Supplementary Materials: The Consortium of Metabolomics Studies (COMETS): Metabolomics in 47 Prospective Cohort Studies

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Population and sample collection

The Health, Aging, and Body Composition Study (Health ABC) is a prospective, longitudinal cohort study of 3075 community-dwelling, initially well-functioning, black and white men and women aged 70-79 years. Participants were recruited from a random sample of white Medicare beneficiaries in selected zip codes and all black Medicare-eligible residents in the Memphis, Tennessee, and Pittsburgh, Pennsylvania areas. Eligibility criteria were 1) no reported difficulty walking one quarter of a mile, climbing 10 steps without resting and performing activities of daily living, 2) no active treatment for cancer in the prior 3 years, 3) planned to stay in the study area for at least 3 years, and 4) were not actively participating in a lifestyle intervention trial. Participants donated blood at multiple time points during the study.

In a prior research effort, we sent 200 µl of blood from 319 black men for metabolomics analysis at the Broad Institute(1). Black men were selected because no studies had examined metabolite-adiposity associations in this population before. The participants in this analysis were selected at random from among all black men in Health ABC. The blood samples were ethylenediaminetetraacetic acid (EDTA) plasma donated at the 12-month study visit and taken after an overnight fast (mean fast = 14 hours). Samples had never been thawed and were stored at −80°C until metabolite profiling. Additionally, a duplicate aliquot was prepared for 40 of these men (selected at random) and sent to Metabolon Inc. for analysis. The current analysis is restricted to just those 40 men whose samples were analyzed by both the Broad Institute and Metabolon Inc.

Metabolomics analysis

A total of 350 metabolites were measured using the metabolite profiling platform of the Broad Institute of Massachusetts Institute of Technology. Detailed methodology is provided in Townsend et al(2). In brief, we used liquid chromatography-mass spectroscopy (LC-MS) to obtain profiles of polar and lipid metabolites. Negative ionization mode results were provided by a ACQUITY ultra-performance liquid

chromatography (Waters) coupled with a 5500 QTRAP triple quadrupole MS (AB SCIEX) using a hydrophilic interaction chromatography method(3). Polar, negatively charged compounds were analyzed by multiple reaction monitoring in the negative ionization mode(4). Positive ionization data were provided by a LC-MS/MS system of a 4000 QTRAP triple quadrupole mass spectrometer (AB SCIEX) with an HTS PAL auto-sampler (Leap Technologies), as described in Wang et al(5). Polar, positively charged metabolites were analyzed with multiple reaction monitoring in the positive ion mode. Lipids were separated using a Prosphere C4 HPLC column and data obtained through a full scan MS analysis in positive ion mode(6). MultiQuant 1.2 software (AB SCIEX) was used to integrate peaks and for manual review of data(6). Reference standards of each metabolite were used to determine chromatographic retention times. Metabolite peaks were compared against known standards to confirm identity. Metabolite signals were measured as LC-MS/MS peak areas that are proportional to metabolite concentrations.

A total of 610 named metabolites were measured using the Orbitrap Elite LC-MS(7) and GC-MS platform(8) of Metabolon Inc. Samples were extracted and prepared for analysis using Metabolon's standard solvent extraction method. The LC/MS portion of the platform was based on a Waters ACQUITY ultra-performance liquid chromatography (UPLC) and a ThermoFisher Scientific Orbitrap Elite high resolution/accurate mass spectrometer, which consisted of a heated electrospray ionization (HESI) source and orbitrap mass analyzer operated at 30 000 mass resolution. The sample extract was dried then reconstituted in acidic or basic LC-compatible solvents, each of which contained 8 or more injection standards at fixed concentrations to ensure injection and chromatographic consistency. One aliquot was analyzed using acidic positive ion optimized conditions and the other using basic negative ion optimized conditions in two independent injections using separate dedicated columns. Extracts reconstituted in acidic conditions were gradient eluted using water and methanol containing 0.1% formic acid, while the basic extracts, which also used water/methanol, contained 6.5mM Ammonium Bicarbonate. The samples destined for GC/MS analysis were re-dried under vacuum desiccation for a minimum of 24 hours prior to being derivatized under dried nitrogen using bistrimethyl-silyl-triflouroacetamide (BSTFA). The GC column was 5% phenyl and the temperature ramp was from 40° to 300° C in a 16-minute period. Samples were analyzed on a Thermo-Finnigan Trace DSQ fast-scanning single-quadrupole mass spectrometer using electron impact ionization. The instrument was tuned and calibrated for mass

