# Supplementary Information

Traceability of cold medications with similar ingredients based on

laser-induced breakdown spectroscopy

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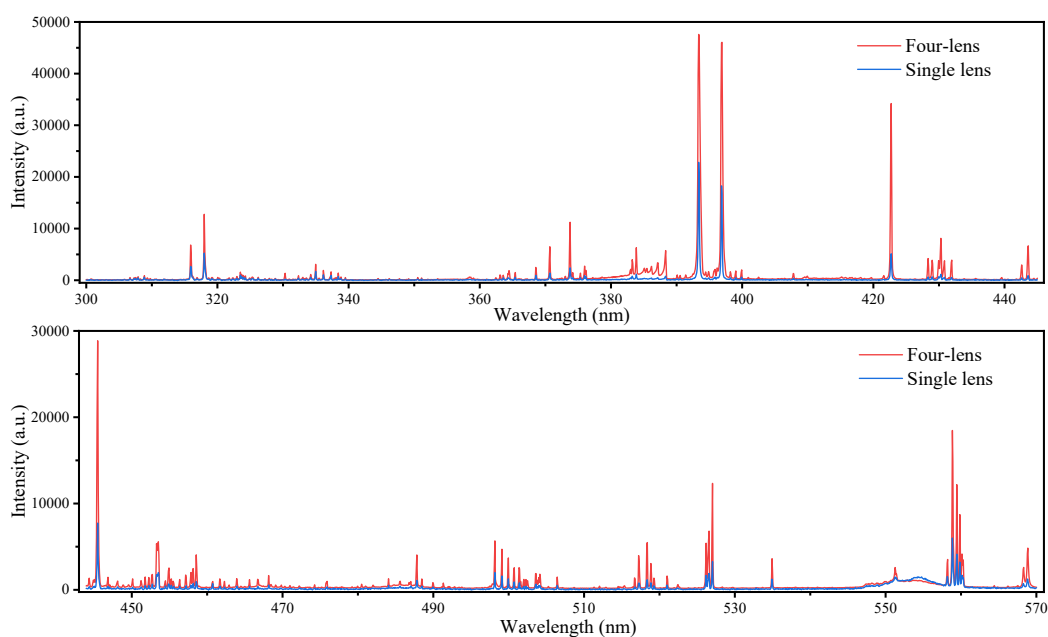
Fig. S1 LIBS spectra for four-lens collection system and single lens collection system.

The diameter of the first three lenses of four-lens collection system was 25.4 cm, and that of the last lens was 10 cm. Firstly, the distance between the first lens (f_1 = 60 mm) and the laser-induced plasma was 60 mm, and this lens converted the light emitted by plasma to collimated light. Secondly, the distance between the second lens (f_2 = 150 mm) and the third lens (f_3 = 60 mm) was 210 mm, and these two lenses reduced the spot to two-fifths of its original size. Lastly, the last lens (f_4 = 10 mm) was used to couple the light into the fiber. Although the four-lens collection system was a bit more complicated than single lens collection system, the field of view (FOV) of four-lens collection system was larger. As shown in Fig. R1, the signal intensity of four-lens collection system was stronger than that of single lens collection system.
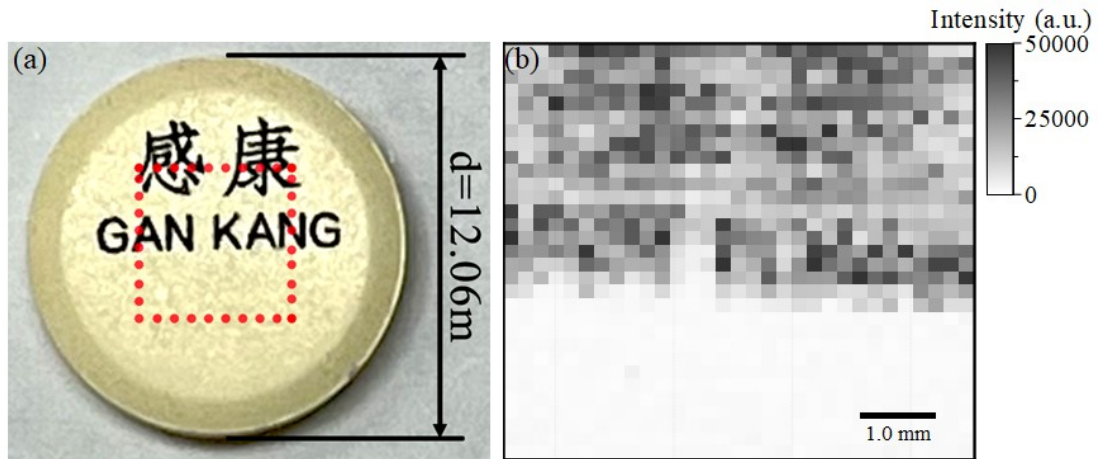
Fig. S2 The photograph of GCPAHT tablet (a) and intensity mapping of Fe I spectra lines of the surface of GCPAHT tablet (b).

