

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.

Band Assignment	HS-Coumarin	HS-Coumarin on AgNPs
	Peak frequency (cm⁻¹)	
u(Ag-S)		310
u(CC) aliph rings	820,900,1020,1070,1110,1170	820,900,1020,1070,1110,1170
δ(CH₂) asym	1330, 1390,1420	1330, 1390,1420
u(CC) arom rings	1500,1560,1610,1660	1500,1560,1610,1660
u(-S-H)	2680	
u(C-H)	3020,3060,3090	3020,3060,3090
HS-Coumarin = HS-(CH ₂) ₁₁ -NHCO-coumarin, AgNPs = silver nanoparticles		
Aliph = aliphatic, arom = aromatic, asym=asymmetric		