Electronic Supplementary Material (ESI) for Analytical Methods.
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Supporting Information

Surface-enhanced Raman spectroscopy for rapid identification and quantification of Flibanserin in different kinds of wine

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1. Repeatability and stability of SERS measurement

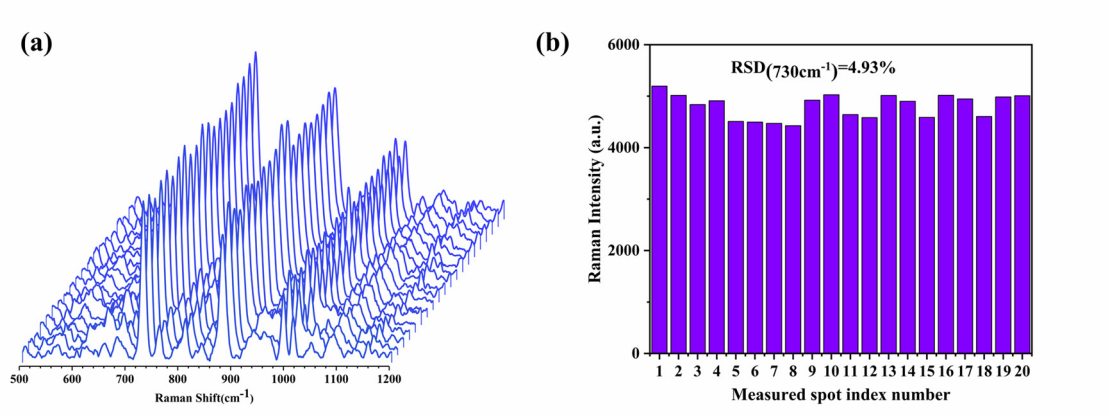

Figure S1 (a) SERS spectra of Flibanserin liquor solution were measured for 20 times under the same condition, (b) Histogram of Raman intensity of Flibanserin characteristic peak.

2. Comparison of PCA and TSNE dimensionality reduction algorithms and SVM classification boundary visualization

We compared the results of PCA dimensionality reduction algorithm with those of other dimensionality reduction algorithms represented by TSNE. The results are shown in Figure S2-S5. After dimensionality reduction is performed on 4 data sets while retaining 2 principal components or dimensions, the dimensionality reduction results of PCA algorithm and TSNE algorithm are similar. According to the previous analysis, if the SVM classifier wants to achieve a good classification effect, it needs to retain a relatively large number of principal components. The PCA algorithm has a clear advantage in this aspect. The TSNE algorithm is more focused on the display of visualized results and generally can retain up to 3 dimensions. Then we input the datasets processed by PCA into the SVM for classification, and the results are shown in Table S1. Table S1 shows that the accuracy of the PCA-SVM model can be higher when the 90% variance is retained, so the PCA-SVM model is selected as the quantitative analysis method.

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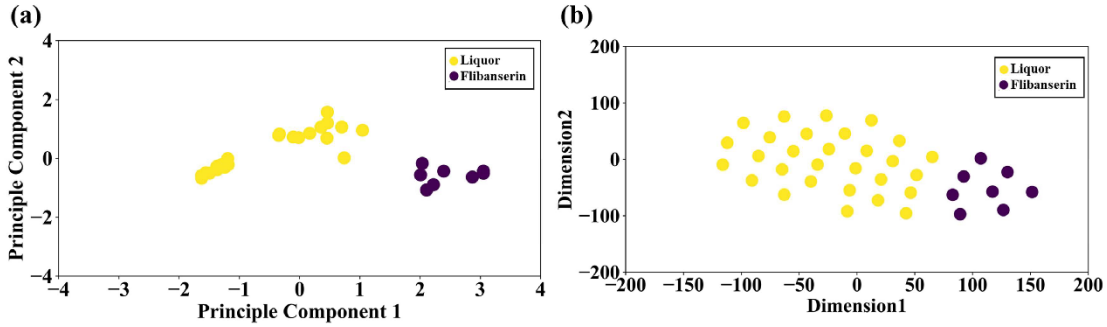

Figure S2 The results of dimensionality reduction of Flibanserin liquor dataset by PCA and TSNE algorithms. (a) PCA score of Flibanserin liquor dataset, (b) TSNE dimensionality reduction result of Flibanserin liquor dataset.

