Supporting Information

Enhancing Substance Identification in Raman Spectroscopy Using Deep Neural Convolutional Networks with Attention Mechanism

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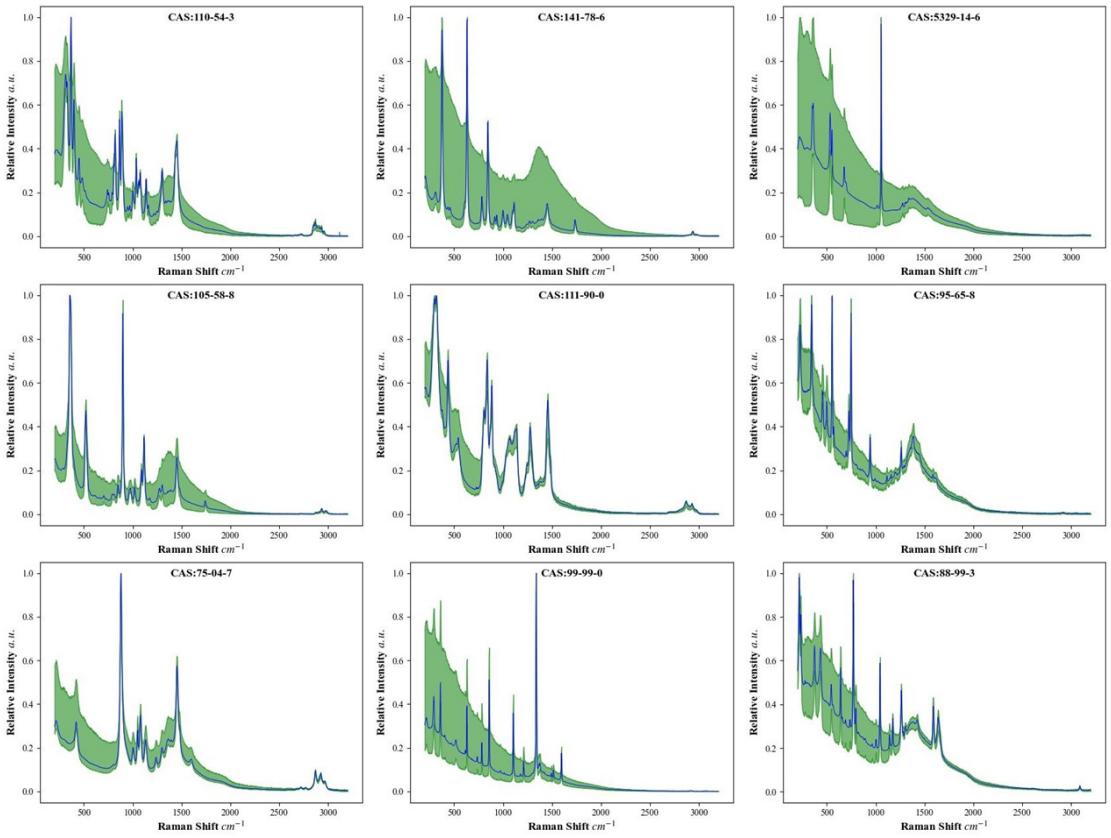

Figure S1 Raman spectroscopy of some hazardous chemicals

We have already made the visualization images of hazardous chemicals in 474 public on GitHub. The website is:
https://github.com/AmarettoSaronno/Raman/tree/ec99a9beceb6785c07a54f92f2487d1

