

# Supplementary tables and figures:

**Table S1.** Weakly transferred metabolites ( $0.1 < R \leq 0.3$ ) with associated biochemical taxonomy and estimated correlations.

Biochemical	Taxonomy	$R_{m24-m1}$	$R_{m1-c}$	$R_{m24-c}$
beta-hydroxyisovalerylcarnitine	Amino Acid	0.42	0.30	0.35
theobromine	Xenobiotics	0.26	0.27	0.26
arachidonoylcarnitine (C20:4)	Lipid	0.41	0.23	0.13
carnitine	Lipid	0.27	0.18	0.23
docosahexaenoate (DHA; 22:6n3)	Lipid	0.09	0.18	0.02
creatinine	Amino Acid	0.50	0.17	0.17
5,6-dihydrouridine	Nucleotide	0.36	0.17	0.09
hexanoylcarnitine (C6)	Lipid	0.29	0.16	0.18
1-methylhistidine	Amino Acid	0.03	0.15	0.10
N-acetylmethionine	Amino Acid	0.20	0.14	0.09
2-aminoheptanoate	Lipid	0.33	0.14	0.11
N2-acetyl.N6-methyllysine	Amino Acid	0.83	0.14	0.07
3-(4-hydroxyphenyl)lactate (HPLA)	Amino Acid	0.44	0.13	0.09
3-methoxytyrosine	Amino Acid	0.40	0.13	0.14
acetylcarnitine (C2)	Lipid	0.28	0.13	0.15
gamma-glutamylphenylalanine	Peptide	0.30	0.13	0.10
palmitoleoylcarnitine (C16:1)*	Lipid	0.16	0.13	0.07
phenylalanine	Amino Acid	0.25	0.13	0.10
arginine	Amino Acid	0.31	0.12	0.08
caproate (6:0)	Lipid	0.16	0.12	0.02
propionylcarnitine (C3)	Lipid	0.31	0.12	0.16
aconitate [cis or trans]	Energy	0.22	0.11	0.02
palmitoylcarnitine (C16)	Lipid	0.28	0.11	0.09
glutamine conjugate of C6H10O2 (1)*	Partially Characterized Molecules	0.30	0.11	0.07
citrate	Energy	0.27	0.11	0.04
cis-4-decenoylcarnitine (C10:1)	Lipid	0.25	0.11	0.02
N-acetylcarnosine	Amino Acid	0.54	0.11	0.05
metronidazole	Xenobiotics	0.00	0.11	-0.01

\*: putative annotation.

**Table S2.** Non-transferred metabolites ( $R \leq 0.1$ ) with associated biochemical taxonomy and estimated correlations.

Biochemical	Taxonomy	$R_{m24-m1}$	$R_{m1-c}$	$R_{m24-c}$
5,6-dihydrothymine	Nucleotide	0.40	0.10	-0.04
hexanoylglutamine	Lipid	0.23	0.10	0.24
(R)-3-hydroxybutyrylcarnitine	Lipid	0.09	0.10	0.08
lysine	Amino Acid	0.30	0.09	0.04
theanine	Xenobiotics	0.54	0.09	0.04
2-aminooctanoate	Lipid	0.21	0.09	0.09
biliverdin	Cofactors and Vitamins	0.45	-0.09	-0.06
glutamine conjugate of C6H10O2 (2)*	Partially Characterized Molecules	0.23	0.09	0.00
linoleoylcarnitine (C18:2)*	Lipid	0.31	0.09	0.05
hydroxycotinine	Xenobiotics	0.75	-0.09	0.00
gamma-glutamylglutamate	Peptide	0.24	0.09	0.00
methyl glucopyranoside (alpha + beta)	Xenobiotics	0.63	-0.09	-0.02
3-methylcytidine	Nucleotide	0.61	0.09	0.06
gamma-glutamylglutamine	Peptide	0.26	-0.09	-0.01
suberoylcarnitine (C8-DC)	Lipid	0.22	0.09	0.02
linoleate (18:2n6)	Lipid	0.12	-0.08	-0.09
3-methoxycatechol sulfate (2)	Xenobiotics	0.29	0.08	0.03
lidocaine	Xenobiotics	0.03	0.08	0.01
octadecanedioylcarnitine (C18-DC)*	Lipid	0.44	0.08	0.02
thiopropine	Xenobiotics	0.27	0.08	-0.01
undecenoylcarnitine (C11:1)	Lipid	0.25	0.08	0.14
tryptophan	Amino Acid	0.32	0.08	0.09
arabitol/xylitol	Carbohydrate	0.26	0.08	0.08
hydroxy-N6,N6,N6-trimethyllysine*	Amino Acid	0.24	0.08	0.09
N2,N2-dimethylguanosine	Nucleotide	0.56	0.07	0.13
3-hydroxyhexanoate	Lipid	0.10	0.07	-0.01
octadecenedioylcarnitine (C18:1-DC)*	Lipid	0.29	0.07	0.06
7-methylguanine	Nucleotide	0.59	0.07	0.16
gamma-glutamylvaline	Peptide	0.39	0.07	0.05
cysteine	Amino Acid	0.43	-0.07	-0.06
cortisol	Lipid	0.30	-0.07	-0.01
3,4-methyleneheptanoate	Xenobiotics	0.22	0.07	0.03
5-hydroxylysine	Amino Acid	0.13	-0.07	0.00
2-ketocaprylate	Amino Acid	0.10	0.07	0.03
myristoleoylcarnitine (C14:1)*	Lipid	0.07	0.07	0.04
isovalerylcarnitine (C5)	Amino Acid	0.32	0.07	-0.03
N-acetylphenylalanine	Amino Acid	0.62	0.07	0.12
nisinate (24:6n3)	Lipid	0.28	-0.07	-0.02
3-methylcrotonylglycine	Amino Acid	0.38	-0.06	-0.09
1-carboxyethylvaline	Amino Acid	0.22	0.06	0.05
dihydroorotate	Nucleotide	0.28	-0.06	-0.01
dimethylarginine (ADMA + SDMA)	Amino Acid	0.41	0.06	0.07
methionine sulfone	Amino Acid	0.65	0.06	0.02
N-acetyl-1-methylhistidine*	Amino Acid	0.61	0.06	0.03
3-hydroxybutyrylglycine	Lipid	0.21	-0.06	-0.06
tridecenedioate (C13:1-DC)*	Lipid	0.27	0.06	-0.03

succinylcarnitine (C4-DC)	Energy	0.48	0.06	0.17
prolylglycine	Peptide	0.19	0.06	0.06
gamma-glutamylglycine	Peptide	0.54	-0.06	-0.03
N-formylmethionine	Amino Acid	0.63	0.06	0.09
2-hydroxylaurate	Lipid	0.28	0.05	-0.01
4-guanidinobutanoate	Amino Acid	0.31	-0.05	0.00
alpha-ketoglutarate	Energy	0.44	0.05	0.04
spermine	Amino Acid	-0.01	0.05	0.02
2-hydroxypalmitate	Lipid	0.07	0.05	-0.01
glutamine	Amino Acid	0.36	0.05	0.05
2-hydroxyibuprofen	Xenobiotics	0.18	0.05	-0.07
4-hydroxyhippurate	Xenobiotics	0.17	-0.05	-0.02
3-methylhistidine	Amino Acid	0.02	0.05	0.02
6-hydroxyindole sulfate	Xenobiotics	0.41	-0.05	0.01
cytosine	Nucleotide	0.15	-0.05	-0.05
2-aminoadipate	Amino Acid	0.49	-0.05	-0.01
3-hydroxykynurenine	Amino Acid	0.37	0.05	0.03
glycine conjugate of C10H14O2 (1)*	Partially Characterized Molecules	0.33	0.05	0.03
7-HOCA	Lipid	0.27	0.05	0.07
3-(N-acetyl-L-cystein-S-yl) acetaminophen	Xenobiotics	-0.02	-0.05	0.01
N-acetyltryptophan	Amino Acid	0.86	-0.05	-0.03
2R,3R-dihydroxybutyrate	Lipid	0.33	0.05	0.02
propionylglycine (C3)	Lipid	0.48	0.05	-0.02
S-methylmethionine	Amino Acid	0.08	-0.05	-0.04
isovalerylglycine	Amino Acid	0.41	0.05	-0.02
iminodiacetate (IDA)	Xenobiotics	0.23	0.05	0.06
quinat	Xenobiotics	0.58	0.05	0.00
palmitoyl ethanolamide	Lipid	0.16	0.05	-0.04
guanosine	Nucleotide	-0.01	-0.05	0.00
(14 or 15)-methylpalmitate (a17:0 or i17:0)	Lipid	0.09	0.05	0.02
3-methyl-2-oxobutyrate	Amino Acid	0.30	0.05	-0.01
histidine	Amino Acid	0.24	-0.05	-0.05
proline	Amino Acid	0.30	0.05	0.02
gamma-glutamyl-2-aminobutyrate	Peptide	0.10	-0.04	0.02
5-methylthioadenosine (MTA)	Amino Acid	0.24	0.04	0.00
N6-acetyllysine	Amino Acid	0.48	0.04	0.01
N-acetylleucine	Amino Acid	0.18	-0.04	0.05
(2 or 3)-decenoate (10:1n7 or n8)	Lipid	0.12	0.04	0.03
4-hydroxy-2-oxoglutaric acid	Lipid	0.40	-0.04	0.01
3beta-hydroxy-5-cholestenoate	Lipid	0.33	-0.04	-0.02
alpha-ketobutyrate	Amino Acid	0.25	-0.04	-0.08
thymol sulfate	Xenobiotics	0.04	-0.04	0.00
phenyllactate (PLA)	Amino Acid	0.24	-0.04	-0.03
gamma-glutamylalanine	Peptide	0.22	-0.04	-0.06
hydroxyproline	Amino Acid	0.15	-0.04	0.02
N-acetyl-2-aminooctanoate*	Lipid	0.27	-0.04	0.00
metoprolol acid metabolite*	Xenobiotics	0.26	0.04	0.03
valylleucine	Peptide	0.04	0.04	0.01
allantoin	Nucleotide	0.27	-0.04	0.02

