Appendix E1

Example of an LCModel control file used in this study. Only common parameters used for all datasets are shown here. Please note that these values should not be considered as a reference for future studies. Control parameters should be always adapted to the data that are being quantified.

```
$LCMODL
.
.
.
DKNTMN = 0.15
DEGZER = 0.0
SDDEGZ = 5.0
DEGPPM = 0.
SDDEGP = 5.0
DOWS = T
SUBBAS = T
NEACH = 99
WDLINE (6) = 0.0
PPMST = 4.0
PPMEND = 0.5
NSIMUL = 12
NCOMBI = 5
CHCOMB (1) = 'PC+GPC'
CHCOMB (2) = 'Cr+PCr'
CHCOMB (3) = 'NAA+NAAG'
CHCOMB (4) = 'Glu+Gln'
CHCOMB (5) = 'Glc+Tau'
NAMREL = 'Cr+PCr'
CONREL = 8.00
DOECC = T (Only for GE and Siemens, Philips spectra were exported already ECC corrected)
.
.
.
$END
```

Table E1. Hardware and software parameters that were used to collect the MRS data

Site ID	Scanner vendor and model	Software release	Tx/Rx hardware	B_0 shimming approach	Phase cycling	Spectral width (Hz)	Data points	Water suppression
G1	GE Discovery MR750w	DV25	Body coil/32-ch head coil	Double-echo GRE	2 steps	5000	4096	CHESS
G2	GE Discovery MR750	DV24	Body coil/8-ch head coil	Double-echo GRE	2 steps	2000	2048	CHESS
G3	GE Discovery MR750	DV24	Body coil/32-ch head coil	Double-echo GRE	8 steps	2000	2048	CHESS
G4	GE Discovery MR750	DV25	Body coil/8-ch head coil	Double-echo GRE	8 steps	5000	4096	CHESS
G5	GE Discovery MR750	DV25	Body coil/32-ch head coil	Double-echo GRE	8 steps	2000	2048	CHESS
G6	GE Signa HDx	HD16	Body coil/8-ch head coil	Double-echo GRE	2 steps	2000	2048	CHESS
G7	GE Discovery MR750	DV24	Body coil/8-ch head coil	Double-echo GRE	8 steps	2000	2048	CHESS
G8	GE Discovery MR750	DV24	Body coil/8-ch head coil	Double-echo GRE	8 steps	2000	2048	CHESS
P1	Philips Achieva	R5.1.7	Body coil/32-ch head coil	PB-auto[a]	16 steps	2000	2048	VAPOR
P2	Philips Achieva	R5.1.7	Body coil/32-ch head coil	PB-auto	16 steps	2000	2048	VAPOR
P3	Philips Achieva	R3.2.2	Body coil/32-ch head coil	PB-auto	16 steps	2000	2048	VAPOR
P4	Philips Ingenia CX	R5.1.7	Body coil/32-ch head coil	PB-auto	16 steps	2000	2048	MOIST
P5	Philips Achieva TX	R5.1.7	Body coil/32-ch head coil	PB-auto	16 steps	2000	2048	MOIST
P6	Philips Achieva	R3.2.3	Body coil/8-ch head coil	PB-auto	16 steps	2000	2048	MOIST
P7	Philips Ingenia	R5.1.8	Body coil/32-ch head coil	PB-auto	16 steps	2000	2048	VAPOR
P8	Philips Ingenia CX	R5.1.8	Body coil/32-ch head coil	PB-auto	16 steps	2000	2048	MOIST
P9	Philips Achieva	R5.1.7	Body coil/32-ch head coil	PB-auto	16 steps	2000	2048	VAPOR
P10	Philips Ingenia	R5.1.9	Body coil/15-ch head coil	PB-auto	16 steps	2000	2048	MOIST
S1	Siemens Trio	VB17	Body coil/32-ch head coil	3D-DESS + manual	16 steps	4000[b]	4096	CHESS
S2	Siemens Verio	VB17	Body coil/32-ch head coil	3D-DESS + manual	16 steps	4000	4096	CHESS
S3	Siemens Prisma	VD13	Body coil/20-ch head coil	FAST (EST)MAP	16 steps	4000	4096	WET
S4	Siemens Prisma	VE11	Body coil/64-ch head coil	3D-DESS	16 steps	4000	4096	WET
S5	Siemens Trio	VB17	Body coil/12-ch head coil	3D-DESS	16 steps	4000	4096	CHESS
S6	Siemens Trio	VB17	Body coil/32-ch head coil	FAST (EST)MAP	16 steps	4000	4096	WET
S7	Siemens Trio	VB17	Body coil/32-ch head coil	FAST (EST)MAP	16 steps	2000	2074[c]	CHESS
S8	Siemens Prisma	VE11	Body coil/64-ch head coil	3D-DESS	16 steps	4000	4096	WET

[a] PB-auto is a Philips pencil-beam projection-based method for automatic voxel shimming.

