

Table S1. Effect of spectral pretreatments and latent variables on the PLS models of GABA and L-Glu on under 10 equidistant intervals.

Spectral pretreatments	LVs	GABA (g/L)				LV s	L-Glu (g/L)			
		RMSEC	RMSECV	RMSEP	Mean		RMSEC	RMSECV	RMSEP	Mean
Smoothing	11	0.63	1.17	5.30	79.49	10	0.48	0.77	8.25	19.00
Auto	11	0.66	1.22	95.43	79.49	11	0.39	0.77	25.82	19.00
Detrend	13	0.48	1.15	4.07	79.49	8	0.68	0.81	2.12	19.00
SNV	11	1.74	3.19	24.70	79.49	11	0.51	0.91	10.95	19.00
Detrend + SNV	12	1.98	3.47	25.21	79.49	11	0.71	1.08	9.44	19.00
SNV + Detrend	12	1.65	2.78	23.11	79.49	13	0.47	0.98	5.44	19.00
MSC	14	0.88	2.94	17.49	79.49	11	0.58	1.05	11.07	19.00
Der1	7	0.47	1.09	7.97	79.49	6	0.43	0.78	5.23	19.00
Der2	8	0.29	1.19	5.66	79.49	5	0.59	0.84	5.63	19.00
Der1 + Detrend	9	0.45	1.13	4.60	79.49	7	0.56	0.80	2.60	19.00
Der1 + SNV	8	1.11	4.33	22.46	79.49	15	0.01	1.54	7.86	19.00
Der1 + MSC	8	1.86	4.77	16.70	79.49	8	0.42	1.69	5.88	19.00

Table S2. Effect of spectral pretreatments and latent variables on the PLS models of GABA and L-Glu on under 20 equidistant intervals.

Spectral pretreatments	LVs	GABA (g/L)				LV s	L-Glu (g/L)			
		RMSEC	RMSECV	RMSEP	Mean		RMSEC	RMSECV	RMSEP	Mean
Smoothing	12	0.60	1.11	6.93	79.49	7	0.65	0.73	1.63	19.00
Auto	10	0.69	1.15	56.83	79.49	11	0.36	0.70	27.95	19.00
Detrend	15	0.10	0.95	5.20	79.49	10	0.54	0.75	1.95	19.00
SNV	12	0.96	2.70	9.58	79.49	13	0.54	0.90	9.19	19.00
Detrend + SNV	12	1.40	3.25	24.22	79.49	14	0.34	1.01	4.08	19.00
SNV + Detrend	12	1.65	2.78	23.11	79.49	13	0.45	0.91	9.58	19.00
MSC	14	0.71	2.47	4.83	79.49	13	0.46	0.97	8.53	19.00
Der1	7	0.51	1.08	7.76	79.49	6	0.41	0.76	5.34	19.00
Der2	6	0.63	1.20	7.24	79.49	3	0.61	0.76	2.65	19.00
Der1 + Detrend	9	0.28	1.10	6.28	79.49	6	0.51	0.78	1.91	19.00
Der1 + SNV	9	0.86	3.99	27.84	79.49	14	0.02	1.39	7.75	19.00
Der1 + MSC	15	0.06	3.73	36.30	79.49	14	0.04	1.52	4.33	19.00

Table S3. Effect of spectral pretreatments and latent variables on the PLS models of GABA and L-Glu on under 30 equidistant intervals.