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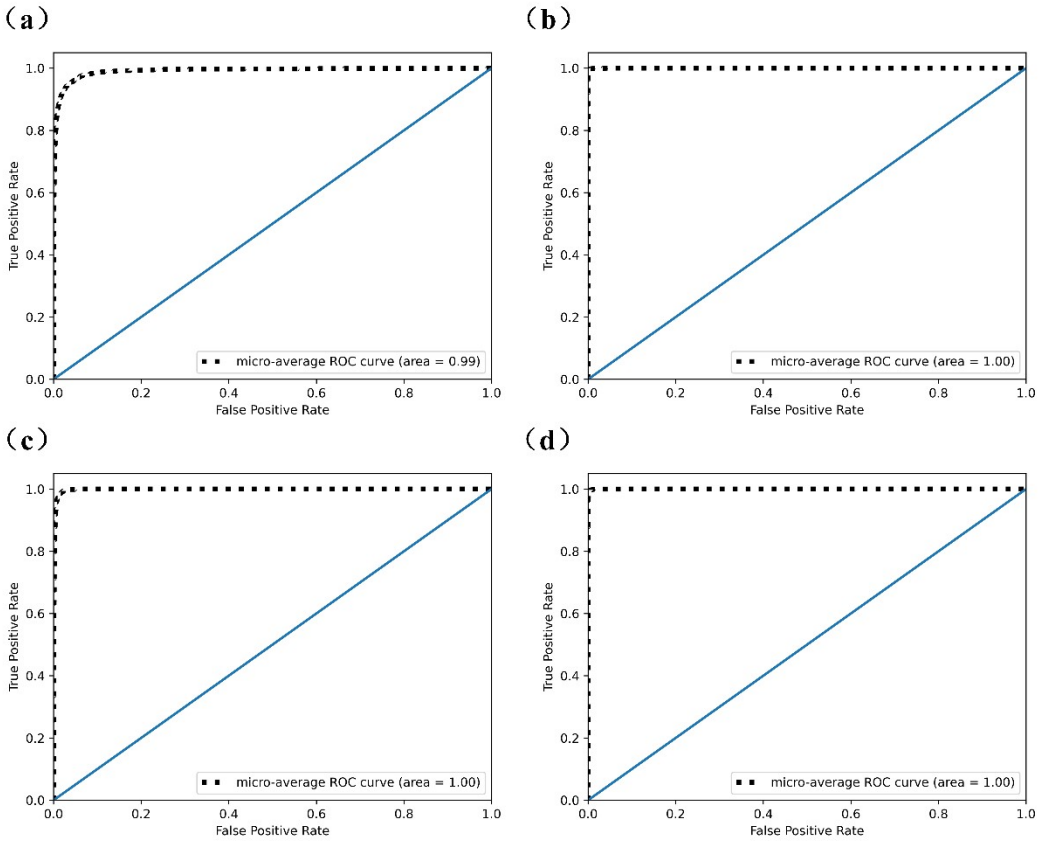


Figure S2 ROC curves of VGG (a), ResNet (b), DenseNet (c), and SE-ResNet (d) models on the original dataset.

