Supplementary Table 1. Age-adjusted baseline population characteristics according to incident diabetes status in the HCHS/SOL*

	Cases (N = 224)	Non-cases (N = 1786)	P value
Age, years	46.7 (43.8-49.6)	37.6 (36.7-38.6)	<0.001
Male, %	46.7 (39.4-54.1)	50.2 (47.0-53.4)	0.38
Study field center			
Bronx	37.2 (27.7-47.9)	30.5 (26.7-34.7)	0.47
Chicago	13.3 (9.2-18.8)	12.2 (10.3-14.4)	
Miami	21.2 (15.4-28.4)	33.8 (29.3-38.6)	
San Diego	28.3 (19.2-40.0)	23.5 (19.8-27.8)	
Hispanic background, %			
Dominican	19.7 (13.5-27.7)	11.3 (9.2-13.9)	0.58
Central/South American	7.0 (4.0-11.9)	12.8 (10.8-15.1)	
Cuban	17.8 (12.0-25.7)	23.3 (19.9-27.2)	
Mexican	39.8 (31.0-49.2)	31.0 (27.5-34.7)	
Puerto-Rican	13.9 (9.4-20.1)	17.5 (14.9-20.5)	
Other heritage	1.8 (0.6-5.1)	4.1 (2.9-5.8)	
Above high school education, %	39.3 (30.7-48.6)	45.0 (41.4-48.6)	0.16
Family yearly income, %			
< $30,000	78.9 (72.7-83.9)	55.5 (52.0-59.0)	0.002
≥ $30,000	18.0 (13.3-23.9)	38.2 (34.7-41.9)	
Not reported	3.1 (1.6-6.3)	6.3 (4.8-8.2)	
Current smoker, %	13.5 (8.6-20.4)	21.4 (18.8-24.2)	0.19
Current drinker, %	53.6 (43.2-63.7)	56.0 (52.5-59.3)	0.48
Total energy intake, kcal/day	2025 (1907-2143)	2041 (1998-2084)	0.79
AHEI-2010 score	47.4 (45.4-49.4)	46.7 (46.2-47.1)	0.46
Physical activity, MET-min/day	12.3 (9.3-15.3)	12.5 (11.2-13.8)	0.86
Use of antihypertensive drugs, %	13.0 (8.8-18.8)	9.4 (7.8-11.4)	0.002
Use of lipid-lowering drugs, %	8.8 (5.4-14.2)	5.8 (4.4-7.6)	0.005
Family history of diabetes, %	53.5 (45.4-61.4)	36.4 (33.3-39.6)	0.007
Fasting time, hours	14.3 (13.7-14.9)	14.4 (14.1-14.6)	0.73
Risk traits			
BMI, kg/m^2	31.7 (30.6-32.8)	28.6 (28.2-29.0)	<0.001
Waist circumference, cm	0.944 (0.932-0.957)	0.908 (0.903-0.913)	<0.001
SBP, mmHg	120.5 (116.5-124.5)	117.6 (116.6-118.5)	0.16
DBP, mmHg	75.3 (72.8-77.9)	71.6 (70.9-72.2)	0.004
Triglyceride, mg/dL	161.2 (144.1-178.3)	118.5 (114.3-122.7)	<0.001
HDL cholesterol, mg/dL	45.0 (42.2-47.9)	49.7 (48.9-50.5)	0.002
CRP, mg/L	4.7 (3.5-5.8)	3.4 (3.0-3.9)	0.071

*All data are age-adjusted mean (95% CI) for continuous variables or percentage (95% CI) for categorical variables.

Supplementary Table 2. Associations of 624 metabolites with incident diabetes in the HCHS/SOL and the related metabolite module detected by topological overlap measures

No.	Sub No.	Metabolites	RR (95% CI)	P value	P value (FDR)	Pathway	Sub-pathway	Modules	Module color
1	1	behenoyl dihydrosphingomyelin (d18:0/22:0)*	1.76 (1.51-2.07)	6.18E-12	3.86E-09	Lipid	Sphingolipid Metabolism	Lipid module 1 (Sphingolipids)	Black
2	2	behenoyl sphingomyelin (d18:1/22:0)*	1.42 (1.17-1.71)	0.000333629	0.003304519	Lipid	Sphingolipid Metabolism	Lipid module 1 (Sphingolipids)	Black
3	3	cholesterol	1.45 (1.16-1.81)	0.001208391	0.009309085	Lipid	Sterol	Lipid module 1 (Sphingolipids)	Black
4	4	lignoceroyl sphingomyelin (d18:1/24:0)	1.32 (1.09-1.59)	0.00428363	0.023865941	Lipid	Sphingolipid Metabolism	Lipid module 1 (Sphingolipids)	Black
5	5	N-palmitoyl-sphingosine (d18:1/16:0)	1.30 (1.09-1.56)	0.00343493	0.022139306	Lipid	Ceramides	Lipid module 1 (Sphingolipids)	Black
6	6	N-stearoyl-sphingosine (d18:1/18:0)*	1.50 (1.25-1.79)	1.37E-05	0.000230677	Lipid	Ceramides	Lipid module 1 (Sphingolipids)	Black
7	7	sphingomyelin (d18:0/18:0, d19:0/17:0)*	1.76 (1.49-2.08)	1.08E-10	2.24E-08	Lipid	Sphingolipid Metabolism	Lipid module 1 (Sphingolipids)	Black
8	8	sphingomyelin (d18:0/20:0, d16:0/22:0)*	1.59 (1.35-1.87)	3.73E-08	2.33E-06	Lipid	Sphingolipid Metabolism	Lipid module 1 (Sphingolipids)	Black
9	1	1,2-dipalmitoyl-GPC (16:0/16:0)	1.28 (1.07-1.53)	0.007623038	0.037162311	Lipid	Phosphatidylcholine (PC)	Lipid module 2 (PC, PI)	Yellow
10	2	1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)	1.35 (1.10-1.66)	0.004181461	0.023806769	Lipid	Phosphatidylcholine (PC)	Lipid module 2 (PC, PI)	Yellow
11	3	1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	1.41 (1.15-1.74)	0.0011846	0.00923988	Lipid	Phosphatidylcholine (PC)	Lipid module 2 (PC, PI)	Yellow
12	4	1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)	1.52 (1.24-1.85)	6.12E-05	0.000867807	Lipid	Phosphatidylinositol (PI)	Lipid module 2 (PC, PI)	Yellow
13	5	1-arachidonoyl-GPI (20:4)*	1.41 (1.15-1.74)	0.001094704	0.008646777	Lipid	Lysophospholipid	Lipid module 2 (PC, PI)	Yellow
14	6	palmitoleate (16:1n7)	1.29 (1.08-1.54)	0.006094009	0.03091595	Lipid	Long Chain Fatty Acid	Lipid module 2 (PC, PI)	Yellow
15	7	1-palmitoleoyl-GPC (16:1)*	1.37 (1.13-1.67)	0.001633252	0.012428647	Lipid	Lysophospholipid	Lipid module 2 (PC, PI)	Yellow
16	8	1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)*	1.58 (1.33-1.88)	2.52E-07	9.83E-06	Lipid	Phosphatidylinositol (PI)	Lipid module 2 (PC, PI)	Yellow
17	9	1-palmitoyl-2-linoleoyl-GPI (16:0/18:2)	1.48 (1.26-1.73)	1.53E-06	3.97E-05	Lipid	Phosphatidylinositol (PI)	Lipid module 2 (PC, PI)	Yellow
18	10	1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	1.41 (1.16-1.70)	0.000435899	0.004000011	Lipid	Phosphatidylcholine (PC)	Lipid module 2 (PC, PI)	Yellow
19	11	1-palmitoyl-2-oleoyl-GPI (16:0/18:1)*	1.48 (1.24-1.76)	1.52E-05	0.000243487	Lipid	Phosphatidylinositol (PI)	Lipid module 2 (PC, PI)	Yellow
20	12	1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*	1.71 (1.45-2.01)	3.62E-10	5.65E-08	Lipid	Phosphatidylcholine (PC)	Lipid module 2 (PC, PI)	Yellow
21	13	1-palmitoyl-GPI (16:0)	1.37 (1.12-1.68)	0.002340935	0.016361789	Lipid	Lysophospholipid	Lipid module 2 (PC, PI)	Yellow
22	14	1-stearoyl-2-oleoyl-GPC (18:0/18:1)	1.47 (1.26-1.73)	2.49E-06	5.56E-05	Lipid	Phosphatidylcholine (PC)	Lipid module 2 (PC, PI)	Yellow
23	1	1-linolenoylglycerol (18:3)	1.36 (1.14-1.61)	0.000508238	0.004530582	Lipid	Monoacylglycerol	Lipid module 3 (MAG, DAG)	Red
24	2	linoleoyl-arachidonoyl-glycerol (18:2/20:4) [1]*	1.47 (1.18-1.83)	0.000695144	0.0057836	Lipid	Diacylglycerol	Lipid module 3 (MAG, DAG)	Red
25	3	1-myristoylglycerol (14:0)	1.44 (1.20-1.72)	9.53E-05	0.001265711	Lipid	Monoacylglycerol	Lipid module 3 (MAG, DAG)	Red
26	4	1-oleoylglycerol (18:1)	1.50 (1.29-1.74)	1.92E-07	7.99E-06	Lipid	Monoacylglycerol	Lipid module 3 (MAG, DAG)	Red
27	5	oleoyl-linoleoyl-glycerol (18:1/18:2) [1]	1.35 (1.11-1.65)	0.00297628	0.019549459	Lipid	Diacylglycerol	Lipid module 3 (MAG, DAG)	Red
28	6	oleoyl-linoleoyl-glycerol (18:1/18:2) [2]	1.41 (1.15-1.72)	0.001094064	0.008646777	Lipid	Diacylglycerol	Lipid module 3 (MAG, DAG)	Red
29	7	1-palmitoleoylglycerol (16:1)*	1.65 (1.42-1.91)	8.89E-11	2.24E-08	Lipid	Monoacylglycerol	Lipid module 3 (MAG, DAG)	Red
30	8	palmitoleoyl-linoleoyl-glycerol (16:1/18:2) [1]*	1.58 (1.32-1.89)	5.93E-07	1.95E-05	Lipid	Diacylglycerol	Lipid module 3 (MAG, DAG)	Red
31	9	palmitoyl-linoleoyl-glycerol (16:0/18:2) [2]*	1.60 (1.31-1.95)	4.51E-06	9.70E-05	Lipid	Diacylglycerol	Lipid module 3 (MAG, DAG)	Red
32	1	1-arachidonoyl-GPE (20:4n6)*	1.25 (1.05-1.48)	0.010396556	0.048413815	Lipid	Lysophospholipid	Lipid module 4 (PE, LPL)	Brown
33	2	1-linoleoyl-GPG (18:2)*	1.33 (1.13-1.57)	0.000723944	0.005943964	Lipid	Lysophospholipid	Lipid module 4 (PE, LPL)	Brown
34	3	1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)*	1.46 (1.20-1.78)	0.000236148	0.002455936	Lipid	Phosphatidylethanolamine (PE)	Lipid module 4 (PE, LPL)	Brown

35	4	1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)	1.41 (1.17-1.69)	0.000235608	0.002455936	Lipid	Phosphatidylethanolamine (PE)	Lipid module 4 (PE, LPL)	Brown
36	5	1-palmitoyl-2-oleoyl-GPE (16:0/18:1)	1.60 (1.33-1.93)	1.04E-06	2.92E-05	Lipid	Phosphatidylethanolamine (PE)	Lipid module 4 (PE, LPL)	Brown
37	6	1-palmitoyl-GPG (16:0)*	1.43 (1.17-1.74)	0.00052003	0.004570405	Lipid	Lysophospholipid	Lipid module 4 (PE, LPL)	Brown
38	7	1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)	1.53 (1.23-1.89)	0.000117313	0.001493943	Lipid	Phosphatidylethanolamine (PE)	Lipid module 4 (PE, LPL)	Brown
39	8	1-stearoyl-2-linoleoyl-GPE (18:0/18:2)*	1.51 (1.25-1.84)	3.46E-05	0.000527167	Lipid	Phosphatidylethanolamine (PE)	Lipid module 4 (PE, LPL)	Brown
40	9	1-stearoyl-2-oleoyl-GPE (18:0/18:1)	1.61 (1.30-1.99)	1.35E-05	0.000230677	Lipid	Phosphatidylethanolamine (PE)	Lipid module 4 (PE, LPL)	Brown
41	10	1-stearoyl-GPE (18:0)	1.36 (1.11-1.67)	0.003653825	0.022701849	Lipid	Lysophospholipid	Lipid module 4 (PE, LPL)	Brown
42	1	alanine	1.49 (1.23-1.81)	5.22E-05	0.000770725	Amino Acid	Alanine and Aspartate Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
43	2	2-aminoadipate	1.70 (1.40-2.07)	1.63E-07	7.84E-06	Amino Acid	Lysine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
44	3	cysteine	1.27 (1.08-1.50)	0.00385684	0.023141042	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
45	4	cysteinylglycine	1.28 (1.07-1.53)	0.006092828	0.03091595	Amino Acid	Glutathione Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
46	5	1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*	0.68 (0.56-0.83)	0.000166398	0.001854149	Lipid	Plasmalogen	AA module 1 (BCAA, AAA, GGAA)	Turquoise
47	6	gamma-glutamylalanine	1.29 (1.10-1.53)	0.002526203	0.017322536	Peptide	Gamma-glutamyl Amino Acid	AA module 1 (BCAA, AAA, GGAA)	Turquoise
48	7	gamma-glutamylisoleucine*	1.69 (1.39-2.05)	1.84E-07	7.99E-06	Peptide	Gamma-glutamyl Amino Acid	AA module 1 (BCAA, AAA, GGAA)	Turquoise
49	8	gamma-glutamylleucine	1.58 (1.29-1.94)	1.22E-05	0.000217752	Peptide	Gamma-glutamyl Amino Acid	AA module 1 (BCAA, AAA, GGAA)	Turquoise
50	9	gamma-glutamylvaline	1.60 (1.30-1.97)	1.12E-05	0.000205242	Peptide	Gamma-glutamyl Amino Acid	AA module 1 (BCAA, AAA, GGAA)	Turquoise
51	10	3-hydroxy-2-ethylpropionate	1.35 (1.10-1.66)	0.004637026	0.025160905	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
52	11	isoleucine	1.65 (1.33-2.05)	8.45E-06	0.000170095	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
53	12	isovalerylcarnitine (C5)	1.55 (1.30-1.85)	2.18E-06	5.03E-05	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
54	13	kynurenate	1.33 (1.11-1.60)	0.002091187	0.014828417	Amino Acid	Tryptophan Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
55	14	kynurenine	1.32 (1.11-1.56)	0.001751037	0.013007704	Amino Acid	Tryptophan Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
56	15	leucine	1.66 (1.32-2.08)	1.82E-05	0.000283347	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
57	16	N-acetylcitrulline	1.31 (1.07-1.59)	0.008025492	0.038820987	Amino Acid	Urea cycle; Arginine and Proline Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
58	17	N-acetylkynurenine (2)	1.43 (1.18-1.74)	0.000286474	0.002919676	Amino Acid	Tryptophan Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
59	18	N-acetylleucine	1.47 (1.20-1.80)	0.000204911	0.00220456	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
60	19	N-acetyltryptophan	1.45 (1.18-1.78)	0.000415894	0.003932092	Amino Acid	Tryptophan Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
61	20	N-acetylvaline	1.36 (1.11-1.66)	0.002686773	0.018223331	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
62	21	2-oxoarginine*	1.27 (1.06-1.53)	0.010027448	0.047046074	Amino Acid	Urea cycle; Arginine and Proline Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
63	22	proline	1.28 (1.08-1.51)	0.004196706	0.023806769	Amino Acid	Urea cycle; Arginine and Proline Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
64	23	tyrosine	1.44 (1.18-1.77)	0.000444944	0.004023841	Amino Acid	Tyrosine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
65	24	urate	1.78 (1.45-2.19)	5.51E-08	3.13E-06	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	AA module 1 (BCAA, AAA, GGAA)	Turquoise
66	25	valine	1.45 (1.21-1.74)	5.31E-05	0.000770725	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
67	26	alpha-hydroxyisocaproate	1.84 (1.44-2.34)	1.08E-06	2.92E-05	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
68	27	alpha-hydroxyisovalerate	1.76 (1.46-2.12)	3.73E-09	3.32E-07	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
69	28	beta-hydroxyisovalerate	1.33 (1.09-1.62)	0.005490607	0.028791082	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
70	29	2-hydroxy-3-methylvalerate	1.87 (1.53-2.28)	1.84E-09	1.92E-07	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
71	30	2-hydroxybutyrate/2-hydroxyisobutyrate	1.49 (1.16-1.92)	0.001939933	0.013914	Amino Acid	Glutathione Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise

72	31	3-hydroxyisobutyrate	1.63 (1.35-1.97)	5.17E-07	1.79E-05	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
73	32	3-(4-hydroxyphenyl)lactate	1.77 (1.43-2.18)	1.43E-07	7.43E-06	Amino Acid	Tyrosine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
74	33	4-hydroxyphenylpyruvate	1.37 (1.13-1.67)	0.0018543	0.013454457	Amino Acid	Tyrosine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
75	34	indolelactate	1.39 (1.13-1.71)	0.001853708	0.013454457	Amino Acid	Tryptophan Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
76	35	3-methyl-2-oxobutyrate	1.64 (1.28-2.11)	0.000102565	0.001333343	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
77	36	4-methyl-2-oxopentanoate	1.56 (1.21-2.00)	0.000659966	0.005565122	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
78	37	3-methyl-2-oxovalerate	1.76 (1.37-2.25)	9.95E-06	0.000194008	Amino Acid	Leucine, Isoleucine and Valine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
79	38	phenyllactate (PLA)	1.43 (1.17-1.74)	0.000401408	0.003853515	Amino Acid	Phenylalanine Metabolism	AA module 1 (BCAA, AAA, GGAA)	Turquoise
80	1	gamma-glutamylglycine	0.69 (0.57-0.83)	7.16E-05	0.000992239	Peptide	Gamma-glutamyl Amino Acid	AA module 2 (Glycine)	Green yellow
81	2	glycine	0.66 (0.56-0.78)	7.33E-07	2.29E-05	Amino Acid	Glycine, Serine and Threonine Metabolism	AA module 2 (Glycine)	Green yellow
82	3	N-acetylglycine	0.64 (0.52-0.77)	6.12E-06	0.000127324	Amino Acid	Glycine, Serine and Threonine Metabolism	AA module 2 (Glycine)	Green yellow
83	4	serine	0.73 (0.59-0.91)	0.005041274	0.026658939	Amino Acid	Glycine, Serine and Threonine Metabolism	AA module 2 (Glycine)	Green yellow
84	1	alpha-ketoglutarate	1.59 (1.32-1.93)	1.77E-06	4.25E-05	Energy	TCA Cycle	Glucose and energy metabolism module	Green
85	2	aspartate	1.41 (1.18-1.67)	0.000140767	0.001689209	Amino Acid	Alanine and Aspartate Metabolism	Glucose and energy metabolism module	Green
86	3	cysteine-glutathione disulfide	0.59 (0.49-0.70)	5.21E-09	3.61E-07	Amino Acid	Glutathione Metabolism	Glucose and energy metabolism module	Green
87	4	glucose	2.69 (1.94-3.72)	5.12E-09	3.61E-07	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	Glucose and energy metabolism module	Green
88	5	glutamate	1.77 (1.41-2.23)	1.63E-06	4.06E-05	Amino Acid	Glutamate Metabolism	Glucose and energy metabolism module	Green
89	6	glycylvaline	1.32 (1.08-1.60)	0.005651091	0.029142817	Peptide	Dipeptide	Glucose and energy metabolism module	Green
90	7	lactate	1.60 (1.34-1.90)	3.09E-07	1.13E-05	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	Glucose and energy metabolism module	Green
91	8	pyruvate	1.79 (1.49-2.15)	1.42E-09	1.77E-07	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	Glucose and energy metabolism module	Green
92	9	xanthine	1.36 (1.15-1.61)	0.000428693	0.003992607	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	Glucose and energy metabolism module	Green
93	1	beta-cryptoxanthin	0.70 (0.59-0.82)	1.43E-05	0.000234947	Xenobiotics	Food Component/Plant	Plant-food metabolite module	Purple
94	2	isocitrate	0.71 (0.60-0.85)	0.000164102	0.001854149	Energy	TCA Cycle	Plant-food metabolite module	Purple
95	3	N-methylproline	0.74 (0.61-0.90)	0.00278378	0.018479558	Amino Acid	Urea cycle; Arginine and Proline Metabolism	Plant-food metabolite module	Purple
96	4	oxalate (ethanedioate)	0.68 (0.57-0.80)	1.06E-05	0.000200056	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	Plant-food metabolite module	Purple
97	5	tartarate	0.74 (0.62-0.88)	0.000598835	0.005118807	Xenobiotics	Food Component/Plant	Plant-food metabolite module	Purple
98	6	threonate	0.76 (0.64-0.91)	0.003441527	0.022139306	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	Plant-food metabolite module	Purple
99	1	5alpha-androstan-3alpha,17beta-diol monosulfate (1)	1.35 (1.10-1.64)	0.003592474	0.022643472	Lipid	Androgenic Steroids	Androgenic steroid module	Magenta
100	2	5alpha-androstan-3beta,17beta-diol disulfate	1.41 (1.12-1.78)	0.004016768	0.023424893	Lipid	Androgenic Steroids	Androgenic steroid module	Magenta
101	3	5alpha-androstan-3beta,17beta-diol monosulfate (2)	1.39 (1.13-1.71)	0.002359873	0.016361789	Lipid	Androgenic Steroids	Androgenic steroid module	Magenta
102	4	androstenediol (3beta,17beta) disulfate (1)	1.46 (1.17-1.81)	0.000822574	0.006666055	Lipid	Androgenic Steroids	Androgenic steroid module	Magenta
103	5	androstenediol (3beta,17beta) monosulfate (1)	1.35 (1.08-1.70)	0.009120974	0.04344647	Lipid	Androgenic Steroids	Androgenic steroid module	Magenta
104	6	androstenediol (3beta,17beta) monosulfate (2)	1.32 (1.09-1.61)	0.005605846	0.029142817	Lipid	Androgenic Steroids	Androgenic steroid module	Magenta
105	1	arabitol/xylitol	1.37 (1.10-1.71)	0.004539419	0.024847348	Carbohydrate	Pentose Metabolism	Mixed metabolite module	Pink
106	2	erythritol	1.32 (1.09-1.59)	0.003852957	0.023141042	Xenobiotics	Food Component/Plant	Mixed metabolite module	Pink

