Supporting Information

Residual Weakly Bound Ligands Influence Biological Compatibility of Mixed Ligand Shell, Thiol-Stabilized Gold Nanoparticles

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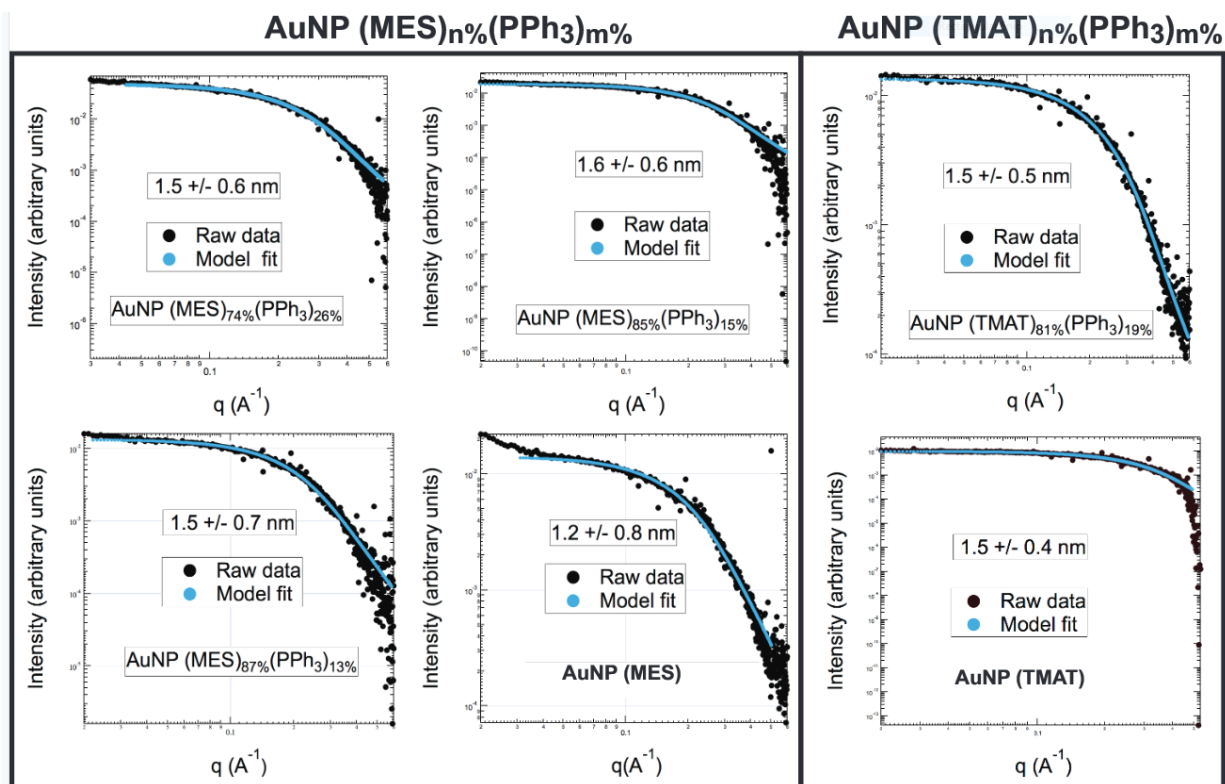Number of figures: 4

Number of tables: 3

AuNP (MES)$_{n\%}$(PPh$_3$)$_{m\%}$

AuNP (TMAT)$_{n\%}$(PPh$_3$)$_{m\%}$

Intensity (arbitrary units) — q (A^{-1})

1.5 +/- 0.6 nm
● Raw data
● Model fit
AuNP (MES)$_{74\%}$(PPh$_3$)$_{26\%}$

1.6 +/- 0.6 nm
● Raw data
● Model fit
AuNP (MES)$_{85\%}$(PPh$_3$)$_{15\%}$

1.5 +/- 0.5 nm
● Raw data
● Model fit
AuNP (TMAT)$_{81\%}$(PPh$_3$)$_{19\%}$

1.5 +/- 0.7 nm
● Raw data
● Model fit
AuNP (MES)$_{87\%}$(PPh$_3$)$_{13\%}$

1.2 +/- 0.8 nm
● Raw data
● Model fit
AuNP (MES)

