THE APPLICATION OF AUTOMATED CORRELATION OPTIMIZED WARPING TO THE QUALITY EVALUATION OF *Radix Puerariae thomsonii*: CORRECTING RETENTION TIME SHIFT IN THE CHROMATOGRAPHIC FINGERPRINTS

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Table 1S. Result of reproducibility test of puerarin

No.	Concentration of puerarin (μg mL^{-1})	RSD (%)
1	35.52	2.0
2	34.00	
3	35.46	
4	35.03	
5	34.22	
6	34.21	

Table 2S. Result of reproducibility test of daidzein

No.	Concentration of daidzein (μg mL^{-1})	RSD (%)
1	3.13	2.6
2	3.09	
3	2.93	
4	3.07	
5	2.95	
6	3.06	

Table 3S. Result of repeatability test of puerarin

No.	Concentration of puerarin (μg mL^{-1})	RSD (%)
1	35.04	1.1
2	35.64	
3	35.76	
4	34.83	
5	34.88	
6	35.34	

Table 4S. Result of repeatability test of daidzein

No.	Concentration of daidzein (μg mL^{-1})	RSD (%)
1	3.13	1.9
2	3.06	
3	3.07	
4	3.11	
5	3.22	
6	3.14	

Table 5S. Result of stability test of puerarin

No.	Concentration of puerarin (μg mL^{-1})	RSD (%)
1	35.59	1.7
2	34.72	
3	35.79	
4	35.27	
5	34.92	
6	34.22	

Table 6S. Result of stability test of daidzein

No.	Concentration of daidzein (μg mL^{-1})	RSD (%)
1	3.06	1.0
2	3.07	
3	2.97	
4	3.04	
5	2.99	
6	3.02	

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Table 7S. Result of recovery test of puerarin

No.	Spiked (μg·mL^{-1})	Found (μg mL^{-1})	Recovery (%)	Average Recovery (%)	RSD (%)
1	14.48	14.94	103.0	101.3	1.9
2	14.48	14.79	102.0		
3	18.35	18.84	102.5		
4	18.35	18.82	102.4		
5	22.22	21.85	98.4		
6	22.22	22.09	99.5		

Table 8S. Result of recovery test of daidzein

No.	Spiked (μg·mL^{-1})	Found (μg mL^{-1})	Recovery (%)	Average Recovery (%)	RSD (%)
1	1.47	1.49	101.5	99.4	2.5
2	1.47	1.44	97.6		
3	1.84	1.85	100.5		
4	1.84	1.89	102.6		
5	2.21	2.14	96.7		
6	2.21	2.16	97.6		

Table 9S. Correlation coefficient between the standard sample and 27 samples

Group	No. of samples	Alignment1[a]		Alignment2[b]		Alignment3[c]	
		Correlation coefficient	Standard deviation	Correlation coefficient	Standard deviation	Correlation coefficient	Standard deviation
A	A1	0.9416	0.0254	0.9552	0.0123	0.9502	0.0005
	A2	0.9498		0.9335		0.9502	
	A3	0.9023		0.9342		0.9494	
B	B1	0.8853	0.0041	0.8747	0.0172	0.8363	0.0345
	B2	0.8933		0.8424		0.9003	
	B3	0.8911		0.8685		0.8908	
C	C1	0.9487	0.0008	0.9221	0.0052	0.9454	0.0055
	C2	0.9472		0.9185		0.9399	
	C3	0.9475		0.9287		0.9509	
D	D1	0.9682	0.0006	0.9685	0.0057	0.9673	0.0042
	D2	0.9669		0.9626		0.9590	
	D3	0.9679		0.9570		0.9642	
E	E1	0.9379	0.0049	0.9047	0.0075	0.9294	0.0038
	E2	0.9362		0.9181		0.9363	
	E3	0.9454		0.9174		0.9301	
F	F1	0.9704	0.0011	0.9730	0.0035	0.9671	0.0019
	F2	0.9683		0.9683		0.9683	
	F3	0.9693		0.9661		0.9708	
G	G1	0.9348	0.0044	0.9068	0.0141	0.9137	0.0043
	G2	0.9281		0.9216		0.9066	
	G3	0.9266		0.9350		0.9058	
H	H1	0.8762	0.0045	0.8361	0.0011	0.8481	0.0013
	H2	0.8737		0.8374		0.8505	
	H3	0.8675		0.8352		0.8502	
I	I1	0.9117	0.0017	0.8852	0.0060	0.8917	0.0015
	I2	0.9109		0.8969		0.8947	
	I3	0.9141		0.8929		0.8937	

[a]The fingerprints were aligned at *segment length*=30 and *slack size*=15. [b]The fingerprints were aligned at *segment length*=55 and *slack size*=2. [c]The fingerprints were aligned at *segment length*=55 and *slack size*=15.

