Supporting information

Standardization of Raman Spectra using Variable Penalty Dynamic Time Warping

Qingyu Xu[1], Hongju Chen [2], Shaoqing Ye[2], Yongming Zeng[2], Hongmei Lu[1], Zhimin Zhang[1,*]

1. College of Chemistry and Chemical Engineering, Central South University, Changsha 410083, PR China.

2. Xiamen PERSer Nanotechnology Co. Ltd., Xiamen 361005, China

E-mail: zmzhang@csu.edu.cn

Contents:

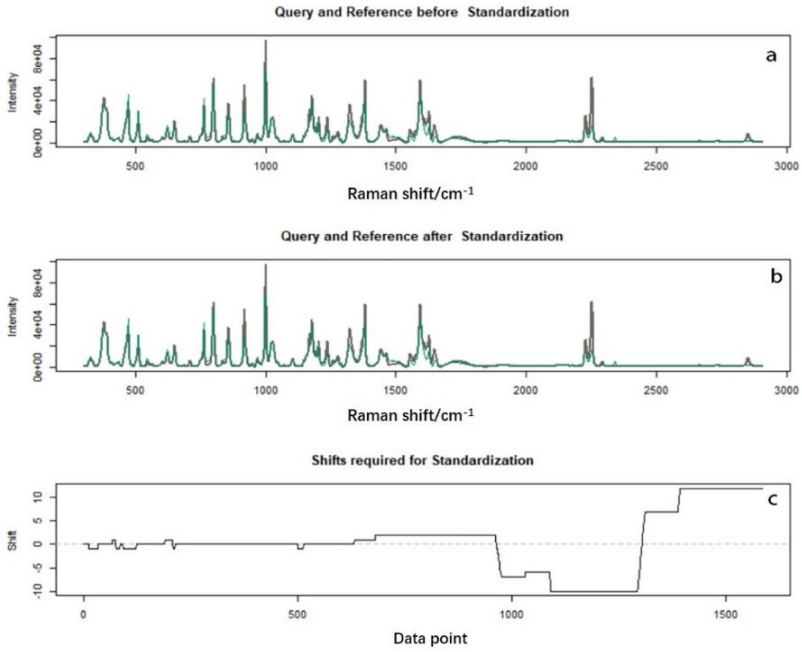

Fig.S1 Standardization result and warping path between i-Raman Plus / PERS-D900-R spectrometer. (a-b) the fused spectra of i-Raman Plus/ PERS-D900-R, which before and after standardization (c) Warping path between i-Raman Plus/ PERS-D900-R spectrometer.