cinnamoylglycine	Xenobiotics	0.33	0.04	0.00
kynurenine	Amino Acid	0.32	0.04	0.02
alpha-hydroxyisocaproate	Amino Acid	0.23	-0.04	-0.08
N-formylanthranilic acid	Amino Acid	0.46	0.04	-0.03
leucine	Amino Acid	0.25	0.04	0.01
glycerol 3-phosphate	Lipid	0.19	-0.04	0.02
6-oxopiperidine-2-carboxylate	Amino Acid	0.36	0.04	-0.04
glycerophosphoethanolamine	Lipid	0.13	-0.04	0.04
choline	Lipid	0.26	0.04	0.05
oleoylcarnitine (C18)	Lipid	0.28	-0.04	0.03
spermidine	Amino Acid	0.00	0.04	0.04
dodecanedioate (C12)	Lipid	-0.01	-0.03	-0.02
citalopram propionate*	Xenobiotics	0.65	0.03	0.01
3-indoleglyoxylic acid	Xenobiotics	0.63	0.03	0.01
4-hydroxyphenylacetate	Amino Acid	0.39	0.03	-0.08
methyl indole-3-acetate	Xenobiotics	0.37	-0.03	0.03
deoxycholic acid (12 or 24)-sulfate*	Lipid	0.37	-0.03	0.11
2-hydroxy-4-(methylthio)butanoic acid	Amino Acid	0.25	-0.03	0.17
3-phenylpropionate (hydrocinnamate)	Xenobiotics	0.40	-0.03	-0.05
N6,N6,N6-trimethyllysine	Amino Acid	0.24	-0.03	0.03
gamma-glutamylhistidine	Peptide	0.28	-0.03	-0.02
2-hydroxyacetaminophen sulfate*	Xenobiotics	0.08	0.03	0.05
phenylalanylhydroxyproline*	Peptide	0.21	0.03	0.04
vanillactate	Amino Acid	0.10	0.03	-0.03
3-hydroxydecanoate	Lipid	0.09	-0.03	-0.01
glucuronate	Carbohydrate	0.30	-0.03	-0.01
glutarate (C5-DC)	Lipid	0.35	0.03	-0.03
indoleacetate	Amino Acid	0.43	0.03	0.02
pipecolate	Amino Acid	0.52	-0.03	-0.02
16-hydroxypalmitate	Lipid	0.13	-0.03	0.11
valine	Amino Acid	0.11	0.03	0.00
gamma-glutamyltyrosine	Peptide	0.19	-0.03	-0.07
N-oleoylserine	Lipid	0.42	0.03	0.04
dihydroferulate	Xenobiotics	0.23	-0.03	-0.02
butyrylcarnitine (C4)	Lipid	0.54	0.03	0.06
asparagine	Amino Acid	0.34	0.03	-0.01
threonine	Amino Acid	0.38	0.03	0.01
inosine 5'-monophosphate (IMP)	Nucleotide	0.15	0.03	0.08
3-amino-2-piperidone	Amino Acid	0.35	-0.03	0.05
3-methylglutaconate	Amino Acid	0.76	-0.03	-0.03
gamma-glutamylthreonine	Peptide	0.35	0.03	0.00
N1-Methyl-4-pyridone-3-carboxamide	Cofactors and Vitamins	0.23	-0.03	-0.01
alpha-ketoglutaramate*	Amino Acid	0.29	-0.03	0.02
betaine	Amino Acid	0.26	-0.03	-0.05
2-oxoarginine*	Amino Acid	0.26	0.03	0.03
pyridoxate	Cofactors and Vitamins	0.27	-0.03	0.06
6-bromotryptophan	Amino Acid	0.58	0.03	0.04
3-hydroxyhippurate	Xenobiotics	0.25	-0.03	0.03
methionine sulfoxide	Amino Acid	0.23	0.03	0.05

phosphoethanolamine (PE)	Lipid	0.24	0.03	-0.02
uracil	Nucleotide	0.13	-0.03	0.05
linolenate (18:3n3 or 3n6)	Lipid	0.50	-0.03	0.08
indolepropionate	Amino Acid	0.38	-0.03	0.19
N-palmitoylglycine	Lipid	0.20	-0.03	-0.01
2-piperidinone	Xenobiotics	0.33	0.02	0.08
N-palmitoylserine	Lipid	0.25	0.02	-0.02
glutamate	Amino Acid	0.26	0.02	0.04
1-methyladenosine	Nucleotide	0.49	0.02	0.04
homocitrulline	Amino Acid	0.18	0.02	0.01
3-formylindole	Xenobiotics	0.48	0.02	-0.03
glycine	Amino Acid	0.60	0.02	-0.02
citraconate/glutaconate	Energy	0.45	-0.02	0.02
N6,N6-dimethyllysine	Amino Acid	0.85	-0.02	-0.04
N,N-dimethylalanine	Amino Acid	0.53	-0.02	-0.05
tyrosine	Amino Acid	0.28	0.02	0.05
1,2,3-benzenetriol sulfate (2)	Xenobiotics	0.20	-0.02	-0.02
3-methylglutarylcarnitine (2)	Amino Acid	0.73	0.02	-0.01
picolinoylglycine	Lipid	0.14	-0.02	-0.01
1-myristoylglycerol (14:0)	Lipid	0.11	-0.02	-0.01
ornithine	Amino Acid	0.27	0.02	0.01
hydroxyasparagine	Amino Acid	0.63	-0.02	0.03
taurine	Amino Acid	0.24	0.02	0.06
N-acetylthearine	Xenobiotics	0.13	0.02	0.09
indolelactate	Amino Acid	0.49	0.02	-0.04
N-acetylserine	Amino Acid	0.60	-0.02	-0.05
arachidonate (20:4n6)	Lipid	0.10	-0.02	0.07
1-carboxyethylphenylalanine	Amino Acid	0.19	-0.02	-0.09
heptenedioate (C7:1-DC)*	Lipid	0.29	0.02	-0.09
1,3,7-trimethylurate	Xenobiotics	0.44	-0.02	-0.01
N-acetylglucosamine/N-acetylgalactosamine	Carbohydrate	0.12	-0.02	-0.11
tartarate	Xenobiotics	0.21	-0.02	-0.06
caprate (10:0)	Lipid	0.09	-0.02	0.00
13-HODE + 9-HODE	Lipid	0.14	-0.02	0.08
3-hydroxyhexanoylcarnitine (1)	Lipid	0.14	0.02	0.05
N-acetylcitrulline	Amino Acid	0.58	-0.01	-0.03
21-hydroxypregnenolone disulfate	Lipid	0.67	0.01	-0.03
cortisone	Lipid	0.23	0.01	0.04
N6-carboxymethyllysine	Carbohydrate	0.27	-0.01	-0.04
erythritol	Xenobiotics	0.05	-0.01	-0.04
N,N,N-trimethyl-alanylproline betaine (TMAP)	Amino Acid	0.21	0.01	0.05
phenylpyruvate	Amino Acid	0.31	-0.01	-0.07
3-phosphoglycerate	Carbohydrate	0.09	0.01	0.10
12-HETE	Lipid	0.04	-0.01	-0.02
gluconate	Xenobiotics	0.46	0.01	-0.02
N-(2-furoyl)glycine	Xenobiotics	0.29	-0.01	0.10
creatine	Amino Acid	0.29	0.01	0.04
8-methoxykynurenate	Amino Acid	0.41	0.01	0.09
sphingosine	Lipid	0.31	-0.01	-0.04

