

Deep Learning-Assisted SERS for Detection of Propoxate and Isopropoxate in E-Cigarettes

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Table S1 Calculation of the enhancement factor.

Project	Isopropoxate
I_{RS} (solid-state)	267.15
C_{RS}	4.26 mol/L
I_{SERS} (1 $\mu\text{g/mL}$)	35431.64
C_{SERS}	3.87×10^{-6} mol/L

Def: EF is 1.46×10^8 .

Table S2 Propoxate characteristic peak attribution.

Propoxate	SERS	DFT x 0.978	Electronic cigarette
$\nu(\text{C}=\text{C}), \gamma(\text{C}-\text{H})$	616	618	611
$\gamma(\text{C}-\text{H})$	783	791	781
$\gamma(\text{C}-\text{H})$	910	913	910
$\nu(\text{C}-\text{O})$	1002	996	999
$\nu(\text{C}-\text{C})$	1028	1034	1023
$\nu(\text{C}-\text{O}), \nu(\text{C}-\text{N}), \delta(\text{C}-\text{H})$	1196	1200	1194
$\nu(\text{C}=\text{C}), \gamma(\text{C}-\text{H})$	1398	1400	1390
$\nu(\text{C}=\text{O})$	1720	1750	1716

Table S3 Isopropoxate characteristic peak attribution.

Isopropoxate	SERS	DFT x 0.968	Electronic cigarette
$\delta(\text{C-H})$	616	613	629
$\gamma(\text{C-H})$	783	784	783
$\nu(\text{C-C})$	844	885	846
$\nu(\text{C-C}), \gamma(\text{C-H})$	1002	986	985
$\delta(\text{C-H})$	1028	1023	1027
$\rho(\text{C-H})$	1196	1207	1192
$\nu(\text{C=C})$	1720	1641	1668

Def: ν : stretching; δ : in plane bending; ρ : rocking. γ : out of plane bending; τ : twisting; β : ring breathing.

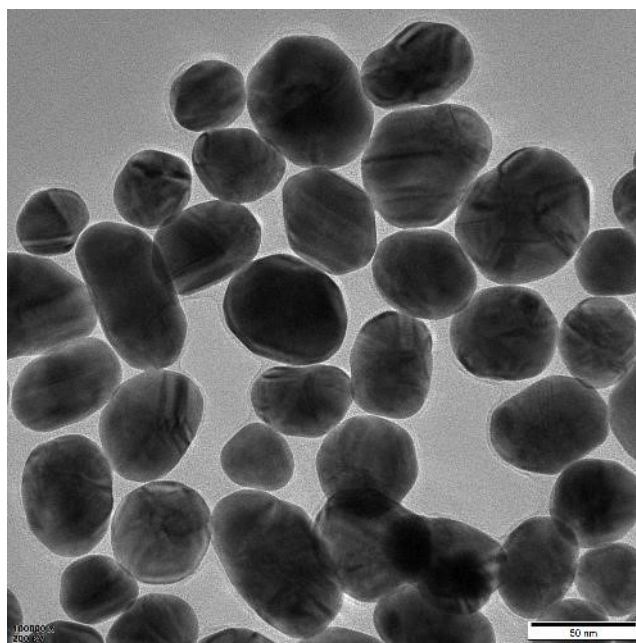


Figure S1 TEM image of AuNPs.

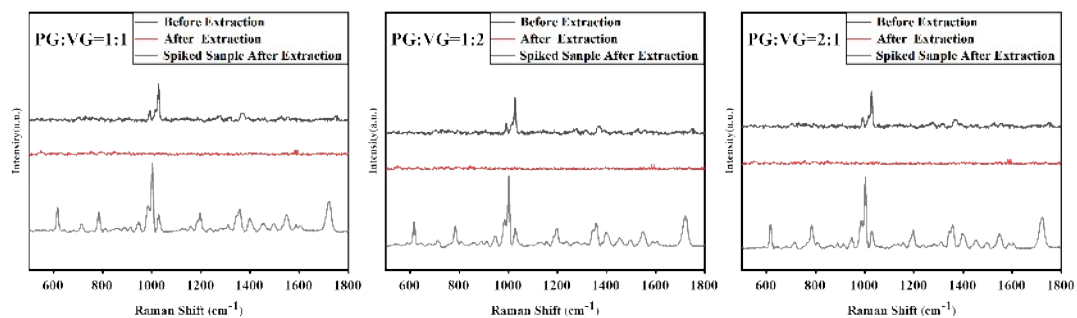


Figure S2 SERS detection results before and after pretreatment under different PG/VG ratios.