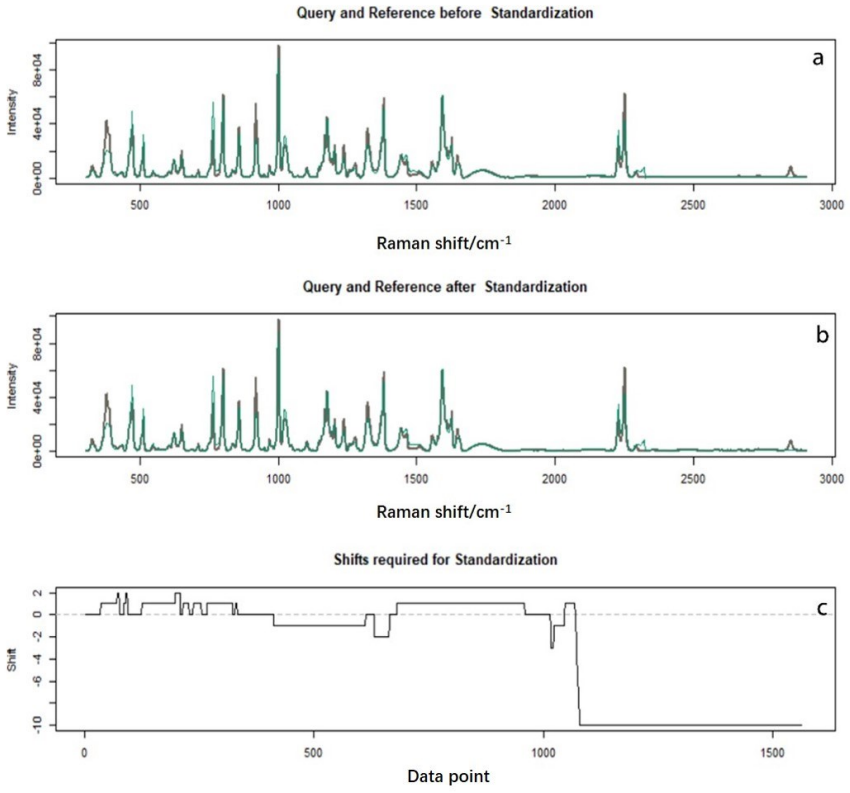

Fig.S2 Standardization result and warping path between i-Raman Plus / A5 268137R spectrometer. (a-b) the fused spectra of i-Raman Plus,/ A5 268137R which before and after standardization (c) Warping path between i-Raman Plus,/ A5 268137R spectrometer.

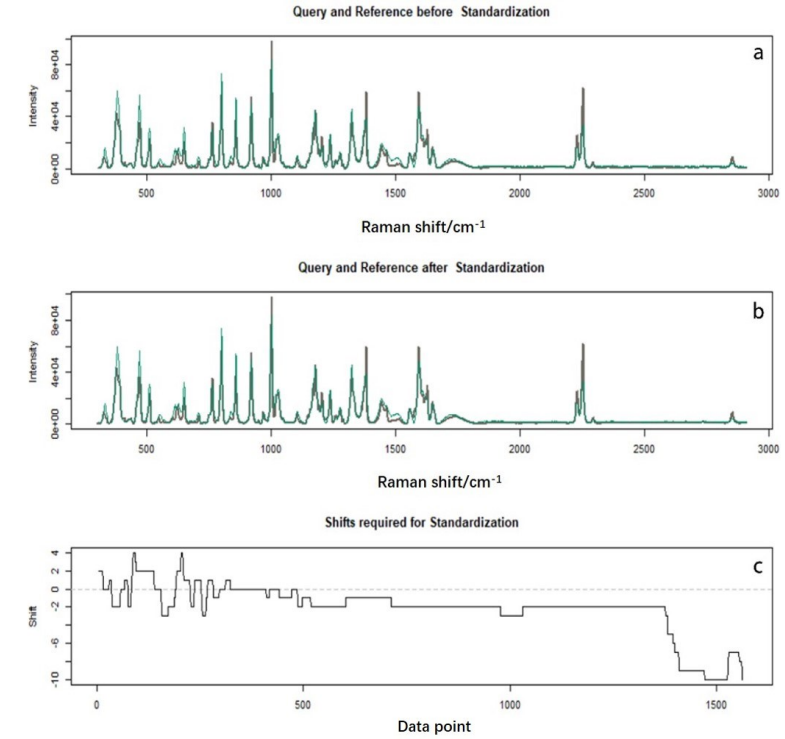

Fig.S3 Standardization result and warping path between i-Raman Plus / PERS-F900 spectrometer. (a-b) the fused spectra of i-Raman Plus,/ PERS-F900, which before and after standardization (c) Warping path between i-Raman Plus,/ PERS-F900 spectrometer.

