a	-0.34	2.4E-03	-0.35	2.3E-03	-0.34	3.0E-03	-0.33	4.6E-03	-0.32	6.3E-03	-0.35	2.5E-03	-0.26	2.6E-01	-0.34	1.5E-04	-0.34	2.4E-04	-0.36	7.0E-05	-0.36	1.6E-04	-0.34	3.0E-04	-0.39	1.8E-05	-0.33	n/a
glycoursodeoxycholate	C18-neg	Bile acids and Bilirubins	HMDB00708	-0.45	5.9E-05	-0.45	1.1E-04	-0.45	5.7E-05	-0.42	3.4E-04	-0.41	5.0E-04	-0.43	1.8E-04	-0.37	7.0E-02	-0.50	6.3E-08	-0.51	5.3E-08	-0.51	4.1E-08	-0.52	1.3E-07	-0.50	1.9E-07	-0.53	1.7E-08	-0.48	n/a
1,7-dimethyluric acid	HILIC-pos	Purines and Pyrimidines	HMDB11103	-0.58	1.3E-07	-0.59	1.2E-07	-0.61	1.5E-08	-0.59	2.2E-07	-0.56	1.1E-06	-0.61	5.2E-08	-0.61	4.1E-03	-0.48	1.0E-07	-0.45	1.0E-06	-0.51	1.3E-08	-0.51	1.1E-07	-0.49	1.6E-07	-0.46	4.2E-07	-0.48	6.5E-08
3-methylxanthine	HILIC-pos	Purines and Pyrimidines	HMDB01886	-0.76	1.2E-12	-0.77	2.4E-12	-0.79	7.6E-14	-0.82	1.8E-13	-0.79	1.5E-12	-0.77	1.4E-12	-0.69	5.3E-04	-0.61	1.9E-11	-0.60	1.1E-10	-0.66	7.7E-13	-0.65	1.7E-11	-0.63	5.6E-11	-0.60	1.8E-10	-0.62	8.8E-12
7-methylxanthine	HILIC-pos	Purines and Pyrimidines	HMDB01991	-0.71	1.4E-11	-0.72	2.7E-11	-0.73	1.5E-12	-0.80	2.9E-13	-0.76	2.8E-12	-0.71	2.7E-11	-0.63	7.4E-04	-0.57	9.8E-10	-0.56	3.5E-09	-0.60	7.3E-11	-0.58	3.2E-09	-0.56	5.8E-09	-0.54	1.5E-08	-0.57	6.2E-10
ADP	HILIC-neg	Purines and Pyrimidines	HMDB01341	0.35	1.6E-03	0.37	1.2E-03	0.35	1.5E-03	0.35	2.6E-03	0.35	2.4E-03	0.33	4.0E-03	0.34	1.2E-01	0.28	3.6E-03	0.24	1.3E-02	0.28	3.2E-03	0.24	1.7E-02	0.25	1.0E-02	0.26	7.6E-03	0.29	n/a
AMP	HILIC-neg	Purines and Pyrimidines	HMDB00045	0.45	4.2E-05	0.47	2.7E-05	0.45	3.9E-05	0.45	8.0E-05	0.46	5.3E-05	0.44	9.3E-05	0.42	4.2E-02	0.48	3.4E-07	0.45	2.2E-06	0.48	2.5E-07	0.46	3.7E-06	0.46	2.4E-06	0.46	1.3E-06	0.48	1.8E-07
CMP	HILIC-neg	Purines and Pyrimidines	HMDB00095	0.47	3.6E-05	0.50	1.6E-05	0.46	4.8E-05	0.47	7.1E-05	0.48	5.0E-05	0.48	4.4E-05	0.44	5.2E-02	0.38	3.2E-06	0.39	2.5E-06	0.37	6.3E-06	0.36	3.6E-05	0.37	1.1E-05	0.36	1.6E-05	0.38	n/a
GDP	HILIC-neg	Purines and Pyrimidines	HMDB01201	0.29	1.0E-02	0.30	8.2E-03	0.29	9.6E-03	0.29	1.5E-02	0.29	1.4E-02	0.27	1.8E-02	0.32	1.4E-01	0.21	3.1E-02	0.17	8.6E-02	0.21	2.9E-02	0.17	1.0E-01	0.18	6.6E-02	0.20	4.3E-02	0.22	n/a
GMP	HILIC-neg	Purines and Pyrimidines	HMDB01397	0.36	9.8E-04	0.38	8.5E-04	0.36	1.0E-03	0.36	1.8E-03	0.37	1.2E-03	0.36	1.8E-03	0.39	7.0E-02	0.41	1.2E-05	0.37	9.4E-05	0.41	1.2E-05	0.39	9.3E-05	0.40	4.0E-05	0.39	4.2E-05	0.42	n/a
hypoxanthine	HILIC-neg	Purines and Pyrimidines	HMDB00157	0.38	4.6E-04	0.36	1.0E-03	0.39	3.2E-04	0.39	4.7E-04	0.40	3.9E-04	0.42	1.5E-04	0.52	5.6E-03	0.34	1.9E-04	0.35	2.3E-04	0.34	2.4E-04	0.32	1.3E-03	0.30	1.9E-03	0.35	1.8E-04	0.33	2.4E-04
IMP	HILIC-neg	Purines and Pyrimidines	HMDB00175	0.30	3.6E-03	0.30	4.5E-03	0.30	3.5E-03	0.29	6.6E-03	0.30	6.0E-03	0.28	7.4E-03	0.33	9.9E-02	0.22	2.0E-02	0.17	8.1E-02	0.22	2.1E-02	0.18	8.3E-02	0.22	3.0E-02	0.23	1.9E-02	0.24	n/a
inosine	HILIC-neg	Purines and Pyrimidines	HMDB00195	0.39	1.3E-04	0.40	1.1E-04	0.39	1.4E-04	0.39	2.5E-04	0.41	9.6E-05	0.41	8.8E-05	0.39	2.6E-02	0.32	9.3E-04	0.34	6.9E-04	0.32	9.5E-04	0.31	2.8E-03	0.30	3.5E-03	0.29	3.0E-03	0.31	1.3E-03
N4-acetylcytidine	HILIC-pos	Purines and Pyrimidines	HMDB05923	-0.40	5.9E-05	-0.35	5.9E-04	-0.42	2.4E-05	-0.44	1.8E-05	-0.42	5.3E-05	-0.46	5.6E-06	-0.20	3.4E-01	-0.38	1.7E-05	-0.30	9.3E-04	-0.44	7.7E-07	-0.41	1.0E-05	-0.37	5.1E-05	-0.40	1.3E-05	-0.39	n/a
UDP	HILIC-neg	Purines and Pyrimidines	HMDB00295	0.37	7.2E-04	0.40	2.6E-04	0.37	6.7E-04	0.35	2.0E-03	0.36	1.6E-03	0.34	2.3E-03	0.37	5.1E-02	0.22	2.1E-02	0.22	2.1E-02	0.22	2.4E-02	0.16	1.0E-01	0.18	7.4E-02	0.20	4.0E-02	0.22	n/a
UMP	HILIC-neg	Purines and Pyrimidines	HMDB00288	0.45	2.0E-05	0.47	1.1E-05	0.44	2.6E-05	0.48	1.4E-05	0.49	7.2E-06	0.42	8.8E-05	0.44	2.8E-02	0.37	4.2E-05	0.35	1.3E-04	0.36	6.6E-05	0.34	3.6E-04	0.36	1.2E-04	0.38	4.8E-05	0.37	3.3E-05
alpha-glycerophosphocholine	HILIC-pos	Quaternary Amines	HMDB00086	0.30	5.2E-03	0.36	1.0E-03	0.31	4.3E-03	0.31	6.6E-03	0.32	5.5E-03	0.28	1.2E-02	0.23	3.2E-01	0.24	1.1E-02	0.25	9.2E-03	0.25	8.6E-03	0.21	3.7E-02	0.22	3.0E-02	0.23	1.9E-02	0.24	n/a
betaine	HILIC-pos	Quaternary Amines	HMDB00043	0.38	2.0E-04	0.38	2.4E-04	0.39	1.4E-04	0.32	2.1E-03	0.33	1.9E-03	0.38	2.2E-04	0.34	4.6E-02	0.38	7.0E-06	0.35	4.7E-05	0.39	3.3E-06	0.40	7.0E-06	0.40	5.4E-06	0.37	1.8E-05	0.37	6.5E-06

Metabolite name	Method	Category	HMDB ID	WHI-OS														WHI-HT											
				Model 1		Model 2		Model 3		Model 4		Model 5		Model 6		Model 7		Model 1		Model 2		Model 3		Model 4		Model 5		Model 6		Model 7	
				Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR
kynurenic acid	HILIC-pos	Indoles and Indole derivatives	HMDB00715	-0.44	2.4E-05	-0.41	1.3E-04	-0.44	2.6E-05	-0.37	6.2E-04	-0.40	1.7E-04	-0.45	2.3E-05	-0.45	9.8E-03	-0.28	2.3E-03	-0.27	3.6E-03	-0.29	1.6E-03	-0.20	4.1E-02	-0.25	1.0E-02	-0.29	1.8E-03	-0.28	2.0E-03
1-methylnicotinamide	HILIC-pos	Pyridines and derivatives	HMDB00699	-0.44	1.8E-05	-0.43	3.9E-05	-0.43	3.1E-05	-0.40	2.0E-04	-0.41	1.4E-04	-0.46	1.5E-05	-0.34	5.3E-02	-0.25	7.4E-03	-0.27	5.3E-03	-0.24	1.1E-02	-0.19	6.0E-02	-0.25	1.2E-02	-0.25	9.4E-03	-0.26	n/a
4-pyridoxate	HILIC-neg	Pyridines and derivatives	HMDB00017	-0.35	6.4E-04	-0.35	8.3E-04	-0.33	1.4E-03	-0.35	8.5E-04	-0.36	6.5E-04	-0.38	2.8E-04	-0.31	1.6E-01	-0.32	5.8E-04	-0.31	9.2E-04	-0.28	2.4E-03	-0.22	2.2E-02	-0.26	7.8E-03	-0.33	4.0E-04	-0.32	n/a
N1-methyl-2-pyridone-5-carboxamide	HILIC-pos	Pyridines and derivatives	HMDB04193	-0.39	2.6E-04	-0.37	7.4E-04	-0.37	4.7E-04	-0.38	5.8E-04	-0.41	2.3E-04	-0.42	1.0E-04	-0.35	9.1E-02	-0.31	1.0E-03	-0.28	3.6E-03	-0.28	2.6E-03	-0.21	3.8E-02	-0.29	3.8E-03	-0.32	7.2E-04	-0.31	n/a
adipate	HILIC-neg	Organic acids and derivatives	HMDB00448	-0.32	1.9E-03	-0.32	2.0E-03	-0.32	1.6E-03	-0.28	9.9E-03	-0.27	1.1E-02	-0.30	5.3E-03	-0.27	1.3E-01	-0.32	1.2E-03	-0.33	1.1E-03	-0.33	7.3E-04	-0.34	1.4E-03	-0.33	1.8E-03	-0.34	7.9E-04	-0.32	n/a
methylmalonate	HILIC-neg	Organic acids and derivatives	HMDB00202	-0.48	3.9E-06	-0.46	1.8E-05	-0.49	2.8E-06	-0.42	1.2E-04	-0.40	2.1E-04	-0.52	1.3E-06	-0.37	5.1E-02	-0.45	1.1E-06	-0.48	6.6E-07	-0.47	3.7E-07	-0.48	1.1E-06	-0.44	5.4E-06	-0.47	7.7E-07	-0.43	n/a
2-phosphoglycerate	HILIC-neg	Organic acids and derivatives	HMDB00362	0.25	1.6E-02	0.27	1.2E-02	0.25	1.7E-02	0.26	1.6E-02	0.26	1.8E-02	0.23	2.9E-02	0.43	2.7E-02	0.39	8.0E-05	0.35	5.2E-04	0.38	1.1E-04	0.37	4.6E-04	0.40	9.5E-05	0.39	1.4E-04	0.40	4.0E-05
hexose monophosphate	HILIC-neg	Carbohydrates and conjugates	HMDB00124	0.32	4.5E-03	0.34	2.9E-03	0.32	4.2E-03	0.34	4.1E-03	0.34	3.6E-03	0.31	7.6E-03	0.29	1.8E-01	0.33	4.3E-04	0.30	2.0E-03	0.33	4.3E-04	0.30	2.8E-03	0.31	1.2E-03	0.33	6.6E-04	0.33	n/a
lactose	HILIC-neg	Carbohydrates and conjugates	HMDB00186	0.23	4.9E-02	0.24	4.4E-02	0.23	4.2E-02	0.22	6.5E-02	0.23	6.3E-02	0.22	6.4E-02	0.24	2.9E-01	0.32	6.3E-04	0.32	7.2E-04	0.32	7.2E-04	0.30	n/a	0.30	n/a	0.29	n/a	0.32	n/a
pentose monophosphate	HILIC-neg	Carbohydrates and conjugates	HMDB01548	0.28	1.0E-02	0.30	7.9E-03	0.29	8.0E-03	0.28	1.7E-02	0.29	1.2E-02	0.27	1.9E-02	0.25	2.4E-01	0.25	6.5E-03	0.23	1.5E-02	0.26	5.5E-03	0.25	8.9E-03	0.25	8.3E-03	0.24	1.2E-02	0.25	n/a
acetaminophen	HILIC-pos	Benzene, Benzenoids, and derivatives	HMDB01859	-0.35	4.3E-03	-0.41	1.0E-03	-0.35	4.8E-03	-0.38	2.7E-03	-0.37	3.4E-03	-0.33	8.9E-03	-0.43	8.4E-02	-0.29	1.4E-04	-0.30	1.3E-04	-0.28	2.7E-04	-0.31	1.7E-04	-0.31	1.0E-04	-0.31	8.5E-05	-0.28	n/a
allantoin	HILIC-pos	Others	HMDB00462	-0.29	1.8E-03	-0.30	1.6E-03	-0.28	3.0E-03	-0.28	3.5E-03	-0.31	1.5E-03	-0.31	1.2E-03	-0.30	9.9E-02	-0.22	2.7E-02	-0.21	3.8E-02	-0.21	3.5E-02	-0.18	9.4E-02	-0.22	3.3E-02	-0.25	1.6E-02	-0.21	n/a
caffeine	HILIC-pos	Others	HMDB01847	-0.53	1.9E-06	-0.52	7.2E-06	-0.57	2.5E-07	-0.53	5.2E-06	-0.50	1.9E-05	-0.56	1.1E-06	-0.57	7.4E-03	-0.32	1.7E-04	-0.26	2.4E-03	-0.34	9.1E-05	-0.36	7.5E-05	-0.36	6.9E-05	-0.32	3.4E-04	-0.34	7.6E-05
carboxyibuprofen	C18-neg	Others	n/a	-0.29	8.9E-03	-0.33	3.2E-03	-0.30	5.5E-03	-0.32	5.9E-03	-0.30	9.0E-03	-0.29	1.2E-02	-0.17	4.3E-01	-0.22	1.5E-02	-0.25	6.9E-03	-0.25	5.1E-03	-0.16	9.0E-02	-0.15	1.2E-01	-0.22	1.7E-02	-0.21	n/a
cortisol	HILIC-pos	Others	HMDB00063	-0.51	3.6E-07	-0.51	6.7E-07	-0.52	3.1E-07	-0.52	1.2E-06	-0.52	8.7E-07	-0.50	1.3E-06	-0.42	1.5E-02	-0.24	1.4E-02	-0.26	8.7E-03	-0.24	1.4E-02	-0.25	1.8E-02	-0.27	8.8E-03	-0.19	6.2E-02	-0.25	8.5E-03
hydroxyectoine	HILIC-pos	Others	n/a	-0.41	9.5E-05	-0.45	2.3E-05	-0.40	1.4E-04	-0.40	2.1E-04	-0.41	1.4E-04	-0.43	6.3E-05	-0.30	1.7E-01	-0.26	4.9E-03	-0.35	2.3E-04	-0.28	2.9E-03	-0.27	5.3E-03	-0.24	1.3E-02	-0.26	5.8E-03	-0.25	n/a
piperine	HILIC-pos	Others	HMDB29377	0.58	6.8E-09	0.57	2.0E-08	0.56	1.3E-08	0.67	6.2E-11	0.66	2.1E-10	0.57	2.1E-08	0.85	1.7E-06	0.48	6.3E-08	0.47	2.8E-07	0.47	1.3E-07	0.51	8.2E-08	0.50	1.0E-07	0.48	1.7E-07	0.48	4.2E-08
pseudouridine	HILIC-pos	Others	HMDB00767	-0.43	1.1E-05	-0.41	5.0E-05	-0.44	6.8E-06	-0.47	4.1E-06	-0.47	3.6E-06	-0.47	2.7E-06	-0.38	3.9E-02	-0.32	5.2E-04	-0.28	3.6E-03	-0.35	1.3E-04	-0.34	4.5E-04	-0.32	8.4E-04	-0.34	3.7E-04	-0.31	5.2E-04
thiamine	HILIC-pos	Others	HMDB00235	-0.35	5.8E-04	-0.38	3.5E-04	-0.33	1.4E-03	-0.36	7.5E-04	-0.36	6.1E-04	-0.38	2.8E-04	-0.41	3.7E-02	-0.42	4.2E-06	-0.42	9.7E-06	-0.39	1.8E-05	-0.36	1.9E-04	-0.40	3.7E-05	-0.45	2.2E-06	-0.42	2.9E-06
trigonelline	HILIC-pos	Others	HMDB00875	-0.58	1.8E-08	-0.59	2.5E-08	-0.58	1.9E-08	-0.54	5.3E-07	-0.53	7.8E-07	-0.59	1.6E-08	-0.60	1.6E-03	-0.50	5.9E-08	-0.53	1.8E-08	-0.49	8.9E-08	-0.45	4.9E-06	-0.47	9.9E-07	-0.50	9.1E-08	-0.50	3.4E-08

Model 1 (fully adjusted model): adjusted for coronary heart disease case-control status, matching factors (age, hysterectomy status, and enrollment window), hormone therapy use status, body mass index, smoking status, alcohol consumption, education, family income, physical activity, baseline health conditions (diabetes, hypertension, and depression), and medication use (aspirin, lipid-lowing, antihyperglycemic, antihypertensive, and antidepressants).

Model 2 (lipid-adjusted model): Model 1 + plasma levels of total cholesterol and high-density lipoprotein cholesterol.

Model 3 (diet quality-adjusted model): Model 1 + Healthy Eating Index-2005.

Model 4 (macronutrient-adjusted model): Model 1 + dietary intake of proteins, total carbohydrates, and total fat.

Model 5 (calorie-adjusted model): Model 1 + total calorie intake.

Model 6 (psychological factor-adjusted model): Model 1 + 8 psychological indicators, including emotional well-being, hostility, general health, optimism, social support, social functioning, social strain, and sleep disturbance.

Model 7 (glucose-adjusted model): Model 1 + blood glucose levels.

