Portable and benchtop Raman spectrometers coupled to cluster analysis to identify quinine sulfate polymorphs in solid dosage forms and antimalarial drug quantification in solution by AuNPs-SERS with MCR-ALS

Supplementary material

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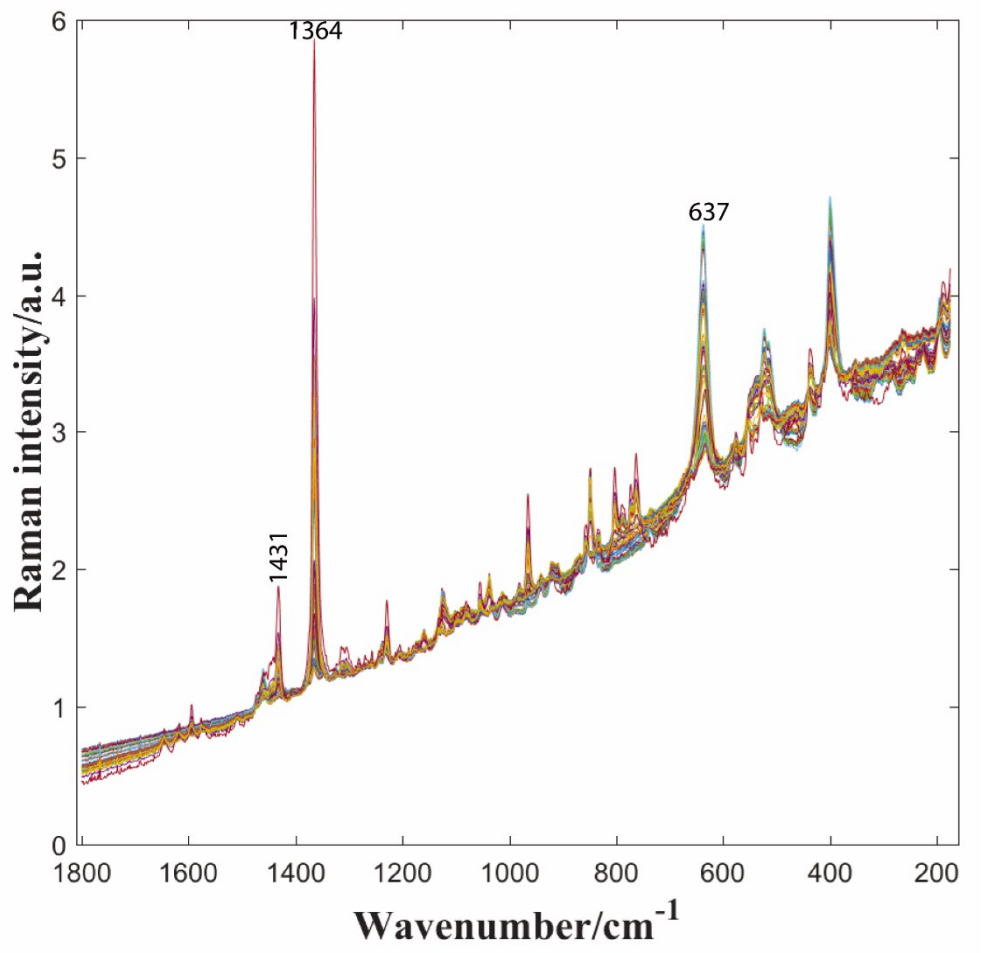

Fig. S1. Raman spectra of 80 commercial quinine sulfate solid dosage forms collected by a portable backscattering Raman spectrometer with excitation laser of 785 nm.

Table S1. MCR-ALS model with concentration correlation constraint on component 2 (quinine sulfate).

Known concentration (C_known) for component 2 in the system (quinine sulfate) used during the concentration correlation constraint on concentration direction, because the first three samples are related to calibration set while sample number four is related to a test sample:

Nan 150.00

Nan 175.00

Nan 200.00

Nan Nan

After the alternating least-squares (ALS) optimization achieves convergence, under application of the various restrictions, the MCR-ALS model reports (output) the concentration and spectra profile as 'copt' and 'sopt', respectively. NaN (Not-a-Number) is the Matlab notation for missing values.

Then, in order to assessment the prediction capacity of the model the authors employed the following commands in Matlab:

```
%Analytical Chemistry

Figure

plot(C_know_2(1:3,2),copt(1:3,2),'-o')
slope=pinv(C_know_2(1:3,2))*copt(1:3,2)
ypred=copt(4,2)/slope
xc=C_know_2(1:3,2);
yc=copt(1:3,2);
CC=corrcoef([xc yc]),R2=CC(1,2)
load C_test_1.txt%containing nominal concentration for test sample
number 1 as: 180.00 ng mL-1
ytest=C_test_1
```