palmitamide (16:0)	Lipid	0.45	-0.01	0.02
citrulline	Amino Acid	0.33	0.01	-0.02
indolin-2-one	Xenobiotics	0.47	-0.01	0.00
O-sulfo-L-tyrosine	Xenobiotics	0.55	0.01	0.02
eicosapentaenoate (EPA; 20:5n3)	Lipid	0.10	-0.01	-0.03
pyroglutamine*	Amino Acid	0.18	0.01	0.03
vanillic acid glycine	Xenobiotics	0.08	-0.01	-0.04
glycoursodeoxycholate	Lipid	0.11	-0.01	0.00
sphinganine	Lipid	0.37	0.01	-0.08
trans-urocanate	Amino Acid	0.14	0.01	0.02
S-allylcysteine	Xenobiotics	0.10	0.01	0.02
trigonelline (N'-methylnicotinate)	Cofactors and Vitamins	0.54	-0.01	0.03
phosphocholine	Lipid	0.22	-0.01	0.00
1-methylnicotinamide	Cofactors and Vitamins	0.21	0.01	0.04
palmitate (16:0)	Lipid	0.12	-0.01	0.07
2-hydroxybutyrate/2-hydroxyisobutyrate	Amino Acid	0.31	0.01	-0.01
azelate (C9-DC)	Lipid	0.25	0.01	0.02
dodecadienoate (12:2)*	Lipid	0.19	0.01	-0.03
lanthionine	Amino Acid	0.22	0.01	0.01
lactose	Carbohydrate	0.28	-0.01	-0.03
nicotinamide	Cofactors and Vitamins	0.07	-0.01	0.02
pantothenate (Vitamin B5)	Cofactors and Vitamins	0.58	-0.01	-0.11
laurate (12:0)	Lipid	0.13	-0.01	-0.02
ectoine	Xenobiotics	0.06	-0.01	0.01
dodecenedioate (C12:1-DC)*	Lipid	0.21	-0.01	0.01
methionine	Amino Acid	0.11	-0.01	0.03
3-(3-hydroxyphenyl)propionate	Xenobiotics	0.25	0.00	0.02
(N(1) + N(8))-acetylspermidine	Amino Acid	0.39	0.00	0.02
2-hydroxydecanoate	Lipid	0.20	0.00	-0.06
pregnenolone sulfate	Lipid	0.50	0.00	0.06
prolylhydroxyproline	Amino Acid	0.33	0.00	0.12
tetradecadienoate (14:2)*	Lipid	0.12	0.00	0.04
4-acetamidobutanoate	Amino Acid	0.31	0.00	0.03
N1-Methyl-2-pyridone-5-carboxamide	Cofactors and Vitamins	0.28	0.00	-0.01
cysteine-glutathione disulfide	Amino Acid	0.10	0.00	0.08
salicylate	Xenobiotics	0.00	0.00	-0.01
1-linoleoyl-GPE (18:2)*	Lipid	0.11	0.00	0.02
AMP	Nucleotide	0.28	0.00	0.12
3-hydroxystachydrine*	Xenobiotics	0.27	-0.21	0.18
dimethylglycine	Amino Acid	-0.60	-0.11	-0.06

\*: putative annotation.

**Table S3.** List of metabolites identified with associated biochemical classes.

Super Pathway	Sub Pathway	Biochemical
Amino Acid	Alanine and Aspartate Metabolism	asparagine
		hydroxyasparagine
		N,N-dimethylalanine
	Creatine Metabolism	creatine
		creatinine
	Glutamate Metabolism	alpha-ketoglutamamate*
		glutamate
		glutamine
		pyroglutamine*
	Glutathione Metabolism	2-hydroxybutyrate/2-hydroxyisobutyrate
		cysteine-glutathione disulfide
	Glycine, Serine and Threonine Metabolism	betaine
		dimethylglycine
		glycine
		N-acetylserine
		threonine
	Guanidino and Acetamido Metabolism	4-guanidinobutanoate
		1-methylhistidine
		3-methylhistidine
	Histidine Metabolism	histidine
		N-acetyl-1-methylhistidine*
		N-acetylcarnosine
		trans-uocanate
		1-carboxyethylvaline
	Leucine, Isoleucine and Valine Metabolism	2-ketocaprylate
		3-methyl-2-oxobutyrate
		3-methylcrotonylglycine
		3-methylglutaconate
		3-methylglutaryl carnitine (2)
		alpha-hydroxyisocaproate
		beta-hydroxyisovaleroyl carnitine
		isovaleryl carnitine (C5)
		isovaleryl glycine
		leucine
		N-acetyl leucine
		valine
	Lysine Metabolism	2-aminoadipate
		5-hydroxylysine
		6-oxopiperidine-2-carboxylate
		hydroxy-N6,N6,N6-trimethyllysine*
		lysine
		N,N,N-trimethyl-5-aminovalerate
		N2-acetyl,N6-methyllysine
		N6,N6,N6-trimethyllysine
		N6,N6-dimethyllysine

	N6-acetyllysine
	N6-methyllysine
	pipecolate
Methionine, Cysteine, SAM and Taurine Metabolism	2-hydroxy-4-(methylthio)butanoic acid
	alpha-ketobutyrate
	cysteine
	lanthionine
	methionine
	methionine sulfone
	methionine sulfoxide
	N-acetylmethionine
	N-formylmethionine
	S-methylmethionine
	taurine
Phenylalanine Metabolism	1-carboxyethylphenylalanine
	4-hydroxyphenylacetate
	N-acetylphenylalanine
	phenylalanine
	phenyllactate (PLA)
Polyamine Metabolism	phenylpyruvate
	(N(1) + N(8))-acetylspermidine
	4-acetamidobutanoate
	5-methylthioadenosine (MTA)
	spermidine
Tryptophan Metabolism	spermine
	3-hydroxykynurenine
	6-bromotryptophan
	8-methoxykynurenate
	indoleacetate
	indolelactate
	indolepropionate
	kynurenine
	N-acetyltryptophan
	N-formylanthranilic acid
	tryptophan
Tyrosine Metabolism	tryptophan betaine
	3-(4-hydroxyphenyl)lactate (HPLA)
	3-methoxytyrosine
	tyrosine
Urea cycle; Arginine and Proline Metabolism	vanillactate
	2-oxoarginine*
	3-amino-2-piperidone
	arginine
	citrulline
	dimethylarginine (ADMA + SDMA)
	homoarginine
	homocitrulline



