Electronic Supplementary Information (ESI)

Dual Colorimetric Sensing of Mercury and Iodide ions by Steroidal 1,2,3-Triazole-Stabilized Silver Nanoparticles

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S1. Synthesis of silver nanoparticles stabilized with ligands 1−4

Silver nanoparticles were synthesized using the reported method[1] by reduction of $AgNO_3$ in sun light in the presence of one of the bile acid-based ligands **1**−**4**. For this, 1 mL (1000 μM) solution of a ligand from **1**−**4** $CHCl_3$/MeOH (1:1) was added to the solution of 1 mL (100 μM) $AgNO_3$ in $CHCl_3$/MeOH (1:1) and the resulting solution was exposed to sun light for 15-20 min. The solution turned dark yellow, indicating the formation of silver nanoparticles. The UV-vis spectrum showed a band around 420 nm for AgNPs (Fig. S1). The HRTEM indicated the formation of highly uniform and monodispersed silver nanoparticles (Figure S2). The average diameter of these particles was found to be 2−10 nm.

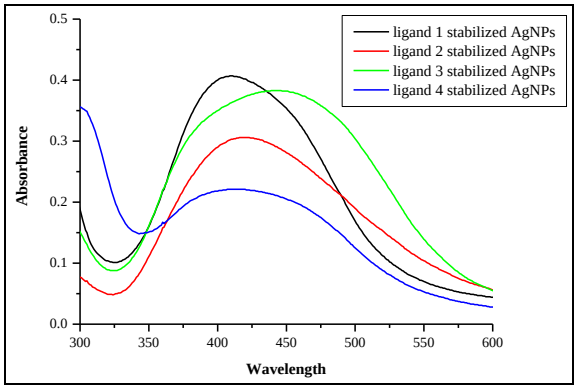

Fig. S1. UV-visible spectra of ligand **1**–**4** stabilized AgNPs

(a) (b)

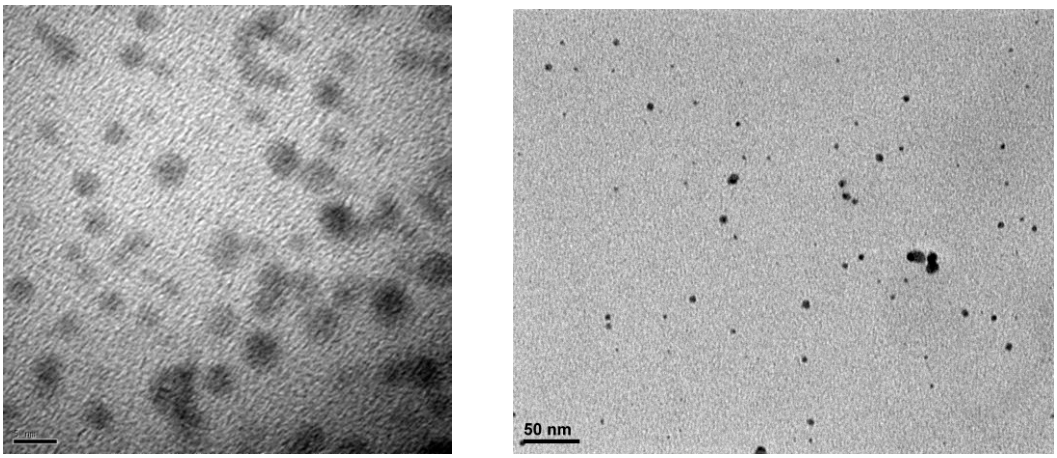

Fig. S2. HRTEM images of AgNPs stabilized with (a) ligand **2** (scale bar 5 nm), (b) ligand **4** (scale bar 50 nm)