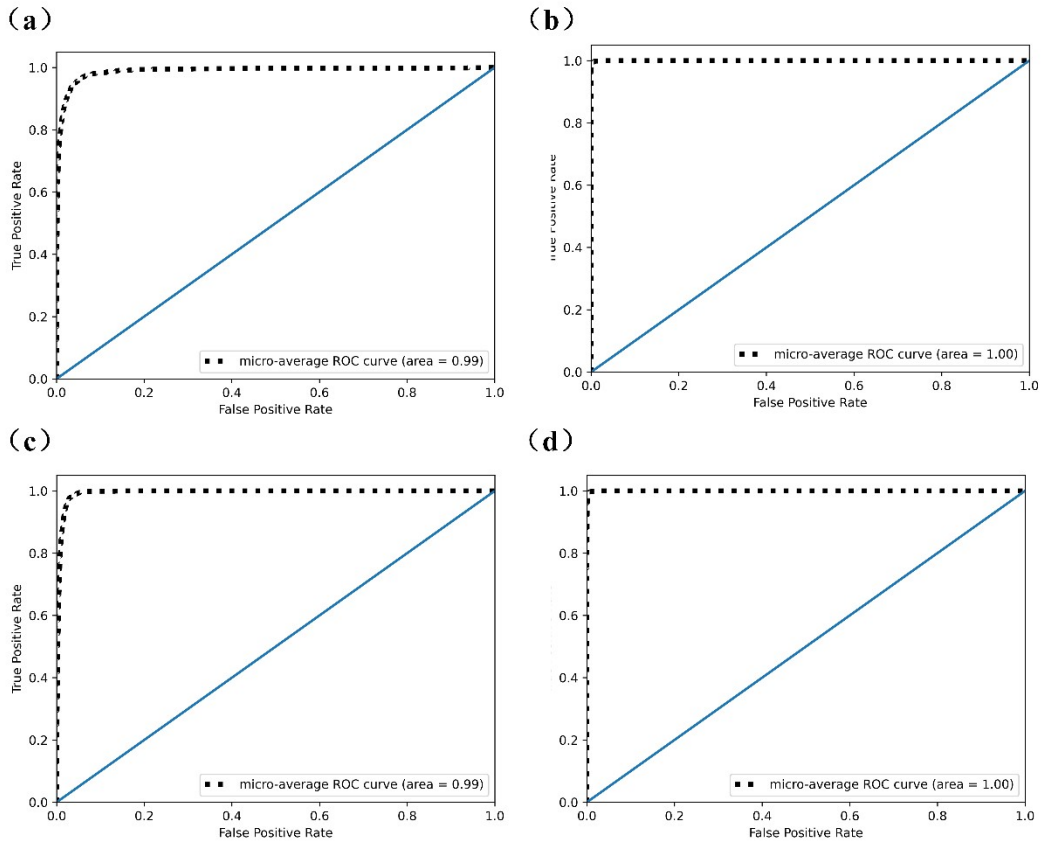


Figure S3 ROC curves of VGG (a), ResNet (b), DenseNet (c), and SE-ResNet (d) models on the Small sample dataset

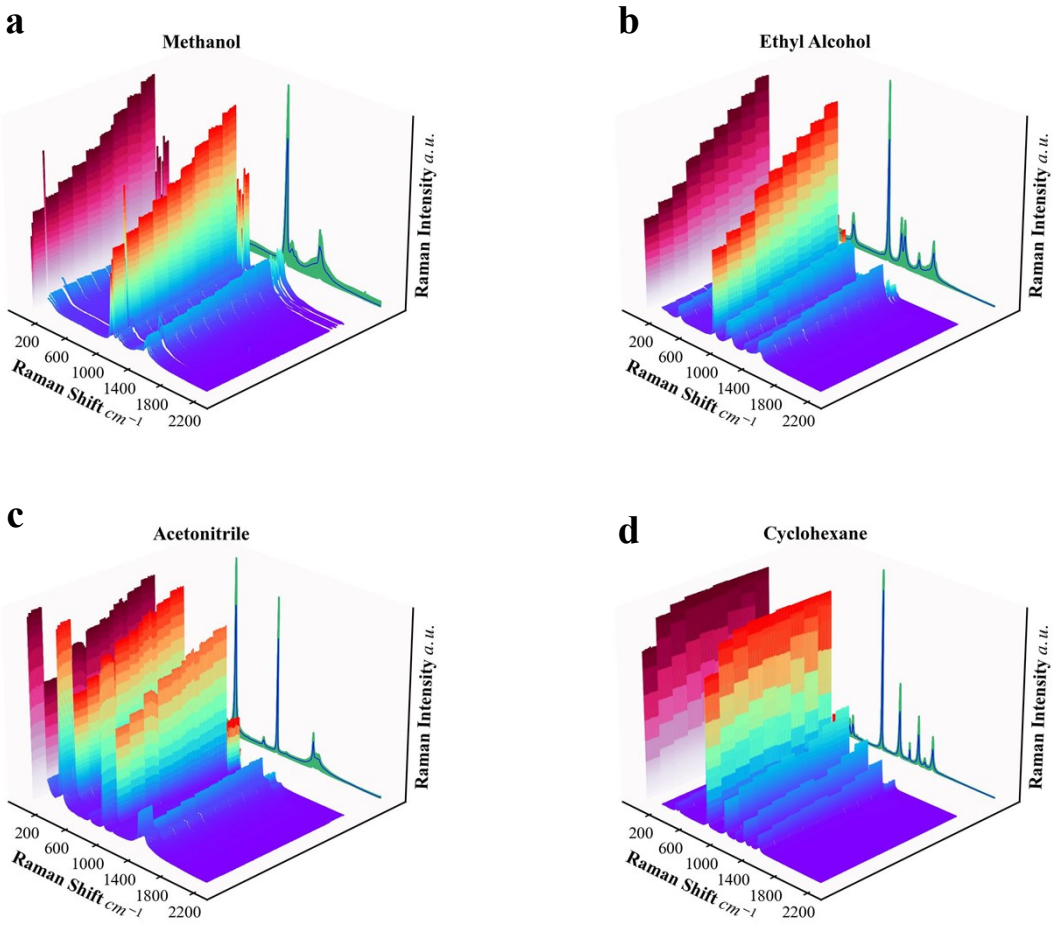
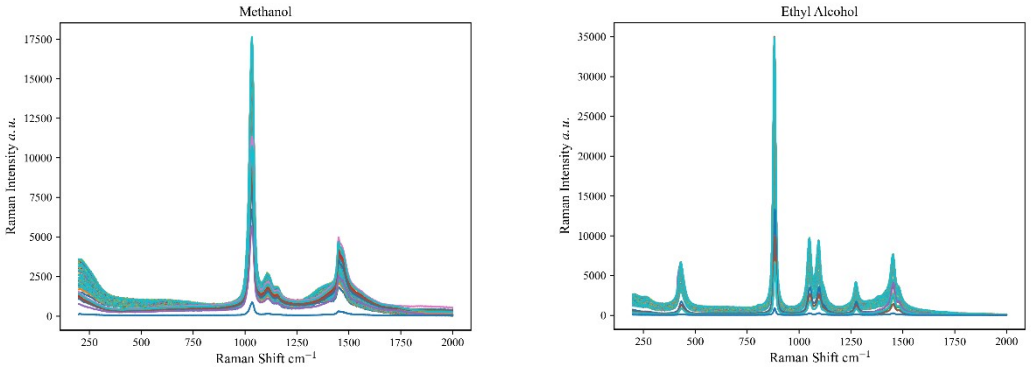