1.5 +/- 0.4 nm
● Raw data
● Model fit
AuNP (TMAT)

Figure S1. SAXS patterns with model fit for 2-mercaptoethanesulfonate (MES)/ triphenylphosphine (PPh$_3$) and *N,N,N* –trimethylammoniumethanethiol (TMAT)/ PPh$_3$- protected AuNPs
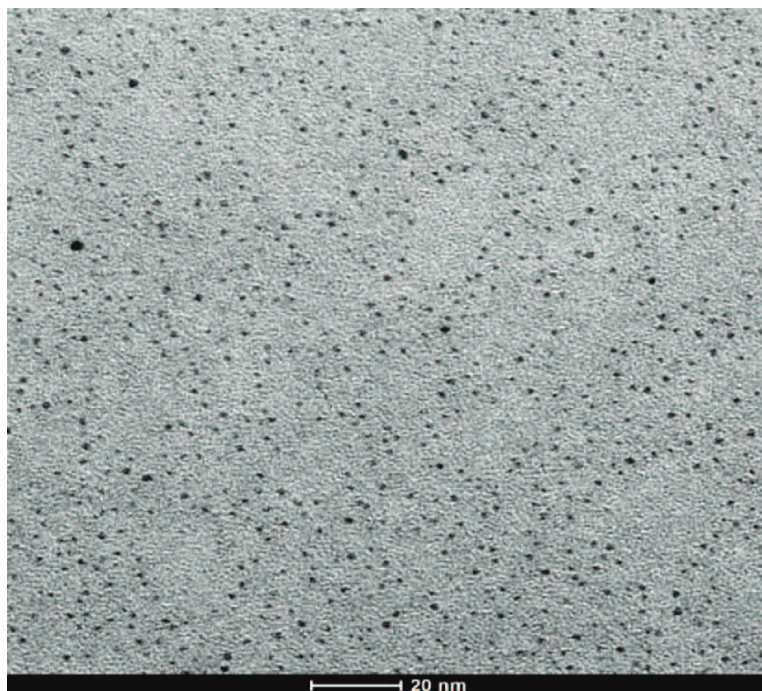
Figure S2. Representative TEM image of AuNP $(MES)_{74\%}(PPh_3)_{26\%}$. Average particles size 1.4 ± 0.4 nm (number of particles analyzed=975)
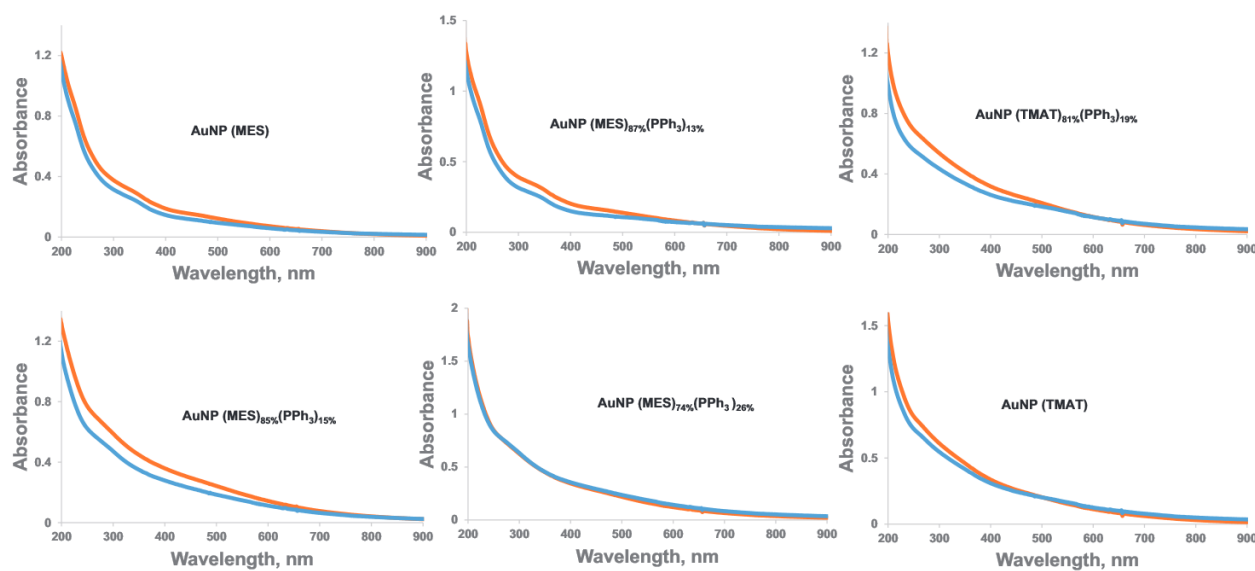