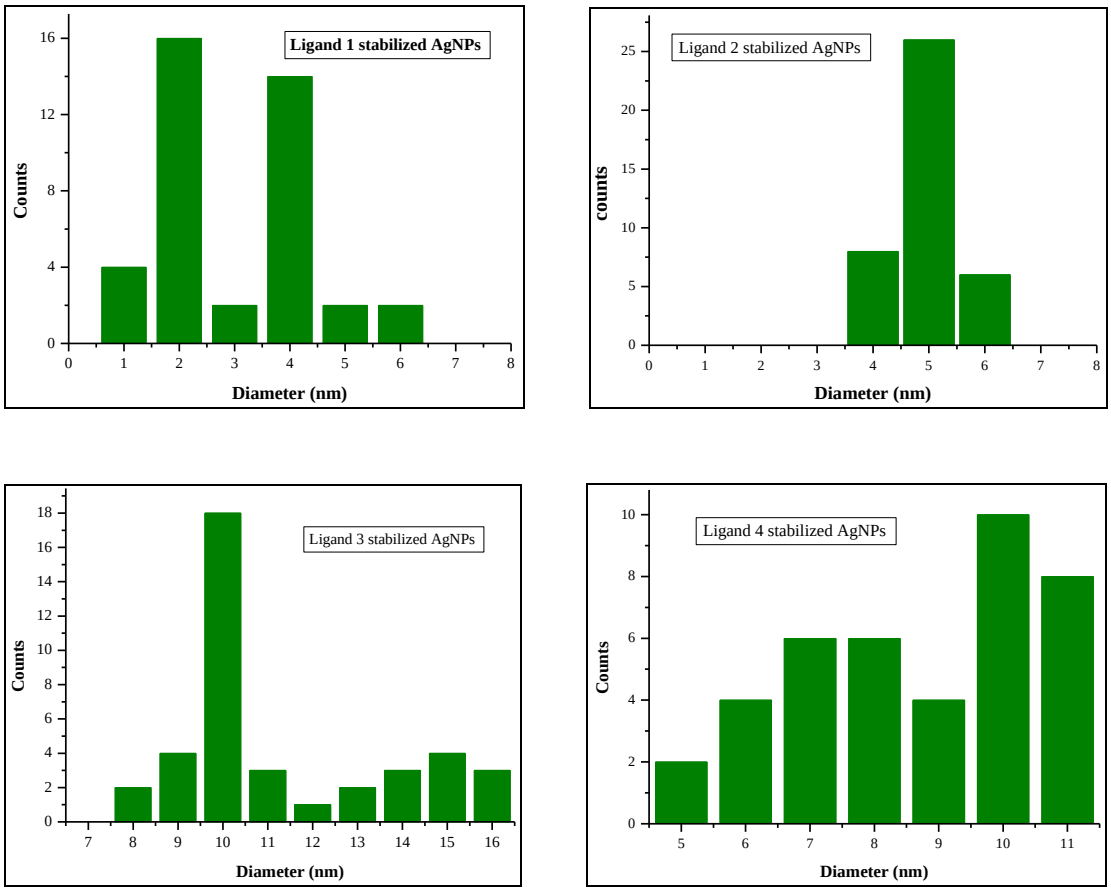

Fig. S3. Size distribution of AgNPs stabilized with ligands **1**−**4**

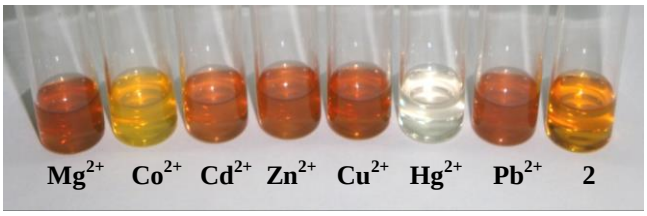

Fig. S4. A photograph of the solutions of AgNPs stabilized with ligand **2** after addition of different metal ions. Ion concentration of Co^{2+}, Cd^{2+}, Zn^{2+}, Cu^{2+} and Pb^{2+} is 1 mM; [Hg^{2+}] = 375 µM.

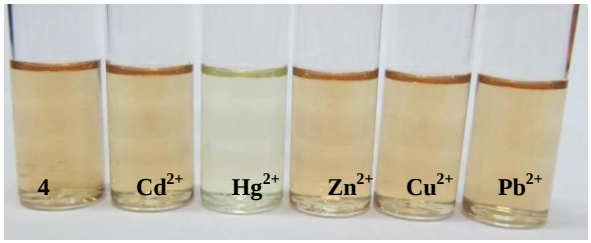

Fig. S5. A photograph of the solutions of AgNPs stabilized with ligand **4** after addition of different metal ions. Ion concentration of Cd^{2+}, Zn^{2+}, Cu^{2+} and Pb^{2+} is 1mM; [Hg^{2+}] = 200 µM.

(a) (b)

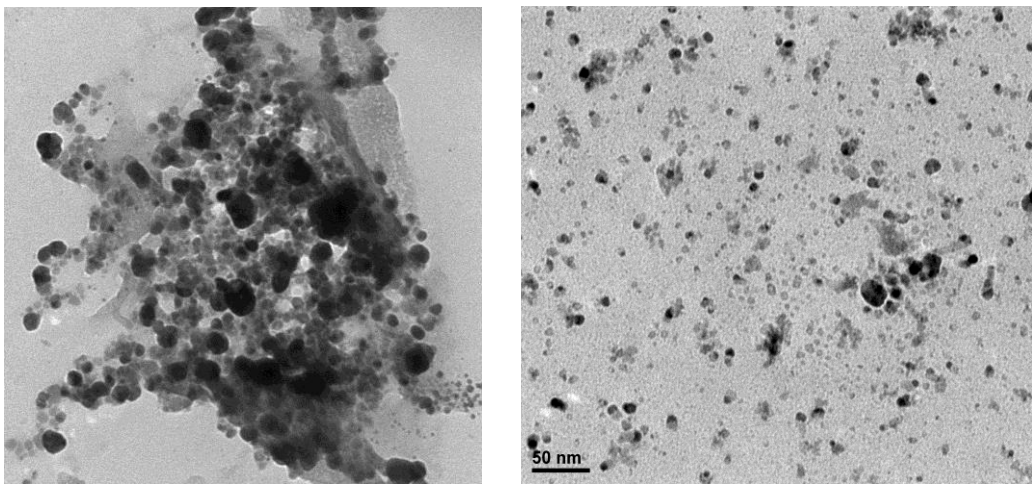

Fig. S6. HRTEM images of ligand-stabilized AgNPs on addition of Hg^{2+} (a) ligand **2**.AgNPs and Hg^{2+} (Scale bar 100 nm), (b) ligand **4**.AgNPs and Hg^{2+} (Scale bar 50 nm)

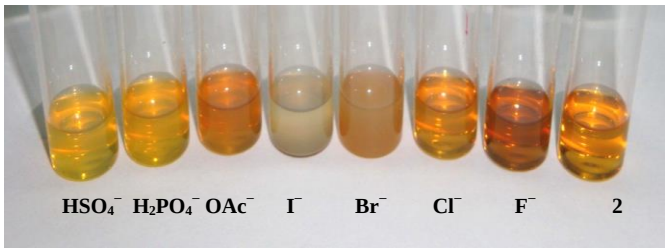

Fig. S7. A photograph of the solutions of AgNPs stabilized with ligand **2** after addition of different anions. Ion concentration of HSO_4^-, $H_2PO_4^-$, OAc^-, Br^-, Cl^- and F^- is 2 mM; $[I^-]$ = 1mM.

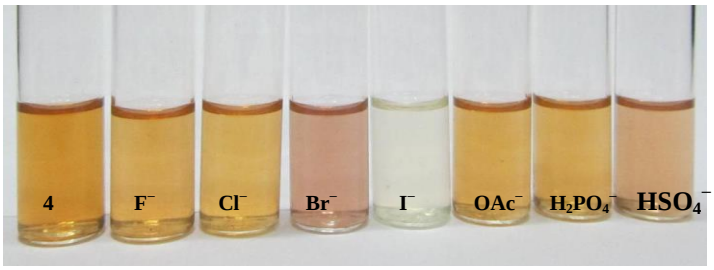

Fig. S8. A photograph of the solutions of AgNPs stabilized with ligand **4** after addition of different anions. Ion concentration of F^-, Cl^- , Br^-, OAc^-, $H_2PO_4^-$ and HSO_4^- is 2 mM; $[I^-]$ = 300 µM.