Carbohydrate	Advanced Glycation End-product	hydroxyproline
		N,N,N-trimethyl-alanylproline betaine (TMAP)
		N-acetylcitrulline
		ornithine
		proline
	Aminosugar Metabolism	prolylhydroxyproline
		N6-carboxymethyllysine
		glucuronate
		N-acetylglucosamine/N-acetylgalactosamine
		lactose
Cofactors and Vitamins	Disaccharides and Oligosaccharides	lactose
	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	3-phosphoglycerate
	Pentose Metabolism	arabitol/xylitol
	Hemoglobin and Porphyrin Metabolism	biliverdin
	Nicotinate and Nicotinamide Metabolism	1-methylnicotinamide
		N1-Methyl-2-pyridone-5-carboxamide
		N1-Methyl-4-pyridone-3-carboxamide
		nicotinamide
		trigonelline (N'-methylnicotinate)
	Pantothenate and CoA Metabolism	pantothenate (Vitamin B5)
Energy	Vitamin B6 Metabolism	pyridoxate
	TCA Cycle	aconitate [cis or trans]
		alpha-ketoglutarate
		citraconate/glutaconate
		citrate
		succinylcarnitine (C4-DC)
Lipid	Carnitine Metabolism	carnitine
	Corticosteroids	cortisol
	Corticosteroids	cortisone
	Eicosanoid	12-HETE
	Endocannabinoid	N-oleoylserine
		N-palmitoylserine
		palmitoyl ethanolamide
	Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)	octadecanedioylcarnitine (C18-DC)*
		octadecenedioylcarnitine (C18:1-DC)*
		suberoylcarnitine (C8-DC)
	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	(R)-3-hydroxybutyrylcarnitine
		3-hydroxyhexanoylcarnitine (1)
	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	palmitoylcarnitine (C16)
	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	hexanoylcarnitine (C6)
	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	cis-4-decenoylcarnitine (C10:1)
		myristoleoylcarnitine (C14:1)*
		oleoylcarnitine (C18)
		palmitoleoylcarnitine (C16:1)*

	undecenoylcarnitine (C11:1)
Fatty Acid Metabolism (Acyl Carnitine. Polyunsaturated)	arachidonoylcarnitine (C20:4)
	linoleoylcarnitine (C18:2)*
Fatty Acid Metabolism (Acyl Carnitine. Short Chain)	acetylcarnitine (C2)
Fatty Acid Metabolism (Acyl Glutamine)	hexanoylglutamine
	3-hydroxybutyrylglycine
Fatty Acid Metabolism (Acyl Glycine)	N-palmitoylglycine
	picolinoylglycine
Fatty Acid Metabolism (also BCAA Metabolism)	butyrylcarnitine (C4)
	propionylcarnitine (C3)
	propionylglycine (C3)
Fatty Acid. Amide	palmitamide (16:0)
Fatty Acid. Amino	2-aminoheptanoate
	2-aminooctanoate
	N-acetyl-2-aminooctanoate*
Fatty Acid. Branched	(14 or 15)-methylpalmitate (a17:0 or i17:0)
Fatty Acid. Dicarboxylate	3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)
	4-hydroxy-2-oxoglutaric acid
	azelate (C9-DC)
	dodecadienoate (12:2)*
	dodecanedioate (C12)
	dodecenedioate (C12:1-DC)*
	glutarate (C5-DC)
	heptenedioate (C7:1-DC)*
	tridecenedioate (C13:1-DC)*
Fatty Acid. Dihydroxy	2R,3R-dihydroxybutyrate
Fatty Acid. Monohydroxy	13-HODE + 9-HODE
	16-hydroxypalmitate
	2-hydroxydecanoate
	2-hydroxylaurate
	2-hydroxypalmitate
	3-hydroxydecanoate
	3-hydroxyhexanoate
Glycerolipid Metabolism	glycerol 3-phosphate
Long Chain Polyunsaturated Fatty Acid (n3 and n6)	arachidonate (20:4n6)
	docosahexaenoate (DHA; 22:6n3)
	eicosapentaenoate (EPA; 20:5n3)
	linoleate (18:2n6)
	linolenate (18:3n3 or 3n6)
	nisinate (24:6n3)
	tetradecadienoate (14:2)*
Long Chain Saturated Fatty Acid	palmitate (16:0)
Lysophospholipid	1-linoleoyl-GPE (18:2)*
Medium Chain Fatty Acid	(2 or 3)-decenoate (10:1n7 or n8)
	caprate (10:0)

		caproate (6:0)
		laurate (12:0)
	Monoacylglycerol	1-myristoylglycerol (14:0)
	Phospholipid Metabolism	choline
		glycerophosphoethanolamine
		phosphocholine
		phosphoethanolamine (PE)
	Pregnenolone Steroids	21-hydroxypregnenolone disulfate
		pregnenolone sulfate
	Secondary Bile Acid Metabolism	deoxycholic acid (12 or 24)-sulfate*
		glycoursodeoxycholate
	Sphingolipid Synthesis	sphinganine
	Sphingosines	sphingosine
	Sterol	3beta-hydroxy-5-cholestenoate
		7-HOCA
Nucleotide	Purine Metabolism. (Hypo)Xanthine/Inosine containing	allantoin
		inosine 5'-monophosphate (IMP)
	Purine Metabolism. Adenine containing	1-methyladenosine
		AMP
	Purine Metabolism. Guanine containing	7-methylguanine
		guanosine
		N2,N2-dimethylguanosine
	Pyrimidine Metabolism. Cytidine containing	3-methylcytidine
		cytosine
	Pyrimidine Metabolism. Orotate containing	dihydroorotate
Peptide	Dipeptide	5,6-dihydrothymine
		5,6-dihydrouridine
		uracil
	Gamma-glutamyl Amino Acid	phenylalanylhydroxyproline*
		prolylglycine
		valylleucine
		gamma-glutamyl-2-aminobutyrate
		gamma-glutamylalanine
		gamma-glutamylglutamate
		gamma-glutamylglutamine
		gamma-glutamylglycine
		gamma-glutamylhistidine
		gamma-glutamylphenylalanine
		gamma-glutamylthreonine
		gamma-glutamyltyrosine
		gamma-glutamylvaline
Xenobiotics	Benzoate Metabolism	3-(3-hydroxyphenyl)propionate
		3-hydroxyhippurate
		3-methoxycatechol sulfate (2)
		3-phenylpropionate (hydrocinnamate)
		4-hydroxyhippurate
	Chemical	1,2,3-benzenetriol sulfate (2)

	6-hydroxyindole sulfate
	ectoine
	iminodiacetate (IDA)
	O-sulfo-L-tyrosine
	thioprolin
Drug - Analgesics. Anesthetics	2-hydroxyacetaminophen sulfate*
	2-hydroxyibuprofen
	3-(N-acetyl-L-cystein-S-yl) acetaminophen
	lidocaine
Drug - Antibiotic	metronidazole
Drug - Cardiovascular	metoprolol acid metabolite*
Drug - Psychoactive	citalopram propionate*
Drug - Topical Agents	salicylate
Food Component/Plant	2-piperidinone
	3,4-methyleneheptanoate
	3-formylindole
	3-hydroxystachydrine*
	3-indoleglyoxylic acid
	cinnamoylglycine
	dihydroferulate
	ergothioneine
	erythritol
	gluconate
	homostachydrine*
	indolin-2-one
	methyl glucopyranoside (alpha + beta)
	methyl indole-3-acetate
	N-(2-furoyl)glycine
	N-acetyltheanine
	quinate
	S-allylcysteine
	stachydrine
	tartarate
	theanine
	thymol sulfate
	vanillic acid glycine
Tobacco Metabolite	cotinine
	hydroxycotinine
Xanthine Metabolism	1,3,7-trimethylurate
	caffeine
	paraxanthine
	theobromine
Partially Characterized Molecules	glutamine conjugate of C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> (1)*
	glutamine conjugate of C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> (2)*
	glycine conjugate of C <sub>10</sub> H <sub>14</sub> O <sub>2</sub> (1)*

\*: putative annotation.

**Table S4.** PLS-R model of metabolites reported. Pathway indicates which metabolites from the mothers were used in the model. w24=plasma from mothers at 24 weeks of pregnancy (N=664). w1=plasma from mothers 1 week postpartum (N=661). LV=number of latent variables included in the model.

