Supplementary materials

One single amino acid for estimation the content of total free amino acids in *Qingkailing injection* using high-performance liquid chromatography-diode array detection

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Supplementary materials

Table S1: Contents of 14 AAs in different batches of *QKLI*

AAs	113901A		RD[a]	110701A		RD[a]	111203A		RD[a]	110505A		RD[a]	010705A		RD[a]	012907A		RD[a]
	a	b	(%)	a	b	(%)	a	b	(%)	a	b	(%)	a	b	(%)	a	b	(%)
Gly	-	1.100	-	-	1.041	-	-	1.126	-	-	1.013	-	-	1.274	-	-	1.073	-
Asp	0.389	0.384	1.31	0.325	0.319	1.74	0.336	0.331	1.65	0.314	0.308	1.83	0.450	0.446	1.02	0.329	0.323	1.71
Glu	1.031	1.060	-2.70	1.008	1.036	-2.69	1.052	1.081	-2.71	0.987	1.014	-2.68	1.311	1.349	-2.81	1.066	1.096	-2.72
Ser	0.288	0.282	2.17	0.282	0.276	2.17	0.307	0.301	2.16	0.285	0.279	2.17	0.324	0.317	2.15	0.248	0.242	2.18
Arg	0.708	0.722	-1.97	0.511	0.520	-1.90	0.487	0.496	-1.89	0.462	0.471	-1.88	0.654	0.667	-1.96	0.595	0.607	-1.94
Ala	1.122	1.169	-4.06	1.127	1.175	-4.06	1.174	1.224	-4.09	1.120	1.167	-4.05	1.262	1.316	-4.15	1.111	1.158	-4.05
Pro	2.381	2.484	-4.14	2.088	2.176	-4.03	2.687	2.806	-4.23	2.095	2.183	-4.03	2.788	2.912	-4.26	2.398	2.501	-4.15
Tyr	0.23	0.23	-2.58	0.25	0.25	-2.68	0.24	0.25	-2.67	0.23	0.24	-2.62	0.28	0.29	-2.81	0.25	0.25	-2.67

	2	8		0	7		8	5		9	6		3	1		0	7	
Val	0.516	0.544	-5.19	0.503	0.530	-5.16	0.531	0.560	-5.24	0.492	0.519	-5.12	0.529	0.558	-5.23	0.493	0.520	-5.13
Ile	0.254	0.264	-3.78	0.246	0.256	-3.69	0.262	0.272	-3.86	0.242	0.251	-3.64	0.264	0.275	-3.88	0.251	0.261	-3.74
Leu	1.127	1.187	-4.99	1.119	1.177	-4.98	1.201	1.265	-5.06	1.081	1.137	-4.94	1.241	1.308	-5.10	1.120	1.179	-4.98
Phe	0.370	0.389	-5.08	0.372	0.392	-5.09	0.406	0.428	-5.23	0.355	0.374	-5.01	0.431	0.455	-5.32	0.375	0.396	-5.11
Orn	0.326	0.330	-1.32	0.328	0.332	-1.31	0.325	0.329	-1.32	0.303	0.307	-1.36	0.521	0.527	-1.10	0.359	0.363	-1.26
Lys	0.240	0.254	-5.72	0.235	0.250	-5.71	0.228	0.242	-5.68	0.213	0.226	-5.63	0.319	0.339	-5.90	0.247	0.262	-5.74

[a] relative deviation=(a-b)/b

a: the content were calculated by One for M method ; b: the content were determined by the traditional Calibration equation method

Table S2: Contents of 14 AAs in different batches of *QKLI*

AAs	113901A		RD[a]	110701A		RD[a]	111203A		RD[a]	110505A		RD[a]	010705A		RD[a]	012907A		RD[a]
	a	b	(%)	a	b	(%)	a	b	(%)	a	b	(%)	a	b	(%)	a	b	(%)
Gly	-	1.100	-	-	1.041	-	-	1.126	-	-	1.013	-	-	1.274	-	-	1.073	-
Asp	0.385	0.384	0.40	0.322	0.319	0.82	0.333	0.331	0.74	0.311	0.308	0.91	0.446	0.446	0.11	0.326	0.323	0.79
Glu	1.041	1.060	-1.74	1.018	1.036	-1.73	1.062	1.081	-1.75	0.997	1.014	-1.71	1.324	1.349	-1.84	1.076	1.096	-1.75
Ser	0.282	0.282	-0.04	0.276	0.276	-0.04	0.301	0.301	-0.05	0.279	0.279	-0.04	0.317	0.317	-0.05	0.242	0.242	-0.02
Arg	0.713	0.722	-1.31	0.514	0.520	-1.25	0.490	0.496	-1.23	0.466	0.471	-1.22	0.658	0.667	-1.30	0.599	0.607	-1.28
Ala	1.159	1.169	-0.83	1.165	1.175	-0.84	1.213	1.224	-0.87	1.157	1.167	-0.83	1.304	1.316	-0.93	1.148	1.158	-0.82
Pro	2.515	2.484	1.25	2.206	2.176	1.37	2.838	2.806	1.15	2.213	2.183	1.37	2.945	2.912	1.13	2.532	2.501	1.24
Tyr	0.24	0.23	0.54	0.25	0.25	0.45	0.25	0.25	0.46	0.24	0.24	0.50	0.29	0.29	0.31	0.25	0.25	0.45

