SUPPLEMENTAL MATERIAL

Supplemental Table 1. Association with CHD for the 371 metabolites in the WHI-OS discovery dataset.

				Matching Adjustment		Full Adjustment	
Metabolite.Name	**Method**	**Category**	**HMDB.ID**	**OR (95 CI%)**	**FDR p**	**OR (95 CI%)**	**FDR p**
glycodeoxycholate	C18-neg	Bile acids	HMDB00631	1.2 (1.38, 1.05)	3.5E-02	1.1 (1.31, 0.99)	2.5E-01
glycocholate	C18-neg	Bile acids	HMDB00138	1.1 (1.29, 0.99)	1.7E-01	1 (1.16, 0.88)	8.9E-01
glycochenodeoxycholate	C18-neg	Bile acids	HMDB00637	1.1 (1.28, 0.99)	1.9E-01	1 (1.18, 0.9)	8.1E-01
glycoursodeoxycholate	C18-neg	Bile acids	HMDB00708	1.1 (1.28, 0.98)	2.2E-01	1 (1.2, 0.91)	7.5E-01
deoxycholate/chenodeoxycholate	C18-neg	Bile acids	HMDB00626	1.1 (1.25, 0.96)	3.3E-01	1.1 (1.21, 0.92)	6.8E-01
taurodeoxycholate	C18-neg	Bile acids	HMDB00896	1 (1.19, 0.92)	5.8E-01	1 (1.17, 0.89)	8.5E-01
taurochenodeoxycholate	C18-neg	Bile acids	HMDB00951	1 (1.19, 0.92)	5.9E-01	1 (1.15, 0.88)	9.2E-01
taurocholate	C18-neg	Bile acids	HMDB00036	1 (1.19, 0.92)	6.0E-01	1 (1.13, 0.86)	8.9E-01
hyodeoxycholate	C18-neg	Bile acids	HMDB00733	1 (1.09, 0.84)	6.1E-01	1 (1.16, 0.88)	9.2E-01
glycolithocholate	C18-neg	Bile acids	HMDB00698	1 (1.18, 0.91)	6.6E-01	1.1 (1.21, 0.92)	6.8E-01
cholate	C18-neg	Bile acids	HMDB00619	1 (1.1, 0.85)	6.6E-01	0.9 (1.07, 0.81)	5.7E-01
taurohyodeoxycholate/ tauroursodeoxycholate	C18-neg	Bile acids	HMDB00874	1 (1.17, 0.91)	6.8E-01	1 (1.12, 0.85)	8.4E-01
ursodeoxycholate	C18-neg	Bile acids	HMDB00946	1 (1.17, 0.9)	7.0E-01	0.9 (1.09, 0.82)	6.8E-01
lithocholate	C18-neg	Bile acids	HMDB00761	1 (1.13, 0.88)	8.4E-01	1 (1.14, 0.87)	9.2E-01
5-HETE	C18-neg	Eicosanoids	HMDB11134	1.4 (1.65, 1.25)	9.9E-06	1.3 (1.55, 1.17)	5.5E-03
11-HETE	C18-neg	Eicosanoids	HMDB04682	1.4 (1.55, 1.19)	3.0E-04	1.3 (1.48, 1.12)	1.7E-02
15-HETE	C18-neg	Eicosanoids	HMDB03876	1.3 (1.53, 1.17)	4.1E-04	1.2 (1.43, 1.08)	3.7E-02
12-HETE	C18-neg	Eicosanoids	HMDB06111	1.2 (1.39, 1.07)	2.2E-02	1.2 (1.36, 1.03)	1.1E-01
LTB4	C18-neg	Eicosanoids	HMDB01085	1.2 (1.36, 1.05)	3.6E-02	1.1 (1.3, 0.99)	2.5E-01
PGE2	C18-neg	Eicosanoids	HMDB01220	1.1 (1.24, 0.95)	3.8E-01	1.1 (1.21, 0.92)	6.8E-01
docosahexaenoic acid	C18-neg	Fatty acids	HMDB02183	0.8 (0.93, 0.71)	1.7E-02	0.8 (0.97, 0.73)	1.1E-01
gamma-linolenic acid	C18-neg	Fatty acids	HMDB03073	0.9 (1.01, 0.78)	2.0E-01	0.9 (0.99, 0.75)	1.7E-01
docosapentaenoic acid	C18-neg	Fatty acids	HMDB01976	0.9 (1.02, 0.78)	2.2E-01	0.9 (1, 0.75)	2.0E-01
eicosapentaenoic acid	C18-neg	Fatty acids	HMDB01999	0.9 (1.04, 0.8)	3.3E-01	0.9 (1.05, 0.8)	4.9E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
palmitoleic acid	C18-neg	Fatty acids	HMDB03229	0.9 (1.06, 0.81)	4.1E-01	0.9 (1.08, 0.81)	6.2E-01
linoleic acid	C18-neg	Fatty acids	HMDB00673	0.9 (1.07, 0.83)	5.0E-01	0.9 (1.04, 0.79)	4.2E-01
myristic acid	C18-neg	Fatty acids	HMDB00806	0.9 (1.08, 0.83)	5.5E-01	0.9 (1.07, 0.82)	6.1E-01
8.11.14-eicosatrienoic acid	C18-neg	Fatty acids	HMDB02925	0.9 (1.08, 0.83)	5.5E-01	0.9 (1.02, 0.77)	3.0E-01
myristoleic acid	C18-neg	Fatty acids	HMDB02000	1.1 (1.2, 0.92)	5.7E-01	1.1 (1.21, 0.92)	6.8E-01
oleic acid	C18-neg	Fatty acids	HMDB00207	1 (1.11, 0.86)	7.2E-01	0.9 (1.08, 0.82)	6.4E-01
stearic acid	C18-neg	Fatty acids	HMDB00827	1 (1.16, 0.9)	7.4E-01	1 (1.11, 0.84)	8.1E-01
palmitic acid	C18-neg	Fatty acids	HMDB00220	1 (1.13, 0.87)	8.0E-01	0.9 (1.06, 0.8)	5.1E-01
adrenic acid	C18-neg	Fatty acids	HMDB02226	1 (1.13, 0.87)	8.0E-01	0.9 (1.04, 0.79)	4.1E-01
arachidonic acid	C18-neg	Fatty acids	HMDB01043	1 (1.15, 0.89)	8.0E-01	0.9 (1.09, 0.83)	6.8E-01
docosatrienoic acid	C18-neg	Fatty acids	HMDB02823	1 (1.14, 0.88)	8.4E-01	1 (1.16, 0.87)	9.2E-01
sphingosine-1-phosphate	C18-neg	Sphingolipids	HMDB00277	0.9 (1.03, 0.79)	2.5E-01	0.9 (1.03, 0.78)	3.5E-01
C16:0 Ceramide (d18:1)	C8-pos	Ceramides	HMDB04949	1.2 (1.33, 1.03)	8.0E-02	1.1 (1.26, 0.92)	6.1E-01
C22:0 Ceramide (d18:1)	C8-pos	Ceramides	HMDB04952	1.2 (1.32, 1.02)	9.0E-02	1 (1.17, 0.84)	9.2E-01
C24:0 Ceramide (d18:1)	C8-pos	Ceramides	HMDB04956	1.1 (1.28, 0.99)	1.8E-01	1 (1.22, 0.89)	7.8E-01
C24:1 Ceramide (d18:1)	C8-pos	Ceramides	HMDB04953	1 (1.17, 0.9)	7.0E-01	1 (1.13, 0.84)	8.4E-01
C22:6 CE	C8-pos	Cholesteryl esters	HMDB06733	0.8 (0.97, 0.74)	6.6E-02	1 (1.1, 0.82)	7.3E-01
C22:4 CE	C8-pos	Cholesteryl esters	HMDB06729	0.9 (0.98, 0.75)	9.8E-02	1 (1.22, 0.89)	7.6E-01
C20:5 CE	C8-pos	Cholesteryl esters	HMDB06731	0.9 (1, 0.77)	1.5E-01	0.9 (1.04, 0.77)	4.1E-01
C18:0 CE	C8-pos	Cholesteryl esters	HMDB10368	1.1 (1.29, 1)	1.6E-01	1.1 (1.27, 0.89)	7.1E-01
C22:5 CE	C8-pos	Cholesteryl esters	HMDB10375	0.9 (1.05, 0.81)	3.8E-01	1.1 (1.25, 0.91)	6.8E-01
C20:4 CE	C8-pos	Cholesteryl esters	HMDB06726	0.9 (1.08, 0.83)	5.5E-01	1 (1.19, 0.85)	9.2E-01
C14:0 CE	C8-pos	Cholesteryl esters	HMDB06725	0.9 (1.08, 0.83)	5.6E-01	1 (1.11, 0.82)	7.5E-01
C20:3 CE	C8-pos	Cholesteryl esters	HMDB06736	1 (1.1, 0.85)	6.7E-01	1 (1.19, 0.88)	8.5E-01
C16:0 CE	C8-pos	Cholesteryl esters	HMDB00885	1 (1.1, 0.85)	6.8E-01	1.1 (1.27, 0.89)	6.9E-01
C18:1 CE	C8-pos	Cholesteryl esters	HMDB00918	1 (1.17, 0.91)	6.8E-01	1.2 (1.48, 1.04)	1.1E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
C18:3 CE	C8-pos	Cholesteryl esters	HMDB10370	1 (1.17, 0.9)	7.0E-01	1 (1.23, 0.89)	7.5E-01
C16:1 CE	C8-pos	Cholesteryl esters	HMDB00658	1 (1.17, 0.88)	7.7E-01	1 (1.14, 0.85)	8.9E-01
C18:2 CE	C8-pos	Cholesteryl esters	HMDB00610	1 (1.14, 0.88)	8.4E-01	1.2 (1.36, 0.97)	3.1E-01
C36:1 DAG	C8-pos	Diacylglycerols	HMDB07216	1.2 (1.42, 1.09)	1.1E-02	0.9 (1.07, 0.76)	4.9E-01
C34:0 DAG	C8-pos	Diacylglycerols	HMDB07100	1.2 (1.39, 1.07)	2.4E-02	0.9 (1.09, 0.79)	6.1E-01
C34:1 DAG	C8-pos	Diacylglycerols	HMDB07102	1.2 (1.38, 1.06)	3.5E-02	0.9 (1.02, 0.72)	2.7E-01
C36:2 DAG	C8-pos	Diacylglycerols	HMDB07218	1.2 (1.38, 1.05)	3.6E-02	0.9 (1.04, 0.72)	3.4E-01
C32:0 DAG	C8-pos	Diacylglycerols	HMDB07098	1.2 (1.35, 1.03)	6.6E-02	0.9 (1.04, 0.76)	3.6E-01
C30:0 DAG	C8-pos	Diacylglycerols	HMDB07011	1.2 (1.32, 1.01)	1.1E-01	0.9 (1.04, 0.76)	3.5E-01
C36:3 DAG	C8-pos	Diacylglycerols	HMDB07219	1.2 (1.31, 1.01)	1.3E-01	0.8 (1, 0.71)	2.2E-01
C34:2 DAG	C8-pos	Diacylglycerols	HMDB07103	1.2 (1.32, 1.01)	1.3E-01	0.8 (0.96, 0.67)	1.1E-01
C32:2 DAG	C8-pos	Diacylglycerols	HMDB07128	1.1 (1.31, 1)	1.7E-01	0.9 (1.01, 0.72)	2.4E-01
C32:1 DAG	C8-pos	Diacylglycerols	HMDB07099	1.1 (1.29, 0.99)	2.0E-01	0.8 (0.97, 0.69)	1.2E-01
C36:4 DAG	C8-pos	Diacylglycerols	HMDB07248	1.1 (1.25, 0.96)	3.3E-01	0.8 (0.98, 0.7)	1.6E-01
C36:0 DAG	C8-pos	Diacylglycerols	HMDB07158	1.1 (1.24, 0.95)	3.8E-01	0.9 (1.09, 0.81)	6.4E-01
C34:3 DAG	C8-pos	Diacylglycerols	HMDB07132	1.1 (1.22, 0.93)	5.2E-01	0.7 (0.88, 0.61)	2.1E-02
C38:5 DAG	C8-pos	Diacylglycerols	HMDB07199	1 (1.19, 0.92)	5.9E-01	0.8 (0.98, 0.72)	1.4E-01
C38:4 DAG	C8-pos	Diacylglycerols	HMDB07170	1 (1.1, 0.85)	6.6E-01	0.8 (0.97, 0.72)	1.1E-01
C36:4 hydroxy-PC	C8-pos	Hydroxy-PC	n/a	1.3 (1.52, 1.17)	4.1E-04	1.3 (1.44, 1.09)	2.7E-02
C34:2 hydroxy-PC	C8-pos	Hydroxy-PC	n/a	1.3 (1.47, 1.12)	2.8E-03	1.2 (1.41, 1.07)	4.6E-02
C20:5 LPC	C8-pos	Lysophosphatidylcholines	HMDB10397	0.9 (1, 0.77)	1.6E-01	0.9 (1.05, 0.78)	4.2E-01
C16:1 LPC	C8-pos	Lysophosphatidylcholines	HMDB10383	0.9 (1.04, 0.79)	3.2E-01	0.9 (1.08, 0.81)	6.1E-01
C20:4 LPC	C8-pos	Lysophosphatidylcholines	HMDB10395	0.9 (1.04, 0.8)	3.5E-01	1 (1.11, 0.83)	7.7E-01
C18:2 LPC	C8-pos	Lysophosphatidylcholines	HMDB10386	0.9 (1.07, 0.82)	4.9E-01	1.1 (1.22, 0.91)	6.8E-01
C14:0 LPC	C8-pos	Lysophosphatidylcholi	HMDB10379	0.9 (1.08, 0.82)	5.1E-01	0.9 (1.03, 0.76)	3.4E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
		nes					
C16:0 LPC	C8-pos	Lysophosphatidylcholines	HMDB10382	1 (1.1, 0.85)	6.7E-01	1 (1.11, 0.83)	7.5E-01
C18:1 LPC	C8-pos	Lysophosphatidylcholines	HMDB02815	1 (1.1, 0.85)	6.8E-01	1.1 (1.22, 0.92)	6.8E-01
C20:3 LPC	C8-pos	Lysophosphatidylcholines	HMDB10393	1 (1.11, 0.85)	6.9E-01	1 (1.1, 0.83)	7.2E-01
C18:0 LPC	C8-pos	Lysophosphatidylcholines	HMDB10384	1 (1.13, 0.87)	8.2E-01	1 (1.17, 0.86)	9.2E-01
C22:6 LPE	C8-pos	Lysophosphatidylethanolamines	HMDB11526	0.8 (0.94, 0.72)	2.5E-02	0.9 (1.01, 0.76)	2.5E-01
C22:6 LPC	C8-pos	Lysophosphatidylethanolamines	HMDB10404	0.9 (0.97, 0.75)	7.7E-02	0.9 (1.06, 0.8)	5.1E-01
C18:1 LPE	C8-pos	Lysophosphatidylethanolamines	HMDB11506	1.1 (1.23, 0.95)	4.1E-01	1.1 (1.25, 0.94)	5.1E-01
C16:1 LPE	C8-pos	Lysophosphatidylethanolamines	HMDB11504	1 (1.09, 0.84)	5.8E-01	0.9 (1.08, 0.82)	6.3E-01
C16:0 LPE	C8-pos	Lysophosphatidylethanolamines	HMDB11503	1 (1.11, 0.85)	6.8E-01	1 (1.14, 0.86)	9.2E-01
C18:2 LPE	C8-pos	Lysophosphatidylethanolamines	HMDB11507	1 (1.18, 0.9)	6.8E-01	1 (1.21, 0.91)	7.2E-01
C18:0 LPE	C8-pos	Lysophosphatidylethanolamines	HMDB11130	1 (1.14, 0.88)	8.4E-01	1 (1.14, 0.86)	9.1E-01
C20:4 LPE	C8-pos	Lysophosphatidylethanolamines	HMDB11517	1 (1.14, 0.88)	8.4E-01	1 (1.17, 0.88)	8.9E-01
C22:1 MAG	C8-pos	Monoacylglycerols	HMDB11582	0.9 (1.06, 0.81)	4.1E-01	0.9 (1.06, 0.81)	5.1E-01
C16:1 MAG	C8-pos	Monoacylglycerols	HMDB11565	1 (1.15, 0.89)	7.7E-01	1 (1.15, 0.88)	9.2E-01