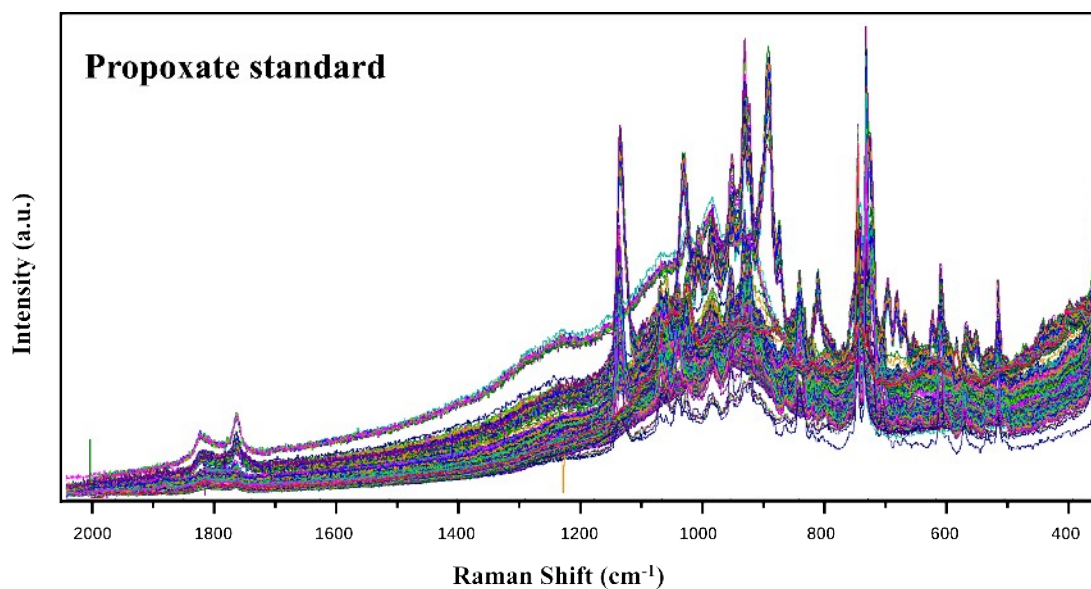


Figure S3 Original Spectral Data of Propoxate Standard.

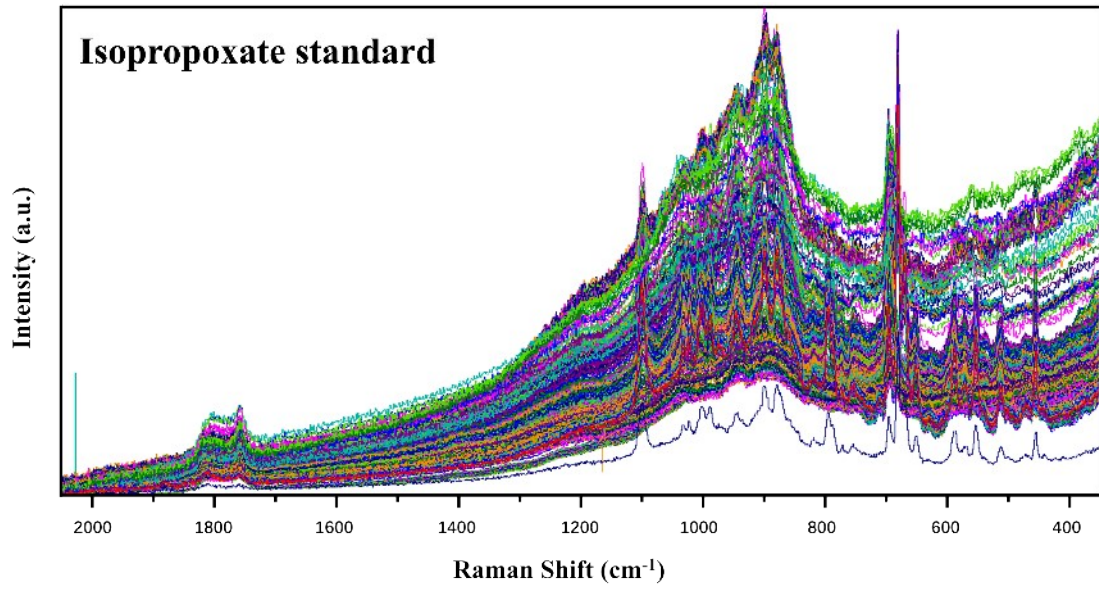


Figure S4 Original Spectral Data of Isopropoxate Standard.

