

Supplementary Information for
Whole-Cell SERS Fingerprints for Rapid Toxicant Attribution in
Water

Ziyang Weng ^{a,#}, Ying Zhou ^{a,#}, Nan Ma ^b, Meikun Fan ^{a,*}

^a School of Environmental Science and Engineering, Southwest Jiaotong University,
Chengdu, Sichuan 611756, China

^b Sichuan Academy of Eco-Environmental Sciences, Chengdu, Sichuan 610041, China

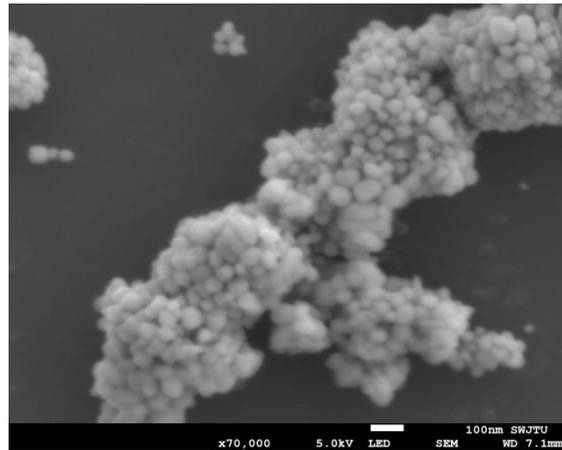


Figure S1. SEM image of Ag NPs (A magnification of 70,000 times)

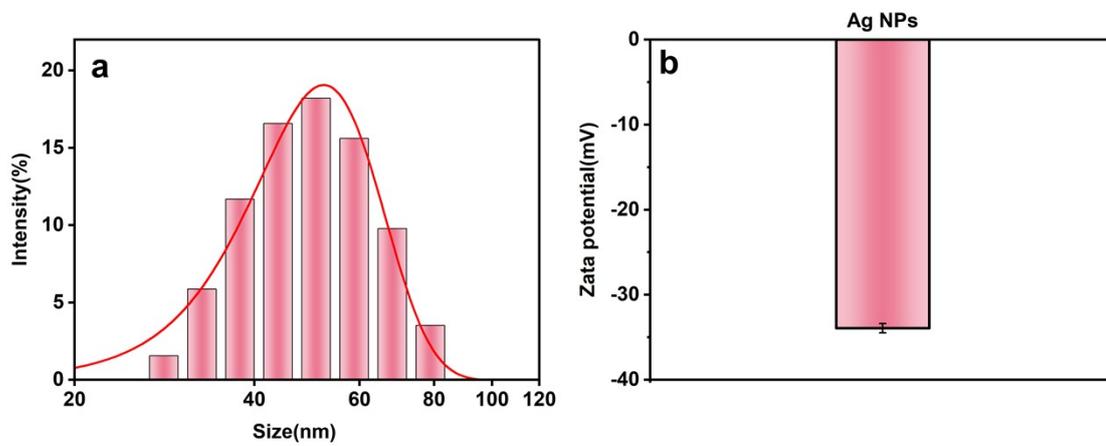


Figure S2. (a) DLS size distribution and (b) Zeta potential of Ag NPs.

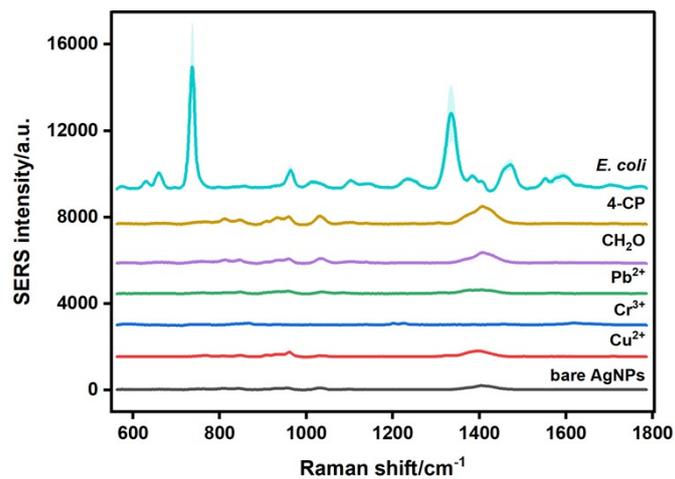


Figure S3. SERS spectra of *Escherichia coli* and toxic substances, with concentrations of Cu^{2+} , Cr^{3+} , Pb^{2+} , and 4-CP at 10 mg/L, and CH_2O at 0.37% (w/v).