[b] TWIX data are oversampled. For example, if the specified spectral width and number of discrete data points are set at 2000 Hz/2048, the data are oversampled to 4000 Hz/4096.

[c] In the Siemens WIP sequence, extra data points are added before and/or after the detected spin echo if the number of data points is specified as 512 or 1024. The additional points before the spin echo were removed during data processing.

GRE, gradient echo; PB, pencil beam; 3D-DESS, Three-dimensional double-echo steady-state; manual, manual shimming, FAST (EST)MAP, Fast, Automatic Shim Technique using Echo-planar Signal readouT for Mapping Along Projections; CHESS, CHEmical Shift Selective; VAPOR, VAriable Power and Optimized Relaxation delays; WET, Water suppression Enhanced through T_1 effects; MOIST, Multiply Optimized Insensitive Suppression Train Rx, receive; Tx, transmit.

Table E2. Number of datasets that were not quantified for a given metabolite based on the quality criteria

	Ala	Asc	Asp	GABA	Glx	Glc+Tau	GSH	Lac	mI	PE	sI	tCho	tCr	tNAA
Count of Not Quant (CRLB > 100%)	115	53	0	12	0	0	0	15	0	6	3	0	0	0
Percentage of all datasets	39.25%	18.09%	0.00%	4.10%	0.00%	0.00%	0.00%	5.12%	0.00%	2.05%	1.02%	0.00%	0.00%	0.00%
Count of datasets with CRLB > 50%	102	26	0	20	0	3	0	31	0	10	2	0	0	0
Percentage of all datasets	34.81%	8.87%	0.00%	6.83%	0.00%	1.02%	0.00%	10.58%	0.00%	3.41%	0.68%	0.00%	0.00%	0.00%
Mean CRLB ± SD (all quantified spectra)	55.3 ± 18%	27.0 ± 18%	13.2 ± 5%	33.2 ± 13%	4.4 ± 1%	13.8 ± 8%	55.3 ± 18%	30.2 ± 16%	3.6 ± 1%	20.7 ± 12%	15.4 ± 8%	2.6 ± 1%	1.2 ± 0.5%	1.6 ± 0.5%

Alanine (Ala) was not reported because the mean CRLB of all quantified spectra was > 50%.

Table E3. Site, vendor and total values (mean ± SD) of metabolite/tCr ratios in arbitrary units (a.u.)