The trademark (感康 GAN KANG) of GCPAHT tablet can be clearly seen from Fig. R2(a). As shown in Fig. R2(b), the signal of Fe I spectra lines was stronger where the trademark is located. It can be inferred that the presence of Fe I lines in spectra of GCPAHT is caused by the surface trademark of the tablet.
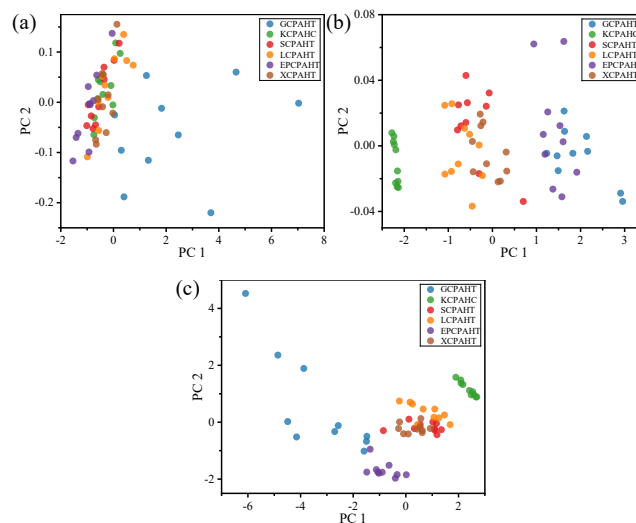

Fig. S3 PCA results of six cold medications using 12 Fe I lines (a), 4 Mg I lines, 12 Fe I and 4 Mg I lines.

Fe was detected only in GCPAHT because of its trademark. In addition, Mg was not detected in KCPAHC because the capsule did not contain magnesium stearate. As shown in Fig. S3 (a), GCPAHT can be distinguished using 12 Fe I lines. If only 4 Mg I lines were used for PCA analysis, KCPAHC was identified (Fig. S3 (b)). In addition, it can be seen from Fig. S4 (c) that both GCPAHT and KCPAHC can be identified using 12 Fe I lines and 4 Mg I lines for PCA analysis. However, other cold medications cannot be identified.
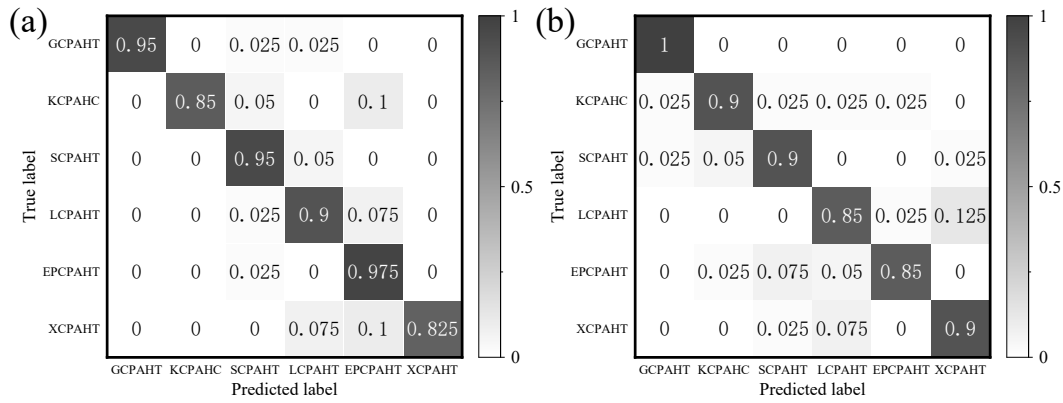
Fig. S4 Confusion matrix of validation and test results with BPNN. (a) 2 hidden layers; 10 and 5 neuros for first and second hidden layer, respectively), (b) 4 hidden layers; 5, 4, 3 and 2 neuros for first to forth hidden layer, respectively.
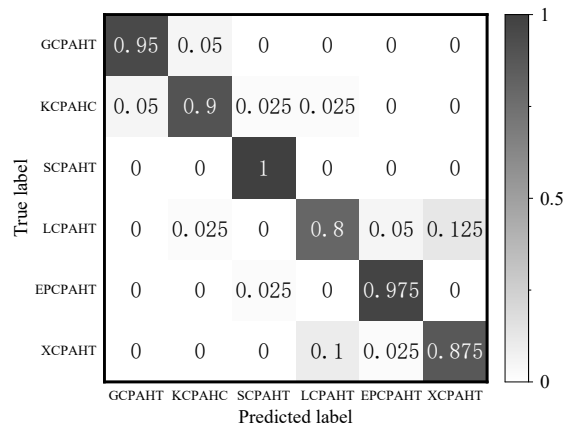
Fig. S5 Confusion matrix of validation and test results with BPNN (5 hidden layers; 6, 5, 4, 3 and 2 neuros for first to fifth hidden layer, respectively).

For LDA analysis, 103 characteristic spectral lines were used as variables. In order to satisfy the condition that the number of data in training set must be greater than the number of variables, every two spectra were averaged, and a total of 220 averaged spectra were obtained for each sample. 140 sets of spectral data were used as the training set for each sample, and other 80 sets of spectral data were used as the test set. It can be seen from Fig. S5 that if the number of hidden layers was set to 5, and the number of neuros for first to fifth hidden layer was set to 6, 5, 4, 3 and 2, respectively, the recognition accuracy of BPNN for SCPAHT was equal to that of LDA (Fig. 9 (b)). For EPCPAHT, LDA accuracy was higher than BPNN. The sample sizes of test set of BPNN and LDA were 40 and 80, respectively. Hence, for both BPNN and LDA, only one sample was misrecognized. From this result, it can be seen that suitable setting of the number of hidden layers and the number of neurons per hidden layer for BPNN can achieve the same accuracy as LDA for SCPAHT and EPCPAHT.