Supplementary Table S4. Regression coefficients of metabolome-wide association analyses in WHI and MESA.

Metabolite name	Method	Category	HMDB ID	WHI-OS				WHI-HT				MESA			
				Model 1		Model 2		Model 1		Model 2		Model 1		Model 2	
				Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	Raw-p	Beta	Raw-p
C30:0 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07011*	-0.467	8.7E-07	-0.320	2.9E-04	-0.591	4.8E-11	-0.318	8.6E-05				
C32:0 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07098*	-0.603	3.5E-09	-0.402	1.5E-05	-0.587	7.8E-12	-0.306	4.1E-05	-0.234	0.677	-0.210	0.703
C32:1 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07099*	-0.872	7.8E-18	-0.653	1.5E-13	-0.864	1.0E-22	-0.548	5.5E-14	-0.562	0.302	-0.483	0.357
C32:2 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07128*	-0.756	3.4E-15	-0.541	2.8E-11	-0.886	5.8E-22	-0.557	4.6E-13				
C34:0 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07100*	-0.593	1.4E-07	-0.427	5.3E-05	-0.427	1.6E-07	-0.238	2.2E-03	-0.618	0.290	-0.507	0.376
C34:1 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07102*	-0.655	3.2E-11	-0.422	5.6E-07	-0.663	3.6E-14	-0.330	2.8E-06	-0.365	0.493	-0.280	0.578
C34:2 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07103*	-0.832	1.0E-16	-0.584	2.4E-12	-0.856	1.3E-22	-0.499	1.3E-13	-0.496	0.342	-0.383	0.436
C34:3 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07132*	-0.948	3.9E-21	-0.710	1.9E-17	-0.975	2.2E-27	-0.618	2.5E-18	-0.783	0.127	-0.572	0.224
C36:1 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07216*	-0.504	1.9E-07	-0.283	8.8E-04	-0.556	7.4E-10	-0.238	1.6E-03	-0.435	0.399	-0.378	0.432
C36:2 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07218*	-0.845	2.8E-17	-0.583	2.5E-12	-0.821	6.3E-20	-0.485	2.0E-11	-0.435	0.386	-0.364	0.437
C36:3 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07219*	-0.788	8.9E-15	-0.522	1.1E-09	-0.783	4.7E-18	-0.451	1.2E-09	-0.617	0.198	-0.493	0.266
C36:4 DAG-A	C8-pos	Glycerolipids - Diacylglycerols	HMDB07248*	-0.590	4.2E-09	-0.361	5.3E-05	-0.611	2.7E-11	-0.313	1.2E-04				
C36:4 DAG-B	C8-pos	Glycerolipids - Diacylglycerols	HMDB07248*	-0.331	1.1E-03	-0.138	1.5E-01	-0.429	1.2E-06	-0.123	n/a				
C38:3 DAG	C8-pos	Glycerolipids - Diacylglycerols	HMDB07168*	-0.717	2.1E-13	-0.500	1.2E-08	-0.683	6.3E-14	-0.373	1.3E-06				
C42:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42061*	-0.481	5.3E-07	-0.342	2.6E-04	-0.537	4.5E-08	-0.337	3.2E-04	-0.337	0.543	-0.342	0.535
C43:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42062*	-0.305	6.2E-04	-0.204	2.2E-02	-0.489	1.4E-06	-0.317	1.3E-03	-0.009	0.988	0.064	0.916
C43:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42098*	-0.589	1.6E-09	-0.446	2.6E-06	-0.485	1.2E-07	-0.292	7.8E-04	-0.554	0.352	-0.542	0.356
C44:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42063*	-0.510	2.5E-07	-0.361	1.6E-04	-0.544	9.1E-09	-0.340	1.5E-04	-0.601	0.285	-0.627	0.264
C44:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42301*	-0.734	1.2E-12	-0.559	1.1E-08	-0.650	1.2E-12	-0.436	2.8E-07	-0.615	0.266	-0.646	0.239
C44:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB47770*	-0.716	2.7E-12	-0.532	3.5E-08	-0.636	6.3E-12	-0.410	1.4E-06	-0.476	0.400	-0.452	0.413
C45:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42093*	-0.213	2.9E-02	-0.159	1.1E-01	-0.398	5.5E-05	-0.252	n/a	-0.181	0.757	-0.057	0.923
C45:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42099*	-0.764	1.2E-13	-0.605	8.2E-10	-0.630	8.2E-12	-0.434	6.0E-07	-0.405	0.484	-0.430	0.458
C45:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB43170*	-0.815	7.2E-15	-0.638	1.6E-10	-0.626	4.9E-12	-0.422	4.9E-07	-0.269	0.643	-0.303	0.599
C45:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	n/a	-0.496	1.1E-07	-0.324	2.9E-04	-0.496	1.1E-07	-0.297	6.3E-04	-0.469	0.409	-0.537	0.338
C46:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10411*	-0.463	4.6E-06	-0.337	7.1E-04	-0.524	1.0E-08	-0.340	1.1E-04	-0.671	0.248	-0.694	0.234
C46:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10412*	-0.759	2.0E-13	-0.584	2.0E-09	-0.689	1.5E-14	-0.471	1.1E-08	-0.718	0.202	-0.742	0.186
C46:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10419*	-0.858	1.4E-16	-0.659	5.5E-12	-0.768	2.2E-17	-0.525	9.6E-11	-0.538	0.335	-0.518	0.343
C46:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42541*	-0.816	3.4E-15	-0.602	2.1E-10	-0.729	1.2E-15	-0.476	3.4E-09	-0.702	0.195	-0.677	0.196
C46:4 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42781*	-0.694	6.9E-12	-0.491	1.8E-07	-0.596	1.9E-10	-0.366	1.8E-05	-0.807	0.142	-0.799	0.134
C47:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42100*	-0.751	2.0E-13	-0.605	8.0E-10	-0.747	4.5E-16	-0.548	2.7E-10	-0.309	0.596	-0.241	0.677
C47:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB48435*	-0.920	6.4E-19	-0.735	4.2E-14	-0.847	1.7E-20	-0.622	6.8E-14	-0.202	0.731	-0.196	0.737
C48:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05356*	-0.401	9.2E-05	-0.273	6.8E-03	-0.431	9.4E-07	-0.246	3.4E-03	0.138	0.815	0.167	0.777
C48:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05359*	-0.742	2.9E-13	-0.578	1.2E-09	-0.750	2.4E-17	-0.509	2.7E-10	-0.571	0.328	-0.519	0.367
C48:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05376*	-0.911	1.7E-18	-0.707	1.2E-13	-0.857	2.7E-22	-0.607	7.5E-15	-0.533	0.349	-0.500	0.367
C48:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05432*	-1.025	7.5E-23	-0.792	1.1E-17	-0.917	1.2E-24	-0.646	3.9E-17	-0.659	0.222	-0.638	0.222
C48:4 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42631*	-0.898	6.2E-18	-0.665	1.0E-12	-0.806	1.1E-18	-0.547	8.0E-12	-0.773	0.141	-0.741	0.143
C48:5 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42841*	-0.720	2.1E-12	-0.505	1.1E-07	-0.631	1.3E-11	-0.408	1.5E-06	-0.788	0.137	-0.791	0.124
C49:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB11705*	-0.632	2.8E-10	-0.508	2.1E-07	-0.747	1.1E-15	-0.552	5.4E-10	-0.016	0.979	0.067	0.908
C49:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB11706*	-0.976	1.1E-21	-0.819	3.1E-17	-0.986	2.8E-27	-0.767	9.7E-20	-0.008	0.989	0.110	0.842
C49:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42103*	**-1.098**	2.3E-27	-0.879	4.4E-22	**-1.061**	1.8E-31	-0.805	2.0E-24	**-0.221**	0.681	-0.179	0.733
C50:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05357*	-0.393	1.2E-04	-0.220	2.5E-02	-0.407	5.6E-06	-0.176	3.1E-02	-0.271	0.634	-0.272	0.629
C50:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB44109*	-0.609	1.1E-09	-0.432	2.6E-06	-0.621	5.2E-13	-0.350	3.7E-06	-0.486	0.392	-0.420	0.446
C50:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05377*	-0.851	6.8E-17	-0.670	4.4E-13	-0.844	8.5E-23	-0.560	3.5E-14	-0.630	0.256	-0.526	0.328
C50:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05433*	**-1.103**	1.1E-26	-0.858	5.4E-22	**-1.046**	1.1E-32	-0.745	7.7E-25	**-0.820**	0.119	-0.747	0.139
C50:4 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05435*	-1.012	1.7E-22	-0.743	4.2E-17	-0.945	5.0E-26	-0.651	2.5E-18	-0.734	0.144	-0.695	0.145
C50:5 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10471*	-0.851	3.3E-16	-0.597	8.3E-11	-0.781	6.8E-18	-0.521	4.6E-11	-0.675	0.192	-0.647	0.188
C50:6 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10497*	-0.639	7.8E-10	-0.420	1.6E-05	-0.529	9.4E-09	-0.321	1.5E-04	-0.652	0.227	-0.676	0.198
C51:0 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB31106*	-0.409	3.4E-05	-0.242	1.1E-02	-0.497	1.9E-07	-0.247	4.2E-03	0.041	0.942	-0.004	0.994
C51:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB42104*	-0.580	1.7E-08	-0.397	4.9E-05	-0.598	2.4E-11	-0.362	8.8E-06	-0.048	0.933	-0.015	0.979
C51:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB49721*	-0.859	8.8E-17	-0.674	2.9E-12	-0.829	3.1E-20	-0.601	3.2E-13	-0.114	0.840	-0.018	0.975
C51:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	n/a	**-0.969**	6.9E-23	-0.778	1.2E-18	**-1.020**	1.8E-29	-0.730	1.9E-20	**-0.170**	0.738	0.035	0.942
C52:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05367*	-0.464	3.8E-06	-0.237	9.0E-03	-0.456	2.8E-07	-0.176	2.0E-02	-0.370	0.491	-0.389	0.444
C52:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05369*	-0.717	1.7E-13	-0.480	6.2E-09	-0.778	6.3E-18	-0.460	1.1E-09	-0.578	0.271	-0.471	0.344

Metabolite name	Method	Category	HMDB ID	WHI-OS				WHI-HT				MESA			
				Model 1		Model 2		Model 1		Model 2		Model 1		Model 2	
				Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	Raw-p	Beta	Raw-p
C52:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05384*	-0.645	1.5E-11	-0.398	1.3E-06	-0.810	5.3E-18	-0.486	7.7E-10	-0.779	0.128	-0.629	0.191
C52:4 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05363*	-0.725	3.1E-13	-0.510	1.1E-08	-0.743	1.1E-15	-0.449	4.1E-08	-0.709	0.146	-0.530	0.252
C52:6 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05436*	-0.725	2.4E-12	-0.471	3.3E-07	-0.663	3.5E-13	-0.428	2.0E-07	-0.585	0.255	-0.598	0.225
C52:7 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10517*	-0.533	3.1E-07	-0.324	1.1E-03	-0.455	6.5E-07	-0.277	1.2E-03	-0.402	0.467	-0.423	0.436
C54:1 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05395*	-0.371	1.8E-04	-0.163	7.8E-02	-0.382	2.8E-05	-0.108	n/a	-0.293	0.574	-0.273	0.583
C54:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05403*	-0.562	1.1E-08	-0.311	2.4E-04	-0.531	4.1E-09	-0.218	3.2E-03	-0.246	0.631	-0.249	0.595
C54:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05405*	-0.720	1.1E-12	-0.476	8.3E-08	-0.695	5.2E-14	-0.406	5.3E-07	-0.111	0.828	-0.067	0.891
C54:4 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05370*	-0.603	6.0E-09	-0.432	1.4E-05	-0.529	9.1E-09	-0.323	2.7E-04	-0.360	0.483	-0.213	0.670
C54:6 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05391*	-0.411	5.9E-05	-0.243	1.6E-02	-0.398	2.9E-05	-0.224	1.6E-02	-0.425	0.434	-0.441	0.414
C54:7 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05447*	-0.363	7.1E-04	-0.152	1.5E-01	-0.230	1.1E-02	-0.074	n/a	0.053	0.923	-0.030	0.956
C54:8 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10518*	-0.326	1.9E-03	-0.144	1.7E-01	-0.239	9.7E-03	-0.100	n/a	-0.041	0.940	-0.114	0.834
C55:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB50319*	-0.657	1.2E-11	-0.439	5.6E-07	-0.651	4.1E-12	-0.375	3.2E-06	0.183	0.732	0.088	0.864
C55:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	n/a	-0.845	1.4E-16	-0.660	1.2E-11	-0.672	3.2E-13	-0.478	4.3E-08	0.587	0.275	0.541	0.309
C56:2 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05404*	-0.529	2.5E-07	-0.318	8.2E-04	-0.525	1.5E-08	-0.287	6.7E-04	0.095	0.858	0.012	0.982
C56:3 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05410*	-0.696	2.7E-12	-0.488	8.9E-08	-0.670	3.2E-13	-0.392	1.2E-06	-0.023	0.966	-0.058	0.909
C56:5 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05406*	-0.561	5.9E-08	-0.422	2.6E-05	-0.429	3.1E-06	-0.222	1.1E-02	0.232	0.679	0.226	0.688
C56:8 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05392*	0.263	1.2E-02	0.370	3.6E-04	0.335	2.4E-04	0.411	6.9E-06	0.285	0.611	0.183	0.746
C58:10 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05476*	0.579	7.6E-09	0.602	3.8E-09	0.651	2.1E-13	0.598	2.1E-11	0.204	0.715	0.073	0.896
C58:11 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB10531*	0.408	6.0E-05	0.453	1.1E-05	0.451	4.0E-07	0.413	3.9E-06	0.840	0.154	0.683	0.248
C58:8 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05413*	0.525	8.8E-09	0.486	1.8E-07	0.699	1.8E-14	0.636	7.4E-12	0.511	0.349	0.413	0.452
C58:9 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05463*	0.525	1.1E-07	0.508	4.6E-07	0.649	1.8E-13	0.583	6.8E-11	0.514	0.365	0.409	0.475
C60:12 TAG	C8-pos	Glycerolipids - Triacylglycerols	HMDB05478*	0.576	9.4E-10	0.569	3.5E-09	0.771	2.8E-18	0.710	1.7E-15	0.476	0.392	0.404	0.472
C16:1 LPC plasmalogen	C8-pos	Glycerophospholipids - Lysophosphatidylcholine plasmalogens	n/a	0.502	4.1E-07	0.543	5.5E-08	0.408	6.1E-06	0.325	3.2E-04				
C18:0 LPC plasmalogen	C8-pos	Glycerophospholipids - Lysophosphatidylcholine plasmalogens	HMDB11149*	0.398	5.9E-05	0.479	1.3E-06	0.270	3.4E-03	0.275	3.2E-03				
C14:0 LPC	HILIC-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10379	-0.882	1.8E-17	-0.753	2.9E-13	-0.784	6.3E-18	-0.707	2.2E-15	0.208	0.708	0.153	0.784
C14:0 LPC-A	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10379*	-0.819	4.8E-16	-0.687	6.5E-12	-0.856	1.7E-20	-0.790	2.0E-18	-0.060	0.918	-0.146	0.803
C14:0 LPC-B	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10379*	-0.695	1.2E-13	-0.581	4.7E-10	-0.618	1.6E-10	-0.571	3.5E-09				
C15:0 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10381	-0.628	2.1E-10	-0.515	1.9E-07	-0.853	2.2E-21	-0.822	5.9E-20				
C16:0 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10382	-0.351	1.6E-03	-0.167	1.4E-01	-0.400	6.4E-06	-0.354	n/a	0.374	0.497	0.179	0.734
C16:1 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10383	-0.829	1.3E-15	-0.734	2.2E-12	-0.962	4.5E-27	-0.959	1.4E-26	-0.339	0.550	-0.495	0.377
C18:1 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB02815	-0.225	3.4E-02	-0.156	1.6E-01	-0.320	2.4E-04	-0.403	n/a	0.366	0.525	0.193	0.733
C18:2 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10386*	-0.223	4.0E-02	-0.196	7.6E-02	-0.283	9.3E-04	-0.409	n/a	0.700	0.208	0.515	0.351
C18:3 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10387*	-0.355	6.2E-04	-0.303	4.0E-03	-0.531	6.7E-09	-0.597	1.1E-10	0.377	0.494	0.175	0.739
C20:3 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10393*	-0.424	8.3E-05	-0.332	2.3E-03	-0.493	1.1E-07	-0.508	4.6E-08				
C20:4 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10395	0.421	5.5E-05	0.480	4.3E-06	0.205	2.2E-02	0.112	2.1E-01	0.192	0.727	0.044	0.936
C22:6 LPC	C8-pos	Glycerophospholipids - Lysophosphatidylcholines	HMDB10404*	0.328	8.2E-04	0.358	3.2E-04	0.473	1.9E-07	0.413	6.9E-06	1.040	0.059	0.895	0.102
C16:0 LPE	C8-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11503	-0.491	1.1E-06	-0.413	5.5E-05	-0.513	3.3E-08	-0.496	1.1E-07	0.243	0.664	0.088	0.874
C18:0 LPE	C8-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11130*	-0.317	3.0E-03	-0.186	8.6E-02	-0.402	1.9E-05	-0.373	n/a	0.234	0.676	0.038	0.944
C18:1 LPE	C8-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11506	-0.432	3.3E-05	-0.360	6.7E-04	-0.530	3.2E-08	-0.548	1.7E-08	-0.186	0.740	-0.291	0.606
C18:2 LPE	C8-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11507*	-0.787	3.5E-14	-0.716	1.0E-11	-0.894	8.7E-23	-0.901	8.1E-23	0.012	0.983	-0.096	0.859
C20:1 LPE	C8-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11512*	-0.481	4.1E-07	-0.429	8.5E-06	-0.488	2.2E-07	-0.546	9.7E-09				
C20:4 LPE	HILIC-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11517	-0.380	4.8E-04	-0.300	6.2E-03	-0.401	1.3E-05	-0.446	1.7E-06	-0.197	0.735	-0.370	0.525
C20:4 LPE-A	C8-pos	Glycerophospholipids - Lysophosphatidylethanolamines	HMDB11517	-0.264	1.7E-02	-0.188	9.6E-02	-0.475	2.8E-07	-0.522	n/a	-0.320	0.586	-0.472	0.422
C32:1 PC plasmalogen-A	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB13404*	-0.493	5.5E-07	-0.521	5.0E-08	-0.500	5.3E-08	-0.628	2.1E-12				
C32:1 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB13404*	0.330	1.2E-03	0.316	9.2E-04	0.403	1.3E-05	0.237	5.4E-03				
C34:1 PC plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11208*	-0.285	8.1E-03	-0.273	7.0E-03	-0.223	1.6E-02	-0.353	5.0E-05	-0.017	0.978	-0.572	0.294
C34:2 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11210*	0.225	2.6E-02	0.170	4.8E-02	0.373	2.6E-05	0.139	6.3E-02				
C34:3 PC plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11211*	0.314	1.9E-03	0.284	1.3E-03	0.487	1.3E-07	0.273	8.3E-04	0.501	0.411	0.015	0.978
C34:4 PC plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11212*	-0.373	5.4E-05	-0.464	2.7E-07	-0.388	1.1E-04	-0.499	9.5E-07	0.074	0.892	-0.143	0.791
C36:2 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11243*	0.502	1.0E-06	0.412	3.6E-06	0.586	7.7E-12	0.356	1.3E-06				
C36:3 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11244*	0.350	7.0E-04	0.308	8.0E-04	0.466	2.5E-07	0.254	1.4E-03				
C36:4 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11310*	0.271	1.2E-02	0.339	8.7E-04	0.334	4.9E-04	0.223	1.0E-02				
C36:5 PC plasmalogen-A	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11221*	0.243	1.7E-02	0.282	5.0E-03	0.240	1.1E-02	0.136	1.2E-01	0.934	0.120	0.609	0.297
C36:5 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11220*	0.583	1.6E-08	0.608	5.9E-10	0.690	2.0E-13	0.527	6.3E-10	0.062	0.920	-0.395	0.493