Site ID	Asc/tCr	Asp/tCr	GABA/tCr	Glx/tCr	GSH/tCr	Glc+Tau/tCr	Lac/tCr	mI/tCr	PE/tCr	sI/tCr	tCho/tCr	tNAA/tCr
G1	1.02 ± 0.39	2.97 ± 0.42	1.08 ± 0.31	13.19 ± 1.40	1.22 ± 0.17	2.14 ± 0.63	0.81 ± 0.42	7.25 ± 0.70	1.88 ± 0.60	0.25 ± 0.10	1.39 ± 0.17	11.54 ± 1.39
G2	0.48 ± 0.14	2.30 ± 0.39	0.89 ± 0.23	12.20 ± 1.13	1.27 ± 0.18	2.12 ± 0.82	0.58 ± 0.21	6.64 ± 0.46	1.99 ± 0.51	0.27 ± 0.11	1.36 ± 0.11	11.31 ± 0.52
G3	0.64 ± 0.22	2.71 ± 0.45	0.86 ± 0.41	12.59 ± 1.04	1.32 ± 0.26	2.22 ± 0.69	0.45 ± 0.08	7.05 ± 0.30	2.20 ± 0.78	0.25 ± 0.15	1.44 ± 0.14	11.40 ± 0.73
G4	1.03 ± 0.61	2.66 ± 0.53	0.84 ± 0.28	12.65 ± 0.66	1.29 ± 0.22	2.07 ± 0.42	0.56 ± 0.28	6.91 ± 0.55	1.93 ± 0.49	0.28 ± 0.06	1.39 ± 0.11	11.49 ± 0.59
G5	0.48 ± 0.14	2.68 ± 0.56	1.01 ± 0.23	12.22 ± 0.76	1.22 ± 0.14	2.13 ± 0.55	0.72 ± 0.19	6.76 ± 0.49	2.06 ± 0.49	0.25 ± 0.09	1.34 ± 0.09	11.22 ± 0.57
G6	0.74 ± 0.35	3.53 ± 0.52	1.03 ± 0.36	15.50 ± 1.08	1.88 ± 0.21	1.92 ± 0.61	0.59 ± 0.24	7.22 ± 0.45	2.36 ± 0.69	0.24 ± 0.13	1.53 ± 0.21	11.53 ± 0.62
G7	0.96 ± 0.75	2.77 ± 0.49	0.80 ± 0.19	11.81 ± 1.30	1.04 ± 0.31	2.58 ± 0.66	0.73 ± 0.32	7.24 ± 0.42	1.89 ± 0.76	0.21 ± 0.09	1.40 ± 0.18	11.40 ± 0.61
G8	1.14 ± 0.41	2.59 ± 0.60	0.71 ± 0.30	11.85 ± 1.71	1.06 ± 0.32	2.61 ± 1.02	0.53 ± 0.32	7.44 ± 0.66	1.98 ± 0.73	0.20 ± 0.05	1.43 ± 0.10	11.35 ± 0.51
GE all	**0.89 ± 0.50**	**2.78 ± 0.59**	**0.91 ± 0.30**	**12.76 ± 1.62**	**1.28 ± 0.34**	**2.22 ± 0.71**	**0.63 ± 0.28**	**7.06 ± 0.57**	**2.03 ± 0.62**	**0.24 ± 0.10**	**1.41 ± 0.15**	**11.41 ± 0.72**
Intersite CV	**32.16%**	**12.92%**	**14.19%**	**9.40%**	**20.22%**	**11.05%**	**19.19%**	**3.88%**	**8.10%**	**11.95%**	**4.20%**	**0.97%**
P1	1.55 ± 0.26	3.20 ± 0.23	0.59 ± 0.10	12.32 ± 0.86	1.19 ± 0.08	3.37 ± 0.44	0.57 ± 0.12	7.04 ± 0.57	2.28 ± 0.52	0.35 ± 0.09	1.28 ± 0.12	11.58 ± 0.85
P2	1.58 ± 0.61	3.32 ± 0.28	0.71 ± 0.10	11.52 ± 0.90	1.25 ± 0.13	3.18 ± 0.49	0.66 ± 0.14	7.20 ± 0.44	3.46 ± 0.63	0.36 ± 0.13	1.44 ± 0.11	11.02 ± 0.72
P3	0.81 ± 0.38	2.19 ± 0.45	0.77 ± 0.26	11.47 ± 0.94	1.31 ± 0.17	2.71 ± 0.67	0.55 ± 0.18	7.13 ± 0.51	2.83 ± 0.71	0.37 ± 0.09	1.33 ± 0.10	10.19 ± 1.06
P4	1.42 ± 0.48	2.95 ± 0.26	0.54 ± 0.12	12.10 ± 0.91	1.32 ± 0.11	3.00 ± 0.77	0.67 ± 0.13	7.06 ± 0.85	3.17 ± 0.58	0.32 ± 0.14	1.36 ± 0.13	10.98 ± 0.67
P5	0.54 ± 0.26	3.21 ± 0.27	0.60 ± 0.13	10.05 ± 0.85	1.22 ± 0.29	1.91 ± 0.38	0.54 ± 0.15	6.35 ± 0.42	1.88 ± 0.51	0.19 ± 0.06	1.14 ± 0.17	10.71 ± 0.35
P6	2.33 ± 1.84	2.59 ± 0.61	0.91 ± 0.23	11.86 ± 0.86	1.58 ± 0.59	3.04 ± 1.58	0.57 ± 0.18	6.23 ± 0.76	2.69 ± 0.84	0.24 ± 0.05	1.28 ± 0.10	10.08 ± 0.62
P7	0.65 ± 0.25	3.88 ± 0.41	0.97 ± 0.52	11.68 ± 1.45	1.35 ± 0.13	2.88 ± 0.61	0.57 ± 0.18	7.27 ± 0.56	3.93 ± 0.99	0.36 ± 0.11	1.50 ± 0.12	11.78 ± 0.61
P8	1.16 ± 0.34	3.15 ± 0.24	0.55 ± 0.22	11.50 ± 0.76	1.29 ± 0.08	2.60 ± 0.32	0.56 ± 0.16	7.08 ± 0.43	2.85 ± 0.58	0.34 ± 0.05	1.30 ± 0.05	10.59 ± 0.37
P9	0.57 ± 0.24	2.79 ± 0.29	0.59 ± 0.13	10.88 ± 0.61	1.38 ± 0.19	2.61 ± 0.36	0.55 ± 0.11	6.76 ± 0.48	2.76 ± 0.56	0.33 ± 0.08	1.36 ± 0.15	10.56 ± 0.65
P10	1.63 ± 0.97	3.55 ± 0.50	0.94 ± 0.35	12.72 ± 1.37	1.53 ± 0.38	2.76 ± 1.17	0.59 ± 0.15	7.48 ± 0.64	3.58 ± 0.91	0.25 ± 0.11	1.48 ± 0.14	11.24 ± 0.50