C18:0 MAG	C8-pos	Monoacylglycerols	HMDB11131	1 (1.15, 0.89)	7.7E-01	1 (1.15, 0.88)	9.2E-01
C14:1 MAG	C8-pos	Monoacylglycerols	HMDB11562	1 (1.13, 0.87)	8.1E-01	1 (1.12, 0.85)	8.5E-01
C34:3 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11211	0.8 (0.91, 0.7)	7.7E-03	1 (1.18, 0.85)	9.3E-01
C38:7 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11229	0.8 (0.95, 0.73)	4.2E-02	0.9 (1.07, 0.8)	5.7E-01
C34:4 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11212	0.8 (0.97, 0.74)	6.4E-02	1 (1.13, 0.84)	8.5E-01
C36:5 PC plasmalogen-A	C8-pos	Phosphatidylcholine	HMDB11221	0.9 (0.97, 0.75)	6.9E-02	0.9 (1.06, 0.79)	4.9E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
		plasmalogens					
C36:3 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11244	0.9 (0.98, 0.75)	9.0E-02	1.1 (1.25, 0.91)	6.8E-01
C34:2 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11210	0.9 (1, 0.78)	1.7E-01	1 (1.16, 0.87)	9.2E-01
C36:5 PC plasmalogen-B	C8-pos	Phosphatidylcholine plasmalogens	HMDB11220	0.9 (1.01, 0.77)	1.7E-01	1 (1.13, 0.84)	8.5E-01
C38:6 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11319	0.9 (1.01, 0.77)	1.8E-01	1 (1.17, 0.86)	9.3E-01
C34:5 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11214	0.9 (1.03, 0.79)	2.6E-01	0.9 (1.06, 0.8)	4.9E-01
C36:4 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11310	0.9 (1.06, 0.82)	4.6E-01	1 (1.13, 0.84)	8.6E-01
C36:2 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11243	1 (1.08, 0.84)	5.7E-01	1.1 (1.29, 0.96)	4.1E-01
C34:1 PC plasmalogen-A	C8-pos	Phosphatidylcholine plasmalogens	HMDB11208	1 (1.09, 0.84)	6.0E-01	1.1 (1.32, 0.97)	3.3E-01
C40:7 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11294	1 (1.1, 0.84)	6.3E-01	1 (1.21, 0.9)	7.5E-01
C36:1 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11241	1 (1.17, 0.91)	6.8E-01	1.2 (1.34, 1.01)	1.8E-01
C38:4 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	HMDB11252	1 (1.16, 0.89)	7.4E-01	1.1 (1.24, 0.92)	6.3E-01
C34:1 PC plasmalogen-B	C8-pos	Phosphatidylcholine plasmalogens	HMDB11239	1 (1.15, 0.89)	8.0E-01	1.2 (1.37, 1.01)	1.7E-01
C40:11 PC plasmalogen	C8-pos	Phosphatidylcholine plasmalogens	n/a	1 (1.14, 0.86)	8.0E-01	1 (1.15, 0.86)	9.2E-01
C40:10 PC	C8-pos	Phosphatidylcholines	HMDB08511	0.7 (0.85, 0.65)	4.1E-04	0.8 (0.96, 0.71)	1.0E-01
C38:6 PC	C8-pos	Phosphatidylcholines	HMDB07991	0.8 (0.92, 0.71)	1.1E-02	0.9 (0.99, 0.74)	1.7E-01
C40:9 PC	C8-pos	Phosphatidylcholines	HMDB08731	0.8 (0.93, 0.72)	2.0E-02	0.9 (0.99, 0.75)	1.7E-01
C36:4 PC-A	C8-pos	Phosphatidylcholines	HMDB07983	0.8 (0.96, 0.73)	5.9E-02	0.9 (1.05, 0.78)	4.5E-01
C40:6 PC	C8-pos	Phosphatidylcholines	HMDB08057	0.9 (0.97, 0.75)	7.7E-02	0.9 (1.02, 0.76)	2.7E-01
C34:4 PC	C8-pos	Phosphatidylcholines	HMDB07883	0.9 (1, 0.76)	1.7E-01	0.9 (1.02, 0.75)	2.8E-01
C36:4 PC-B	C8-pos	Phosphatidylcholines	HMDB08138	0.9 (1.01, 0.77)	1.8E-01	0.9 (1.02, 0.75)	2.7E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
C38:2 PC	C8-pos	Phosphatidylcholines	HMDB08270	0.9 (1.03, 0.79)	2.9E-01	0.9 (1.09, 0.81)	6.7E-01
C34:3 PC	C8-pos	Phosphatidylcholines	HMDB08006	0.9 (1.04, 0.78)	2.9E-01	0.9 (1.07, 0.77)	5.1E-01
C32:2 PC	C8-pos	Phosphatidylcholines	HMDB07874	0.9 (1.04, 0.78)	3.3E-01	0.9 (1.04, 0.75)	3.5E-01
C38:4 PC	C8-pos	Phosphatidylcholines	HMDB08048	0.9 (1.04, 0.8)	3.3E-01	0.9 (1.04, 0.77)	4.1E-01
C36:0 PC	C8-pos	Phosphatidylcholines	HMDB08036	0.9 (1.05, 0.81)	3.6E-01	0.9 (1.1, 0.81)	6.8E-01
C30:0 PC	C8-pos	Phosphatidylcholines	HMDB07869	0.9 (1.05, 0.8)	3.8E-01	0.9 (1.05, 0.77)	4.2E-01
C30:1 PC	C8-pos	Phosphatidylcholines	HMDB07870	0.9 (1.08, 0.81)	4.9E-01	0.9 (1.06, 0.78)	5.0E-01
C32:0 PC	C8-pos	Phosphatidylcholines	HMDB07871	0.9 (1.07, 0.82)	4.9E-01	1 (1.11, 0.82)	7.5E-01
C32:1 PC	C8-pos	Phosphatidylcholines	HMDB07873	1 (1.11, 0.83)	6.5E-01	0.9 (1.08, 0.8)	6.1E-01
C38:3 PC	C8-pos	Phosphatidylcholines	HMDB08047	1 (1.18, 0.91)	6.8E-01	0.9 (1.1, 0.81)	6.8E-01
C34:2 PC	C8-pos	Phosphatidylcholines	HMDB07973	1 (1.12, 0.85)	7.1E-01	1 (1.15, 0.84)	8.9E-01
C34:1 PC	C8-pos	Phosphatidylcholines	HMDB07972	1 (1.12, 0.85)	7.3E-01	1 (1.14, 0.85)	8.9E-01
C34:0 PC	C8-pos	Phosphatidylcholines	HMDB07970	1 (1.16, 0.89)	7.6E-01	1 (1.16, 0.87)	9.2E-01
C36:2 PC	C8-pos	Phosphatidylcholines	HMDB08039	1 (1.15, 0.89)	8.0E-01	1 (1.19, 0.88)	8.5E-01
C36:3 PC	C8-pos	Phosphatidylcholines	HMDB08105	1 (1.14, 0.87)	8.1E-01	1 (1.17, 0.86)	9.3E-01
C36:1 PC	C8-pos	Phosphatidylcholines	HMDB08038	1 (1.14, 0.88)	8.4E-01	1 (1.16, 0.87)	9.2E-01
C38:3 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB11384	0.8 (0.97, 0.74)	6.0E-02	1 (1.11, 0.83)	7.7E-01
C38:7 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB11420	0.9 (0.98, 0.75)	9.0E-02	0.9 (1.03, 0.77)	3.5E-01
C44:13 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	n/a	0.9 (1, 0.77)	1.6E-01	1 (1.1, 0.83)	7.5E-01
C36:3 PS plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	n/a	1.1 (1.27, 0.98)	2.4E-01	1.1 (1.26, 0.96)	4.2E-01
C40:7 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB11394	0.9 (1.04, 0.79)	3.0E-01	1 (1.1, 0.82)	7.3E-01
C38:6 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB11387	0.9 (1.04, 0.79)	3.0E-01	0.9 (1.08, 0.81)	6.0E-01
C36:3 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB11441	1.1 (1.24, 0.96)	3.5E-01	1.1 (1.29, 0.97)	3.4E-01
C36:1 PE plasmalogen	C8-pos	Phosphatidylethanola	HMDB09016	0.9 (1.04, 0.81)	3.6E-01	1 (1.2, 0.9)	7.6E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
		mine plasmalogens					
C36:5 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB11410	0.9 (1.05, 0.81)	3.8E-01	0.9 (1.06, 0.8)	5.1E-01
C36:2 PS plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	n/a	1.1 (1.21, 0.94)	4.8E-01	1 (1.18, 0.87)	8.9E-01
C42:11 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	n/a	0.9 (1.07, 0.82)	5.0E-01	1 (1.11, 0.84)	7.9E-01
C36:1 PS plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	n/a	1 (1.08, 0.84)	5.7E-01	1 (1.21, 0.89)	8.0E-01
C38:5 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB11386	1 (1.09, 0.84)	5.9E-01	1 (1.11, 0.84)	7.8E-01
C34:2 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB08952	1 (1.09, 0.84)	5.9E-01	1 (1.13, 0.86)	8.9E-01
C36:2 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB09082	1 (1.19, 0.92)	5.9E-01	1.1 (1.23, 0.93)	6.1E-01
C34:3 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB11343	1 (1.09, 0.84)	6.0E-01	1 (1.11, 0.84)	8.0E-01
C36:4 PE plasmalogen	C8-pos	Phosphatidylethanolamine plasmalogens	HMDB11442	1 (1.12, 0.87)	7.7E-01	1 (1.17, 0.89)	8.8E-01
C36:1 PE	C8-pos	Phosphatidylethanolamines	HMDB08993	1.1 (1.28, 0.98)	2.2E-01	1 (1.13, 0.84)	8.5E-01
C36:2 PE	C8-pos	Phosphatidylethanolamines	HMDB08994	1.1 (1.28, 0.97)	2.5E-01	1 (1.11, 0.83)	7.5E-01
C36:0 PE	C8-pos	Phosphatidylethanolamines	HMDB08991	0.9 (1.03, 0.79)	2.9E-01	0.9 (1.09, 0.8)	6.4E-01
C38:2 PE	C8-pos	Phosphatidylethanolamines	HMDB08942	0.9 (1.03, 0.79)	2.9E-01	1 (1.17, 0.86)	9.3E-01
C38:6 PE	C8-pos	Phosphatidylethanolamines	HMDB09102	0.9 (1.04, 0.8)	3.2E-01	0.9 (1.02, 0.77)	3.1E-01
C34:2 PE	C8-pos	Phosphatidylethanolamines	HMDB08928	1.1 (1.25, 0.95)	3.8E-01	1 (1.13, 0.85)	8.5E-01
C36:3 PE	C8-pos	Phosphatidylethanolamines	HMDB09060	1.1 (1.23, 0.94)	4.8E-01	1 (1.16, 0.87)	9.2E-01
C38:5 PE	C8-pos	Phosphatidylethanolamines	HMDB09069	0.9 (1.08, 0.83)	5.7E-01	0.9 (1.07, 0.8)	5.5E-01
C40:6 PE	C8-pos	Phosphatidylethanolamines	HMDB09012	1 (1.11, 0.85)	6.8E-01	0.9 (0.99, 0.74)	1.7E-01
C34:0 PE	C8-pos	Phosphatidylethanola	HMDB08925	1 (1.11, 0.86)	7.0E-01	1 (1.16, 0.88)	8.9E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
		mines					
C36:4 PE	C8-pos	Phosphatidylethanolamines	HMDB08937	1 (1.12, 0.86)	7.3E-01	0.9 (1.06, 0.8)	5.1E-01
C38:4 PE	C8-pos	Phosphatidylethanolamines	HMDB09003	1 (1.14, 0.87)	8.4E-01	0.9 (1.05, 0.79)	4.2E-01
sphingosine	C8-pos	Sphingolipids	HMDB00252	1 (1.13, 0.87)	8.0E-01	0.9 (1.08, 0.82)	6.4E-01
C14:0 SM	C8-pos	Sphingomyelins	HMDB12097	0.9 (1.01, 0.77)	1.7E-01	0.9 (1.06, 0.77)	4.9E-01
C22:1 SM	C8-pos	Sphingomyelins	HMDB12104	0.9 (1.01, 0.78)	1.9E-01	1 (1.16, 0.83)	8.7E-01
C16:1 SM	C8-pos	Sphingomyelins	n/a	0.9 (1.05, 0.81)	3.7E-01	1 (1.12, 0.81)	7.5E-01
C20:0 SM	C8-pos	Sphingomyelins	HMDB12102	0.9 (1.07, 0.82)	4.8E-01	1 (1.14, 0.82)	8.4E-01
C18:2 SM	C8-pos	Sphingomyelins	HMDB12101	1 (1.08, 0.83)	5.7E-01	0.9 (1.09, 0.81)	6.8E-01
C18:1 SM	C8-pos	Sphingomyelins	HMDB12101	1 (1.09, 0.84)	6.0E-01	1 (1.14, 0.83)	8.5E-01
C24:1 SM	C8-pos	Sphingomyelins	HMDB12107	1 (1.09, 0.84)	6.2E-01	1.1 (1.3, 0.95)	4.3E-01
C18:0 SM	C8-pos	Sphingomyelins	HMDB01348	1 (1.16, 0.89)	7.5E-01	1 (1.21, 0.88)	8.4E-01
C16:0 SM	C8-pos	Sphingomyelins	HMDB10169	1 (1.13, 0.87)	8.0E-01	1.1 (1.35, 0.96)	3.8E-01
C22:0 SM	C8-pos	Sphingomyelins	HMDB12103	1 (1.14, 0.88)	8.4E-01	1 (1.2, 0.86)	8.9E-01
C24:0 SM	C8-pos	Sphingomyelins	HMDB11697	1 (1.14, 0.88)	8.4E-01	1.1 (1.26, 0.91)	6.4E-01
C54:1 TAG	C8-pos	Triacylglycerols	HMDB05395	1.3 (1.49, 1.14)	1.7E-03	1 (1.17, 0.85)	9.3E-01