107	3	erythronate*	1.36 (1.09-1.70)	0.006268304	0.031543726	Carbohydrate	Aminosugar Metabolism	Mixed metabolite module	Pink
108	4	2-keto-3-deoxy-gluconate	1.35 (1.11-1.63)	0.002754138	0.018479377	Xenobiotics	Food Component/Plant	Mixed metabolite module	Pink
109	5	5-methylthioadenosine (MTA)	1.44 (1.18-1.76)	0.000290096	0.002919676	Amino Acid	Polyamine Metabolism	Mixed metabolite module	Pink
110	6	N1-methylinosine	1.31 (1.08-1.60)	0.006326152	0.031580153	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	Mixed metabolite module	Pink
111	7	N-acetylputrescine	1.35 (1.10-1.65)	0.004503978	0.024847348	Amino Acid	Polyamine Metabolism	Mixed metabolite module	Pink
112	8	orotidine	1.45 (1.20-1.76)	0.000164528	0.001854149	Nucleotide	Pyrimidine Metabolism, Orotate containing	Mixed metabolite module	Pink
113	9	ribitol	1.47 (1.21-1.77)	8.02E-05	0.001088352	Carbohydrate	Pentose Metabolism	Mixed metabolite module	Pink
114	1	4-acetamidobutanoate	1.22 (1.00-1.48)	0.04626131	0.155199233	Amino Acid	Polyamine Metabolism	NA	NA
115	2	5-acetylamino-6-amino-3-methyluracil	1.09 (0.90-1.31)	0.396225745	0.591494892	Xenobiotics	Xanthine Metabolism	NA	NA
116	3	5-acetylamino-6-formylamino-3-methyluracil	1.26 (1.04-1.53)	0.017206485	0.070637148	Xenobiotics	Xanthine Metabolism	NA	NA
117	4	acetylcarnitine (C2)	0.88 (0.74-1.06)	0.182877978	0.385526547	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
118	5	acisoga	1.18 (0.94-1.49)	0.148340794	0.343619182	Amino Acid	Polyamine Metabolism	NA	NA
119	6	aconitate [cis or trans]	1.14 (0.90-1.44)	0.289872813	0.484934679	Energy	TCA Cycle	NA	NA
120	7	adenine	1.13 (0.94-1.37)	0.19690089	0.402839854	Nucleotide	Purine Metabolism, Adenine containing	NA	NA
121	8	adenosine	0.86 (0.70-1.07)	0.189107347	0.391740712	Nucleotide	Purine Metabolism, Adenine containing	NA	NA
122	9	adipoylcarnitine (C6-DC)	0.94 (0.78-1.12)	0.471794092	0.670613926	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
123	10	ADpSGEGDFXAEGGGVR*	1.07 (0.88-1.30)	0.477343698	0.675425096	Peptide	Fibrinogen Cleavage Peptide	NA	NA
124	11	adrenate (22:4n6)	1.27 (1.03-1.56)	0.025459128	0.098064791	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
125	12	16a-hydroxy DHEA 3-sulfate	1.13 (0.92-1.37)	0.240725281	0.45549379	Lipid	Androgenic Steroids	NA	NA
126	13	allantoin	1.26 (1.02-1.55)	0.031168534	0.117163646	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	NA	NA
127	14	alliin	1.07 (0.88-1.29)	0.505476924	0.700928002	Xenobiotics	Food Component/Plant	NA	NA
128	15	4-allylphenol sulfate	1.01 (0.87-1.17)	0.932004673	0.96928486	Xenobiotics	Food Component/Plant	NA	NA
129	16	5alpha-androstan-3beta,17alpha-diol disulfate	1.04 (0.85-1.28)	0.686399859	0.834919126	Lipid	Androgenic Steroids	NA	NA
130	17	7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)	1.11 (0.91-1.36)	0.294066984	0.489327461	Lipid	Sterol	NA	NA
131	18	5alpha-pregnan-3beta,20alpha-diol disulfate	0.97 (0.81-1.16)	0.752681913	0.872999097	Lipid	Progestin Steroids	NA	NA
132	19	5alpha-pregnan-3beta,20alpha-diol monosulfate (2)	0.87 (0.70-1.07)	0.177756274	0.377278621	Lipid	Progestin Steroids	NA	NA
133	20	5alpha-pregnan-3beta,20beta-diol monosulfate (1)	1.01 (0.83-1.23)	0.90272211	0.955694566	Lipid	Progestin Steroids	NA	NA
134	21	alpha-tocopherol	1.12 (0.91-1.39)	0.288022745	0.483134927	Cofactors and Vitamins	Tocopherol Metabolism	NA	NA
135	22	2-aminobutyrate	1.05 (0.88-1.27)	0.58585997	0.746074738	Amino Acid	Glutathione Metabolism	NA	NA
136	23	2-aminoheptanoate	1.10 (0.94-1.29)	0.243757738	0.45549379	Lipid	Fatty Acid, Amino	NA	NA
137	24	3-aminoisobutyrate	0.79 (0.68-0.93)	0.003930216	0.023350512	Nucleotide	Pyrimidine Metabolism, Thymine containing	NA	NA
138	25	2-aminooctanoate	0.74 (0.63-0.86)	0.000149929	0.001765208	Lipid	Fatty Acid, Amino	NA	NA
139	26	2-aminophenol sulfate	1.01 (0.83-1.23)	0.906684588	0.955694566	Xenobiotics	Chemical	NA	NA
140	27	androstenediol (3alpha, 17alpha) monosulfate (2)	1.15 (0.98-1.36)	0.096619328	0.264833116	Lipid	Androgenic Steroids	NA	NA
141	28	androstenediol (3alpha, 17alpha) monosulfate (3)	1.17 (0.94-1.44)	0.15725357	0.355529809	Lipid	Androgenic Steroids	NA	NA
142	29	androstenediol (3beta,17beta) disulfate (2)	1.18 (0.98-1.44)	0.086468967	0.247535973	Lipid	Androgenic Steroids	NA	NA

143	30	andro steroid monosulfate C19H28O6S (1)*	1.09 (0.86-1.38)	0.482602617	0.676728164	Lipid	Androgenic Steroids	NA	NA
144	31	androsterone sulfate	1.19 (0.94-1.51)	0.152406836	0.349639211	Lipid	Androgenic Steroids	NA	NA
145	32	1,5-anhydroglucitol (1,5-AG)	0.90 (0.72-1.13)	0.373408862	0.568310072	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	NA	NA
146	33	arabinose	1.22 (1.00-1.48)	0.050452918	0.165526236	Carbohydrate	Pentose Metabolism	NA	NA
147	34	arabonate/xylonate	1.20 (1.00-1.43)	0.047553977	0.157838731	Carbohydrate	Pentose Metabolism	NA	NA
148	35	arachidate (20:0)	0.99 (0.83-1.18)	0.886243014	0.943712698	Lipid	Long Chain Fatty Acid	NA	NA
149	36	arachidonate (20:4n6)	1.00 (0.82-1.23)	0.971486582	0.987308839	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
150	37	arachidonoylcholine	0.93 (0.72-1.20)	0.574121568	0.744125616	Lipid	Fatty Acid Metabolism (Acyl Choline)	NA	NA
151	38	1-arachidonoyl-GPA (20:4)	1.04 (0.84-1.29)	0.701403614	0.839465052	Lipid	Lysophospholipid	NA	NA
152	39	1-arachidonoyl-GPC (20:4n6)*	1.08 (0.87-1.32)	0.491711522	0.686416085	Lipid	Lysophospholipid	NA	NA
153	40	1-arachidonylglycerol (20:4)	1.01 (0.85-1.21)	0.879411745	0.938039194	Lipid	Monoacylglycerol	NA	NA
154	41	argininate*	1.10 (0.92-1.32)	0.305754852	0.501807948	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
155	42	arginine	1.03 (0.82-1.29)	0.789221621	0.892260414	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
156	43	asparagine	0.69 (0.54-0.87)	0.001694254	0.012737523	Amino Acid	Alanine and Aspartate Metabolism	NA	NA
157	44	azelate (nonanedioate)	0.95 (0.79-1.14)	0.584533436	0.746074738	Lipid	Fatty Acid, Dicarboxylate	NA	NA
158	45	benzoate	0.97 (0.83-1.13)	0.701992213	0.839465052	Xenobiotics	Benzoate Metabolism	NA	NA
159	46	beta-citrylglutamate	1.15 (0.96-1.38)	0.13589003	0.324886508	Amino Acid	Glutamate Metabolism	NA	NA
160	47	3beta-hydroxy-5-cholestenoate	0.72 (0.60-0.87)	0.000562398	0.004874119	Lipid	Sterol	NA	NA
161	48	betaine	0.87 (0.72-1.05)	0.15065654	0.346899191	Amino Acid	Glycine, Serine and Threonine Metabolism	NA	NA
162	49	bilirubin (E,E)*	1.02 (0.84-1.24)	0.848211469	0.929711349	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	NA	NA
163	50	bilirubin (E,Z or Z,E)*	0.87 (0.71-1.07)	0.196025529	0.402368191	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	NA	NA
164	51	bilirubin (Z,Z)	0.85 (0.71-1.02)	0.078112921	0.232106965	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	NA	NA
165	52	biliverdin	0.96 (0.79-1.16)	0.647564061	0.808159948	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	NA	NA
166	53	5-bromotryptophan	1.04 (0.86-1.26)	0.68281278	0.832178076	Amino Acid	Tryptophan Metabolism	NA	NA
167	54	butyrylcarnitine (C4)	1.29 (1.09-1.53)	0.003966593	0.023350512	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	NA	NA
168	55	caffeine	1.26 (1.07-1.50)	0.006760184	0.033479007	Xenobiotics	Xanthine Metabolism	NA	NA
169	56	caprate (10:0)	0.95 (0.81-1.11)	0.513650906	0.705987148	Lipid	Medium Chain Fatty Acid	NA	NA
170	57	caproate (6:0)	1.10 (0.91-1.33)	0.324447348	0.521791611	Lipid	Medium Chain Fatty Acid	NA	NA
171	58	caprylate (8:0)	0.87 (0.72-1.06)	0.173697068	0.375041421	Lipid	Medium Chain Fatty Acid	NA	NA
172	59	3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)	0.91 (0.75-1.10)	0.329337212	0.52829414	Lipid	Fatty Acid, Dicarboxylate	NA	NA
173	60	carboxyethyl-GABA	0.83 (0.69-0.99)	0.043280153	0.147109107	Amino Acid	Glutamate Metabolism	NA	NA
174	61	carnitine	1.00 (0.82-1.23)	0.996252284	0.998055376	Lipid	Carnitine Metabolism	NA	NA
175	62	carotene diol (1)	0.86 (0.69-1.08)	0.203979596	0.413109699	Xenobiotics	Food Component/Plant	NA	NA
176	63	carotene diol (2)	0.87 (0.74-1.03)	0.104742948	0.279314528	Xenobiotics	Food Component/Plant	NA	NA
177	64	catechol sulfate	1.03 (0.83-1.27)	0.815397184	0.911842012	Xenobiotics	Benzoate Metabolism	NA	NA
178	65	ceramide (d18:2/24:1, d18:1/24:2)*	1.15 (0.96-1.39)	0.135787783	0.324886508	Lipid	Ceramides	NA	NA

179	66	cerotoylcarnitine (C26)*	1.16 (0.98-1.37)	0.079840171	0.235001259	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
180	67	C-glycosyltryptophan	1.13 (0.89-1.44)	0.320316392	0.516479144	Amino Acid	Tryptophan Metabolism	NA	NA
181	68	cholate	1.13 (0.92-1.38)	0.262689019	0.466868106	Lipid	Primary Bile Acid Metabolism	NA	NA
182	69	choline phosphate	0.90 (0.76-1.07)	0.232820706	0.449340296	Lipid	Phospholipid Metabolism	NA	NA
183	70	choline	0.89 (0.75-1.07)	0.21938846	0.435982163	Lipid	Phospholipid Metabolism	NA	NA
184	71	cinnamoylglycine	0.79 (0.68-0.93)	0.003674498	0.022701849	Xenobiotics	Food Component/Plant	NA	NA
185	72	cis-4-decenoylcarnitine (C10:1)	0.92 (0.77-1.09)	0.330381218	0.528609948	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
186	73	citrate	1.01 (0.80-1.28)	0.912321026	0.958397846	Energy	TCA Cycle	NA	NA
187	74	citrulline	0.84 (0.68-1.03)	0.096456465	0.264833116	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
188	75	cortisol	1.02 (0.83-1.25)	0.868252233	0.932055413	Lipid	Corticosteroids	NA	NA
189	76	cortisone	1.10 (0.89-1.35)	0.376652917	0.570464613	Lipid	Corticosteroids	NA	NA
190	77	creatine	1.10 (0.89-1.36)	0.368757306	0.563981761	Amino Acid	Creatine Metabolism	NA	NA
191	78	creatinine	0.85 (0.69-1.05)	0.140879449	0.332987788	Amino Acid	Creatine Metabolism	NA	NA
192	79	cys-gly, oxidized	0.97 (0.80-1.18)	0.743641325	0.864734146	Amino Acid	Glutathione Metabolism	NA	NA
193	80	cysteine s-sulfate	1.20 (0.98-1.46)	0.078788496	0.23300484	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
194	81	cysteine sulfinic acid	1.06 (0.87-1.30)	0.5363236	0.718167224	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
195	82	cystine	1.29 (1.05-1.60)	0.017510188	0.070950372	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
196	83	cytidine	1.17 (0.98-1.41)	0.091177006	0.256281314	Nucleotide	Pyrimidine Metabolism, Cytidine containing	NA	NA
197	84	decanoylcarnitine (C10)	0.88 (0.75-1.03)	0.113757007	0.289464251	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
198	85	dehydroisoandrosterone sulfate (DHEA-S)	1.09 (0.85-1.40)	0.491417297	0.686416085	Lipid	Androgenic Steroids	NA	NA
199	86	deoxycarnitine	0.88 (0.69-1.12)	0.283967114	0.481509454	Lipid	Carnitine Metabolism	NA	NA
200	87	2'-deoxyuridine	0.86 (0.74-1.01)	0.062017109	0.193493379	Nucleotide	Pyrimidine Metabolism, Uracil containing	NA	NA
201	88	12,13-DiHOME	0.80 (0.65-0.99)	0.045019997	0.151851233	Lipid	Fatty Acid, Dihydroxy	NA	NA
202	89	9,10-DiHOME	0.73 (0.58-0.91)	0.004765557	0.025635412	Lipid	Fatty Acid, Dihydroxy	NA	NA
203	90	dihomo-linoleate (20:2n6)	1.17 (0.95-1.44)	0.138801243	0.329323102	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
204	91	dihomo-linolenate (20:3n3 or n6)	1.15 (0.97-1.36)	0.115048788	0.289477596	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
205	92	dihomo-linolenoyl-choline	1.10 (0.90-1.33)	0.350119877	0.546187008	Lipid	Fatty Acid Metabolism (Acyl Choline)	NA	NA
206	93	1-dihomo-linolenylglycerol (20:3)	1.08 (0.90-1.29)	0.429439982	0.623573889	Lipid	Monoacylglycerol	NA	NA
207	94	dihydroorotate	1.03 (0.84-1.26)	0.770889821	0.885884435	Nucleotide	Pyrimidine Metabolism, Orotate containing	NA	NA
208	95	5,6-dihydrothymine	1.03 (0.82-1.31)	0.784199671	0.889710172	Nucleotide	Pyrimidine Metabolism, Thymine containing	NA	NA
209	96	2,3-dihydroxy-2-methylbutyrate	1.18 (0.93-1.49)	0.167828251	0.367455539	Amino Acid	Leucine, Isoleucine and Valine Metabolism	NA	NA
210	97	2,3-dihydroxyisovalerate	0.99 (0.82-1.20)	0.904362223	0.955694566	Xenobiotics	Food Component/Plant	NA	NA
211	98	1,2-dilinoleoyl-GPC (18:2/18:2)	0.83 (0.68-1.01)	0.069691619	0.211104711	Lipid	Phosphatidylcholine (PC)	NA	NA
212	99	dimethylarginine (SDMA + ADMA)	0.93 (0.70-1.22)	0.583712977	0.746074738	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
213	100	dimethylglycine	1.02 (0.84-1.23)	0.843397319	0.929711349	Amino Acid	Glycine, Serine and Threonine Metabolism	NA	NA
214	101	1,3-dimethylurate	1.11 (0.91-1.37)	0.299210324	0.496561814	Xenobiotics	Xanthine Metabolism	NA	NA
215	102	1,7-dimethylurate	1.20 (0.99-1.46)	0.067096386	0.206258212	Xenobiotics	Xanthine Metabolism	NA	NA

