Supporting Information for

Emerging investigator series: quantitative insights into the relationship between the concentrations and SERS intensities of neonicotinoids in water

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A Summary of Tables and Figures in Supporting Information:

Table S1. High-performance liquid chromatography (HPLC) method for imidacloprid (IMD) and clothianidin (CLO) quantification

HPLC Instrument Conditions	
HPLC	Agilent 1260 Infinity
Analytical Column	Agilent Poroshell 120 EC-C18 3x50mm, 2.7 μm
Guard column	Agilent Eclipse Plus C18 4.6x5mm, 1.8 μm
Column Temperature	30 °C
Injection Volume	25 μL
Mobile Phase	85% (0.1% Formic acid in water); 15% (0.1% Formic acid in acetonitrile)
Flow rate	1 mL/min
Stop time	2.5
Detector settings	
Wavelength	269 nm
Bandwidth	4 nm
Reference wavelength	360 nm
Reference Bandwidth	100 nm
Collection frequency	2.5 Hz

The retention times for CLO and IMD are 1.83 and 2.07 min, respectively.

Table S2. Freundlich and Langmuir adsorption isotherm fitting parameters for CLO data shown in **Fig. 2a**

Equation	y = a*x^b	y = a*b*x/(1+b*x)
a	0.61326 ± 0.02718	1.60831 ± 0.11761
b	0.44599 ± 0.02744	0.75315 ± 0.19734

Table S3. Langmuir adsorption isotherm fitting parameters for CLO data shown in **Fig. S4a**

Equation	y = a*b*x/(1+b*x)
a	0.16193 ± 0.02861
b	1.18373 ± 0.50669

Table S4. Freundlich and Langmuir adsorption isotherm fitting parameters for CLO data shown in **Fig. 2b**

Equation	y = a*x^b	y = a*b*x/(1+b*x)
a	0.09486 ± 0.00732	0.1491 ± 0.02718
b	0.23464 ± 0.04558	3.36684 ± 1.82347

Table S5. Linear fitting parameters for CLO data shown in **Fig. 2c**

Equation	y = a + b*x
Intercept	0.00179 ± 2.196E-4
Slope	0.17556 ± 0.00929

Table S6. Freundlich and Langmuir adsorption isotherm fitting parameters for IMD data shown in **Fig. 3a**

Equation	y = a*x^b	y = a*b*x/(1+b*x)
a	0.53749 ± 0.01573	1.36125 ± 0.1183
b	0.4044 ± 0.0138	0.78953 ± 0.25545

Table S7. Langmuir adsorption isotherm fitting parameters for IMD data shown in **Fig. S6a**

Equation	y = a*b*x/(1+b*x)
a	0.06282 ± 0.0024
b	2.27209 ± 0.35542

Table S8. Freundlich and Langmuir isotherm fitting parameters for IMD data shown in **Fig. 3b**

Equation	y = a*x^b	y = a*b*x/(1+b*x)
a	0.04213 ± 0.00269	0.05843 ± 0.00237
b	0.2089 ± 0.03405	8.79693 ± 1.92877