C54:2 TAG	C8-pos	Triacylglycerols	HMDB05403	1.3 (1.48, 1.13)	2.3E-03	1 (1.14, 0.8)	7.7E-01
C56:10 TAG	C8-pos	Triacylglycerols	HMDB10513	0.8 (0.89, 0.68)	3.6E-03	0.8 (0.88, 0.66)	1.1E-02
C56:2 TAG	C8-pos	Triacylglycerols	HMDB05404	1.3 (1.44, 1.1)	8.2E-03	1 (1.17, 0.85)	9.3E-01
C52:1 TAG	C8-pos	Triacylglycerols	HMDB05367	1.2 (1.43, 1.09)	9.9E-03	0.9 (1.08, 0.77)	5.4E-01
C52:0 TAG	C8-pos	Triacylglycerols	HMDB05365	1.2 (1.42, 1.09)	1.0E-02	1 (1.13, 0.83)	8.2E-01
C54:3 TAG	C8-pos	Triacylglycerols	HMDB05405	1.2 (1.41, 1.08)	1.8E-02	0.9 (1.11, 0.79)	6.8E-01
C56:3 TAG	C8-pos	Triacylglycerols	HMDB05410	1.2 (1.41, 1.07)	2.0E-02	1 (1.16, 0.84)	8.9E-01
C58:11 TAG	C8-pos	Triacylglycerols	HMDB10531	0.8 (0.93, 0.72)	2.0E-02	0.8 (0.91, 0.69)	2.6E-02
C52:2 TAG	C8-pos	Triacylglycerols	HMDB05369	1.2 (1.4, 1.07)	2.4E-02	0.9 (1.03, 0.72)	3.2E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
C50:0 TAG	C8-pos	Triacylglycerols	HMDB05357	1.2 (1.38, 1.06)	3.0E-02	0.9 (1.09, 0.79)	6.1E-01
C50:1 TAG	C8-pos	Triacylglycerols	HMDB05360	1.2 (1.38, 1.05)	3.6E-02	0.9 (1.05, 0.76)	4.1E-01
C48:0 TAG	C8-pos	Triacylglycerols	HMDB05356	1.2 (1.34, 1.02)	8.9E-02	0.9 (1.07, 0.79)	5.2E-01
C52:3 TAG	C8-pos	Triacylglycerols	HMDB05384	1.2 (1.33, 1.02)	9.0E-02	0.8 (0.97, 0.67)	1.3E-01
C56:4 TAG	C8-pos	Triacylglycerols	HMDB05398	1.2 (1.33, 1.02)	9.6E-02	0.9 (1.07, 0.77)	5.2E-01
C58:9 TAG	C8-pos	Triacylglycerols	HMDB05463	0.9 (0.99, 0.76)	1.1E-01	0.8 (0.94, 0.71)	4.8E-02
C50:2 TAG	C8-pos	Triacylglycerols	HMDB05377	1.2 (1.33, 1.01)	1.2E-01	0.8 (0.99, 0.71)	1.8E-01
C54:4 TAG	C8-pos	Triacylglycerols	HMDB05370	1.2 (1.31, 1.01)	1.2E-01	0.9 (1.08, 0.78)	5.9E-01
C58:10 TAG	C8-pos	Triacylglycerols	HMDB05476	0.9 (0.99, 0.77)	1.4E-01	0.8 (0.92, 0.69)	3.6E-02
C48:1 TAG	C8-pos	Triacylglycerols	HMDB05359	1.1 (1.31, 1)	1.7E-01	0.9 (1.02, 0.74)	2.7E-01
C46:0 TAG	C8-pos	Triacylglycerols	HMDB10411	1.1 (1.29, 0.99)	1.9E-01	0.9 (1.04, 0.77)	4.0E-01
C56:9 TAG	C8-pos	Triacylglycerols	HMDB05448	0.9 (1.01, 0.78)	1.9E-01	0.8 (0.89, 0.66)	1.7E-02
C60:12 TAG	C8-pos	Triacylglycerols	HMDB05478	0.9 (1.02, 0.78)	2.0E-01	0.9 (1.03, 0.78)	3.5E-01
C56:1 TAG	C8-pos	Triacylglycerols	HMDB05396	1.1 (1.27, 0.98)	2.3E-01	1 (1.18, 0.89)	8.4E-01
C52:4 TAG	C8-pos	Triacylglycerols	HMDB05363	1.1 (1.27, 0.97)	2.5E-01	0.8 (0.96, 0.68)	1.1E-01
C54:9 TAG	C8-pos	Triacylglycerols	HMDB10498	0.9 (1.02, 0.79)	2.5E-01	0.9 (1.03, 0.79)	3.8E-01
C58:8 TAG	C8-pos	Triacylglycerols	HMDB05413	0.9 (1.03, 0.79)	2.5E-01	0.8 (0.93, 0.69)	3.7E-02
C54:5 TAG	C8-pos	Triacylglycerols	HMDB05385	1.1 (1.26, 0.97)	2.9E-01	0.9 (1.02, 0.74)	2.7E-01
C46:1 TAG	C8-pos	Triacylglycerols	HMDB10412	1.1 (1.25, 0.95)	3.6E-01	0.8 (0.99, 0.72)	1.7E-01
C58:7 TAG	C8-pos	Triacylglycerols	HMDB05471	0.9 (1.05, 0.8)	3.6E-01	0.8 (0.94, 0.7)	5.0E-02
C44:0 TAG	C8-pos	Triacylglycerols	HMDB42063	1.1 (1.24, 0.95)	3.7E-01	0.9 (1, 0.73)	2.0E-01
C50:3 TAG	C8-pos	Triacylglycerols	HMDB05433	1.1 (1.25, 0.95)	3.7E-01	0.8 (0.93, 0.65)	5.0E-02
C52:7 TAG	C8-pos	Triacylglycerols	HMDB10517	0.9 (1.05, 0.8)	3.7E-01	0.8 (0.9, 0.66)	2.1E-02
C56:8 TAG	C8-pos	Triacylglycerols	HMDB05392	0.9 (1.05, 0.81)	3.8E-01	0.8 (0.89, 0.66)	1.7E-02
C48:2 TAG	C8-pos	Triacylglycerols	HMDB05376	1.1 (1.25, 0.95)	3.9E-01	0.8 (0.96, 0.69)	1.1E-01
C44:1 TAG	C8-pos	Triacylglycerols	n/a	1.1 (1.24, 0.95)	4.1E-01	0.9 (1.01, 0.74)	2.5E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
C42:0 TAG	C8-pos	Triacylglycerols	n/a	1.1 (1.23, 0.95)	4.1E-01	0.9 (1.04, 0.77)	4.0E-01
C56:5 TAG	C8-pos	Triacylglycerols	HMDB05406	1.1 (1.22, 0.94)	4.7E-01	0.8 (0.97, 0.7)	1.2E-01
C46:2 TAG	C8-pos	Triacylglycerols	HMDB10419	1.1 (1.23, 0.94)	4.8E-01	0.8 (0.97, 0.7)	1.3E-01
C54:8 TAG	C8-pos	Triacylglycerols	HMDB10518	0.9 (1.07, 0.82)	4.8E-01	0.8 (0.93, 0.69)	4.8E-02
C46:3 TAG	C8-pos	Triacylglycerols	n/a	1.1 (1.22, 0.93)	5.1E-01	0.8 (0.97, 0.7)	1.2E-01
C44:2 TAG	C8-pos	Triacylglycerols	n/a	1.1 (1.21, 0.93)	5.2E-01	0.9 (1, 0.73)	1.9E-01
C56:7 TAG	C8-pos	Triacylglycerols	HMDB05462	0.9 (1.08, 0.83)	5.4E-01	0.8 (0.91, 0.67)	2.6E-02
C54:6 TAG	C8-pos	Triacylglycerols	HMDB05391	1.1 (1.2, 0.92)	5.7E-01	0.8 (1, 0.72)	1.9E-01
C48:3 TAG	C8-pos	Triacylglycerols	HMDB05432	1.1 (1.21, 0.92)	5.9E-01	0.8 (0.92, 0.66)	4.8E-02
C48:4 TAG	C8-pos	Triacylglycerols	n/a	1 (1.19, 0.91)	6.6E-01	0.8 (0.94, 0.67)	6.3E-02
C46:4 TAG	C8-pos	Triacylglycerols	n/a	1 (1.18, 0.9)	6.8E-01	0.8 (0.97, 0.72)	1.2E-01
C48:5 TAG	C8-pos	Triacylglycerols	n/a	1 (1.18, 0.91)	6.8E-01	0.8 (0.99, 0.73)	1.8E-01
C50:4 TAG	C8-pos	Triacylglycerols	HMDB05435	1 (1.18, 0.9)	6.8E-01	0.7 (0.89, 0.62)	2.1E-02
C52:5 TAG	C8-pos	Triacylglycerols	HMDB05380	1 (1.18, 0.91)	6.8E-01	0.8 (0.94, 0.68)	6.3E-02
C58:6 TAG	C8-pos	Triacylglycerols	HMDB05458	1 (1.18, 0.91)	6.8E-01	0.8 (0.98, 0.72)	1.6E-01
C54:10 TAG	C8-pos	Triacylglycerols	n/a	1 (1.11, 0.85)	6.9E-01	1 (1.13, 0.85)	8.6E-01
C50:6 TAG	C8-pos	Triacylglycerols	HMDB10497	1 (1.11, 0.85)	7.0E-01	0.8 (0.94, 0.69)	5.0E-02
C56:6 TAG	C8-pos	Triacylglycerols	HMDB05456	1 (1.16, 0.9)	7.2E-01	0.8 (0.92, 0.67)	3.7E-02
C52:6 TAG	C8-pos	Triacylglycerols	HMDB05436	1 (1.12, 0.86)	7.5E-01	0.7 (0.88, 0.63)	1.7E-02
C50:5 TAG	C8-pos	Triacylglycerols	HMDB10471	1 (1.16, 0.88)	8.0E-01	0.8 (0.9, 0.64)	2.6E-02
C54:7 TAG	C8-pos	Triacylglycerols	HMDB05447	1 (1.14, 0.88)	8.5E-01	0.8 (0.95, 0.69)	6.6E-02
alpha-glycerophosphate	HILIC-neg	Acyl Phosphates	HMDB00126	0.9 (1.02, 0.79)	2.2E-01	0.9 (1.01, 0.77)	2.4E-01
sorbitol	HILIC-neg	Alcohols and Polyols	HMDB00247	1.3 (1.47, 1.12)	3.6E-03	1.1 (1.32, 0.99)	2.5E-01
inositol	HILIC-neg	Alcohols and Polyols	HMDB00211	1.1 (1.31, 1)	1.4E-01	1.2 (1.37, 1.03)	1.2E-01
cystathionine	HILIC-neg	Amino Acids	HMDB00099	1.3 (1.44, 1.1)	7.5E-03	1.1 (1.31, 0.99)	2.5E-01
2-aminoadipate	HILIC-neg	Amino Acids	HMDB00510	1.2 (1.35, 1.04)	4.8E-02	1 (1.19, 0.89)	8.4E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
kynurenine	HILIC-neg	Amino Acids	HMDB00684	1.2 (1.33, 1.02)	9.0E-02	1 (1.21, 0.9)	7.5E-01
pantothenate	HILIC-neg	Amino Acids	HMDB00210	1 (1.1, 0.85)	6.8E-01	1 (1.16, 0.88)	9.0E-01
hydroxyphenylacetate	HILIC-neg	Aromatic Acids	HMDB00020	1.2 (1.38, 1.06)	2.6E-02	1.2 (1.34, 1.01)	1.7E-01
gentisate	HILIC-neg	Aromatic Acids	HMDB00152	1 (1.12, 0.86)	7.5E-01	1 (1.11, 0.84)	8.0E-01
fructose/glucose/galactose	HILIC-neg	Carbohydrates	HMDB00122	1.4 (1.56, 1.19)	3.0E-04	1.1 (1.25, 0.9)	6.9E-01
sucrose	HILIC-neg	Carbohydrates	HMDB00258	1.2 (1.42, 1.1)	8.5E-03	1.2 (1.33, 1.01)	1.7E-01
glucuronate	HILIC-neg	Carbohydrates	HMDB00127	1.2 (1.36, 1.04)	4.9E-02	1.1 (1.3, 0.98)	3.0E-01
lactose	HILIC-neg	Carbohydrates	HMDB00186	1.1 (1.22, 0.94)	4.3E-01	1.1 (1.24, 0.94)	5.5E-01
2-hydroxyglutarate	HILIC-neg	Dicarboxylic Acids	HMDB00694	1.3 (1.51, 1.16)	5.8E-04	1.2 (1.39, 1.05)	6.6E-02
fumarate/maleate	HILIC-neg	Dicarboxylic Acids	HMDB00134	1.3 (1.44, 1.1)	8.1E-03	1.2 (1.35, 1.02)	1.6E-01
3-methyladipate/pimelate	HILIC-neg	Dicarboxylic Acids	HMDB00555	1.2 (1.39, 1.07)	2.2E-02	1.2 (1.39, 1.05)	6.6E-02
methylmalonate	HILIC-neg	Dicarboxylic Acids	HMDB00202	1.2 (1.37, 1.04)	5.6E-02	1.2 (1.36, 1.01)	1.7E-01
malate	HILIC-neg	Dicarboxylic Acids	HMDB00156	1.1 (1.3, 1.01)	1.4E-01	1.1 (1.23, 0.94)	5.8E-01
succinate	HILIC-neg	Dicarboxylic Acids	HMDB00254	1.1 (1.26, 0.97)	2.9E-01	1.1 (1.26, 0.95)	4.5E-01
adipate	HILIC-neg	Dicarboxylic Acids	HMDB00448	1.1 (1.24, 0.96)	3.6E-01	1.1 (1.27, 0.96)	4.1E-01
oxalate	HILIC-neg	Dicarboxylic Acids	HMDB02329	1.1 (1.23, 0.95)	3.8E-01	1.1 (1.29, 0.98)	3.2E-01
alpha-ketoglutarate	HILIC-neg	Dicarboxylic Acids	HMDB00208	1 (1.1, 0.85)	6.8E-01	1 (1.09, 0.83)	7.0E-01
lactate	HILIC-neg	Hydroxy Acids	HMDB00190	1.1 (1.29, 1)	1.6E-01	1 (1.14, 0.87)	9.2E-01
alpha-hydroxybutyrate	HILIC-neg	Hydroxy Acids	HMDB00008	1.1 (1.25, 0.97)	3.0E-01	1 (1.14, 0.86)	9.2E-01
beta-hydroxybutyrate	HILIC-neg	Hydroxy Acids	HMDB00011	1 (1.19, 0.92)	5.8E-01	1.1 (1.21, 0.92)	6.8E-01
2-phosphoglycerate	HILIC-neg	Organic acids	HMDB00362	0.8 (0.95, 0.73)	3.5E-02	0.8 (0.94, 0.71)	5.0E-02
pyruvate	HILIC-neg	Organic acids	HMDB00243	0.9 (0.99, 0.76)	1.3E-01	0.9 (1, 0.76)	2.2E-01
phosphocreatine	HILIC-neg	Other	HMDB01511	0.7 (0.85, 0.64)	4.1E-04	0.8 (0.93, 0.69)	3.7E-02
indole-3-propionate	HILIC-neg	Other	HMDB02302	0.9 (1.02, 0.79)	2.5E-01	1 (1.16, 0.87)	9.2E-01
indoxylsulfate	HILIC-neg	Other	HMDB00682	1.1 (1.26, 0.98)	2.5E-01	1.1 (1.28, 0.97)	3.3E-01
hippurate	HILIC-neg	Other	HMDB00714	0.9 (1.08, 0.83)	5.6E-01	1 (1.14, 0.86)	8.9E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
4-pyridoxate	HILIC-neg	Other	HMDB00017	1 (1.09, 0.84)	6.2E-01	1 (1.19, 0.9)	8.0E-01
salicylurate	HILIC-neg	Other	HMDB00840	1 (1.15, 0.89)	8.1E-01	0.9 (1.09, 0.81)	6.6E-01
uracil	HILIC-neg	Purines and Pyrimidines	HMDB00300	0.7 (0.85, 0.66)	4.1E-04	0.8 (0.95, 0.72)	6.3E-02
uridine	HILIC-neg	Purines and Pyrimidines	HMDB00296	0.8 (0.86, 0.66)	5.3E-04	0.8 (0.94, 0.71)	5.0E-02
CMP	HILIC-neg	Purines and Pyrimidines	HMDB00095	1.3 (1.46, 1.13)	2.8E-03	1.2 (1.43, 1.09)	2.7E-02