216	103	docosadienoate (22:2n6)	1.26 (1.01-1.58)	0.039265431	0.138427284	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
217	104	docosadioate	0.95 (0.76-1.19)	0.652210535	0.810409667	Lipid	Fatty Acid, Dicarboxylate	NA	NA
218	105	docosahexaenoate (DHA; 22:6n3)	0.96 (0.76-1.20)	0.705635603	0.839465052	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
219	106	docosahexaenoylcholine	0.90 (0.72-1.13)	0.361309066	0.555312456	Lipid	Fatty Acid Metabolism (Acyl Choline)	NA	NA
220	107	1-docosahexaenoylglycerol (22:6)	0.96 (0.79-1.17)	0.663456335	0.818175401	Lipid	Monoacylglycerol	NA	NA
221	108	docosapentaenoate (n3 DPA; 22:5n3)	1.15 (0.92-1.42)	0.220428779	0.436658915	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
222	109	docosapentaenoate (n6 DPA; 22:5n6)	1.02 (0.85-1.22)	0.850745481	0.929711349	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
223	110	5-dodecenoate (12:1n7)	1.10 (0.89-1.37)	0.357969937	0.552638468	Lipid	Medium Chain Fatty Acid	NA	NA
224	111	dopamine 3-O-sulfate	1.13 (0.92-1.38)	0.235666476	0.451091661	Amino Acid	Tyrosine Metabolism	NA	NA
225	112	DSGEGDFXAEGGGVR*	0.97 (0.80-1.18)	0.775038092	0.887383063	Peptide	Fibrinogen Cleavage Peptide	NA	NA
226	113	ectoine	1.09 (0.91-1.29)	0.353460379	0.548654917	Xenobiotics	Chemical	NA	NA
227	114	eicosanodioate	0.86 (0.68-1.08)	0.18959246	0.391740712	Lipid	Fatty Acid, Dicarboxylate	NA	NA
228	115	eicosapentaenoate (EPA; 20:5n3)	1.12 (0.90-1.38)	0.31768131	0.513557351	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
229	116	eicosenoate (20:1)	1.09 (0.90-1.32)	0.392261301	0.587404935	Lipid	Long Chain Fatty Acid	NA	NA
230	117	1-(1-enyl-oleoyl)-GPE (P-18:1)*	0.90 (0.74-1.09)	0.27279132	0.471528487	Lipid	Lysoplasmalogen	NA	NA
231	118	1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*	0.98 (0.83-1.17)	0.848149102	0.929711349	Lipid	Plasmalogen	NA	NA
232	119	1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*	1.15 (0.94-1.41)	0.165401317	0.364701138	Lipid	Plasmalogen	NA	NA
233	120	1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*	0.76 (0.61-0.95)	0.014320391	0.0607886	Lipid	Plasmalogen	NA	NA
234	121	1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)*	0.97 (0.79-1.18)	0.764852504	0.881560257	Lipid	Plasmalogen	NA	NA
235	122	1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)*	1.04 (0.87-1.24)	0.696672815	0.839465052	Lipid	Plasmalogen	NA	NA
236	123	1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)*	0.98 (0.83-1.15)	0.780101478	0.889710172	Lipid	Plasmalogen	NA	NA
237	124	1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*	0.89 (0.75-1.06)	0.1845116	0.387147974	Lipid	Plasmalogen	NA	NA
238	125	1-(1-enyl-palmitoyl)-GPC (P-16:0)*	0.79 (0.66-0.95)	0.012399567	0.055664245	Lipid	Lysoplasmalogen	NA	NA
239	126	1-(1-enyl-palmitoyl)-GPE (P-16:0)*	1.01 (0.83-1.23)	0.948124328	0.976517187	Lipid	Lysoplasmalogen	NA	NA
240	127	1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*	1.04 (0.82-1.32)	0.72359	0.849269705	Lipid	Plasmalogen	NA	NA
241	128	1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)*	0.97 (0.79-1.19)	0.783430643	0.889710172	Lipid	Plasmalogen	NA	NA
242	129	1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)	1.05 (0.86-1.27)	0.637663748	0.802090852	Lipid	Plasmalogen	NA	NA
243	130	1-(1-enyl-stearoyl)-GPE (P-18:0)*	0.89 (0.71-1.11)	0.300741497	0.497779029	Lipid	Lysoplasmalogen	NA	NA
244	131	epiandrosterone sulfate	1.15 (0.90-1.48)	0.270530778	0.470727632	Lipid	Androgenic Steroids	NA	NA
245	132	ergothioneine	1.09 (0.89-1.33)	0.424779919	0.619305302	Xenobiotics	Food Component/Plant	NA	NA
246	133	erucate (22:1n9)	1.03 (0.85-1.25)	0.765714197	0.881560257	Lipid	Long Chain Fatty Acid	NA	NA
247	134	ethylmalonate	1.22 (1.01-1.48)	0.037260247	0.132859397	Amino Acid	Leucine, Isoleucine and Valine Metabolism	NA	NA
248	135	4-ethylphenylsulfate	0.86 (0.74-1.00)	0.051695029	0.167138332	Xenobiotics	Benzoate Metabolism	NA	NA
249	136	etiocholanolone glucuronide	0.98 (0.79-1.22)	0.870814593	0.932055413	Lipid	Androgenic Steroids	NA	NA
250	137	fructose	1.30 (1.08-1.57)	0.006845225	0.033633232	Carbohydrate	Fructose, Mannose and Galactose Metabolism	NA	NA
251	138	fumarate	1.08 (0.88-1.32)	0.48116278	0.676728164	Energy	TCA Cycle	NA	NA

252	139	5-(galactosylhydroxy)-L-lysine	1.14 (0.94-1.37)	0.17443001	0.375325264	Amino Acid	Lysine Metabolism	NA	NA
253	140	gamma-CEHC glucuronide*	1.15 (0.95-1.38)	0.147507825	0.343451055	Cofactors and Vitamins	Tocopherol Metabolism	NA	NA
254	141	gamma-CEHC	1.02 (0.85-1.22)	0.869621359	0.932055413	Cofactors and Vitamins	Tocopherol Metabolism	NA	NA
255	142	gamma-glutamyl-2-aminobutyrate	0.97 (0.80-1.17)	0.739088606	0.862039795	Peptide	Gamma-glutamyl Amino Acid	NA	NA
256	143	gamma-glutamyl-alpha-lysine	1.05 (0.82-1.34)	0.703393416	0.839465052	Peptide	Gamma-glutamyl Amino Acid	NA	NA
257	144	gamma-glutamyl-epsilon-lysine	1.08 (0.91-1.27)	0.404685284	0.598574078	Peptide	Gamma-glutamyl Amino Acid	NA	NA
258	145	gamma-glutamylglutamate	1.28 (1.05-1.55)	0.013763231	0.059136113	Peptide	Gamma-glutamyl Amino Acid	NA	NA
259	146	gamma-glutamylglutamine	0.75 (0.60-0.95)	0.01561363	0.065388623	Peptide	Gamma-glutamyl Amino Acid	NA	NA
260	147	gamma-glutamylhistidine	0.90 (0.72-1.11)	0.316756688	0.513392659	Peptide	Gamma-glutamyl Amino Acid	NA	NA
261	148	gamma-glutamylmethionine	1.12 (0.88-1.43)	0.351063212	0.546292879	Peptide	Gamma-glutamyl Amino Acid	NA	NA
262	149	gamma-glutamylphenylalanine	1.30 (1.01-1.67)	0.042769936	0.147109107	Peptide	Gamma-glutamyl Amino Acid	NA	NA
263	150	gamma-glutamylthreonine	1.00 (0.84-1.20)	0.968010874	0.98699148	Peptide	Gamma-glutamyl Amino Acid	NA	NA
264	151	gamma-glutamyltryptophan	1.16 (0.93-1.45)	0.18031366	0.381409232	Peptide	Gamma-glutamyl Amino Acid	NA	NA
265	152	gamma-glutamyltyrosine	1.25 (0.98-1.58)	0.067525616	0.206258212	Peptide	Gamma-glutamyl Amino Acid	NA	NA
266	153	gamma-tocopherol/beta-tocopherol	1.59 (1.32-1.91)	1.02E-06	2.92E-05	Cofactors and Vitamins	Tocopherol Metabolism	NA	NA
267	154	gentisate	0.81 (0.62-1.05)	0.11135293	0.285943326	Amino Acid	Tyrosine Metabolism	NA	NA
268	155	gluconate	1.14 (0.92-1.42)	0.241833196	0.45549379	Xenobiotics	Food Component/Plant	NA	NA
269	156	glucuronate	1.21 (0.99-1.49)	0.061835993	0.193493379	Carbohydrate	Aminosugar Metabolism	NA	NA
270	157	glutamate, gamma-methyl ester	0.93 (0.75-1.17)	0.550437486	0.730793599	Amino Acid	Glutamate Metabolism	NA	NA
271	158	glutamine	0.74 (0.57-0.96)	0.024824144	0.09621283	Amino Acid	Glutamate Metabolism	NA	NA
272	159	glutarate (pentanedioate)	0.95 (0.81-1.13)	0.582313061	0.746074738	Lipid	Fatty Acid, Dicarboxylate	NA	NA
273	160	glutarylcarnitine (C5-DC)	1.03 (0.84-1.26)	0.781103647	0.889710172	Amino Acid	Lysine Metabolism	NA	NA
274	161	glycerate	0.90 (0.74-1.08)	0.246964766	0.458648851	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	NA	NA
275	162	glycerol 3-phosphate	1.09 (0.89-1.34)	0.407335559	0.600892172	Lipid	Glycerolipid Metabolism	NA	NA
276	163	glycerol	1.18 (0.97-1.44)	0.106184912	0.281954831	Lipid	Glycerolipid Metabolism	NA	NA
277	164	glycerophosphoethanolamine	0.94 (0.78-1.13)	0.507292321	0.701885605	Lipid	Phospholipid Metabolism	NA	NA
278	165	glycerophosphoinositol*	0.94 (0.79-1.13)	0.521699692	0.710787353	Lipid	Phospholipid Metabolism	NA	NA
279	166	glycerophosphorylcholine (GPC)	0.80 (0.66-0.98)	0.03318529	0.1224482	Lipid	Phospholipid Metabolism	NA	NA
280	167	glycochenodeoxycholate glucuronide (1)	1.03 (0.87-1.22)	0.731474127	0.854756283	Lipid	Primary Bile Acid Metabolism	NA	NA
281	168	glycochenodeoxycholate	1.03 (0.86-1.23)	0.74417025	0.864734146	Lipid	Primary Bile Acid Metabolism	NA	NA
282	169	glycochenodeoxycholate sulfate	1.05 (0.87-1.27)	0.61960321	0.785838217	Lipid	Primary Bile Acid Metabolism	NA	NA
283	170	glycocholate	1.07 (0.91-1.26)	0.415752141	0.607562848	Lipid	Primary Bile Acid Metabolism	NA	NA
284	171	glycocholenate sulfate*	1.02 (0.80-1.31)	0.864270411	0.931441686	Lipid	Secondary Bile Acid Metabolism	NA	NA
285	172	glycodeoxycholate sulfate	1.10 (0.95-1.29)	0.205400531	0.413109699	Lipid	Secondary Bile Acid Metabolism	NA	NA
286	173	glycohyocholate	0.72 (0.57-0.90)	0.004999429	0.026658939	Lipid	Secondary Bile Acid Metabolism	NA	NA
287	174	glycolithocholate sulfate*	1.05 (0.90-1.22)	0.566839938	0.74152646	Lipid	Secondary Bile Acid Metabolism	NA	NA

288	175	glycosyl ceramide (d18:1/20:0, d16:1/22:0)*	1.09 (0.89-1.33)	0.398349043	0.593245353	Lipid	Ceramides	NA	NA
289	176	glycosyl ceramide (d18:2/24:1, d18:1/24:2)*	0.88 (0.70-1.10)	0.251092363	0.461034008	Lipid	Ceramides	NA	NA
290	177	glycosyl-N-(2-hydroxynervonoyl)-sphingosine (d18:1/24:1(2OH))*	1.46 (1.20-1.79)	0.000188107	0.002059278	Lipid	Ceramides	NA	NA
291	178	glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	1.22 (1.02-1.45)	0.031939438	0.118632198	Lipid	Ceramides	NA	NA
292	179	glycosyl-N-stearoyl-sphingosine (d18:1/18:0)	1.17 (0.96-1.42)	0.132618297	0.321999289	Lipid	Ceramides	NA	NA
293	180	glycoursodeoxycholate	0.98 (0.82-1.17)	0.808229008	0.905604463	Lipid	Secondary Bile Acid Metabolism	NA	NA
294	181	guanidinoacetate	0.97 (0.80-1.16)	0.706280693	0.839465052	Amino Acid	Creatine Metabolism	NA	NA
295	182	4-guanidinobutanoate	1.18 (0.97-1.45)	0.10435271	0.279314528	Amino Acid	Guanidino and Acetamido Metabolism	NA	NA
296	183	guanosine	1.14 (0.91-1.43)	0.264029356	0.466868106	Nucleotide	Purine Metabolism, Guanine containing	NA	NA
297	184	gulonate*	1.10 (0.90-1.36)	0.340724939	0.536899904	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	NA	NA
298	185	10-heptadecenoate (17:1n7)	1.20 (1.01-1.43)	0.042493704	0.147109107	Lipid	Long Chain Fatty Acid	NA	NA
299	186	12-HETE	1.00 (0.82-1.22)	0.995923536	0.998055376	Lipid	Eicosanoid	NA	NA
300	187	hexadecadienoate (16:2n6)	1.13 (0.91-1.40)	0.258024812	0.465344732	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
301	188	hexadecanedioate	0.87 (0.71-1.06)	0.155882769	0.353712175	Lipid	Fatty Acid, Dicarboxylate	NA	NA
302	189	hexanoylcarnitine (C6)	1.00 (0.85-1.17)	0.965848355	0.98639832	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
303	190	hexanoylglutamine	1.02 (0.83-1.25)	0.853065974	0.929823454	Lipid	Fatty Acid Metabolism (Acyl Glutamine)	NA	NA
304	191	hippurate	0.94 (0.79-1.11)	0.461244335	0.658618914	Xenobiotics	Benzoate Metabolism	NA	NA
305	192	histidine	0.74 (0.60-0.92)	0.008155835	0.039148009	Amino Acid	Histidine Metabolism	NA	NA
306	193	13-HODE + 9-HODE	0.94 (0.77-1.14)	0.531818187	0.717217269	Lipid	Fatty Acid, Monohydroxy	NA	NA
307	194	homoarginine	1.28 (0.97-1.70)	0.085121729	0.245907218	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
308	195	homocitrulline	0.90 (0.74-1.10)	0.304938762	0.501807948	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
309	196	homostachydrine*	0.93 (0.74-1.17)	0.548035199	0.730713599	Xenobiotics	Food Component/Plant	NA	NA
310	197	hydantoin-5-propionic acid	1.26 (1.02-1.55)	0.034876119	0.12507298	Amino Acid	Histidine Metabolism	NA	NA
311	198	hydroquinone sulfate	0.90 (0.75-1.07)	0.225846283	0.443170065	Xenobiotics	Drug	NA	NA
312	199	3-hydroxy-3-methylglutarate	1.15 (0.97-1.37)	0.104612847	0.279314528	Lipid	Mevalonate Metabolism	NA	NA
313	200	4-hydroxybenzoate	1.13 (0.98-1.30)	0.099281358	0.268188603	Xenobiotics	Benzoate Metabolism	NA	NA
314	201	3-hydroxybutyrate (BHBA)	0.84 (0.71-1.00)	0.047135471	0.157286277	Lipid	Ketone Bodies	NA	NA
315	202	3-hydroxybutyrylcarnitine (1)	1.03 (0.82-1.28)	0.803748617	0.90367412	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
316	203	3-hydroxybutyrylcarnitine (2)	0.99 (0.82-1.20)	0.917641573	0.961380664	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
317	204	4-hydroxychlorothalonil	0.97 (0.81-1.15)	0.703886419	0.839465052	Xenobiotics	Chemical	NA	NA
318	205	2-hydroxydecanoate	0.97 (0.82-1.14)	0.701708342	0.839465052	Lipid	Fatty Acid, Monohydroxy	NA	NA
319	206	3-hydroxydecanoate	1.03 (0.84-1.28)	0.761074381	0.879463729	Lipid	Fatty Acid, Monohydroxy	NA	NA
320	207	2-hydroxyglutarate	1.07 (0.86-1.34)	0.550313631	0.730793599	Lipid	Fatty Acid, Dicarboxylate	NA	NA
321	208	3-hydroxyhexanoate	0.88 (0.73-1.07)	0.205864599	0.413109699	Lipid	Fatty Acid, Monohydroxy	NA	NA
322	209	3-hydroxyhippurate	1.00 (0.80-1.25)	0.991909777	0.998055376	Xenobiotics	Benzoate Metabolism	NA	NA
323	210	4-hydroxyhippurate	1.00 (0.84-1.20)	0.963935166	0.986058268	Xenobiotics	Benzoate Metabolism	NA	NA

324	211	2-hydroxyhippurate (salicylurate)	0.94 (0.78-1.15)	0.560071932	0.74152646	Xenobiotics	Benzoate Metabolism	NA	NA
325	212	6-hydroxyindole sulfate	0.89 (0.76-1.05)	0.16039529	0.356563236	Xenobiotics	Chemical	NA	NA
326	213	3-hydroxylaurate	1.08 (0.87-1.34)	0.48260153	0.676728164	Lipid	Fatty Acid, Monohydroxy	NA	NA
327	214	5-hydroxylysine	1.33 (1.09-1.61)	0.004254194	0.023865941	Amino Acid	Lysine Metabolism	NA	NA
328	215	2-hydroxyoctanoate	0.90 (0.75-1.08)	0.247720651	0.458687496	Lipid	Fatty Acid, Monohydroxy	NA	NA
329	216	3-hydroxyoctanoate	0.87 (0.72-1.05)	0.154516519	0.352190979	Lipid	Fatty Acid, Monohydroxy	NA	NA
330	217	16-hydroxypalmitate	1.02 (0.83-1.25)	0.879409464	0.938039194	Lipid	Fatty Acid, Monohydroxy	NA	NA
331	218	2-hydroxypalmitate	1.06 (0.91-1.25)	0.44415689	0.638603455	Lipid	Fatty Acid, Monohydroxy	NA	NA
332	219	2-hydroxyphenylacetate	1.01 (0.78-1.32)	0.920085026	0.961380664	Amino Acid	Tyrosine Metabolism	NA	NA
333	220	21-hydroxypregnenolone disulfate	0.96 (0.79-1.17)	0.700560816	0.839465052	Lipid	Pregnenolone Steroids	NA	NA
334	221	3-hydroxypyridine sulfate	0.88 (0.74-1.06)	0.184887975	0.387147974	Xenobiotics	Chemical	NA	NA
335	222	2-hydroxystearate	1.02 (0.86-1.22)	0.808368087	0.905604463	Lipid	Fatty Acid, Monohydroxy	NA	NA
336	223	hyocholate	1.02 (0.84-1.22)	0.861132589	0.931441686	Lipid	Secondary Bile Acid Metabolism	NA	NA
337	224	hypotaurine	0.76 (0.62-0.94)	0.009599222	0.045378142	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
338	225	hypoxanthine	1.15 (0.96-1.39)	0.130510594	0.319367101	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	NA	NA
339	226	imidazole lactate	0.91 (0.76-1.09)	0.287155815	0.483134927	Amino Acid	Histidine Metabolism	NA	NA
340	227	imidazole propionate	1.03 (0.87-1.22)	0.724056863	0.849269705	Amino Acid	Histidine Metabolism	NA	NA
341	228	indole-3-carboxylic acid	0.97 (0.82-1.15)	0.722193142	0.849269705	Amino Acid	Tryptophan Metabolism	NA	NA
342	229	indoleacetate	0.94 (0.75-1.17)	0.575981847	0.744125616	Amino Acid	Tryptophan Metabolism	NA	NA
343	230	indoleacetylglutamine	1.20 (0.94-1.52)	0.137932449	0.328510871	Amino Acid	Tryptophan Metabolism	NA	NA
344	231	indolepropionate	0.81 (0.66-0.99)	0.043378326	0.147109107	Amino Acid	Tryptophan Metabolism	NA	NA
345	232	3-indoxyl sulfate	0.90 (0.77-1.04)	0.160567739	0.356563236	Amino Acid	Tryptophan Metabolism	NA	NA
346	233	inosine	1.11 (0.90-1.38)	0.331246612	0.528639094	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	NA	NA
347	234	isobutyrylcarnitine (C4)	0.89 (0.74-1.07)	0.199143983	0.405494578	Amino Acid	Leucine, Isoleucine and Valine Metabolism	NA	NA
348	235	isobutyrylglycine	0.94 (0.77-1.15)	0.541021811	0.722907089	Amino Acid	Leucine, Isoleucine and Valine Metabolism	NA	NA
349	236	isoursodeoxycholate	1.05 (0.89-1.23)	0.566179377	0.74152646	Lipid	Secondary Bile Acid Metabolism	NA	NA
350	237	isovalerate	0.96 (0.79-1.18)	0.726540035	0.850583456	Amino Acid	Leucine, Isoleucine and Valine Metabolism	NA	NA
351	238	isovalerylglycine	0.89 (0.71-1.13)	0.344122706	0.538176864	Amino Acid	Leucine, Isoleucine and Valine Metabolism	NA	NA
352	239	lactosyl-N-behenoyl-sphingosine (d18:1/22:0)*	0.99 (0.82-1.19)	0.9273746	0.966079717	Lipid	Sphingolipid Metabolism	NA	NA
353	240	lactosyl-N-nervonoyl-sphingosine (d18:1/24:1)*	0.87 (0.73-1.04)	0.124016694	0.307088957	Lipid	Ceramides	NA	NA
354	241	lactosyl-N-palmitoyl-sphingosine (d18:1/16:0)	0.87 (0.73-1.03)	0.108554888	0.282242708	Lipid	Ceramides	NA	NA
355	242	lanthionine	1.20 (0.99-1.45)	0.067424849	0.206258212	Xenobiotics	Chemical	NA	NA
356	243	laurate (12:0)	0.96 (0.81-1.14)	0.678458622	0.82848959	Lipid	Medium Chain Fatty Acid	NA	NA
357	244	laurylcarnitine (C12)	0.90 (0.76-1.07)	0.243805971	0.45549379	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
358	245	leucylalanine	1.04 (0.85-1.27)	0.711314218	0.842239226	Peptide	Dipeptide	NA	NA
359	246	leucylglycine	0.87 (0.70-1.09)	0.231907875	0.449340296	Peptide	Dipeptide	NA	NA
360	247	1-lignoceroyl-GPC (24:0)	1.00 (0.77-1.30)	0.996455929	0.998055376	Lipid	Lysophospholipid	NA	NA