Spectral pretreatments	LVs	GABA (g/L)				LV s	L-Glu (g/L)			
		RMSEC	RMSECV	RMSEP	Mean		RMSEC	RMSECV	RMSEP	Mean
Smoothing	13	0.30	0.97	6.83	79.49	13	0.16	0.66	3.54	19.00
Auto	14	0.25	1.00	44.27	79.49	14	0.13	0.62	31.94	19.00
Detrend	15	0.18	1.01	9.29	79.49	11	0.38	0.73	4.77	19.00
SNV	14	0.81	2.29	23.23	79.49	13	0.39	0.86	2.09	19.00
Detrend + SNV	12	1.57	2.91	16.89	79.49	14	0.34	0.82	2.79	19.00
SNV + Detrend	14	1.04	2.46	12.83	79.49	13	0.30	0.78	5.06	19.00
MSC	9	2.22	2.66	10.25	79.49	13	0.44	0.90	2.33	19.00
Der1	15	0.02	0.91	10.75	79.49	12	0.04	0.62	2.97	19.00
Der2	15	0.07	1.08	10.74	79.49	15	0.01	0.62	4.28	19.00
Der1 + Detrend	15	0.02	1.06	4.08	79.49	14	0.08	0.68	1.64	19.00
Der1 + SNV	15	0.05	3.65	37.31	79.49	12	0.33	1.39	10.19	19.00
Der1 + MSC	13	0.20	3.57	11.52	79.49	13	0.08	1.34	5.58	19.00

Table S4. Effect of spectral pretreatments and latent variables on the PLS models of GABA and L-Glu on under 40 equidistant intervals.

Spectral pretreatments	LVs	GABA (g/L)				LV s	L-Glu (g/L)			
		RMSEC	RMSECV	RMSEP	Mean		RMSEC	RMSECV	RMSEP	Mean
Smoothing	14	0.25	0.93	6.71	79.49	12	0.31	0.64	7.24	19.00
Auto	9	0.90	1.11	84.00	79.49	11	0.34	0.67	12.25	19.00
Detrend	15	0.14	0.81	4.20	79.49	14	0.07	0.64	3.29	19.00
SNV	13	0.77	2.16	29.84	79.49	13	0.51	0.83	7.78	19.00
Detrend + SNV	13	1.09	2.94	19.69	79.49	14	0.32	0.86	2.54	19.00
SNV + Detrend	14	0.77	2.39	16.78	79.49	15	0.21	0.69	2.17	19.00
MSC	12	1.81	2.61	26.19	79.49	13	0.58	0.99	9.81	19.00
Der1	15	0.02	0.80	7.82	79.49	15	0.05	0.57	3.43	19.00
Der2	15	0.02	0.90	7.49	79.49	13	0.06	0.56	3.52	19.00
Der1 + Detrend	15	0.04	0.86	6.12	79.49	15	0.05	0.59	2.52	19.00
Der1 + SNV	15	0.09	3.37	32.89	79.49	15	0.02	1.21	7.36	19.00
Der1 + MSC	15	0.10	3.52	23.31	79.49	15	0.04	1.31	3.62	19.00

Table S5. Effect of spectral pretreatments and latent variables on the PLS models of GABA and L-Glu on under 50 equidistant intervals.

Spectral pretreatments	LVs	GABA (g/L)				LV s	L-Glu (g/L)			
		RMSEC	RMSECV	RMSEP	Mean		RMSEC	RMSECV	RMSEP	Mean
Smoothing	14	0.29	0.89	8.24	79.49	13	0.34	0.61	1.27	19.00
Auto	15	0.12	0.79	186.21	79.49	14	0.11	0.54	103.81	19.00
Detrend	15	0.11	0.85	5.66	79.49	11	0.35	0.62	1.52	19.00
SNV	14	0.62	1.93	19.82	79.49	14	0.42	0.82	3.44	19.00
Detrend + SNV	9	2.35	3.17	9.31	79.49	12	0.64	1.03	5.07	19.00
SNV + Detrend	9	2.13	2.78	6.80	79.49	15	0.44	0.91	4.27	19.00
MSC	14	0.83	2.03	17.71	79.49	13	0.55	0.85	2.54	19.00
Der1	15	0.06	0.82	7.87	79.49	15	0.01	0.59	2.88	19.00
Der2	11	0.10	0.96	6.60	79.49	15	0.01	0.55	3.87	19.00
Der1 + Detrend	15	0.03	0.85	9.46	79.49	14	0.02	0.64	3.46	19.00
Der1 + SNV	15	0.10	3.16	33.54	79.49	14	0.05	1.21	8.47	19.00
Der1 + MSC	15	0.22	3.02	11.04	79.49	15	0.14	1.22	2.43	19.00