inosine	HILIC-neg	Purines and Pyrimidines	HMDB00195	1.2 (1.35, 1.04)	5.7E-02	1.1 (1.27, 0.96)	4.0E-01
IMP	HILIC-neg	Purines and Pyrimidines	HMDB00175	0.9 (0.98, 0.75)	9.0E-02	0.9 (1.01, 0.77)	2.5E-01
urate	HILIC-neg	Purines and Pyrimidines	HMDB00289	1.2 (1.31, 1.01)	1.2E-01	1.1 (1.21, 0.92)	6.8E-01
thymine	HILIC-neg	Purines and Pyrimidines	HMDB00262	1.1 (1.28, 0.99)	2.0E-01	1.1 (1.23, 0.93)	6.0E-01
UDP-glucuronate	HILIC-neg	Purines and Pyrimidines	HMDB00935	1.1 (1.25, 0.96)	3.3E-01	1.1 (1.25, 0.95)	4.9E-01
UMP	HILIC-neg	Purines and Pyrimidines	HMDB00288	1.1 (1.24, 0.96)	3.5E-01	1.1 (1.24, 0.94)	5.2E-01
UDP-galactose/UDP-glucose	HILIC-neg	Purines and Pyrimidines	HMDB00286	1.1 (1.23, 0.95)	4.1E-01	1.1 (1.24, 0.94)	5.2E-01
cytidine	HILIC-neg	Purines and Pyrimidines	HMDB00089	1.1 (1.22, 0.94)	4.7E-01	1 (1.2, 0.91)	7.4E-01
UDP	HILIC-neg	Purines and Pyrimidines	HMDB00295	1.1 (1.22, 0.94)	4.8E-01	1 (1.19, 0.9)	7.7E-01
hypoxanthine	HILIC-neg	Purines and Pyrimidines	HMDB00157	0.9 (1.07, 0.83)	5.0E-01	0.9 (1.03, 0.78)	3.3E-01
cAMP	HILIC-neg	Purines and Pyrimidines	HMDB00058	0.9 (1.07, 0.83)	5.1E-01	0.9 (1.08, 0.82)	6.6E-01
GMP	HILIC-neg	Purines and Pyrimidines	HMDB01397	1.1 (1.2, 0.93)	5.4E-01	1.1 (1.23, 0.94)	5.8E-01
AMP	HILIC-neg	Purines and Pyrimidines	HMDB00045	1 (1.19, 0.92)	6.0E-01	1.1 (1.21, 0.92)	6.8E-01
ADP	HILIC-neg	Purines and Pyrimidines	HMDB01341	1 (1.11, 0.85)	6.9E-01	1 (1.13, 0.86)	8.9E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
OR (95 CI%)	FDR p	Purines and Pyrimidines	HMDB01201	1 (1.12, 0.87)	7.7E-01	1 (1.14, 0.87)	9.2E-01
xanthine	HILIC-neg	Purines and Pyrimidines	HMDB00292	1 (1.15, 0.89)	8.0E-01	0.9 (1.07, 0.81)	6.0E-01
xanthurenate	HILIC-neg	Purines and Pyrimidines	HMDB00881	1 (1.14, 0.88)	8.4E-01	1 (1.1, 0.84)	7.5E-01
hexose monophosphate	HILIC-neg	Sugar Phosphates	HMDB00124	1.1 (1.26, 0.98)	2.5E-01	1.1 (1.21, 0.92)	6.8E-01
hexose diphosphate	HILIC-neg	Sugar Phosphates	HMDB01058	0.9 (1.05, 0.81)	3.7E-01	0.9 (1.07, 0.81)	5.7E-01
pentose monophosphate	HILIC-neg	Sugar Phosphates	HMDB01548	1.1 (1.23, 0.95)	4.1E-01	1.1 (1.24, 0.95)	5.1E-01
6-phosphogluconate	HILIC-neg	Sugar Phosphates	HMDB01316	1.1 (1.22, 0.94)	4.5E-01	1.1 (1.25, 0.95)	4.9E-01
isocitrate	HILIC-neg	Tricarboxylic Acids	HMDB00193	1.2 (1.37, 1.05)	3.5E-02	1.1 (1.23, 0.93)	6.1E-01
aconitate	HILIC-neg	Tricarboxylic Acids	HMDB00072	1.1 (1.3, 1)	1.6E-01	1 (1.19, 0.9)	7.7E-01
citrate	HILIC-neg	Tricarboxylic Acids	HMDB00094	1 (1.11, 0.86)	7.2E-01	1 (1.15, 0.88)	9.2E-01
C4-OH carnitine	HILIC-pos	Acylcarnitines	HMDB13127	1.2 (1.4, 1.07)	2.0E-02	1.1 (1.27, 0.96)	4.2E-01
C18 carnitine	HILIC-pos	Acylcarnitines	HMDB00848	1.1 (1.31, 1)	1.7E-01	1.1 (1.28, 0.96)	4.2E-01
C26 carnitine	HILIC-pos	Acylcarnitines	HMDB06347	1.1 (1.28, 0.99)	1.9E-01	1 (1.21, 0.9)	7.5E-01
C3 carnitine	HILIC-pos	Acylcarnitines	HMDB00824	1.1 (1.28, 0.99)	2.0E-01	1 (1.2, 0.9)	7.7E-01
C14 carnitine	HILIC-pos	Acylcarnitines	HMDB05066	1.1 (1.24, 0.95)	3.8E-01	1 (1.18, 0.89)	8.4E-01
C5 carnitine	HILIC-pos	Acylcarnitines	HMDB00688	1.1 (1.22, 0.94)	4.7E-01	1 (1.1, 0.83)	7.5E-01
C10 carnitine	HILIC-pos	Acylcarnitines	HMDB00651	0.9 (1.07, 0.82)	4.9E-01	0.9 (1.07, 0.82)	6.1E-01
C5-DC carnitine	HILIC-pos	Acylcarnitines	HMDB13130	1.1 (1.21, 0.93)	5.1E-01	1 (1.18, 0.9)	8.4E-01
C2 carnitine	HILIC-pos	Acylcarnitines	HMDB00201	1.1 (1.2, 0.93)	5.2E-01	1.1 (1.22, 0.93)	6.4E-01
C18:1-OH carnitine	HILIC-pos	Acylcarnitines	HMDB13339	1.1 (1.21, 0.93)	5.3E-01	1 (1.18, 0.89)	8.4E-01
C8 carnitine	HILIC-pos	Acylcarnitines	HMDB00791	0.9 (1.08, 0.83)	5.5E-01	0.9 (1.07, 0.82)	6.0E-01
C9 carnitine	HILIC-pos	Acylcarnitines	HMDB13288	0.9 (1.08, 0.83)	5.6E-01	0.9 (1.06, 0.8)	5.1E-01
C16 carnitine	HILIC-pos	Acylcarnitines	HMDB00222	1.1 (1.2, 0.92)	5.7E-01	1 (1.13, 0.85)	8.6E-01
C3-DC-CH3 carnitine	HILIC-pos	Acylcarnitines	HMDB13133	1 (1.09, 0.84)	5.8E-01	0.9 (1.03, 0.76)	3.3E-01
C10:2 carnitine	HILIC-pos	Acylcarnitines	HMDB13325	1 (1.2, 0.92)	5.9E-01	1 (1.15, 0.87)	9.3E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
C12 carnitine	HILIC-pos	Acylcarnitines	HMDB02250	1 (1.19, 0.92)	5.9E-01	1 (1.19, 0.9)	8.0E-01
C14:1 carnitine	HILIC-pos	Acylcarnitines	HMDB02014	1 (1.19, 0.92)	6.0E-01	1 (1.2, 0.91)	7.5E-01
C7 carnitine	HILIC-pos	Acylcarnitines	HMDB13238	1 (1.19, 0.91)	6.2E-01	1 (1.14, 0.87)	9.2E-01
C4 carnitine	HILIC-pos	Acylcarnitines	HMDB02013	1 (1.18, 0.91)	6.3E-01	1 (1.13, 0.86)	8.6E-01
C18:1 carnitine	HILIC-pos	Acylcarnitines	HMDB05065	1 (1.19, 0.91)	6.6E-01	1 (1.18, 0.89)	8.5E-01
C12:1 carnitine	HILIC-pos	Acylcarnitines	HMDB13326	1 (1.17, 0.9)	6.9E-01	1 (1.16, 0.88)	8.9E-01
C18:2 carnitine	HILIC-pos	Acylcarnitines	HMDB06469	1 (1.11, 0.85)	7.0E-01	1 (1.12, 0.85)	8.4E-01
C20 carnitine	HILIC-pos	Acylcarnitines	HMDB06460	1 (1.17, 0.9)	7.2E-01	1 (1.2, 0.91)	7.5E-01
C5:1 carnitine	HILIC-pos	Acylcarnitines	HMDB02366	1 (1.16, 0.9)	7.3E-01	1 (1.16, 0.88)	8.9E-01
C6 carnitine	HILIC-pos	Acylcarnitines	HMDB00705	1 (1.15, 0.89)	7.7E-01	1 (1.1, 0.84)	7.5E-01
C14:2 carnitine	HILIC-pos	Acylcarnitines	HMDB13331	1 (1.15, 0.88)	8.0E-01	1 (1.16, 0.88)	9.2E-01
glutamate	HILIC-pos	Amino Acids	HMDB00148	1.6 (1.8, 1.36)	1.9E-08	1.4 (1.6, 1.18)	5.5E-03
asparagine	HILIC-pos	Amino Acids	HMDB00168	0.6 (0.74, 0.56)	3.6E-08	0.8 (0.87, 0.64)	1.1E-02
glutamine	HILIC-pos	Amino Acids	HMDB00641	0.7 (0.77, 0.58)	1.2E-06	0.7 (0.87, 0.64)	1.1E-02
methionine	HILIC-pos	Amino Acids	HMDB00696	0.7 (0.85, 0.65)	3.0E-04	0.8 (0.88, 0.66)	1.1E-02
histidine	HILIC-pos	Amino Acids	HMDB00177	0.7 (0.86, 0.65)	5.8E-04	0.8 (0.95, 0.71)	6.6E-02
threonine	HILIC-pos	Amino Acids	HMDB00167	0.8 (0.86, 0.66)	5.8E-04	0.8 (0.95, 0.71)	6.1E-02
serine	HILIC-pos	Amino Acids	HMDB00187	0.8 (0.9, 0.68)	4.2E-03	0.9 (1.01, 0.76)	2.5E-01
glycine	HILIC-pos	Amino Acids	HMDB00123	0.8 (0.91, 0.69)	6.7E-03	0.9 (1.07, 0.8)	5.7E-01
lysine	HILIC-pos	Amino Acids	HMDB00182	0.8 (0.91, 0.7)	8.7E-03	0.8 (0.92, 0.69)	2.7E-02
1-methylhistamine	HILIC-pos	Amino Acids	HMDB00898	0.8 (0.93, 0.7)	1.4E-02	0.8 (0.94, 0.71)	5.0E-02
tryptophan	HILIC-pos	Amino Acids	HMDB00929	0.8 (0.96, 0.74)	5.6E-02	0.9 (0.99, 0.75)	1.8E-01
dimethylglycine	HILIC-pos	Amino Acids	HMDB00092	1.2 (1.34, 1.03)	8.2E-02	1.1 (1.26, 0.95)	4.9E-01
arginine	HILIC-pos	Amino Acids	HMDB00517	0.9 (1.01, 0.78)	1.8E-01	1 (1.11, 0.84)	7.9E-01
creatine	HILIC-pos	Amino Acids	HMDB00064	0.9 (1.01, 0.78)	2.0E-01	0.9 (1.08, 0.81)	6.1E-01
methionine sulfoxide	HILIC-pos	Amino Acids	HMDB02005	1.1 (1.28, 0.98)	2.1E-01	1.2 (1.34, 1.02)	1.5E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
pipecolic acid	HILIC-pos	Amino Acids	HMDB00716	0.9 (1.02, 0.79)	2.4E-01	0.9 (1.03, 0.78)	3.7E-01
isoleucine	HILIC-pos	Amino Acids	HMDB00172	1.1 (1.23, 0.95)	4.1E-01	0.9 (0.99, 0.74)	1.7E-01
aminoisobutyric acid	HILIC-pos	Amino Acids	HMDB01906	0.9 (1.06, 0.82)	4.4E-01	0.9 (1.09, 0.83)	6.8E-01
pyroglutamic acid	HILIC-pos	Amino Acids	HMDB00267	1.1 (1.22, 0.94)	4.8E-01	1.1 (1.23, 0.93)	6.1E-01
taurine	HILIC-pos	Amino Acids	HMDB00251	0.9 (1.07, 0.83)	5.1E-01	1 (1.12, 0.85)	8.5E-01
phenylalanine	HILIC-pos	Amino Acids	HMDB00159	0.9 (1.07, 0.83)	5.2E-01	0.9 (1.01, 0.76)	2.5E-01
leucine	HILIC-pos	Amino Acids	HMDB00687	1 (1.08, 0.84)	5.8E-01	0.8 (0.92, 0.69)	2.7E-02
SDMA	HILIC-pos	Amino Acids	HMDB03334	1 (1.09, 0.84)	6.1E-01	1 (1.19, 0.89)	8.4E-01
ornithine	HILIC-pos	Amino Acids	HMDB00214	1 (1.17, 0.91)	6.8E-01	1 (1.15, 0.88)	9.2E-01
valine	HILIC-pos	Amino Acids	HMDB00883	1 (1.17, 0.9)	6.9E-01	0.8 (0.94, 0.7)	5.0E-02
proline	HILIC-pos	Amino Acids	HMDB00162	1 (1.16, 0.9)	7.1E-01	0.9 (1.05, 0.79)	4.6E-01
alanine	HILIC-pos	Amino Acids	HMDB00161	1 (1.12, 0.86)	7.4E-01	0.9 (1, 0.75)	2.3E-01
hydroxyproline	HILIC-pos	Amino Acids	HMDB00725	1 (1.12, 0.86)	7.5E-01	0.9 (1.09, 0.83)	6.8E-01
tyrosine	HILIC-pos	Amino Acids	HMDB00158	1 (1.12, 0.87)	7.7E-01	0.9 (1.04, 0.79)	4.1E-01
citrulline	HILIC-pos	Amino Acids	HMDB00904	1 (1.14, 0.88)	8.5E-01	1.1 (1.23, 0.93)	6.2E-01
allantoin	HILIC-pos	Amino Ketones	HMDB00462	1.1 (1.31, 1.01)	1.3E-01	1.1 (1.32, 0.99)	2.5E-01
cotinine	HILIC-pos	Amino Ketones	HMDB01046	1.1 (1.26, 0.97)	2.6E-01	1 (1.23, 0.86)	8.5E-01
creatinine	HILIC-pos	Amino Ketones	HMDB00562	1 (1.19, 0.92)	5.9E-01	1.1 (1.23, 0.93)	6.0E-01
serotonin	HILIC-pos	Indoles and Indole Derivatives	HMDB00259	0.9 (1.05, 0.81)	3.6E-01	1 (1.1, 0.83)	7.5E-01
kynurenic acid	HILIC-pos	Indoles and Indole Derivatives	HMDB00715	1.1 (1.21, 0.94)	4.8E-01	0.9 (1.09, 0.82)	6.8E-01
5-hydroxytryptophan	HILIC-pos	Indoles and Indole Derivatives	HMDB00472	0.9 (1.07, 0.82)	4.8E-01	0.9 (1.04, 0.79)	4.2E-01
1-methylnicotinamide	HILIC-pos	Other	HMDB00699	0.8 (0.97, 0.74)	6.5E-02	0.9 (1.03, 0.78)	3.5E-01
thyroxine	HILIC-pos	Other	HMDB00248	0.9 (1, 0.77)	1.6E-01	0.9 (1.01, 0.76)	2.5E-01
NMMA	HILIC-pos	Other	HMDB29416	0.9 (1.02, 0.78)	2.2E-01	0.9 (1.05, 0.8)	4.6E-01
N-carbamoyl-beta-alanine	HILIC-pos	Other	HMDB00026	1.1 (1.27, 0.97)	2.5E-01	1.1 (1.23, 0.93)	6.1E-01