resolution and mass accuracy on a daily basis. Metabolite signals were measured as LC-MS peak areas, with prior data indicating that peak areas are proportion to metabolite concentrations over much of the linear dynamic range(9). To account for variability by run day, values were standardized as a proportion of the median observed value for that day. Thus, the median value for each metabolite for each run day was set to 1, and metabolite values twice that of the median for that day were to 2, and so on.

Statistical analysis

The current analysis utilizes data from the 40 men whose samples were analyzed at both the Broad Institute and Metabolon Inc. For both sets of data, the distribution of metabolites was skewed and we thus log transformed metabolite values to approximate a normal distribution. Metabolite values were then grand mean centered (mean=0, standard deviation=1). Missing values were assumed to be below the limit of detection and were imputed with half of the minimum observed value for that metabolite.

We identified the metabolites constituting matches between the Broad Institute and Metabolon Inc. metabolomics platforms by using Human Metabolome Database(10) identifiers that each lab reported for their metabolites. These unique identifiers served as keys linking the different metabolite naming systems of the Broad Institute and Metabolon.

In our analysis, we compared metabolite values between the Broad Institute and Metabolon Inc. using both Spearman and Pearson correlations. We focus primarily on Spearman correlations because metabolomics data sometimes contain outliers (even after log-transformation) and because there is no guarantee that peak area values will be linearly proportional across platforms. Spearman correlations, unlike Pearson correlations, are not sensitive to outliers and do not assume linearly proportional relationships. We report Pearson correlations as complementary data because they have more statistical power when the assumption of linear proportionality is met.

References

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Web Table 1. Location of cohorts and contributing study authors.

Cohort	Location	Contributing study authors and research group[a]
AIRWAVE	United Kingdom	Abbas Dehghan; Paul Elliott; Ioanna Tzoulaki
ATBC	Finland	Demetrius Albanes; Rachael Stolzenberg-Solomon
ARIC	United States	Eric Boerwinkle; Bing Yu
ALSPAC	United Kingdom	Deborah A. Lawlor
BHS	Brazil	Alexandre C. Pereira
BIB	United Kingdom	Deborah A. Lawlor
BCFR	Australia; United States	Ann W. Hsing
BWHHS	United Kingdom	Juan P. Casas; Caroline Dale
CaPS	United Kingdom	Yoav Ben-Shlomo
CPS-II	United States	Victoria L. Stevens; Ying Wang
CATHGEN	United States	Svati H. Shah
CAMP	United States	Clary Clish; Jessica Lasky-Su
COLO	United States	Cornelia M. Ulrich
KORA	Germany	Christian Gieger
DIPP	Finland	Matej Oresic
DPP	United States	Marinella Temprosa; Naji Younes; DPP Research Group[b]
ET2DS	United Kingdom	Jackie Price
Estonia OE	Estonia	Joel N. Hirschhorn
EPIC	Denmark; France; Germany; Greece; Italy; Norway; Spain; Sweden; The Netherlands; United Kingdom	Ruth Travis; Marc Gunter
Fenland	United Kingdom	Claudia Langenberg; Luca A. Lotta; Nick J. Wareham
FHS2	United States	Ramachandran S. Vasan
FHS3	United States	Ramachandran S. Vasan
GDM	Spain	Clara Barrios Barrera
HABC	United States	Tamara Harris; Rachel Murphy
HPFS	United States	A. Heather Eliassen
MAC	United States	Hua Zhao
MRC NSHD	United Kingdom	Andrew Wong
MrOS	United States	Eric Orwoll
MEC	United States	Bruce S. Kristal; Loic LeMarchand
MESA	United States	David Herrington
NHS	United States	A. Heather Eliassen