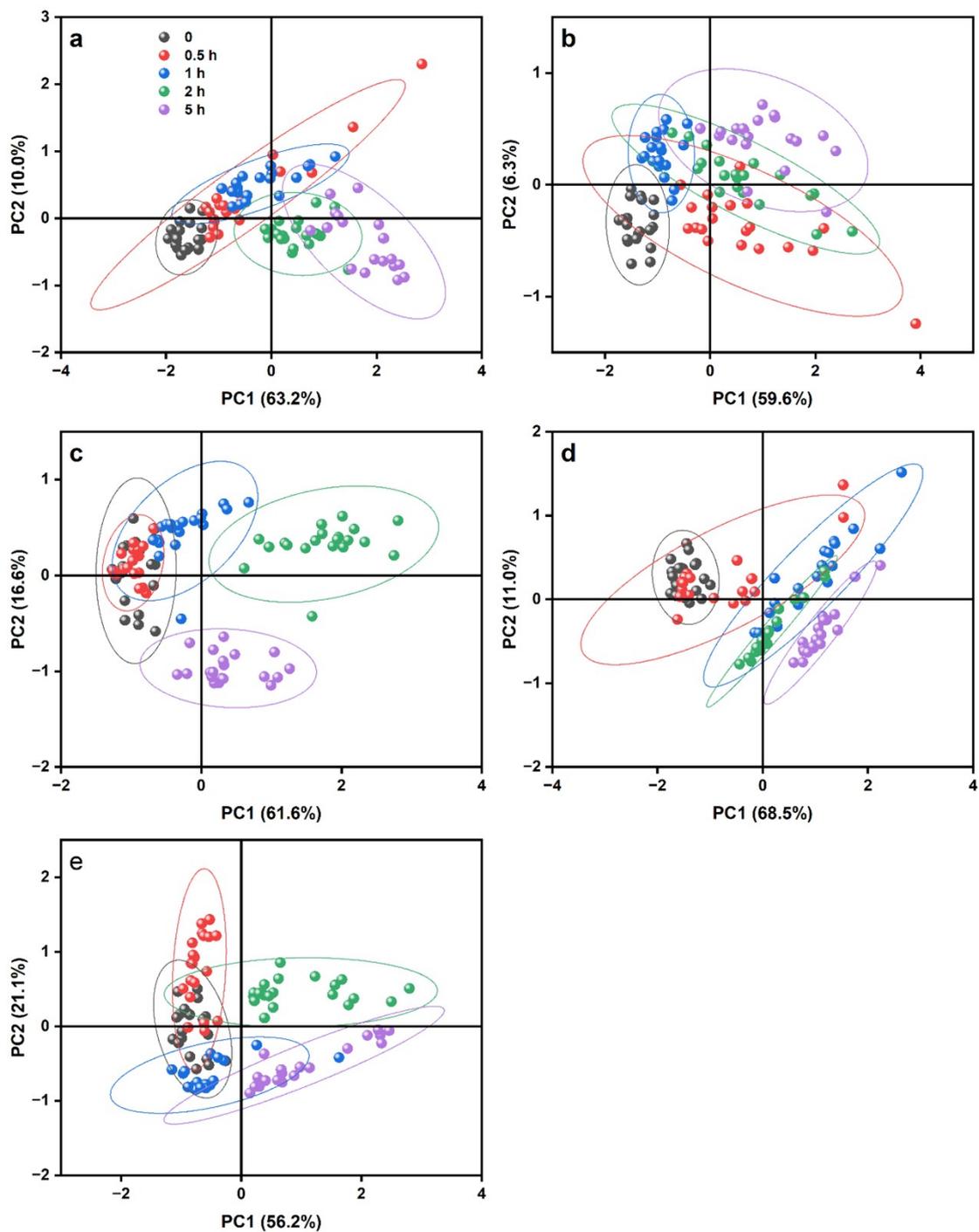


Figure S4. Principal Component Analysis (PCA) scatter plots of SERS spectra for *Escherichia coli* at different exposure times. a–e represent bacteria treated with Cu^{2+} , Cr^{3+} , Pb^{2+} , CH_2O and 4-CP, respectively.