Metabolite.Name	Method	Category	HMDB.ID	Matching Adjustment		Full Adjustment	
				OR (95 CI%)	FDR p	OR (95 CI%)	FDR p
histamine	HILIC-pos	Other	HMDB00870	0.9 (1.03, 0.79)	2.8E-01	0.9 (1.04, 0.79)	4.2E-01
trimethylamine-N-oxide	HILIC-pos	Other	HMDB00925	1.1 (1.23, 0.95)	3.8E-01	1 (1.17, 0.89)	8.8E-01
thiamine	HILIC-pos	Other	HMDB00235	0.9 (1.07, 0.82)	5.1E-01	1 (1.17, 0.88)	8.9E-01
carnosine	HILIC-pos	Other	HMDB00033	1 (1.09, 0.84)	6.1E-01	1 (1.11, 0.85)	8.4E-01
niacinamide	HILIC-pos	Other	HMDB01406	1 (1.13, 0.88)	8.4E-01	1 (1.14, 0.87)	9.2E-01
putrescine	HILIC-pos	Polyamines	HMDB01414	0.9 (1.05, 0.81)	3.7E-01	1 (1.13, 0.85)	8.6E-01
xanthosine	HILIC-pos	Purines and Pyrimidines	HMDB00299	0.8 (0.9, 0.68)	3.7E-03	0.9 (1.02, 0.74)	2.6E-01
cytosine	HILIC-pos	Purines and Pyrimidines	HMDB00630	1.2 (1.35, 1.01)	1.1E-01	1.1 (1.29, 0.95)	4.0E-01
adenosine	HILIC-pos	Purines and Pyrimidines	HMDB00050	0.9 (1.05, 0.81)	3.7E-01	1 (1.11, 0.84)	7.7E-01
sarcosine	HILIC-pos	Quaternary Amines	HMDB00271	0.8 (0.96, 0.74)	4.9E-02	0.9 (0.99, 0.74)	1.6E-01
betaine	HILIC-pos	Quaternary Amines	HMDB00043	1 (1.18, 0.9)	6.8E-01	1 (1.2, 0.9)	7.6E-01
butyrobetaine	HILIC-pos	Quaternary Amines	HMDB01161	1 (1.1, 0.85)	6.8E-01	1 (1.14, 0.87)	9.2E-01
carnitine	HILIC-pos	Quaternary Amines	HMDB00062	1 (1.11, 0.86)	7.0E-01	1 (1.14, 0.86)	8.9E-01
phosphocholine	HILIC-pos	Quaternary Amines	HMDB01565	1 (1.11, 0.86)	7.1E-01	1 (1.17, 0.89)	8.6E-01
choline	HILIC-pos	Quaternary Amines	HMDB00097	1 (1.15, 0.89)	8.0E-01	0.9 (1.09, 0.83)	6.8E-01
alpha-glycerophosphocholine	HILIC-pos	Quaternary Amines	HMDB00086	1 (1.14, 0.88)	8.2E-01	1 (1.15, 0.87)	9.3E-01