361	248	linoleate (18:2n6)	1.07 (0.87-1.32)	0.519860383	0.710787353	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
362	249	linolenate [alpha or gamma; (18:3n3 or 6)]	1.06 (0.87-1.30)	0.561769892	0.74152646	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
363	250	1-linolenoyl-GPC (18:3)*	1.10 (0.93-1.32)	0.264082233	0.466868106	Lipid	Lysophospholipid	NA	NA
364	251	1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4n6)*	1.02 (0.78-1.33)	0.904233404	0.955694566	Lipid	Phosphatidylcholine (PC)	NA	NA
365	252	1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)*	0.79 (0.66-0.95)	0.012376867	0.055664245	Lipid	Phosphatidylcholine (PC)	NA	NA
366	253	linoleoylcarnitine (C18:2)*	0.86 (0.73-1.03)	0.096229488	0.264833116	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
367	254	linoleoylcholine*	0.84 (0.66-1.07)	0.158208192	0.356396794	Lipid	Fatty Acid Metabolism (Acyl Choline)	NA	NA
368	255	linoleoyl ethanolamide	1.02 (0.84-1.23)	0.836518887	0.928803889	Lipid	Endocannabinoid	NA	NA
369	256	1-linoleoylglycerol (18:2)	1.15 (0.99-1.35)	0.070911225	0.213761373	Lipid	Monoacylglycerol	NA	NA
370	257	2-linoleoylglycerol (18:2)	1.04 (0.89-1.21)	0.646328921	0.808159948	Lipid	Monoacylglycerol	NA	NA
371	258	1-linoleoyl-GPA (18:2)*	1.11 (0.90-1.37)	0.31353413	0.509492961	Lipid	Lysophospholipid	NA	NA
372	259	1-linoleoyl-GPC (18:2)	0.90 (0.75-1.08)	0.271740128	0.471016222	Lipid	Lysophospholipid	NA	NA
373	260	1-linoleoyl-GPE (18:2)*	1.16 (0.99-1.34)	0.063007989	0.19560689	Lipid	Lysophospholipid	NA	NA
374	261	1-linoleoyl-GPI (18:2)*	1.26 (1.05-1.52)	0.013813212	0.059136113	Lipid	Lysophospholipid	NA	NA
375	262	linoleoyl-linoleoyl-glycerol (18:2/18:2) [1]*	1.21 (0.99-1.46)	0.058939312	0.185748133	Lipid	Diacylglycerol	NA	NA
376	263	lysine	1.17 (0.89-1.54)	0.261727152	0.466868106	Amino Acid	Lysine Metabolism	NA	NA
377	264	malate	1.26 (1.03-1.54)	0.022586295	0.088640555	Energy	TCA Cycle	NA	NA
378	265	maleate	1.07 (0.86-1.34)	0.529231344	0.717044079	Lipid	Fatty Acid, Dicarboxylate	NA	NA
379	266	maltose	1.03 (0.84-1.28)	0.758488298	0.878101481	Carbohydrate	Glycogen Metabolism	NA	NA
380	267	mannitol/sorbitol	1.13 (0.91-1.41)	0.270819263	0.470727632	Carbohydrate	Fructose, Mannose and Galactose Metabolism	NA	NA
381	268	margarate (17:0)	1.12 (0.92-1.36)	0.257108497	0.465344732	Lipid	Long Chain Fatty Acid	NA	NA
382	269	methionine	1.02 (0.80-1.30)	0.848714619	0.929711349	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
383	270	methionine sulfone	0.84 (0.69-1.01)	0.067761111	0.206258212	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
384	271	methionine sulfoxide	1.01 (0.82-1.23)	0.950179296	0.976790578	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
385	272	3-methoxytyramine sulfate	1.13 (0.88-1.43)	0.337450315	0.534439078	Amino Acid	Tyrosine Metabolism	NA	NA
386	273	3-methoxytyrosine	0.93 (0.79-1.11)	0.429706366	0.623573889	Amino Acid	Tyrosine Metabolism	NA	NA
387	274	methyl-4-hydroxybenzoate sulfate	1.01 (0.81-1.25)	0.953188509	0.978272417	Xenobiotics	Benzoate Metabolism	NA	NA
388	275	2-methylbutyrylcarnitine (C5)	1.17 (0.92-1.48)	0.199498134	0.405494578	Amino Acid	Leucine, Isoleucine and Valine Metabolism	NA	NA
389	276	3-methyl catechol sulfate (1)	0.94 (0.79-1.13)	0.524042937	0.712424385	Xenobiotics	Benzoate Metabolism	NA	NA
390	277	4-methylcatechol sulfate	0.95 (0.81-1.12)	0.574193271	0.744125616	Xenobiotics	Benzoate Metabolism	NA	NA
391	278	2-methylcitrate/homocitrate	1.02 (0.86-1.22)	0.793882571	0.895809628	Energy	TCA Cycle	NA	NA
392	279	methyl glucopyranoside (alpha + beta)	0.91 (0.73-1.13)	0.376134455	0.570464613	Xenobiotics	Food Component/Plant	NA	NA
393	280	3-methylglutaconate	1.05 (0.86-1.29)	0.638844797	0.802090852	Amino Acid	Leucine, Isoleucine and Valine Metabolism	NA	NA
394	281	3-methylglutarylcarnitine (2)	0.86 (0.70-1.06)	0.163698547	0.362226573	Amino Acid	Leucine, Isoleucine and Valine Metabolism	NA	NA
395	282	7-methylguanine	1.18 (0.94-1.48)	0.159999617	0.356563236	Nucleotide	Purine Metabolism, Guanine containing	NA	NA
396	283	1-methylhistamine	1.40 (1.16-1.68)	0.00038991	0.003801627	Amino Acid	Histidine Metabolism	NA	NA
397	284	1-methylhistidine	1.00 (0.83-1.22)	0.975038262	0.989307115	Amino Acid	Histidine Metabolism	NA	NA

398	285	3-methylhistidine	0.98 (0.84-1.15)	0.84750424	0.929711349	Amino Acid	Histidine Metabolism	NA	NA
399	286	1-methylimidazoleacetate	1.17 (0.91-1.50)	0.230265487	0.4490177	Amino Acid	Histidine Metabolism	NA	NA
400	287	methyl indole-3-acetate	1.07 (0.86-1.32)	0.564948275	0.74152646	Xenobiotics	Food Component/Plant	NA	NA
401	288	1-methylnicotinamide	0.90 (0.72-1.12)	0.339083097	0.535665449	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	NA	NA
402	289	15-methylpalmitate	0.95 (0.80-1.13)	0.57837207	0.745669777	Lipid	Fatty Acid, Branched	NA	NA
403	290	17-methylstearate	1.09 (0.87-1.37)	0.437980007	0.631176731	Lipid	Fatty Acid, Branched	NA	NA
404	291	methylsuccinate	0.93 (0.72-1.20)	0.574245272	0.744125616	Amino Acid	Leucine, Isoleucine and Valine Metabolism	NA	NA
405	292	5-methyluridine (ribothymidine)	0.97 (0.82-1.14)	0.713508137	0.843236889	Nucleotide	Pyrimidine Metabolism, Uracil containing	NA	NA
406	293	1-methylxanthine	0.92 (0.76-1.12)	0.414465895	0.607562848	Xenobiotics	Xanthine Metabolism	NA	NA
407	294	3-methylxanthine	0.86 (0.71-1.04)	0.119823121	0.299078509	Xenobiotics	Xanthine Metabolism	NA	NA
408	295	7-methylxanthine	0.87 (0.71-1.05)	0.154647962	0.352190979	Xenobiotics	Xanthine Metabolism	NA	NA
409	296	myo-inositol	1.16 (0.90-1.49)	0.256310857	0.465344732	Lipid	Inositol Metabolism	NA	NA
410	297	myristate (14:0)	1.10 (0.92-1.32)	0.279420457	0.476388976	Lipid	Long Chain Fatty Acid	NA	NA
411	298	myristoleate (14:1n5)	1.13 (0.93-1.36)	0.222042427	0.438463527	Lipid	Long Chain Fatty Acid	NA	NA
412	299	myristoleoylcarnitine (C14:1)*	0.95 (0.80-1.14)	0.590574519	0.750546842	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
413	300	myristoyl dihydrosphingomyelin (d18:0/14:0)*	1.24 (1.04-1.47)	0.017349725	0.070759665	Lipid	Sphingolipid Metabolism	NA	NA
414	301	N('1)-acetylspermidine	1.14 (0.92-1.40)	0.243606389	0.45549379	Amino Acid	Polyamine Metabolism	NA	NA
415	302	N1-Methyl-2-pyridone-5-carboxamide	1.06 (0.87-1.29)	0.575466025	0.744125616	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	NA	NA
416	303	N1-methyladenosine	1.23 (1.02-1.47)	0.030275491	0.115194552	Nucleotide	Purine Metabolism, Adenine containing	NA	NA
417	304	N1,N12-diacetylspermine	1.11 (0.91-1.35)	0.291020914	0.485553611	Amino Acid	Polyamine Metabolism	NA	NA
418	305	N2-acetyllysine	1.08 (0.91-1.29)	0.381282712	0.57607848	Amino Acid	Lysine Metabolism	NA	NA
419	306	N2,N2-dimethylguanosine	1.33 (1.06-1.66)	0.01275164	0.056432788	Nucleotide	Purine Metabolism, Guanine containing	NA	NA
420	307	N2,N5-diacetylornithine	1.12 (0.91-1.39)	0.270167934	0.470727632	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
421	308	N4-acetylcytidine	1.28 (1.06-1.55)	0.011435363	0.052468137	Nucleotide	Pyrimidine Metabolism, Cytidine containing	NA	NA
422	309	N6-acetyllysine	1.24 (1.05-1.47)	0.013836334	0.059136113	Amino Acid	Lysine Metabolism	NA	NA
423	310	N6-carbamoylthreonyladenosine	1.18 (0.88-1.57)	0.26893553	0.470727632	Nucleotide	Purine Metabolism, Adenine containing	NA	NA
424	311	N6-carboxymethyllysine	1.06 (0.88-1.28)	0.518833076	0.710787353	Carbohydrate	Advanced Glycation End-product	NA	NA
425	312	N6,N6,N6-trimethyllysine	1.22 (0.94-1.57)	0.134587741	0.324257723	Amino Acid	Lysine Metabolism	NA	NA
426	313	N6-succinyladenosine	1.33 (1.06-1.68)	0.015731792	0.065444255	Nucleotide	Purine Metabolism, Adenine containing	NA	NA
427	314	N-acetyl-1-methylhistidine*	1.14 (0.93-1.39)	0.215678268	0.431356536	Amino Acid	Histidine Metabolism	NA	NA
428	315	N-acetylalanine	1.18 (0.97-1.44)	0.090148432	0.254536749	Amino Acid	Alanine and Aspartate Metabolism	NA	NA
429	316	N-acetylalliin	1.19 (0.97-1.46)	0.098155907	0.266434133	Xenobiotics	Food Component/Plant	NA	NA
430	317	N-acetylarginine	1.03 (0.87-1.22)	0.708913666	0.840992638	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
431	318	N-acetylasparagine	0.89 (0.74-1.09)	0.258773433	0.465344732	Amino Acid	Alanine and Aspartate Metabolism	NA	NA
432	319	N-acetylaspartate (NAA)	0.91 (0.77-1.07)	0.240734561	0.45549379	Amino Acid	Alanine and Aspartate Metabolism	NA	NA
433	320	N-acetyl-aspartyl-glutamate (NAAG)	0.99 (0.82-1.21)	0.946243237	0.976517187	Amino Acid	Glutamate Metabolism	NA	NA

434	321	N-acetyl-beta-alanine	1.18 (0.99-1.39)	0.058438059	0.185103294	Nucleotide	Pyrimidine Metabolism, Uracil containing	NA	NA
435	322	N-acetyl-cadaverine	1.24 (1.02-1.52)	0.031128959	0.117163646	Amino Acid	Lysine Metabolism	NA	NA
436	323	N-acetylcarnosine	1.24 (0.95-1.63)	0.109451103	0.283110459	Peptide	Dipeptide Derivative	NA	NA
437	324	N-acetylglucosamine/N-acetylgalactosamine	1.28 (0.99-1.65)	0.058058027	0.184837801	Carbohydrate	Aminosugar Metabolism	NA	NA
438	325	N-acetylglucosaminylasparagine	1.02 (0.85-1.22)	0.850593684	0.929711349	Carbohydrate	Aminosugar Metabolism	NA	NA
439	326	N-acetylglutamate	1.11 (0.93-1.32)	0.251204428	0.461034008	Amino Acid	Glutamate Metabolism	NA	NA
440	327	N-acetylglutamine	1.25 (1.02-1.52)	0.031475083	0.117607497	Amino Acid	Glutamate Metabolism	NA	NA
441	328	N-acetylhistidine	1.09 (0.87-1.36)	0.455685469	0.652173698	Amino Acid	Histidine Metabolism	NA	NA
442	329	N-acetylmethionine	0.88 (0.71-1.09)	0.243776504	0.45549379	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
443	330	N-acetylneuraminate	1.10 (0.90-1.34)	0.358683621	0.552638468	Carbohydrate	Aminosugar Metabolism	NA	NA
444	331	N-acetylphenylalanine	1.28 (1.01-1.63)	0.042522576	0.147109107	Amino Acid	Phenylalanine Metabolism	NA	NA
445	332	N-acetylproline	1.20 (1.00-1.45)	0.050665883	0.165526236	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
446	333	N-acetylserine	1.04 (0.85-1.27)	0.704530254	0.839465052	Amino Acid	Glycine, Serine and Threonine Metabolism	NA	NA
447	334	N-acetyltaurine	1.24 (0.95-1.61)	0.107413966	0.282242708	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
448	335	N-acetylthreonine	1.09 (0.85-1.39)	0.49521983	0.689770477	Amino Acid	Glycine, Serine and Threonine Metabolism	NA	NA
449	336	N-acetyltyrosine	1.23 (0.96-1.57)	0.109796044	0.283110459	Amino Acid	Tyrosine Metabolism	NA	NA
450	337	N-delta-acetylornithine	0.91 (0.78-1.08)	0.287910307	0.483134927	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
451	338	N-formylmethionine	1.11 (0.93-1.34)	0.252219601	0.461539681	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
452	339	nicotinamide N-oxide	1.21 (0.97-1.51)	0.086875606	0.247535973	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	NA	NA
453	340	nicotinamide	1.07 (0.88-1.30)	0.512966217	0.705987148	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	NA	NA
454	341	N-methylpipecolate	1.19 (0.95-1.47)	0.12523233	0.308873414	Xenobiotics	Chemical	NA	NA
455	342	N-oleoylserine	0.90 (0.76-1.08)	0.266361304	0.469518231	Lipid	Endocannabinoid	NA	NA
456	343	N-oleoyltaurine	1.14 (0.93-1.41)	0.205892815	0.413109699	Lipid	Endocannabinoid	NA	NA
457	344	nonadecanoate (19:0)	0.94 (0.77-1.14)	0.532255866	0.717217269	Lipid	Long Chain Fatty Acid	NA	NA
458	345	10-nonadecenoate (19:1n9)	1.14 (0.95-1.37)	0.168422535	0.367467349	Lipid	Long Chain Fatty Acid	NA	NA
459	346	N-palmitoylglycine	0.85 (0.69-1.04)	0.112705407	0.288230221	Lipid	Fatty Acid Metabolism(Acyl Glycine)	NA	NA
460	347	N-trimethyl 5-aminovalerate	1.04 (0.88-1.24)	0.636886034	0.802090852	Amino Acid	Lysine Metabolism	NA	NA
461	348	o-cresol sulfate	0.91 (0.70-1.19)	0.500266489	0.695247861	Xenobiotics	Benzoate Metabolism	NA	NA
462	349	octadecanedioate	0.92 (0.77-1.09)	0.336420753	0.534164249	Lipid	Fatty Acid, Dicarboxylate	NA	NA
463	350	octanoylcarnitine (C8)	0.94 (0.80-1.10)	0.413759892	0.607562848	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
464	351	oleate/vaccenate (18:1)	1.14 (0.94-1.37)	0.176468203	0.377278621	Lipid	Long Chain Fatty Acid	NA	NA
465	352	oleoylcarnitine (C18:1)	0.96 (0.80-1.16)	0.676104821	0.827234134	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
466	353	oleoylcholine	0.88 (0.70-1.10)	0.257968949	0.465344732	Lipid	Fatty Acid Metabolism (Acyl Choline)	NA	NA
467	354	oleoyl ethanolamide	1.14 (0.94-1.39)	0.186223335	0.388640004	Lipid	Endocannabinoid	NA	NA
468	355	1-oleoyl-GPC (18:1)	0.96 (0.79-1.16)	0.655916336	0.8104788	Lipid	Lysophospholipid	NA	NA
469	356	1-oleoyl-GPE (18:1)	1.13 (0.97-1.31)	0.114115714	0.289464251	Lipid	Lysophospholipid	NA	NA

