Supporting Information

Peptide-mediated Synthesis of Gold Nanoparticles: Effects of Peptide Sequence and Nature of Binding on Physicochemical Properties

Yue Li,[1,#] Zhenghua Tang,[2,#] Paras N. Prasad,[3,4] Marc R. Knecht,[2,*] and Mark T. Swihart[1,*]

[1] *Department of Chemical and Biological Engineering, University at Buffalo (SUNY), Buffalo, NY 14260, Email: swihart@buffalo.edu*

[2] *Department of Chemistry, University of Miami. 1301 Memorial Drive, Coral Gables, Florida 33146, Email: knecht@miami.edu*

[3] *Department of Chemistry and Institute for Laser Photonics and Biophotonics, University at Buffalo (SUNY), Buffalo, NY 14260*

[4] *Department of Chemistry, Korea University, Seoul, Korea*

#: These authors contributed equally.

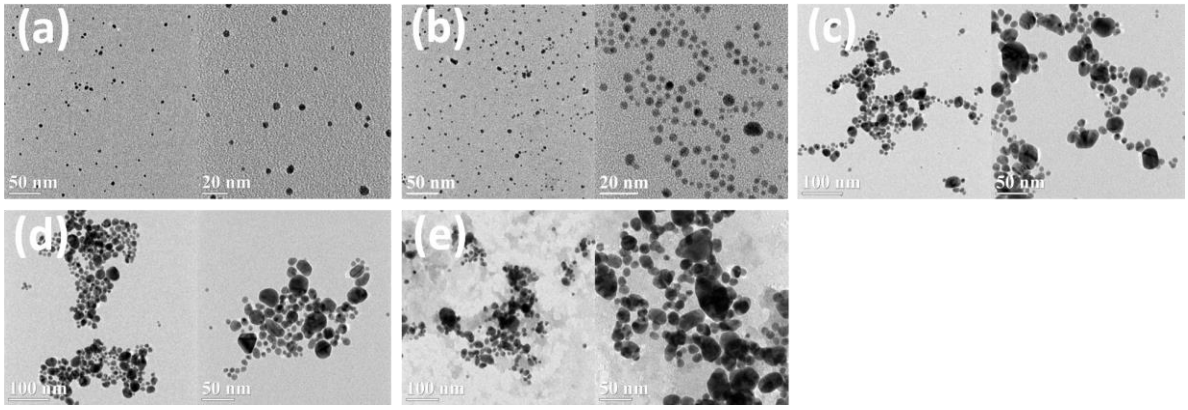

Fig. S1. TEM analysis of the gold nanoparticles prepared using AuBP1 at an Au/peptide ratio of (a) 2:1, (b) 4:1, (c) 10:1, (d) 20:1, (e) 40:1 with peptide concentration fixed at 0.1 mM.

