Supporting information for

Paper/GO/e-Au Flexible SERS Sensors for In-situ Detection of Tricyclazole in Orange Juice and on Cucumber Skin at Sub-ppb Level: Machine Learning-Assisted Data Analysis

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Calculation of limit of detection (LOD) and limit of quantification (LOQ)

The standard curve of linear detecting range was given as:

$$Y = A + B \times Log(X) \quad (1)$$

where A and B are intercept and slope of regression equation obtained through the plot of the logarithmic SERS intensity (Y) – logarithmic concentration (X).

The LOD is calculated using the following equation [1]:

$$LOD = 10^{\left[(Y_{blank} + 3SD)/Y_{blank} - A\right]/B} \quad (2)$$

The LOQ is calculated as

$$LOQ = 10^{\left[(Y_{blank} + 10SD)/Y_{blank} - A\right]/B} \quad (3)$$

where Y_{blank} and SD are the SERS signal and the standard deviation of blank sample, respectively.

SD is calculated via the well-known formula:

$$SD = \sqrt{\frac{1}{n-1} \times \sum_{i}^{n} (x_i - x_{average})^2} \quad (4)$$

where x_i if the "i" sample of the series of measurements, $x_{average}$ is the average value of SERS signal obtained from the blank sample repeated n times.

Calculation of relative standard deviation (RSD)

The RSD value of repeatability and reproducibility is calculated via the well-known formula:

$$\text{RSD} = \frac{SD \times 100}{x_{average}} \quad (5)$$

where SD is the standard deviation that calculates using equation 4 and $x_{average}$ is the average value of SERS signal obtained from each measurement.

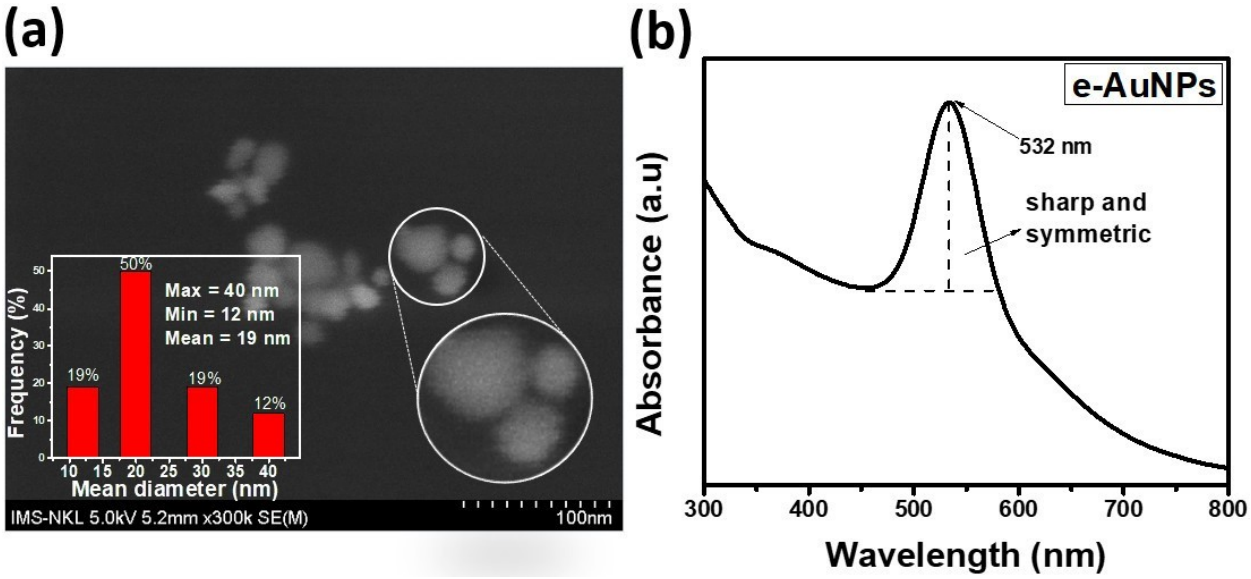

Figure S1. (a) SEM images and particle size distribution histograms of e-AuNPs (b) Absorbance spectra of e-AuNPs (Images adapted from ref [2])

