**Electronic Supplementary Information for:**

**A size-controlled synthesis and characterization of mixed monolayer protected silver-S-(CH2)11-NHCO-coumarin nanoparticles and their Raman activities**

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**Density Functional Theory (DFT) calculations and models**

All calculations were carried out with Gaussian 03 programs [24] within the DFT framework. In this study the ligand-metal system structures of silver were optimized using the Becke’s three parameter hybrid functional [25] with the Lee et al. [26] (B3LYP) correlation functional employed with the electron core potential basis set LANL2DZ developed by Hay and Wadt [27-29]. For silver (Ag), the LANL2DZ set electron core potential simulates the 60 of the total 79 (Ag) electrons. The remaining 19 electrons are described by all electron basis sets consisting of a (8s6p4d) set of primitive Gaussian type functions contracted to the [3s3p2d]. For C, S and O the LANL2DZ basis consists of a (10s5p) set contracted to the [3s2p] set, while for H a (4s) set contracted to the [2s] basis set was used.



**FIG. S1.** Zeta potentials of AgNPs 16nm stabilized by (a) Citrate (b) 1% HS-(CH2)11-NHCO-coumarin (c) 50% HS-(CH2)11-NHCO-coumarin.



**FIG. S2.** Zeta potentials of AgNPs 30 nm stabilized by (a) Citrate (b) 1% HS-(CH2)11-NHCO-coumarin (c) 50% HS-(CH2)11-NHCO-coumarin.



**FIG. S3.** Zeta potentials of AgNPs 40 nm stabilized by (a) Citrate (b) 1% HS-(CH2)11-NHCO-coumarin (c) 50% HS-(CH2)11-NHCO-coumarin.

**Table S1.** Summary of the potentials





**FIG. S4.** Optimized geometries of (a) HS-(CH2)11-NHCO-coumarin and (b) Ag-S-(CH2)11-NHCO-coumarin.



**FIG. S5.** DFT calculated Raman spectra of (a) HS-(CH2)11-NHCO-coumarin and (b) Ag-S-(CH2)11-NHCO-coumarin.

**Table S2.** Summary of the peak assignments of DFT calculated Raman spectra of HS-(CH2)11-NHCO-coumarin and Ag-S-(CH2)11-NHCO-coumarin.