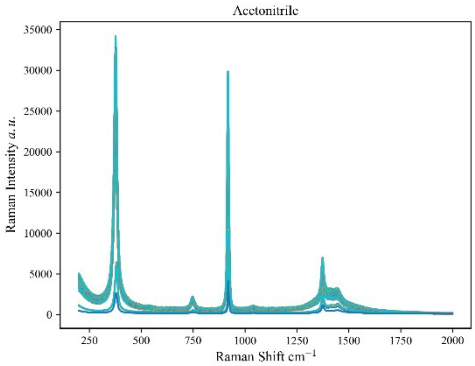
Figure S4 Raman spectra of chemical substances under different instrument parameters: methanol, ethanol, acetonitrile, and cyclohexane

Among the 100 selected acetonitrile test samples, there was only one misclassification of the model. Among the 100 selected ethanol test samples, there were only two misclassifications of the model. Among the 100 selected methanol test samples, there were only three misclassifications of the model. Among the 100 selected cyclohexane test samples, there was only one misclassification of the model. It can be concluded that the model has significant value in actual hazardous chemical detection. The misclassification of the model may be due to significant differences in different detection data, and the detected data may contain certain noise interference. Among them, the most common reason for the detection error of methanol can be found to be the Raman scattering of methanol by observing the chart. The fluctuation of the spectrum is significant, as it leads to certain misclassifications in the model.