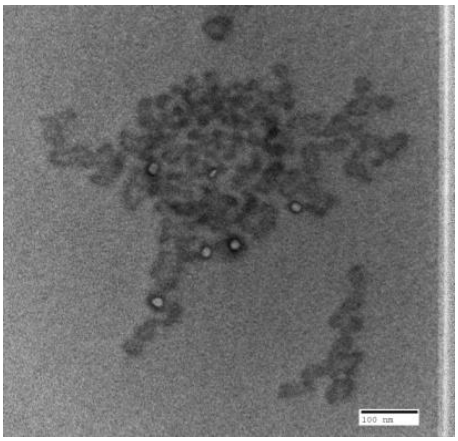

Fig. S9. HRTEM images of ligand 4.AgNPs on addition of I^- (Scale bar 100 nm)

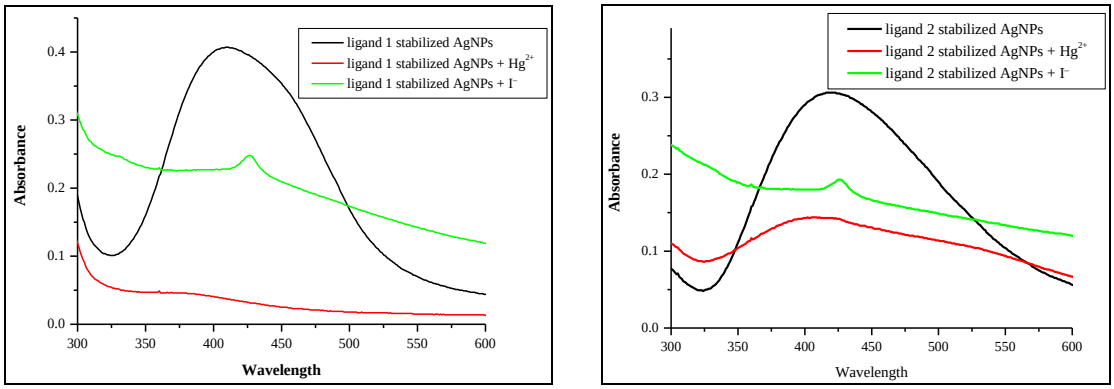

Fig. S10. UV-vis spectra on addition of Hg^{2+} / I^- to ligand-stabilized **1** and **2**.AgNPs respectively

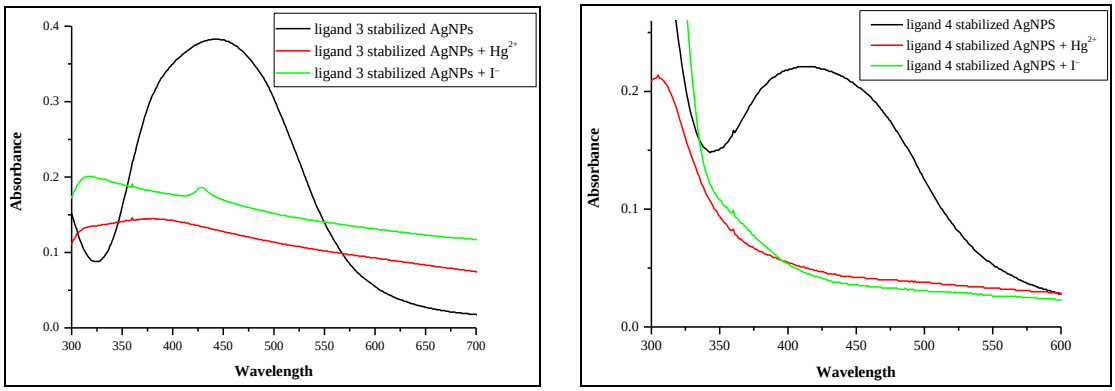

Fig. S11. UV-vis spectra on addition of Hg^{2+} / I^- to ligand-stabilized **3** and **4**.AgNPs respectively