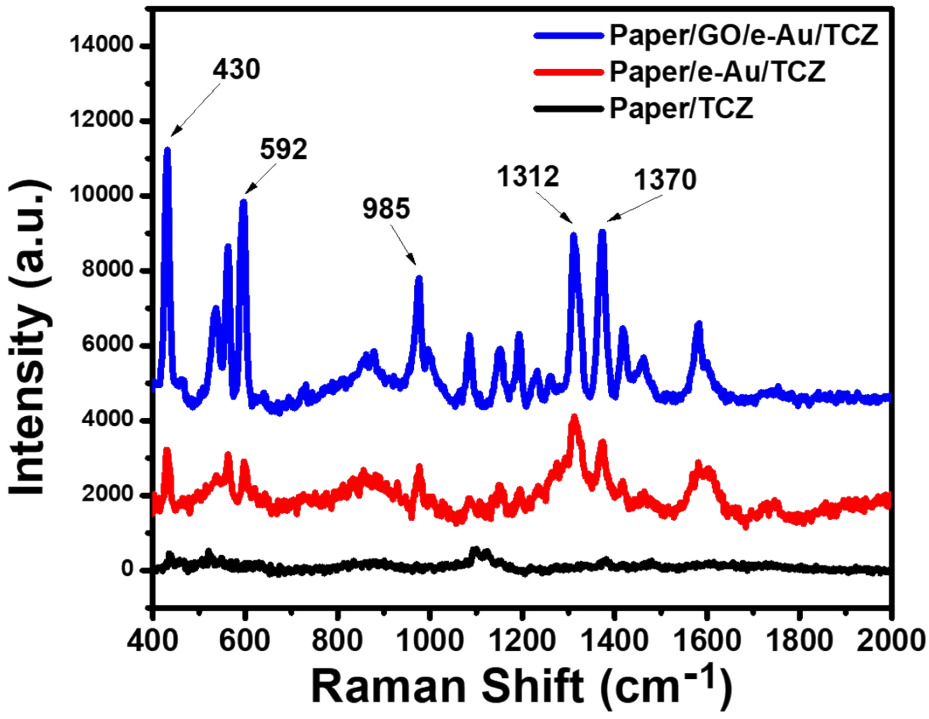

Figure S2. SERS spectra of TCZ on paper/GO/e-Au, paper/e-Au and paper.