Biochemical	Pathway	Mothers	LV	R <sup>2</sup> Cal	R <sup>2</sup> CV	RMSE Cal	RMSE CV
3-carboxy-4-methyl-5-propyl-2-furanpropanoate	all	w24	2	0.31	0.00	5.22X10 <sup>-4</sup>	7.75X10 <sup>-3</sup>
	Lipids	w24	2	0.23	0.10	5.50X10 <sup>-4</sup>	6.00X10 <sup>-4</sup>
	Fatty Acid. Dicarboxylate	w24	2	0.25	0.20	5.40X10 <sup>-4</sup>	5.60X10 <sup>-4</sup>
	all	w1	2	0.60	0.49	3.90X10 <sup>-4</sup>	4.40X10 <sup>-4</sup>
	Lipids	w1	2	0.59	0.53	3.90X10 <sup>-4</sup>	4.20X10 <sup>-4</sup>
	Fatty Acid. Dicarboxylate	w1	4	0.76	0.74	3.00X10 <sup>-4</sup>	3.20X10 <sup>-4</sup>
tryptophan betaine	all	w24	4	0.62	0.18	4.60X10 <sup>-4</sup>	7.12X10 <sup>-4</sup>
	Amino Acids	w24	4	0.56	0.35	4.92X10 <sup>-4</sup>	6.06X10 <sup>-4</sup>
	Tryptophan Metabolism	w24	4	0.47	0.43	5.42X10 <sup>-4</sup>	5.63X10 <sup>-4</sup>
	all	w1	2	0.41	0.12	6.18X10 <sup>-4</sup>	7.82X10 <sup>-4</sup>
	Amino Acids	w1	2	0.60	0.44	5.08X10 <sup>-4</sup>	6.05X10 <sup>-4</sup>
	Tryptophan Metabolism	w1	2	0.70	0.68	4.05X10 <sup>-4</sup>	4.18X10 <sup>-4</sup>
ergothioneine	all	w24	11	0.89	0.20	4.60X10 <sup>-5</sup>	1.37X10 <sup>-4</sup>
	Xenobiotics	w24	3	0.51	0.31	9.60X10 <sup>-5</sup>	1.16X10 <sup>-4</sup>
	Food component/ plant	w24	3	0.53	0.45	9.40X10 <sup>-5</sup>	1.02X10 <sup>-4</sup>
	all	w1	2	0.37	0.12	1.09X10 <sup>-4</sup>	1.36X10 <sup>-4</sup>
	Xenobiotics	w1	3	0.49	0.20	9.78X10 <sup>-5</sup>	1.40X10 <sup>-4</sup>
	Food component/ plant	w1	3	0.51	0.43	9.60X10 <sup>-5</sup>	1.04X10 <sup>-4</sup>
N6-methyllysine	all	w24	3	0.59	0.09	1.85X10 <sup>-5</sup>	3.63X10 <sup>-5</sup>
	Amino Acids	w24	3	0.45	0.29	2.14X10 <sup>-5</sup>	2.43X10 <sup>-5</sup>
	Lysin Metabolism	w24	4	0.38	0.35	2.26X10 <sup>-5</sup>	2.31X10 <sup>-5</sup>
	all	w1	2	0.42	0.15	2.22X10 <sup>-5</sup>	2.74X10 <sup>-5</sup>
	Amino Acids	w1	2	0.38	0.27	2.50X10 <sup>-5</sup>	2.49X10 <sup>-5</sup>
	Lysin Metabolism	w1	2	0.37	0.35	2.30X10 <sup>-5</sup>	2.35X10 <sup>-5</sup>
N,N,N-trimethyl-5-aminovalerate	all	w24	2	0.19	0.05	1.20X10 <sup>-3</sup>	1.30X10 <sup>-3</sup>
	Amino Acids	w24	2	0.29	0.13	1.10X10 <sup>-3</sup>	1.20X10 <sup>-3</sup>
	Lysin Metabolism	w24	2	0.31	0.28	1.10X10 <sup>-3</sup>	1.10X10 <sup>-3</sup>
	all	w1	2	0.35	0.07	1.10X10 <sup>-3</sup>	1.40X10 <sup>-3</sup>
	Amino Acids	w1	3	0.43	0.20	9.90X10 <sup>-4</sup>	1.20X10 <sup>-3</sup>
	Lysin Metabolism	w1	3	0.32	0.29	1.10X10 <sup>-3</sup>	1.20X10 <sup>-3</sup>
stachydrine	all	w24	2	0.33	0.12	4.35X10 <sup>-3</sup>	5.15X10 <sup>-3</sup>

	Xenobiotics	w24	2	0.26	0.14	4.58X10 <sup>-3</sup>	5.00X10 <sup>-3</sup>
	Food component/ plant	w24	2	0.21	0.14	4.73X10 <sup>-3</sup>	4.98X10 <sup>-3</sup>
	all	w1	3	0.51	0.23	3.73X10 <sup>-3</sup>	4.82X10 <sup>-3</sup>
	Xenobiotics	w1	2	0.34	0.20	4.33X10 <sup>-3</sup>	4.83X10 <sup>-3</sup>
	Food component/ plant	w1	2	0.30	0.25	4.45X10 <sup>-3</sup>	4.62X10 <sup>-3</sup>
	all	w24	1	0.19	0.06	3.00X10 <sup>-5</sup>	3.00X10 <sup>-5</sup>
<b>homostachydrine*</b>	Xenobiotics	w24	2	0.23	0.05	3.00X10 <sup>-5</sup>	3.70X10 <sup>-5</sup>
	Food component/ plant	w24	2	0.16	0.07	3.20X10 <sup>-5</sup>	3.40X10 <sup>-5</sup>
	all	w1	1	0.20	0.04	3.10X10 <sup>-5</sup>	3.50X10 <sup>-5</sup>
	Xenobiotics	w1	1	0.11	0.03	3.20X10 <sup>-5</sup>	3.60X10 <sup>-5</sup>
	Food component/ plant	w1	2	0.27	0.12	3.00X10 <sup>-5</sup>	3.30X10 <sup>-5</sup>
	all	w24	1	0.18	0.03	2.26X10 <sup>-5</sup>	2.53X10 <sup>-5</sup>
<b>homoarginine</b>	Amino Acids	w24	2	0.36	0.17	2.00X10 <sup>-5</sup>	2.31X10 <sup>-5</sup>
	Urea cycle; Arginine and Proline Metabolism	w24	3	0.29	0.25	2.11X10 <sup>-5</sup>	2.16X10 <sup>-5</sup>
	all	w1	2	0.32	0.02	2.06X10 <sup>-5</sup>	3.13X10 <sup>-5</sup>
	Amino Acids	w1	2	0.27	0.11	2.12X10 <sup>-5</sup>	2.37X10 <sup>-5</sup>
	Urea cycle; Arginine and Proline Metabolism	w1	3	0.21	0.16	2.21X10 <sup>-5</sup>	2.28X10 <sup>-5</sup>
	all	w24	2	0.38	0.00	1.50X10 <sup>-4</sup>	3.70X10 <sup>-3</sup>
<b>paraxanthine</b>	Xenobiotics	w24	2	0.31	0.00	1.60X10 <sup>-4</sup>	1.10X10 <sup>-2</sup>
	Xanthine Metabolism	w24	2	0.23	0.21	1.70X10 <sup>-4</sup>	1.70X10 <sup>-4</sup>
	all	w1	2	0.34	0.06	1.50X10 <sup>-4</sup>	2.00X10 <sup>-4</sup>
	Xenobiotics	w1	2	0.29	0.01	1.60X10 <sup>-4</sup>	3.70X10 <sup>-4</sup>
	Xanthine Metabolism	w1	2	0.21	0.16	1.70X10 <sup>-4</sup>	1.80X10 <sup>-4</sup>
	all	w24	2	0.38	0.00	2.36X10 <sup>-5</sup>	3.70X10 <sup>-3</sup>
<b>cotinine</b>	Xenobiotics	w24	2	0.45	0.01	2.21X10 <sup>-5</sup>	1.00X10 <sup>-3</sup>
	all	w1	2	0.32	0.06	2.40X10 <sup>-5</sup>	2.97X10 <sup>-5</sup>
	Xenobiotics	w1	2	0.22	0.04	2.57X10 <sup>-5</sup>	3.42X10 <sup>-5</sup>
	all	w24	1	0.27	0.09	8.54X10 <sup>-1</sup>	9.70X10 <sup>-1</sup>
<b>caffeine</b>	Xenobiotics	w24	1	0.19	0.07	9.00X10 <sup>-1</sup>	1
	Xanthine Metabolism	w24	1	0.21	0.20	8.80X10 <sup>-1</sup>	8.90X10 <sup>-1</sup>
	all	w1	1	0.24	0.07	8.70X10 <sup>-1</sup>	9.80X10 <sup>-1</sup>
	Xenobiotics	w1	1	0.15	0.07	9.10X10 <sup>-1</sup>	9.70X10 <sup>-1</sup>
	Xanthine Metabolism	w1	1	0.01	0.00	9.90X10 <sup>-1</sup>	1
	all	w24	1	0.19	0.07	9.00X10 <sup>-1</sup>	1