NHS-II	United States	A. Heather Eliassen
PHS	United States	Howard D. Sesso; Lorelei Mucci
POPS	United Kingdom	Gordon C.S. Smith; Ulla Sovio
PLCO	United States	Steven C. Moore
SMHS	China	Wei Zheng; Xiao-Ou Shu
SPA	China	Charles E. Matthews
SWHS	China	Xiao-Ou Shu
SP2	Singapore	Deron R. Herr; Chin Meng Khoo; Wei Jie Seow
SABRE	United Kingdom	Therese Tillin
TMCS	Japan	Sei Harada; Toru Takebayashi
TwinsUK	United Kingdom	Massimo Mangino; Cristina Menni
UPBEAT	United Kingdom	Lucilla Poston
VDAART	United States	Rachel S. Kelly; Jessica Lasky-Su
WH-II	United Kingdom	Mika Kivimäki
WHI	United States	Kathryn Rexrode
WIHS	United States	Qibin Qi

[a] For each research group, footnotes provide references that include complete lists of research group members.

[b] Knowler WC, Barrett-Connor E, Fowler SE, et al. Reduction in the incidence of type 2 diabetes with lifestyle intervention or metformin. N Engl J Med. 2002;346(6):393-403.

Web Table 2. Methods of follow-up for outcomes in participating COMETS studies[a].

Cohort	Follow-up questionnaire	Protocol-based clinic or home visit[b]	Medical record confirmation	Death registry	Cancer registry
AIRWAVE	P	P	✓	✓	✓
ATBC	✓	✓	✓	✓	✓
ARIC	✓	✓	✓	✓	X
ALSPAC	✓	✓	✓	✓	✓
BHS	✓	✓	X	X	X
BIB	✓	✓	✓	✓	✓
BCFR	✓	X	X	✓	✓
BWHHS	✓	✓	✓	✓	✓
CaPS	✓	✓	✓	✓	✓
CPS-II	✓	X	✓	✓	✓
CATHGEN	✓	✓	✓	✓	X
CAMP	✓	✓	X	X	X
COLO	✓	X	✓	✓	X
KORA	X	P	X	✓	X
DIPP	✓	✓	X	X	X
DPP	✓	✓	✓	✓	X
ET2DS	✓	✓	✓	✓	X
Estonia OE	P	P	✓	✓	✓
EPIC	P	X	P	✓	✓
Fenland	✓	✓	X	X	X
FHS2	✓	✓	✓	X	X
FHS3	✓	✓	✓	X	X
GDM	✓	✓	✓	✓	X
HABC	✓	✓	✓	X	X
HPFS	✓	X	✓	✓	X
MAC	✓	X	X	✓	✓
MRC NSHD	✓	✓	✓	✓	✓
MrOS	✓	✓	X	X	X
MEC	✓	X	X	✓	✓
MESA	✓	✓	✓	✓	X
NHS	✓	X	✓	✓	✓
NHSII	✓	X	✓	✓	✓
PHS	✓	X	✓	✓	X

POPS	✓	X	X	X	X
PLCO	✓	✓	✓	X	X
SMHS	✓	✓	✓	✓	✓
SPA	✓	✓	✓	✓	✓
SWHS	✓	✓	✓	✓	✓
SP2	✓	✓	X	✓	✓
SABRE	P	P	P	✓	✓
TMCS	✓	✓	✓	✓	✓
TwinsUK	✓	✓	X	X	X
UPBEAT	✓	✓	✓	✓	✓
VDAART	✓	✓	X	X	X
WH-II	✓	✓	✓	✓	✓
WHI	✓	✓	✓	✓	X
WIHS	✓	✓	✓	✓	✓

[a] ✓indicates that the measurement is available in all participants, P indicates that the measurement is available in a portion of participants, X indicates that the measurement is not available in any of the participants.

[b] Does not include incidental hospital visits.

Web Table 3. Title, legend, and table provided separately in Excel.

Web Table 4. Correlations (Spearman and Pearson) between log-transformed metabolite values measured at the Broad Institute and Metabolon, Inc. for 111 overlapping metabolites.

