Supplementary Information

MCR-ALS with Sample Insertion Constraint to Enhance the Sensitivity of Surface-Enhanced Raman Scattering Detection

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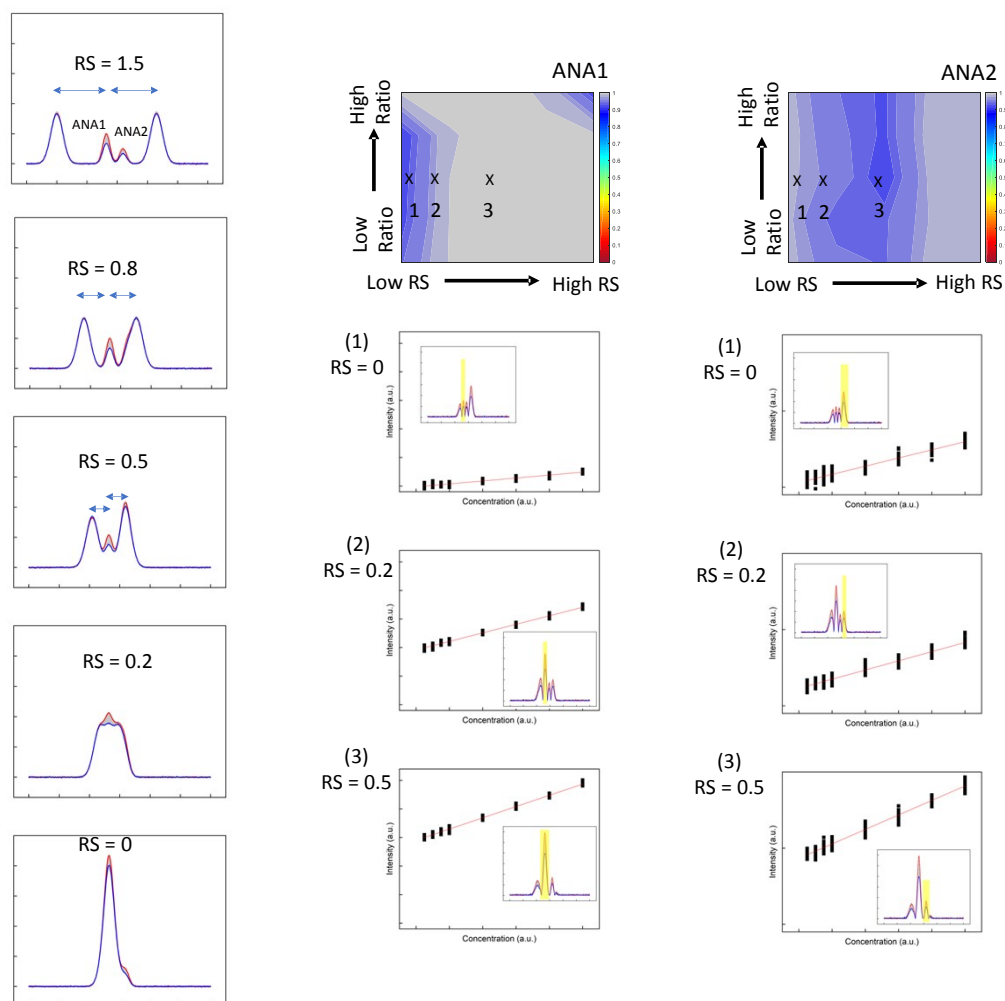
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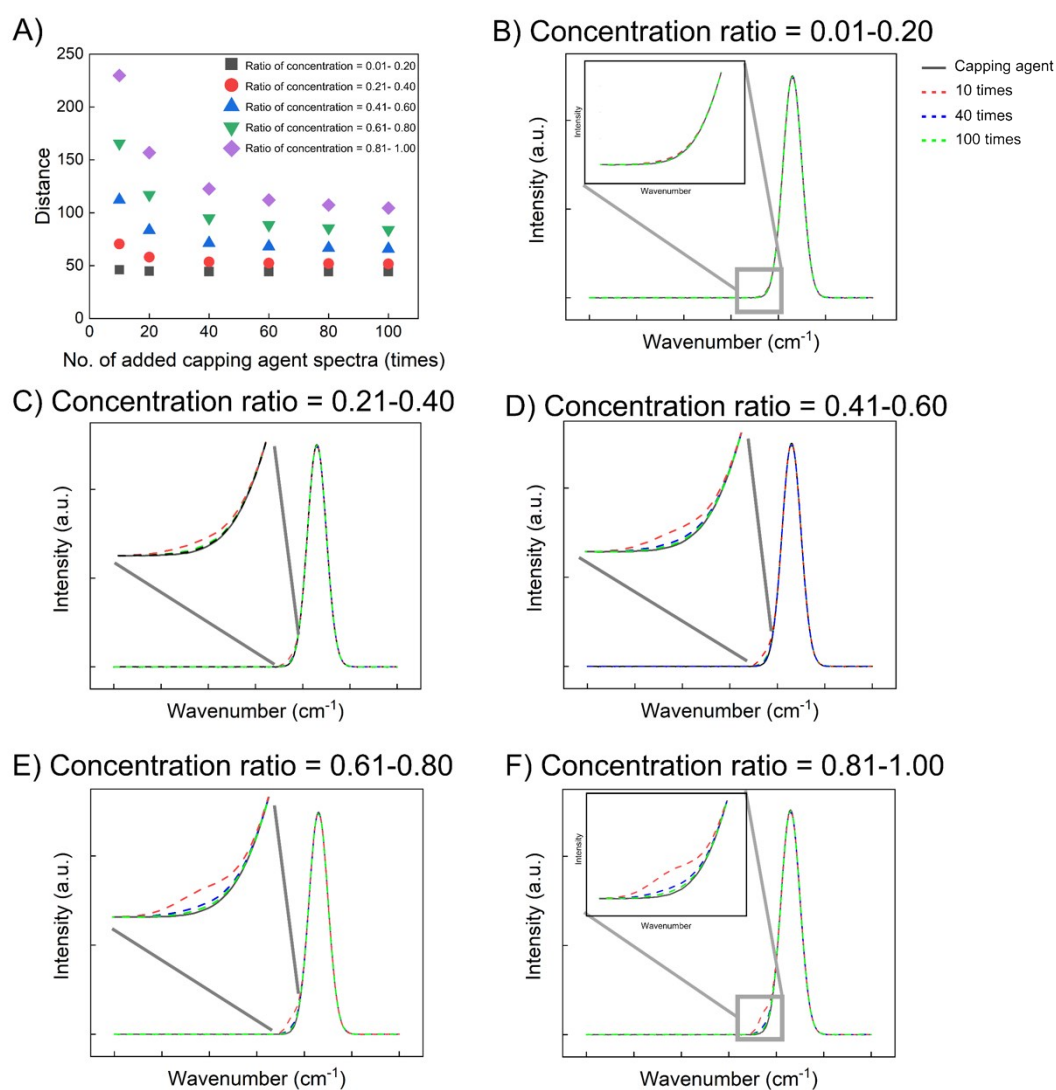
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Figure S1 (Left) The simulated spectra with different overlapping characteristics between two analytes (ANA1, ANA2) and a capping agent (CAP). (Right) The contour map of R^2 value of the calibration curves calculated from the analyte peaks (ANA1 and ANA2) extracted with MCR-ALS with the sample insertion constrain. The calibration curve plots from point (1), (2) and (3) on the contour maps with the inset figures as the analyte peaks after extraction.

Figure S2 (A) The Euclidean distances of the pre-set spectra and the extracted spectra of capping agent at the various numbers of the added capping agent. The black square, red circle, blue triangle, green triangle, and purple diamond are the distance at the different concentration ratios from 0.01-0.20, 0.21-0.40, 0.41-0.60, 0.61-0.80, and 0.81-1.00, respectively. (B) the pre-set spectra (black line) and the extracted spectra of the capping agent using sample insertion at 10 (red dash line), 40 (blue dash line) and 100 (green dash line) times, respectively. The inset figures show the spectra at the 1700 cm-1 with condition of RS = 0.5.

Figure S3 Predicted concentration versus presetting concentration in the carbofuran derived azo-compound at the 1570 cm^{-1} peaks the black square and red circle represent the calibration and validation set, respectively by the *RMSEC* is the *RMSE* values of calibration and *RMSEP* is the *RMSE* of the validation sets.