Figure S3. UV-vis spectra of MES, MES/TPP, TMAT and TMAT/TPP AuNPs in EM: starting solution (red) and after 5 days (blue). The concentration was 50 mg/L.
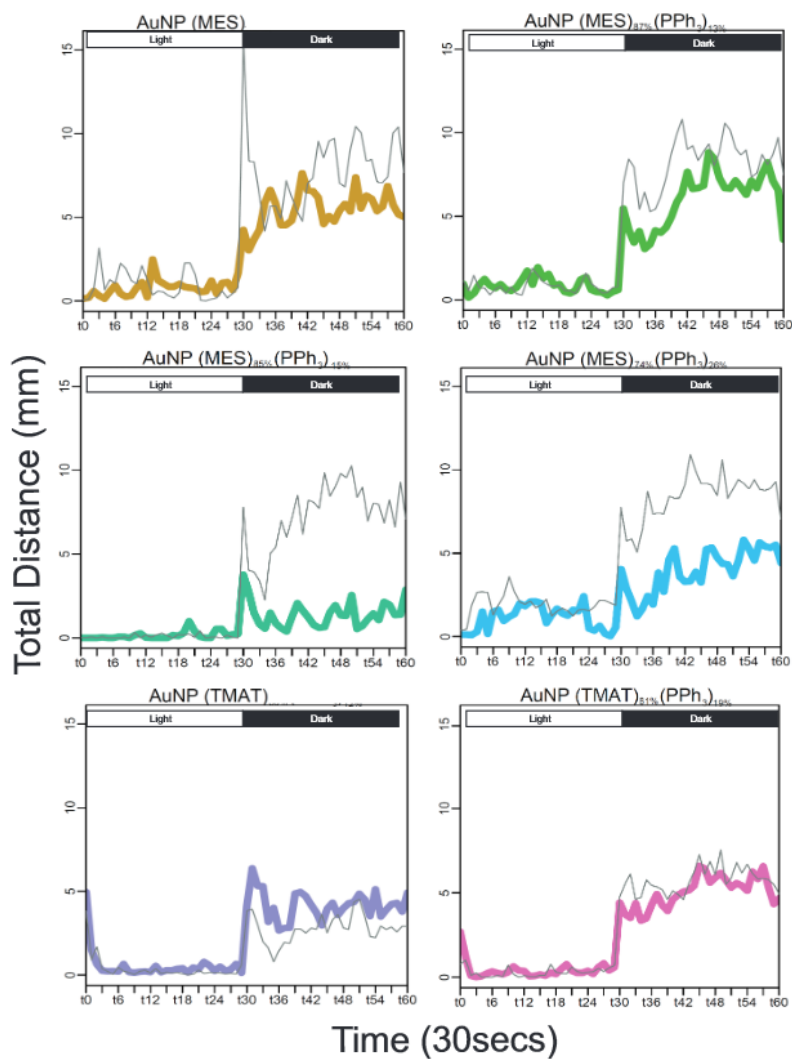
Figure S4. TPP content impacts larval photomotor response.