Table S9. Linear fitting parameters for IMD data shown in **Fig. 3c**

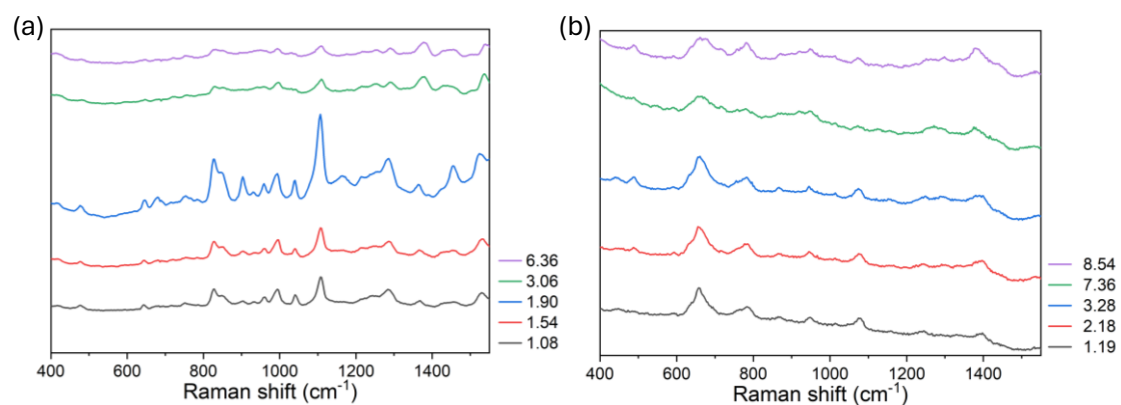| Equation	y = a + b*x
Intercept	0.00579 ± 0.00144
Slope	0.00874 ± 4.71822E-4