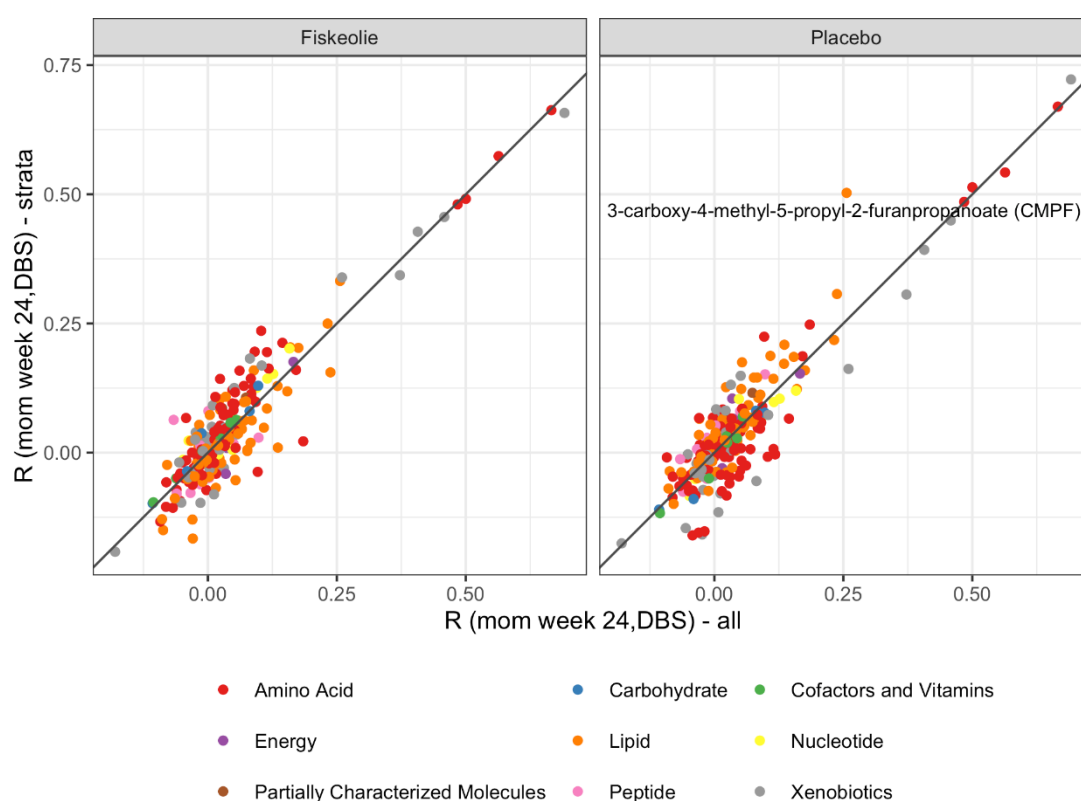
\*: putative annotation.

**Table S5.** Bootstrapped replication results for top 11 metabolites exhibiting vertical transfer.  $R_{m1-c}$  refers to the observed Pearson correlations, with bootstrapped 95% confidence bounds. # Discovery shows the discovery rate at the level of  $R_{m1-c} > 0.3$ , # replication shows the rate of the out of bag replication results at level  $R_{m1-c} > 0.3$  as well as plain significance  $p < 0.05$ . From a total of 1000 bootstraps.

BIOCHEMICAL	$R_{m1-c}$	# Discovery	# replication ( $r > 0.3$ )	# replication ( $p < 0.05$ )
CMPF	0.87 (0.84-0.89)	1000 (100%)	1000 (100%)	1000 (100%)
tryptophan betaine	0.82 (0.71-0.86)	1000 (100%)	1000 (100%)	1000 (100%)
ergothioneine	0.68 (0.61-0.74)	1000 (100%)	1000 (100%)	1000 (100%)
N6-methyllysine	0.6 (0.54-0.65)	1000 (100%)	1000 (100%)	1000 (100%)
N,N,N-trimethyl-5-aminovalerate	0.54 (0.48-0.6)	1000 (100%)	1000 (100%)	1000 (100%)
stachydrine	0.5 (0.43-0.56)	1000 (100%)	1000 (100%)	1000 (100%)
homostachydrine*	0.43 (0.31-0.54)	988 (99%)	941 (95%)	987 (100%)
homoarginine	0.42 (0.34-0.49)	997 (100%)	985 (99%)	997 (100%)
paraxanthine	0.4 (0.32-0.47)	995 (100%)	974 (98%)	995 (100%)
cotinine	0.36 (0.26-0.66)	943 (94%)	771 (82%)	932 (99%)
caffeine	0.35 (0.26-0.44)	867 (87%)	677 (78%)	867 (100%)

\*: putative annotation.

**Figure S1.** Robustness analysis for the transfer results given the fish oil intervention.

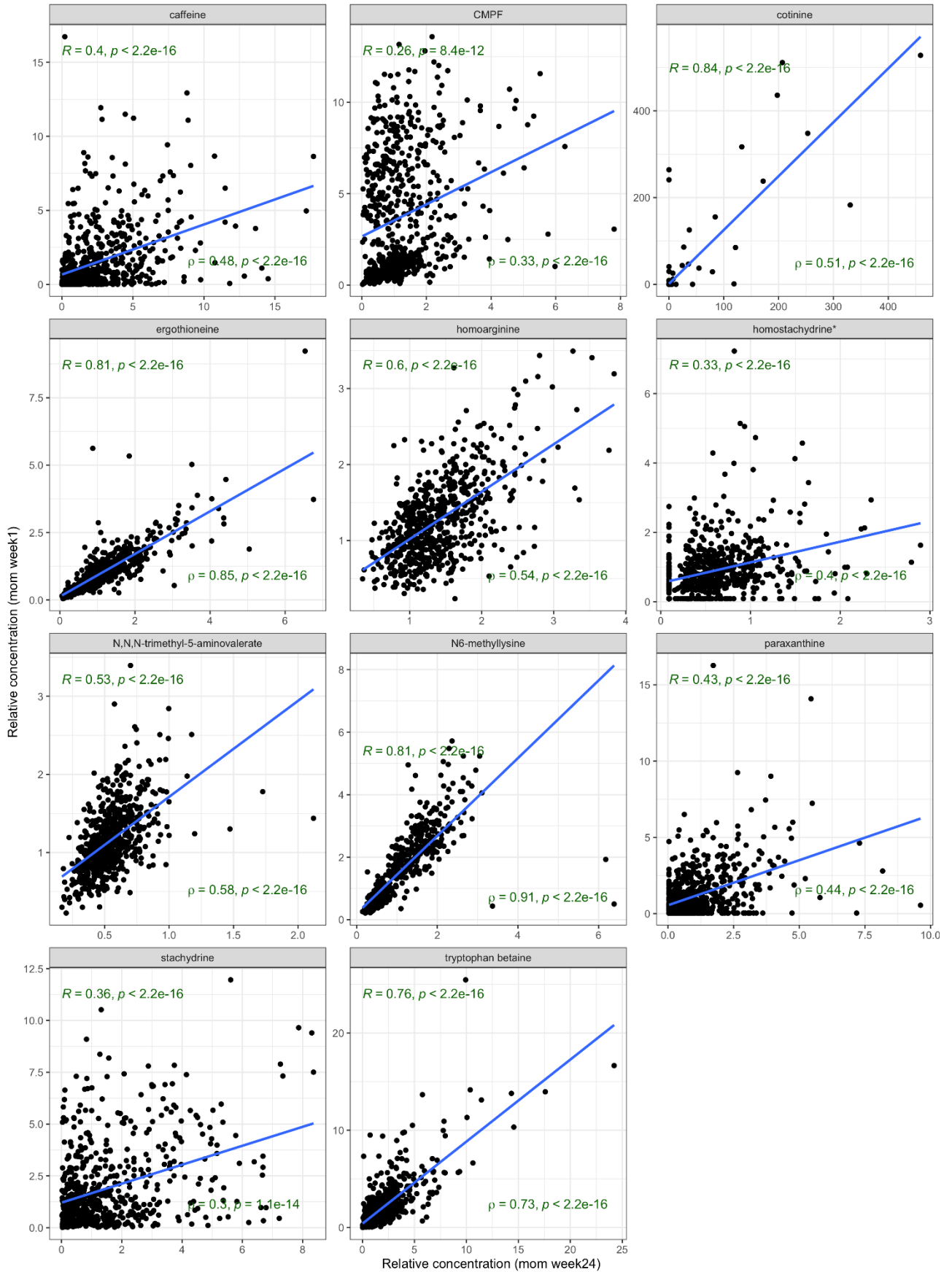


**Figure S2.** Child metabolite level from DBS as function of maternal week 24 mid pregnancy (red) and one week postpartum (blue) blood levels of the 11 metabolites with strong transfer merits ( $R_{m1-c} > 0.3$ ). The correlations denoted  $R$  and  $\rho$  refers to Pearson and Spearman correlation coefficients respectively.