Metabolite name	Method	Category	HMDB ID	WHI-OS				WHI-HT				MESA			
				Model 1		Model 2		Model 1		Model 2		Model 1		Model 2	
				Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	Raw-p	Beta	Raw-p
C38:4 PC plasmalogen-A	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11252*	-0.240	3.1E-02	-0.134	2.3E-01	-0.254	7.0E-03	-0.289	n/a				
C38:4 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11252*	0.341	1.7E-03	0.414	5.5E-05	0.382	4.2E-05	0.298	5.6E-04				
C38:6 PC plasmalogen-A	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11319*	0.578	3.2E-08	0.643	7.3E-10	0.687	3.8E-14	0.615	8.5E-13				
C38:6 PC plasmalogen-B	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11319*	0.454	1.3E-05	0.469	1.3E-06	0.516	4.5E-08	0.334	7.2E-05				
C38:7 PC plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11229*	0.621	1.9E-10	0.633	3.9E-11	0.910	1.4E-23	0.775	5.3E-20	0.393	0.474	0.011	0.983
C40:11 PC plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	n/a	-0.776	5.8E-14	-0.738	2.7E-12	-0.823	2.3E-19	-0.833	1.6E-19				
C40:7 PC plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylcholine plasmalogens	HMDB11294*	0.494	1.5E-06	0.527	6.8E-08	0.659	2.6E-12	0.529	8.8E-10	0.140	0.813	-0.383	0.465
C28:0 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07866*	-0.700	5.5E-14	-0.641	1.3E-11	-0.598	7.4E-10	-0.572	2.1E-09				
C30:0 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07869*	-0.791	1.3E-15	-0.695	2.2E-12	-0.678	1.1E-14	-0.667	1.9E-15	-0.256	0.688	-0.427	0.506
C30:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07870*	-0.983	4.2E-24	-0.917	6.7E-21	-0.912	1.1E-24	-0.890	1.6E-24	-0.645	0.296	-0.816	0.188
C31:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07936*	**-1.064**	1.2E-28	-1.009	1.4E-25	**-1.087**	2.1E-33	-1.065	1.4E-33				
C32:0 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07871*	-0.462	5.3E-06	-0.329	7.7E-04	-0.375	3.3E-05	-0.402	9.5E-07	-0.051	0.936	-0.531	0.363
C32:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07873*	-1.002	1.1E-23	-0.921	3.6E-20	-0.916	2.2E-27	-0.876	8.4E-27	-0.542	0.351	-0.806	0.160
C32:2 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07874*	**-1.137**	1.2E-28	-1.011	1.9E-24	**-1.050**	2.6E-35	-1.025	8.1E-40	**-0.273**	0.635	-0.538	0.340
C34:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07972*	-0.691	8.2E-12	-0.556	1.4E-08	-0.526	4.3E-09	-0.496	1.8E-09	-0.172	0.769	-0.566	0.302
C34:2 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07973*	-0.857	1.1E-17	-0.716	2.7E-14	-0.734	4.3E-16	-0.728	8.1E-20	-0.084	0.875	-0.623	0.164
C34:3 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08006*	**-1.116**	2.3E-27	-0.969	1.0E-23	**-1.004**	1.2E-32	-1.012	3.2E-40	**-0.734**	0.185	-1.152	0.025
C34:4 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07883*	-0.657	1.5E-11	-0.554	6.2E-09	-0.818	4.0E-20	-0.843	5.3E-23	-0.418	0.493	-0.641	0.291
C34:5 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07885*	-0.411	2.2E-05	-0.323	8.0E-04	-0.444	1.2E-06	-0.480	5.0E-08				
C36:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08038*	-0.431	5.5E-05	-0.290	5.4E-03	-0.327	5.7E-04	-0.302	6.0E-04	-0.004	0.995	-0.375	0.501
C36:2 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08039*	-0.666	1.1E-10	-0.508	1.1E-07	-0.557	4.5E-09	-0.559	4.3E-11	-0.193	0.739	-0.737	0.142
C36:3 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08105*	-0.844	9.4E-16	-0.696	2.4E-12	-0.821	3.4E-20	-0.821	1.1E-24	-0.644	0.246	-1.045	0.042
C36:4 PC-A	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07983*	-0.754	6.6E-12	-0.656	1.0E-09	-0.267	2.3E-03	-0.321	9.9E-05	-0.326	0.544	-0.719	0.151
C36:5 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07890*	-0.282	7.8E-03	-0.173	1.0E-01	-0.351	4.0E-05	-0.393	n/a				
C37:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB07952*	-0.395	1.4E-04	-0.267	7.9E-03	-0.262	5.4E-03	-0.284	1.1E-03				
C38:2 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08270*	-0.394	1.9E-04	-0.235	2.1E-02	-0.238	1.2E-02	-0.196	2.1E-02	0.107	0.856	-0.353	0.504
C38:3 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08047*	-0.496	2.5E-06	-0.295	3.5E-03	-0.480	3.0E-07	-0.358	2.6E-05	-0.171	0.752	-0.456	0.363
C40:1 PC	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08026*	-0.209	3.6E-02	-0.133	1.9E-01	-0.212	2.7E-02	-0.278	n/a				
C40:6 PC-A	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08057*	-0.408	1.3E-04	-0.212	4.1E-02	-0.385	4.2E-05	-0.276	1.4E-03				
C40:6 PC-B	C8-pos	Glycerophospholipids - Phosphatidylcholines	HMDB08057*	0.287	3.8E-03	0.408	2.3E-05	0.584	2.5E-10	0.613	6.3E-12				
C34:2 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB08952*	0.301	4.7E-03	0.337	1.2E-03	0.451	3.4E-06	0.319	5.2E-04	0.982	0.094	0.578	0.294
C34:3 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB11343*	0.233	3.2E-02	0.254	2.0E-02	0.332	5.1E-04	0.219	1.8E-02	0.456	0.437	0.142	0.803
C36:2 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB09082*	0.307	3.6E-03	0.343	8.8E-04	0.443	4.0E-06	0.332	3.0E-04	0.542	0.368	0.180	0.756
C36:5 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB11410*	0.752	3.0E-12	0.796	5.4E-13	0.824	1.0E-19	0.736	1.0E-16	0.620	0.298	0.308	0.596
C38:5 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB11386*	0.638	1.4E-09	0.678	1.5E-10	0.746	9.4E-16	0.642	6.0E-13	0.501	0.414	0.153	0.798
C38:6 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB11387*	0.702	1.7E-11	0.740	1.9E-12	0.766	1.6E-16	0.623	6.7E-13	0.499	0.402	0.074	0.894
C38:7 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB11420*	0.656	2.2E-11	0.701	1.0E-12	0.986	1.8E-27	0.889	2.7E-25	0.973	0.067	0.607	0.228
C40:7 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	HMDB11394*	**0.766**	2.4E-14	0.797	1.4E-15	**1.057**	6.4E-30	0.945	3.3E-27	**0.640**	0.244	0.240	0.642
C42:11 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	n/a	-0.612	9.8E-09	-0.630	7.2E-09	-0.657	2.7E-13	-0.633	6.2E-12				
C44:13 PE plasmalogen	C8-pos	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	n/a	0.749	1.9E-12	0.729	2.5E-11	0.482	1.6E-08	0.437	5.6E-07	-0.072	0.897	-0.400	0.452
C34:2 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB08928*	-0.744	1.6E-13	-0.658	9.8E-11	-0.608	6.5E-12	-0.434	3.8E-07	-0.897	0.109	-0.850	0.129
C36:0 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB08991*	-0.625	2.2E-09	-0.513	4.6E-07	-0.511	3.2E-08	-0.541	3.8E-10	1.027	0.086	0.783	0.181
C36:1 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB08993*	-0.425	1.9E-05	-0.296	2.7E-03	-0.362	9.4E-05	-0.185	3.6E-02	-0.681	0.227	-0.752	0.181
C36:2 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB08994*	-0.874	6.4E-18	-0.743	1.2E-13	-0.699	8.5E-15	-0.519	1.0E-09	-0.853	0.109	-0.925	0.082
C36:3 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB09060*	-0.828	3.5E-16	-0.741	6.3E-13	-0.662	1.8E-13	-0.557	3.6E-10	-1.123	0.050	-1.176	0.042
C38:2 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB08942*	-0.724	4.3E-12	-0.624	2.1E-10	-0.596	3.7E-11	-0.667	7.7E-16	0.659	0.217	0.252	0.605
C38:5 PE	C8-pos	Glycerophospholipids - Phosphatidylethanolamines	HMDB09069*	-0.361	4.5E-04	-0.277	7.7E-03	-0.292	1.3E-03	-0.279	2.0E-03	-0.941	0.129	-1.090	0.078
C40:6 PS	C8-pos	Glycerophospholipids - phosphatidylserine	HMDB10167*	-0.843	8.9E-17	-0.773	5.2E-14	-0.949	1.5E-25	-0.921	2.5E-24	0.241	0.672	0.147	0.798
4-cholesten-3-one	C8-pos	Sterol lipids - Cholesteryl	HMDB00921	-0.725	1.1E-15	-0.501	6.9E-10	-0.909	2.5E-20	-0.748	2.6E-18				
C14:0 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06725	-0.499	1.9E-07	-0.436	6.4E-06	-0.563	1.7E-09	-0.591	2.4E-10	0.919	0.109	0.754	0.186
C16:0 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB00885	0.603	1.3E-10	0.616	2.4E-12	0.728	3.9E-14	0.517	1.2E-08	0.248	0.652	-0.168	0.738
C16:1 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB00658*	-0.680	2.0E-12	-0.653	2.5E-11	-0.583	1.0E-10	-0.655	4.6E-13	-0.151	0.769	-0.410	0.416
C18:0 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB10368	0.210	4.4E-02	0.499	1.1E-09	0.283	2.2E-03	0.380	3.8E-07	0.671	0.254	0.237	0.613
C18:1 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB00918	0.480	2.5E-07	0.452	5.7E-08	0.611	7.3E-11	0.329	7.9E-05	0.322	0.559	-0.114	0.814

Metabolite name	Method	Category	HMDB ID	WHI-OS				WHI-HT				MESA			
				Model 1		Model 2		Model 1		Model 2		Model 1		Model 2	
				Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	Raw-p	Beta	Raw-p
C18:2 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB00610*	0.539	1.3E-08	0.456	1.8E-07	0.538	9.4E-09	0.240	3.7E-03	0.179	0.747	-0.140	0.786
C20:1 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB05193	0.234	2.5E-02	0.368	1.3E-04	0.627	4.4E-12	0.530	1.3E-10				
C20:2 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06734	0.502	1.6E-07	0.479	7.0E-08	0.794	1.8E-18	0.543	2.5E-11				
C20:3 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06736*	0.490	1.9E-06	0.484	6.9E-07	0.534	2.0E-08	0.301	6.2E-04	0.268	0.623	0.015	0.977
C20:4 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06726	**1.065**	6.9E-28	1.016	6.5E-29	**1.121**	2.1E-33	0.851	7.7E-25	**-0.121**	0.819	-0.387	0.444
C20:5 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06731	0.469	5.0E-06	0.530	7.3E-08	0.403	4.6E-06	0.235	4.0E-03	1.145	0.045	0.817	0.137
C22:4 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06729*	**0.840**	1.4E-20	0.756	2.7E-19	**1.072**	1.7E-30	0.782	2.4E-21	**0.176**	0.740	0.027	0.958
C22:5 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB10375*	0.932	4.9E-19	0.906	2.7E-19	0.936	4.5E-27	0.739	1.6E-19	0.430	0.425	0.221	0.676
C22:6 CE	C8-pos	Sterol lipids - Cholesteryl esters	HMDB06733	**0.963**	1.5E-23	0.927	5.8E-23	**1.241**	4.9E-44	1.055	4.1E-36	**0.637**	0.239	0.419	0.428
C16:0 Ceramide (d18:1)	C8-pos	Sphingolipids - Ceramides	HMDB04949	-0.258	1.2E-02	-0.031	7.6E-01	-0.272	5.0E-03	-0.144	n/a	0.378	0.515	0.032	0.948
C22:0 Ceramide (d18:1)	C8-pos	Sphingolipids - Ceramides	HMDB04952	-0.277	6.7E-03	-0.013	9.0E-01	-0.376	8.1E-05	-0.210	n/a	0.845	0.096	0.559	0.193
C23:0 Ceramide (d18:1)	C8-pos	Sphingolipids - Ceramides	HMDB00950	-0.363	3.4E-04	-0.098	3.0E-01	-0.495	1.8E-07	-0.353	n/a				
C24:0 Ceramide (d18:1)	C8-pos	Sphingolipids - Ceramides	HMDB04956	-0.213	4.9E-02	0.058	5.6E-01	-0.212	2.6E-02	-0.088	n/a	1.171	0.027	0.769	0.073
C24:1 Ceramide (d18:1)	C8-pos	Sphingolipids - Ceramides	HMDB04953	-0.305	4.1E-03	-0.106	3.3E-01	-0.307	1.0E-03	-0.160	n/a	0.443	0.422	0.189	0.709
sphinganine	HILIC-pos	Sphingolipids - Sphingolipids	HMDB00269	0.334	6.9E-05	0.347	5.5E-05	0.240	2.5E-02	0.260	1.6E-02	-0.388	0.508	-0.573	0.320
sphingosine-1-phosphate	C18-neg	Sphingolipids - Sphingolipids	HMDB00277	0.220	4.9E-02	0.233	4.3E-02	0.203	3.2E-02	0.163	9.3E-02				
C14:0 SM	C8-pos	Sphingolipids - Sphingomyelins	HMDB12097	-0.530	2.8E-07	-0.370	9.2E-05	-0.472	3.8E-07	-0.524	2.3E-11	0.563	0.321	0.120	0.814
C18:0 SM	C8-pos	Sphingolipids - Sphingomyelins	HMDB01348	0.297	4.8E-03	0.485	1.0E-07	0.206	2.9E-02	0.208	9.8E-03	0.549	0.373	0.110	0.843
C18:1 SM	C8-pos	Sphingolipids - Sphingomyelins	HMDB12101	0.343	1.1E-03	0.490	1.6E-07	0.280	2.3E-03	0.243	2.9E-03	0.186	0.766	-0.343	0.533
C24:1 SM	C8-pos	Sphingolipids - Sphingomyelins	HMDB12107	0.308	6.5E-03	0.440	1.3E-05	0.421	2.4E-06	0.350	8.8E-06	0.432	0.466	-0.190	0.695
2-hydroxyhexadecanoate	C18-neg	Fatty acids	HMDB31057	-0.303	6.4E-03	-0.295	9.3E-03	-0.283	1.9E-03	-0.280	2.7E-03				
8,11,14-eicosatrienoic acid	C18-neg	Fatty acids	HMDB02925	-0.288	5.5E-03	-0.281	7.9E-03	-0.298	7.0E-04	-0.255	4.3E-03				
eicosanedioate	C18-neg	Fatty acids	n/a	0.335	1.4E-03	0.311	3.8E-03	0.338	3.8E-04	0.294	2.5E-03				
gamma-linolenic acid	C18-neg	Fatty acids	HMDB03073	-0.374	8.5E-04	-0.391	6.0E-04	-0.379	3.2E-05	-0.398	2.2E-05				
hexadecanedioate	C18-neg	Fatty acids	HMDB00672	-0.607	6.2E-09	-0.629	4.4E-09	-0.587	4.3E-11	-0.604	4.1E-11				
hydroxymyristate	C18-neg	Fatty acids	HMDB02261	-0.673	4.1E-10	-0.682	6.0E-10	-0.688	7.1E-14	-0.717	2.8E-14				
myristic acid	C18-neg	Fatty acids	HMDB00806	-0.206	3.4E-02	-0.226	2.2E-02	-0.214	1.4E-02	-0.230	1.0E-02				
oleate	C18-neg	Fatty acids	HMDB00207	-0.298	3.1E-03	-0.330	1.2E-03	-0.288	3.2E-03	-0.322	1.4E-03				
palmitoleic acid	C18-neg	Fatty acids	HMDB03229	-0.844	2.6E-15	-0.908	4.8E-17	-0.738	2.1E-17	-0.794	3.2E-19				
sebacate	C18-neg	Fatty acids	HMDB00792	-0.294	2.9E-03	-0.315	1.7E-03	-0.374	1.4E-04	-0.364	3.2E-04				
C12:1 carnitine	HILIC-pos	Acylcarnitines	HMDB13326	-0.503	1.5E-06	-0.537	4.1E-07	-0.311	7.6E-04	-0.343	3.0E-04	-0.385	0.476	-0.499	0.355
C14 carnitine	HILIC-pos	Acylcarnitines	HMDB05066	-0.354	6.9E-04	-0.350	9.2E-04	-0.267	3.5E-03	-0.295	1.5E-03	0.505	0.346	0.436	0.414
C14:1 carnitine	HILIC-pos	Acylcarnitines	HMDB02014	-0.321	2.4E-03	-0.365	6.4E-04	-0.192	3.7E-02	-0.254	7.0E-03	-0.077	0.885	-0.145	0.785
C18 carnitine	HILIC-pos	Acylcarnitines	HMDB00848	0.351	1.5E-03	0.396	4.4E-04	0.321	4.3E-05	0.307	1.3E-04	1.268	0.020	1.287	0.016
C5:1 carnitine	HILIC-pos	Acylcarnitines	HMDB02366	-0.241	1.1E-02	-0.232	1.7E-02	-0.321	1.6E-03	-0.316	2.5E-03	0.716	0.201	0.597	0.287
2-aminooctanoate	HILIC-pos	Amino Acids	HMDB00991	-0.324	3.6E-03	-0.364	1.2E-03	-0.282	2.2E-03	-0.330	4.9E-04	-0.224	0.680	-0.192	0.724
4-acetamidobutanoate	HILIC-pos	Amino Acids	HMDB03681	-0.495	5.3E-07	-0.514	2.7E-07	-0.271	2.8E-03	-0.297	1.4E-03	0.013	0.979	-0.024	0.962
5-acetylamino-6-amino-3-methyluracil	HILIC-pos	Amino Acids	HMDB04400	-0.650	2.6E-10	-0.659	4.3E-10	-0.546	8.7E-10	-0.534	3.9E-09	-0.160	0.772	-0.212	0.704
ADMA	HILIC-pos	Amino Acids	HMDB01539	-0.511	4.1E-07	-0.529	3.0E-07	-0.547	1.4E-08	-0.511	2.1E-07	0.595	0.337	0.775	0.205
alanine	HILIC-pos	Amino Acids	HMDB00161	-0.465	1.9E-05	-0.363	9.2E-04	-0.434	2.4E-06	-0.306	8.7E-04	-0.860	0.123	-0.929	0.093
arginine	HILIC-pos	Amino Acids	HMDB00517	0.280	5.1E-03	0.237	2.1E-02	0.282	4.0E-03	0.254	1.1E-02	-0.703	0.211	-0.830	0.142
citrulline	HILIC-pos	Amino Acids	HMDB00904	-0.370	3.9E-04	-0.414	8.9E-05	-0.245	7.9E-03	-0.335	3.6E-04	0.720	0.209	0.632	0.272
creatinine	HILIC-pos	Amino Acids	HMDB00562	0.290	5.7E-03	0.243	2.4E-02	0.289	2.5E-03	0.315	1.3E-03	0.357	0.447	0.485	0.302
homoarginine	HILIC-pos	Amino Acids	HMDB00670	0.611	1.5E-09	0.574	3.1E-08	0.634	2.2E-13	0.667	4.6E-14	-0.502	0.319	-0.471	0.357
hydroxyproline	HILIC-pos	Amino Acids	HMDB00725	0.318	7.0E-03	0.293	1.6E-02	0.587	1.4E-11	0.510	6.8E-09	-0.026	0.966	-0.119	0.846
kynurenine	HILIC-neg	Amino Acids	HMDB00684	-0.594	3.8E-09	-0.544	9.9E-08	-0.422	2.1E-06	-0.340	1.7E-04	0.035	0.952	0.009	0.988
lysine	HILIC-pos	Amino Acids	HMDB00182	-0.338	1.8E-03	-0.347	1.7E-03	-0.417	5.9E-06	-0.378	6.6E-05	-0.602	0.279	-0.595	0.291
N-acetylornithine	HILIC-pos	Amino Acids	HMDB03357	-0.718	3.6E-11	-0.707	2.5E-10	-0.707	1.6E-15	-0.713	4.2E-15	0.701	0.215	0.727	0.197
N-alpha-acetylarginine	HILIC-pos	Amino Acids	HMDB04620	0.596	1.5E-08	0.590	4.1E-08	0.751	8.7E-16	0.717	4.9E-14	0.192	0.734	0.064	0.911
N6,N6-dimethyllysine	HILIC-pos	Amino Acids	HMDB13287	-1.060	1.5E-24	-1.058	1.9E-23	-0.953	6.1E-25	-0.965	1.6E-24				
ornithine	HILIC-pos	Amino Acids	HMDB00214	-0.362	6.2E-04	-0.369	6.4E-04	-0.624	2.2E-11	-0.629	5.0E-11	0.010	0.986	0.014	0.980
pantothenate	HILIC-neg	Amino Acids	HMDB00210	-0.247	1.9E-02	-0.224	4.1E-02	-0.436	3.0E-06	-0.415	1.5E-05	1.464	0.021	1.397	0.029
phenylalanine	HILIC-pos	Amino Acids	HMDB00159	-0.246	2.6E-02	-0.193	9.2E-02	-0.261	4.3E-03	-0.195	n/a	0.529	0.333	0.781	0.143
proline	HILIC-pos	Amino Acids	HMDB00162	-0.352	1.4E-03	-0.283	1.1E-02	-0.297	1.2E-03	-0.212	2.1E-02	-1.113	0.043	-1.062	0.053

