

Supporting Information (SI) for
Development of a Postcolumn Infused-internal Standard Liquid Chromatography Mass Spectrometry Method for Quantitative Metabolomics Studies

Hsiao-Wei Liao^{a,b}, Guan-Yuan Chen^{a,b}, Ming-Shiang Wu^c, Wei-Chih Liao^c,
Ching-Hung Lin^{*,†,c,d,e}, and Ching-Hua Kuo^{*,†,a,b,f}

^aSchool of Pharmacy, College of Medicine, National Taiwan University, Taiwan

^bThe Metabolomics Core Laboratory, Center of Genomic Medicine, National Taiwan University, Taiwan

^cDepartment of Internal Medicine, National Taiwan University Hospital, Taiwan

^dDepartment of Oncology, National Taiwan University Hospital, Taiwan

^eOncology Center, National Taiwan University Hospital Hsin-Chu Branch, Taiwan

^fDepartment of Pharmacy, National Taiwan University Hospital, Taiwan

*Corresponding Author

Ching-Hung Lin

Address: Department of Oncology, National Taiwan University Hospital, Taiwan(R.O.C.)

Tel:+886.2.3123456 ext 67513

Fax: +886.2.23711174

E-mail:chinghlin@ntu.edu.tw

*Corresponding Author

Ching-Hua Kuo

Address: School of Pharmacy, College of Medicine, National Taiwan University, Rm. 418, 4F., No.33, Linsen S. Rd., Chongsheng Dist., Taipei City 100, Taiwan (R.O.C.)

Tel: +886.2.33668766

Fax: +886.2.23919098

E-mail: kuoch@ntu.edu.tw

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Table S1. The optimized mass spectrometer parameters and MRM transitions for 11 AAs

Compound Name	Precursor Ion (m/z)	Product Ion (m/z)	Fragmentor (V)	Collision Energy (V)
Alanine	90.1	44.2	55	9
Alanine-15N,13C	94.1	47.2	55	9
Glutamate	148.1	130	73	5
Glutamate-15N,13C	154.1	136	73	5
Glutamine	147.1	130	78	5
Glutamine-d5	152.1	135	78	5
Histidine	156.1	110	75	9
Histidine-15N,13C	165.1	118	75	9
Leucine	132.1	86.1	80	5
Leucine-15N,13C	139.1	92.1	80	5
Methionine	150.1	104	60	5
Methionine-15N,13C	156.1	109	60	5
Phenylalanine	166.1	120	88	9
Phenylalanine-15N,13C	176.1	129	88	9
Threonine	120.1	74.1	65	5
Threonine-15N,13C	125.1	78.1	65	5
Tryptophan	205.1	188	83	4
Tryptophan-d5	210.1	192	83	4
Valine	118.1	72.1	50	9
Valine-15N,13C	124.1	77.1	50	9
Phenylalanine-d8	174.1	128.2	95	9

Table S2. Concentration of 16 amino acids in 3 plasma samples quantified by PCI-IS method, and SIL-IS method ($n = 3$ runs, $\mu\text{g mL}^{-1}$).

Plasma sample 1	SIL-IS method	PCI-IS +MNF method
alanine	24.38 \pm 1.73	26.40 \pm 0.64
glutamic acid	3.37 \pm 1.62	3.70 \pm 0.54
glutamine	74.25 \pm 14.08	78.49 \pm 9.67
histidine	8.78 \pm 1.36	10.23 \pm 1.05
leucine/isoleucine	17.93 \pm 0.43	16.22 \pm 0.55
methionine	2.64 \pm 0.39	3.13 \pm 0.06
phenylalanine	8.15 \pm 0.26	8.45 \pm 0.18
threonine	12.58 \pm 3.91	12.93 \pm 0.14
tryptophan	6.09 \pm 1.45	5.45 \pm 0.12
valine	15.88 \pm 1.95	15.01 \pm 0.10

Plasma sample 2	SIL-IS method	PCI-IS +MNF method
alanine	37.62 \pm 1.54	32.63 \pm 3.21
glutamic acid	4.75 \pm 1.63	4.66 \pm 0.76
glutamine	81.81 \pm 16.77	90.94 \pm 7.91
histidine	13.43 \pm 1.26	12.61 \pm 0.37
leucine/isoleucine	26.25 \pm 0.07	24.43 \pm 0.55
methionine	4.53 \pm 0.40	3.37 \pm 0.23
phenylalanine	10.54 \pm 0.13	10.37 \pm 0.38
threonine	20.52 \pm 3.33	19.20 \pm 1.88
tryptophan	12.69 \pm 1.29	14.69 \pm 0.82
valine	23.81 \pm 1.46	22.54 \pm 1.50

Plasma sample 3	SIL-IS method	PCI-IS +MNF method
alanine	32.72 \pm 1.76	28.60 \pm 3.14
glutamic acid	7.40 \pm 0.23	7.22 \pm 1.15
glutamine	63.92 \pm 3.51	63.95 \pm 3.81
histidine	9.47 \pm 0.67	10.89 \pm 0.17
leucine/isoleucine	22.79 \pm 0.48	22.35 \pm 1.17
methionine	3.18 \pm 0.49	3.22 \pm 0.23
phenylalanine	9.84 \pm 0.33	9.50 \pm 0.83
threonine	14.79 \pm 1.02	17.23 \pm 0.78
tryptophan	10.24 \pm 0.25	10.83 \pm 0.31
valine	24.20 \pm 0.33	19.64 \pm 1.61

Before PCI-IS combined with *MNF* correction After PCI-IS combined with *MNF* correction

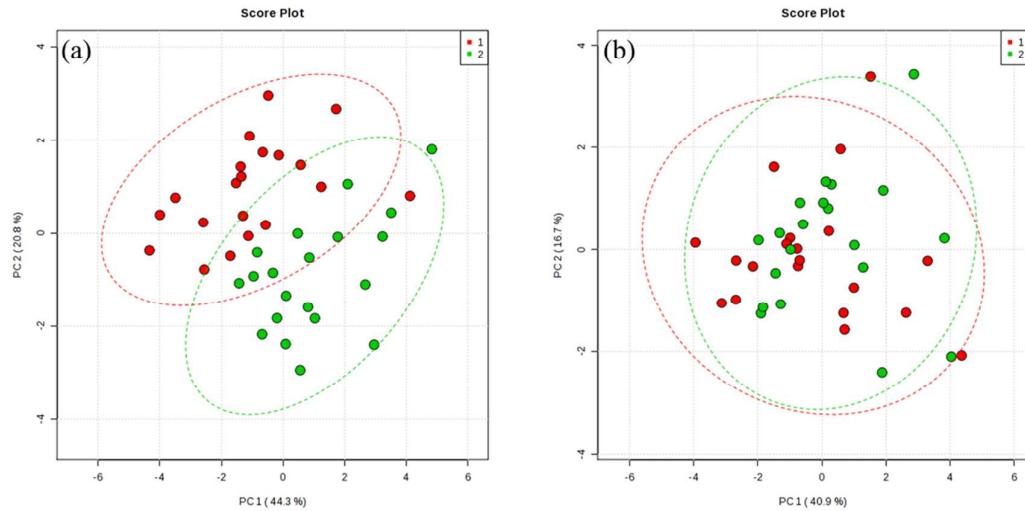


Figure S1. The PCA results of the first 20 samples (red dots) and the last 20 samples (green dots) (a) before and (b) after the implementation of the PCI-IS in combination with *MNF* correction method.