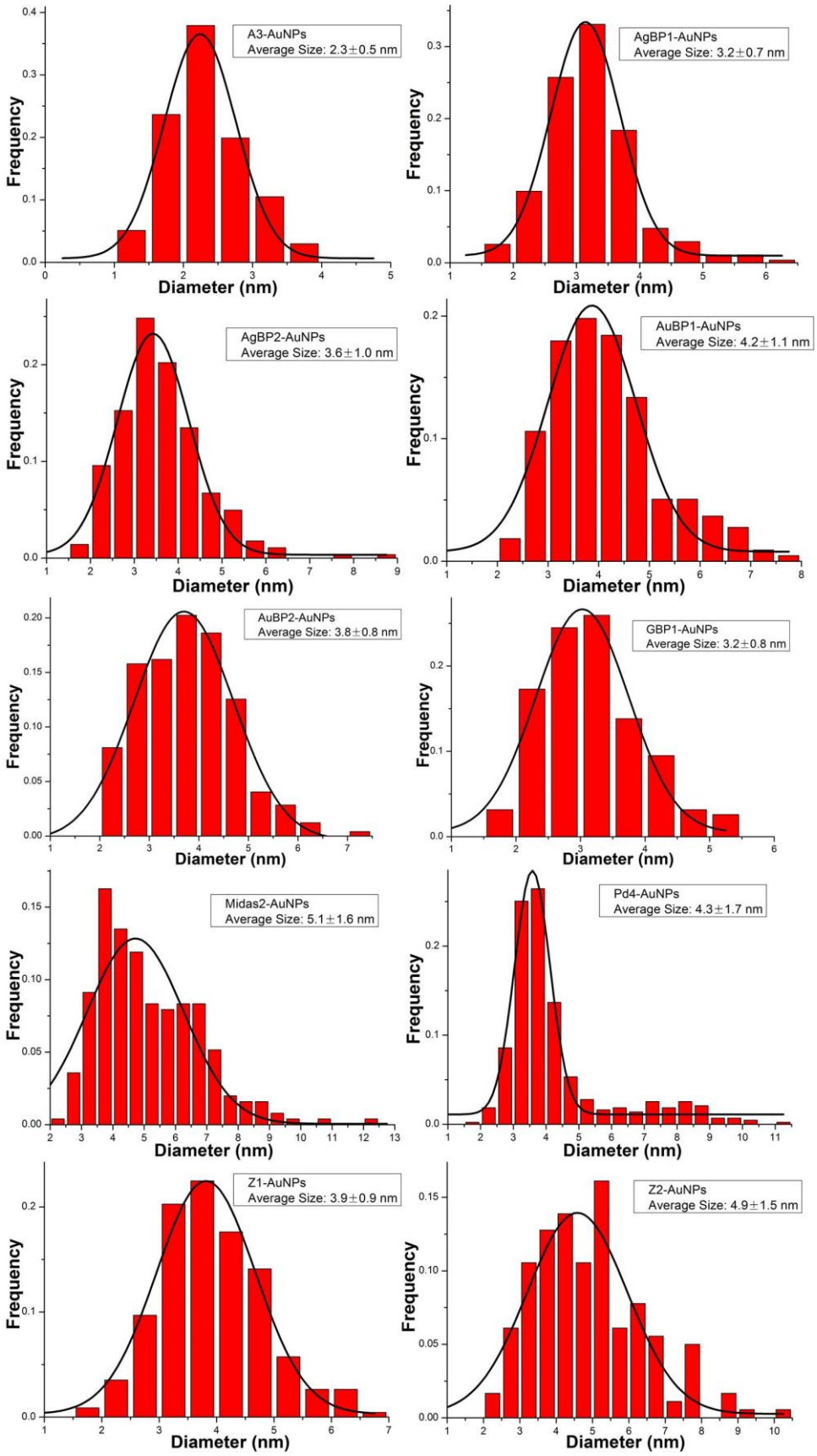

Fig. S2. Size distributions obtained from TEM analysis of the Au nanoparticles prepared using the indicated peptides.