Name | HMDB ID	Spearman Correlation	Pearson Correlation
X_1_METHYLNICOTINAMIDE | HMDB00699	0.93	0.95
X_2_AMINOADIPATE | HMDB00510	0.77	0.75
X_2_HYDROXYGLUTARATE | HMDB00694	0.46	0.45
X_4_PYRIDOXATE | HMDB00017	0.95	0.96
ACETYLGLYCINE | HMDB00532	0.82	0.88
ADENINE | HMDB00034	-0.30	-0.14
ADMA | HMDB01539	0.49	0.43
ADP | HMDB01341	0.87	0.90
ALANINE | HMDB00161	0.61	0.43
ALPHA_GLYCEROPHOSPHATE | HMDB00126	0.14	0.32
ALPHA_GLYCEROPHOSPHOCHOLINE | HMDB00086	0.49	0.47
ALPHA_HYDROXYBUTYRATE | HMDB00008	0.97	0.98
ALPHA_KETOGLUTARATE | HMDB00208	0.23	0.14
AMP | HMDB00045	0.87	0.91
ARGININE | HMDB00517	0.80	0.76
ASPARAGINE | HMDB00168	0.60	0.65
BENZOATE | HMDB01870	0.10	0.12
BETA_ALANINE | HMDB00056	0.12	0.18
BETAINE | HMDB00043	0.75	0.76
BUTYROBETAINE | HMDB01161	0.43	0.29
C10_CARNITINE | HMDB00651	0.93	0.95
C12_CARNITINE | HMDB02250	0.74	0.77
C14_CARNITINE | HMDB05066	0.54	0.54
C14_0_LPC | HMDB10379	0.76	0.75
C16_CARNITINE | HMDB00222	0.32	0.29
C16_0_LPC | HMDB10382	0.48	0.70
C16_0_LPE | HMDB11503	0.52	0.64
C16_1_LPC | HMDB10383	0.75	0.70
C18_CARNITINE | HMDB00848	0.46	0.41
C18_0_LPC | HMDB10384	0.45	0.71
C18_0_LPE | HMDB11130	0.71	0.78
C18_0_SM | HMDB01348	0.70	0.72
C18_1_CARNITINE | HMDB05065	0.24	0.18
C18_1_LPC | HMDB02815	0.75	0.75
C18_1_LPE | HMDB11506	0.79	0.83
C18_2_LPC | HMDB10386	0.71	0.78
C18_2_LPE | HMDB11507	0.86	0.85

C2_CARNITINE | HMDB00201	0.90	0.92
C20_4_LPC | HMDB10395	0.63	0.76
C20_4_LPE | HMDB11517	0.80	0.78
C3_CARNITINE | HMDB00824	0.91	0.93
C3_DC_CH3_CARNITINE | HMDB13133	0.50	0.65
C4_CARNITINE | HMDB02013	0.78	0.70
C4_OH_CARNITINE | HMDB13127	0.92	0.88
C5_CARNITINE | HMDB00688	0.83	0.83
C5_DC_CARNITINE | HMDB13130	0.96	0.97
C5_1_CARNITINE | HMDB02366	0.95	0.94
C6_CARNITINE | HMDB00705	0.92	0.92
C8_CARNITINE | HMDB00791	0.97	0.99
CAMP | HMDB00058	0.08	0.22
CARNITINE | HMDB00062	0.62	0.63
CHOLATE | HMDB00619	0.94	0.93
CHOLINE | HMDB00097	0.91	0.93
CITRATE | HMDB00094	0.77	0.83
CITRULLINE | HMDB00904	0.86	0.90
COTININE | HMDB01046	0.68	0.94
CREATINE | HMDB00064	0.90	0.92
CREATININE | HMDB00562	0.93	0.93
DIMETHYLGLYCINE | HMDB00092	0.90	0.87
FRUCTOSE_GLUCOSE_GALACTOSE | HMDB00122	0.86	0.92
GENTISATE | HMDB00152	0.89	0.90
GLUTAMATE | HMDB00148	0.79	0.85
GLUTAMINE | HMDB00641	0.46	0.54
GLYCINE | HMDB00123	0.31	0.27
GLYCOCHOLATE | HMDB00138	0.76	0.76
GLYCODEOXYCHOLATE_GLYCOCHENODEOX | HMDB00631	0.76	0.66
HIPPURATE | HMDB00714	0.96	0.98
HISTIDINE | HMDB00177	0.44	0.48
HYDROXYPHENYLACETATE | HMDB00020	0.15	0.21
HYDROXYPROLINE | HMDB00725	0.96	0.98
HYPOXANTHINE | HMDB00157	0.88	0.91
INDOLE_3_PROPIONATE | HMDB02302	0.95	0.94
INDOXYLSULFATE | HMDB00682	0.96	0.98
INOSINE | HMDB00195	0.03	0.08
INOSITOL | HMDB00211	0.67	0.74
ISOLEUCINE | HMDB00172	0.89	0.88
KYNURENIC_ACID | HMDB00715	0.77	0.77
KYNURENINE | HMDB00684	0.89	0.89