Metabolite name	Method	Category	HMDB ID	WHI-OS				WHI-HT				MESA			
				Model 1		Model 2		Model 1		Model 2		Model 1		Model 2	
				Beta	FDR	Beta	FDR	Beta	FDR	Beta	FDR	Beta	Raw-p	Beta	Raw-p
serine	HILIC-pos	Amino Acids	HMDB00187	0.293	3.9E-03	0.246	1.7E-02	0.313	1.0E-03	0.235	1.5E-02	-0.257	0.667	-0.256	0.672
taurine	HILIC-pos	Amino Acids	HMDB00251	0.307	6.8E-03	0.314	6.8E-03	0.263	4.5E-03	0.207	2.7E-02	0.511	0.369	0.410	0.475
bilirubin	HILIC-pos	Bile acids and Bilirubins	HMDB00054	-0.356	1.8E-04	-0.377	9.2E-05	-0.401	2.5E-05	-0.457	2.6E-06	0.016	0.974	-0.061	0.905
biliverdin	HILIC-pos	Bile acids and Bilirubins	HMDB01008	-0.388	1.8E-04	-0.429	4.8E-05	-0.352	1.8E-04	-0.392	5.0E-05	0.108	0.817	0.122	0.795
glycochenodeoxycholate	C18-neg	Bile acids and Bilirubins	HMDB00637	-0.289	1.0E-02	-0.299	9.5E-03	-0.320	5.2E-04	-0.329	5.1E-04				
glycodeoxycholate	C18-neg	Bile acids and Bilirubins	HMDB00631	-0.239	2.8E-02	-0.247	2.6E-02	-0.257	6.1E-03	-0.257	7.3E-03				
glycodeoxycholate/glycochenodeoxycholate	HILIC-pos	Bile acids and Bilirubins	n/a	-0.343	2.4E-03	-0.351	2.3E-03	-0.341	1.5E-04	-0.340	2.4E-04	0.757	0.193	0.731	0.212
glycoursodeoxycholate	C18-neg	Bile acids and Bilirubins	HMDB00708	-0.451	5.9E-05	-0.446	1.1E-04	-0.497	6.3E-08	-0.513	5.3E-08				
1,7-dimethyluric acid	HILIC-pos	Purines and Pyrimidines	HMDB11103	-0.578	1.3E-07	-0.591	1.2E-07	-0.477	1.0E-07	-0.446	1.0E-06				
3-methylxanthine	HILIC-pos	Purines and Pyrimidines	HMDB01886	-0.756	1.2E-12	-0.767	2.4E-12	-0.614	1.9E-11	-0.602	1.1E-10	0.117	0.826	0.021	0.969
7-methylxanthine	HILIC-pos	Purines and Pyrimidines	HMDB01991	-0.706	1.4E-11	-0.716	2.7E-11	-0.565	9.8E-10	-0.559	3.5E-09	0.500	0.379	0.462	0.421
ADP	HILIC-neg	Purines and Pyrimidines	HMDB01341	0.351	1.6E-03	0.367	1.2E-03	0.275	3.6E-03	0.241	1.3E-02	0.942	0.100	0.966	0.094
AMP	HILIC-neg	Purines and Pyrimidines	HMDB00045	0.446	4.2E-05	0.467	2.7E-05	0.476	3.4E-07	0.452	2.2E-06				
CMP	HILIC-neg	Purines and Pyrimidines	HMDB00095	0.467	3.6E-05	0.498	1.6E-05	0.380	3.2E-06	0.394	2.5E-06				
GDP	HILIC-neg	Purines and Pyrimidines	HMDB01201	0.287	1.0E-02	0.301	8.2E-03	0.206	3.1E-02	0.167	8.6E-02				
GMP	HILIC-neg	Purines and Pyrimidines	HMDB01397	0.364	9.8E-04	0.376	8.5E-04	0.406	1.2E-05	0.372	9.4E-05				
hypoxanthine	HILIC-neg	Purines and Pyrimidines	HMDB00157	0.379	4.6E-04	0.363	1.0E-03	0.344	1.9E-04	0.350	2.3E-04	1.557	0.008	1.602	0.007
IMP	HILIC-neg	Purines and Pyrimidines	HMDB00175	0.297	3.6E-03	0.296	4.5E-03	0.219	2.0E-02	0.168	8.1E-02				
inosine	HILIC-neg	Purines and Pyrimidines	HMDB00195	0.390	1.3E-04	0.404	1.1E-04	0.321	9.3E-04	0.338	6.9E-04	0.595	0.323	0.716	0.233
N4-acetylcytidine	HILIC-pos	Purines and Pyrimidines	HMDB05923	-0.400	5.9E-05	-0.351	5.9E-04	-0.385	1.7E-05	-0.301	9.3E-04	-0.480	0.417	-0.538	0.367
UDP	HILIC-neg	Purines and Pyrimidines	HMDB00295	0.365	7.2E-04	0.402	2.6E-04	0.219	2.1E-02	0.221	2.1E-02				
UMP	HILIC-neg	Purines and Pyrimidines	HMDB00288	0.447	2.0E-05	0.472	1.1E-05	0.369	4.2E-05	0.355	1.3E-04				
alpha-glycerophosphocholine	HILIC-pos	Quaternary Amines	HMDB00086	0.304	5.2E-03	0.360	1.0E-03	0.241	1.1E-02	0.252	9.2E-03	0.314	0.590	0.214	0.715
betaine	HILIC-pos	Quaternary Amines	HMDB00043	0.377	2.0E-04	0.382	2.4E-04	0.377	7.0E-06	0.351	4.7E-05	0.807	0.144	0.880	0.112
kynurenic acid	HILIC-pos	Indoles and Indole derivatives	HMDB00715	-0.437	2.4E-05	-0.406	1.3E-04	-0.278	2.3E-03	-0.272	3.6E-03	-0.964	0.081	-0.967	0.082
1-methylnicotinamide	HILIC-pos	Pyridines and derivatives	HMDB00699	-0.442	1.8E-05	-0.435	3.9E-05	-0.249	7.4E-03	-0.265	5.3E-03	-0.092	0.865	-0.238	0.663
4-pyridoxate	HILIC-neg	Pyridines and derivatives	HMDB00017	-0.351	6.4E-04	-0.351	8.3E-04	-0.316	5.8E-04	-0.313	9.2E-04				
N1-methyl-2-pyridone-5-carboxamide	HILIC-pos	Pyridines and derivatives	HMDB04193	-0.388	2.6E-04	-0.368	7.4E-04	-0.308	1.0E-03	-0.279	3.6E-03	1.219	0.035	1.049	0.070
adipate	HILIC-neg	Dicarboxylic acids	HMDB00448	-0.317	1.9E-03	-0.323	2.0E-03	-0.319	1.2E-03	-0.330	1.1E-03				
methylmalonate	HILIC-neg	Dicarboxylic acids	HMDB00202	-0.480	3.9E-06	-0.458	1.8E-05	-0.453	1.1E-06	-0.475	6.6E-07				
2-phosphoglycerate	HILIC-neg	Organic acids	HMDB00362	0.249	1.6E-02	0.267	1.2E-02	0.389	8.0E-05	0.351	5.2E-04				
hexose monophosphate	HILIC-neg	Carbohydrates and conjugates	HMDB00124	0.315	4.5E-03	0.337	2.9E-03	0.329	4.3E-04	0.295	2.0E-03				
lactose	HILIC-neg	Carbohydrates and conjugates	HMDB00186	0.226	4.9E-02	0.238	4.4E-02	0.317	6.3E-04	0.322	7.2E-04				
pentose monophosphate	HILIC-neg	Carbohydrates and conjugates	HMDB01548	0.285	1.0E-02	0.301	7.9E-03	0.249	6.5E-03	0.226	1.5E-02				
acetaminophen	HILIC-pos	Benzenoids	HMDB01859	-0.351	4.3E-03	-0.406	1.0E-03	-0.292	1.4E-04	-0.302	1.3E-04	0.548	0.389	0.553	0.389
allantoin	HILIC-pos	Others	HMDB00462	-0.290	1.8E-03	-0.300	1.6E-03	-0.221	2.7E-02	-0.213	3.8E-02				
caffeine	HILIC-pos	Others	HMDB01847	-0.532	1.9E-06	-0.515	7.2E-06	-0.325	1.7E-04	-0.265	2.4E-03	-0.820	0.133	-0.908	0.095
carboxyibuprofen	C18-neg	Others	n/a	-0.288	8.9E-03	-0.329	3.2E-03	-0.218	1.5E-02	-0.249	6.9E-03				
cortisol	HILIC-pos	Others	HMDB00063	-0.514	3.6E-07	-0.513	6.7E-07	-0.238	1.4E-02	-0.262	8.7E-03	0.359	0.545	0.180	0.762
hydroxyectoine	HILIC-pos	Others	n/a	-0.407	9.5E-05	-0.448	2.3E-05	-0.259	4.9E-03	-0.346	2.3E-04				
piperine	HILIC-pos	Others	HMDB29377	0.576	6.8E-09	0.572	2.0E-08	0.481	6.3E-08	0.469	2.8E-07	-0.788	0.149	-0.798	0.148
pseudouridine	HILIC-pos	Others	HMDB00767	-0.433	1.1E-05	-0.409	5.0E-05	-0.321	5.2E-04	-0.275	3.6E-03	-0.225	0.676	-0.214	0.695
thiamine	HILIC-pos	Others	HMDB00235	-0.354	5.8E-04	-0.375	3.5E-04	-0.422	4.2E-06	-0.417	9.7E-06				
trigonelline	HILIC-pos	Others	HMDB00875	-0.577	1.8E-08	-0.586	2.5E-08	-0.499	5.9E-08	-0.530	1.8E-08	0.635	0.281	0.661	0.267

Model 1 (fully adjusted model) is adjusted for coronary heart disease case-control status (WHI only), age (a matching factor in the WHI), enrollment window (WHI only; a matching factor in the WHI), hysterectomy status, hormone therapy use status, body mass index, smoking status, alcohol consumption, education, family income, physical activity, baseline diseases (diabetes, hypertension, and depression), and medication use (aspirin, lipid-lowing, antihyperglycemic, antihypertensive, and antidepressants).

Model 2 (lipid-adjusted model) is adjusted for variables in Model 1 plus plasma levels of total cholesterol and high-density lipoprotein cholesterol.

Supplementary Table S5. Magnitude of difference in metabolites that were more than 0.5-SD between Black and White women, and their associations with risk of coronary heart disease in the WHI, JHS, and NHS.