Figure S1. a) SERS spectra of 100 µM imidacloprid measured by AuNP/BC substrates at different pH values ranging from 1.08 to 6.36. b) SERS spectra of 10 µM clothianidin measured by AuNP/BC substrates at different pH values ranging from 1.19 to 8.54.
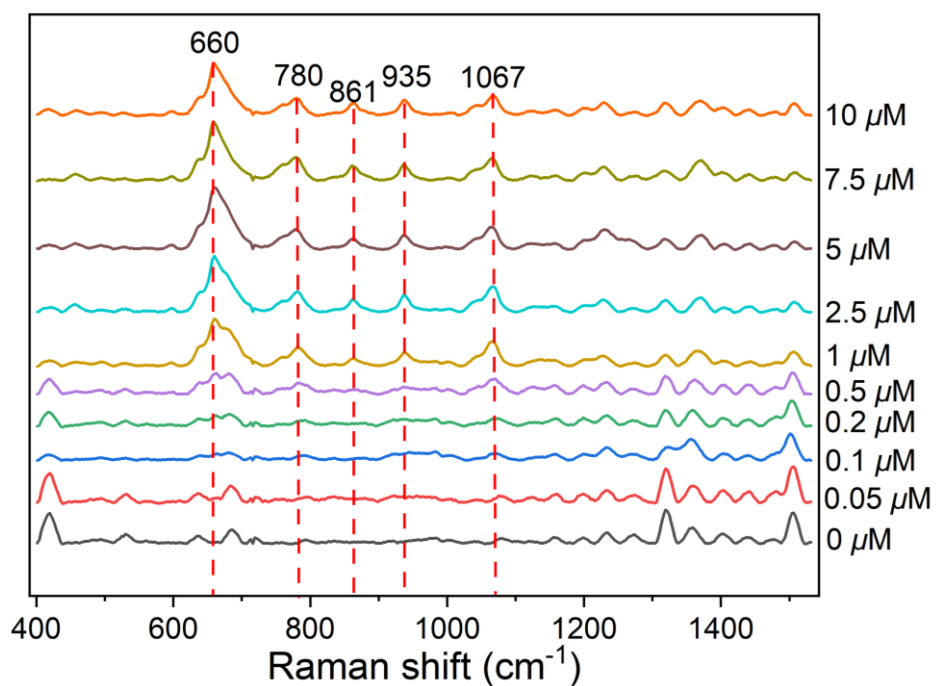
Figure S2. Hot-spot normalized SERS spectra of CLO collected from AuNP/BC substrates incubated in CLO solutions with concentrations ranging from 0 to 10 μM. Raman bands at 660, 780, 861, 935 and 1067 cm^{-1} are identified as the fingerprint features of CLO.
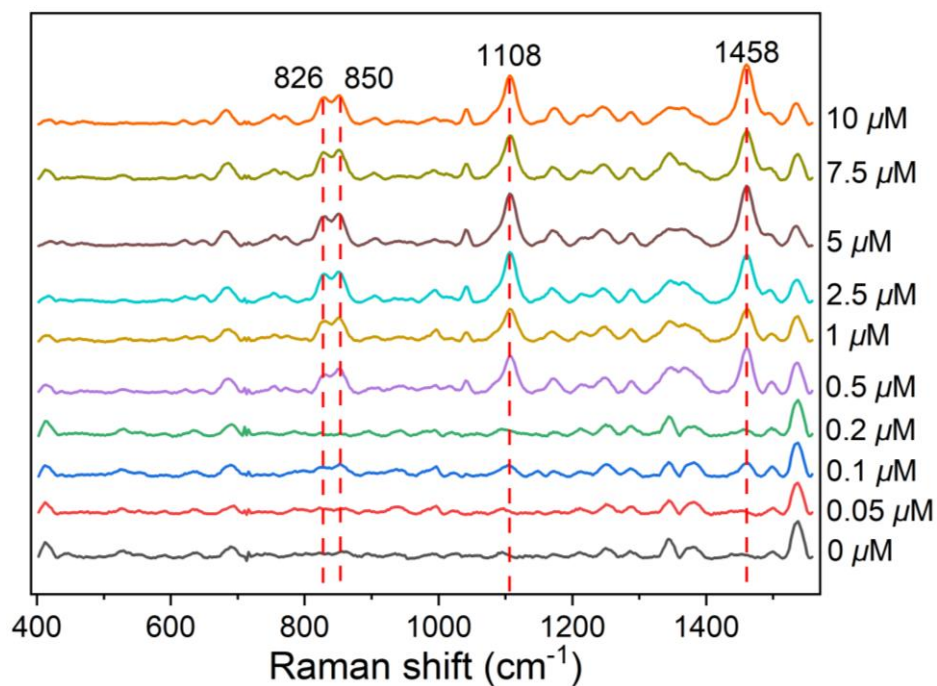
Figure S3. Hot-spot normalized SERS spectra of IMD collected from AuNP/BC substrates incubated in IMD solutions with concentrations ranging from 0 to 10 µM. Raman bands at 826, 850, 1108, and 1458 cm^{-1} are identified as the fingerprint features of IMD.
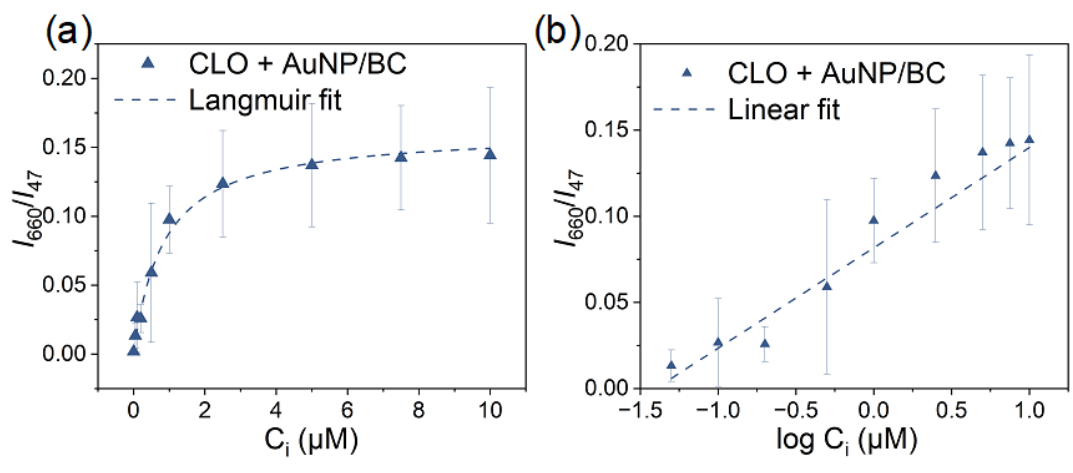
Figure S4. (a) Variation of the normalized CLO SERS intensities as a function of initial solution concentrations, C_i. (b) Variation of normalized CLO SERS intensities as a function of logarithmic initial solution concentrations, log C_i.