Embryos exposed to 10 µg/mL of varying AuNPs were evaluated for a predictable photomotor response following 180s in the light, and then the dark. Typical behavior is low movement in the light, and then a sharp increase in the dark that levels out. Each panel represents the response to a particular AuNP, and the respective control.

Table S1. Zeta potential measurements for AuNPs Day 0 (10 minutes after suspension made) and Day 5 (the time when the zebrafish experiment is completed). Measurements are represented as the mean of triplicate measurements with 10 scans ± the standard deviation.

Sample	0 day	5 day
AuNP (MES)	-18.62 ± 2.33	-22.56 ± 1.18
AuNP (MES)$_{87\%}$(PPh$_3$)$_{13\%}$	-16.24 ± 1.74	-20.94 ± 1.42
AuNP (MES)$_{85\%}$(PPh$_3$)$_{15\%}$	-18.62 ± 1.14	-20.58 ± 1.11
AuNP (MES)$_{74\%}$(PPh$_3$)$_{26\%}$	-16.08 ± 0.92	-21.44 ± 1.59
AuNP (TMAT)	9.87 ± 3.59	13.42 ± 0.50
AuNP (MES)$_{81\%}$(PPh$_3$)$_{19\%}$	10.83 ± 2.98	12.15 ± 1.85

Table S2. Atomic percentages and standard deviation for elements present in AuNPs determined by X-ray photoelectron spectroscopy (XPS).   nd = not detected.

% (SD)	Au4f	S2p (reduced)	S2p (oxidized)	P2p	C1s	N1s	F1s	O1s
Mica	nd	nd	nd	nd	1.7(0.2)	nd	nd	68.5(0.3)
1.5 nm AuNP (MES)$_{74\%}$(PPh$_3$)$_{26\%}$	14.6(0.8)	5.7(0.4)	7.6(0.4)	2.0(0.3)	44.4(1.0)	nd	nd	18.5(0.9)
1.6 nm AuNP (MES)$_{85\%}$(PPh$_3$)$_{15\%}$	10.7(0.8)	4.6(0.4)	6.0(0.4)	0.8(0.1)	44.1(2.8)	nd	nd	23.0(0.6)
1.5 nm AuNP (MES)$_{87\%}$(PPh$_3$)$_{13\%}$	5.7(0)	4.1(0.1)	4.9(0.1)	0.6(0.1)	49.2(0.5)	nd	nd	24.2(0.2)
1.2 nm AuNP (MES)	5.5(0)	3.9(0.3)	6.0(0.4)	nd	49.7(6.6)	nd	nd	29.0(5.5)
1.5 nm AuNP (TMAT)$_{81\%}$(PPh$_3$)$_{19\%}$	6.6(0.7)	2.6(0.2)	nd	0.6(0)	53.6(1.5)	2.3(0.4)	5.0(1.1)	19.6(0.3)
1.5 nm AuNP (TMAT)	5.2(1.1)	2.8(0.5)	nd	Traces (below detection limit)	49.1(3.5)	2.9(0.5)	4.0(0.9)	25.8(3.5)

Table S3. Primer Sequences

Gene	Forward Primer (5'- 3')	Reverse Primer (5'- 3')
gst p1	TTCAGTCCAACGCCATGC	ATGAGATCTGATCGCCAACC
gclc	CTATCTGGAGAACATGGAGG	CATTTTCCTCTGTTGACCGG
gclm	TGGCTTCGTCAGCACACTAAAGT	TCACGGGAACATTAAAACAGGC
gpx3	AAGAACGCATGTCCGCCTGTAG	ACCTGCAGAAACCCTGTGTTGAC
β-actin	AAGCAGGAGTACGATGAGTC	TGGAGTCCTCAGATGCATTG