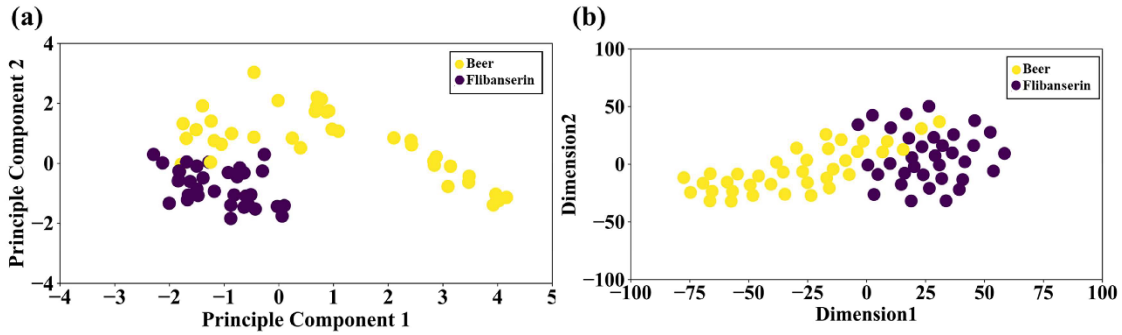

Figure S3 The results of dimensionality reduction of Flibanserin beer dataset by PCA and TSNE algorithms. (a) PCA score of Flibanserin beer dataset, (b) TSNE dimensionality reduction result of Flibanserin beer dataset.

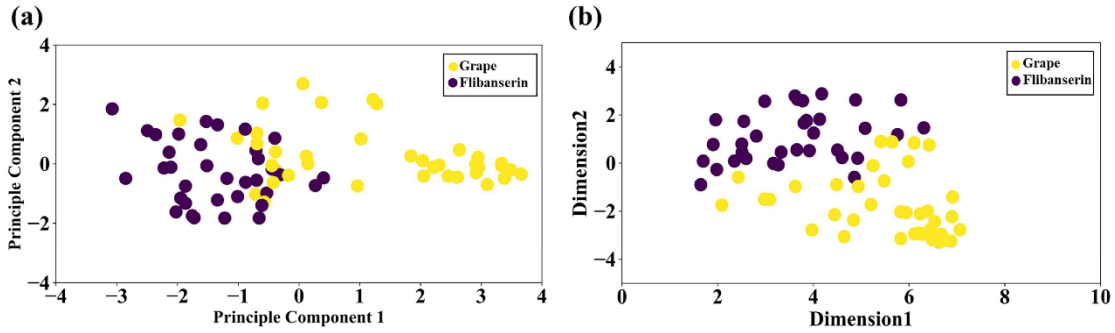

Figure S4 The results of dimensionality reduction of Flibanserin grape wine dataset by PCA and TSNE algorithms. (a) PCA score of Flibanserin grape wine dataset, (b) TSNE dimensionality reduction result of Flibanserin grape wine dataset.

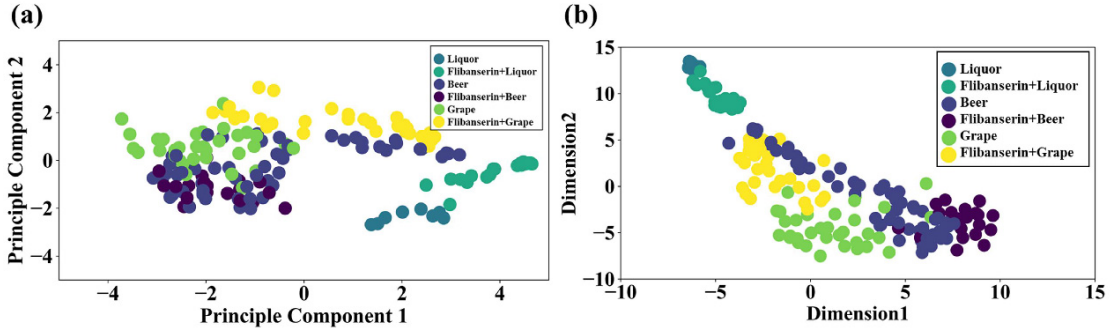

Figure S5 The results of dimensionality reduction of Flibanserin total dataset by PCA and TSNE algorithms. (a) PCA

score of Flibanserin total dataset, (b) TSNE dimensionality reduction result of Flibanserin total dataset.