Philips all	1.31 ± 0.93	3.08 ± 0.59	0.72 ± 0.29	11.66 ± 1.16	1.35 ± 0.28	2.84 ± 0.84	0.59 ± 0.15	6.98 ± 0.68	2.98 ± 0.88	0.32 ± 0.11	1.35 ± 0.15	10.88 ± 0.85
Intersite CV	47.54%	15.59%	23.53%	6.45%	9.38%	14.32%	7.91%	5.75%	20.85%	20.12%	7.95%	5.11%
S1	1.30 ± 0.48	2.41 ± 0.76	0.50 ± 0.14	12.71 ± 0.54	1.50 ± 0.14	2.90 ± 0.61	0.52 ± 0.12	7.05 ± 0.52	3.56 ± 0.59	0.27 ± 0.05	1.53 ± 0.10	10.88 ± 1.14
S2	1.16 ± 0.17	2.34 ± 0.60	0.52 ± 0.08	12.97 ± 1.10	1.48 ± 0.16	2.34 ± 0.47	0.67 ± 0.20	7.09 ± 0.31	3.75 ± 0.48	0.30 ± 0.14	1.66 ± 0.22	11.65 ± 0.43
S3	1.82 ± 0.21	3.16 ± 0.29	0.44 ± 0.09	10.71 ± 0.74	1.10 ± 0.11	2.67 ± 0.42	0.59 ± 0.26	7.21 ± 0.45	2.88 ± 0.37	0.31 ± 0.12	1.47 ± 0.10	10.09 ± 0.67
S4	1.36 ± 0.23	3.25 ± 0.28	0.44 ± 0.12	11.86 ± 0.85	1.16 ± 0.07	2.83 ± 0.44	0.50 ± 0.11	7.06 ± 0.54	2.84 ± 0.35	0.40 ± 0.09	1.45 ± 0.17	11.46 ± 0.72
S5	1.46 ± 0.30	3.05 ± 0.66	0.61 ± 0.30	13.41 ± 0.99	1.50 ± 0.16	2.48 ± 0.52	0.50 ± 0.18	7.37 ± 0.63	3.24 ± 0.47	0.27 ± 0.08	1.57 ± 0.14	12.21 ± 0.78
S6	1.18 ± 0.13	2.72 ± 0.44	0.63 ± 0.19	13.72 ± 0.74	1.33 ± 0.12	2.56 ± 0.43	0.57 ± 0.11	7.15 ± 0.48	3.12 ± 0.43	0.30 ± 0.04	1.54 ± 0.20	12.24 ± 0.73
S7	1.37 ± 0.31	3.20 ± 0.50	0.49 ± 0.20	12.64 ± 0.79	1.43 ± 0.13	2.66 ± 0.44	0.57 ± 0.14	6.80 ± 0.39	2.96 ± 0.44	0.28 ± 0.07	1.52 ± 0.16	11.39 ± 0.87
S8	1.54 ± 0.18	2.92 ± 0.21	0.55 ± 0.08	11.29 ± 0.64	1.06 ± 0.10	2.72 ± 0.53	0.56 ± 0.17	7.20 ± 0.41	2.63 ± 0.30	0.29 ± 0.05	1.50 ± 0.18	10.90 ± 0.67
Siemens all	1.41 ± 0.33	2.92 ± 0.57	0.52 ± 0.18	12.40 ± 1.25	1.31 ± 0.21	2.67 ± 0.49	0.55 ± 0.16	7.12 ± 0.49	3.08 ± 0.53	0.30 ± 0.09	1.52 ± 0.16	11.35 ± 1.04
Intersite CV	15.20%	12.34%	13.75%	8.40%	14.20%	6.97%	10.15%	2.29%	12.16%	13.35%	4.13%	6.37%
Total	1.26 ± 0.71	2.94 ± 0.60	0.72 ± 0.31	12.22 ± 1.42	1.32 ± 0.28	2.60 ± 0.75	0.59 ± 0.20	7.05 ± 0.60	2.73 ± 0.85	0.29 ± 0.10	1.42 ± 0.17	11.18 ± 0.90