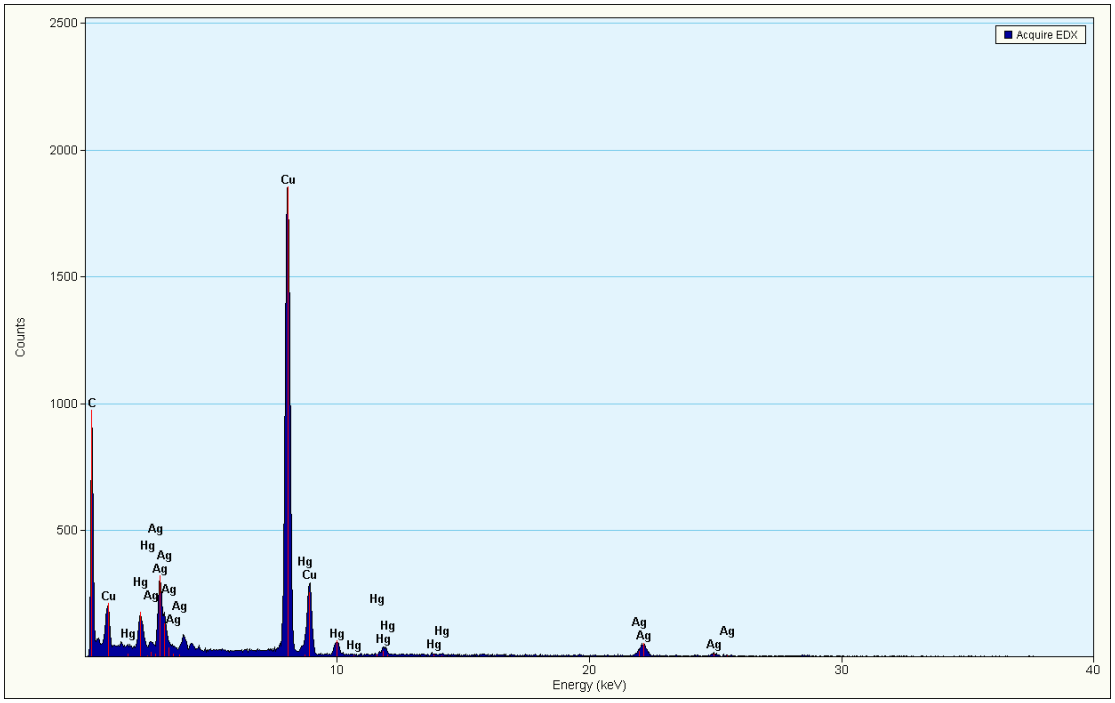

Fig. S12. TEM-EDX **3**.AgNPs after addition of Hg^{2+}

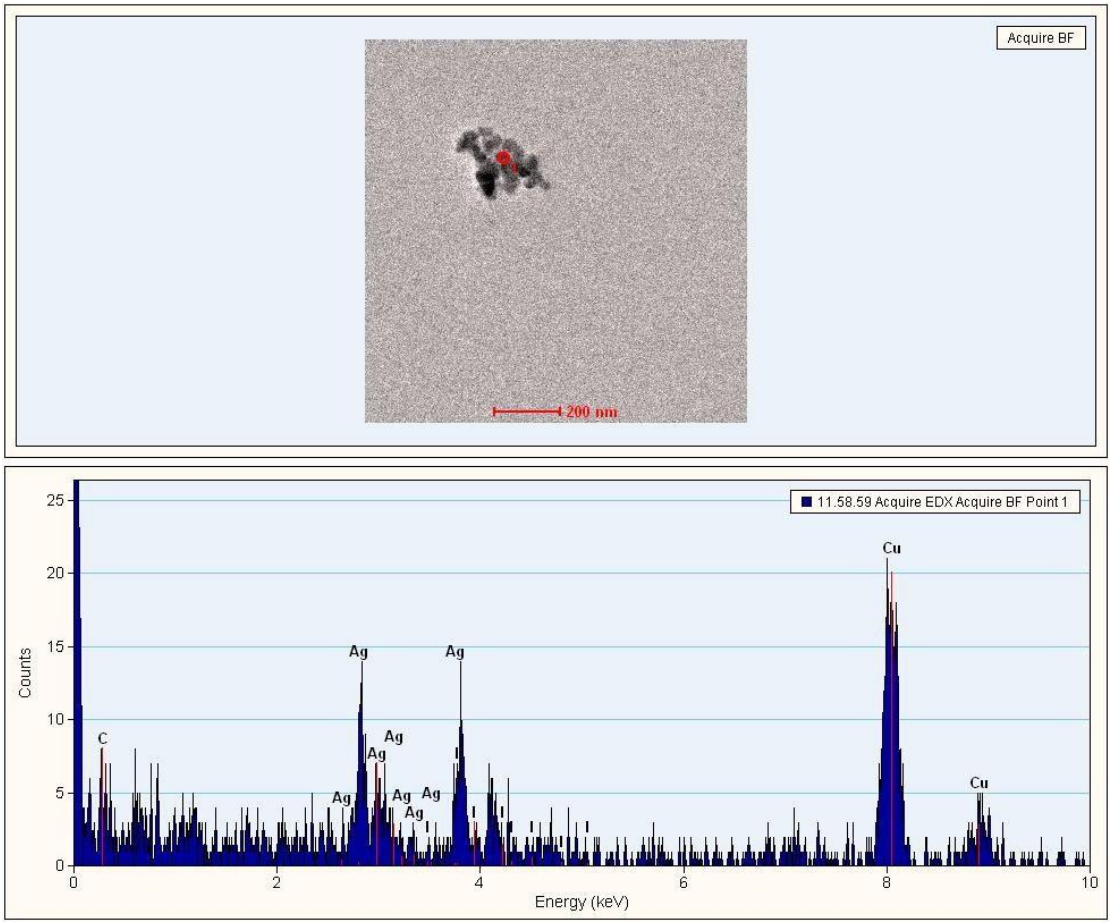

Fig. S13. TEM-EDX **3**.AgNPs after addition of I^-

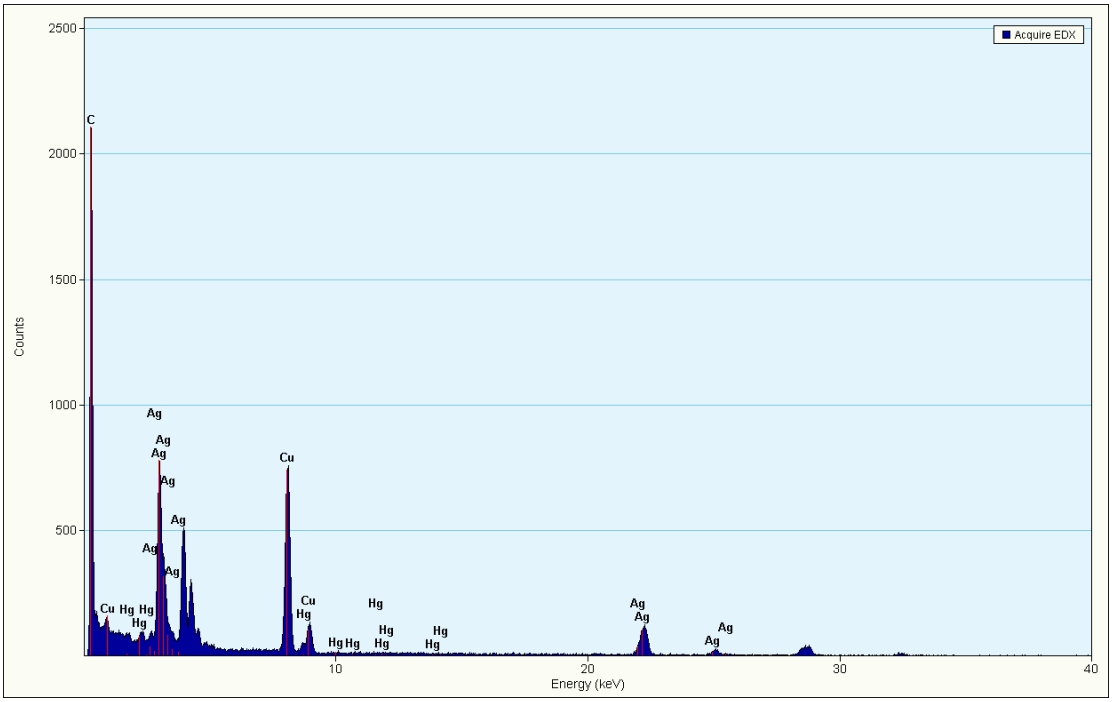

Fig. S14. TEM-EDX **4**.AgNPs after addition of Hg^{2+}

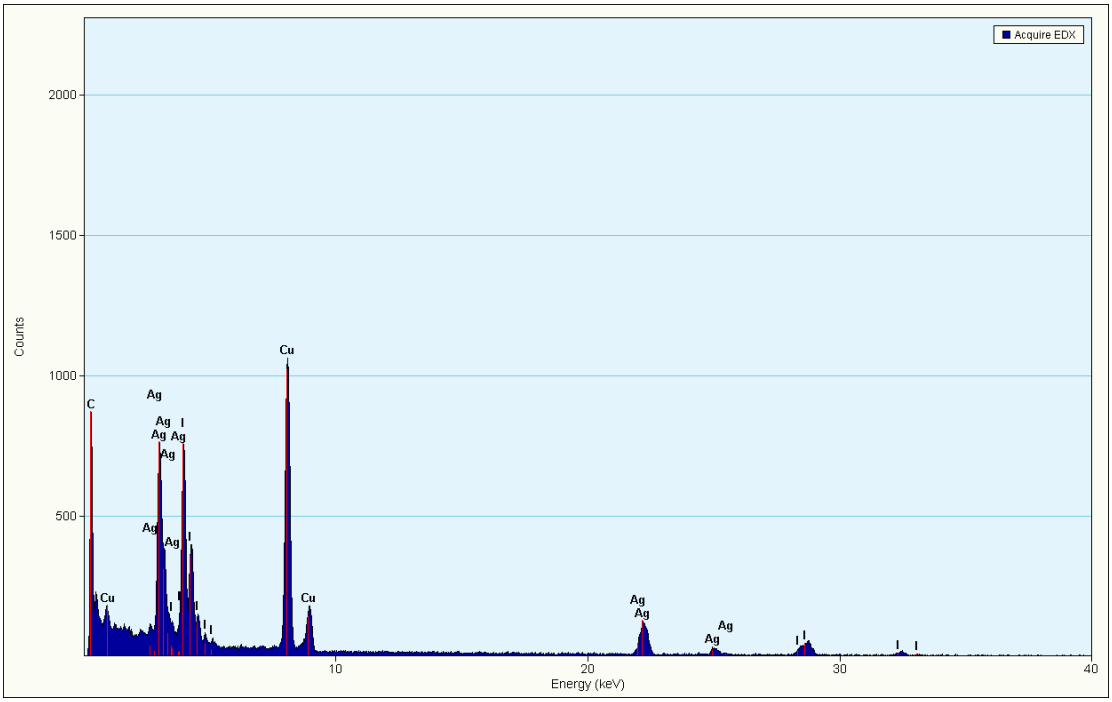

Fig. S15. TEM-EDX **4**.AgNPs after addition of I^-

S2. General procedure for the synthesis of bile acid based receptors

To a solution of 3β, 12β-bis-(azidoacetyl)deoxycholate in 30 mL of *t*-BuOH was added propargyl derivative. To this solution, $CuSO_4.5H_2O$ (10 mol %) and sodium ascorbate (20 mol %) were added in 3.0 mL of H_2O. The solutions was stirred at 60 $^{\circ}$C for 14 h and evaporated under vacuum. The residue was dissolved in 30 mL of $CHCl_3$ and washed with H_2O (10 mL) followed by brine (10 mL). The chloroform layer was dried over anhydrous Na_2SO_4 and evaporated completely. The crude product was purified by column chromatography over silica-gel to give the 1,2,3-triazole receptors.

*Compound **1***

Compound **1** was synthesized by reported literature procedure.[2]

*Compound **2***

The 3β, 12β-bis-(azidoacetyl)deoxycholate (250 mg, 0.43 mmol) and prop-2-ynyloxy-benzene (126 mg, 0.95 mmol) were taken. The product **2** was isolated as 338

mg of white solid. Yield: 94%; mp 90−91 °C; ^{1}H NMR (300 MHz, $CDCl_3$, TMS): δ (ppm): 0.71 (s, 3H, 18-Me), 0.81 (d, 3H, J = 4.8 Hz, 21-Me), 0.89 (s, 3H, 19-Me), 1.01-2.39 (26H, steroidal H), 3.67 (s, 3H, -OCH_3), 4.79 (m, 1H, 3β-H), 5.15−5.2 7 (m, 9H, 12β-H, -$OCOCH_2$ × 2, -OCH_2 × 2), 6.94−7.01 (m, 