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Developing an AI algorithm for Raman spectrum analysis

Raman spectroscopy detects molecular vibrations via photon scattering, while Surface-enhanced Raman spectroscopy (SERS) enhances signals using nanostructured metals like gold or silver. Our study focuses on developing an algorithm to identify mi17RNA signatures in blood, a complex medium where overlapping peaks present significant challenges. The process includes comprehensive data preprocessing techniques such as moving average, convolution, moving median, moving max, normalization, baseline correction, and deconvolution for noise reduction and signal enhancement. Calibration is performed to ensure accuracy and consistency across different datasets. The algorithm's performance is validated on diverse datasets, with results displayed through clustered models to accurately distinguish molecular species and variations. This research advances automated Raman spectrum analysis for applications in materials science and biomedical diagnostics.

References

[1] Premachandran et al. (2022). ACS Nano.
[2] Koo et al. (2018). ACS Nano.
[3] Rusciano et al. (2014). ACS.Nano.
[4] Matschulat et al. (2010). ACS.Nano.

Figures
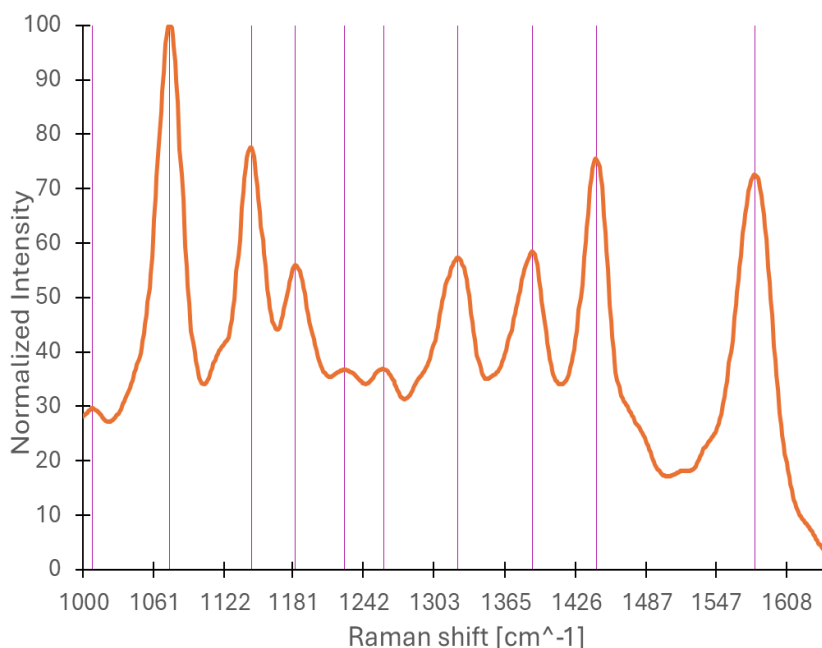
Figure 1: Normalized intensity (a.u) vs Raman shift (cm^{-1}), the Orange function represents the molecule 4-ATP after smoothing. the purple line represents the normalized model using a moving max window width of $n \pm 7$, with the parameter of the normalized threshold value set to 99.99 for peak detection resolution.