Supplementary Information

Between-person comparison of metabolite fitting for NMR-based quantitative metabolomics

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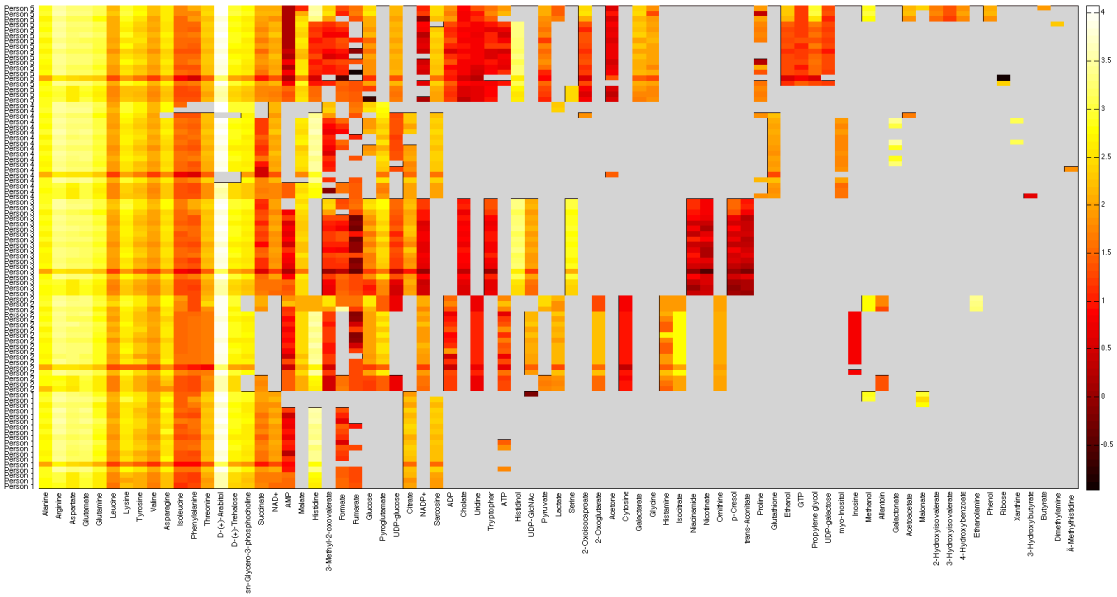

Figure S1 Log scaled concentrations of metabolites in each sample that were assigned and fitted by each individual in round one.