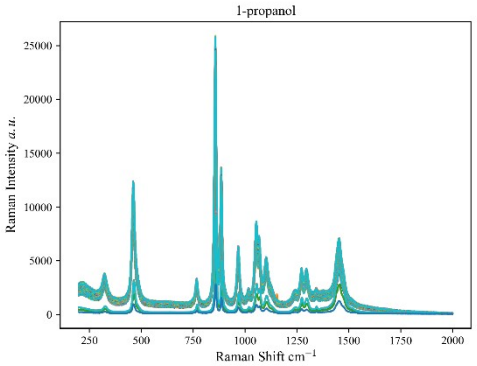


(a)

(b)

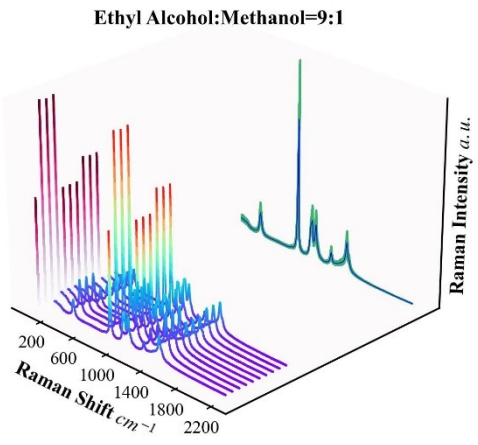


(c)

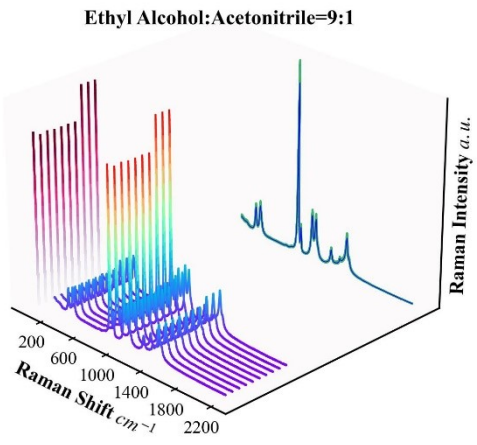


(d)

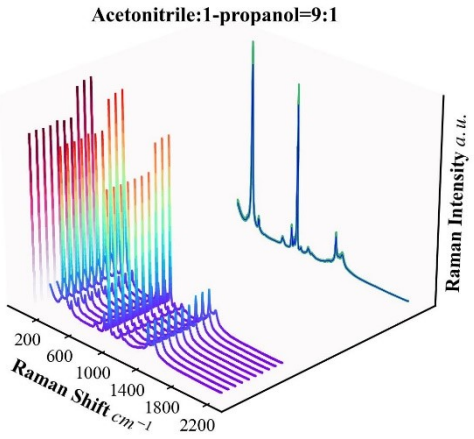
Figure S5 Raman spectra of the four substances used to prepare the mixture; (a) Methanol, (b) Ethyl Alcohol, (c) Acetonitrile, (d) 1-propanol



(a)



(b)



(c)

Figure S6 Raman spectra of three mixtures; (a) Ethyl Alcohol : Methanol =9:1, (b) Ethyl Alcohol : Acetonitrile =9:1, (c) Acetonitrile : 1-propanol =9:1

The model was verified by configuring a mixture of three main components with a concentration of about 90%. From the verification results, it can be seen that when the impurity content is low (about 10%), the Raman spectrum of the main component is still very obvious, so the final output of the model is not greatly affected and can still maintain a confidence output of more than 0.75.

For the first data enhancement method, the implementation steps are as follows: First step, generate random noise with a normal distribution using the (np.random.normal) method with a mean of 0, standard deviation of 100, and the data point length is equal to the Raman spectrum length.

Second step, filter the noise generated in the first step using a Savitzky-Golay filter. The Savitzky-Golay filter is a filtering method based on local polynomial least squares fitting in the time domain. We set the window length to be equal to the length of the noise and the order of polynomial fitting to be 4. Therefore, the Savitzky-Golay filter will smooth the noise generated in the first step into a smoothed baseline fitted with a fourth-order polynomial.

Third step, normalize the baseline obtained in the second step to the maximum and minimum values, then add it to the original spectral data. This results in the newly augmented spectral data.

The distinctive feature of this filter is its ability to remove noise while preserving the shape and width of the signal. Additionally, the effectiveness of smoothing is more apparent with a larger window set for the filter, while a smaller window aligns more closely with the original curve. In this context, we increased the window size to ensure the smoothing of the baseline noise. The window size was set to be consistent with the length of the Raman spectra data, and all data were normalized to serve as training data after data augmentation. The randomness observed in the data augmentation process is well-suited for large-scale augmentation.