Table E4. Site, vendor and total values (mean ± SD) of relative metabolite CRLBs in percentage

Site ID	Asc	Asp	GABA	Glc+Tau	Glx	GSH	Lac	mI	PE	sI	tCho	tCr	tNAA
G1	37.90 ± 15.26	15.17 ± 2.66	29.75 ± 7.33	17.67 ± 4.25	4.83 ± 0.58	10.08 ± 1.44	34.25 ± 20.01	4.08 ± 0.29	34.64 ± 17.51	21.00 ± 9.26	3.67 ± 0.49	1.58 ± 0.51	2.00 ± 0.00
G2	62.67 ± 19.35	19.42 ± 4.98	33.58 ± 6.91	20.08 ± 10.90	4.92 ± 0.51	9.00 ± 1.65	44.20 ± 20.33	4.17 ± 0.39	29.82 ± 7.35	17.83 ± 6.09	3.33 ± 0.49	1.67 ± 0.49	1.83 ± 0.39
G3	46.80 ± 19.38	14.57 ± 4.50	35.71 ± 20.10	16.86 ± 9.12	4.43 ± 0.53	8.29 ± 1.25	36.83 ± 10.03	3.71 ± 0.49	28.00 ± 17.29	24.14 ± 20.95	3.14 ± 0.38	1.14 ± 0.38	1.71 ± 0.49
G4	42.75 ± 20.62	17.75 ± 3.57	40.91 ± 9.97	19.00 ± 4.22	5.08 ± 0.67	9.83 ± 2.86	52.11 ± 25.20	4.00 ± 0.00	34.82 ± 13.91	17.50 ± 4.30	3.50 ± 0.52	1.83 ± 0.39	2.00 ± 0.00
G5	67.40 ± 24.49	14.50 ± 2.97	25.33 ± 3.31	16.33 ± 5.96	4.42 ± 0.51	8.67 ± 1.15	29.33 ± 9.56	3.83 ± 0.39	25.75 ± 5.14	17.75 ± 5.56	3.08 ± 0.29	1.17 ± 0.39	1.92 ± 0.29
G6	55.75 ± 25.64	14.75 ± 2.26	38.50 ± 20.22	21.25 ± 9.04	4.33 ± 0.49	7.33 ± 0.89	48.36 ± 20.73	4.00 ± 0.00	30.17 ± 10.72	25.18 ± 9.77	3.67 ± 0.65	1.92 ± 0.29	1.92 ± 0.29
G7	40.67 ± 15.63	16.17 ± 6.78	32.82 ± 7.87	14.92 ± 6.42	4.92 ± 0.79	12.08 ± 6.01	31.36 ± 16.05	3.92 ± 0.51	36.73 ± 23.66	23.09 ± 6.74	3.42 ± 0.51	1.42 ± 0.51	1.83 ± 0.39
G8	30.50 ± 12.46	17.33 ± 4.10	44.27 ± 23.56	15.33 ± 4.75	4.92 ± 0.67	12 25 ± 5.21	42.17 ± 17.59	3.83 ± 0.58	31.46 ± 13.22	22.58 ± 5.99	3.33 ± 0.49	1.67 ± 0.49	1.75 ± 0.45
GE all	44.48 ± 20.31	16.30 ± 4.37	34.93 ± 14.52	17.73 ± 7.16	4.75 ± 0.64	9.77 ± 3.52	39.76 ± 19.02	3.96 ± 0.39	31.54 ± 14.22	20.90 ± 8.96	3.41 ± 0.52	1.57 ± 0.50	1.88 ± 0.33