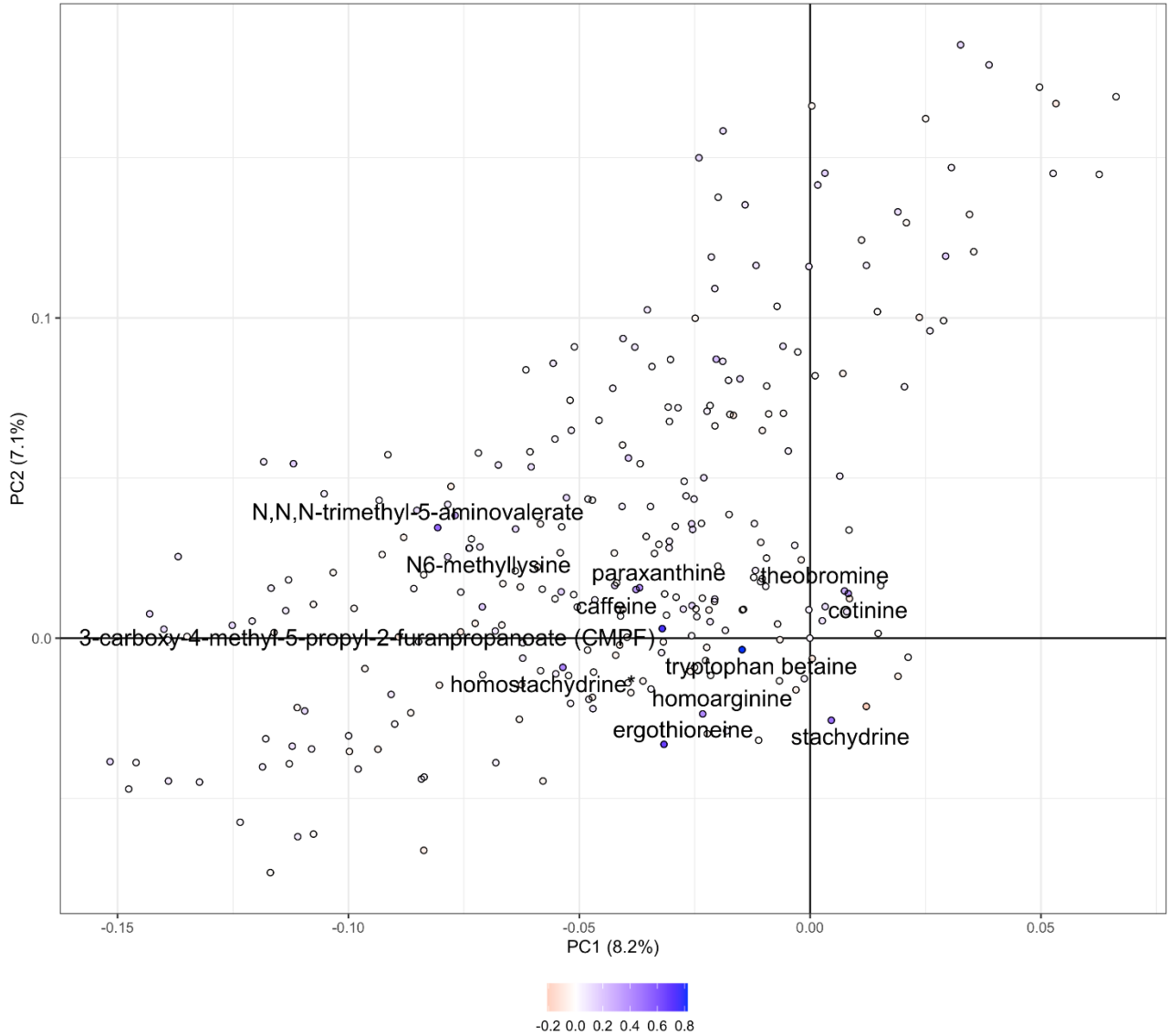




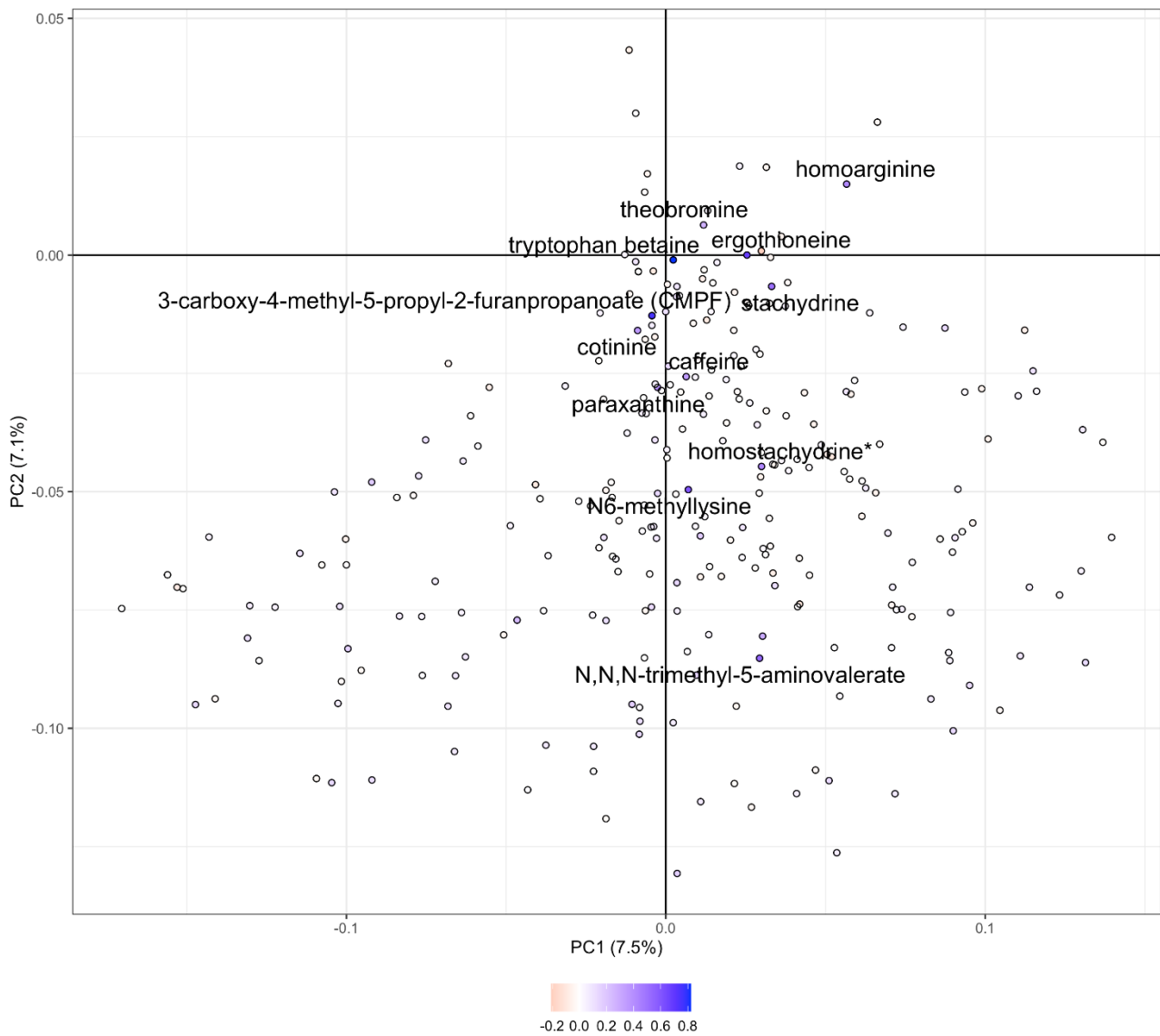
**Figure S3.** Maternal levels of one week postpartum samples versus week 24 mid pregnancy samples of the 11 metabolites with strong transfer merits ( $R_{m1-c} > 0.3$ ). The correlations denoted  $R$  and  $\rho$  refers to Pearson and Spearman correlation coefficients respectively.



