Sensing Antibiotics in Wastewater using Surface Enhanced Raman Scattering

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Supplementary Information

Summary:

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Parameter	Concentration	Description	Reference
Aluminum (mg/L)	19	Secondary effluent	Project No. SP-173,
NH ₃ -N (mg/L N)	22.6	water quality based on	Effluent Reuse Study
Iron (mg/L)	350	2008 and 2009 annual	GWRS Final Expansion
Manganese (mg/L)	45	average data.	FINAL Implementation
TDS (mg/L)	935		Plan Volume 1 of 3
TOC (mg/L)	14		
Turbidity (NTU)	3.2		
TBOD (mg/L)	11.1	Annual average	FACILITIES
CBOD (mg/L)	6.3	activated sludge	OPERATION AND
		effluent biochemical	MAINTENANCE
		oxygen demand for	
		fiscal year 2004 -2005	

Table S1. Water quality parameters in the secondary effluent used for seeding study

Table S2. The assignment of SERS bands of quinoline

Experiment (cm ⁻¹)	Literature (cm ⁻¹)	Vibrational assignment
770	760	ring deformation
1019	1014	ring breathing
1030	1034	ring breathing
1057	-	CH bending
1133	-	CH bending
1264	-	CNC bending
1314	-	CH bending
1376	1372	CCC stretching
1391	1392	CCC stretching
1440	1433	CH rocking
1463	-	CH rocking
1579	1571	CCC stretching

Figure S1. Comparison of SERS detection of quinoline in DI water with the quantification results by UPLC-MS/MS.



Figure S2. PCA plot of SERS spectra of DI water, treated wastewater, 50 ppm quinoline spiked in DI water or in treated wastewater. (a) Data collected on Self-Assembled SERS substrate; (b) Data collected on SEStrate.





Figure S3. SERS spectra collected using Self-assembly SERS substrate for erythromycin, humic acid, Microcystin-LR, glycine, L-arginine and quinoline spiked DI water in the concentration of 5 ppm.

Figure S4. Microscopy image of (a) fresh Self-Assembly SERS substrate and (b) washed Self-Assembly SERS substrate.

