

**Note to readers with disabilities:** *EHP* strives to ensure that all journal content is accessible to all readers. However, some figures and Supplemental Material published in *EHP* articles may not conform to [508 standards](#) due to the complexity of the information being presented. If you need assistance accessing journal content, please contact [ehp508@niehs.nih.gov](mailto:ehp508@niehs.nih.gov). Our staff will work with you to assess and meet your accessibility needs within 3 working days.

### **Supplemental Material**

#### **Metabolomics Profiling before, during, and after the Beijing Olympics: A Panel Study of Within-Individual Differences during Periods of High and Low Air Pollution**

Lina Mu, Zhongzheng Niu, Rachael Hageman Blair, Han Yu, Richard W. Browne, Matthew R. Bonner, Tiffany Fanter, Furong Deng, and Mya Swanson

#### **Table of Contents**

**Table S1.** Subclasses of 74 out of 886 metabolites that were different before, during, and after 2008 Beijing Olympics in 26 non-smoking adults.

**Table S2.** ANOVA test of modules for times before, during, and after the Olympics, sex, and interaction in 26 non-smoking adults.

**Table S3.** Metabolites and associated classes detected from module 1-4 with significant differences (adjusted  $P < 0.05$ ) before, during and after the Beijing 2008 Olympics in 26 non-smoking adults.

**Supplemental Table S1. Subclasses of 74 out of 886 metabolites that were different before, during, and after 2008 Beijing Olympics in 26 non-smoking adults \***

<b>Super class</b>	<b>Class</b>	<b># of metabolites in subclass</b>	<b># of metabolites changed with P&lt;0.05 *</b>
<b>Amino Acid Super Class</b>			
	<i>Alanine and Aspartate Metabolism</i>	5	0
	<i>Creatine Metabolism</i>	2	0
	<i>Glutamate Metabolism</i>	5	1
	<i>Glutathione Metabolism</i>	3	0
	<i>Glycine, Serine and Threonine Metabolism</i>	10	0
	<i>Guanidino and Acetamido Metabolism</i>	1	0
	<i>Histidine Metabolism</i>	7	0
	<i>Leucine, Isoleucine and Valine Metabolism</i>	21	0
	<i>Lysine Metabolism</i>	5	0
	<i>Methionine, Cysteine, SAM and Taurine Metabolism</i>	11	0
	<i>Phenylalanine and Tyrosine Metabolism</i>	19	1
	<i>Polyamine Metabolism</i>	4	0
	<i>Tryptophan Metabolism</i>	14	0
	<i>Urea cycle; Arginine and Proline Metabolism</i>	13	0
<b>Carbohydrate Super Class</b>			
	<i>Aminosugar Metabolism</i>	2	0
	<i>Fructose, Mannose and Galactose Metabolism</i>	4	1
	<i>Glycolysis, Gluconeogenesis, and Pyruvate Metabolism</i>	5	1
	<i>Pentose Metabolism</i>	11	1
<b>Cofactors and Vitamins Super Class</b>			
	<i>Ascorbate and Aldarate Metabolism</i>	4	2
	<i>Hemoglobin and Porphyrin Metabolism</i>	5	0
	<i>Nicotinate and Nicotinamide Metabolism</i>	4	1
	<i>Pantothenate and CoA Metabolism</i>	1	0
	<i>Riboflavin Metabolism</i>	1	0
	<i>Tocopherol Metabolism</i>	6	0
	<i>Vitamin B6 Metabolism</i>	1	0
<b>Energy Super Class</b>			
	<i>Oxidative Phosphorylation</i>	2	0
	<i>TCA Cycle</i>	6	0
<b>Lipid Super Class</b>			
	<i>Carnitine Metabolism</i>	3	0
	<i>Diacylglycerol</i>	2	0
	<i>Eicosanoid</i>	2	0
	<i>Endocannabinoid</i>	5	1
	<i>Fatty Acid Metabolism (also BCAA Metabolism)</i>	2	0
	<i>Fatty Acid Metabolism(Acyl Carnitine)</i>	12	1
	<i>Fatty Acid Synthesis</i>	1	0
	<i>Fatty Acid, Amide</i>	2	0
	<i>Fatty Acid, Amino</i>	2	0
	<i>Fatty Acid, Branched</i>	1	0
	<i>Fatty Acid, Dicarboxylate</i>	7	2
	<i>Fatty Acid, Methyl Ester</i>	1	0
	<i>Fatty Acid, Monohydroxy</i>	6	2
	<i>Glycerolipid Metabolism</i>	2	1
	<i>Inositol Metabolism</i>	3	0
	<i>Ketone Bodies</i>	2	0
	<i>Long Chain Fatty Acid</i>	17	8
	<i>Lysolipid</i>	63	1
	<i>Medium Chain Fatty Acid</i>	8	4
	<i>Monoacylglycerol</i>	10	0
	<i>Phospholipid Metabolism</i>	4	0
	<i>Polyunsaturated Fatty Acid (n3 and n6)</i>	14	5
	<i>Primary Bile Acid Metabolism</i>	5	0
	<i>Secondary Bile Acid Metabolism</i>	10	0
	<i>Short Chain Fatty Acid</i>	1	0