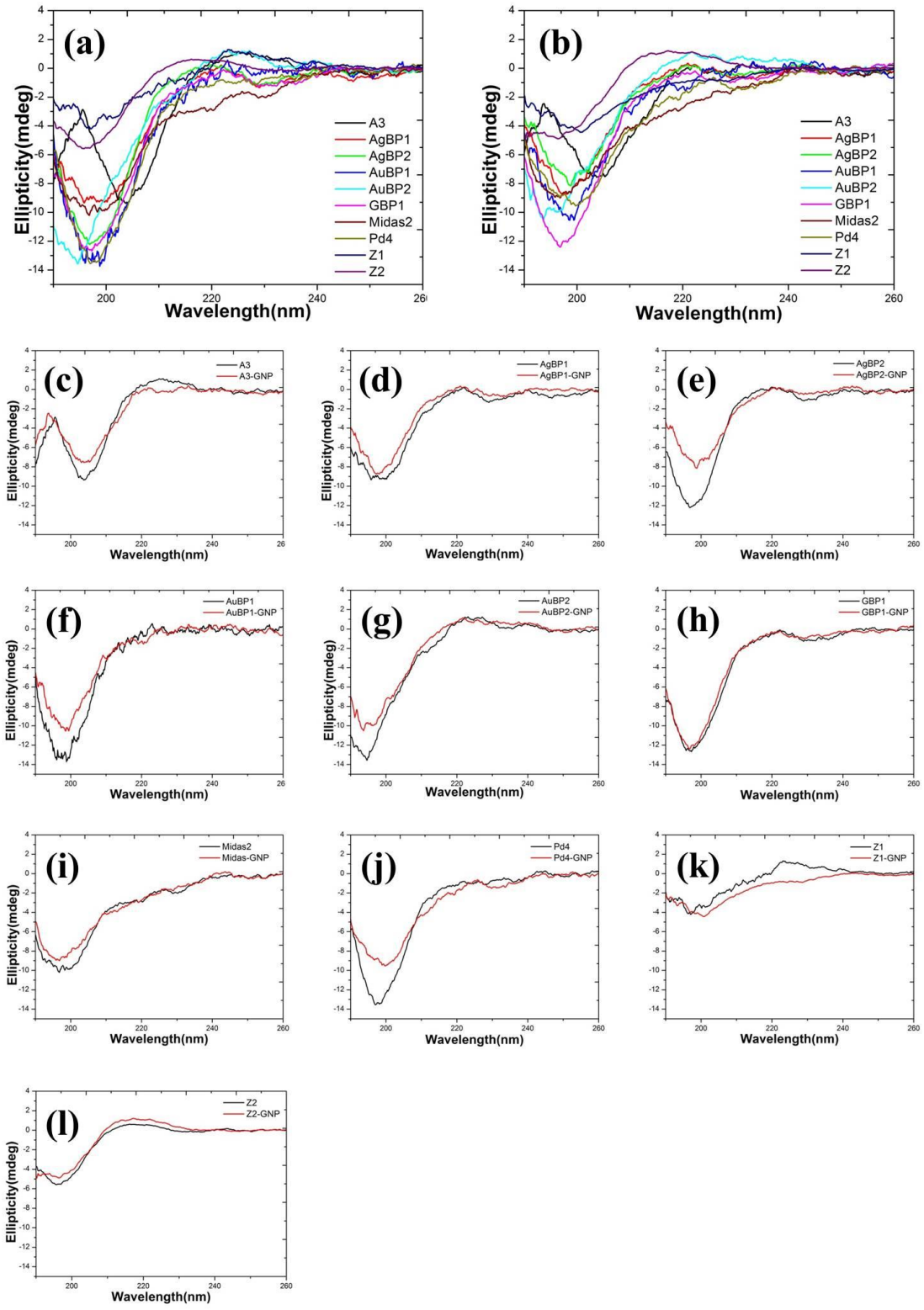

Fig. S3. CD analysis of (a) free peptides and (b) Au nanoparticle dispersions containing the same amount of peptide, part of which is bound on the nanoparticle surface. Parts (c-l) compare the CD spectra of free peptide and Au nanoparticle dispersion for each peptide separately.