	0	8		9	7		6	5		7	6		2	1		8	7	
Val	0.539	0.544	-0.91	0.525	0.530	-0.87	0.555	0.560	-0.95	0.514	0.519	-0.84	0.553	0.558	-0.95	0.515	0.520	-0.84
Ile	0.265	0.264	0.31	0.257	0.256	0.40	0.273	0.272	0.22	0.253	0.251	0.45	0.276	0.275	0.20	0.261	0.261	0.35
Leu	1.184	1.187	-0.21	1.175	1.177	-0.20	1.261	1.265	-0.29	1.135	1.137	-0.16	1.303	1.308	-0.33	1.176	1.179	-0.21
Phe	0.394	0.389	1.26	0.397	0.392	1.25	0.433	0.428	1.10	0.379	0.374	1.34	0.460	0.455	1.01	0.400	0.396	1.24
Orn	0.328	0.330	-0.62	0.330	0.332	-0.61	0.327	0.329	-0.62	0.305	0.307	-0.66	0.525	0.527	-0.40	0.361	0.363	-0.56
Lys	0.245	0.254	-3.50	0.241	0.250	-3.49	0.233	0.242	-3.46	0.218	0.226	-3.41	0.326	0.339	-3.69	0.253	0.262	-3.52

[a] relative deviation=(a-b)/b

a: the content were calculated by One for M method ; b: the content were determined by the traditional Calibration equation method

Table S3: Contents of 14 AAs in different batches of *QKLI*

AAs	113901A		RD[a]	110701A		RD[a]	111203A		RD[a]	110505A		RD[a]	010705A		RD[a]	012907A		RD[a]
	a	b	(%)	a	b	(%)	a	b	(%)	a	b	(%)	a	b	(%)	a	b	(%)
Gly	-	1.100	-	-	1.041	-	-	1.126	-	-	1.013	-	-	1.274	-	-	1.073	-
Asp	0.386	0.384	0.69	0.323	0.319	1.17	0.334	0.331	1.07	0.312	0.308	1.28	0.447	0.446	0.36	0.327	0.323	1.13
Glu	1.037	1.060	-2.11	1.014	1.036	-2.11	1.058	1.081	-2.11	0.993	1.014	-2.10	1.320	1.349	-2.14	1.073	1.096	-2.11
Ser	0.286	0.282	1.15	0.279	0.276	1.17	0.304	0.301	1.07	0.282	0.279	1.16	0.320	0.317	1.00	0.246	0.242	1.36
Arg	0.711	0.722	-1.62	0.512	0.520	-1.66	0.488	0.496	-1.67	0.463	0.471	-1.68	0.656	0.667	-1.63	0.597	0.607	-1.64
Ala	1.146	1.169	-1.95	1.152	1.175	-1.95	1.200	1.224	-1.94	1.144	1.167	-1.95	1.291	1.316	-1.92	1.135	1.158	-1.96
Pro	2.477	2.484	-0.26	2.168	2.176	-0.36	2.801	2.806	-0.19	2.176	2.183	-0.36	2.907	2.912	-0.17	2.495	2.501	-0.26
Tyr	0.23	0.23	-1.23	0.25	0.25	-1.19	0.25	0.25	-1.19	0.24	0.24	-1.21	0.28	0.29	-1.14	0.25	0.25	-1.19

	6	8		4	7		2	5		3	6		8	1		4	7	
Val	0.531	0.544	-2.43	0.517	0.530	-2.43	0.547	0.560	-2.43	0.506	0.519	-2.43	0.545	0.558	-2.43	0.507	0.520	-2.43
Ile	0.261	0.264	-1.18	0.253	0.256	-1.14	0.269	0.272	-1.22	0.249	0.251	-1.12	0.272	0.275	-1.23	0.258	0.261	-1.17
Leu	1.167	1.187	-1.67	1.158	1.177	-1.68	1.244	1.265	-1.66	1.118	1.137	-1.68	1.286	1.308	-1.66	1.159	1.179	-1.68
Phe	0.383	0.389	-1.65	0.386	0.392	-1.64	0.421	0.428	-1.55	0.368	0.374	-1.70	0.448	0.455	-1.49	0.389	0.396	-1.64
Orn	0.327	0.330	-1.14	0.329	0.332	-1.14	0.326	0.329	-1.15	0.304	0.307	-1.23	0.523	0.527	-0.73	0.360	0.363	-1.04
Lys	0.243	0.254	-4.58	0.238	0.250	-4.59	0.231	0.242	-4.60	0.216	0.226	-4.62	0.323	0.339	-4.50	0.250	0.262	-4.57