LACTATE | HMDB00190	0.95	0.95
LEUCINE | HMDB00687	0.89	0.90
LYSINE | HMDB00182	0.83	0.57
MALATE | HMDB00156	0.80	0.66
METHIONINE | HMDB00696	0.83	0.80
N_CARBAMOYL_BETA_ALANINE | HMDB00026	0.80	0.86
NIACINAMIDE | HMDB01406	0.92	0.91
ORNITHINE | HMDB00214	0.83	0.81
OROTATE | HMDB00226	0.41	0.76
OXALATE | HMDB02329	0.11	0.09
PANTOTHENATE | HMDB00210	0.81	0.83
PHENYLALANINE | HMDB00159	0.81	0.78
PROLINE | HMDB00162	0.84	0.82
PYROGLUTAMIC_ACID | HMDB00267	0.30	0.25
PYRUVATE | HMDB00243	0.71	0.70
SALICYLURATE | HMDB00840	0.97	0.97
SDMA | HMDB03334	0.69	0.77
SERINE | HMDB00187	0.82	0.78
SEROTONIN | HMDB00259	0.89	0.93
SUCROSE | HMDB00258	NA	NA
TAURINE | HMDB00251	0.95	0.95
TAURODEOXYCHOLATE_TAUROCHENODEO | HMDB00896	0.74	0.88
THREONINE | HMDB00167	0.86	0.65
TRIMETHYLAMINE_N_OXIDE | HMDB00925	0.93	0.96
TRYPTOPHAN | HMDB00929	0.67	0.79
TYROSINE | HMDB00158	0.83	0.85
URACIL | HMDB00300	0.39	0.27
URATE | HMDB00289	0.82	0.87
URIDINE | HMDB00296	0.78	0.76
VALINE | HMDB00883	0.92	0.9
XANTHINE | HMDB00292	0.75	0.91
XANTHOSINE | HMDB00299	-0.02	0.00
XANTHURENATE | HMDB00881	0.60	0.69

Web Table 5. Metabolite pairs that are highly correlated across the Broad Institute and Metabolon, Inc. metabolomics platforms.