Supplemental Table 2. Logistic regression results in the validation WHI-HT dataset for all discovered markers

	WHI-HT Adjust for matching*		WHI-HT Adjusted for risk factors†	
Metabolite	Odds Ratio‡	P- Value	Odds Ratio‡	P-value
C34:2 hydroxy-PC	1.83 (1.54 ,2.17)	5.4E-13	1.76 (1.47 ,2.1)	2.5E-10
15-HETE	1.73 (1.44 ,2.07)	2.3E-10	1.65 (1.36 ,1.99)	5.6E-08
5-HETE	1.71 (1.43 ,2.04)	3.0E-10	1.65 (1.37 ,1.99)	2.6E-08
11-HETE	1.68 (1.41 ,2)	9.0E-10	1.64 (1.36 ,1.97)	4.3E-08
C36:4 hydroxy-PC	1.66 (1.39 ,1.99)	2.4E-09	1.56 (1.3 ,1.87)	7.0E-07
12-HETE	1.64 (1.38 ,1.95)	3.9E-09	-	-
glutamate	1.64 (1.38 ,1.95)	5.5E-09	1.5 (1.25 ,1.8)	8.3E-06
glutamine	0.61 (0.5 ,0.73)	1.4E-08	0.67 (0.55 ,0.82)	2.5E-05
2-hydroxyglutarate	1.45 (1.22 ,1.72)	1.0E-05	-	-
C52:0 TAG	1.42 (1.2 ,1.67)	2.5E-05	-	-
glucose	1.42 (1.19 ,1.69)	3.4E-05	-	-
C36:1 DAG	1.41 (1.19 ,1.67)	3.9E-05	-	-
C34:1 DAG	1.4 (1.18 ,1.65)	5.9E-05	-	-
sucrose	1.4 (1.18 ,1.65)	7.2E-05	-	-
C52:1 TAG	1.38 (1.17 ,1.63)	8.1E-05	-	-
CMP	1.38 (1.17 ,1.63)	1.1E-04	1.33 (1.11 ,1.59)	1.4E-03
C50:0 TAG	1.37 (1.16 ,1.61)	1.4E-04	-	-
C54:2 TAG	1.36 (1.15 ,1.6)	2.0E-04	-	-
C54:1 TAG	1.34 (1.14 ,1.58)	3.3E-04	-	-
C56:2 TAG	1.34 (1.14 ,1.59)	3.4E-04	-	-
C50:1 TAG	1.34 (1.14 ,1.58)	3.6E-04	-	-
asparagine	0.75 (0.64 ,0.88)	4.2E-04	0.87 (0.73 ,1.05)	1.4E-01
C52:2 TAG	1.32 (1.12 ,1.55)	7.8E-04	-	-
C36:2 DAG	1.31 (1.11 ,1.54)	1.3E-03	-	-
sorbitol	1.28 (1.08 ,1.51)	3.4E-03	-	-
C34:0 DAG	1.26 (1.06 ,1.49)	6.5E-03	-	-
uracil	0.8 (0.68 ,0.94)	6.5E-03	-	-
C54:3 TAG	1.25 (1.06 ,1.47)	6.7E-03	-	-
xanthosine	0.8 (0.68 ,0.95)	7.5E-03	-	-
C56:3 TAG	1.23 (1.05 ,1.45)	1.2E-02	-	-
C40:10 PC	0.82 (0.7 ,0.97)	1.8E-02	-	-
fumarate/maleate	1.22 (1.03 ,1.44)	2.1E-02	-	-
isocitrate	1.21 (1.02 ,1.42)	2.4E-02	-	-
hydroxyphenylacetate	1.17 (1 ,1.38)	5.2E-02	-	-