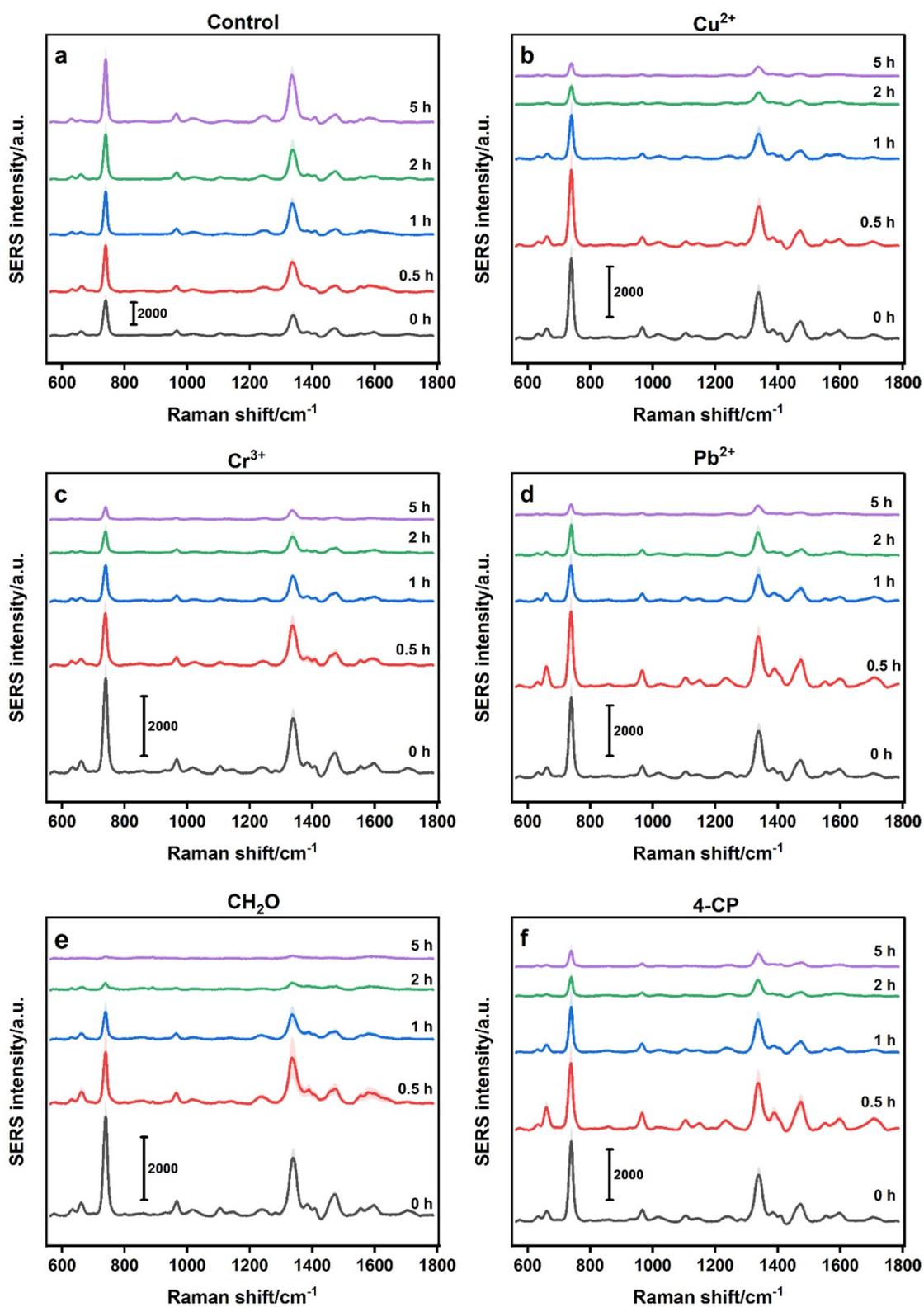


Figure S5. Changes in SERS spectra of *Staphylococcus aureus* under different toxicant treatments over exposure time. a–f represent the control group and experimental groups treated with Cu²⁺, Cr³⁺, Pb²⁺, CH₂O and 4-CP, respectively.

Table S1 Classification Accuracy of PCA–LDA for E. coli SERS Spectra

Time	Actual Class	Predicted Class					Class Accuracy	Overall Accuracy
		Cu ²⁺	Cr ³⁺	Pb ²⁺	CH ₂ O	4-CP		
0.5 h	Cu ²⁺	19	0	0	0	1	95%	95%
	Cr ³⁺	0	20	0	0	0	100%	
	Pb ²⁺	1	0	19	0	0	95%	
	CH ₂ O	0	0	0	20	0	100%	
	4-CP	3	0	1	0	17	85%	
1 h	Cu ²⁺	20	0	0	0	0	100%	98%
	Cr ³⁺	0	19	1	0	0	95%	
	Pb ²⁺	0	1	19	0	0	95%	
	CH ₂ O	0	0	0	20	0	100%	
	4-CP	0	0	0	0	20	100%	
2 h	Cu ²⁺	20	0	0	0	0	100%	99%
	Cr ³⁺	0	20	0	0	0	100%	
	Pb ²⁺	0	0	20	0	0	100%	
	CH ₂ O	0	0	0	20	0	100%	
	4-CP	1	0	0	0	19	95%	
5 h	Cu ²⁺	20	0	0	0	0	100%	95%
	Cr ³⁺	0	20	0	0	0	100%	
	Pb ²⁺	0	0	18	0	2	90%	
	CH ₂ O	0	0	0	20	0	100%	
	4-CP	0	0	4	0	16	80%	

Table S2. 5-fold cross-validation accuracy of PCA-LDA classification

Bacterial Strain	Exposure Time	Mean Accuracy (%)	SD (%)
E. coli	2h	96.59	3.24
S. aureus	1h	100.0	0.00