6H, Ar-H), 7.26−7.33 (m, 4H, Ar-H), 7.82 (s, 1H, Ar-H),7.89 (s, 1H, Ar-H); ^{13}C NMR (75 MHz, $CDCl_3$, TMS): δ (ppm): 11.79, 17.21, 22.31, 22.88, 24.88, 25.39, 25.66, 26.19, 26.82, 30.31, 30.47, 31.17, 33.39, 33.57, 34.17, 34.91, 41.11, 44.59, 46.86, 48.79, 50.84, 51.10, 61.27, 76.21, 77.86, 114.25, 114.29, 120.76, 120.86, 124.19, 124.39, 129.10, 129.18, 143.76, 143.98, 157.80, 157.86, 164.94, 165.57, 174.17; ES-HRMS calcd for $C_{47}H_{60}N_6O_8Na$ 859.4370, found 859.4365, $(M + Na)^+$.

*Compound **3***

The 3β, 12β-bis-(azidoacetyl)deoxycholate (300 mg, 0.52 mmol) and prop-2-ynylsulfanyl-benzene (169 mg, 1.14 mmol) were taken. The crude product was purified by column chromatography over silica-gel (40% ethyl acetate in hexane) to give 379 mg of **3**. Yield: 84%; mp: 103−105 ºC; IR (KBr): 3072, 2923, 1743, 1452, 1223 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, TMS): δ (ppm): 0.70 (s, 3H, 18−Me), 0.79 (s, 3H, 21−Me), 0.87 (s, 3H, 19−Me), 1.02−2.35 (26H, steroidal H), 3.66 (s, 3H, −OCH_3), 4.21 (s, 2H, −SCH_2), 4.28 (s, 2H, −SCH_2), 4.75 (m, 1H, 3β-H), 5.09−5.16 (m, 5H, 12β-H, −$OCOCH_2$ × 2), 6.87−7.36 (m, 10H, Ar−H), 7.60 (s, 1H, triazole-H), 7.64 (s, 1H, triazole-H); ^{13}C NMR (75 MHz, $CDCl_3$, TMS): δ (ppm): 11.96, 17.35, 22.45, 22.99, 25.02, 25.46, 25.73, 26.31, 26.93, 28.29, 28.44, 29.37, 30.44, 30.61, 31.32, 33.52, 33.71, 34.27, 35.05, 41.24, 44.69, 47.01, 48.92, 50.94, 51.24, 76.28, 78.03, 123.49, 123.68, 126.08, 128.68, 128.76, 129.02, 135.35, 135.54, 144.71, 144.87, 165.03, 165.61, 174.31; ES-HRMS calcd for $C_{47}H_{63}N_6O_6S_2$ 869.4089, found 869.4068, $(M + H)^+$.