[a] relative deviation=(a-b)/b

a: the content were calculated by One for M method ; b: the content were determined by the traditional Calibration equation method

Table S4: Contents of 14 AAs in different batches of *QKLI*

AAs	113901A		RD [a]	110701A		RD [a]	111203A		RD [a]	110505A		RD [a]	010705A		RD [a]	012907A		RD [a]
	a	b	(%)	a	b	(%)	a	b	(%)	a	b	(%)	a	b	(%)	a	b	(%)
Gly	-	1.100	-	-	1.041	-	-	1.126	-	-	1.013	-	-	1.274	-	-	1.073	-
Asp	0.392	0.384	2.19	0.329	0.319	2.98	0.340	0.331	2.82	0.318	0.308	3.15	0.453	0.446	1.65	0.333	0.323	2.92
Glu	1.044	1.060	-1.51	1.021	1.036	-1.49	1.065	1.081	-1.52	0.999	1.014	-1.48	1.327	1.349	-1.67	1.079	1.096	-1.53
Ser	0.290	0.282	2.77	0.284	0.276	2.83	0.308	0.301	2.59	0.287	0.279	2.80	0.325	0.317	2.45	0.250	0.242	3.25
Arg	0.718	0.722	-0.64	0.519	0.520	-0.30	0.495	0.496	-0.25	0.470	0.471	-0.18	0.663	0.667	-0.56	0.604	0.607	-0.47
Ala	1.150	1.169	-1.65	1.156	1.175	-1.65	1.204	1.224	-1.65	1.148	1.167	-1.65	1.295	1.316	-1.65	1.139	1.158	-1.65
Pro	2.48	2.48	-0.09	2.17	2.17	-0.16	2.80	2.80	-0.03	2.18	2.18	-0.16	2.91	2.91	-0.02	2.49	2.50	-0.09

	1	4		3	6		5	6		0	3		2	2		9	1	
Tyr	0.242	0.238	1.62	0.261	0.257	1.45	0.259	0.255	1.46	0.249	0.246	1.55	0.295	0.291	1.19	0.261	0.257	1.45
Val	0.535	0.544	-1.55	0.522	0.530	-1.53	0.551	0.560	-1.57	0.511	0.519	-1.51	0.550	0.558	-1.57	0.512	0.520	-1.51
Ile	0.266	0.264	0.74	0.258	0.256	0.84	0.274	0.272	0.64	0.254	0.251	0.90	0.277	0.275	0.61	0.263	0.261	0.78
Leu	1.172	1.187	-1.25	1.163	1.177	-1.25	1.249	1.265	-1.26	1.123	1.137	-1.24	1.291	1.308	-1.27	1.164	1.179	-1.25
Phe	0.389	0.389	-0.06	0.392	0.392	-0.06	0.427	0.428	-0.10	0.374	0.374	-0.04	0.454	0.455	-0.13	0.395	0.396	-0.07
Orn	0.330	0.330	-0.11	0.332	0.332	-0.11	0.329	0.329	-0.11	0.307	0.307	-0.11	0.526	0.527	-0.08	0.363	0.363	-0.10
Lys	0.246	0.254	-3.31	0.241	0.250	-3.29	0.234	0.242	-3.26	0.219	0.226	-3.19	0.327	0.339	-3.54	0.254	0.262	-3.34

[a] relative deviation=(a-b)/b

a: the content were calculated by One for M method ; b: the content were determined by the traditional Calibration equation method

Table S5: RCFs in different instruments and columns

AAs	Agilent			RSD %	Wasters			RSD %
	luna column	Hypersil column	Diamonsi column		luna column	Hypersil column	Diamonsi column	
Asp	0.564	0.560	0.542	2.14	0.548	0.545	0.572	2.67
Glu	0.502	0.497	0.490	1.23	0.483	0.488	0.507	2.53
Ser	0.691	0.688	0.695	0.51	0.693	0.690	0.693	0.24
Arg	0.452	0.441	0.444	1.23	0.456	0.451	0.471	2.27
Ala	0.890	0.881	0.876	0.80	0.885	0.877	0.885	0.48
Pro	0.734	0.724	0.733	0.74	0.685	0.673	0.683	0.91
Tyr	0.468	0.464	0.466	0.37	0.472	0.468	0.470	0.41
Val	0.674	0.663	0.650	1.80	0.680	0.673	0.678	0.52
Ile	0.631	0.647	0.613	2.68	0.655	0.655	0.611	3.96
Leu	0.633	0.637	0.623	1.11	0.641	0.639	0.642	0.23
Phe	0.512	0.512	0.511	0.14	0.520	0.518	0.517	0.25
Orn	0.935	0.929	0.932	0.33	0.940	0.931	0.941	0.57
Lys	0.972	0.977	0.945	1.82	0.975	0.977	0.988	0.75