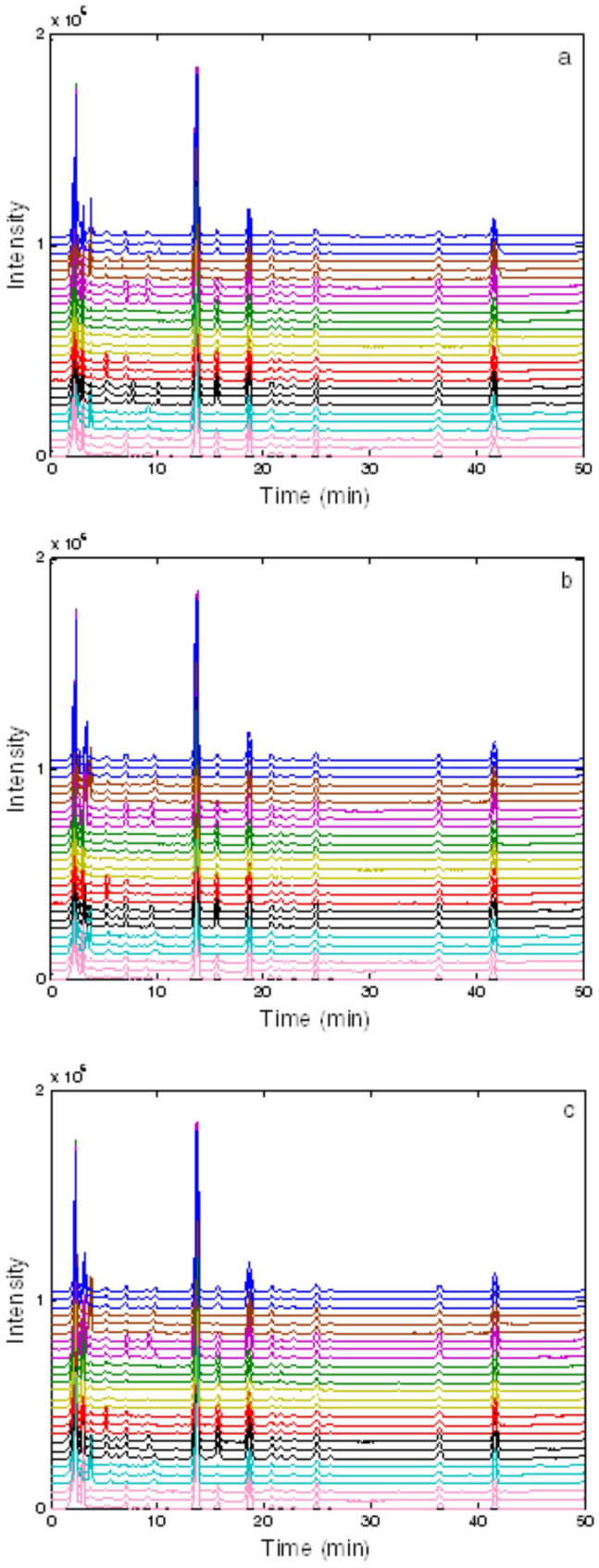

Figure 1S. *Chromatographic fingerprints of RPT samples (a) after Alignment1; (b) after Alignment2; (c) after Alignment3. The chromatographic profile from bottom to up is the fingerprint of A1, A2, A3, B1 …… to I3 respectively*

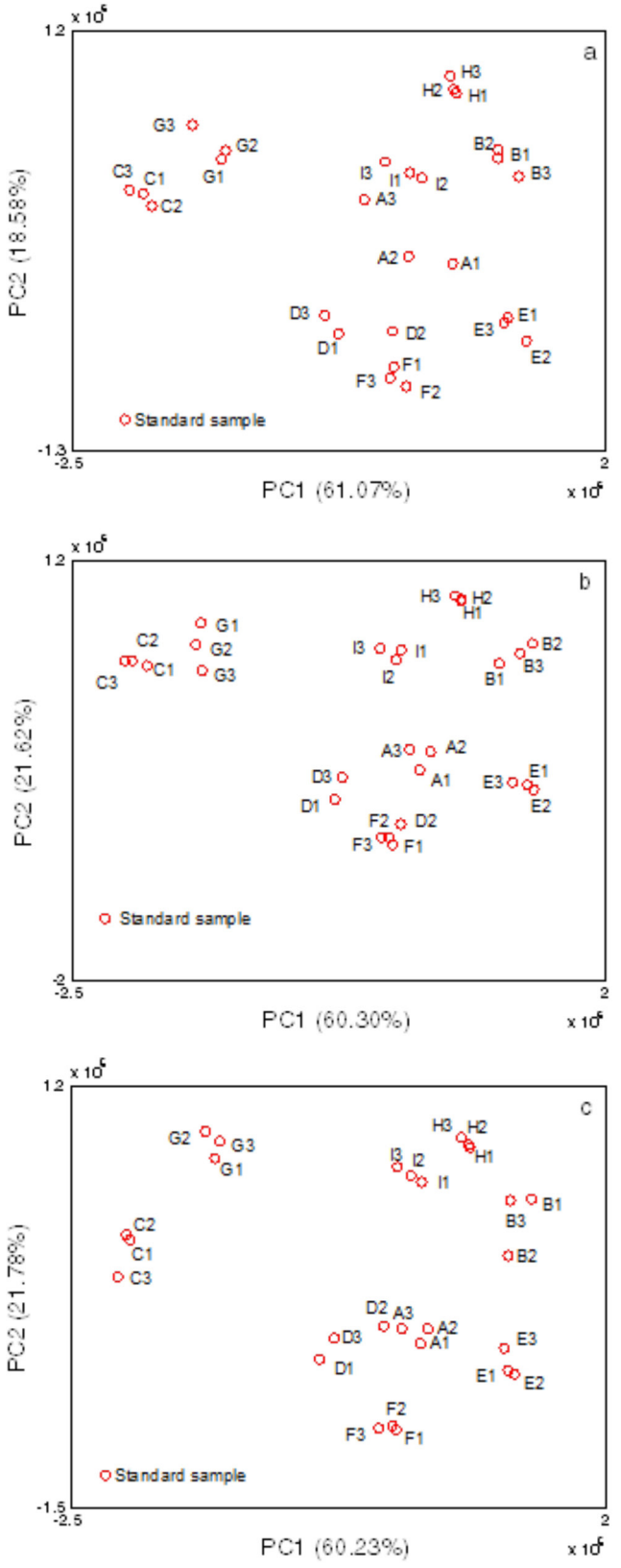

Figure 2S. *Score plot of PCA resulted from (a) fingerprints after Alignment1; (b) fingerprints after Alignment2; (c) fingerprints after Alignment3*