<i>Sphingolipid Metabolism</i>	5	0
<i>Steroid</i>	21	4
<i>Sterol</i>	6	1
<b>Nucleotide Super Class</b>		
<i>Purine and Pyrimidine Metabolism</i>	1	0
<i>Purine Metabolism, (Hypo)Xanthine/Inosine containing</i>	6	0
<i>Purine Metabolism, Adenine containing</i>	6	0
<i>Purine Metabolism, Guanine containing</i>	4	0
<i>Pyrimidine Metabolism, Cytidine containing</i>	2	0
<i>Pyrimidine Metabolism, Thymine containing</i>	2	0
<i>Pyrimidine Metabolism, Uracil containing</i>	8	0
<b>Peptide Super Class</b>		
<i>Dipeptide</i>	61	2
<i>Dipeptide Derivative</i>	1	0
<i>Fibrinogen Cleavage Peptide</i>	2	0
<i>Gamma-glutamyl Amino Acid</i>	12	1
<i>Polypeptide</i>	3	0
<b>Xenobiotics Super Class</b>		
<i>Benzoate Metabolism</i>	12	0
<i>Chemical</i>	10	1
<i>Drug</i>	18	0
<i>Food Component/Plant</i>	19	1
<i>Tobacco Metabolite</i>	2	0
<i>Xanthine Metabolism</i>	12	0
<b>Unidentified</b>	316	23

**Notes:**

Statistical comparisons were all adjusted for time-invariant variables including age, sex, BMI, and time-varying variables including diet and transportation mode.

\*: Number of metabolites changed significantly ( $p < 0.05$  prior to adjustment for multiple comparisons) for three-time points comparison or any two-time points contrast.

**Supplemental Table S2. ANOVA test of modules for times before, during, and after the Olympics, sex, and interaction in 26 non-smoking adults.**

Module	Size	P value					
		Overall comparison	Adjusted overall comparison	During vs. Before the Olympics	After vs. During the Olympics	Main effect of sex	Interaction between sex and study visits
1	38	0.0000	0.0000	0.0001	0.0000	0.0000	0.0629
2	37	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
3	23	0.0000	0.0000	0.0000	0.0118	0.0000	0.0018
4	5	0.0000	0.0001	0.0000	0.0004	0.0000	0.9787

**Notes:**

Four modules that were significantly different between both pairs of time points (before vs. during, and during vs. after the Olympics) after multiple comparison adjustment. Size is the number of metabolites (of both known and unknown identity) in each module.

Statistical comparisons were all adjusted for time-invariant variables including age, sex, BMI, and time-varying variables including diet and transportation mode.