Method	Metabolite	HMDB ID	Category	SD-difference in the WHI-HT		Associations between metabolite with large race differences and CHD risk in women from WHI, JHS, and NHS									
						All women (WHI)		Black women (WHI)		Black women (JHS)		White women (WHI)		White women (NHS)	
				Beta	FDR-P	OR (95% CI)	FDR	OR (95% CI)	FDR	HR (95% CI)	raw-P	OR (95% CI)	FDR	HR (95% CI)	raw-P
Metabolites with >1 SD higher in Black women															
C8-pos	C40:7 PE plasmalogen	HMDB11394*	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	**1.057**	**6.4E-30**	0.95 (0.83, 1.09)	0.770	0.77 (0.47, 1.26)	0.867	1.09 (0.88, 1.36)	0.413	0.97 (0.84, 1.12)	0.906	1.02 (0.85, 1.23)	0.821
C8-pos	C20:4 CE	HMDB06726	Sterol lipids - Cholesteryl esters	**1.121**	**2.1E-33**	1.06 (0.91, 1.24)	0.775	0.87 (0.49, 1.55)	0.963	-	-	1.08 (0.91, 1.27)	0.733	0.97 (0.80, 1.19)	0.778
C8-pos	C22:4 CE	HMDB06729*	Sterol lipids - Cholesteryl esters	**1.072**	**1.7E-30**	1.02 (0.88, 1.18)	0.929	1.04 (0.58, 1.85)	0.998	-	-	1.03 (0.88, 1.20)	0.921	0.96 (0.70, 1.31)	0.785
C8-pos	C22:6 CE	HMDB06733	Sterol lipids - Cholesteryl esters	**1.241**	**4.9E-44**	1.01 (0.88, 1.17)	0.938	0.86 (0.52, 1.40)	0.932	-	-	1.04 (0.89, 1.20)	0.883	0.98 (0.80, 1.20)	0.861
Metabolites with 0.5-1 SD higher in Black women															
C8-pos	C36:2 PC plasmalogen-B	HMDB11243*	Glycerophospholipids - Phosphatidylcholine plasmalogens	0.586	7.7E-12	**1.28 (1.09, 1.49)**	**0.032**	1.62 (0.94, 2.80)	0.867	-	-	**1.25 (1.06, 1.47)**	**0.080**	1.07 (0.88, 1.31)	0.476
C8-pos	C18:1 CE	HMDB00918	Sterol lipids - Cholesteryl esters	0.611	7.3E-11	**1.24 (1.06, 1.46)**	**0.074**	1.47 (0.82, 2.65)	0.867	-	-	1.24 (1.04, 1.47)	0.128	0.99 (0.80, 1.22)	0.916
C8-pos	C36:5 PE plasmalogen	HMDB11410*	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	0.824	1.0E-19	**0.84 (0.74, 0.96)**	**0.078**	0.66 (0.44, 1.01)	0.867	1.05 (0.86, 1.29)	0.638	0.87 (0.76, 1.00)	0.268	0.98 (0.81, 1.18)	0.814
C8-pos	C58:9 TAG	HMDB05463*	Glycerolipids - Triacylglycerols	0.649	1.8E-13	0.85 (0.74, 0.97)	0.117	0.99 (0.65, 1.52)	0.998	-	-	0.84 (0.73, 0.96)	0.119	0.89 (0.71, 1.10)	0.270
C8-pos	C58:10 TAG	HMDB05476*	Glycerolipids - Triacylglycerols	0.651	2.1E-13	0.85 (0.75, 0.97)	0.124	0.99 (0.65, 1.52)	0.998	-	-	0.84 (0.73, 0.97)	0.127	0.93 (0.77, 1.14)	0.494
C8-pos	C60:12 TAG	HMDB05478*	Glycerolipids - Triacylglycerols	0.771	2.8E-18	0.86 (0.75, 0.98)	0.182	0.97 (0.63, 1.50)	0.998	-	-	0.85 (0.73, 0.98)	0.152	1.01 (0.82, 1.25)	0.918
C8-pos	C38:6 PE plasmalogen	HMDB11387*	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	0.766	1.6E-16	0.86 (0.75, 0.98)	0.185	0.59 (0.38, 0.94)	0.867	1.08 (0.87, 1.35)	0.464	0.89 (0.77, 1.03)	0.472	1.01 (0.84, 1.22)	0.917
C8-pos	C18:2 CE	HMDB00610*	Sterol lipids - Cholesteryl esters	0.538	9.4E-09	1.16 (0.99, 1.35)	0.320	1.34 (0.76, 2.35)	0.867	-	-	1.16 (0.98, 1.37)	0.397	1.06 (0.83, 1.36)	0.649
C8-pos	C58:8 TAG	HMDB05413*	Glycerolipids - Triacylglycerols	0.699	1.8E-14	0.88 (0.77, 1.01)	0.320	1.06 (0.66, 1.70)	0.998	-	-	0.87 (0.75, 1.00)	0.268	**0.51 (0.32, 0.80)**	**0.004**
HILIC-pos	homoarginine	HMDB00670	Amino Acids	0.634	2.2E-13	0.89 (0.78, 1.02)	0.363	0.94 (0.60, 1.46)	0.991	**0.81 (0.65, 1.00)**	**0.049**	0.89 (0.77, 1.02)	0.429	0.96 (0.80, 1.15)	0.640
C8-pos	C20:3 CE	HMDB06736*	Sterol lipids - Cholesteryl esters	0.534	2.0E-08	1.12 (0.97, 1.28)	0.398	1.47 (0.89, 2.42)	0.867	-	-	1.08 (0.94, 1.25)	0.646	1.13 (0.93, 1.36)	0.214
C8-pos	C38:7 PE plasmalogen	HMDB11420*	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	0.986	1.8E-27	0.90 (0.78, 1.03)	0.398	0.64 (0.39, 1.04)	0.867	1.09 (0.89, 1.34)	0.414	0.93 (0.80, 1.07)	0.696	0.99 (0.82, 1.20)	0.914
HILIC-pos	hydroxyproline	HMDB00725	Amino Acids	0.587	1.4E-11	0.91 (0.80, 1.03)	0.422	0.90 (0.63, 1.28)	0.946	1.08 (0.89, 1.31)	0.451	0.91 (0.79, 1.04)	0.508	0.94 (0.78, 1.12)	0.463
C8-pos	C38:5 PE plasmalogen	HMDB11386*	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	0.746	9.4E-16	0.91 (0.80, 1.04)	0.473	0.76 (0.50, 1.15)	0.867	1.06 (0.86, 1.30)	0.604	0.93 (0.80, 1.07)	0.654	1.01 (0.84, 1.22)	0.911
C8-pos	C40:6 PC-B	HMDB08057*	Glycerophospholipids - Phosphatidylcholines	0.584	2.5E-10	0.92 (0.81, 1.06)	0.587	0.87 (0.56, 1.34)	0.931	-	-	0.93 (0.81, 1.07)	0.706	1.00 (0.82, 1.21)	0.989
C8-pos	C16:0 CE	HMDB00885	Sterol lipids - Cholesteryl esters	0.728	3.9E-14	1.08 (0.93, 1.27)	0.662	0.98 (0.56, 1.75)	0.998	-	-	1.08 (0.92, 1.28)	0.707	1.00 (0.81, 1.23)	0.994
C8-pos	C38:6 PC plasmalogen-A	HMDB11319*	Glycerophospholipids - Phosphatidylcholine plasmalogens	0.687	3.8E-14	0.95 (0.83, 1.08)	0.743	0.97 (0.64, 1.47)	0.998	1.20 (0.97, 1.49)	0.088	0.94 (0.82, 1.08)	0.739	-	-
C8-pos	C36:5 PC plasmalogen-B	HMDB11220*	Glycerophospholipids - Phosphatidylcholine plasmalogens	0.690	2.0E-13	0.95 (0.82, 1.09)	0.770	0.98 (0.68, 1.40)	0.998	1.07 (0.88, 1.31)	0.501	0.93 (0.80, 1.09)	0.733	0.90 (0.74, 1.10)	0.306
C8-pos	C40:7 PC plasmalogen	HMDB11294*	Glycerophospholipids - Phosphatidylcholine plasmalogens	0.659	2.6E-12	1.06 (0.92, 1.21)	0.770	1.19 (0.77, 1.83)	0.919	-	-	1.04 (0.89, 1.21)	0.883	-	-
C8-pos	C38:7 PC plasmalogen	HMDB11229*	Glycerophospholipids - Phosphatidylcholine plasmalogens	0.910	1.4E-23	0.95 (0.83, 1.09)	0.785	0.86 (0.55, 1.32)	0.927	1.14 (0.92, 1.40)	0.226	0.96 (0.83, 1.11)	0.867	0.99 (0.79, 1.23)	0.911
C8-pos	C22:5 CE	HMDB10375*	Sterol lipids - Cholesteryl esters	0.936	4.5E-27	1.04 (0.91, 1.20)	0.819	0.93 (0.58, 1.50)	0.991	-	-	1.06 (0.92, 1.23)	0.768	1.00 (0.80, 1.25)	0.989
C8-pos	C38:6 PC plasmalogen-B	HMDB11319*	Glycerophospholipids - Phosphatidylcholine plasmalogens	0.516	4.5E-08	0.97 (0.84, 1.12)	0.881	0.88 (0.55, 1.42)	0.959	-	-	0.97 (0.84, 1.13)	0.921	-	-
HILIC-pos	N-alpha-acetylarginine	HMDB04620	Amino Acids	0.751	8.7E-16	0.98 (0.86, 1.11)	0.904	0.88 (0.58, 1.35)	0.948	0.89 (0.73, 1.08)	0.233	0.99 (0.87, 1.14)	0.988	0.87 (0.71, 1.06)	0.155
C8-pos	C20:2 CE	HMDB06734	Sterol lipids - Cholesteryl esters	0.794	1.8E-18	1.02 (0.88, 1.18)	0.934	1.38 (0.80, 2.36)	0.867	-	-	0.99 (0.85, 1.16)	0.988	-	-
C8-pos	C20:1 CE	HMDB05193	Sterol lipids - Cholesteryl esters	0.627	4.4E-12	1.00 (0.87, 1.15)	0.977	1.47 (0.82, 2.65)	0.867	-	-	0.97 (0.84, 1.13)	0.921	-	-
Metabolites with >1 SD lower in Black women															
C8-pos	C51:3 TAG	n/a	Glycerolipids - Triacylglycerols	**-1.020**	**1.8E-29**	**0.81 (0.70, 0.94)**	**0.066**	0.99 (0.58, 1.70)	0.998	-	-	**0.78 (0.67, 0.92)**	**0.049**	-	-
C8-pos	C49:3 TAG	HMDB42103*	Glycerolipids - Triacylglycerols	**-1.061**	**1.8E-31**	0.87 (0.75, 1.01)	0.320	1.17 (0.70, 1.94)	0.944	-	-	0.83 (0.71, 0.97)	0.138	0.99 (0.81, 1.20)	0.883
C8-pos	C50:3 TAG	HMDB05433*	Glycerolipids - Triacylglycerols	**-1.046**	**1.1E-32**	0.87 (0.74, 1.01)	0.328	0.96 (0.59, 1.56)	0.998	-	-	0.83 (0.70, 0.98)	0.192	1.03 (0.83, 1.29)	0.793
C8-pos	C32:2 PC	HMDB07874*	Glycerophospholipids - Phosphatidylcholines	**-1.050**	**2.6E-35**	0.90 (0.78, 1.03)	0.431	1.22 (0.74, 2.00)	0.917	1.10 (0.89, 1.37)	0.373	0.87 (0.75, 1.01)	0.359	1.00 (0.81, 1.24)	0.975
C8-pos	C34:3 PC	HMDB08006*	Glycerophospholipids - Phosphatidylcholines	**-1.004**	**1.2E-32**	0.96 (0.83, 1.11)	0.848	1.01 (0.63, 1.61)	0.998	1.22 (0.98, 1.51)	0.081	0.95 (0.82, 1.11)	0.829	1.00 (0.80, 1.23)	0.964
C8-pos	C31:1 PC	HMDB07936*	Glycerophospholipids - Phosphatidylcholines	**-1.087**	**2.1E-33**	0.98 (0.85, 1.13)	0.929	1.62 (0.92, 2.83)	0.867	-	-	0.93 (0.80, 1.08)	0.706	-	-
Metabolites with 0.5-1 SD lower in Black women															
C8-pos	C36:4 DAG-A	HMDB07248*	Glycerolipids - Diacylglycerols	-0.611	2.7E-11	**0.80 (0.69, 0.92)**	**0.032**	0.68 (0.40, 1.16)	0.867	-	-	**0.81 (0.69, 0.94)**	**0.072**	0.98 (0.79, 1.21)	0.846
C8-pos	C52:6 TAG	HMDB05436*	Glycerolipids - Triacylglycerols	-0.663	3.5E-13	**0.80 (0.70, 0.92)**	**0.032**	0.85 (0.55, 1.32)	0.927	-	-	**0.79 (0.68, 0.92)**	**0.049**	0.94 (0.74, 1.19)	0.608
C8-pos	C50:4 TAG	HMDB05435*	Glycerolipids - Triacylglycerols	-0.945	5.0E-26	**0.80 (0.69, 0.94)**	**0.063**	0.84 (0.52, 1.37)	0.927	-	-	**0.78 (0.67, 0.93)**	**0.054**	0.93 (0.71, 1.22)	0.590
C8-pos	C50:6 TAG	HMDB10497*	Glycerolipids - Triacylglycerols	-0.529	9.4E-09	**0.83 (0.72, 0.95)**	**0.064**	0.97 (0.64, 1.45)	0.998	-	-	**0.80 (0.69, 0.93)**	**0.049**	0.97 (0.79, 1.20)	0.773
C8-pos	C50:5 TAG	HMDB10471*	Glycerolipids - Triacylglycerols	-0.781	6.8E-18	**0.82 (0.71, 0.94)**	**0.066**	0.87 (0.56, 1.36)	0.946	-	-	**0.80 (0.69, 0.94)**	**0.066**	0.99 (0.79, 1.24)	0.931
C8-pos	C36:3 DAG	HMDB07219*	Glycerolipids - Diacylglycerols	-0.783	4.7E-18	**0.81 (0.69, 0.94)**	**0.069**	0.75 (0.44, 1.29)	0.867	-	-	**0.80 (0.68, 0.94)**	**0.080**	0.99 (0.79, 1.24)	0.917
C8-pos	C34:3 DAG	HMDB07132*	Glycerolipids - Diacylglycerols	-0.975	2.2E-27	**0.80 (0.68, 0.94)**	**0.072**	0.84 (0.49, 1.41)	0.930	-	-	**0.77 (0.65, 0.92)**	**0.057**	0.90 (0.69, 1.18)	0.452
C8-pos	C52:4 TAG	HMDB05363*	Glycerolipids - Triacylglycerols	-0.743	1.1E-15	**0.82 (0.71, 0.96)**	**0.093**	0.70 (0.42, 1.19)	0.867	-	-	0.83 (0.71, 0.98)	0.157	0.97 (0.80, 1.19)	0.787
C8-pos	C18:1 LPE	HMDB11506	Glycerophospholipids - Lysophosphatidylethanolamines	-0.530	3.2E-08	1.17 (1.03, 1.33)	0.124	1.27 (0.84, 1.91)	0.867	1.03 (0.84, 1.28)	0.750	1.15 (1.01, 1.32)	0.244	1.03 (0.86, 1.24)	0.737
C8-pos	C38:3 DAG	HMDB07168*	Glycerolipids - Diacylglycerols	-0.683	6.3E-14	0.85 (0.73, 0.98)	0.185	0.95 (0.58, 1.55)	0.998	-	-	0.82 (0.70, 0.97)	0.130	-	-
C8-pos	C48:4 TAG	HMDB42631*	Glycerolipids - Triacylglycerols	-0.806	1.1E-18	0.85 (0.74, 0.98)	0.185	0.95 (0.62, 1.47)	0.998	-	-	0.83 (0.71, 0.97)	0.129	-	-
C8-pos	C48:5 TAG	HMDB42841*	Glycerolipids - Triacylglycerols	-0.631	1.3E-11	0.86 (0.75, 0.98)	0.185	0.99 (0.67, 1.48)	0.998	-	-	0.83 (0.71, 0.96)	0.125	-	-
C8-pos	C54:4 TAG	HMDB05370*	Glycerolipids - Triacylglycerols	-0.529	9.1E-09	0.86 (0.75, 0.99)	0.197	0.60 (0.36, 1.01)	0.867	-	-	0.89 (0.77, 1.03)	0.435	0.98 (0.81, 1.19)	0.851
C8-pos	C55:3 TAG	n/a	Glycerolipids - Triacylglycerols	-0.672	3.2E-13	0.87 (0.76, 1.00)	0.277	1.12 (0.66, 1.91)	0.972	-	-	0.85 (0.74, 0.99)	0.206	-	-
C8-pos	C48:3 TAG	HMDB05432*	Glycerolipids - Triacylglycerols	-0.917	1.2E-24	0.87 (0.75, 1.01)	0.320	1.03 (0.65, 1.62)	0.998	-	-	0.83 (0.71, 0.98)	0.176	1.02 (0.82, 1.26)	0.884
C8-pos	C34:2 DAG	HMDB07103*	Glycerolipids - Diacylglycerols	-0.856	1.3E-22	0.86 (0.73, 1.02)	0.342	0.96 (0.56, 1.65)	0.998	-	-	0.82 (0.69, 0.98)	0.202	1.07 (0.84, 1.37)	0.565
C8-pos	C52:3 TAG	HMDB05384*	Glycerolipids - Triacylglycerols	-0.810	5.3E-18	0.87 (0.74, 1.02)	0.354	0.87 (0.52, 1.44)	0.951	-	-	0.85 (0.72, 1.01)	0.344	0.96 (0.74, 1.24)	0.739
C8-pos	C16:1 CE	HMDB00658*	Sterol lipids - Cholesteryl esters	-0.583	1.0E-10	1.12 (0.98, 1.27)	0.370	1.28 (0.79, 2.07)	0.867	-	-	1.08 (0.95, 1.24)	0.609	1.02 (0.84, 1.23)	0.850
C8-pos	C34:4 PC	HMDB07883*	Glycerophospholipids - Phosphatidylcholines	-0.818	4.0E-20	0.89 (0.78, 1.02)	0.387	0.78 (0.46, 1.34)	0.867	0.94 (0.75, 1.17)	0.562	0.90 (0.78, 1.04)	0.508	1.04 (0.84, 1.29)	0.698
C18-neg	hydroxymyristate	HMDB02261	Fatty acids	-0.688	7.1E-14	0.90 (0.79, 1.02)	0.398	0.88 (0.57, 1.37)	0.949	-	-	0.92 (0.80, 1.05)	0.609	**1.50 (1.01, 2.23)**	**0.044**
C8-pos	C46:4 TAG	HMDB42781*	Glycerolipids - Triacylglycerols	-0.596	1.9E-10	0.90 (0.78, 1.03)	0.435	0.99 (0.66, 1.50)	0.998	-	-	0.88 (0.75, 1.02)	0.411	-	-
C8-pos	C46:3 TAG	HMDB42541*	Glycerolipids - Triacylglycerols	-0.729	1.2E-15	0.90 (0.78, 1.04)	0.469	1.02 (0.67, 1.57)	0.998	1.10 (0.89, 1.37)	0.372	0.87 (0.75, 1.01)	0.392	-	-