P1	13.92 ± 2.15	9.58 ± 0.79	28.08 ± 6.67	9.00 ± 0.85	4.00 ± 0.00	7.33 ± 0.65	21.92 ± 7.53	3.67 ± 0.49	17.83 ± 3.71	10.67 ± 2.42	2.08 ± 0.29	1.00 ± 0.00	1.00 ± 0.00
P2	18.75 ± 11.92	10.08 ± 1.16	25.75 ± 5.82	10.25 ± 1.82	4.33 ± 0.49	7.67 ± 0.78	21.08 ± 5.45	3.83 ± 0.39	13.00 ± 2.30	12.08 ± 4.83	2.00 ± 0.00	1.00 ± 0.00	1.83 ± 0.39
P3	40.13 ± 17.13	18.25 ± 4.61	36.83 ± 11.00	15.42 ± 4.58	5.17 ± 0.39	8.08 ± 1.08	38.73 ± 16.38	4.00 ± 0.00	22.58 ± 8.10	14.08 ± 3.26	2.83 ± 0.39	1.25 ± 0.45	2.00 ± 0.00
P4	18.83 ± 10.95	10.92 ± 2.78	32.10 ± 5.65	12.67 ± 13.38	4.25 ± 0.75	7.25 ± 1.82	21.25 ± 8.90	3.50 ± 0.67	14.25 ± 4.33	12.58 ± 5.48	2.33 ± 0.49	1.17 ± 0.39	1.42 ± 0.51
P5	48.00 ± 26.66	9.38 ± 1.06	28.88 ± 5.44	15.25 ± 3.77	4.50 ± 0.53	7.00 ± 1.07	24.25 ± 7.72	3.63 ± 0.52	22.50 ± 5.55	19.00 ± 7.54	2.50 ± 0.53	1.00 ± 0.00	1.50 ± 0.53
P6	14.75 ± 6.12	13.92 ± 4.62	22.58 ± 3.32	11.33 ± 3.47	4.42 ± 0.67	7.17 ± 1.19	29.50 ± 16.20	3.92 ± 0.51	19.17 ± 12.15	16.08 ± 4.44	2.50 ± 0.67	1.08 ± 0.29	1.58 ± 0.51
P7	46.00 ± 20.48	9.17 ± 0.94	29.64 ± 11 27	14.33 ± 3.70	4.83 ± 0.39	7.42 ± 0.79	33.73 ± 12.36	3.75 ± 0.45	17.25 ± 5.29	13.25 ± 2.73	2.83 ± 0.39	1.08 ± 0.29	1.83 ± 0.39
P8	17.00 ± 6.42	8.08 ± 0.51	30.50 ± 13.81	10.08 ± 1.83	4.00 ± 0.00	5.92 ± 0.29	20.08 ± 6.29	3.00 ± 0.00	12.83 ± 1.34	9.58 ± 1.16	2.00 ± 0.00	1.00 ± 0.00	1.25 ± 0.45
P9	40.00 ± 20.80	10.00 ± 0.60	25.67 ± 4.94	10.25 ± 1.48	4.00 ± 0.00	6.25 ± 0.87	19.83 ± 3.76	3.08 ± 0.29	13.50 ± 1.62	9.83 ± 1.59	2.00 ± 0.00	1.00 ± 0.00	1.00 ± 0.00
P10	26.64 ± 10.81	13.58 ± 2.39	34.09 ± 10.25	21.00 ± 23.58	5.50 ± 0.90	9.08 ± 1.93	40.75 ± 14.40	4.33 ± 0.49	20.58 ± 10.90	23.64 ± 11.59	3.00 ± 0.00	1.67 ± 0.49	1.92 ± 0.29