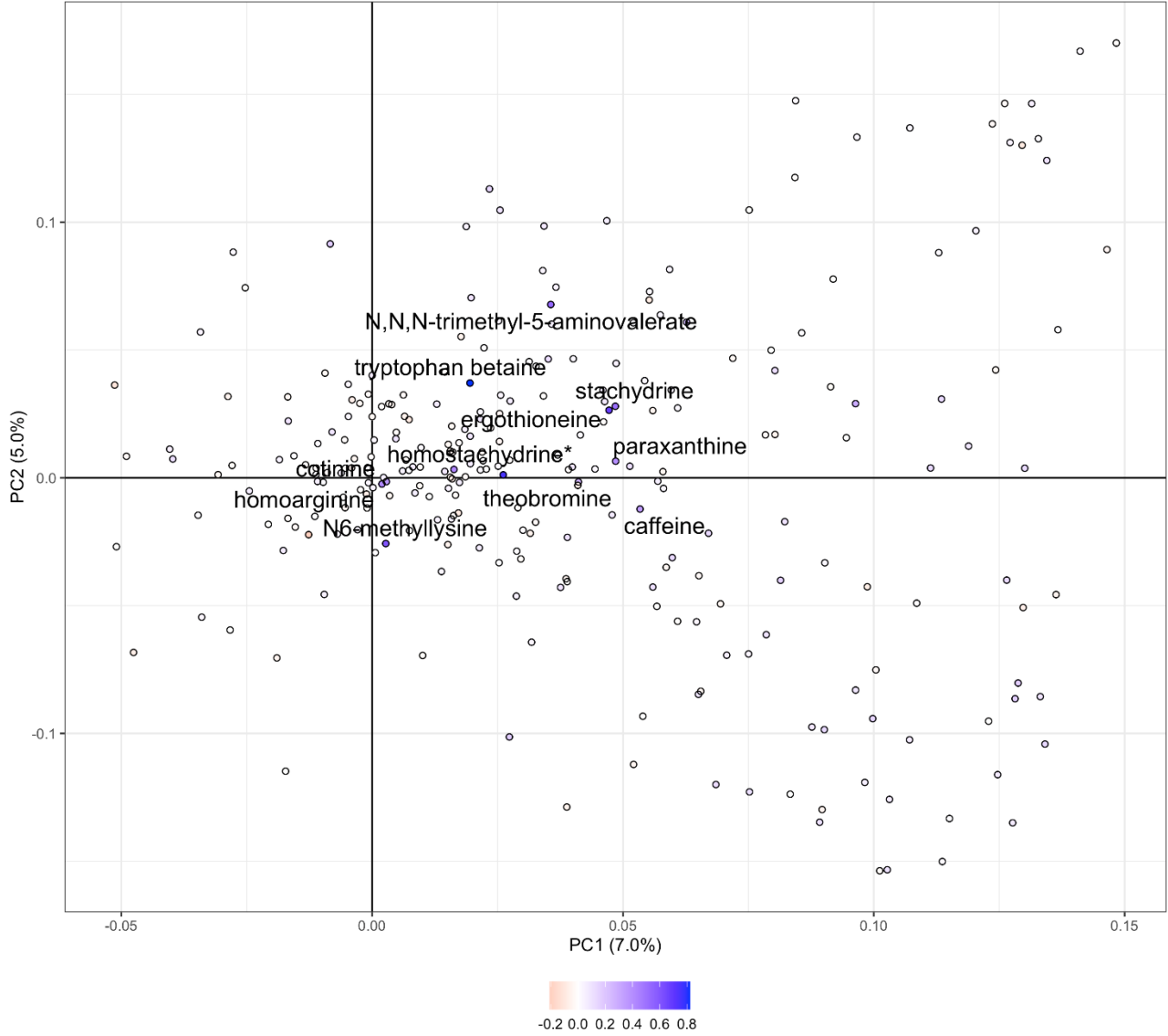
**Figure S4.** PCA loading plot of plasma from mothers at 24 weeks of pregnancy. Loadings were color-coded by correlation  $R_{m1-c}$ .



**Figure S5.** PCA loading plot of plasma from mothers 1 week postpartum. Loadings were color-coded by correlation  $R_{m1-c}$ .

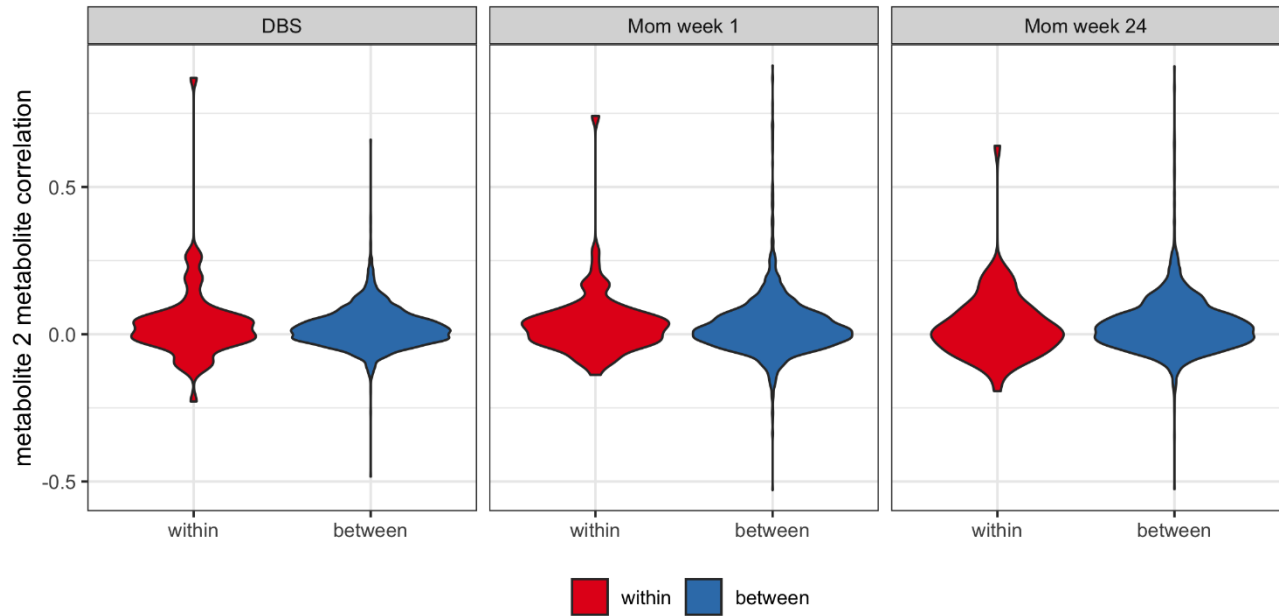


**Figure S6.** PCA loading plot of DBS samples from newborns. Loadings were color-coded by correlation  $R_{m1-c}$ .



In addition to the PCA analysis the correlation between the metabolites with transfer statistics  $R_{m1-c} > 0.3$  (denoted within in Figure S7) is compared with the correlations between metabolites with  $R_{m1-c} > 0.3$  and metabolites with  $R_{m1-c} \leq 0.3$  (denoted between in Figure S7). This analysis is in agreement with the interpretation of the loadings plot, namely that there is not a particular pattern characterizing the metabolites exhibiting strong transfer statistics.

**Figure S7.** Metabolite to metabolite correlation computed within each time point and partitioned into within transferred metabolites ( $R_{m1-c} > 0.3$ ) and between none-to weak transferred ( $R_{m1-c} \leq 0.3$ ) and transferred ( $R_{m1-c} > 0.3$ ) metabolites.



**Table S6.** Descriptive (median and IQR) for metabolite to metabolite correlations within each time point, and partitioned into within transferred metabolites ( $R_{m1-c} > 0.3$ ) and between none-to weak transferred ( $R_{m1-c} \leq 0.3$ ) and transferred ( $R_{m1-c} > 0.3$ ) metabolites.

time	between	within
DBS	0.02 (-0.02;0.06)	0.02 (-0.03;0.06)
Mom week 1	0.01 (-0.03;0.06)	0.02 (-0.03;0.06)
Mom week 24	0.02 (-0.03;0.07)	0.01 (-0.05;0.08)