Method	Metabolite	HMDB ID	Category	SD-difference in the WHI-HT		Associations between metabolite with large race differences and CHD risk in women from WHI, JHS, and NHS									
						All women (WHI)		Black women (WHI)		Black women (JHS)		White women (WHI)		White women (NHS)	
				Beta	FDR-P	OR (95% CI)	FDR	OR (95% CI)	FDR	HR (95% CI)	raw-P	OR (95% CI)	FDR	HR (95% CI)	raw-P
C8-pos	C36:2 DAG	HMDB07218*	Glycerolipids - Diacylglycerols	-0.821	6.3E-20	0.90 (0.77, 1.05)	0.501	0.88 (0.55, 1.41)	0.954	-	-	0.87 (0.73, 1.04)	0.455	1.02 (0.80, 1.30)	0.904
HILIC-pos	3-methylxanthine	HMDB01886	Purines and Pyrimidines	-0.614	1.9E-11	1.09 (0.96, 1.23)	0.517	1.47 (1.03, 2.10)	0.867	-	-	1.03 (0.90, 1.18)	0.903	-	-
HILIC-pos	5-acetylamino-6-amino-3-methyluracil	HMDB04400	Amino Acids	-0.546	8.7E-10	1.09 (0.96, 1.24)	0.521	1.47 (0.96, 2.26)	0.867	-	-	1.04 (0.91, 1.20)	0.856	1.00 (0.82, 1.22)	0.994
C8-pos	C16:0 LPE	HMDB11503	Glycerophospholipids - Lysophosphatidylethanolamines	-0.513	3.3E-08	1.08 (0.95, 1.23)	0.555	1.61 (1.01, 2.54)	0.867	0.94 (0.76, 1.15)	0.539	1.04 (0.90, 1.19)	0.876	1.12 (0.94, 1.35)	0.210
C8-pos	C52:2 TAG	HMDB05369*	Glycerolipids - Triacylglycerols	-0.778	6.3E-18	0.91 (0.78, 1.06)	0.564	0.94 (0.59, 1.47)	0.991	-	-	0.88 (0.74, 1.04)	0.472	1.00 (0.79, 1.27)	0.984
C8-pos	4-cholesten-3-one	HMDB00921	Sterol lipids - Cholesterol and derivatives	-0.909	2.5E-20	1.10 (0.94, 1.29)	0.595	1.09 (0.64, 1.86)	0.991	-	-	1.10 (0.93, 1.30)	0.648	-	-
C8-pos	C42:11 PE plasmalogen	n/a	Glycerophospholipids - Phosphatidylethanolamine plasmalogens	-0.657	2.7E-13	1.09 (0.94, 1.26)	0.595	1.21 (0.75, 1.97)	0.917	-	-	1.07 (0.92, 1.25)	0.717	-	-
C8-pos	C56:3 TAG	HMDB05410*	Glycerolipids - Triacylglycerols	-0.670	3.2E-13	0.92 (0.80, 1.06)	0.595	0.91 (0.58, 1.42)	0.977	-	-	0.91 (0.78, 1.06)	0.609	0.98 (0.78, 1.22)	0.842
C8-pos	C18:2 LPE	HMDB11507*	Glycerophospholipids - Lysophosphatidylethanolamines	-0.894	8.7E-23	1.08 (0.95, 1.23)	0.603	1.26 (0.82, 1.94)	0.867	1.16 (0.93, 1.44)	0.178	1.06 (0.92, 1.22)	0.768	0.96 (0.80, 1.16)	0.692
C8-pos	C34:1 PC	HMDB07972*	Glycerophospholipids - Phosphatidylcholines	-0.526	4.3E-09	1.08 (0.94, 1.23)	0.638	1.33 (0.82, 2.17)	0.867	-	-	1.04 (0.90, 1.20)	0.867	0.96 (0.78, 1.19)	0.706
C8-pos	C51:2 TAG	HMDB49721*	Glycerolipids - Triacylglycerols	-0.829	3.1E-20	0.93 (0.81, 1.06)	0.638	1.17 (0.74, 1.84)	0.927	-	-	0.88 (0.76, 1.02)	0.421	-	-
C8-pos	C54:3 TAG	HMDB05405*	Glycerolipids - Triacylglycerols	-0.695	5.2E-14	0.92 (0.80, 1.07)	0.651	0.74 (0.46, 1.19)	0.867	-	-	0.94 (0.80, 1.10)	0.769	1.00 (0.81, 1.24)	0.967
C8-pos	C14:0 LPC-B	HMDB10379*	Glycerophospholipids - Lysophosphatidylcholines	-0.618	1.6E-10	0.93 (0.81, 1.07)	0.654	1.31 (0.77, 2.24)	0.867	-	-	0.90 (0.78, 1.04)	0.516	1.01 (0.83, 1.22)	0.917
HILIC-pos	ADMA	HMDB01539	Amino Acids	-0.547	1.4E-08	0.93 (0.82, 1.06)	0.657	1.00 (0.59, 1.68)	0.998	1.08 (0.89, 1.33)	0.438	0.93 (0.81, 1.06)	0.654	0.99 (0.81, 1.21)	0.938
C8-pos	C14:0 CE	HMDB06725	Sterol lipids - Cholesteryl esters	-0.563	1.7E-09	1.07 (0.94, 1.22)	0.662	1.35 (0.82, 2.23)	0.867	-	-	1.04 (0.91, 1.20)	0.861	1.08 (0.89, 1.30)	0.426
C8-pos	C32:2 DAG	HMDB07128*	Glycerolipids - Diacylglycerols	-0.886	5.8E-22	0.92 (0.78, 1.08)	0.662	1.13 (0.64, 1.96)	0.977	-	-	0.88 (0.74, 1.05)	0.508	-	-
HILIC-pos	N-acetylornithine	HMDB03357	Amino Acids	-0.707	1.6E-15	0.94 (0.83, 1.06)	0.681	1.01 (0.66, 1.57)	0.998	1.18 (0.97, 1.44)	0.103	0.93 (0.82, 1.07)	0.686	1.14 (0.95, 1.36)	0.153
HILIC-pos	7-methylxanthine	HMDB01991	Purines and Pyrimidines	-0.565	9.8E-10	1.06 (0.94, 1.20)	0.693	1.44 (1.00, 2.08)	0.867	-	-	1.00 (0.88, 1.15)	0.989	-	-
C8-pos	C40:11 PC plasmalogen	n/a	Glycerophospholipids - Phosphatidylcholine plasmalogens	-0.823	2.3E-19	1.06 (0.94, 1.21)	0.693	1.76 (1.11, 2.79)	0.867	-	-	1.00 (0.87, 1.14)	0.989	-	-
C8-pos	C46:2 TAG	HMDB10419*	Glycerolipids - Triacylglycerols	-0.768	2.2E-17	0.93 (0.81, 1.08)	0.693	1.14 (0.72, 1.79)	0.951	1.05 (0.85, 1.30)	0.631	0.89 (0.77, 1.04)	0.508	0.99 (0.80, 1.22)	0.905
HILIC-pos	N6,N6-dimethyllysine	HMDB13287	Amino Acids	-0.953	6.1E-25	1.06 (0.94, 1.20)	0.693	1.31 (0.89, 1.92)	0.867	0.96 (0.79, 1.18)	0.720	1.04 (0.91, 1.19)	0.867	1.02 (0.85, 1.22)	0.825
HILIC-pos	C14:0 LPC	HMDB10379	Glycerophospholipids - Lysophosphatidylcholines	-0.784	6.3E-18	0.94 (0.83, 1.07)	0.714	1.46 (0.88, 2.42)	0.867	0.85 (0.68, 1.04)	0.117	0.91 (0.80, 1.04)	0.528	1.01 (0.83, 1.22)	0.917
C8-pos	C32:1 DAG	HMDB07099*	Glycerolipids - Diacylglycerols	-0.864	1.0E-22	0.93 (0.80, 1.09)	0.714	1.13 (0.68, 1.90)	0.963	-	-	0.89 (0.75, 1.05)	0.508	1.03 (0.82, 1.29)	0.786
C8-pos	C34:1 DAG	HMDB07102*	Glycerolipids - Diacylglycerols	-0.663	3.6E-14	0.94 (0.80, 1.09)	0.743	0.97 (0.59, 1.62)	0.998	0.86 (0.69, 1.08)	0.190	0.90 (0.76, 1.07)	0.609	1.04 (0.81, 1.32)	0.777
C8-pos	C36:0 PE	HMDB08991*	Glycerophospholipids - Phosphatidylethanolamines	-0.511	3.2E-08	1.06 (0.92, 1.21)	0.743	1.80 (1.05, 3.09)	0.867	-	-	1.01 (0.87, 1.16)	0.988	0.99 (0.82, 1.19)	0.901
C8-pos	C40:6 PS	HMDB10167*	Glycerophospholipids - phosphatidylserine	-0.949	1.5E-25	1.06 (0.93, 1.20)	0.743	1.57 (0.96, 2.57)	0.867	-	-	1.01 (0.88, 1.15)	0.988	1.23 (0.81, 1.89)	0.331
C8-pos	C47:2 TAG	HMDB48435*	Glycerolipids - Triacylglycerols	-0.847	1.7E-20	0.94 (0.82, 1.08)	0.743	1.32 (0.80, 2.17)	0.867	-	-	0.90 (0.77, 1.04)	0.508	-	-
HILIC-pos	ornithine	HMDB00214	Amino Acids	-0.624	2.2E-11	0.95 (0.84, 1.08)	0.743	0.94 (0.60, 1.48)	0.991	1.00 (0.82, 1.23)	0.978	0.96 (0.84, 1.10)	0.865	-	-
C8-pos	C55:2 TAG	HMDB50319*	Glycerolipids - Triacylglycerols	-0.651	4.1E-12	0.95 (0.82, 1.09)	0.770	1.24 (0.79, 1.96)	0.867	-	-	0.90 (0.77, 1.05)	0.547	-	-
C8-pos	C15:0 LPC	HMDB10381	Glycerophospholipids - Lysophosphatidylcholines	-0.853	2.2E-21	0.96 (0.84, 1.09)	0.790	1.34 (0.84, 2.16)	0.867	-	-	0.93 (0.81, 1.06)	0.642	-	-
C8-pos	C32:1 PC	HMDB07873*	Glycerophospholipids - Phosphatidylcholines	-0.916	2.2E-27	1.04 (0.91, 1.19)	0.811	1.31 (0.83, 2.08)	0.867	-	-	1.00 (0.87, 1.16)	0.997	1.02 (0.82, 1.26)	0.852
C8-pos	C44:2 TAG	HMDB47770*	Glycerolipids - Triacylglycerols	-0.636	6.3E-12	0.96 (0.83, 1.10)	0.813	1.17 (0.74, 1.86)	0.927	1.08 (0.88, 1.34)	0.459	0.92 (0.79, 1.07)	0.648	-	-
C8-pos	C50:2 TAG	HMDB05377*	Glycerolipids - Triacylglycerols	-0.844	8.5E-23	0.95 (0.83, 1.10)	0.813	1.11 (0.69, 1.78)	0.977	-	-	0.91 (0.78, 1.07)	0.609	1.00 (0.80, 1.26)	0.994
C8-pos	C48:2 TAG	HMDB05376*	Glycerolipids - Triacylglycerols	-0.857	2.7E-22	0.96 (0.83, 1.10)	0.813	1.19 (0.74, 1.92)	0.927	-	-	0.91 (0.78, 1.06)	0.604	1.01 (0.82, 1.25)	0.905
C8-pos	C18:3 LPC	HMDB10387*	Glycerophospholipids - Lysophosphatidylcholines	-0.531	6.7E-09	1.04 (0.92, 1.18)	0.819	1.11 (0.70, 1.77)	0.963	0.82 (0.66, 1.01)	0.056	1.03 (0.90, 1.18)	0.883	0.87 (0.66, 1.15)	0.322
C8-pos	C14:0 LPC-A	HMDB10379*	Glycerophospholipids - Lysophosphatidylcholines	-0.856	1.7E-20	0.96 (0.84, 1.10)	0.822	1.34 (0.83, 2.16)	0.867	-	-	0.93 (0.81, 1.07)	0.648	1.01 (0.83, 1.22)	0.917
C8-pos	C45:2 TAG	HMDB43170*	Glycerolipids - Triacylglycerols	-0.626	4.9E-12	0.96 (0.83, 1.10)	0.824	1.32 (0.80, 2.16)	0.867	-	-	0.92 (0.79, 1.07)	0.642	0.95 (0.75, 1.20)	0.690
C8-pos	C30:0 DAG	HMDB07011*	Glycerolipids - Diacylglycerols	-0.591	4.8E-11	0.96 (0.82, 1.12)	0.839	1.32 (0.69, 2.55)	0.896	-	-	0.93 (0.79, 1.09)	0.706	0.70 (0.37, 1.32)	0.269
C8-pos	C56:2 TAG	HMDB05404*	Glycerolipids - Triacylglycerols	-0.525	1.5E-08	1.04 (0.90, 1.19)	0.856	1.21 (0.80, 1.84)	0.869	-	-	1.00 (0.86, 1.17)	0.993	0.84 (0.66, 1.07)	0.156
C8-pos	C36:2 PC	HMDB08039*	Glycerophospholipids - Phosphatidylcholines	-0.557	4.5E-09	1.03 (0.90, 1.18)	0.881	1.05 (0.65, 1.69)	0.998	1.14 (0.91, 1.44)	0.255	1.03 (0.89, 1.20)	0.900	0.99 (0.82, 1.20)	0.911
C8-pos	C36:2 PE	HMDB08994*	Glycerophospholipids - Phosphatidylethanolamines	-0.699	8.5E-15	0.97 (0.85, 1.11)	0.881	0.97 (0.64, 1.46)	0.998	**1.40 (1.13, 1.74)**	**0.002**	0.97 (0.84, 1.11)	0.883	1.12 (0.91, 1.36)	0.280
C8-pos	C49:2 TAG	HMDB11706*	Glycerolipids - Triacylglycerols	-0.986	2.8E-27	0.97 (0.85, 1.11)	0.881	1.38 (0.84, 2.26)	0.867	-	-	0.92 (0.80, 1.06)	0.634	0.96 (0.79, 1.16)	0.656
C8-pos	C54:2 TAG	HMDB05403*	Glycerolipids - Triacylglycerols	-0.531	4.1E-09	0.97 (0.83, 1.13)	0.881	0.92 (0.59, 1.43)	0.988	-	-	0.95 (0.80, 1.13)	0.870	0.96 (0.76, 1.22)	0.746
C8-pos	C32:0 DAG	HMDB07098*	Glycerolipids - Diacylglycerols	-0.587	7.8E-12	0.97 (0.84, 1.12)	0.882	1.20 (0.72, 2.00)	0.927	-	-	0.93 (0.79, 1.08)	0.706	0.97 (0.75, 1.24)	0.785
C8-pos	C28:0 PC	HMDB07866*	Glycerophospholipids - Phosphatidylcholines	-0.598	7.4E-10	1.03 (0.90, 1.17)	0.894	1.76 (1.04, 2.98)	0.867	-	-	0.97 (0.85, 1.12)	0.917	-	-
C8-pos	C30:0 PC	HMDB07869*	Glycerophospholipids - Phosphatidylcholines	-0.678	1.1E-14	1.03 (0.90, 1.17)	0.904	1.61 (0.97, 2.68)	0.867	1.10 (0.89, 1.37)	0.372	0.97 (0.84, 1.12)	0.906	1.01 (0.83, 1.24)	0.904
C8-pos	C36:3 PC	HMDB08105*	Glycerophospholipids - Phosphatidylcholines	-0.821	3.4E-20	1.02 (0.89, 1.18)	0.906	1.35 (0.80, 2.29)	0.867	-	-	0.99 (0.86, 1.15)	0.988	1.17 (0.96, 1.44)	0.128
C8-pos	C46:0 TAG	HMDB10411*	Glycerolipids - Triacylglycerols	-0.524	1.0E-08	1.02 (0.89, 1.17)	0.906	1.35 (0.79, 2.32)	0.867	-	-	0.98 (0.85, 1.13)	0.959	0.97 (0.80, 1.18)	0.760
C8-pos	C50:1 TAG	HMDB44109*	Glycerolipids - Triacylglycerols	-0.621	5.2E-13	0.98 (0.84, 1.13)	0.906	1.10 (0.68, 1.79)	0.982	-	-	0.93 (0.80, 1.09)	0.733	-	-
C8-pos	C51:1 TAG	HMDB42104*	Glycerolipids - Triacylglycerols	-0.598	2.4E-11	0.98 (0.85, 1.12)	0.906	1.26 (0.79, 2.02)	0.867	-	-	0.93 (0.80, 1.08)	0.696	1.01 (0.81, 1.25)	0.946
C8-pos	C36:1 DAG	HMDB07216*	Glycerolipids - Diacylglycerols	-0.556	7.4E-10	0.98 (0.84, 1.14)	0.929	1.01 (0.63, 1.63)	0.998	-	-	0.95 (0.81, 1.12)	0.861	1.03 (0.80, 1.33)	0.828
C8-pos	C42:0 TAG	HMDB42061*	Glycerolipids - Triacylglycerols	-0.537	4.5E-08	0.98 (0.85, 1.13)	0.929	1.38 (0.77, 2.47)	0.867	-	-	0.95 (0.82, 1.10)	0.812	-	-
C8-pos	C16:1 LPC	HMDB10383	Glycerophospholipids - Lysophosphatidylcholines	-0.962	4.5E-27	1.01 (0.89, 1.15)	0.938	1.15 (0.75, 1.77)	0.932	0.81 (0.66, 1.00)	0.052	0.99 (0.86, 1.13)	0.984	1.05 (0.87, 1.26)	0.635
C8-pos	C44:1 TAG	HMDB42301*	Glycerolipids - Triacylglycerols	-0.650	1.2E-12	0.98 (0.86, 1.13)	0.938	1.30 (0.81, 2.10)	0.867	1.04 (0.85, 1.28)	0.694	0.94 (0.81, 1.09)	0.769	0.86 (0.57, 1.29)	0.464
C8-pos	C45:1 TAG	HMDB42099*	Glycerolipids - Triacylglycerols	-0.630	8.2E-12	0.98 (0.86, 1.13)	0.938	1.40 (0.83, 2.34)	0.867	-	-	0.94 (0.81, 1.09)	0.733	1.03 (0.79, 1.34)	0.815
C8-pos	C46:1 TAG	HMDB10412*	Glycerolipids - Triacylglycerols	-0.689	1.5E-14	0.98 (0.86, 1.13)	0.938	1.27 (0.79, 2.05)	0.867	-	-	0.94 (0.81, 1.09)	0.756	1.01 (0.83, 1.24)	0.914
C8-pos	C48:1 TAG	HMDB05359*	Glycerolipids - Triacylglycerols	-0.750	2.4E-17	0.99 (0.86, 1.13)	0.938	1.27 (0.78, 2.07)	0.867	-	-	0.94 (0.81, 1.09)	0.756	1.00 (0.81, 1.23)	0.982
C18-neg	palmitoleic acid	HMDB03229	Fatty acids	-0.738	2.1E-17	0.99 (0.87, 1.12)	0.938	0.96 (0.64, 1.44)	0.998	-	-	0.99 (0.86, 1.13)	0.971	1.19 (0.81, 1.77)	0.376
C8-pos	C30:1 PC	HMDB07870*	Glycerophospholipids - Phosphatidylcholines	-0.912	1.1E-24	1.01 (0.88, 1.16)	0.954	1.54 (0.92, 2.56)	0.867	-	-	0.96 (0.83, 1.11)	0.867	1.07 (0.87, 1.31)	0.536
C8-pos	C47:1 TAG	HMDB42100*	Glycerolipids - Triacylglycerols	-0.747	4.5E-16	0.99 (0.87, 1.13)	0.954	1.49 (0.89, 2.49)	0.867	-	-	0.94 (0.81, 1.08)	0.726	1.03 (0.84, 1.25)	0.800
C18-neg	hexadecanedioate	HMDB00672	Fatty acids	-0.587	4.3E-11	1.01 (0.89, 1.14)	0.954	0.97 (0.61, 1.53)	0.998	-	-	1.00 (0.88, 1.14)	0.988	0.91 (0.65, 1.27)	0.595
C8-pos	C44:0 TAG	HMDB42063*	Glycerolipids - Triacylglycerols	-0.544	9.1E-09	0.99 (0.86, 1.14)	0.972	1.30 (0.75, 2.25)	0.867	-	-	0.96 (0.83, 1.11)	0.867	0.94 (0.73, 1.21)	0.620

Method	Metabolite	HMDB ID	Category	SD-difference in the WHI-HT		Associations between metabolite with large race differences and CHD risk in women from WHI, JHS, and NHS									
						All women (WHI)		Black women (WHI)		Black women (JHS)		White women (WHI)		White women (NHS)	
				Beta	FDR-P	OR (95% CI)	FDR	OR (95% CI)	FDR	HR (95% CI)	raw-P	OR (95% CI)	FDR	HR (95% CI)	raw-P
C8-pos	C36:3 PE	HMDB09060*	Glycerophospholipids - Phosphatidylethanolamines	-0.662	1.8E-13	0.99 (0.88, 1.13)	0.972	1.00 (0.67, 1.51)	0.998	-	-	0.99 (0.87, 1.14)	0.988	1.16 (0.96, 1.40)	0.135
C8-pos	C38:2 PE	HMDB08942*	Glycerophospholipids - Phosphatidylethanolamines	-0.596	3.7E-11	1.00 (0.87, 1.14)	0.977	1.41 (0.81, 2.43)	0.867	-	-	0.98 (0.84, 1.13)	0.921	0.92 (0.76, 1.12)	0.408
C8-pos	C34:2 PC	HMDB07973*	Glycerophospholipids - Phosphatidylcholines	-0.734	4.3E-16	1.00 (0.86, 1.16)	0.992	1.08 (0.65, 1.82)	0.991	-	-	0.99 (0.85, 1.15)	0.986	0.98 (0.80, 1.19)	0.804
C8-pos	C34:2 PE	HMDB08928*	Glycerophospholipids - Phosphatidylethanolamines	-0.608	6.5E-12	1.00 (0.88, 1.14)	0.995	1.17 (0.76, 1.81)	0.927	**1.29 (1.03, 1.60)**	**0.024**	0.98 (0.85, 1.12)	0.921	**1.25 (1.03, 1.52)**	**0.026**
C8-pos	C49:1 TAG	HMDB11705*	Glycerolipids - Triacylglycerols	-0.747	1.1E-15	1.00 (0.88, 1.14)	0.995	1.43 (0.88, 2.34)	0.867	-	-	0.95 (0.83, 1.09)	0.795	1.15 (0.88, 1.50)	0.312

Associations between selected metabolites (>0.5 SD difference in levels between Black and White women in the WHI-HT) and CHD risk in the WHI (combining WHI-OS and placebo arms of WHI-HT; analyses were also stratified by self-reported race), JHS (Black women only), and NHS (White women only). Levels of individual metabolites in each cohort were inverse-normal transformed.
In the WHI, CHD cases were matched to an equal number of healthy controls on baseline age, self-reported race (Black and White), hysterectomy status, and enrollment window, and conditional logistic regression models were used to estimate the associations between metabolites and CHD risk.
In the JHS and NHS, incident CHD cases were documented, and cox proportional-hazards models were used for available metabolites.
Models were adjusted for sub-studies (OS/Estrogen-alone trial/Estrogen-plus-progestin trial; WHI only), batch (JHS only), age (JHS and NHS), body mass index, menopausal status (JHS and NHS), hormone therapy use status, smoking status, diabetes, antihyperglycemic medication use, systolic blood pressure, antihypertensive medication use, aspirin use, lipid-lowing medication use, and plasma levels of total and high-density lipoprotein cholesterol.