470	357	1-oleoyl-GPI (18:1)*	1.18 (0.95-1.47)	0.142466454	0.335468178	Lipid	Lysophospholipid	NA	NA
471	358	O-methylcatechol sulfate	1.14 (0.92-1.41)	0.228989383	0.447929075	Xenobiotics	Benzoate Metabolism	NA	NA
472	359	2'-O-methylcytidine	0.99 (0.84-1.17)	0.948334935	0.976517187	Nucleotide	Pyrimidine Metabolism, Cytidine containing	NA	NA
473	360	2'-O-methyluridine	1.06 (0.91-1.23)	0.45086982	0.646764983	Nucleotide	Pyrimidine Metabolism, Uracil containing	NA	NA
474	361	ornithine	1.16 (0.94-1.42)	0.167739652	0.367455539	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
475	362	orotate	0.84 (0.69-1.03)	0.098204889	0.266434133	Nucleotide	Pyrimidine Metabolism, Orotate containing	NA	NA
476	363	O-sulfo-L-tyrosine	1.15 (0.94-1.40)	0.177298467	0.377278621	Xenobiotics	Chemical	NA	NA
477	364	2-oxindole-3-acetate	1.17 (0.96-1.43)	0.129406149	0.31791117	Xenobiotics	Food Component/Plant	NA	NA
478	365	6-oxopiperidine-2-carboxylate	1.10 (0.85-1.42)	0.474882753	0.673470086	Amino Acid	Lysine Metabolism	NA	NA
479	366	5-oxoproline	0.99 (0.80-1.22)	0.893922835	0.950268908	Amino Acid	Glutathione Metabolism	NA	NA
480	367	palmitate (16:0)	1.24 (1.04-1.49)	0.01818675	0.073216337	Lipid	Long Chain Fatty Acid	NA	NA
481	368	1-palmitoleoyl-2-linolenoyl-GPC (16:1/18:3)*	0.95 (0.78-1.15)	0.585020953	0.746074738	Lipid	Phosphatidylcholine (PC)	NA	NA
482	369	palmitoleoylcarnitine (C16:1)*	1.04 (0.85-1.27)	0.700761125	0.839465052	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
483	370	1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	1.29 (1.06-1.58)	0.012046729	0.054869771	Lipid	Phosphatidylcholine (PC)	NA	NA
484	371	1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	1.31 (1.06-1.63)	0.013444036	0.058664885	Lipid	Phosphatidylcholine (PC)	NA	NA
485	372	palmitoylcarnitine (C16)	1.11 (0.91-1.35)	0.286694878	0.483134927	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
486	373	palmitoylcholine	0.90 (0.70-1.15)	0.40009489	0.594426694	Lipid	Fatty Acid Metabolism (Acyl Choline)	NA	NA
487	374	palmitoyl dihydrosphingomyelin (d18:0/16:0)*	1.15 (0.96-1.39)	0.133529867	0.322955959	Lipid	Sphingolipid Metabolism	NA	NA
488	375	palmitoyl ethanolamide	1.11 (0.93-1.33)	0.246108472	0.458422945	Lipid	Endocannabinoid	NA	NA
489	376	1-palmitoylglycerol (16:0)	1.23 (1.00-1.50)	0.04831454	0.159514673	Lipid	Monoacylglycerol	NA	NA
490	377	1-palmitoyl-GPA (16:0)	1.26 (1.02-1.55)	0.033359285	0.1224482	Lipid	Lysophospholipid	NA	NA
491	378	1-palmitoyl-GPC (16:0)	1.14 (0.92-1.42)	0.233311308	0.449340296	Lipid	Lysophospholipid	NA	NA
492	379	2-palmitoyl-GPC (16:0)*	1.08 (0.85-1.38)	0.511499056	0.705987148	Lipid	Lysophospholipid	NA	NA
493	380	1-palmitoyl-GPE (16:0)	1.24 (1.03-1.50)	0.023386805	0.091208538	Lipid	Lysophospholipid	NA	NA
494	381	palmitoyl sphingomyelin (d18:1/16:0)	0.96 (0.80-1.16)	0.668662143	0.821348774	Lipid	Sphingolipid Metabolism	NA	NA
495	382	pantothenate	1.15 (0.96-1.37)	0.120840663	0.300416627	Cofactors and Vitamins	Pantothenate and CoA Metabolism	NA	NA
496	383	paraxanthine	1.09 (0.90-1.31)	0.38343108	0.57710959	Xenobiotics	Xanthine Metabolism	NA	NA
497	384	p-cresol-glucuronide*	1.02 (0.85-1.22)	0.861625712	0.931441686	Amino Acid	Tyrosine Metabolism	NA	NA
498	385	p-cresol sulfate	0.91 (0.77-1.06)	0.224098059	0.44112678	Xenobiotics	Benzoate Metabolism	NA	NA
499	386	pentadecanoate (15:0)	1.00 (0.84-1.19)	0.970884499	0.987308839	Lipid	Long Chain Fatty Acid	NA	NA
500	387	1-pentadecanoylglycerol (15:0)	0.98 (0.82-1.17)	0.857758665	0.930854621	Lipid	Monoacylglycerol	NA	NA
501	388	perfluorooctanesulfonic acid (PFOS)	1.16 (0.95-1.41)	0.145917354	0.342302365	Xenobiotics	Chemical	NA	NA
502	389	phenol sulfate	0.92 (0.77-1.10)	0.355586864	0.550586111	Amino Acid	Tyrosine Metabolism	NA	NA
503	390	phenylacetate	0.77 (0.64-0.92)	0.003809463	0.023141042	Amino Acid	Phenylalanine Metabolism	NA	NA
504	391	phenylacetylcarnitine	0.90 (0.77-1.04)	0.158955487	0.356563236	Peptide	Acetylated Peptides	NA	NA
505	392	phenylacetylglutamine	0.85 (0.73-1.00)	0.051410213	0.167083191	Peptide	Acetylated Peptides	NA	NA

506	393	phenylalanine	1.27 (0.97-1.66)	0.080908556	0.235920276	Amino Acid	Phenylalanine Metabolism	NA	NA
507	394	3-phenylpropionate (hydrocinnamate)	0.82 (0.70-0.96)	0.011402012	0.052468137	Xenobiotics	Benzoate Metabolism	NA	NA
508	395	phenylpyruvate	1.10 (0.93-1.31)	0.264109682	0.466868106	Amino Acid	Phenylalanine Metabolism	NA	NA
509	396	phosphate	0.95 (0.80-1.12)	0.533315405	0.717217269	Energy	Oxidative Phosphorylation	NA	NA
510	397	phosphoethanolamine	0.96 (0.79-1.17)	0.693663601	0.839465052	Lipid	Phospholipid Metabolism	NA	NA
511	398	picolinate	1.04 (0.88-1.22)	0.651815057	0.810409667	Amino Acid	Tryptophan Metabolism	NA	NA
512	399	pimeloylcarnitine/3-methyladipoylcarnitine (C7-DC)	0.78 (0.65-0.95)	0.012688669	0.056432788	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
513	400	pipecolate	1.11 (0.93-1.33)	0.231011425	0.449068939	Amino Acid	Lysine Metabolism	NA	NA
514	401	2-piperidinone	1.00 (0.86-1.17)	0.979588155	0.990701797	Xenobiotics	Food Component/Plant	NA	NA
515	402	piperine	1.21 (1.01-1.44)	0.033914654	0.123415741	Xenobiotics	Food Component/Plant	NA	NA
516	403	pregnanediol-3-glucuronide	0.91 (0.76-1.08)	0.277624865	0.474763489	Lipid	Progestin Steroids	NA	NA
517	404	pregnen-diol disulfate C21H34O8S2*	1.01 (0.84-1.21)	0.948348422	0.976517187	Lipid	Progestin Steroids	NA	NA
518	405	pregnenolone sulfate	0.93 (0.76-1.15)	0.521336216	0.710787353	Lipid	Pregnenolone Steroids	NA	NA
519	406	pregn steroid monosulfate C21H34O5S*	0.89 (0.72-1.10)	0.282053362	0.479567569	Lipid	Progestin Steroids	NA	NA
520	407	pro-hydroxy-pro	0.97 (0.82-1.15)	0.72009552	0.849269705	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
521	408	prolylglycine	1.21 (1.01-1.45)	0.0429682	0.147109107	Peptide	Dipeptide	NA	NA
522	409	propionylcarnitine (C3)	1.12 (0.94-1.34)	0.187734152	0.390487036	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	NA	NA
523	410	propionylglycine	0.84 (0.69-1.02)	0.086536401	0.247535973	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	NA	NA
524	411	propyl 4-hydroxybenzoate	0.93 (0.79-1.11)	0.434035617	0.628394954	Xenobiotics	Benzoate Metabolism	NA	NA
525	412	propyl 4-hydroxybenzoate sulfate	1.02 (0.85-1.22)	0.820620192	0.916041144	Xenobiotics	Benzoate Metabolism	NA	NA
526	413	pseudouridine	0.95 (0.77-1.18)	0.645816393	0.808159948	Nucleotide	Pyrimidine Metabolism, Uracil containing	NA	NA
527	414	pyridoxate	0.93 (0.77-1.13)	0.468688786	0.667721011	Cofactors and Vitamins	Vitamin B6 Metabolism	NA	NA
528	415	pyroglutamine*	0.71 (0.53-0.94)	0.016883527	0.069770338	Amino Acid	Glutamate Metabolism	NA	NA
529	416	pyrraline	0.97 (0.76-1.23)	0.783664155	0.889710172	Xenobiotics	Food Component/Plant	NA	NA
530	417	2-pyrrolidinone	1.01 (0.82-1.24)	0.944199035	0.976517187	Amino Acid	Glutamate Metabolism	NA	NA
531	418	quinate	0.91 (0.76-1.09)	0.309967398	0.505012158	Xenobiotics	Food Component/Plant	NA	NA
532	419	quinolinate	1.30 (1.02-1.65)	0.034216223	0.123415741	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	NA	NA
533	420	retinol (Vitamin A)	1.05 (0.88-1.26)	0.563745101	0.74152646	Cofactors and Vitamins	Vitamin A Metabolism	NA	NA
534	421	S-1-pyrroline-5-carboxylate	1.12 (0.92-1.36)	0.24889506	0.459498572	Amino Acid	Glutamate Metabolism	NA	NA
535	422	S-adenosylhomocysteine (SAH)	1.08 (0.85-1.36)	0.534537124	0.717314334	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
536	423	salicylate	0.90 (0.73-1.11)	0.342467338	0.538176864	Xenobiotics	Drug	NA	NA
537	424	S-allylcysteine	1.18 (0.94-1.47)	0.148681377	0.343619182	Xenobiotics	Food Component/Plant	NA	NA
538	425	sarcosine	1.03 (0.85-1.24)	0.797352749	0.898101292	Amino Acid	Glycine, Serine and Threonine Metabolism	NA	NA
539	426	S-carboxymethyl-L-cysteine	0.96 (0.80-1.15)	0.653262921	0.810409667	Xenobiotics	Drug	NA	NA
540	427	serotonin	1.14 (0.94-1.39)	0.195426229	0.402368191	Amino Acid	Tryptophan Metabolism	NA	NA
541	428	S-methylcysteine	0.96 (0.80-1.15)	0.655873996	0.8104788	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA

542	429	S-methylcysteine sulfoxide	0.87 (0.74-1.03)	0.108501804	0.282242708	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
543	430	spermidine	0.77 (0.64-0.92)	0.003559731	0.022643472	Amino Acid	Polyamine Metabolism	NA	NA
544	431	sphinganine-1-phosphate	1.07 (0.87-1.30)	0.529739296	0.717044079	Lipid	Sphingolipid Metabolism	NA	NA
545	432	sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)*	0.92 (0.78-1.09)	0.335741769	0.534164249	Lipid	Sphingolipid Metabolism	NA	NA
546	433	sphingomyelin (d17:2/16:0, d18:2/15:0)*	1.02 (0.82-1.28)	0.856979362	0.930854621	Lipid	Sphingolipid Metabolism	NA	NA
547	434	sphingomyelin (d18:1/14:0, d16:1/16:0)*	1.17 (0.99-1.39)	0.073244186	0.219732558	Lipid	Sphingolipid Metabolism	NA	NA
548	435	sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)	0.96 (0.81-1.15)	0.670799867	0.822355829	Lipid	Sphingolipid Metabolism	NA	NA
549	436	sphingomyelin (d18:1/18:1, d18:2/18:0)	1.30 (1.04-1.62)	0.0218879	0.086443351	Lipid	Sphingolipid Metabolism	NA	NA
550	437	sphingomyelin (d18:1/19:0, d19:1/18:0)*	1.09 (0.90-1.32)	0.372386392	0.56813963	Lipid	Sphingolipid Metabolism	NA	NA
551	438	sphingomyelin (d18:1/20:0, d16:1/22:0)*	1.17 (0.98-1.40)	0.074632983	0.222827661	Lipid	Sphingolipid Metabolism	NA	NA
552	439	sphingomyelin (d18:1/20:1, d18:2/20:0)*	0.91 (0.73-1.14)	0.404804905	0.598574078	Lipid	Sphingolipid Metabolism	NA	NA
553	440	sphingomyelin (d18:1/20:2, d18:2/20:1, d16:1/22:2)*	0.94 (0.76-1.17)	0.582321498	0.746074738	Lipid	Sphingolipid Metabolism	NA	NA
554	441	sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)*	1.11 (0.92-1.35)	0.276700603	0.474763489	Lipid	Sphingolipid Metabolism	NA	NA
555	442	sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)*	0.98 (0.81-1.19)	0.853828268	0.929823454	Lipid	Sphingolipid Metabolism	NA	NA
556	443	sphingomyelin (d18:1/22:2, d18:2/22:1, d16:1/24:2)*	0.90 (0.75-1.09)	0.277706207	0.474763489	Lipid	Sphingolipid Metabolism	NA	NA
557	444	sphingomyelin (d18:1/24:1, d18:2/24:0)*	1.16 (0.94-1.43)	0.170899114	0.370281414	Lipid	Sphingolipid Metabolism	NA	NA
558	445	sphingomyelin (d18:1/25:0, d19:0/24:1, d20:1/23:0, d19:1/24:0)*	1.00 (0.87-1.16)	0.978565637	0.990701797	Lipid	Sphingolipid Metabolism	NA	NA
559	446	sphingomyelin (d18:2/14:0, d18:1/14:1)*	1.13 (0.93-1.38)	0.218879726	0.435982163	Lipid	Sphingolipid Metabolism	NA	NA
560	447	sphingomyelin (d18:2/16:0, d18:1/16:1)*	1.23 (0.97-1.57)	0.093065883	0.260417538	Lipid	Sphingolipid Metabolism	NA	NA
561	448	sphingomyelin (d18:2/18:1)*	0.95 (0.76-1.19)	0.667357644	0.821348774	Lipid	Sphingolipid Metabolism	NA	NA
562	449	sphingomyelin (d18:2/21:0, d16:2/23:0)*	1.02 (0.77-1.34)	0.905416874	0.955694566	Lipid	Sphingolipid Metabolism	NA	NA
563	450	sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)*	0.98 (0.80-1.21)	0.868265326	0.932055413	Lipid	Sphingolipid Metabolism	NA	NA
564	451	sphingomyelin (d18:2/23:1)*	0.98 (0.79-1.22)	0.842470182	0.929711349	Lipid	Sphingolipid Metabolism	NA	NA
565	452	sphingomyelin (d18:2/24:1, d18:1/24:2)*	0.90 (0.74-1.10)	0.306392353	0.501807948	Lipid	Sphingolipid Metabolism	NA	NA
566	453	sphingomyelin (d18:2/24:2)*	0.81 (0.66-0.99)	0.038137056	0.135213199	Lipid	Sphingolipid Metabolism	NA	NA
567	454	sphingosine 1-phosphate	1.16 (0.98-1.38)	0.080669756	0.235920276	Lipid	Sphingolipid Metabolism	NA	NA
568	455	stachydrine	0.87 (0.73-1.03)	0.106910473	0.282242708	Xenobiotics	Food Component/Plant	NA	NA
569	456	stearate (18:0)	1.19 (0.98-1.46)	0.083831962	0.243307648	Lipid	Long Chain Fatty Acid	NA	NA
570	457	stearidonate (18:4n3)	1.18 (0.94-1.49)	0.14706235	0.343451055	Lipid	Polyunsaturated Fatty Acid (n3 and n6)	NA	NA
571	458	1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*	1.28 (1.05-1.56)	0.013335567	0.058601367	Lipid	Phosphatidylcholine (PC)	NA	NA
572	459	1-stearoyl-2-linoleoyl-GPI (18:0/18:2)	1.23 (0.99-1.51)	0.057417402	0.183735686	Lipid	Phosphatidylinositol (PI)	NA	NA
573	460	1-stearoyl-2-oleoyl-GPI (18:0/18:1)*	1.22 (1.03-1.44)	0.018987974	0.075468128	Lipid	Phosphatidylinositol (PI)	NA	NA
574	461	stearoylcarnitine (C18)	1.01 (0.85-1.19)	0.911118297	0.958397846	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
575	462	stearoylcholine*	0.93 (0.74-1.18)	0.56880731	0.742543434	Lipid	Fatty Acid Metabolism (Acyl Choline)	NA	NA
576	463	1-stearoyl-GPC (18:0)	1.21 (0.96-1.53)	0.108500408	0.282242708	Lipid	Lysophospholipid	NA	NA