	WHI-HT Adjust for matching*		WHI-HT Adjusted for risk factors†	
Metabolite	Odds Ratio‡	P- Value	Odds Ratio‡	P-value
uridine	0.86 (0.73 ,1)	5.5E-02	0.93 (0.78 ,1.1)	3.8E-01
glycine	0.85 (0.73 ,1)	5.5E-02	-	-
histidine	0.86 (0.73 ,1.01)	0.073	-	-
glycodeoxycholate	1.14 (0.97 ,1.34)	0.108	-	-
3-methyladipate/pimelate	1.14 (0.97 ,1.34)	0.108	-	-
serine	0.88 (0.75 ,1.04)	0.131	-	-
cystathionine	1.13 (0.96 ,1.32)	0.134	-	-
1-methylhistamine	0.89 (0.76 ,1.04)	0.14	0.91 (0.77 ,1.08)	2.7E-01
LTB4	1.12 (0.95 ,1.31)	0.171	-	-
2-phosphoglycerate	0.9 (0.76 ,1.05)	0.176	0.9 (0.76 ,1.06)	2.1E-01
C40:9 PC	0.91 (0.77 ,1.07)	0.233	-	-
C4-OH carnitine	1.1 (0.94 ,1.29)	0.251	-	-
glucuronate	1.09 (0.93 ,1.28)	0.271	-	-
C34:3 PC plasmalogen	0.92 (0.78 ,1.08)	0.286	-	-
C38:7 PC plasmalogen	0.93 (0.79 ,1.09)	0.368	-	-
C38:6 PC	0.93 (0.79 ,1.1)	0.409	-	-
phosphocreatine	0.94 (0.8 ,1.1)	0.46	1.04 (0.87 ,1.23)	6.9E-01
threonine	1.06 (0.9 ,1.25)	0.461	-	-
C56:10 TAG	1.05 (0.9 ,1.24)	0.514	1.04 (0.87 ,1.24)	6.5E-01
sarcosine	0.95 (0.81 ,1.12)	0.566	-	-
docosahexaenoic acid	1.04 (0.89 ,1.23)	0.607	-	-
C58:11 TAG	0.96 (0.82 ,1.13)	0.611	0.93 (0.78 ,1.11)	4.2E-01
lysine	0.98 (0.83 ,1.15)	0.789	1.02 (0.85 ,1.22)	8.3E-01
methionine	0.98 (0.84 ,1.15)	0.816	1.07 (0.9 ,1.27)	4.3E-01
C22:6 LPE	1.02 (0.87 ,1.19)	0.842	-	-
2-aminoadipate	1.01 (0.87 ,1.19)	0.861	-	-
C34:3 DAG	-	-	0.96 (0.76 ,1.2)	7.0E-01
C48:3 TAG	-	-	1.02 (0.83 ,1.27)	8.2E-01
C50:3 TAG	-	-	1 (0.79 ,1.25)	9.7E-01
C50:4 TAG	-	-	0.97 (0.78 ,1.21)	7.7E-01
C50:5 TAG	-	-	1 (0.81 ,1.23)	9.9E-01
C50:6 TAG	-	-	1.03 (0.86 ,1.24)	7.4E-01
C52:6 TAG	-	-	0.94 (0.76 ,1.15)	5.5E-01
C52:7 TAG	-	-	0.94 (0.78 ,1.14)	5.5E-01
C54:8 TAG	-	-	0.89 (0.73 ,1.07)	2.0E-01
C56:6 TAG	-	-	0.88 (0.72 ,1.08)	2.1E-01