Table S6. Components and their coefficients (estimated using elastic net) in the Racial Difference Metabolomic Pattern (RDMP).

Metabolite name and other components	Method	Category	HMDB ID	Coefficient	Avaliable in MESA	Avaliable in JHS	Avaliable in NHS
Intercept				-2.816	Yes	Yes	Yes
Baseline age				-0.034	Yes	Yes	Yes
C36:4 DAG-B	C8-pos	Diacylglycerols	HMDB07248*	0.091			Yes
C38:5 DAG	C8-pos	Diacylglycerols	HMDB07199*	0.037	Yes		Yes
C16:1 MAG	C8-pos	Monoacylglycerols	HMDB11534*	0.021	Yes		
C22:1 MAG	C8-pos	Monoacylglycerols	HMDB11582*	-0.002			
C45:3 TAG	C8-pos	Triacylglycerols	n/a	0.194	Yes		
C52:0 TAG	C8-pos	Triacylglycerols	HMDB05365*	0.356	Yes		Yes
C54:3 TAG	C8-pos	Triacylglycerols	HMDB05405*	-0.096	Yes		Yes
C54:4 TAG	C8-pos	Triacylglycerols	HMDB05370*	-0.328	Yes		Yes
C55:3 TAG	C8-pos	Triacylglycerols	n/a	-0.131	Yes		
C58:10 TAG	C8-pos	Triacylglycerols	HMDB05476*	0.059	Yes		Yes
C60:12 TAG	C8-pos	Triacylglycerols	HMDB05478*	0.077	Yes		Yes
C18:0 LPC	HILIC-pos	Lysophosphatidylcholines	HMDB10384	0.175	Yes	Yes	Yes
C22:4 LPC	C8-pos	Lysophosphatidylcholines	HMDB10401*	0.323		Yes	
C32:1 PC plasmalogen-A	C8-pos	Phosphatidylcholine plasmalogens	HMDB13404*	-0.249			
C34:4 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11212*	-0.423	Yes		Yes
C36:2 PC plasmalogen-A	C8-pos	Phosphatidylcholine plasmalogens	HMDB11243*	0.037			Yes
C36:2 PC plasmalogen-B	C8-pos	Phosphatidylcholine plasmalogens	HMDB11243*	0.193			Yes
C36:3 PC plasmalogen-B	C8-pos	Phosphatidylcholine plasmalogens	HMDB11244*	0.221			Yes
C36:4 PC plasmalogen-A	C8-pos	Phosphatidylcholine plasmalogens	HMDB11310*	-0.121			Yes
C38:4 PC plasmalogen-B	C8-pos	Phosphatidylcholine plasmalogens	HMDB11252*	0.374			Yes
C38:6 PC plasmalogen-A	C8-pos	Phosphatidylcholine plasmalogens	HMDB11319*	0.501		Yes	
C40:11 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	n/a	-0.212			
C40:7 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11294*	0.029	Yes		
C30:1 PC	C8-pos	Phosphatidylcholines	HMDB07870*	-0.049	Yes		Yes
C31:1 PC	C8-pos	Phosphatidylcholines	HMDB07936*	-0.378			
C32:0 PC	C8-pos	Phosphatidylcholines	HMDB07871*	-0.076	Yes		Yes
C32:2 PC	C8-pos	Phosphatidylcholines	HMDB07874*	-0.227	Yes	Yes	Yes
C34:3 PC	C8-pos	Phosphatidylcholines	HMDB08006*	-0.243	Yes	Yes	Yes
C34:5 PC	C8-pos	Phosphatidylcholines	HMDB07885*	-0.224			
C36:4 PC-B	C8-pos	Phosphatidylcholines	HMDB08138*	0.014	Yes		Yes
C34:2 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB08952*	-0.046	Yes	Yes	Yes
C36:2 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB09082*	-0.166	Yes		Yes
C42:11 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	n/a	-0.193			
C34:2 PE	C8-pos	Phosphatidylethanolamines	HMDB08928*	0.026	Yes	Yes	Yes
C36:0 PE	C8-pos	Phosphatidylethanolamines	HMDB08991*	-0.073	Yes		Yes
C40:6 PS	C8-pos	phosphatidylserine	HMDB10167*	-0.041	Yes		Yes
4-cholesten-3-one	C8-pos	Cholesteryl	HMDB00921	-0.512			
C16:0 CE	C8-pos	Cholesteryl esters	HMDB00885	0.425	Yes		Yes
C16:1 CE	C8-pos	Cholesteryl esters	HMDB00658*	-0.263	Yes		Yes
C20:1 CE	C8-pos	Cholesteryl esters	HMDB05193	0.101			
C20:2 CE	C8-pos	Cholesteryl esters	HMDB06734	0.224			
C20:4 CE	C8-pos	Cholesteryl esters	HMDB06726	0.313	Yes		Yes
C20:5 CE	C8-pos	Cholesteryl esters	HMDB06731	-0.306	Yes		Yes
C22:4 CE	C8-pos	Cholesteryl esters	HMDB06729*	0.198	Yes		Yes
C16:0 Ceramide (d18:1)	C8-pos	Ceramides	HMDB04949	-0.328	Yes	Yes	Yes
sphingosine	HILIC-pos	Sphingolipids	HMDB00252	0.147	Yes		
C18:1 SM	C8-pos	Sphingomyelins	HMDB12101	0.108	Yes	Yes	Yes
C22:1 SM	C8-pos	Sphingomyelins	HMDB12104	0.387	Yes		
15-HETE	C18-neg	Fatty acids	HMDB03876	-0.198			
2-hydroxyhexadecanoate	C18-neg	Fatty acids	HMDB31057	-0.169			Yes
8,11,14-eicosatrienoic acid	C18-neg	Fatty acids	HMDB02925	-0.005			Yes
docosapentaenoic acid	C18-neg	Fatty acids	HMDB01976	-0.234			
eicosanedioate	C18-neg	Fatty acids	n/a	0.038			
hexadecanedioate	C18-neg	Fatty acids	HMDB00672	-0.525			Yes
hydroxymyristate	C18-neg	Fatty acids	HMDB02261	-0.297			Yes
LTB4	C18-neg	Fatty acids	HMDB01085	0.167			
palmitoleic acid	C18-neg	Fatty acids	HMDB03229	-0.101			Yes
PGE2	C18-neg	Fatty acids	HMDB01220	0.645			
stearate	C18-neg	Fatty acids	HMDB00827	0.364			Yes
C12 carnitine	HILIC-pos	Acylcarnitines	HMDB02250	-0.006	Yes	Yes	Yes
C12:1 carnitine	HILIC-pos	Acylcarnitines	HMDB13326	-0.042	Yes	Yes	Yes
C18 carnitine	HILIC-pos	Acylcarnitines	HMDB00848	0.346	Yes	Yes	
C2 carnitine	HILIC-pos	Acylcarnitines	HMDB00201	-0.086	Yes	Yes	Yes
C3 carnitine	HILIC-pos	Acylcarnitines	HMDB00824	0.066	Yes	Yes	Yes
C3-DC-CH3 carnitine	HILIC-pos	Acylcarnitines	HMDB13133	0.356	Yes	Yes	
C4 carnitine	HILIC-pos	Acylcarnitines	HMDB02013	-0.333	Yes	Yes	Yes
C5 carnitine	HILIC-pos	Acylcarnitines	HMDB00688	0.268	Yes	Yes	Yes
C5-DC carnitine	HILIC-pos	Acylcarnitines	HMDB13130	-0.060	Yes	Yes	Yes
C7 carnitine	HILIC-pos	Acylcarnitines	HMDB13238	0.037		Yes	Yes

Metabolite name and other components	Method	Category	HMDB ID	Coefficient	Avaliable in MESA	Avaliable in JHS	Avaliable in NHS
4-hydroxyhippurate	HILIC-pos	Amino Acids	HMDB13678	-0.069			Yes
5-acetylamino-6-amino-3-methyluracil	HILIC-pos	Amino Acids	HMDB04400	-0.005	Yes		Yes
ADMA	HILIC-pos	Amino Acids	HMDB01539	-0.134	Yes	Yes	Yes
alanine	HILIC-pos	Amino Acids	HMDB00161	-0.296	Yes	Yes	Yes
aminoisobutyric acid	HILIC-pos	Amino Acids	HMDB03911	-0.086			
asparagine	HILIC-pos	Amino Acids	HMDB00168	-0.127		Yes	Yes
creatinine	HILIC-pos	Amino Acids	HMDB00562	0.375	Yes	Yes	Yes
cystathionine	HILIC-neg	Amino Acids	HMDB00099	0.021			
dimethylglycine	HILIC-pos	Amino Acids	HMDB00092	0.094	Yes	Yes	Yes
glutamine	HILIC-pos	Amino Acids	HMDB00641	-0.406	Yes	Yes	Yes
glycine	HILIC-pos	Amino Acids	HMDB00123	-0.045	Yes	Yes	Yes
histidine	HILIC-pos	Amino Acids	HMDB00177	-0.406	Yes	Yes	Yes
homoarginine	HILIC-pos	Amino Acids	HMDB00670	0.476	Yes	Yes	Yes
hydroxyproline	HILIC-pos	Amino Acids	HMDB00725	0.047	Yes	Yes	Yes
isoleucine	HILIC-pos	Amino Acids	HMDB00172	0.212	Yes	Yes	Yes
kynurenine	HILIC-neg	Amino Acids	HMDB00684	-0.297	Yes	Yes	Yes
lysine	HILIC-pos	Amino Acids	HMDB00182	-0.387	Yes	Yes	Yes
methionine	HILIC-pos	Amino Acids	HMDB00696	0.510	Yes	Yes	Yes
N-acetylaspartic acid	HILIC-pos	Amino Acids	HMDB00812	0.243	Yes	Yes	Yes
N-acetylornithine	HILIC-pos	Amino Acids	HMDB03357	-0.304	Yes	Yes	Yes
N-alpha-acetylarginine	HILIC-pos	Amino Acids	HMDB04620	0.440	Yes	Yes	Yes
N6-acetyllysine	HILIC-pos	Amino Acids	HMDB00206	-0.012	Yes	Yes	Yes
N6,N6-dimethyllysine	HILIC-pos	Amino Acids	HMDB13287	-0.701		Yes	Yes
ornithine	HILIC-pos	Amino Acids	HMDB00214	-0.092	Yes	Yes	
phenylacetylglutamine	HILIC-pos	Amino Acids	HMDB06344	-0.135	Yes	Yes	Yes
phenylalanine	HILIC-pos	Amino Acids	HMDB00159	-0.080	Yes	Yes	
phosphocreatine	HILIC-neg	Amino Acids	HMDB01511	-0.019	Yes		
pyroglutamate	HILIC-pos	Amino Acids	HMDB00267	-0.186		Yes	
SDMA	HILIC-pos	Amino Acids	HMDB03334	-0.012	Yes	Yes	Yes
threonine	HILIC-pos	Amino Acids	HMDB00167	0.045	Yes	Yes	Yes
trimethylamine-N-oxide	HILIC-pos	Amino Acids	HMDB00925	0.357	Yes	Yes	Yes
valine	HILIC-pos	Amino Acids	HMDB00883	0.263	Yes	Yes	Yes
bilirubin	HILIC-pos	Bile acids and Bilirubins	HMDB00054	-0.123	Yes	Yes	Yes
deoxycholate	C18-neg	Bile acids and Bilirubins	HMDB00626	0.031			
glycochenodeoxycholate	C18-neg	Bile acids and Bilirubins	HMDB00637	-0.050		Yes	Yes
glycodeoxycholate/glycochenodeoxycholate	HILIC-pos	Bile acids and Bilirubins	n/a	-0.072	Yes	Yes	
glycoursodeoxycholate	C18-neg	Bile acids and Bilirubins	HMDB00708	-0.389			Yes
taurocholate	C18-neg	Bile acids and Bilirubins	HMDB00036	0.369		Yes	Yes
1-methylguanine	HILIC-pos	Purines and Pyrimidines	HMDB03282	0.161	Yes	Yes	Yes
3-methylxanthine	HILIC-pos	Purines and Pyrimidines	HMDB01886	-0.309	Yes		
7-methylguanine	HILIC-pos	Purines and Pyrimidines	HMDB00897	0.083	Yes	Yes	Yes
7-methylxanthine	HILIC-pos	Purines and Pyrimidines	HMDB01991	-0.487	Yes		
AMP	HILIC-neg	Purines and Pyrimidines	HMDB00045	0.246			
cAMP	HILIC-neg	Purines and Pyrimidines	HMDB00058	0.233	Yes	Yes	
CMP	HILIC-neg	Purines and Pyrimidines	HMDB00095	0.267			
cytidine	HILIC-neg	Purines and Pyrimidines	HMDB00089	-0.062			
cytosine	HILIC-pos	Purines and Pyrimidines	HMDB00630	-0.032			Yes
hypoxanthine	HILIC-neg	Purines and Pyrimidines	HMDB00157	0.196	Yes	Yes	
inosine	HILIC-neg	Purines and Pyrimidines	HMDB00195	0.327	Yes	Yes	
N2,N2-dimethylguanosine	HILIC-pos	Purines and Pyrimidines	HMDB04824	0.033		Yes	Yes
UDP-galactose/UDP-glucose	HILIC-neg	Purines and Pyrimidines	HMDB00286	-0.141	Yes		
UDP-glucuronate	HILIC-neg	Purines and Pyrimidines	HMDB00935	-0.002			
uracil	HILIC-neg	Purines and Pyrimidines	HMDB00300	-0.073			Yes
urate	HILIC-neg	Purines and Pyrimidines	HMDB00289	0.468	Yes	Yes	Yes
xanthosine	HILIC-pos	Purines and Pyrimidines	HMDB00299	0.204		Yes	
xanthurenate	HILIC-neg	Purines and Pyrimidines	HMDB00881	0.082	Yes	Yes	Yes
betaine	HILIC-pos	Quaternary Amines	HMDB00043	0.009	Yes	Yes	Yes
kynurenic acid	HILIC-pos	Indoles and Indole derivatives	HMDB00715	-0.227	Yes	Yes	Yes
tryptamine	HILIC-pos	Indoles and Indole derivatives	HMDB00303	-0.226			
N1-methyl-2-pyridone-5-carboxamide	HILIC-pos	Pyridines and derivatives	HMDB04193	0.007	Yes	Yes	Yes
indoxylsulfate	HILIC-neg	Arylsulfates	HMDB00682	-0.215	Yes	Yes	Yes
alpha-ketoglutarate	HILIC-neg	Dicarboxylic acids	HMDB00208	0.120			
fumarate/maleate	HILIC-neg	Dicarboxylic acids	HMDB00134	0.207	Yes	Yes	
methylmalonate	HILIC-neg	Dicarboxylic acids	HMDB00202	-0.125			
oxalate	HILIC-neg	Dicarboxylic acids	HMDB02329	0.124	Yes	Yes	
succinate	HILIC-neg	Dicarboxylic acids	HMDB00254	0.210	Yes	Yes	
alpha-hydroxybutyrate	HILIC-neg	Hydroxy acids and derivatives	HMDB00008	-0.222	Yes	Yes	Yes
lactate	HILIC-neg	Hydroxy acids and derivatives	HMDB00190	0.028	Yes	Yes	
6-phosphogluconate	HILIC-neg	Carbohydrates and conjugates	HMDB01316	-0.154			
glucose	HILIC-pos	Carbohydrates and conjugates	HMDB00122	0.539		Yes	
hydroxyphenylacetate	HILIC-neg	Aromatic acids	HMDB00020	-0.308			Yes
trimethylbenzene	HILIC-pos	Benzene and derivatives	HMDB13733	0.228	Yes	Yes	Yes

Metabolite name and other components	Method	Category	HMDB ID	Coefficient	Avaliable in MESA	Avaliable in JHS	Avaliable in NHS
acetaminophen	HILIC-pos	Benzenoids	HMDB01859	-0.147	Yes	Yes	Yes
hippurate	HILIC-neg	Benzenoids	HMDB00714	-0.058	Yes	Yes	Yes
salicylurate	HILIC-neg	Benzenoids	HMDB00840	0.325		Yes	Yes
allantoin	HILIC-pos	Others	HMDB00462	0.099		Yes	Yes
cortisol	HILIC-pos	Others	HMDB00063	-0.372	Yes	Yes	Yes
hydroxyectoine	HILIC-pos	Others	n/a	-0.065		Yes	
L-threo-Sphingosine	HILIC-pos	Others	n/a	0.275			
piperine	HILIC-pos	Others	HMDB29377	0.395	Yes	Yes	Yes
putrescine	HILIC-pos	Others	HMDB01414	-0.297			Yes
thiamine	HILIC-pos	Others	HMDB00235	-0.292		Yes	Yes
trigonelline	HILIC-pos	Others	HMDB00875	-0.053	Yes	Yes	Yes

Supplemental Figures

Figure S1. Flow chart for the statistical analysis approaches of this study.

This study aimed to examine differences between Black and White women in metabolomic profiles and investigate whether such differences explain racial differences in CHD risk. **First**, we performed metabolome-wide association analysis to estimate differences in metabolomic profiles between Black and White women in the WHI-OS (discovery); findings were replicated in the WHI-HT (replication) and MESA (validation). **Second**, we constructed the Racial Difference Metabolomic Pattern (RDMP) that represents differences in metabolomic profiles between Black and White women in the WHI-OS (training). We then compared the distribution of the RDMP between Black and White women from the WHI-OS, WHI-HT (internal testing), and MESA (external testing). **Third**, we estimated associations of metabolites with large race differences and the RDMP (quartiles) with the risk of CHD in the WHI (combining WHI-OS and placebo arms of the WHI-HT), adjusting for baseline characteristics and known CHD risk factors. We also performed race-stratified analyses in the WHI and replicated in the JHS (Black women) and NHS (White women).