577	464	2-stearoyl-GPE (18:0)*	1.25 (1.02-1.54)	0.034081658	0.123415741	Lipid	Lysophospholipid	NA	NA
578	465	1-stearoyl-GPI (18:0)	1.23 (0.95-1.60)	0.119044564	0.298328546	Lipid	Lysophospholipid	NA	NA
579	466	stearoyl sphingomyelin (d18:1/18:0)	1.23 (1.04-1.45)	0.018585442	0.074341769	Lipid	Sphingolipid Metabolism	NA	NA
580	467	suberate (octanedioate)	1.07 (0.90-1.26)	0.436773474	0.630895018	Lipid	Fatty Acid, Dicarboxylate	NA	NA
581	468	suberoylcarnitine (C8-DC)	0.90 (0.74-1.09)	0.267957535	0.470727632	Lipid	Fatty Acid Metabolism(Acyl Carnitine)	NA	NA
582	469	succinate	1.00 (0.83-1.21)	0.985217661	0.994205724	Energy	TCA Cycle	NA	NA
583	470	succinimide	0.98 (0.82-1.17)	0.830706342	0.92399422	Xenobiotics	Chemical	NA	NA
584	471	succinylcarnitine (C4-DC)	1.19 (0.97-1.45)	0.096462927	0.264833116	Energy	TCA Cycle	NA	NA
585	472	sulfate*	1.19 (0.97-1.45)	0.089045997	0.252566828	Xenobiotics	Chemical	NA	NA
586	473	tartronate (hydroxymalonate)	0.80 (0.66-0.98)	0.028751693	0.110067831	Xenobiotics	Bacterial/Fungal	NA	NA
587	474	taurine	0.98 (0.79-1.21)	0.826605424	0.921074616	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	NA	NA
588	475	taurochenodeoxycholate	1.11 (0.93-1.33)	0.239408089	0.45549379	Lipid	Primary Bile Acid Metabolism	NA	NA
589	476	taurocholate	1.06 (0.85-1.31)	0.631800458	0.798063736	Lipid	Primary Bile Acid Metabolism	NA	NA
590	477	taurocholenate sulfate	0.96 (0.73-1.27)	0.789307289	0.892260414	Lipid	Secondary Bile Acid Metabolism	NA	NA
591	478	taurodeoxycholate	1.21 (1.04-1.42)	0.01460059	0.061559245	Lipid	Secondary Bile Acid Metabolism	NA	NA
592	479	taurolithocholate 3-sulfate	0.99 (0.85-1.16)	0.921323136	0.961380664	Lipid	Secondary Bile Acid Metabolism	NA	NA
593	480	tetradecanedioate	0.82 (0.67-0.99)	0.042477156	0.147109107	Lipid	Fatty Acid, Dicarboxylate	NA	NA
594	481	theobromine	0.96 (0.79-1.15)	0.629329429	0.796554897	Xenobiotics	Xanthine Metabolism	NA	NA
595	482	theophylline	1.11 (0.92-1.35)	0.277146342	0.474763489	Xenobiotics	Xanthine Metabolism	NA	NA
596	483	thioproline	1.12 (0.90-1.39)	0.305342518	0.501807948	Xenobiotics	Chemical	NA	NA
597	484	threonine	0.98 (0.85-1.14)	0.842887886	0.929711349	Amino Acid	Glycine, Serine and Threonine Metabolism	NA	NA
598	485	threonylphenylalanine	1.11 (0.93-1.33)	0.234764061	0.450746998	Peptide	Dipeptide	NA	NA
599	486	thymol sulfate	0.90 (0.75-1.08)	0.260524332	0.466868106	Xenobiotics	Food Component/Plant	NA	NA
600	487	thyroxine	1.00 (0.81-1.22)	0.986239332	0.994205724	Amino Acid	Tyrosine Metabolism	NA	NA
601	488	tiglylcarnitine (C5:1-DC)	1.01 (0.86-1.17)	0.937009032	0.972867947	Amino Acid	Leucine, Isoleucine and Valine Metabolism	NA	NA
602	489	trans-4-hydroxyproline	1.06 (0.88-1.27)	0.566240776	0.74152646	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA
603	490	trans-urocanate	1.08 (0.92-1.26)	0.343808205	0.538176864	Amino Acid	Histidine Metabolism	NA	NA
604	491	tricosanoyl sphingomyelin (d18:1/23:0)*	1.22 (1.00-1.50)	0.052364023	0.168428609	Lipid	Sphingolipid Metabolism	NA	NA
605	492	trigonelline (N'-methylnicotinate)	0.99 (0.82-1.20)	0.918342756	0.961380664	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	NA	NA
606	493	trimethylamine N-oxide	1.11 (0.89-1.38)	0.363609462	0.557474949	Lipid	Phospholipid Metabolism	NA	NA
607	494	tryptophan betaine	1.00 (0.85-1.16)	0.962046573	0.985742302	Amino Acid	Tryptophan Metabolism	NA	NA
608	495	tryptophan	1.16 (0.93-1.44)	0.177746068	0.377278621	Amino Acid	Tryptophan Metabolism	NA	NA
609	496	tyramine O-sulfate	1.14 (0.95-1.36)	0.169329242	0.368158351	Amino Acid	Tyrosine Metabolism	NA	NA
610	497	10-undecenoate (11:1n1)	0.87 (0.73-1.03)	0.096765946	0.264833116	Lipid	Medium Chain Fatty Acid	NA	NA
611	498	uracil	0.96 (0.73-1.26)	0.773536592	0.887291973	Nucleotide	Pyrimidine Metabolism, Uracil containing	NA	NA
612	499	urea	0.89 (0.73-1.09)	0.258682342	0.465344732	Amino Acid	Urea cycle; Arginine and Proline Metabolism	NA	NA

613	500	3-ureidopropionate	1.11 (0.86-1.45)	0.415282148	0.607562848	Nucleotide	Pyrimidine Metabolism, Uracil containing	NA	NA
614	501	uridine	1.16 (0.96-1.40)	0.131565075	0.32068987	Nucleotide	Pyrimidine Metabolism, Uracil containing	NA	NA
615	502	ursodeoxycholate	1.26 (1.08-1.48)	0.004165365	0.023806769	Lipid	Secondary Bile Acid Metabolism	NA	NA
616	503	valylglycine	0.82 (0.64-1.05)	0.114581311	0.289468576	Peptide	Dipeptide	NA	NA
617	504	valylleucine	0.91 (0.73-1.13)	0.383814872	0.57710959	Peptide	Dipeptide	NA	NA
618	505	vanillactate	1.02 (0.83-1.24)	0.863541146	0.931441686	Amino Acid	Tyrosine Metabolism	NA	NA
619	506	vanillylmandelate (VMA)	0.89 (0.71-1.11)	0.309369939	0.505012158	Amino Acid	Tyrosine Metabolism	NA	NA
620	507	4-vinylphenol sulfate	1.00 (0.81-1.23)	0.998835714	0.998835714	Xenobiotics	Benzoate Metabolism	NA	NA
621	508	1,2,3-benzenetriol sulfate (2)	1.07 (0.88-1.30)	0.482495551	0.676728164	Xenobiotics	Chemical	NA	NA
622	509	xylose	1.10 (0.89-1.36)	0.392544644	0.587404935	Carbohydrate	Pentose Metabolism	NA	NA
623	510	dodecanedioate	0.75 (0.65-0.87)	0.000125677	0.001568453	Lipid	Fatty Acid, Dicarboxylate	NA	NA
624	511	mannose	1.92 (1.38-2.67)	0.000128731	0.001575059	Carbohydrate	Fructose, Mannose and Galactose Metabolism	NA	NA

Supplementary Table 3: Metabolite modules in relation to 6-y changes in cardiometabolic traits

Module	Traits	Model 1				Model 2			
		Beta	CI_lower	CI_upper	P value	Beta	CI_lower	CI_upper	P value
Black	Fasting glucose	1.015991	0.2073324	1.82465	0.0139	0.6624337	-0.2081055	1.532973	0.1356
Lipid module 1 (Sphingolipids)	2-h OGTT	5.01673	2.433505	7.599956	0.0002	3.671139	0.9357791	6.406499	0.0086
	HbA1c	2.006547	0.9618069	3.051287	0.0002	1.723865	0.6267047	2.821024	0.0021
	Fasting insulin	3.544094	0.9382538	6.149933	0.0078	1.51101	-0.4005529	3.422572	0.1211
	HOMA IR	2.739088	0.8865773	4.591599	0.0038	1.251884	-0.146888	2.650657	0.0793
	Triglycerides	3.065142	1.15559	4.974695	0.0017	2.90362	0.8746591	4.93258	0.0051
	Total cholesterol	-1.940539	-5.107484	1.226406	0.2293	-0.1763426	-3.756562	3.403876	0.923
	LDL cholesterol	-2.395852	-5.960355	1.16865	0.1873	-0.7789972	-4.736737	3.178742	0.6992
	HDL cholesterol	-1.784403	-4.632107	1.0633	0.219	-2.5693	-5.535604	0.3970049	0.0895
	SBP	1.383715	-0.6742612	3.441692	0.1872	1.818736	-0.2844767	3.921948	0.09
	DBP	2.030287	-0.7729605	4.833535	0.1554	2.242488	-0.5966803	5.081657	0.1214
Yellow	Fasting glucose	1.22226	0.2234879	2.221032	0.0165	1.157908	0.1476325	2.168183	0.0247
Lipid module 2 (PC, PI)	2-h OGTT	2.054102	-0.7393471	4.847552	0.1492	1.723237	-1.057176	4.503651	0.224
	HbA1c	1.163495	-0.0620584	2.389049	0.0627	1.094272	-0.1177428	2.306287	0.0767
	Fasting insulin	-0.4900869	-2.784095	1.803922	0.675	-0.9612288	-3.115766	1.193308	0.3813
	HOMA IR	0.3132134	-1.475832	2.102258	0.7311	0.0111856	-1.720044	1.742416	0.989
	Triglycerides	-0.8868123	-3.376763	1.603138	0.4846	-0.8243071	-3.31811	1.669496	0.5165
	Total cholesterol	-1.004679	-3.658677	1.649318	0.4575	-0.6345604	-3.288514	2.019394	0.6389
	LDL cholesterol	0.178088	-2.370636	2.726812	0.8909	0.7381267	-1.766735	3.242988	0.563
	HDL cholesterol	0.3820983	-3.120587	3.884784	0.8304	-0.5961466	-3.662489	2.470196	0.7028
	SBP	1.019217	-1.574461	3.612894	0.4406	0.9018365	-1.663883	3.467556	0.4903
	DBP	0.9852455	-1.939916	3.910407	0.5086	0.6432364	-2.229671	3.516144	0.6603
Red	Fasting glucose	1.238655	0.3567577	2.120552	0.006	1.0207	0.1236057	1.917794	0.0258
Lipid module 3 (MAG, DAG)	2-h OGTT	3.003096	0.1132731	5.892918	0.0417	2.28755	-0.6168812	5.191982	0.1224
	HbA1c	1.572832	0.5515829	2.594081	0.0026	1.327742	0.2732154	2.382268	0.0137
	Fasting insulin	0.7115246	-1.819844	3.242893	0.5812	-0.2683548	-2.800827	2.264117	0.8352
	HOMA IR	1.124933	-0.8039293	3.053796	0.2525	0.4118183	-1.561907	2.385543	0.6821
	Triglycerides	3.85186	0.2455276	7.458193	0.0364	3.626833	-0.0014042	7.255071	0.0501
	Total cholesterol	-1.372889	-3.728729	0.9829507	0.2529	-0.8336034	-3.240124	1.572917	0.4966
	LDL cholesterol	0.3305319	-2.03102	2.692084	0.7835	0.8966	-1.492136	3.285336	0.4614
	HDL cholesterol	-0.2210291	-3.42599	2.983932	0.8923	-0.3340623	-3.55278	2.884656	0.8386
	SBP	0.6316801	-1.986477	3.249837	0.6358	0.7055241	-1.923672	3.33472	0.5984
	DBP	0.4633257	-2.347605	3.274257	0.7463	0.3444464	-2.481825	3.170718	0.8109

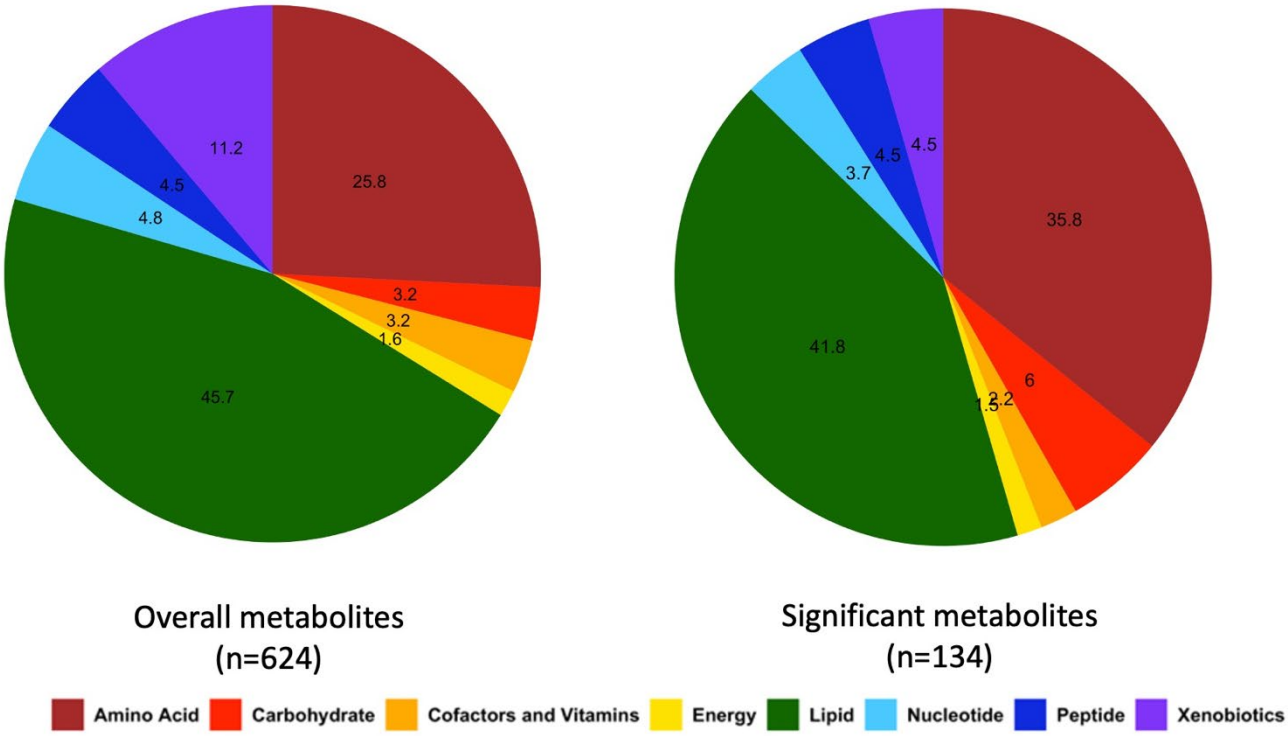
Brown	Fasting glucose	0.9633461	0.0147136	1.911978	0.0466	0.8888139	-0.0623785	1.840006	0.067
Lipid module 4 (PE, LPL)	2-h OGTT	2.99787	-0.0647763	6.060517	0.055	2.690404	-0.3932242	5.774032	0.0871
	HbA1c	1.135207	0.0556135	2.2148	0.0393	1.041865	-0.0418396	2.12557	0.0595
	Fasting insulin	0.0425998	-2.281464	2.366664	0.9713	-0.3878263	-2.614153	1.838501	0.7324
	HOMA IR	0.7227135	-1.175185	2.620612	0.4549	0.4625854	-1.396303	2.321474	0.6252
	Triglycerides	-0.6937413	-3.204198	1.816715	0.5876	-0.5428344	-3.048919	1.96325	0.6707
	Total cholesterol	-0.9551788	-3.220953	1.310596	0.4081	-0.5550251	-2.826094	1.716043	0.6315
	LDL cholesterol	0.4442113	-2.011221	2.899644	0.7225	0.9844334	-1.46707	3.435937	0.4307
	HDL cholesterol	0.2471465	-2.803231	3.297524	0.8736	-0.3901532	-3.221415	2.441108	0.7868
	SBP	0.2747483	-2.379601	2.929098	0.839	0.1175917	-2.498459	2.733642	0.9297
	DBP	0.9511615	-1.988141	3.890464	0.5254	0.6310656	-2.279033	3.541164	0.6704
Turquoise	Fasting glucose	2.22496	1.033192	3.416727	0.0003	1.793618	0.4944304	3.092805	0.0069
AA module 1 (BCAA, AAA, GGAA)	2-h OGTT	7.863194	4.096337	11.63005	<0.0001	6.035096	1.941791	10.1284	0.0039
	HbA1c	1.730615	0.2769877	3.184242	0.0197	1.125776	-0.4970724	2.748625	0.1736
	Fasting insulin	5.935657	1.422219	10.4491	0.01	3.137561	-0.4418896	6.717012	0.0857
	HOMA IR	5.337174	1.809614	8.864735	0.0031	3.349879	0.3193961	6.380362	0.0303
	Triglycerides	0.6918158	-1.676975	3.060607	0.5665	-0.0795907	-2.677021	2.51784	0.952
	Total cholesterol	-3.925408	-6.597984	-1.252832	0.0041	-3.00057	-5.817628	-0.1835129	0.0369
	LDL cholesterol	-3.330447	-6.156528	-0.504365	0.021	-2.253536	-5.217383	0.7103106	0.1359
	HDL cholesterol	-0.0587611	-4.0057	3.888177	0.9767	-0.301773	-4.545085	3.941539	0.889
	SBP	-0.7043946	-3.403882	1.995093	0.6085	-0.2766011	-3.269446	2.716244	0.856
	DBP	-2.248846	-5.505771	1.00808	0.1756	-2.481368	-5.917179	0.9544434	0.1566
Green yellow	Fasting glucose	-0.7981864	-1.51048	-0.0858925	0.0281	-0.4880137	-1.189422	0.2133952	0.1723
AA module 2 (Glycine)	2-h OGTT	-3.98285	-6.577818	-1.387883	0.0027	-2.782558	-5.416153	-0.1489639	0.0384
	HbA1c	-1.246009	-2.13445	-0.3575674	0.0061	-0.9473888	-1.874659	-0.0201189	0.0452
	Fasting insulin	-1.901351	-5.000438	1.197735	0.2287	-0.4873779	-2.732584	1.757828	0.6701
	HOMA IR	-1.563238	-3.834165	0.7076885	0.1769	-0.5268417	-2.265944	1.212261	0.5521
	Triglycerides	0.9545462	-0.721522	2.630615	0.2638	1.481954	-0.2971456	3.261054	0.1024
	Total cholesterol	2.406449	0.1817106	4.631187	0.034	1.874575	-0.5749649	4.324115	0.1334
	LDL cholesterol	2.089773	-0.2434662	4.423011	0.0791	1.313339	-1.184485	3.811163	0.3022
	HDL cholesterol	-1.423938	-4.271381	1.423505	0.3265	-0.8734094	-3.528653	1.781834	0.5186
	SBP	0.5809602	-1.49782	2.65974	0.5833	0.2198235	-1.892382	2.332029	0.8381
	DBP	1.804484	-0.7191212	4.328088	0.1608	1.690049	-0.9212072	4.301305	0.2042
Green	Fasting glucose	1.638047	0.6647729	2.611321	0.001	1.360171	0.3008124	2.41953	0.0119
Glucose and energy metabolism module	2-h OGTT	4.800724	1.766614	7.834833	0.002	3.306784	0.1011316	6.512437	0.0432
	HbA1c	2.550391	1.137576	3.963206	0.0004	2.377399	0.8584198	3.896378	0.0022

	Fasting insulin	4.287259	0.5015993	8.072918	0.0265	2.371838	-0.6956849	5.439361	0.1294
	HOMA IR	3.687423	0.9674275	6.407418	0.008	2.331629	0.0690891	4.594168	0.0434
	Triglycerides	1.413019	-0.8551378	3.681176	0.2216	1.045907	-1.381991	3.473805	0.3979
	Total cholesterol	-2.334964	-4.886223	0.2162948	0.0728	-1.514559	-4.36767	1.338553	0.2976
	LDL cholesterol	-2.063519	-4.672316	0.5452781	0.1209	-0.9734631	-3.927205	1.980279	0.5177
	HDL cholesterol	-1.045563	-4.190672	2.099546	0.5141	-2.157552	-4.949181	0.6340782	0.1296
	SBP	2.276336	-0.0973258	4.649999	0.0601	3.115009	0.5831417	5.646876	0.016
	DBP	2.103372	-0.7000321	4.906776	0.1411	2.414647	-0.3692013	5.198496	0.089
Purple	Fasting glucose	-2.106926	-3.226393	-0.9874593	0.0002	-1.96071	-3.088599	-0.8328216	0.0007
Plant-food metabolite module	2-h OGTT	-2.897093	-6.141775	0.3475881	0.08	-2.036042	-5.317928	1.245843	0.2236
	HbA1c	-2.156403	-3.572565	-0.7402419	0.0029	-1.985036	-3.404076	-0.5659958	0.0062
	Fasting insulin	-4.030848	-6.702909	-1.358787	0.0032	-3.043567	-5.244413	-0.8427218	0.0068
	HOMA IR	-3.765934	-5.848161	-1.683707	0.0004	-3.065632	-4.859012	-1.272252	0.0008
	Triglycerides	-1.301382	-2.73063	0.1278661	0.0742	-1.091074	-2.516679	0.3345304	0.1334
	Total cholesterol	-0.532066	-2.694755	1.630623	0.6292	-1.130637	-3.276421	1.015147	0.3012
	LDL cholesterol	0.1334497	-2.076014	2.342913	0.9056	-0.6009134	-2.767375	1.565549	0.5862
	HDL cholesterol	-0.656323	-3.784632	2.471986	0.6805	-0.0609371	-3.016161	2.894286	0.9677
	SBP	-0.8951823	-3.468478	1.678114	0.4948	-1.242931	-3.808635	1.322772	0.3418
	DBP	-1.569964	-4.548645	1.408718	0.3011	-1.899425	-4.846622	1.047772	0.2061
Magenta	Fasting glucose	1.509688	0.59821	2.421164	0.0012	1.432386	0.5341454	2.330627	0.0018
Androgenic steroid module	2-h OGTT	5.510037	2.793068	8.227006	0.0001	5.225643	2.495291	7.955995	0.0002
	HbA1c	1.064405	0.019303	2.1095	0.0459	0.968759	-0.0685777	2.006096	0.0671
	Fasting insulin	1.151437	-1.055558	3.358433	0.306	0.2874981	-1.892748	2.467744	0.7958
	HOMA IR	1.317608	-0.4897947	3.12501	0.1528	0.7191008	-1.064105	2.502307	0.4287
	Triglycerides	1.279116	-0.5364551	3.094687	0.167	1.241777	-0.5606178	3.044173	0.1766
	Total cholesterol	1.712686	-0.8318794	4.257251	0.1867	2.130039	-0.4448815	4.70496	0.1048
	LDL cholesterol	1.252731	-1.499104	4.004566	0.3717	1.783172	-1.002098	4.568442	0.2091
	HDL cholesterol	1.228946	-2.720733	5.178625	0.5414	0.6735511	-3.057153	4.404255	0.7231
	SBP	1.814498	-1.020582	4.649579	0.2093	1.761295	-1.038266	4.560855	0.2171
	DBP	2.430581	-0.6299904	5.491153	0.1194	2.252201	-0.7414193	5.245822	0.1401
Pink	Fasting glucose	0.6903446	-0.1642198	1.544909	0.1132	0.4154303	-0.4701526	1.301013	0.3573
Mixed metabolite module	2-h OGTT	4.508121	1.508978	7.507265	0.0033	3.280188	0.1661967	6.39418	0.039
	HbA1c	0.259876	-1.03901	1.558762	0.6945	-0.1034554	-1.401321	1.19441	0.8757
	Fasting insulin	0.2868042	-3.508944	4.082552	0.8821	-1.09828	-4.849651	2.65309	0.5656
	HOMA IR	0.5698954	-2.328051	3.467841	0.6995	-0.410112	-3.337857	2.517633	0.7833
	Triglycerides	-0.5367012	-2.571905	1.498503	0.6047	-0.9191844	-3.039501	1.201132	0.3949

