Supplementary information

Label-free detection of cytotoxicity effect of cisplatin in human leukemic cells using Raman spectroscopy in conjunction with multivariate analysis

Weiwei Chen, [*a] Shenghe Weng, [*a] Weixiong Zhong, [a] Hao Huang, [b] Chuanhe Yang, [a] Jian Yang, [a] Liangling Ye, [a] Wenshan Chen, [a] Chunge Song, [a] Shiyuan Du, [a] Xiaohu Chen, [a] and Yun Yu[*b]

[a] School of Medical Technology and Engineering, Fujian Health College, Fuzhou, 350101, China. E-mail: wwchen072@163.com; shengheweng3322@163.com

[b] College of Integrative Medicine, Laboratory of Pathophysiology, Key Laboratory of Integrative Medicine on Chronic Diseases (Fujian Province University), Synthesized Laboratory of Integrative Medicine, Fujian University of Traditional Chinese Medicine, Fuzhou, 350122, China. E-mail: yuyunsatan@163.com

For detection, the laser was applied to the entire cell (as shown in Fig. S1). An average Raman spectrum was generated after 10 detections per cell, and a total of 300 cells were divided into 10 groups to obtain a total of 300 average spectra. Specific cellular assay details are shown in Table S1.

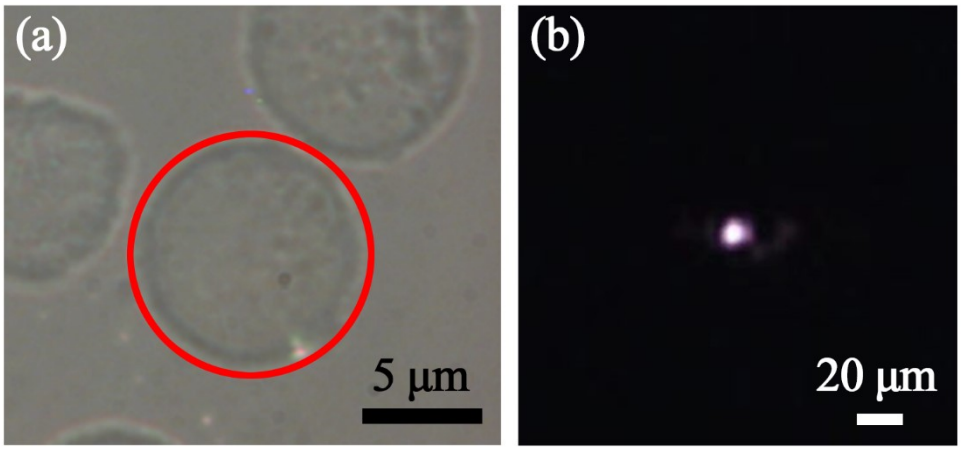

Fig.S1 Micrographs of cells treated with 10.5 μmol/L cisplatin under white light (a) and laser (b).

Table S1. Details of cellular assay

Groups	Number of tested cell per group	Number of spectral detections per cell	Average spectrum used per cell	Entire cell measurements
0 μmol/L	30	10	√	√
3.5 μmol/L	30	10	√	√
7.0 μmol/L	30	10	√	√
10.5 μmol/L	30	10	√	√
14.0 μmol/L	30	10	√	√
0 hour	30	10	√	√
6 hours	30	10	√	√
12 hours	30	10	√	√
24 hours	30	10	√	√
36 hours	30	10	√	√

As can be seen in Fig. S2, guanine has a characteristic band at 1303 cm^{-1} in its Raman spectrum, so the 1303 cm^{-1} band in Fig. 1 and 4 was assigned to guanine.

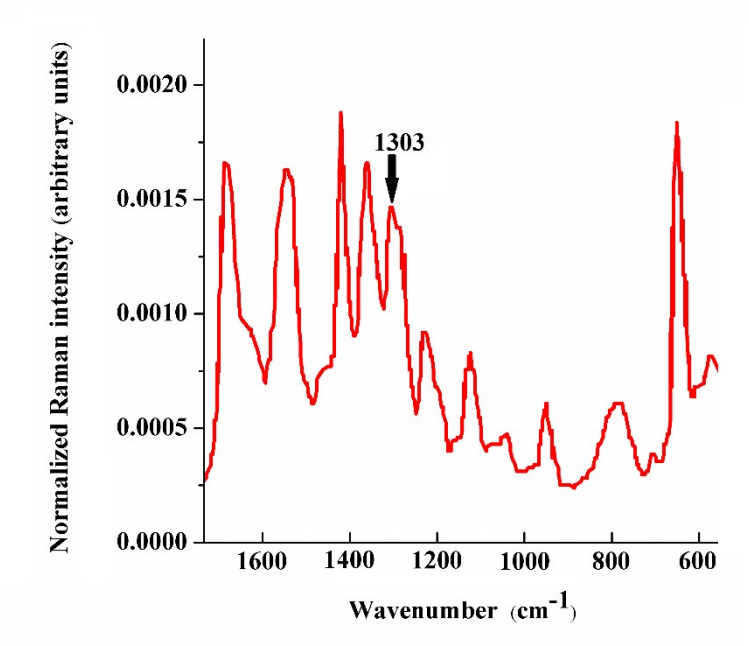

Fig. S2 Raman spectrum of guanine.

Code：

```
x=xlsread('c:/2.xlsx');
y=xlsread('c:/1.xlsx');
[XL,YL,XS,YS,BETA,PCTVAR,MSE,stats] = plsregress(x,y,20,'cv',10);
add=cumsum(100*PCTVAR(2,:))；
figure
plot(1:20,cumsum(100*PCTVAR(2,:)),'-bo');
xlabel('Number of PLS components');
ylabel('Percent Variance Explained');
figure
plot(0:20, (MSE(2,:)),'-bo');
xlabel('Number of PLS components');
ylabel('Estimated mean squared prediction error');
a=XS(:,1:2);
b=xlsread('c:/1.xlsx');
test=XS(:,1:2);
y_test=xlsread('c:/1.xlsx');
[train,pstrain] = mapminmax(a',-1 ,1);
x1 = train';
[train_labels,pslabels] = mapminmax(b',-1 ,1);
y1=train_labels';
[test_w,pstest] = mapminmax(test',-1 ,1);
test1 = test_w';
[test_w_labels,pslabels] = mapminmax(y_test',-1 ,1);
y_test1 = test_w_labels';
[bestacc,bestc,bestg] = SVMcg(y1,x1,-10,10,-10,10,10,1,1,0.5);
cmd = ['-c ',num2str(bestc),' -g ',num2str(bestg)];
model = libsvmtrain(y1,x1,cmd);
[predict_label, accuracy, decision_values] = libsvmpredict(y_test1, test1, model);
```