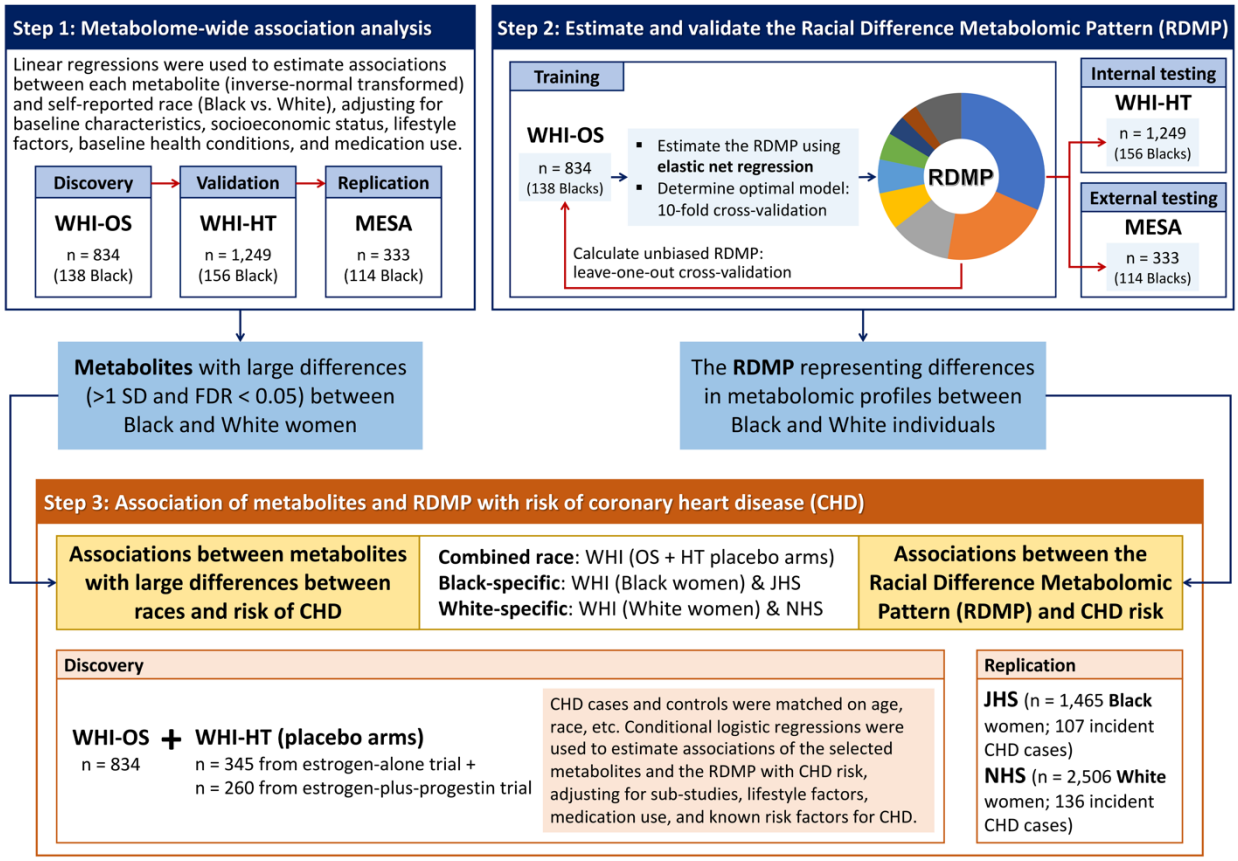
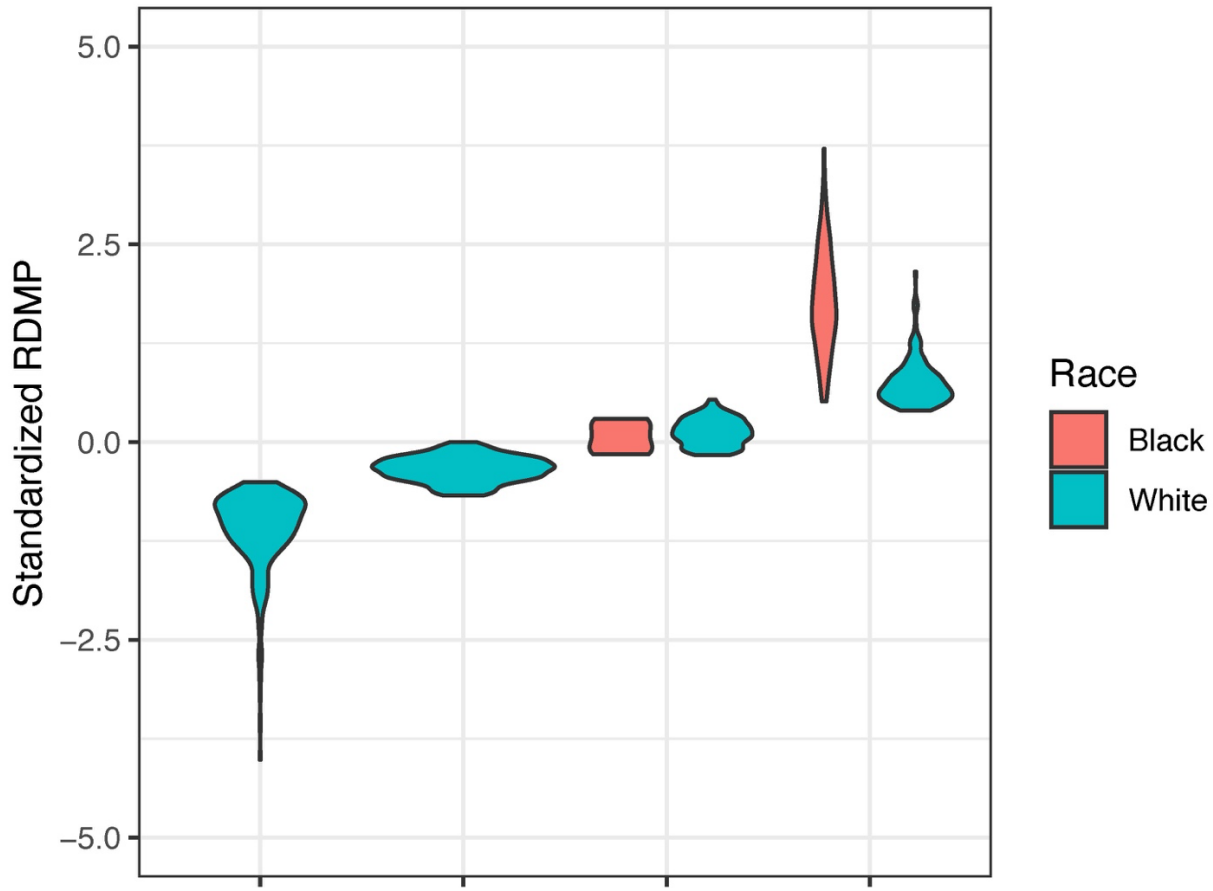


Figure S2. Distributions of Racial Difference Metabolomic Pattern (RDMP) z-score in each RDMP quartile in the WHI by race.

The violin plot showed distributions of the RDMP in WHI participants that were used to estimate associations between RDMP and CHD risk (i.e., combined datasets for WHI-OS and placebo arms of the WHI-HT). The table below showed the numbers (percentages) of all women and women of each race group in each RDMP quartile category.



	Quartile 1	Quartile 2	Quartile 3	Quartile 4
Total N	359 (25.0%)	359 (25.0%)	359 (25.0%)	359 (25.0%)
Black	0 (0%)	1 (0.5%)	6 (2.8%)	210 (96.8%)
White	359 (29.5%)	358 (29.4%)	353 (29.0%)	149 (12.2%)

Figure S3. Concordance of regression coefficients associated with self-reported race (Black vs White) between WHI-OS, WHI-HT, and MESA.

Regression coefficients associated with self-reported race (Black vs White) were estimated using linear regression models in the metabolome-wide association analysis, and represented difference in SD units for each metabolite between Black and White participants. Models were adjusted for baseline age, coronary heart disease case-control status (WHI only), hysterectomy status, hormone therapy status (never/past/current users), enrollment window (WHI only), body mass index, smoking status, alcohol consumption, education, family income, physical activity, baseline health conditions (diabetes, hypertension, and depression), and medication use (aspirin, statin or other lipid-lowing, antihyperglycemic, and antihypertensive). Concordance of association coefficients between the discovery set (WHI-OS) and A) WHI-HT and B) women from the MESA were evaluated by Pearson correlation coefficients (r).

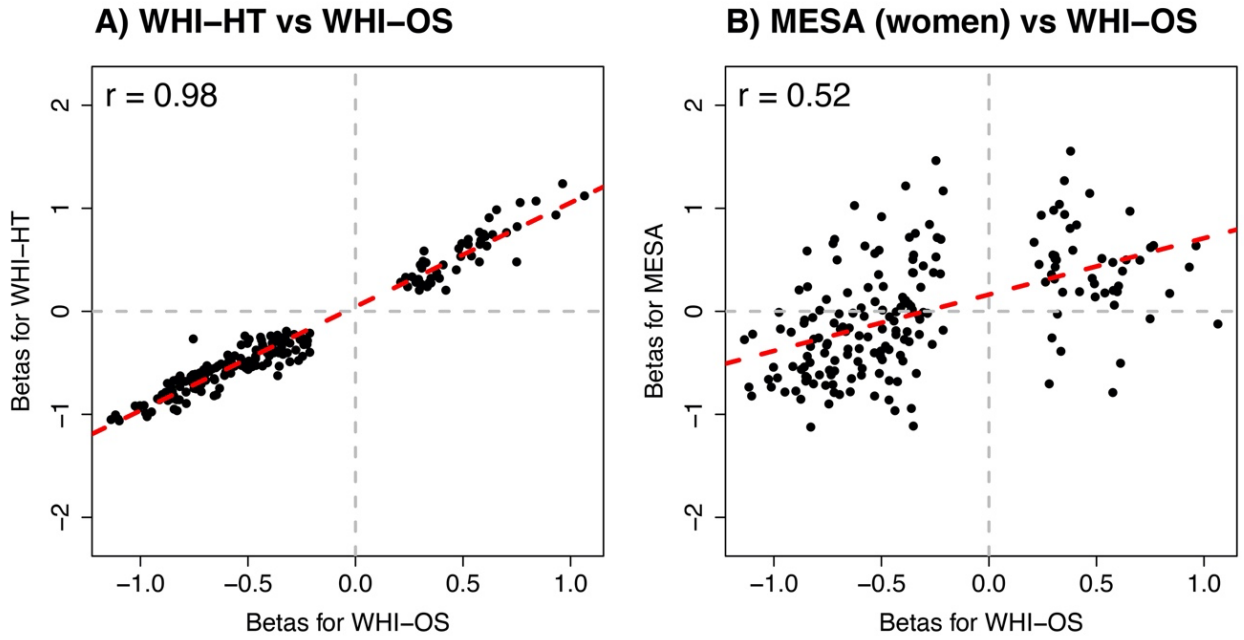
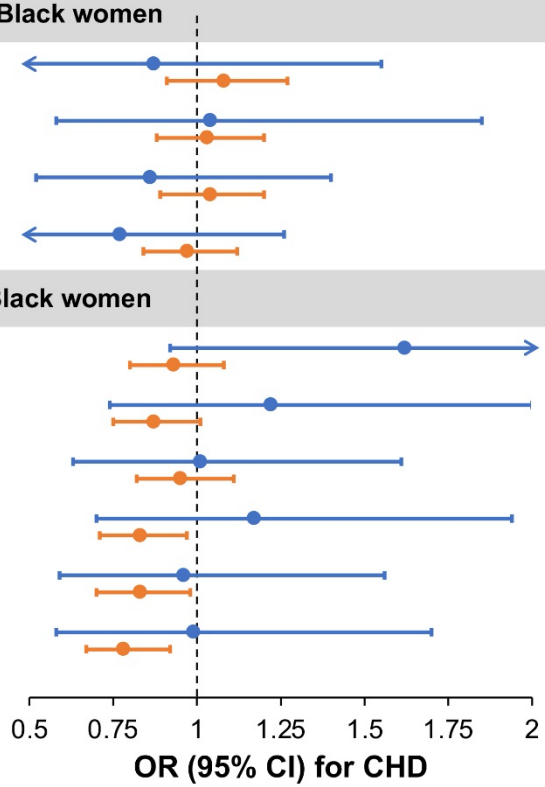


Figure S4. Associations between metabolites with >1 SD difference by race and with CHD risk in the WHI, stratified by self-reported race.

Associations were estimated in the combined dataset of WHI-OS and placebo arms of WHI-HT, stratified by self-reported race. CHD cases were matched to controls on age, self-reported race, hysterectomy, and enrollment window. Conditional logistic regression models were adjusted for sub-studies (OS/estrogen-alone trial/estrogen-plus-progestin trial), body mass index, hormone therapy use status, smoking, diabetes, antihyperglycemic medication use, systolic blood pressure, antihypertensive medication use, aspirin use, lipid-lowing medication use, and total and high-density lipoprotein cholesterol.



Metabolite	Black women		White women	
	OR (95% CI)	FDR	OR (95% CI)	FDR
More than 1-SD higher in Black women				
C20:4 CE	0.87 (0.49, 1.55)	0.963	1.08 (0.91, 1.27)	0.733
C22:4 CE	1.04 (0.58, 1.85)	0.998	1.03 (0.88, 1.20)	0.921
C22:6 CE	0.86 (0.52, 1.40)	0.932	1.04 (0.89, 1.20)	0.883
C40:7 PE plasmalogen	0.77 (0.47, 1.26)	0.867	0.97 (0.84, 1.12)	0.906
More than 1-SD lower in Black women				
C31:1 PC	1.62 (0.92, 2.83)	0.867	0.93 (0.80, 1.08)	0.706
C32:2 PC	1.22 (0.74, 2.00)	0.917	0.87 (0.75, 1.01)	0.359
C34:3 PC	1.01 (0.63, 1.61)	0.998	0.95 (0.82, 1.11)	0.829
C49:3 TAG	1.17 (0.70, 1.94)	0.944	0.83 (0.71, 0.97)	0.138
C50:3 TAG	0.96 (0.59, 1.56)	0.998	0.83 (0.70, 0.98)	0.192
C51:3 TAG	0.99 (0.58, 1.70)	0.998	0.78 (0.67, 0.92)	0.049

Figure S5. Receiver operating characteristic (ROC) performance of the Racial Difference Metabolomic Pattern (RDMP) and the restricted RDMP (rRDMP) and self-reported race in WHI and MESA.

ROC curves were used and the area under the ROC curves (AUC) were calculated. The RDMP were estimated using elastic net regression in the WHI-OS (training set). The RDMP composed of 152 metabolites, but only 93 of these metabolites were available in the MESA (used to calculate rRDMP1), 79 were available in the JHS (used to calculate rRDMP2), and 98 were available in the NHS (used to calculate rRDMP3). To evaluate changes in the ROC performance when reducing the number of metabolites, we calculated RDMP, rRDMP1, rRDMP2, and rRDMP3 in the WHI-HT. The red line is the ROC curve for WHI-OS in which the RDMP was calculated using a leave-one-out cross-validation approach to avoid overfitting. The blue lines are ROCs for RDMP, rRDMP1, rRDMP2, and rRDMP3 in the WHI-HT (internal testing). The orange line is the ROC for rRDMP1 in women from the MESA (external testing).

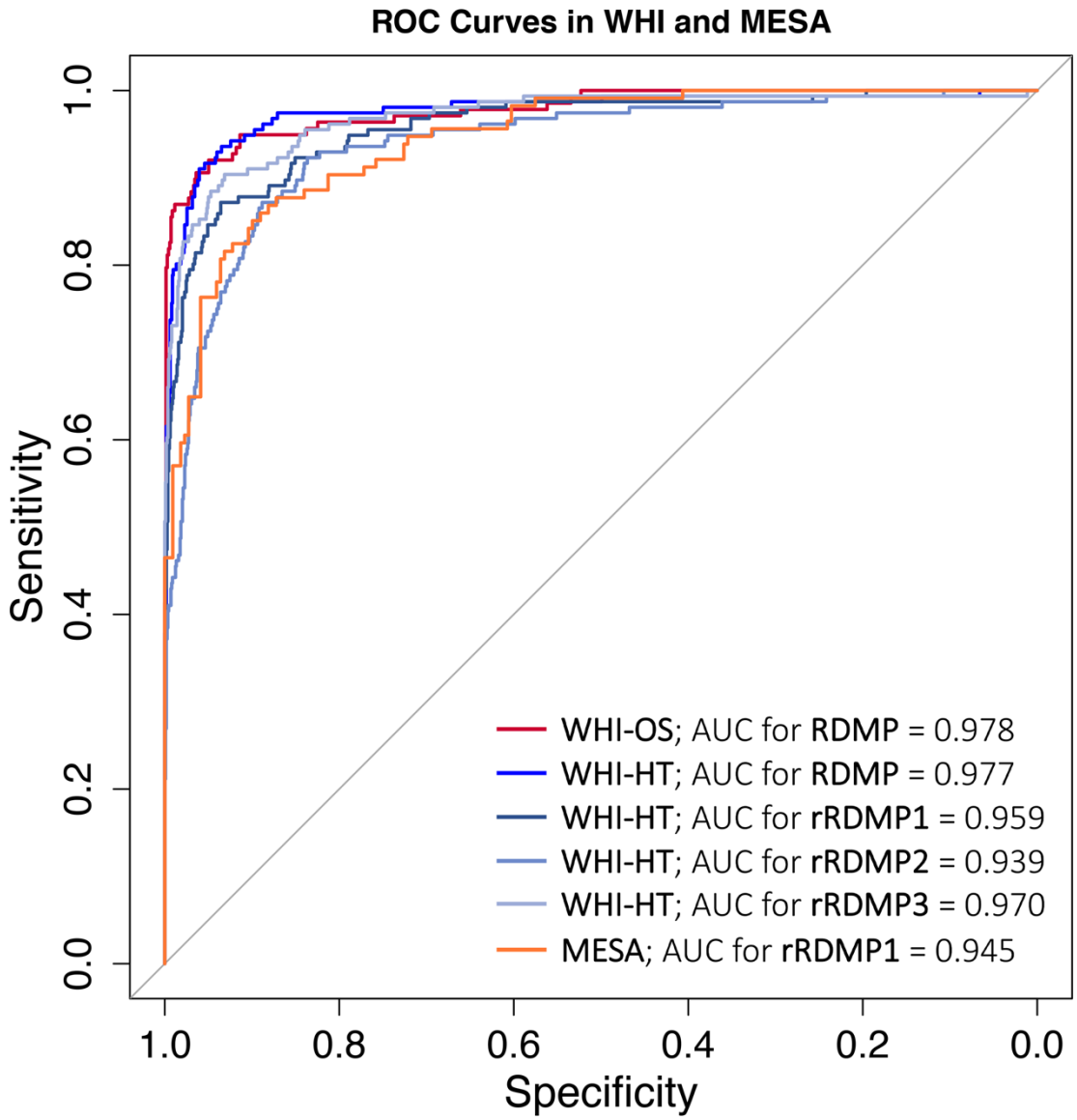


Figure S6. Distributions of restricted Racial Difference Metabolomic Pattern (rRDMP) that were calculated using the overlapping metabolites with MESA, JHS, or NHS in the WHI-HT.

The RDMP was calculated based on 152 metabolites in the WHI-OS, only 93 of these metabolites were available in the MESA (used to calculate rRDMP1), 79 were available in the JHS (used to calculate rRDMP2), and 98 were available in the NHS (used to calculate rRDMP3). We then compared the distributions of A) rRDMP1, B) rRDMP2, and C) rRDMP3 between Black and White women from the WHI-HT using violin plots. *P*-values were calculated using Wilcoxon signed-rank test, indicating whether median rRDMPs were different between Black and White women.