*Compound **4***

The 3β, 12β-bis-(azidoacetyl)deoxycholate (300 mg, 0.52 mmol) and 2-prop-2-ynylsulfanyl-phenylamine (215 mg, 1.14 mmol) were taken. The crude product was purified by column chromatography over silica-gel (70% ethyl acetate in hexane) to give 397 mg of **4**. Yield: 85%; mp: 155−157 ºC; IR (KBr) 3433, 3329, 2942, 1741, 1612, 1474, 1218 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, TMS): δ (ppm): 0.72 (s, 3H, 18−Me), 0.79 (s, 3H, 21−Me), 0.89 (s, 3H, 19−Me), 1.02−2.36 (26H, steroidal H), 3.68 (s, 3H, $-OCH_3$), 4.01 (s, 2H, $-SCH_2$), 4.05 (s, 2H, $-SCH_2$), 4.31 (bs, 2H, $-NH_2$), 4.38 (bs, 2H, $-NH_2$), 4.76 (m, 1H, 3β-H), 5.12−5.20 (m, 5H, 12β-H, $-OCOCH_2 \times 2$), 6.62−6.70 (m, 4H, Ar−H), 7.08−7.13 (m, 2H, Ar−H), 7.26−7.28 (m, 3H, Ar−H), 7.29 (s, 1H, triazole-H), 7.30 (s, 1H, triazole-H); ^{13}C NMR (75 MHz, $CDCl_3$, TMS): δ (ppm): 12.16, 17.57, 22.67, 23.18, 25.28, 25.67, 25.99, 26.51, 27.14, 29.04, 29.30, 29.59, 30.63, 30.86, 31.60, 33.74, 33.97, 34.38, 34.50, 35.27, 41.43, 44.92, 47.31, 49.15, 50.99, 51.06, 51.50, 76.44, 78.30, 114.99, 116.56, 116.64, 118.29, 123.35, 123.57, 130.23, 130.26, 136.24, 136.44, 144.80, 144.93, 148.73, 148.94, 165.32, 165.92, 174.56; ES-HRMS calcd for $C_{47}H_{63}N_8O_6S_2$ 899.4306, found 899.4319, $(M + H)^+$.

Reference

1. A. Kumar, R. K. Chhatra and P. S. Pandey, *Org. Lett.* 2010, **12**, 24.
2. A. Kumar and P. S. Pandey, *Org. Lett*. 2008, **10**, 165.