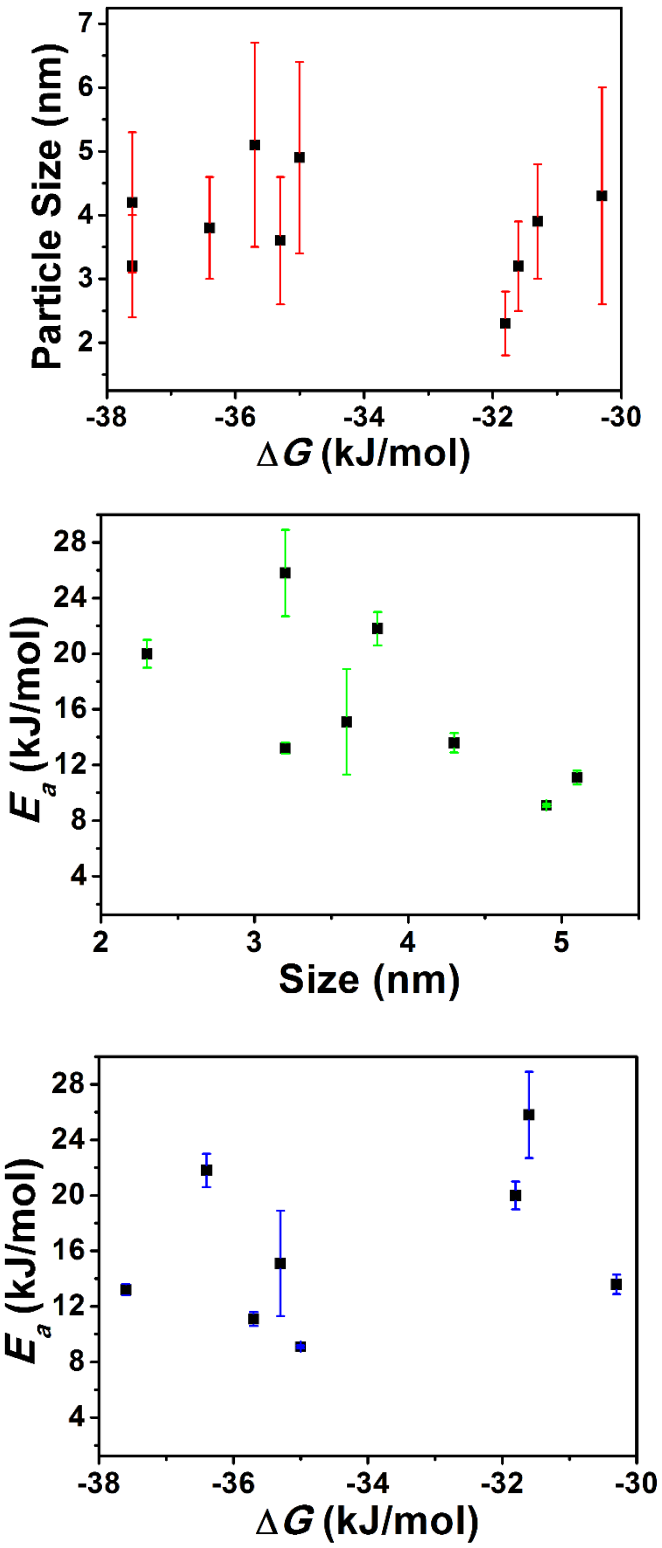

Fig. S4. Relationships between (top) nanoparticle size and peptide-Au binding free energy; (middle) nanoparticle size and the reaction activation energy, and (bottom) peptide-Au binding free energy and the reaction activation energy.

Table S1: Relationship of Anchor Assignment and Entropy Assignment (from Ref. 3) to Activation Energy for 4-Nitrophenol Reduction

Peptide	Sequence	Δ*G* (kJ/mol)	anchor assignment	entropy assignment	Activation Energy (kJ/mol)
Z2	RMRMKMK	-35.0 ± 0.6	Medium	Low	9.1 ± 0.1
Midas2	TGTSVLIATPYV	-35.7 ± 1.2	Weak	High	11.1 ± 0.5
GBP1	MHGKTQATSGTIQS	-37.6 ± 1.0	Medium	High	13.2 ± 0.4
Pd4	TSNAVHPTLRHL	-30.3 ± 0.2	Weak	High	13.6 ± 0.7
AgBP2	EQLGVRKELRGV	-35.3 ± 1.2	Medium	Medium	15.1 ± 3.8
A3	AYSSGAPPMPPF	-31.8 ± 0.3	Strong	High	20.0 ± 1.0
AuBP2	WALRRSIRRQSY	-36.4 ± 0.3	Strong	Medium	21.8 ± 1.2
AgBP1	TGIFKSARAMRN	-31.6 ± 0.2	Strong	High	25.8 ± 3.1