## In Solution SERS Sensing using Mesoporous Silica-coated Gold Nanorods

Zhe Gao,<sup>a</sup> Nathan D. Burrows,<sup>b</sup> Nicholas A. Valley,<sup>c</sup> George C. Schatz,<sup>d</sup> Catherine J. Murphy<sup>b</sup> and Christy L. Haynes<sup>\*a</sup>

a.Department of Chemistry, University of Minnesota 207 Pleasant St SE, Minneapolis, MN 55455, USA. Email: chaynes@umn.edu

b.Department of Chemistry, University of Illinois at Urbana-Champaign, 600 S Mathews Ave, Urbana, IL 61801, USA. c.College of Health Sciences, California Northstate University 2910 Prospect Park Drive, Rancho Cordova, CA 95670, USA.

d.Department of Chemistry, Northwestern University 2145 Sheridan Rd, Evanston, IL 60208, USA.



Fig. S1 Colorimetric and ion-selective electrode calibration curves for [Br-] determination using NaBr (A, C, E, G) and CTAB (B, D, F, H). A,B) Color photographs of the colorimetric standards in order of decreasing concentration from left to right. C, D) Vis-NIR absorption spectra for the colorimetric standard. E, F) colorimetric standard curves. G, H) ion-selective electrode standard curves.



Fig. S2 MS spectra (from top to bottom) of synthesized 9-anthracenethiol, benz[a]anthrancenethiol, and thiolated  $\beta$ -cyclodextrin. The MS spectra were acquire to confirm the products synthesized according to literature procedures.



Fig. S3 TEM images of AuNR@MS with a MS shell of 50 nm. The AuNR@MS was synthesized by adding 200  $\mu$ L 0.88 M TEOS twice during the coating process. Due to the excess TEOS, AuNR-free MS NPs were found mixed with the AuNR@MS.



Fig. S4 XRD data for AuNR@MS.



Fig. S5 SERS spectra of molecules on bare AuNRs.  $\lambda$  ex=785 nm, P=9 mW, and t=30 s. The normal Raman signal for each analyte molecule at the same 1 mM concentration yielded no measurable Raman signal under the same collection conditions. The spectra shown are the average of 5 spectra.



Fig. S6 Computed dimensions of thiolated molecules.