	Total cholesterol	-1.928907	-4.277054	0.4192402	0.1072	-1.176848	-3.62585	1.272153	0.3457
	LDL cholesterol	-1.882188	-4.436558	0.6721812	0.1484	-0.8047093	-3.390362	1.780943	0.5413
	HDL cholesterol	1.762955	-2.397823	5.923734	0.4057	0.6749747	-2.980763	4.330713	0.717
	SBP	-0.8723044	-3.876292	2.131683	0.5687	-0.556527	-3.683196	2.570142	0.7268
	DBP	-0.9238016	-5.088645	3.241041	0.6633	-0.8271497	-4.925285	3.270986	0.692

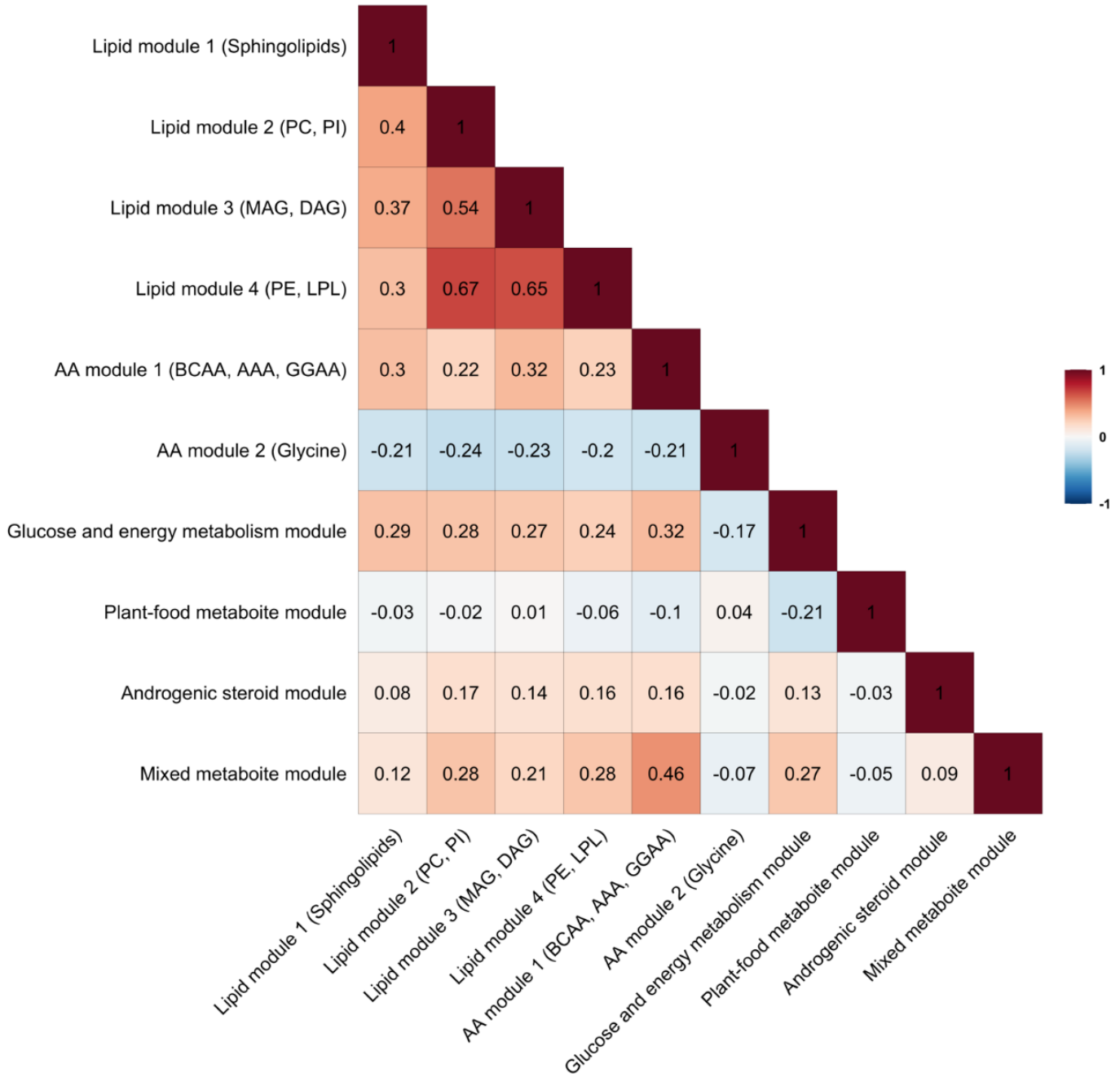
Results were from multivariable survey linear regression models; participants who were treated for diabetes, dyslipidemia, or hypertension at V1 or V2 were excluded from the analyses of changes in glycemic traits, serum lipids, or blood pressure, respectively.
Model 1 was adjusted for age, sex, study field center, Hispanic/Latino background, education, annual household income, smoking status, drinking status, total physical activity, AHEI-2010 score, family history of diabetes, fasting hours for the blood samples at V1 and V2 (for changes in blood biomarkers), baseline levels of the assessed cardiometabolic traits.
Model 2 was further adjusted for BMI and WHR.

Supplementary Figure 1. Pathway-specific proportions for all tested metabolites and for metabolites significantly associated with incident diabetes.



Supplementary Figure 2. Correlations among 10 metabolite modules.

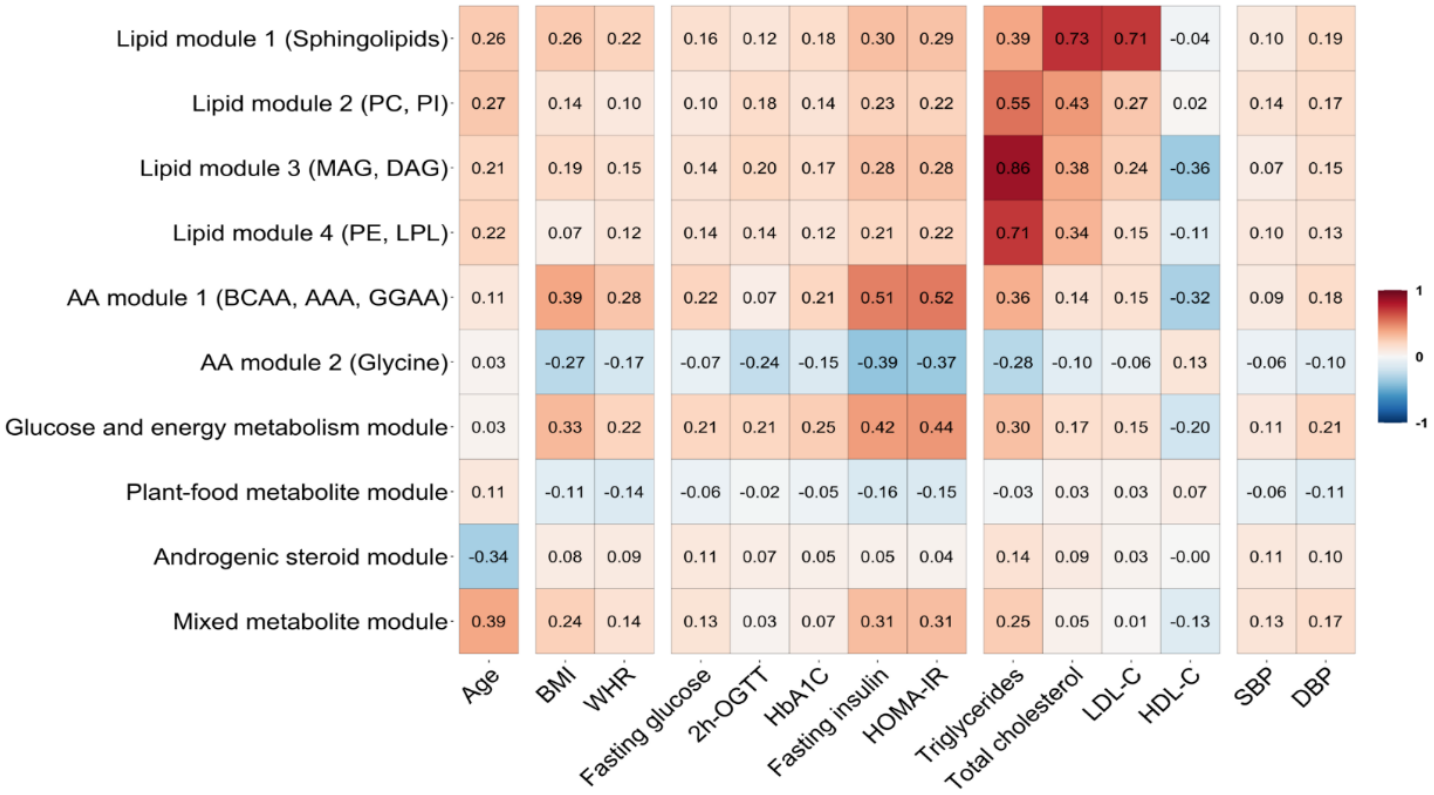
Results were partial Spearman correlations with adjustment for age, sex, study field center, and Hispanic/Latino background.



Supplementary Figure 3. correlations between 10 metabolite modules and diabetes risk factors.

Results were partial Spearman correlations with adjustment for age (where appliable), sex, study field center, and Hispanic/Latino background.

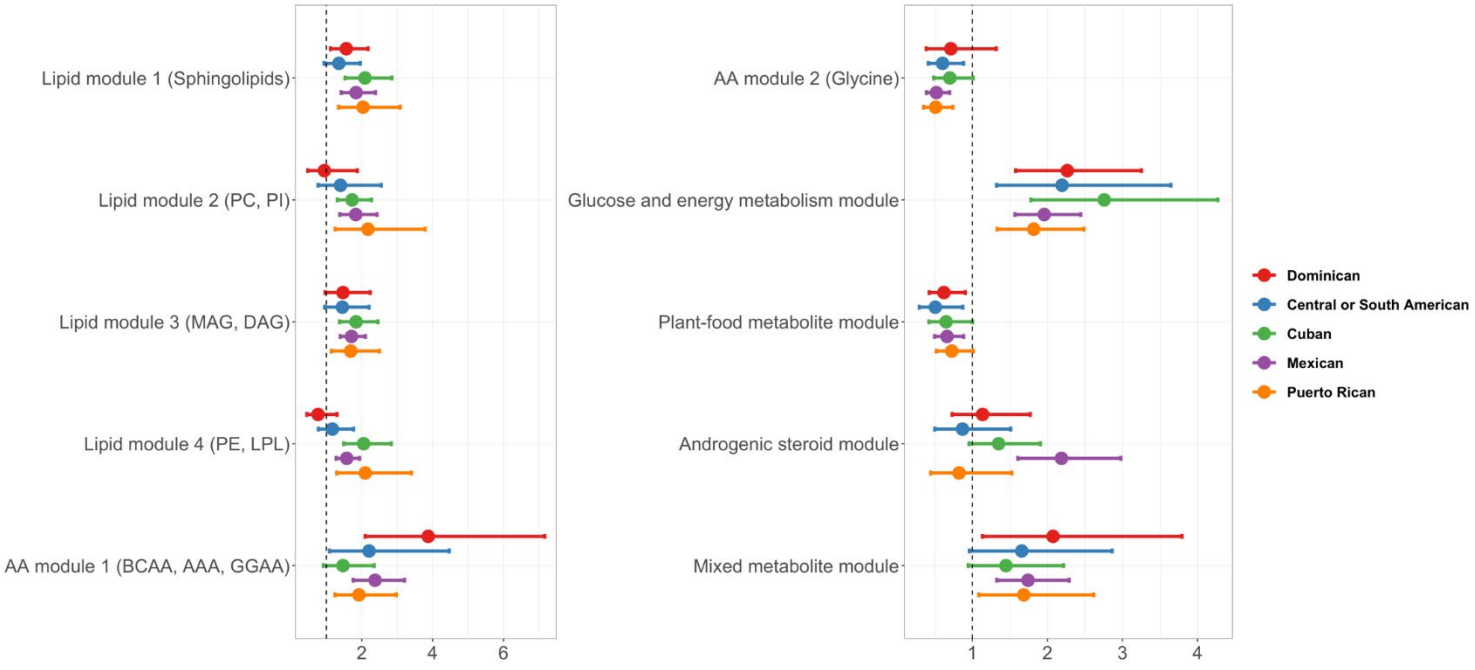
AA, amino acids; AAA, aromatic amino acids; BCAA, Branched-chain amino acids; BMI, body mass index; DAG, Diacylglycerol; DBP, diastolic blood pressure; GGAA, gamma-glutamyl amino acids; HbA1c, hemoglobin A1c; HDL-C, high-density lipoprotein cholesterol; HOMA-IR, homeostatic model assessment of insulin resistance; LDL-C, low-density lipoprotein cholesterol; MAG, monoacylglycerol; OGTT, oral glucose tolerance test; PC, phosphatidylcholine; PE, phosphatidylethanolamine; PI, phosphatidylinositol; SBP, systolic blood pressure; WHR, waist-to-hip ratio.



Supplementary Figure 4. Association of 10 metabolite modules with incident diabetes by Hispanic/Latino background.

Results are relative risks and 95% confidence intervals of incident diabetes associated with per SD increment of the module scores in multivariable survey Poisson regression models.

Models were adjusted for age, sex, study field center, Hispanic/Latino background, education, annual household income, smoking status, drinking status, total physical activity, AHEI-2010 score, lipid lowering medication use, antihypertensive medication use, family history of diabetes, and fasting hours for the blood samples.



Supplementary Figure 5. Association of 10 metabolite modules with incident diabetes.

Results are relative risks and 95% confidence intervals of incident diabetes associated with per SD increment of the module scores in multivariable survey Poisson regression models.

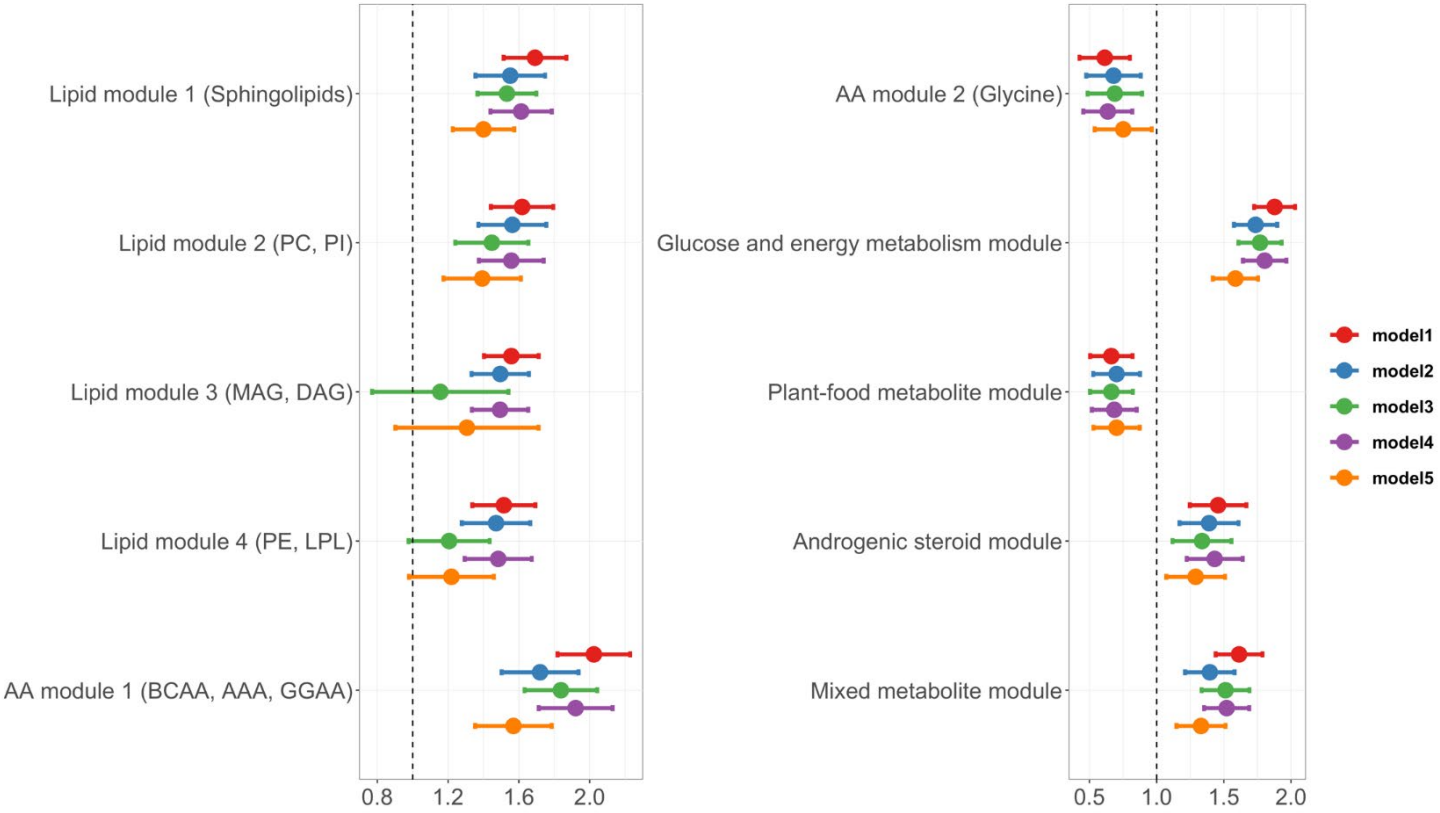
Model 1: age, sex, study field center, Hispanic/Latino background, education, annual household income, smoking status, drinking status, total physical activity, AHEI-2010 score, lipid lowering medication use, antihypertensive medication use, family history of diabetes, and fasting hours for the blood samples.

Model 2: model 1 + BMI and waist-to-hip ratio.

Model 3: model 1 + HDL cholesterol and triglycerides.