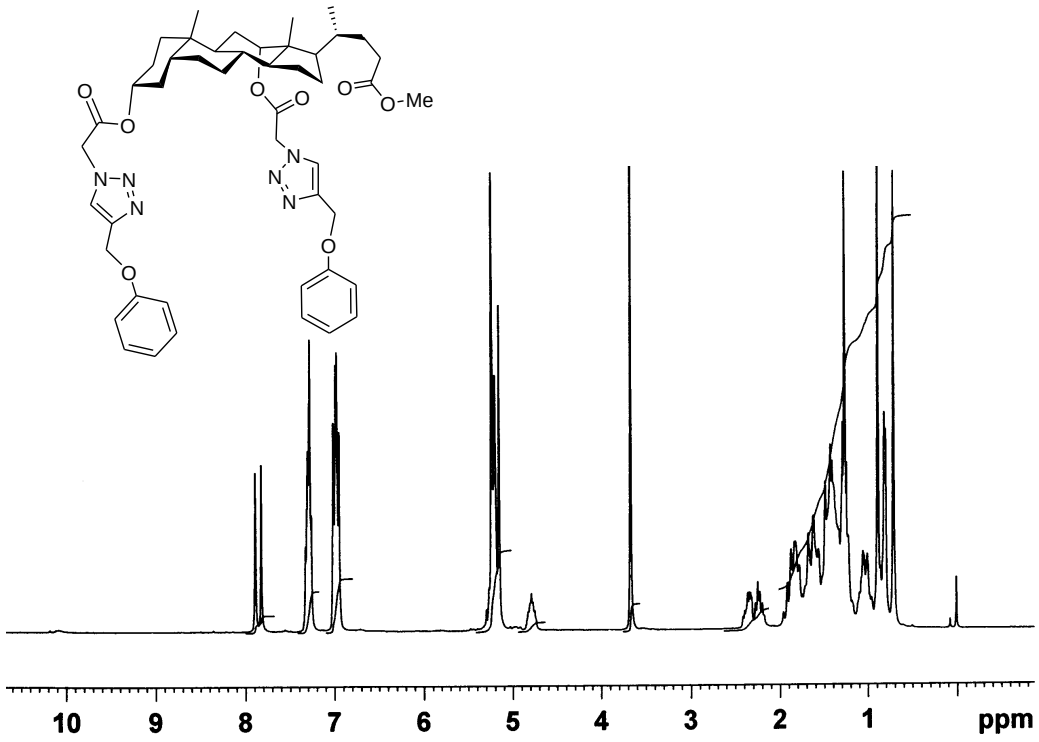

Fig. S16. ^{1}H NMR spectrum of ligand **2**

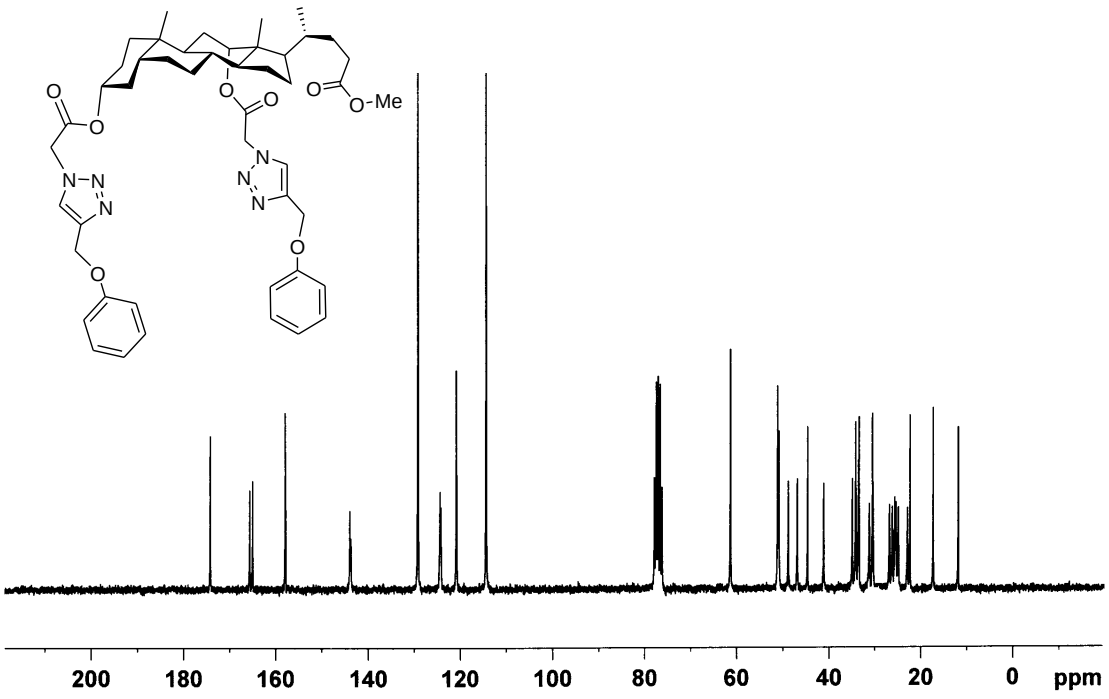

Fig. S17. ^{13}C NMR spectrum of ligand **2**

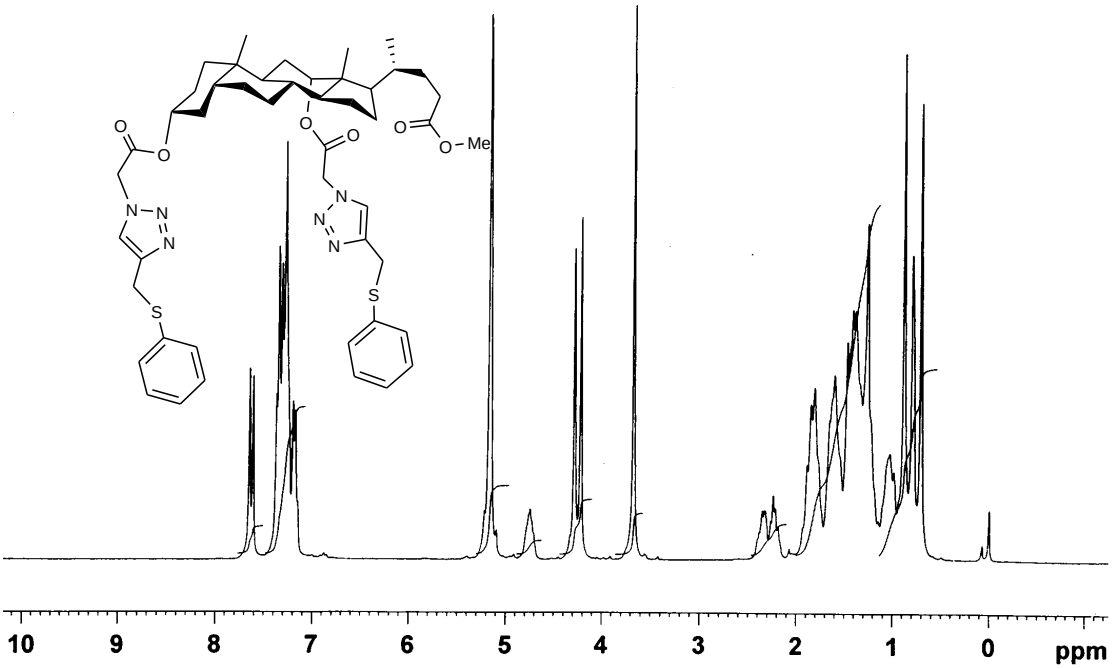

Fig. S18. ^{1}H NMR spectrum of ligand **3**