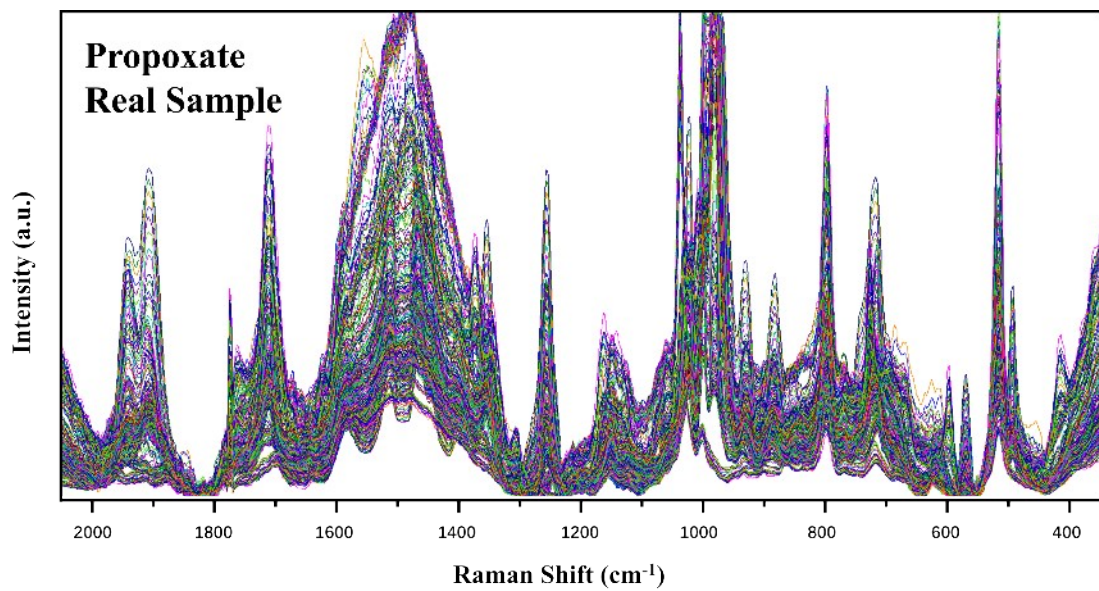


Figure S5 Original Spectral Data of Propoxate Real Sample.

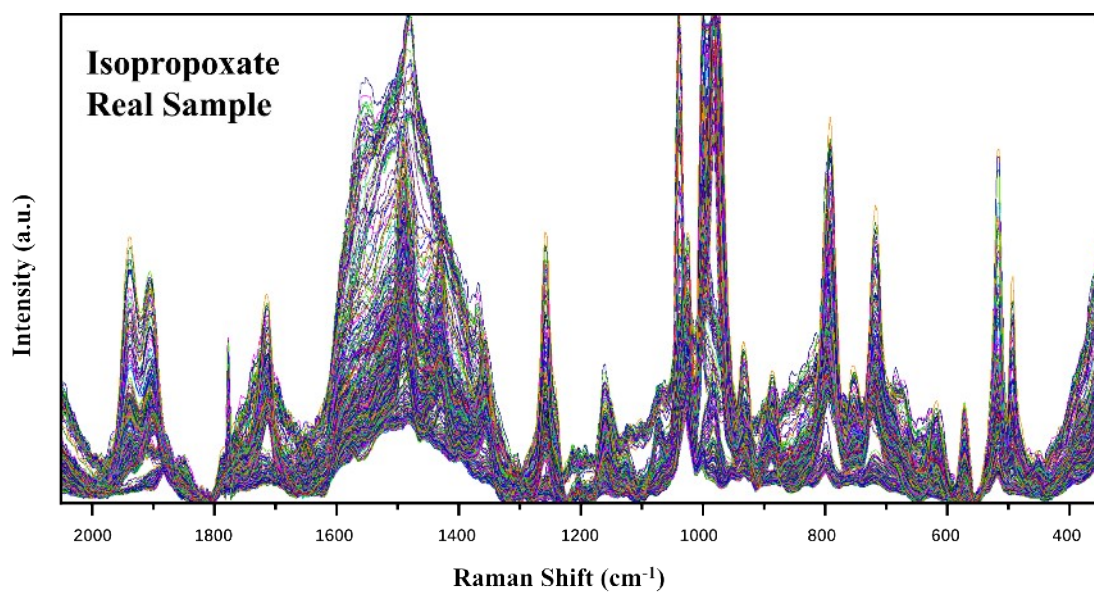


Figure S6 Original Spectral Data of Isopropoxate Real Sample.