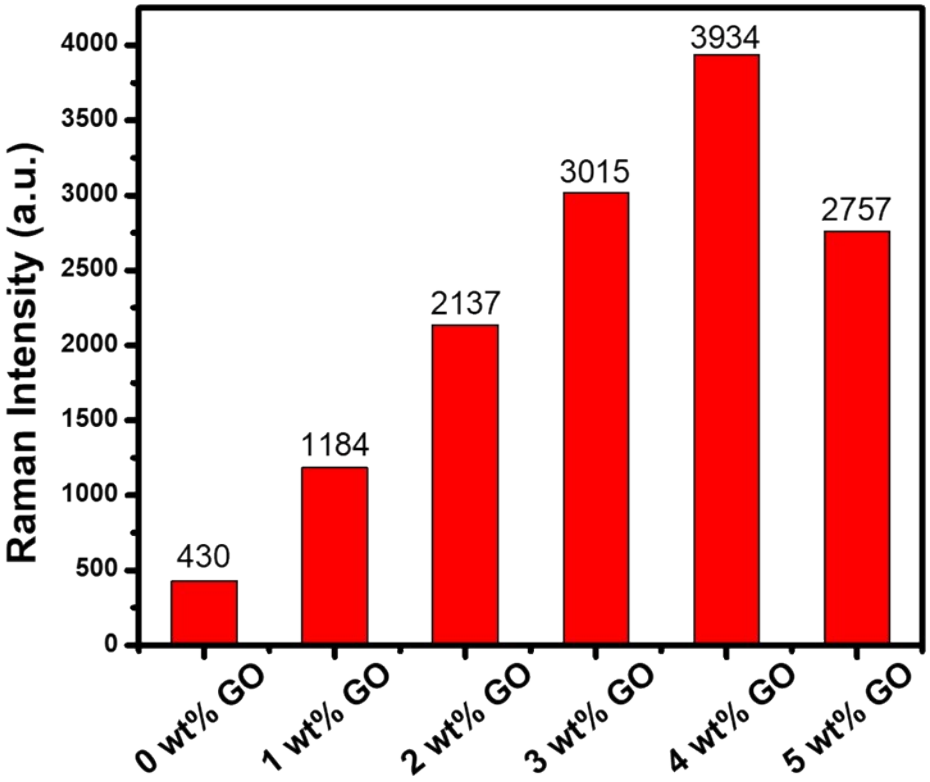

Figure S3. SERS intensity at the peak of 592 cm^{-1} of TCZ (10^{-5} M) on Paper/GO/e-Au substrate with different GO contents.

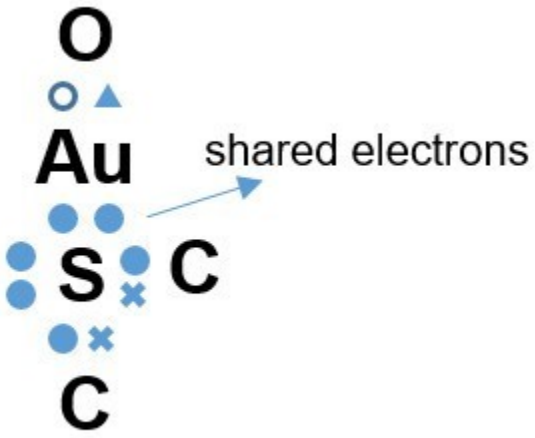

Figure S4. Lewis dot diagram of dative bond between Au atom in paper/GO/e-Au and S atom in TCZ.

Table S1. Characteristic peaks of ten organic molecules for feeding the machine learning model

Compound	**Characteristic peak (cm^{-1})**	**Assignment**
4-nitrophenol	491	C=O out-plane bending [3]
	1248	O–C stretching [3]
	1322	NO_2 symmetric stretching [3]
Carbaryl	424	C–C bending [4]
	485	C–C bending [4]
	1230	Ring vibration [4]
	1443	C–C wagging [4]
Chloramphenicol	1163	N–H in plane bending [5]
	1347	N–O_2 symmetric stretching [5]
	1605	Ring stretching [5]
Congo red	1159	C–N stretching [6]

	1368	(C=C) naphthyl stretching [6]
	1589	C–C aromatic ring stretching [6]
Crystal violet	424	phenyl-C^{+}-phenyl bending [7]
	534	skeletal ring vibrations and ring C–H deformations [7]
	915	ring skeletal vibration of radical orientation [7]
	1172	C-H in-plane bending [7]
Glyphosate	455	O-P=O bending [8]
	774	P-O bending [8]
	860	P-O stretching [8]
	1035	C-OH stretching [8]
Methylene blue	450	C-N-C deformation [9]
	505	C-N-C deformation [9]
	1390	C-H in-plane ring deformation [9]
	1600	C-C ring stretching [9]
Thiram	440	CSS symmetric stretching [10]

	562	S-S stretching [10]
	1143	CH3 rocking [10]
	1365	CH3 bending; C-C stretching [10]
Tricyclazole	430	C-N-C deformation [11, 12]
	985	C-C symmetric stretching [11, 12]
	592	C-S-C deformation vibration [11, 12]
	1312	C-N stretching [11, 12]
	1372	C-N stretching [11, 12]
Urea	1000	C-N stretching [13]

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