Broad Institute name	Metabolon, Inc. name	Spearman correlation	Pearson correlation
ACETYLCHOLINE	DEOXYCARNITINE	0.92	0.97
ACONITATE	X_18886	0.78	0.78
AMINOISOBUTYRIC_ACID	X_12824	0.64	0.70
BETA_HYDROXYBUTYRATE	X_3_HYDROXYBUTYRATE__BHBA_	0.98	0.99
C10_2_CARNITINE	X_13435	0.79	0.75
C12_1_CARNITINE	X_13743	0.76	0.74
C14_1_CARNITINE	X_13743	0.77	0.77
C14_2_CARNITINE	X_13743	0.78	0.80
C16_0_SM	PALMITOYL_SPHINGOMYELIN	0.75	0.74
C18_1_OH_CARNITINE	HYDROXYBUTYRYLCARNITINE	0.75	0.76
C20_5_LPC	X_2_LINOLEOYLGLYCEROPHOSPHOETH	0.76	0.78
C22_6_LPC	X_1_DOCOSAHEXAENOYLGLYCEROPHOS	0.57	0.73
C22_6_LPE	X_1_DOCOSAHEXAENOYLGLYCEROPETH	0.85	0.86
C32_0_DAG	X_15497	0.72	0.47
C32_1_PC	X_1_PALMITOLEOYLGLYCEROPEA	0.66	0.71
C32_1_PI	PALMITOYL_SPHINGOMYELIN	0.75	0.65
C32_2_PC	X_1_MYRISTOYLGLYCEROPHOSPHOCHO	0.70	0.66
C34_0_PS	X_1_EICOSAPENTAENOYLGLYCEROPHO	0.68	0.76
C34_3_PC	X_2_MYRISTOYLGLYCEROPHOSPHOCHO	0.71	0.65
C34_3_PE_PLASMALOGEN	X_2_ARACHIDONOYLGLYCEROPHOSCHO	0.59	0.79
C34_4_PC	X_1_MYRISTOYLGLYCEROPHOSPHOCHO	0.77	0.80
C36_1_PC	X_1_PALMITOLEOYLGLYCEROPEA	0.58	0.71
C36_3_PC	X_1_EICOSATRIENOYLGLYCEROPPETH	0.70	0.64
C36_3_PE_PLASMALOGEN	X_2_ARACHIDONOYLGLYCEROPHOSCHO	0.69	0.75
C36_4_PC_A	X_1_LINOLEOYLGLYCEROPHOSPHOETH	0.72	0.60
C36_4_PE_PLASMALOGEN	X_2_LINOLEOYLGLYCEROPHOSPHOCHO	0.66	0.78
C36_5_PC_PLASMALOGEN_B	X_2_ARACHIDONOYLGLYCEROPHOSCHO	0.74	0.68
C36_5_PE_PLASMALOGEN	X_2_ARACHIDONOYLGLYCEROPHOSCHO	0.61	0.71
C38_5_PE_PLASMALOGEN	X_2_ARACHIDONOYLGLYCEROPHOSCHO	0.73	0.77
C38_6_PC	DOCOSAHEXAENOATE	0.69	0.73
C38_6_PC_PLASMALOGEN	X_2_ARACHIDONOYLGLYCEROPHOSCHO	0.72	0.80
C38_6_PE_PLASMALOGEN	X_2_ARACHIDONOYLGLYCEROPHOSCHO	0.73	0.79
C38_7_PE_PLASMALOGEN	CMPF	0.69	0.70
C40_7_PC_PLASMALOGEN	BETA_ALANINE	0.70	0.60
C40_9_PC	DOCOSAHEXAENOATE	0.71	0.75
C44_13_PE_PLASMALOGEN	X_2_LINOLEOYLGLYCEROPHOSPHOETH	0.68	0.70
C44_2_TAG	X_1_MYRISTOLEOYLGLYCEROPHOSPHO	0.71	0.63

C56_10_TAG	EICOSAPENTAENOATE	0.66	0.76
C56_8_TAG	EICOSAPENTAENOATE	0.70	0.74
C56_9_TAG	EICOSAPENTAENOATE	0.70	0.77
C58_10_TAG	DOCOSAHEXAENOATE	0.69	0.71
C58_11_TAG	EICOSAPENTAENOATE	0.72	0.69
C58_9_TAG	DOCOSAHEXAENOATE	0.70	0.71
C7_CARNITINE	X_17335	0.73	0.67
C9_CARNITINE	X_13431	0.80	0.80
GABA	X_2_AMINOBUTYRATE	0.82	0.76
GDP	ADENOSINE_5__DIPHOSPHATE__ADP	0.87	0.89
GLUTATHIONE_OXIDIZED	CIS_VACCENATE__18_1N7_	0.82	0.81
GMP	ADENOSINE_5__MONOPHOSPHATE__A	0.79	0.88
ISOCITRATE	X_12819	0.71	0.76
LACTOSE	MALTOSE	0.80	0.72
PIPECOLIC_ACID	PIPECOLATE	0.94	0.98
PROPIONATE	GUANOSINE	0.78	0.74
QUINOLINATE	X_15503	0.77	0.84
SORBITOL	MANNITOL	0.86	0.88
UDP	ADENOSINE_5__DIPHOSPHATE__ADP	0.77	0.76
X_5_AMINOLEVULINIC_ACID	N_ACETYLVALINE	0.83	0.89