	WHI-HT Adjust for matching*		WHI-HT Adjusted for risk factors†	
Metabolite	Odds Ratio‡	P- Value	Odds Ratio‡	P-value
C56:7 TAG	-	-	0.86 (0.7 ,1.04)	1.2E-01
C56:8 TAG	-	-	0.87 (0.71 ,1.05)	1.5E-01
C56:9 TAG	-	-	0.91 (0.75 ,1.1)	3.4E-01
C58:10 TAG	-	-	0.9 (0.75 ,1.09)	2.9E-01
C58:7 TAG	-	-	0.84 (0.7 ,1.01)	6.4E-02
C58:8 TAG	-	-	0.86 (0.71 ,1.03)	1.0E-01
C58:9 TAG	-	-	0.87 (0.73 ,1.05)	1.5E-01
leucine	-	-	0.93 (0.78 ,1.11)	4.2E-01
valine	-	-	1 (0.84 ,1.21)	9.6E-01

* adjusted for baseline age, race/ethnicity, hysterectomy status, and enrollment window

† adjusted for baseline age, race/ethnicity, hysterectomy status, enrollment window, aspirin use, statin use, anti-diabetic use, anti-hypertensive use, smoking, systolic blood pressure, diabetes, total and HDL cholesterol.

‡ odds ratios are per 1 standard deviation of log transformed value

Supplemental Table 3. CVs and number below the limit of detection for validated markers

Metabolite	Coefficient of Variation*	Percent below the limit of detection
11-HETE	-	0%
12-HETE	9.6	0%
15-HETE	10.3	0%
2-hydroxyglutarate	7.5	0%
5-HETE	9.7	0%
asparagine	5.4	0%
C34:0 DAG	4.8	0%
C34:1 DAG	3.1	0%
C34:2 hydroxy-PC	12.9	19%
C36:1 DAG	3.7	0%
C36:2 DAG	3.0	0%
C36:4 hydroxy-PC	8.9	2%
C40:10 PC	6.0	0%
C50:0 TAG	4.9	0%
C50:1 TAG	3.5	0%
C52:0 TAG	6.7	0%
C52:1 TAG	4.2	0%
C52:2 TAG	3.9	0%
C54:1 TAG	5.8	0%
C54:2 TAG	4.2	0%
C54:3 TAG	4.3	0%
C56:2 TAG	23.7	0%
C56:3 TAG	10.1	0%
CMP	58.1	21%
fumarate/maleate	12.3	0%
glucose	3.5	0%
glutamate	4.4	0%
glutamine	6.2	0%
isocitrate	6.8	0%
sorbitol	3.9	0%
sucrose	10.5	0%
uracil	8.8	0%
xanthosine	33.8	0%

*Calculated using pooled plasma samples

Supplemental Table 4. Baseline characteristics for the PREDIMED replication cohort.

	Sub-cohort * (n=787)	Cases (n=230)	*P*-value†
Intervention group, %			
Control	234 (29.7)	83 (36.1)	0.15
Mediterranean diet + EVOO	291 (37.0)	82 (35.7)	
Mediterranean diet + Nuts	262 (33.3)	65 (28.3)	
Women, %	450 (57.2)	91 (39.6)	<0.0001
Family history of premature CHD, %	196 (24.9)	44 (19.1)	0.070
Smoking, %			
Never	491 (62.4)	104 (45.2)	<0.0001
Current	96 (12.2)	46 (20.0)	
Former	200 (25.4)	80 (34.8)	
Baseline prevalent disease, %			
Hypertension	659 (83.7)	190 (82.6)	0.69
Dyslipidemia	579 (73.6)	134 (58.3)	<0.0001
Diabetes	372 (47.3)	149 (64.8)	<0.0001
Age (years)	67.2±5.9	69.5±6.5	<0.0001
Body mass index (kg/m^2)	29.8±3.6	29.6±3.7	0.63
Fasting glucose (mg/dL)	121.9±41.0	136.2±48.9	<0.0001
Total cholesterol (mg/dl)	210.3±37.1	212.1±35.7	0.086
HDL cholesterol (mg/dL)	54.0±15.4	51.9±16.4	0.43
LDL cholesterol (mg/dL)	130.8±33.4	131.4±33.4	0.81
Triglyceride (mg/dL)	135.0±79.3	151.5±83.4	0.0065
Systolic blood pressure (mmHg)	147.3±20.3	154.9±23.1	<0.0001
Diastolic blood pressure (mmHg)	82.0±10.5	83.0±11.6	0.25
Statin use	317 (40.3)	57 (24.8)	<0.0001

Abbreviations: EVOO, extra-virgin olive oil; CHD, coronary heart disease; HDL, high-density lipoprotein; LDL, low-density lipoprotein;

*The sub-cohort also included 37 cases.

† For categorical and binary variables, *P*-values were calculated from χ^2-test. For continuous variables, *P*-values were calculated from t-test.