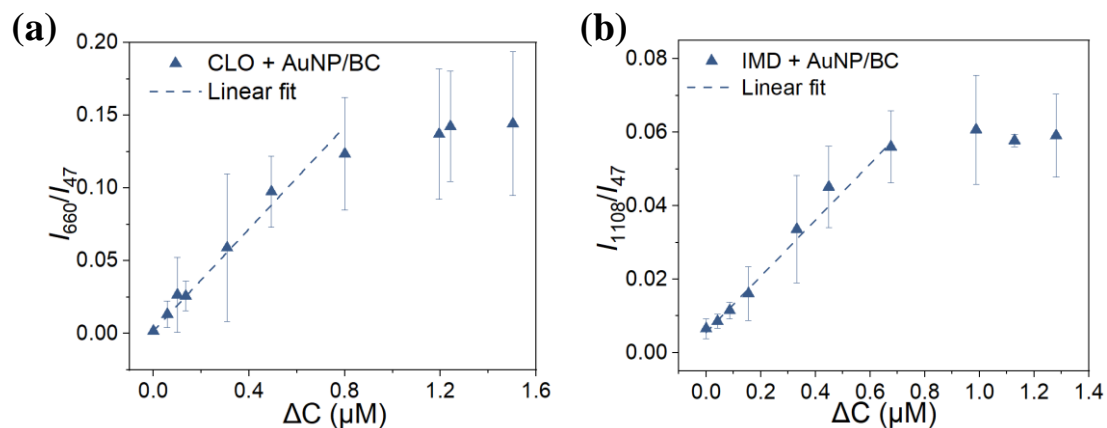
Figure S5. (a) Variation of the normalized SERS intensities of CLO as a function of its differential concentrations, $\triangle C$, with an extended initial concentration range from 0 to 10 μM. Within the range of 0.05 to 2.5 μM, a linear relationship was observed. Beyond 2.5 μM, there was a notable deviation from the linear fitting curve. (b) Variation of the normalized SERS intensities of IMD as a function of its differential concentrations, $\triangle C$, with an extended initial concentration range from 0 to 10 μM. Similar relationships with CLO were observed for IMD.
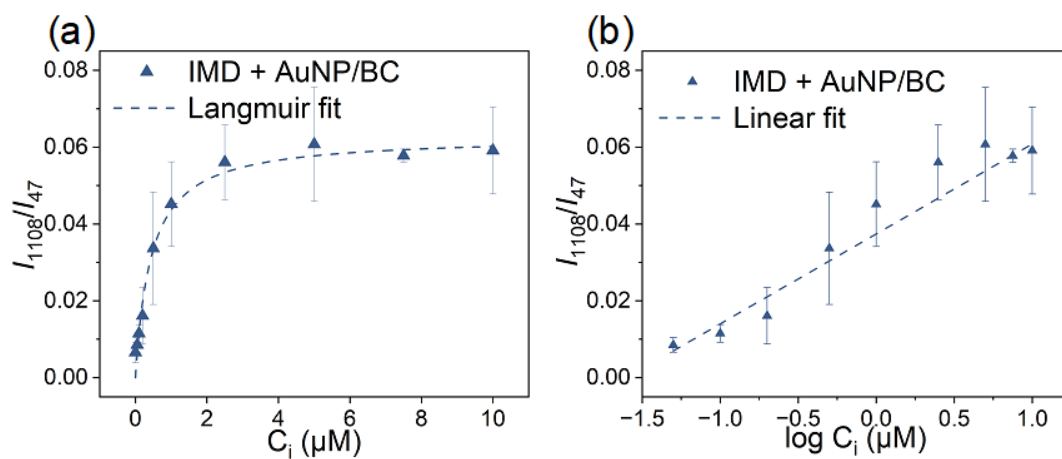
Figure S6. (a) Variation of normalized IMD SERS intensities as a function of initial solution concentration, C_i. (b) Variation of normalized IMD SERS intensities as a function of logarithmic initial IMD concentrations, $\log C_i$.