Surface Selective Binding of 2,5-Dimercapto-1,3,4-thiadiazole (DMTD) on Silver and Gold nanoparticles. A Raman and DFT study

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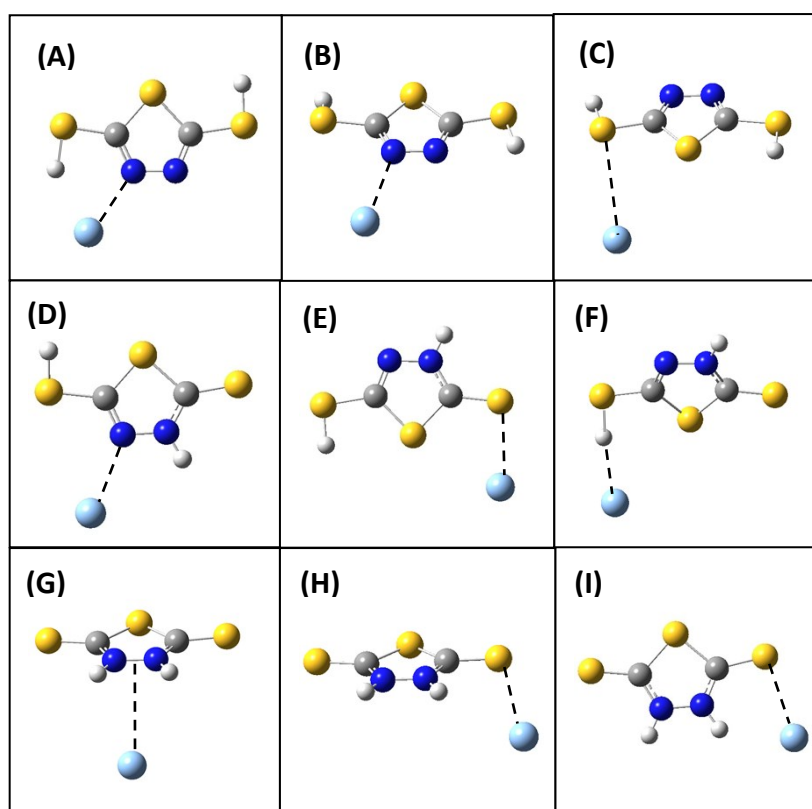
Supplementary Information

Figure S1. Optimized structures of three possible dithiol-Ag complexes (A) bound through ring N (S-H pointing towards Ag), (B) bound through ring N (S-H pointing away from Ag), (C) bound through thiol S; three possible thione-thiol-Ag complexes (D) bound through ring N, (E) bound through thione S, (F) bound through thiol S-H and three possible dithione-Ag complexes (G) bound through ring N-N bond, (H) bound through thione S S (Ag out of plane with dithione) and (I) bound through thione S (Ag in plane with dithione).
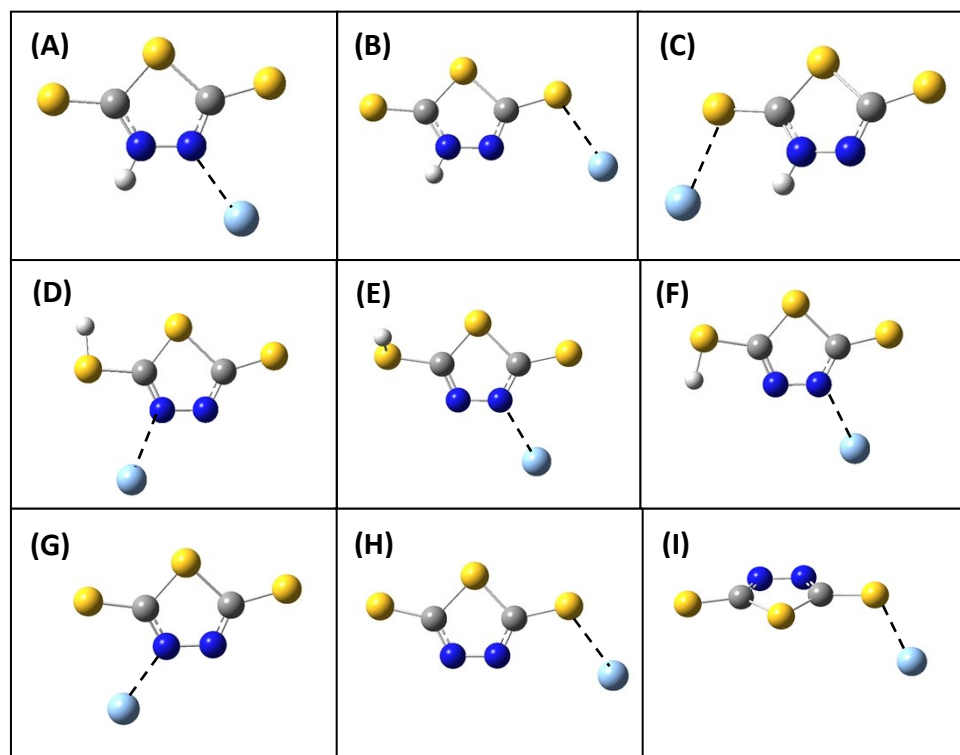
Figure S2. Optimized structures of three possible thione-thiolate-Ag complexes (A) bound through ring N, (B) bound through thione S, (C) bound through thione S with N-H in proximity, (C); three possible thiol-thiolate-Ag complexes (D) bound through ring N with S-H facing towards ring S, (E) bound through ring N with S-H out of plane with the ring, (F) bound through ring N with S-H facing towards ring N; and three possible dithiolate-Ag complexes (G) bound through ring N, (H) bound through thione S (Ag in plane with dithiolate) and (I) bound through thione S (Ag out of plane with dithiolate).