Table S1 Accuracy of the PCA-SVM model for classification of the four Flibanserin spectrum datasets

Model	Liquor	Beer	Grape Wine	Total dataset
PCA-SVM (2 Principle Components)	0.923	0.917	0.909	0.723
PCA-SVM (90% Principle Component)	1.000	0.958	0.920	0.932

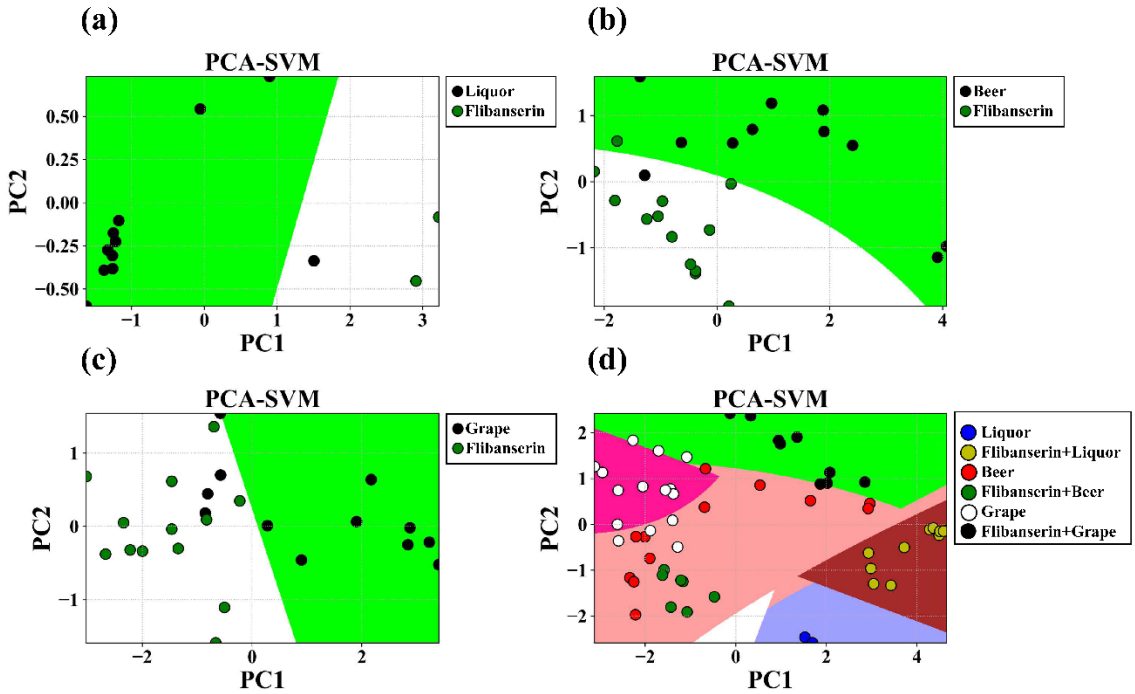

Figure S6 Classification boundary of the four datasets after classification by PCA-SVM model (a) Classification boundary of Flibanserin liquor dataset, (b) Classification boundary of Flibanserin beer dataset, (c) Classification boundary of Flibanserin grape wine dataset, (d) Classification boundary of Flibanserin total dataset.

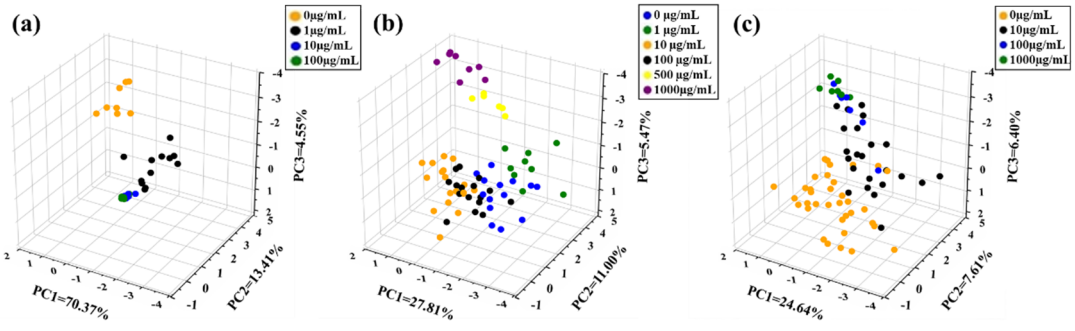

Figure S7 PCA score plots of the first three principal components of the spectral data sets of three wine solutions of Flibanserin at different concentrations. (a) PCA score plots of the data set of Flibanserin liquor solution, (b) PCA score plots of the data set of Flibanserin beer solution, (c) PCA score plots of the data set of Flibanserin grape wine solution.