Philips all	25.85 ± 17.81	11.36 ± 3.81	29.34 ± 9.20	12.88 ± 9.42	4.50 ± 0.70	7.33 ± 1.40	27.05 ± 12.95	3.67 ± 0.57	17.17 ± 7.29	13.83 ± 6.47	2.41 ± 0.51	1.13 ± 0.34	1.53 ± 0.50
S1	23.25 ± 12.51	16.42 ± 6.08	40.90 ± 14.02	10.92 ± 1.68	4.25 ± 0.62	6.83 ± 1.11	32.08 ± 18.43	3.25 ± 0.45	15.17 ± 5.67	13.58 ± 4.48	2.25 ± 0.45	1.08 ± 0.29	1.67 ± 0.49
S2	24.00 ± 4.42	18.60 ± 9.29	44.40 ± 12.05	14.00 ± 3.08	4.40 ± 0.55	7.60 ± 0.89	25.80 ± 6.80	3.20 ± 0.45	15.20 ± 1.64	14.80 ± 8.44	2.20 ± 0.45	1.20 ± 0.45	2.00 ± 0.00
S3	13.36 ± 1.91	10.82 ± 1.40	40.27 ± 9.03	11.09 ± 2.39	4.45 ± 0.52	8.36 ± 1.03	23.70 ± 7.70	3.18 ± 0.40	15.46 ± 2.70	11.73 ± 3.90	2.09 ± 0.30	1.09 ± 0.30	1.64 ± 0.50
S4	15.33 ± 2.39	9.58 ± 1.08	37.92 ± 19.36	9.67 ± 1.61	4.00 ± 0.43	7.00 ± 0.74	22.42 ± 5.99	2.92 ± 0.29	13.67 ± 1.78	8.25 ± 1.91	2.08 ± 0.29	1.00 ± 0.00	1.25 ± 0.45
S5	19.64 ± 6.85	13.08 ± 4.32	38.00 ± 15.90	13.33 ± 2.81	4.08 ± 0.29	7.08 ± 1.16	34.58 ± 20.97	3.33 ± 0.49	16.17 ± 1.85	14.67 ± 6.96	2.08 ± 0.29	1.08 ± 0.29	1.67 ± 0.49
S6	19.83 ± 2.44	12.42 ± 2.11	30.00 ± 9.62	10.92 ± 1.44	3.58 ± 0.51	6.92 ± 0.29	22.33 ± 5.14	3.00 ± 0.00	13.75 ± 1.60	10.58 ± 1.51	2.00 ± 0.00	1.00 ± 0.00	1.17 ± 0.39
S7	15.82 ± 3.25	9.64 ± 1.69	38.55 ± 21.31	9.82 ± 1.60	3.45 ± 0.52	6.09 ± 0.54	21.55 ± 9.55	3.00 ± 0.45	13.55 ± 1.86	10.91 ± 2.81	2.00 ± 0.00	1.00 ± 0.00	1.18 ± 0.40
S8	13.73 ± 1.85	10.64 ± 0.92	27.27 ± 4.67	10.00 ± 2.00	4.09 ± 0.30	7.91 ± 0.54	20.46 ± 5.09	3.00 ± 0.00	14.36 ± 1.63	10.27 ± 2.10	2.00 ± 0.00	1.00 ± 0.00	1.09 ± 0.30
Siemens all	17.75 ± 6.66	12.24 ± 4.48	36.58 ± 14.75	11.02 ± 2.40	4.01 ± 0.56	7.19 ± 1.05	25.47 ± 12.62	3.10 ± 0.38	14.63 ± 2.82	11.64 ± 4.55	2.08 ± 0.28	1.05 ± 0.21	1.42 ± 0.50
Total	27.02 ± 18.34	13.15 ± 4.69	33.18 ± 13.09	13.84 ± 7.74	4.43 ± 0.71	8.04 ± 2.50	30.18 ± 15.99	3.59 ± 0.58	20.67 ± 11.58	15.35 ± 7.85	2.62 ± 0.71	1.24 ± 0.43	1.61 ± 0.49