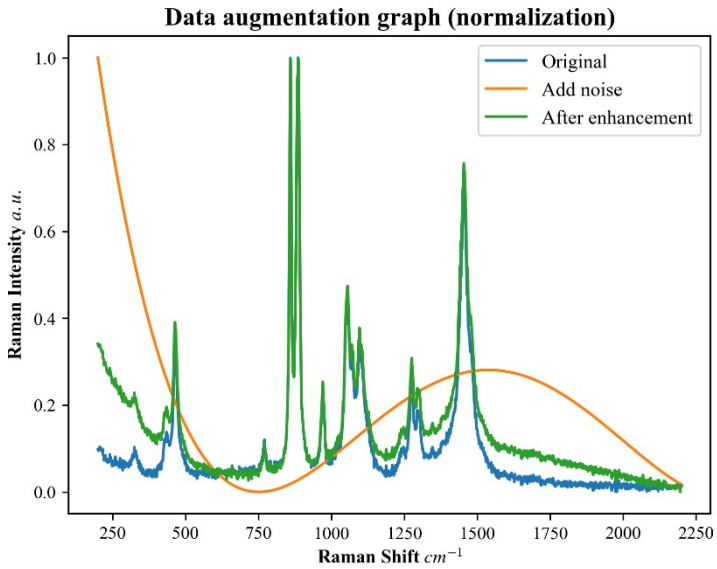


Figure S7 Random baseline data enhancement method；the final enhanced data is equal to 0.2*baseline+0.8*Raman spectrum

For the second data enhancement method, the implementation steps are as follows:

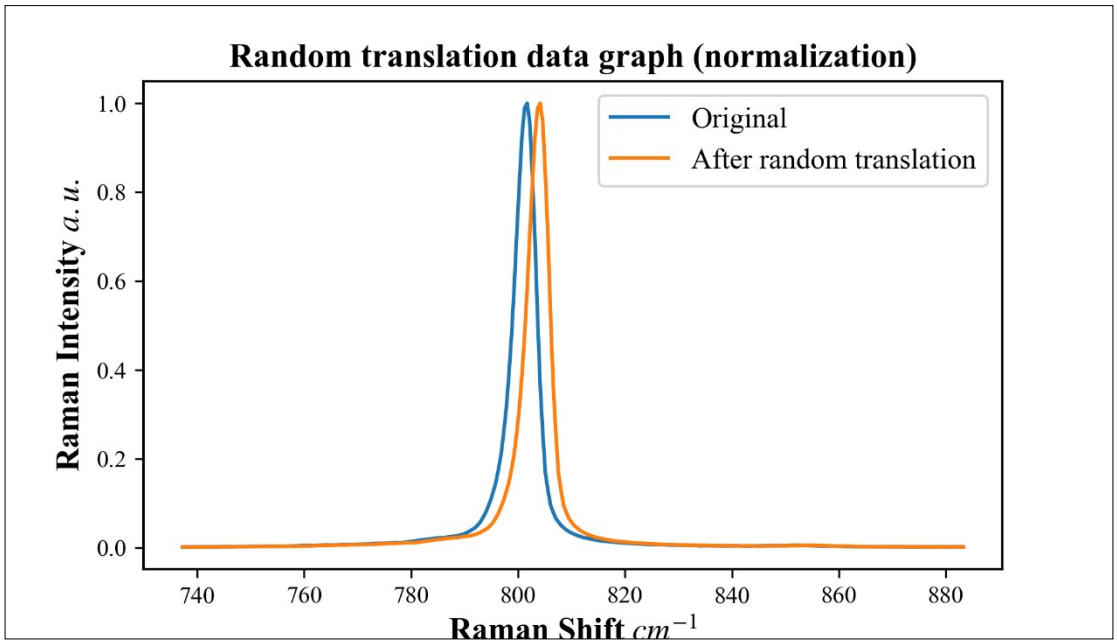


Figure S8 Random Translation Data Augmentation