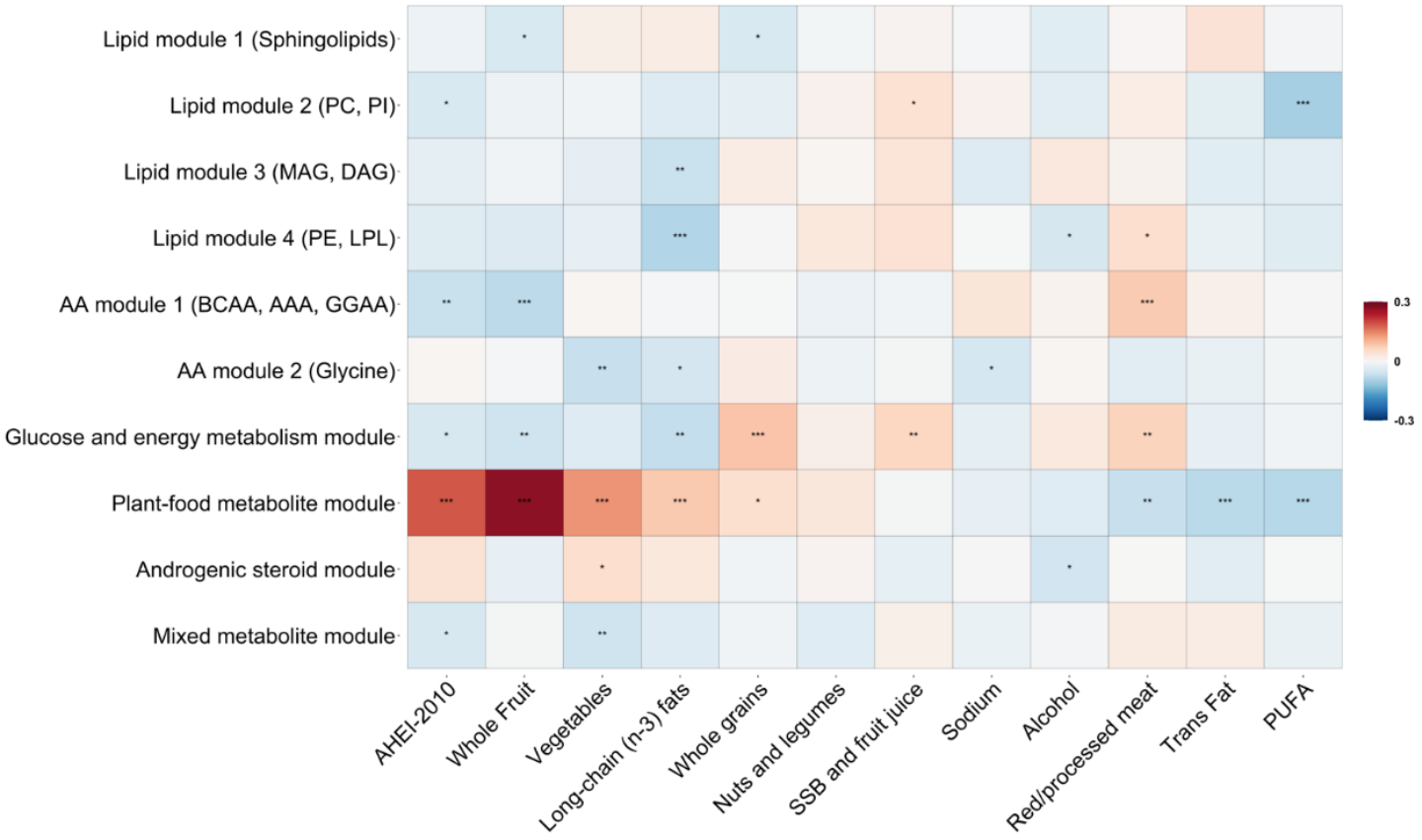
Model 4: model 1 + SBP and DBP.

Model 5: all above.



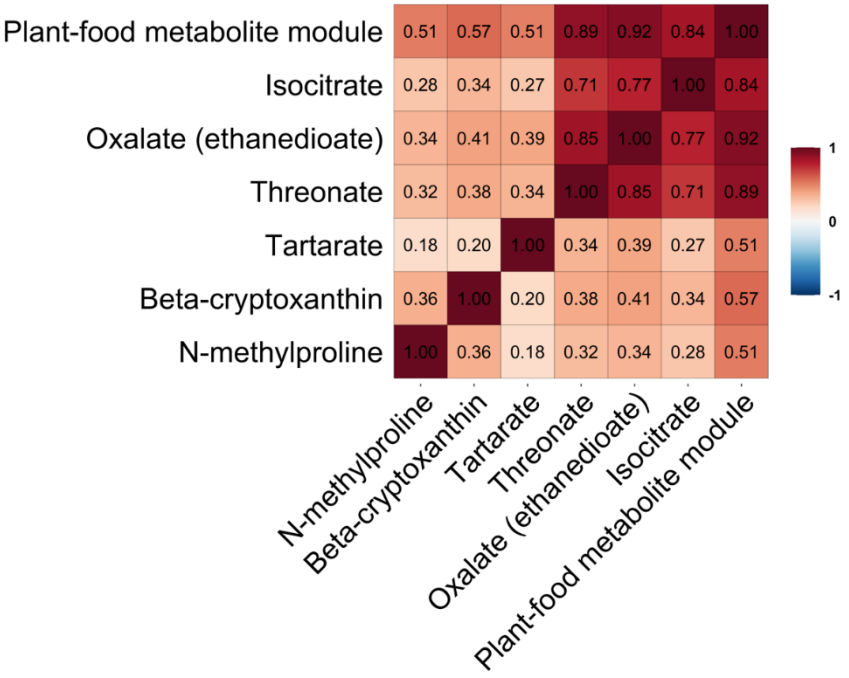
Supplementary Figure 6. Correlations between 10 metabolite modules and AHEI-2010 score and its component food groups/nutrients.

Results were partial Spearman correlations with adjustment for age, sex, study field center, and Hispanic/Latino background. *P<0.05; **P<0.01; *** P< 0.001.



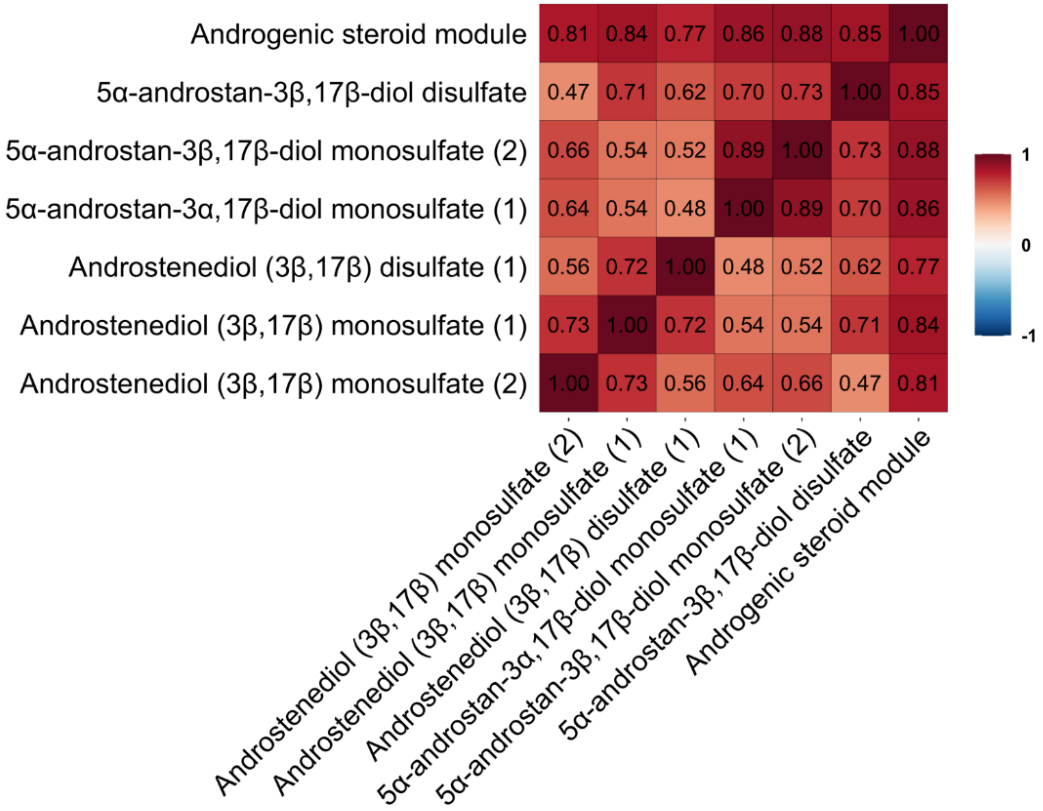
Supplementary Figure 7. Correlations among component metabolites within the plant-food metabolite module

Results were partial Spearman correlations with adjustment for age, sex, study field center, and Hispanic/Latino background.

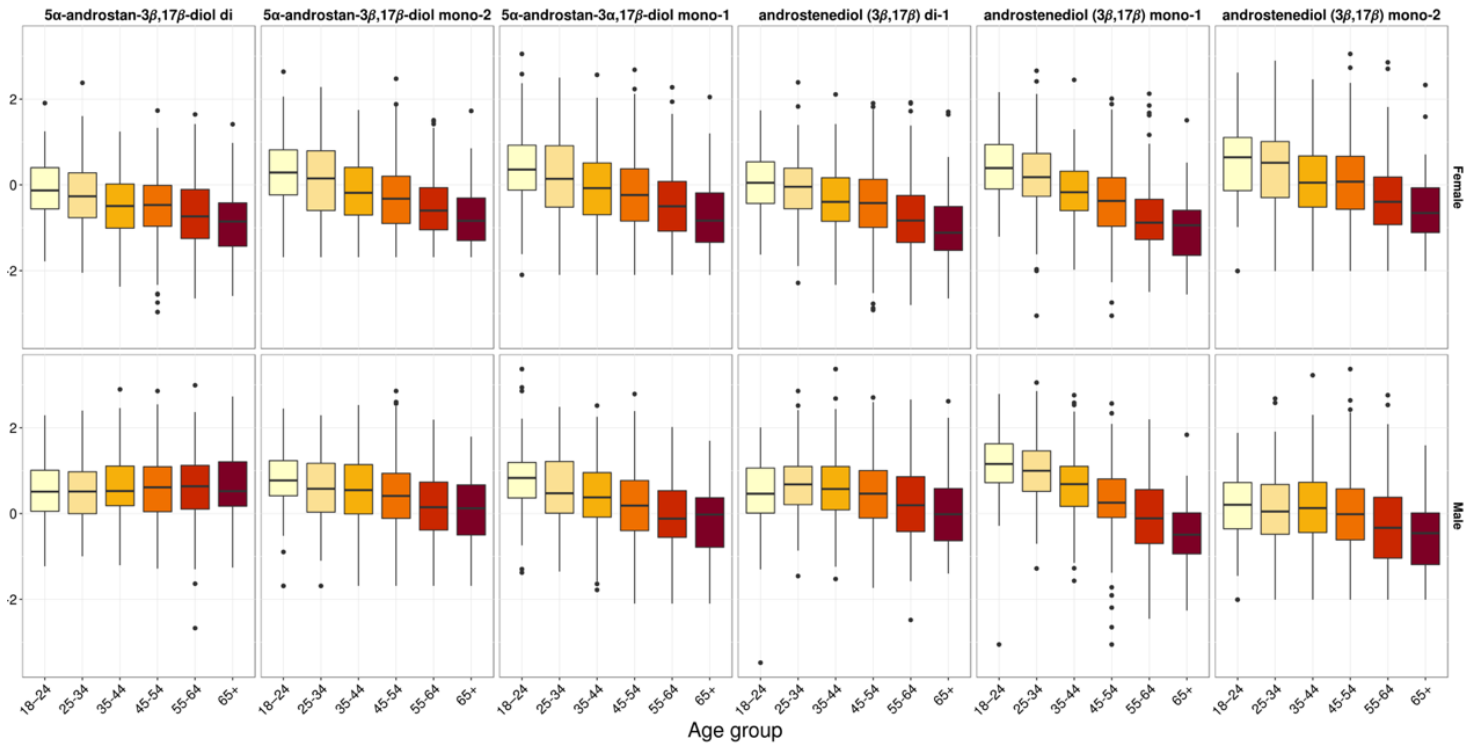


Supplementary Figure 8. Correlations among metabolites of androgenic steroid module

Results were partial Spearman correlations with adjustment for age, sex, study field center, and Hispanic/Latino background.



Supplementary Figure 9. Distribution of metabolites in the androgenic steroid module in women and men according to age groups

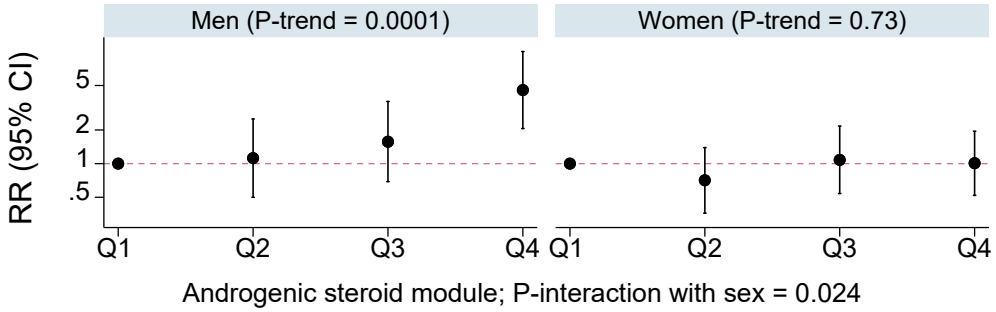


Supplementary Figure 10. Sex-specific association of androgenic steroid module and its component metabolites with risk of diabetes in the SOL study.

A: Androgenic steroid module score and risk of diabetes in men and women; B: Component metabolites for the Androgenic steroid module and risk of diabetes.

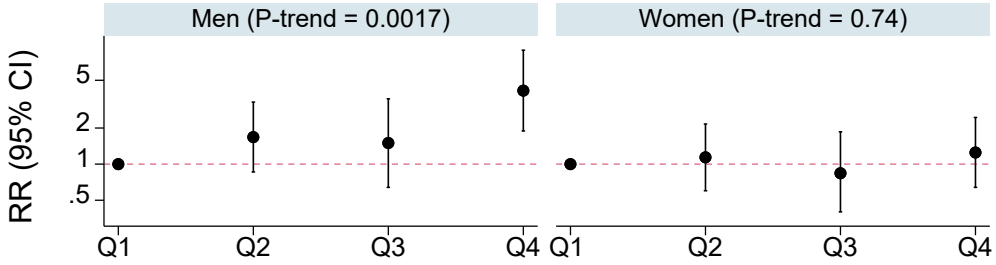
Results were adjusted for age, sex, study field center, Hispanic/Latino background, education, annual household income, smoking status, drinking status, total physical activity, AHEI-2010 score, lipid lowering medication use, antihypertensive medication use, family history of diabetes, and fasting hours for the blood samples.

A

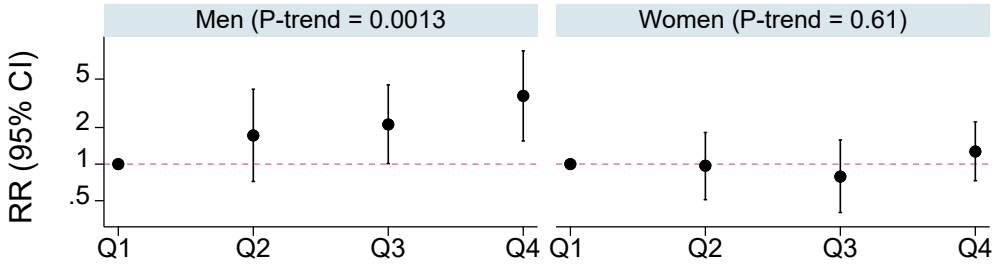


Androgenic steroid module; P-interaction with sex = 0.024

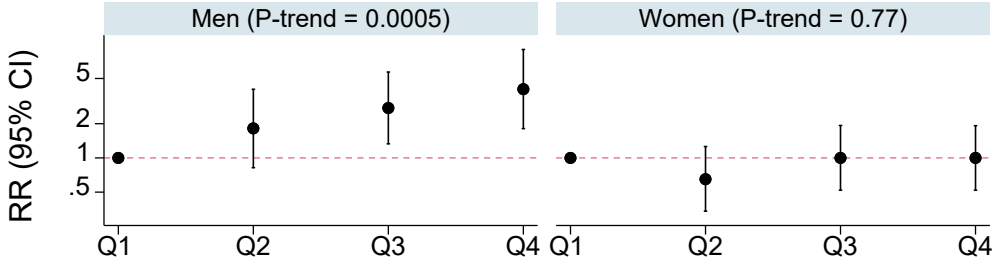
B



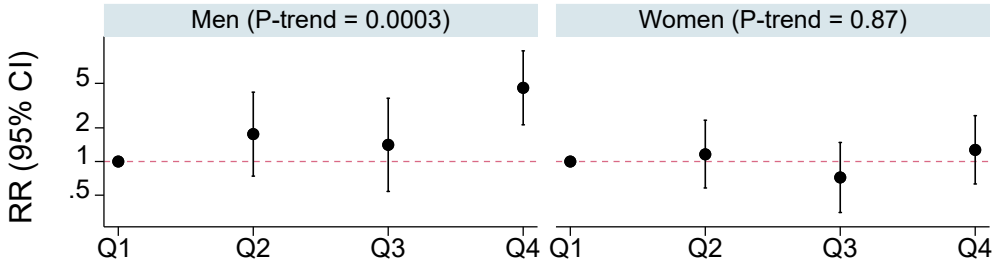
5alpha-androstan-3alpha,17beta-diol monosulfate (1) ; P-interaction = 0.092



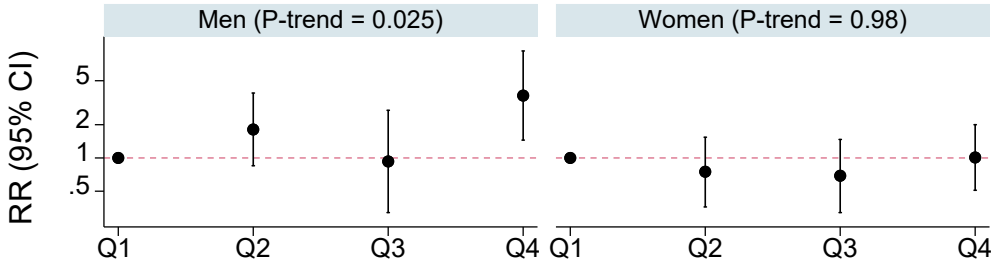
5alpha-androstan-3beta,17beta-diol disulfate ; P-interaction = 0.11



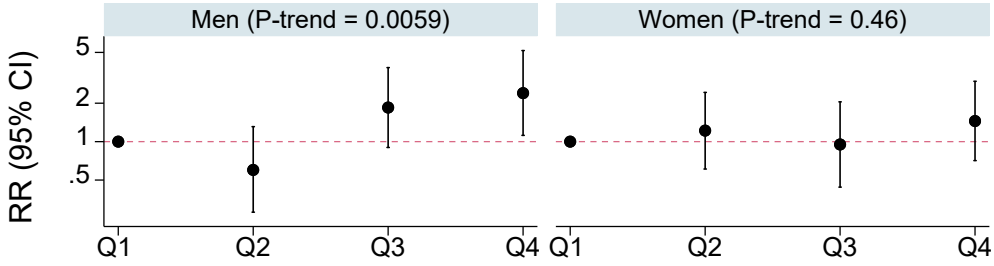
5alpha-androstan-3beta,17beta-diol monosulfate (2) ; P-interaction = 0.056



Androstenediol (3beta,17beta) disulfate (1) ; P-interaction = 0.025



Androstenediol (3beta,17beta) monosulfate (1) ; P-interaction = 0.17



Androstenediol (3beta,17beta) monosulfate (2) ; P-interaction = 0.51