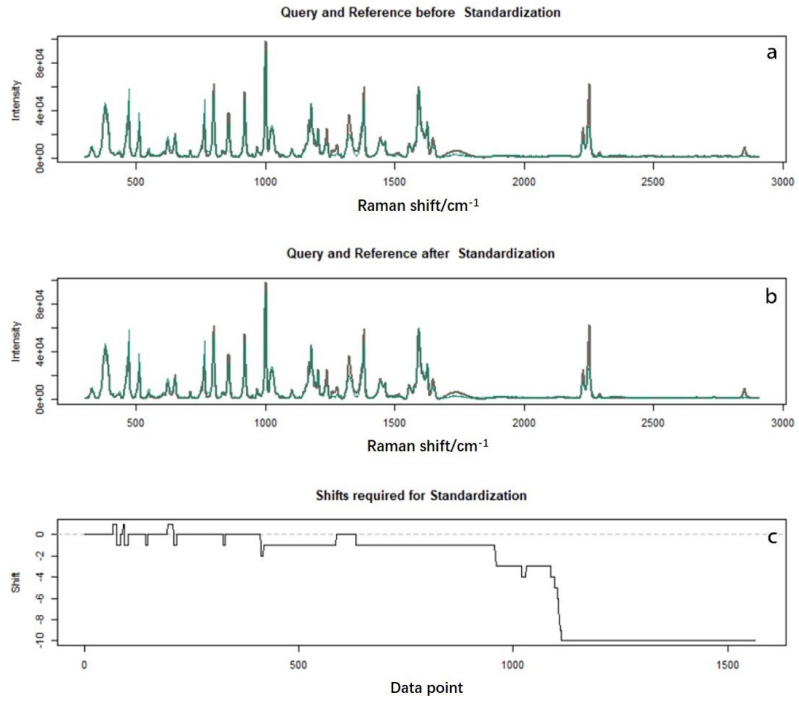

Fig.S4 Standardization result and warping path between i-Raman Plus / PERS-D600 spectrometer. (a-b) the fused spectra of i-Raman Plus / PERS-D600, which before and after standardization (c) Warping path between i-Raman Plus / PERS-D600 spectrometers.

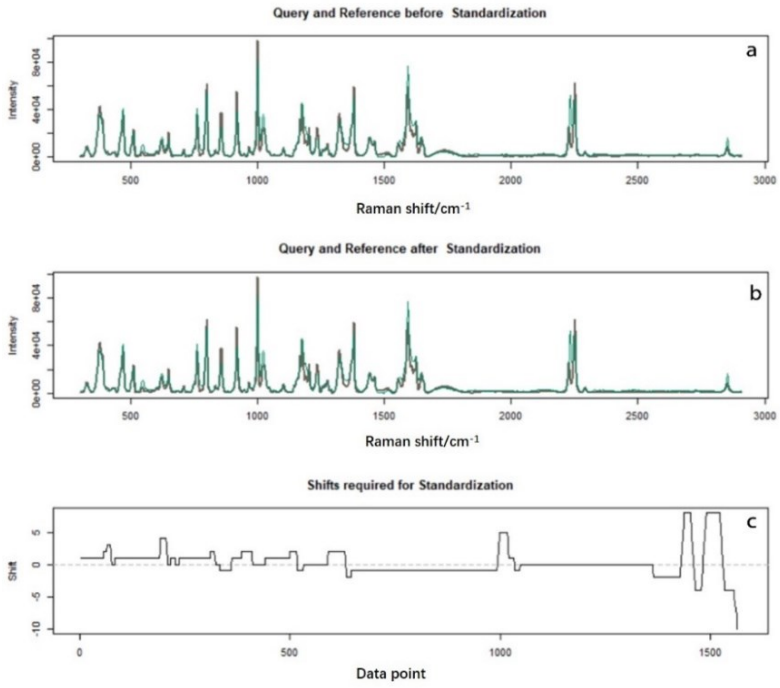

Fig.S5 Standardization result and warping path between i-Raman Plus / PERS-SR530 spectrometer. (a-b) the fused spectra of i-Raman Plus / PERS-SR530, which before and after standardization (c) Warping path between i-Raman Plus / PERS-SR530 spectrometer.

Table S1. Details of the standardized results of each group of Raman instruments
Please see "Table S1.xlsx" for more details

Table S2. Results of Raman standardization between RS-VPdtw and MWFFT
Please see "Table S2.xlsx" for more details

Table S3. The resules of control experiment using RS-VPdtw

i-Raman Plus	PERS-F900	
	Samples	After
aspirin	Pymetrozine	0.4736
	acetone	0.0864
	carbendazim	0.1625
	Enrofloxacin	0.2465
	ascorbic acid	0.1087
	hexamethylenetetramine	0.1747
	Chloramphenicol	0.0402
	Lemon yellow	0.1634
	Trichloromethane	0.0213
	Sudan 1	0.1432
	Sodium nitrate	0.0278
	Ethanol	0.0521

Table S4. MWFFT standardized results preprocessed by airPLS and ALS method

Samples	RS-VPdtw	MWFFT	
		airPLS	ALS
aspirin	0.9553	0.8785	0.8968
Pymetrozine	0.9571	0.8344	0.8516
acetone	0.991	0.9684	0.9770
carbendazim	0.9842	0.8454	0.8562
Enrofloxacin	0.9677	0.9366	0.9603
ascorbic acid	0.9707	0.9461	0.9601
hexamethylenetetramine	0.9514	0.9055	0.8597
Chloramphenicol	0.9834	0.9585	0.9435
Lemon yellow	0.9879	0.9643	0.9785
Trichloromethane	0.9688	0.9512	0.8974
Sudan 1	0.9189	0.9553	0.9143
Sodium nitrate	0.9705	0.9059	0.9079
Ethanol	0.9679	0.9598	0.9650