

Supporting Information:

Surface-Enhanced Raman Scattering Based Detection of Bacterial Biomarker and Potential Surface Reaction Species

Han-Wen Cheng, Wei-Qi Luo, Guo-Li Wen, Shuang-Yan Huan*, Guo-Li Shen, and Ru-Qin Yu*

State Key Laboratory for Chemo/Biosensing and Chemometrics, College of Chemistry and Chemical Engineering, Hunan University, Changsha 410082, China (* Corresponding authors: Professors R.Q. Yu (email: rqyu@hnu.cn) and S.Y. Huan (email: huanshuangyan@yahoo.com.cn))

Table S1. Raman bands and assignments

Mode Assignment	DPA _(S)	DPA/AuNPs
C-C ring bend	644	661
C-H out-of-plane	759	825 (& 755)
Sym. ring breathing	994	999
Trig. ring breathing	-	1054
C-H bend	1154	1170
C-C ring mode	1269	-
C-C bend	1293	1300
C-O stretch	1328	1352
C-C ring stretch	1448	1420
ring stretch	1573	1571
C=O stretch	1640	~1639(sh.)

Table S2. Concentrations used for the solutions with mixed DPA and Py in different concentration ratios for the SERS experiment

[DPA] (mM)	[Py] (mM)	C ₀ (mM)	X _{DPA}	X _{Py}
0	0.30	0.30	0	1.00
0.15	0.15	0.30	0.50	0.50
0.20	0.10	0.30	0.67	0.33
0.25	0.05	0.30	0.83	0.17
0.27	0.03	0.30	0.92	0.08
0.29	0.01	0.30	0.98	0.02
0.30	0	0.30	1.00	0

(C₀ is the total concentration of Py and DPA)

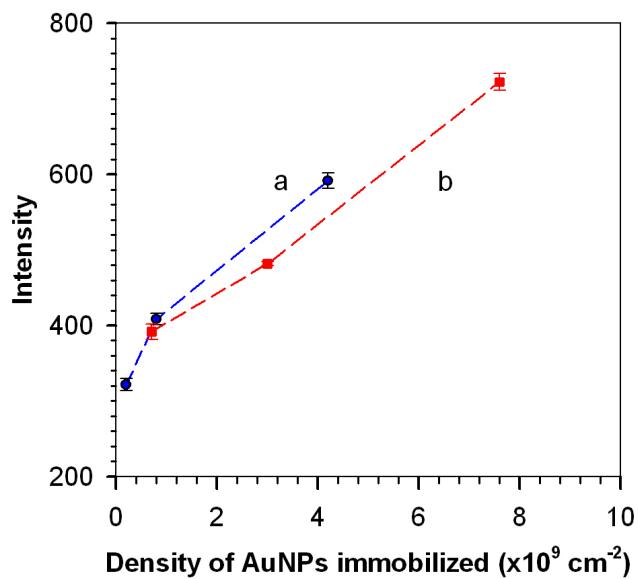


Figure S1. Plots of the SERS intensity (peak height at 999 cm⁻¹) for an AuNPs/Au substrate in a DPA solution ([DPA] = 50 ppm) vs. the surface density of particles as determined from the FE-SEM analysis for Au NPs on conducting glass substrate. Sizes of Au nanoparticles: 50 (a) and 60 (b) nm.

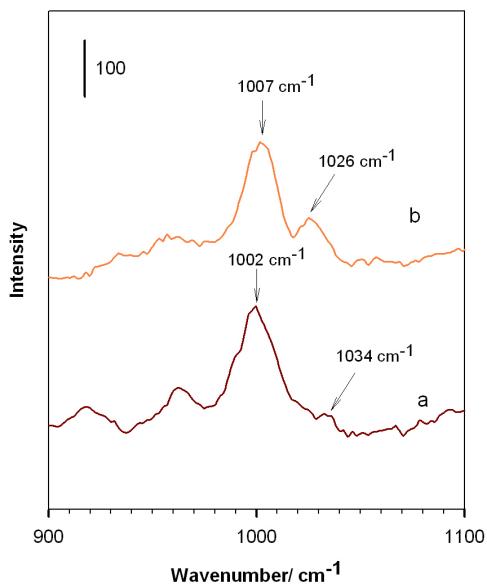


Figure S2. SERS spectra for DPA (0.01 mM) on an AuNPs/Au substrate before (a) and after exposure to a laser power of 12 mW (b).