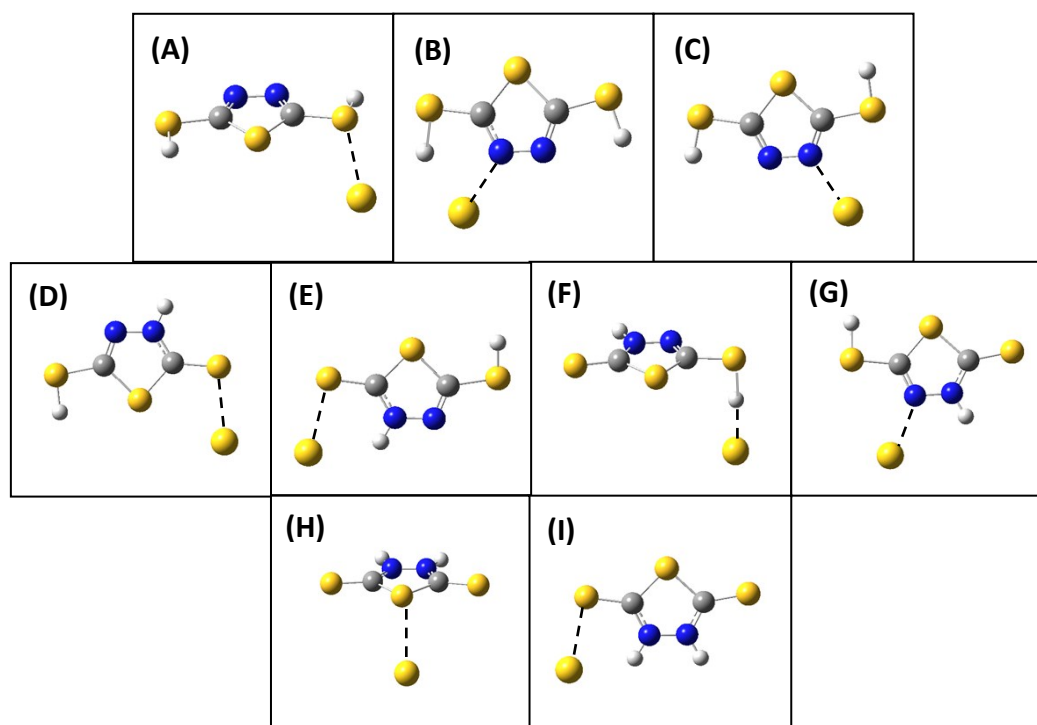
Figure S3. Optimized structures of three possible dithiol-Au complexes (A) bound through thiol S (B) bound through ring N with S-H facing the ring N atoms, (C) bound through ring N with S-H facing away from the ring N atoms; four possible thione-thiol-Ag complexes (D) bound through thione S, (E) bound through thione S with N-H in proximity, (F) bound through thiol S-H, (H) bound through ring N and two possible dithione-Ag complexes (H) bound through ring S (Ag out of plane with dithione) and (I) bound through thione S (Ag in plane with dithione).
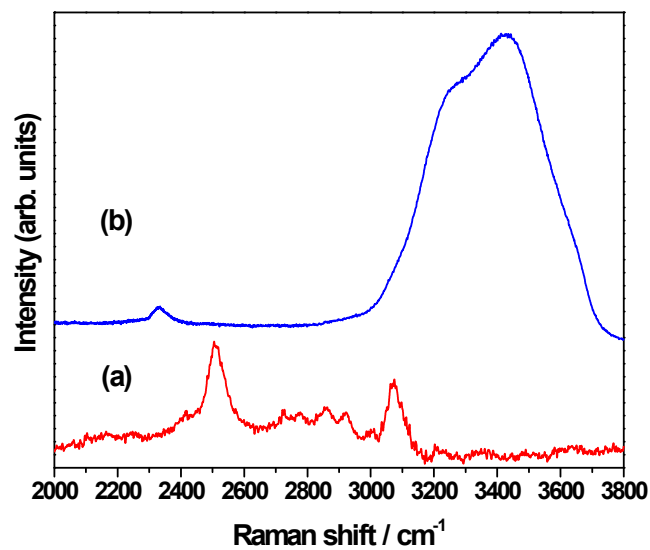
Figure S4. Raman spectra of (a) solid DMTD and (b) 10^{-2} M DMTD solution at pH 1.5 in the higher frequency region from 2000-3800 cm^{-1}.