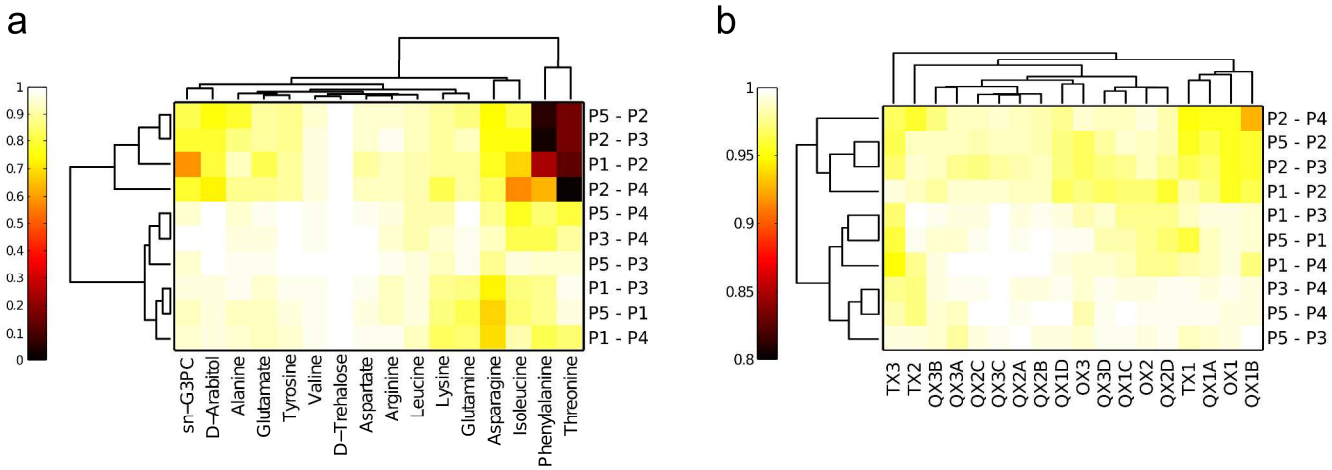

Figure S2 Correlations (Spearman's ρ) between people for both metabolites and samples ordered by hierarchical clustering in both dimensions for round one data. a) association between different people for individual metabolites; b) association between different people for individual samples.

Table S1. Metabolites fitted in the current study, and comparison of the contribution of individual variability in fitting (factor "person") and experimental treatment (factor "method") on variance; ANOVA carried out on log-transformed data from round one, i.e. metabolites fitted independently. One outlying sample (QXB1) was excluded from the analyses. PCID: PubChem ID.

		Method			Person			Interaction		
Metabolite	PCID	Mean Square	F	p	Mean Square	F	p	Mean Square	F	p
Alanine	5950	0.028	3.073	0.016	0.006	0.659	0.623	0.005	0.592	0.902
Arginine	6322	0.572	95.951	<0.001	0.037	6.216	0.000	0.003	0.560	0.923
Aspartate	5960	0.931	182.727	<0.001	0.012	2.310	0.069	0.001	0.124	1.000
Glutamate	33032	0.216	38.322	<0.001	0.035	6.242	0.000	0.001	0.242	1.000
Glutamine	5961	0.263	31.841	<0.001	0.039	4.686	0.003	0.001	0.159	1.000
Leucine	6106	0.298	40.253	<0.001	0.012	1.562	0.197	0.005	0.672	0.835
Lysine	5962	0.484	42.784	<0.001	0.032	2.803	0.034	0.010	0.890	0.600
Tyrosine	6057	0.471	64.175	<0.001	0.089	12.072	<0.001	0.003	0.405	0.986
Valine	6287	0.170	28.374	<0.001	0.014	2.306	0.070	0.001	0.177	1.000
Asparagine	6267	0.326	29.061	<0.001	0.005	0.430	0.786	0.009	0.835	0.662
Isoleucine	6306	0.167	31.291	<0.001	0.035	6.559	0.000	0.011	1.967	0.025
Phenylalanine	6140	0.241	31.962	<0.001	0.022	2.929	0.029	0.053	7.063	0.000
Threonine	6288	0.146	16.754	<0.001	0.728	83.634	<0.001	0.030	3.446	0.000
D-Arabitol	94154	0.374	79.540	<0.001	0.005	1.098	0.367	0.002	0.418	0.983
D-Trehalose	7427	0.391	79.910	<0.001	0.000	0.067	0.991	0.001	0.122	1.000
sn-G3PC	439285	0.012	2.399	0.079	0.012	2.290	0.089	0.001	0.162	1.000

Table S2. Metabolites fitted in the current study, and comparison of the contribution of individual variability in fitting (factor "person") and experimental treatment (factor "method") on variance; ANOVA carried out on log-transformed data from round two, i.e. with shared information on metabolite assignment. One outlying sample (QXB1) was excluded from the analyses. PCID: PubChem ID.