Table E5. Site between-participant coefficients of variation (CVs) and vendor-mean between-participant CVs for quantified metabolites in percentage

Site ID	Asc/tCr	Asp/tCr	GABA/tCr	Glc+Tau/tCr	Glx/tCr	GSH/tCr	Lac/tCr	ml/tCr	PE/tCr	sl/tCr	tCho/tCr	tNAA/tCr
G1	38.45	14.11	28.93	29.51	10.63	14.12	51.74	9.6	31.91	38.82	12.16	12.08
G2	28.22	17.15	26.29	38.9	9.22	14.15	36.87	6.87	25.72	40.31	8.26	4.64
G3	33.71	16.55	47.96	31.14	8.3	19.6	18.45	4.25	35.68	60.58	9.49	6.4
G4	58.83	19.89	32.85	20.54	5.21	16.71	50.83	7.95	25.56	22.01	8.16	5.18
G5	29.99	21.1	22.64	25.54	6.25	11.61	25.78	7.18	23.59	37.41	6.72	5.05
G6	47.42	14.66	35.31	31.7	6.98	11.24	39.95	6.23	29.2	56.15	13.84	5.38
G7	77.75	17.63	24.18	25.49	11.01	29.85	44.48	5.78	40.22	45.61	13.02	5.39
G8	35.96	23.22	42.33	39.06	14.4	30.31	60.04	8.92	37.06	24.24	6.64	4.46
GE Mean	**43.79**	**18.04**	**32.56**	**30.23**	**9**	**18.45**	**41.02**	**7.1**	**31.12**	**40.64**	**9.79**	**6.07**
P1	16.82	7.16	17.58	13.13	7	6.89	21.12	8.06	22.91	27.09	9.58	7.36
P2	38.39	8.55	13.93	15.42	7.8	10.14	21.39	6.09	18.3	36.47	7.97	6.52
P3	46.5	20.67	33.98	24.63	8.17	12.98	32.11	7.19	25.31	23.44	7.47	10.4
P4	33.38	8.7	22.7	25.79	7.5	8.19	19.48	12.08	18.36	43.52	9.92	6.12
P5	47.59	8.28	22.27	20.12	8.42	23.89	28.37	6.6	26.91	32.47	15.06	3.24
P6	79.17	23.57	25.39	52.09	7.25	37.58	31.18	12.27	31	19.95	7.57	6.18
P7	39.08	10.52	53.85	21.12	12.41	9.54	32.19	7.75	25.34	29.78	7.95	5.17
P8	29.18	7.58	39.2	12.16	6.6	6.03	27.94	6.07	20.34	15.71	4.04	3.5
P9	42.49	10.21	21.95	13.92	5.62	14.02	19.29	7.14	20.29	23.32	10.82	6.15
P10	59.48	14.23	37.74	42.21	10.75	24.6	24.75	8.54	25.27	46.03	9.43	4.49
Philips Mean	**43.21**	**11.95**	**28.86**	**24.06**	**8.15**	**15.39**	**25.78**	**8.18**	**23.4**	**29.78**	**8.98**	**5.91**
S1	36.45	31.4	27.24	20.93	4.23	9.4	23.17	7.32	16.63	17.83	6.42	10.47

S2	14.65	25.53	15.52	20.23	8.46	11.02	30.08	4.43	12.78	46.21	13.27	3.7
S3	11.32	9.01	20.33	15.66	6.86	10.24	44.09	6.19	12.9	39.56	7.07	6.69
S4	17.12	8.67	27.72	15.43	7.16	6.13	22.87	7.61	12.37	21.63	11.7	6.24
S5	20.47	21.71	48.54	21.01	7.35	11.01	35.88	8.5	14.61	28.31	8.66	6.36
S6	11.14	16.35	30.8	16.76	5.41	8.69	18.53	6.65	13.79	14.66	12.86	5.94
S7	22.7	15.77	40.77	16.46	6.26	8.88	24.82	5.69	14.84	25.74	10.8	7.61
S8	11.99	7.26	14.93	19.41	5.67	9.12	30.15	5.73	11.24	17.16	12.25	6.17
Siemens Mean	**18.23**	**16.96**	**28.23**	**18.23**	**6.42**	**9.31**	**28.7**	**6.51**	**13.65**	**26.39**	**10.38**	**6.65**

Table E6. Variance partition coefficients (shown as percentages) for site-, vendor- and participant-level effects for the metabolite ratios

	Metabolite											
	Asc/tCr	Asp/tCr	GABA/tCr	Glc+Tau/tCr	Glx/tCr	GSH/tCr	Lac/tCr	mI/tCr	PE/tCr	sI/tCr	tCho/tCr	tNAA/tCr
Vendor	6.40%	Negligible	23.2%*	9.7%*	6.20%	Negligible	0.50%	Negligible	27.1%*	6.0%*	16.0%	3.50%
Site	25.7%*	41.2%*	13.4%*	7.2%*	44.2%*	37.7%*	3.20%	17.1%*	21.4%*	13.4%*	15.3%	29.4%
Participant	67.90%	58.80%	63.40%	83.10%	49.70%	62.30%	96.40%	82.90%	51.50%	80.60%	68.70%	67.10%

	Macromolecule				
	MM09/tCr	MM20/tCr	MM12/tCr	MM14/tCr	MM17/tCr
Vendor	Negligible	0.03	0.009	0.046	8.6%*
Site	13.8%*	37.8%*	5.9%*	14.6%*	0.024
Participant	0.862	0.592	0.931	0.808	0.891

* Significant based on linear mixed effect modeling ($P < .05$).