**Supplemental Table S3. Metabolites and associated classes detected from module 1 -4 with significant differences (adjusted P < 0.05) before, during and after the Beijing 2008 Olympics in 26 non-smoking adults.**

<b>Super class</b>	<b>Class</b>	<b>Metabolite</b>	<b>Module</b>
NA	NA	X - 11540	1
NA	NA	X - 12450	1
NA	NA	X - 13435	1
NA	NA	X - 13891	1
NA	NA	X - 18938	1
Lipid	Fatty Acid Metabolism(Acyl Carnitine)	cis-4-decenoyl carnitine	1
Lipid	Fatty Acid Metabolism(Acyl Carnitine)	decanoylcarnitine	1
Lipid	Fatty Acid Metabolism(Acyl Carnitine)	hexanoylcarnitine	1
Lipid	Fatty Acid Metabolism(Acyl Carnitine)	octanoylcarnitine	1
Lipid	Fatty Acid, Branched	17-methylstearate	1
Lipid	Fatty Acid, Monohydroxy	3-hydroxydecanoate	1
Lipid	Glycerolipid Metabolism	glycerol	1
Lipid	Long Chain Fatty Acid	10-heptadecenoate (17:1n7)	1
Lipid	Long Chain Fatty Acid	10-nonadecenoate (19:1n9)	1
Lipid	Long Chain Fatty Acid	cis-vaccenate (18:1n7)	1
Lipid	Long Chain Fatty Acid	eicosenoate (20:1n9 or 11)	1
Lipid	Long Chain Fatty Acid	margarate (17:0)	1
Lipid	Long Chain Fatty Acid	myristate (14:0)	1
Lipid	Long Chain Fatty Acid	myristoleate (14:1n5)	1
Lipid	Long Chain Fatty Acid	nonadecanoate (19:0)	1
Lipid	Long Chain Fatty Acid	oleate (18:1n9)	1
Lipid	Long Chain Fatty Acid	palmitate (16:0)	1
Lipid	Long Chain Fatty Acid	palmitoleate (16:1n7)	1
Lipid	Long Chain Fatty Acid	stearate (18:0)	1
Lipid	Lysolipid	1- eicosapentaenoylglycerophosphocholine (20:5n3)*	1
Lipid	Medium Chain Fatty Acid	5-dodecenoate (12:1n7)	1
Lipid	Medium Chain Fatty Acid	caprate (10:0)	1
Lipid	Medium Chain Fatty Acid	caprylate (8:0)	1
Lipid	Medium Chain Fatty Acid	laurate (12:0)	1
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	dihomo-linoleate (20:2n6)	1
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	dihomo-linolenate (20:3n3 or n6)	1
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	docosadienoate (22:2n6)	1
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	docosapentaenoate (n3 DPA; 22:5n3)	1
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	docosatrienoate (22:3n3)	1
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	eicosapentaenoate (EPA; 20:5n3)	1
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	linoleate (18:2n6)	1
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	linolenate [alpha or gamma; (18:3n3 or 6)]	1
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	stearidonate (18:4n3)	1
NA	NA	X - 10445	2
NA	NA	X - 11449	2
NA	NA	X - 15168	2
NA	NA	X - 16036	2
NA	NA	X - 17115	2
Peptide	Dipeptide	asparagylleucine	2
Peptide	Dipeptide	aspartylleucine	2
Peptide	Dipeptide	histidylleucine	2
Peptide	Dipeptide	histidylvaline	2
Peptide	Dipeptide	isoleucylalanine	2
Peptide	Dipeptide	isoleucylaspartate	2
Peptide	Dipeptide	isoleucylglycine	2
Peptide	Dipeptide	isoleucylvaline	2
Peptide	Dipeptide	leucylglutamate	2
Peptide	Dipeptide	leucylglycine	2
Peptide	Dipeptide	leucylphenylalanine	2

