

SUPPLEMENTARY MATERIAL for

Plasma and serum metabolite association networks: comparability within and between studies using NMR and MS profiling

Maria Suarez-Diez<sup>1,\*†</sup>, Jonathan Adam<sup>2,3,4</sup>, Jerzy Adamski<sup>4,5,6</sup>, Styliani A. Chasapi<sup>7</sup>, Claudio Luchinat<sup>8,9</sup>, Annette Peters<sup>2,3,4,10</sup>, Cornelia Prehn<sup>5</sup>, Claudio Santucci<sup>8</sup>, Alexandros Spyridonidis<sup>11</sup>, Georgios A. Spyroulias<sup>7</sup>, Leonardo Tenori<sup>12</sup>, Rui Wang-Sattler<sup>2,3,4</sup>, Edoardo Saccenti<sup>1,\*†</sup>

<sup>1</sup>Laboratory of Systems and Synthetic Biology, Wageningen University & Research, Stippeneng 4 6708 WE, Wageningen, the Netherlands.

<sup>2</sup>Research Unit of Molecular Epidemiology, Helmholtz Zentrum München, 85764 München-Neuherberg, Germany.

<sup>3</sup>Institute of Epidemiology II, Helmholtz Zentrum München, 85764 München-Neuherberg, Germany.

<sup>4</sup>German Center for Diabetes Research (DZD), Helmholtz Zentrum München, 85764 München-Neuherberg, Germany.

<sup>5</sup>Institute of Experimental Genetics, Helmholtz Zentrum München, 85764 München-Neuherberg, Germany.

<sup>6</sup>Chair of Experimental Genetics, Center of Life and Food Sciences Weihenstephan, Technische Universität München, 85353 Freising, Germany.

<sup>7</sup>Department of Pharmacy, University of Patras, GR-26504, Patras, Greece.

<sup>8</sup>Magnetic Resonance Center (CERM), University of Florence, Via L. Sacconi 6, 50019 Sesto Fiorentino, Italy.

<sup>9</sup>Department of Chemistry, University of Florence, Via della Lastruccia 3, 50019 Sesto Fiorentino, Italy.

<sup>10</sup>Department of Environmental Health, Harvard School of Public Health, 02115, Boston, USA.

<sup>11</sup>Bone Marrow Transplantation Unit, University Hospital Patras, 26500 Rio, Greece.

<sup>12</sup>Department of Experimental and Clinical Medicine, University of Florence, Largo Brambilla 3, 501134, Florence, Italy.

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**Table S1** Observed metabolite degree, in the plasma and serum consensus network obtained for data in study I (serum and plasma obtained from different blood samples).

#	Metabolite	Metabolite degree	
		Plasma	Serum
1	Alanine	3	0
2	Citrate	6	0
3	Proline	3	0
4	Oxoglutarate	9	3
5	Histidine	13	8
6	Acetate	11	8
7	HDL	9	7
8	Threonine	9	7
9	Methionine	3	3
10	Acetoacetate	7	7
11	Pyruvate	6	7
12	Arginine	15	18
13	3-Hydroxybutyrate	9	11
14	LDL	6	8
15	Creatinine	7	10
16	Serine	7	10
17	Isoleucine	9	14
18	Formate	24	42
19	Glutamine	6	11
20	Leucine	9	17
21	Tyrosine	13	25
22	Glucose	4	8
23	Dimethylglycine	11	24
24	Lysine	7	16
25	Valine	9	24
26	Phenylalanine	3	10
27	Creatine	6	23
28	NAG1	6	40
29	VLDL	0	3

**Table S2** Average plasma and serum concentration (expressed in arbitrary units) and standard error (S.E.) of 29 metabolites measured using NMR. All difference are significant ( $P < 10^{-4}$ ) after Bonferroni correction for multiple testing except for 3-Hydroxybutyrate. For Plasma and serum data obtain via FIA-MS please refer to the paper <http://journals.plos.org/plosone/article?id=10.1371/journal.pone.0021230>.

Metabolite	Plasma		Serum	
	Mean	S.E.	Mean	S.E.
3-Hydroxybutyrate	6.63E-05	0.000294	6.72E-05	0.000531
Acetate	0.000204	9.94E-05	0.000305	0.000153
Acetoacetate	0.003214	0.002644	0.005893	0.003923
Alanine	0.00508	0.000638	0.004292	0.001053
Arginine	0.002531	0.000421	0.003727	0.000868
Citrate	0.000315	0.000396	0.002029	0.00345
Creatine	7.27E-05	6.43E-05	0.004237	0.00094
Creatinine	0.00038	7.43E-05	0.000524	0.000131
Dimethylglycine	5.13E-05	4.45E-05	8.89E-05	8.49E-05
Formate	0.000124	7.88E-05	2.91E-05	2.44E-05
Glucose	0.00437	0.00101	0.007124	0.001537
Glutamine	0.001767	0.001008	0.003891	0.000948
HDL	0.005826	0.002665	0.048072	0.028138
Histidine	0.000263	9.91E-05	0.000637	0.000194
Isoleucine	0.000219	4.86E-05	0.000308	8.5E-05
LDL	0.06845	0.006462	0.109332	0.014234
Leucine	0.001022	0.000298	0.001395	0.000398
Lysine	2.23E-05	3.87E-05	4.35E-05	2.23E-05
Methionine	0.005932	0.000858	0.000471	0.000186
NAG1	0.005945	0.000859	0.008942	0.001839
Oxoglutarate	0.000123	3.96E-05	9.09E-05	6.32E-05
Phenylalanine	0.000256	5.34E-05	0.000555	0.00012
Proline	0.000907	0.000238	0.001388	0.000413
Pyruvate	0.000704	0.000201	0.000542	0.000325
Serine	0.000855	0.000432	0.001877	0.000528
Threonine	0.031093	0.012221	0.029297	0.012401
Tyrosine	0.000321	6.53E-05	0.000427	0.00011
Valine	0.001818	0.000336	0.002723	0.000667
VLDL	0.003199	0.002934	0.006186	0.004341