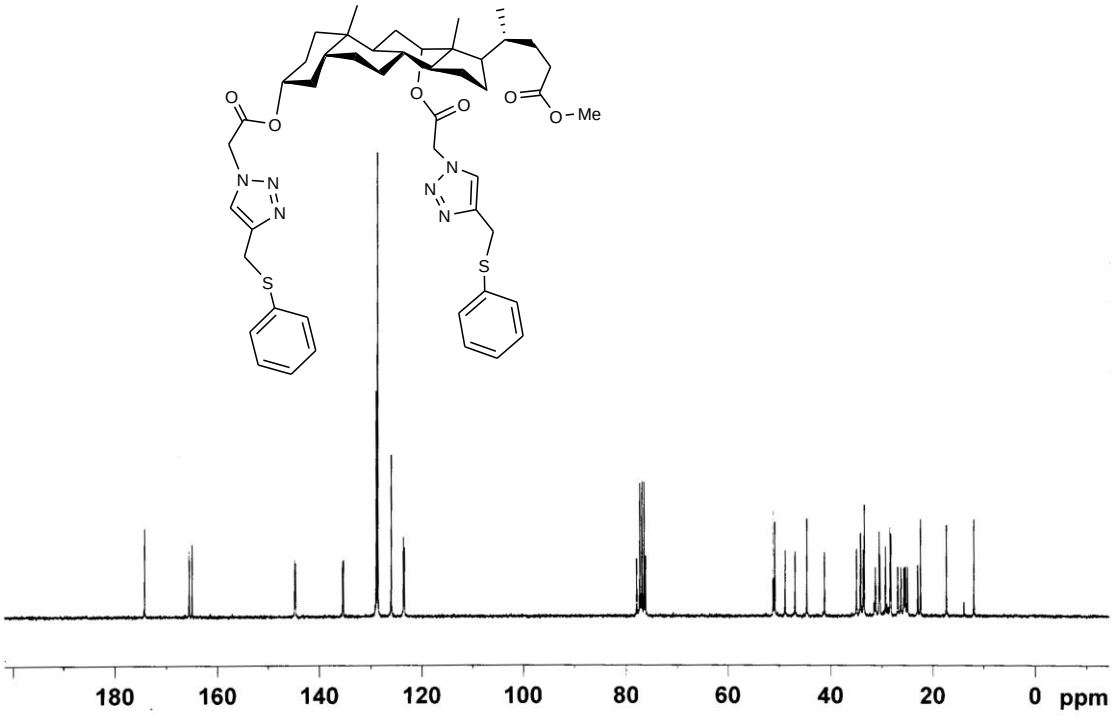

Fig. S19. ^{13}C NMR spectrum of ligand **3**

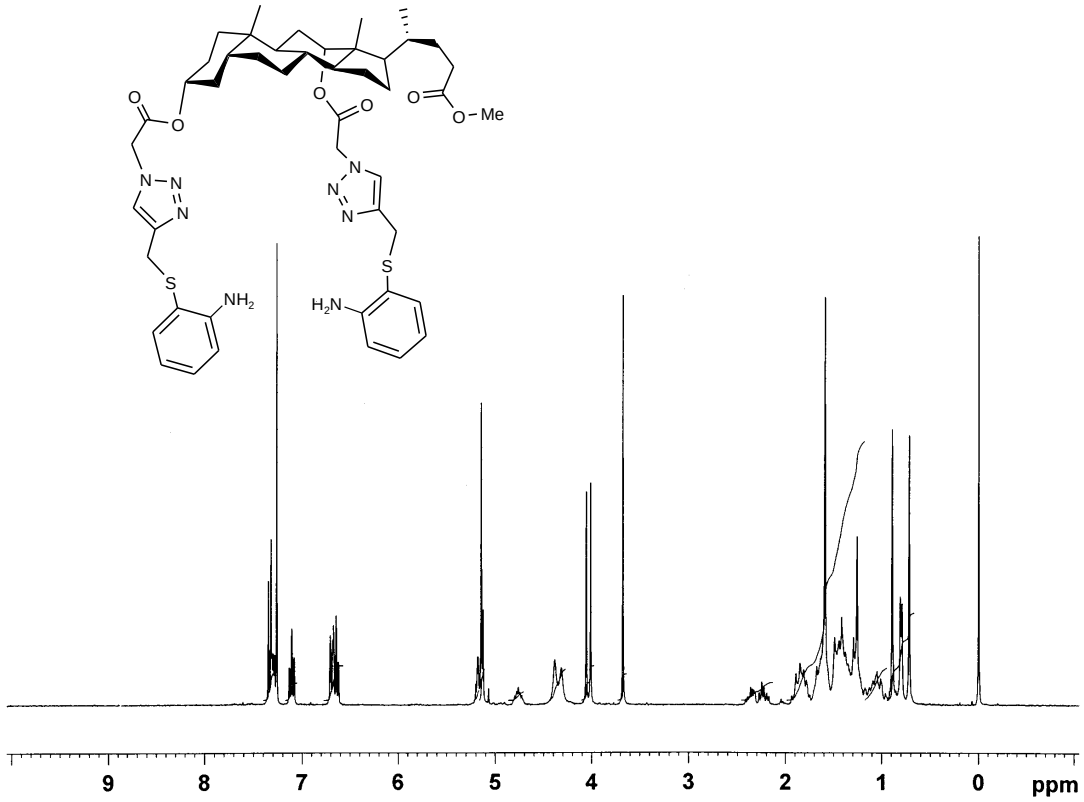

Fig. S20. ^{1}H NMR spectrum of ligand **4**

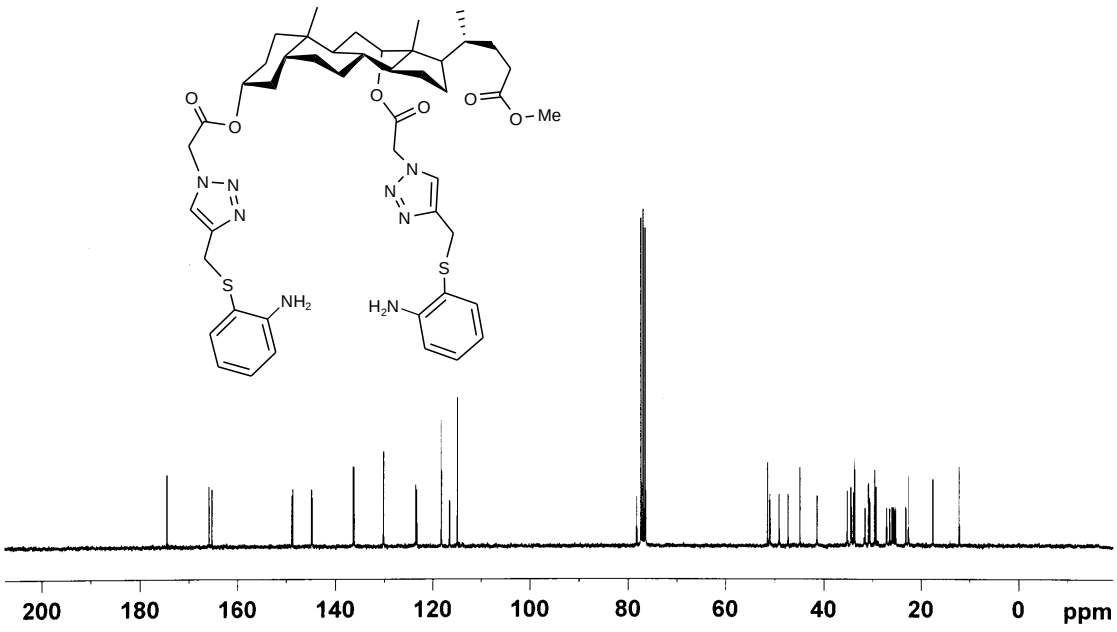

Fig. S21. ^{13}C NMR spectrum of ligand **4**