<b>Peptide</b>	<i>Dipeptide</i>	phenylalanylalanine	2
<b>Peptide</b>	<i>Dipeptide</i>	phenylalanylaspargate	2
<b>Peptide</b>	<i>Dipeptide</i>	phenylalanylglycine	2
<b>Peptide</b>	<i>Dipeptide</i>	prolylalanine	2
<b>Peptide</b>	<i>Dipeptide</i>	prolylglycine	2
<b>Peptide</b>	<i>Dipeptide</i>	prolylphenylalanine	2
<b>Peptide</b>	<i>Dipeptide</i>	threonylleucine	2
<b>Peptide</b>	<i>Dipeptide</i>	tyrosylglutamate	2
<b>Peptide</b>	<i>Dipeptide</i>	valylaspargate	2
<b>Peptide</b>	<i>Dipeptide</i>	valylglutamate	2
<b>Peptide</b>	<i>Dipeptide</i>	valylglutamine	2
<b>Peptide</b>	<i>Dipeptide</i>	valylglycine	2
<b>Peptide</b>	<i>Dipeptide</i>	valylleucine	2
<b>Lipid</b>	<i>Eicosanoid</i>	12-HEPE	2
<b>Lipid</b>	<i>Eicosanoid</i>	12-HETE	2
<b>Carbohydrate</b>	<i>Glycolysis, Gluconeogenesis, and Pyruvate Metabolism</i>	lactate	2
<b>Amino Acid</b>	<i>Methionine, Cysteine, SAM and Taurine Metabolism</i>	S-adenosylhomocysteine (SAH)	2
<b>Amino Acid</b>	<i>Methionine, Cysteine, SAM and Taurine Metabolism</i>	taurine	2
<b>Nucleotide</b>	<i>Purine Metabolism, (Hypo)Xanthine/Inosine containing</i>	hypoxanthine	2
<b>Nucleotide</b>	<i>Purine Metabolism, (Hypo)Xanthine/Inosine containing</i>	xanthine	2
<b>Nucleotide</b>	<i>Purine Metabolism, (Hypo)Xanthine/Inosine containing</i>	xanthosine	2
<b>NA</b>	NA	X - 11261	3
<b>NA</b>	NA	X - 11478	3
<b>NA</b>	NA	X - 11521	3
<b>NA</b>	NA	X - 11949	3
<b>NA</b>	NA	X - 12742	3
<b>NA</b>	NA	X - 12802	3
<b>NA</b>	NA	X - 12824	3
<b>NA</b>	NA	X - 12855	3
<b>NA</b>	NA	X - 12860	3
<b>NA</b>	NA	X - 13743	3
<b>NA</b>	NA	X - 14939	3
<b>NA</b>	NA	X - 15486	3
<b>NA</b>	NA	X - 16397	3
<b>NA</b>	NA	X - 16570	3
<b>NA</b>	NA	X - 16580	3
<b>NA</b>	NA	X - 17001	3
<b>NA</b>	NA	X - 17138	3
<b>NA</b>	NA	X - 18888	3
<b>NA</b>	NA	X - 18921	3
<b>Lipid</b>	<i>Fatty Acid Metabolism(Acyl Carnitine)</i>	acetylcarnitine	3
<b>Lipid</b>	<i>Fatty Acid Metabolism(Acyl Carnitine)</i>	hydroxybutyrylcarnitine*	3
<b>Lipid</b>	<i>Fatty Acid, Monohydroxy</i>	3-hydroxyoctanoate	3
<b>Lipid</b>	<i>Ketone Bodies</i>	3-hydroxybutyrate (BHBA)	3
<b>NA</b>	NA	X - 15664	4
<b>NA</b>	NA	X - 16932	4
<b>NA</b>	NA	X - 16938	4
<b>NA</b>	NA	X - 17137	4
<b>NA</b>	NA	X - 18752	4

**Note:**

NA: Not applicable, compound not identified; \* indicates compounds with level 3 identity confidence (lack authenticated standards but had characteristics correlated with known metabolites).