		Method			Person			Interaction		
Metabolite	PCID	Mean Square	F	p	Mean Square	F	p	Mean Square	F	p
3M2OV	47	5.02	186	<0.001	0.077	2.86	0.067	0.026	0.980	0.497
AMP	6083	1.16	18.3	<0.001	0.11	1.79	0.146	0.091	1.44	0.145
Alanine	5950	0.027	4.48	0.002	0.0013	0.212	0.930	0.0013	0.0504	1.000
Arginine	6322	0.56	96.4	<0.001	0.0075	1.29	0.285	0.0011	0.186	1.000
Asparagine	6267	0.29	67.8	<0.001	0.023	5.27	0.001	0.0046	1.08	0.386
Aspartate	5960	0.93	139	<0.001	0.020	2.97	0.027	0.0022	0.325	0.996
NAM	14180	0.18	6.11	<0.001	0.070	2.37	0.081	0.062	2.10	0.018
Citrate	311	0.45	17.6	<0.001	0.13	5.15	0.001	0.039	1.51	0.115
Met. sulfox.	847	0.31	59.1	<0.001	0.0080	1.52	0.208	0.0014	0.0850	1.000
D-Arabitol	94154	0.41	53.5	<0.001	0.0077	1.01	0.409	0.0020	0.125	1.000
D-Trehalose	7427	0.40	71.6	<0.001	0.0018	0.151	0.962	0.0012	0.226	1.000
Formate	284	1.00	60.4	<0.001	0.15	9.33	<0.001	0.040	2.42	0.007
Fumarate	444972	3.86	47.5	<0.001	0	0	NaN	0.11	1.33	0.234
Glucose	5793	2.08	137	<0.001	0.040	2.65	0.043	0.0051	0.337	0.995
Glutamate	33032	0.22	41.6	<0.001	0.0027	0.503	0.734	0.0046	0.857	0.637
Glutamine	5961	0.29	31.9	<0.001	0.013	1.49	0.216	0.0023	0.252	0.999
Histidinol	776	1.32	310	<0.001	0.014	3.26	0.018	0.0018	0.418	0.983
Isoleucine	6306	0.25	35.8	<0.001	0.069	9.83	<0.001	0.023	3.26	<0.001
Leucine	6106	0.26	37.2	<0.001	0.028	4.04	0.006	0.0044	0.637	0.866
Lysine	5962	0.53	46.0	<0.001	0.088	7.58	<0.001	0.011	0.993	0.484
Malate	525	0.048	2.35	0.066	0.28	13.6	<0.001	0.043	2.08	0.019
NAD+	5893	0.28	28.2	<0.001	0.069	6.87	<0.001	0.0044	0.436	0.978
NADP+	5886	1.16	11.4	<0.001	0.92	9.06	<0.001	0.12	1.23	0.263
Niacinamide	936	0.28	5.03	0.002	0.23	4.03	0.013	0.057	1.02	0.459
Nicotinate	938	0.31	4.37	0.005	0.79	11.0	<0.001	0.15	2.10	0.021
Phenylalanine	6140	0.54	51.6	<0.001	0.043	4.07	0.006	0.025	2.40	0.005
Pyroglutamate	7405	1.20	86.8	<0.001	0.019	1.38	0.253	0.0094	0.676	0.832

Serine	5951	0.39	19.9	<0.001	0.22	11.5	<0.001	0.024	1.21	0.276
Succinate	1110	0.66	8.67	<0.001	0.10	1.34	0.267	0.077	1.01	0.464
Threonine	6288	0.24	38.2	<0.001	0.053	8.40	<0.001	0.0039	0.619	0.881
Tryptophan	6305	0.77	21.9	<0.001	0.23	6.44	<0.001	0.11	3.04	0.001
Tyrosine	6057	0.47	63.1	<0.001	0.0058	0.789	0.537	0.0028	0.379	0.990
UDP-GlcNAc	16667373	0.47	41.5	<0.001	0.026	2.28	0.072	0.0090	0.795	0.708
UDP-glucose	8629	0.024	0.56	0.691	1.39	33.1	<0.001	0.079	1.89	0.038
Valine	6287	0.17	30.0	<0.001	0.0093	1.63	0.180	0.0026	0.453	0.973
sn-G3PC	439285	0.49	75.6	<0.001	0.022	3.34	0.016	0.0015	0.232	1.000
trans-Aconitate	444212	0.39	2.41	0.080	0.073	0.446	0.643	0.15	0.923	0.553