

Towards the Identification of the Gold Binding Region within Trypsin Stabilized Nanoclusters using Microwave Synthesis Routes

Mark H. Griep[†], Michael S. Sellers[†], Bijil Subhash[‡], Alexis M. Fakner[†], Abby L. West[†],
Nicholas M. Bedford^{‡*}

[†] Weapons and Materials Research Directorate, US Army Research Laboratory, Aberdeen
Proving Ground, MD 21005, USA

[‡]School of Chemical Engineering, University of New South Wales, Sydney, NSW 2052,
Australia

*Corresponding author: n.bedford@unsw.edu

Supporting Information Figures

Figure S1. Fluorescent emission of BSA, lysozyme etc PNC

Figure S2. CD of BSA, lysozyme, etc PNC

Figure S3. k^2 -space Au PNC data

Figure S4. EXAFS modelling fits

Figure S5. Atomic PDF at 30 Å

Figure S6. 4-NP reduction data for standard trypsin Au PNC

Table S1. Summary of synchrotron characterization results on Au PNCs.

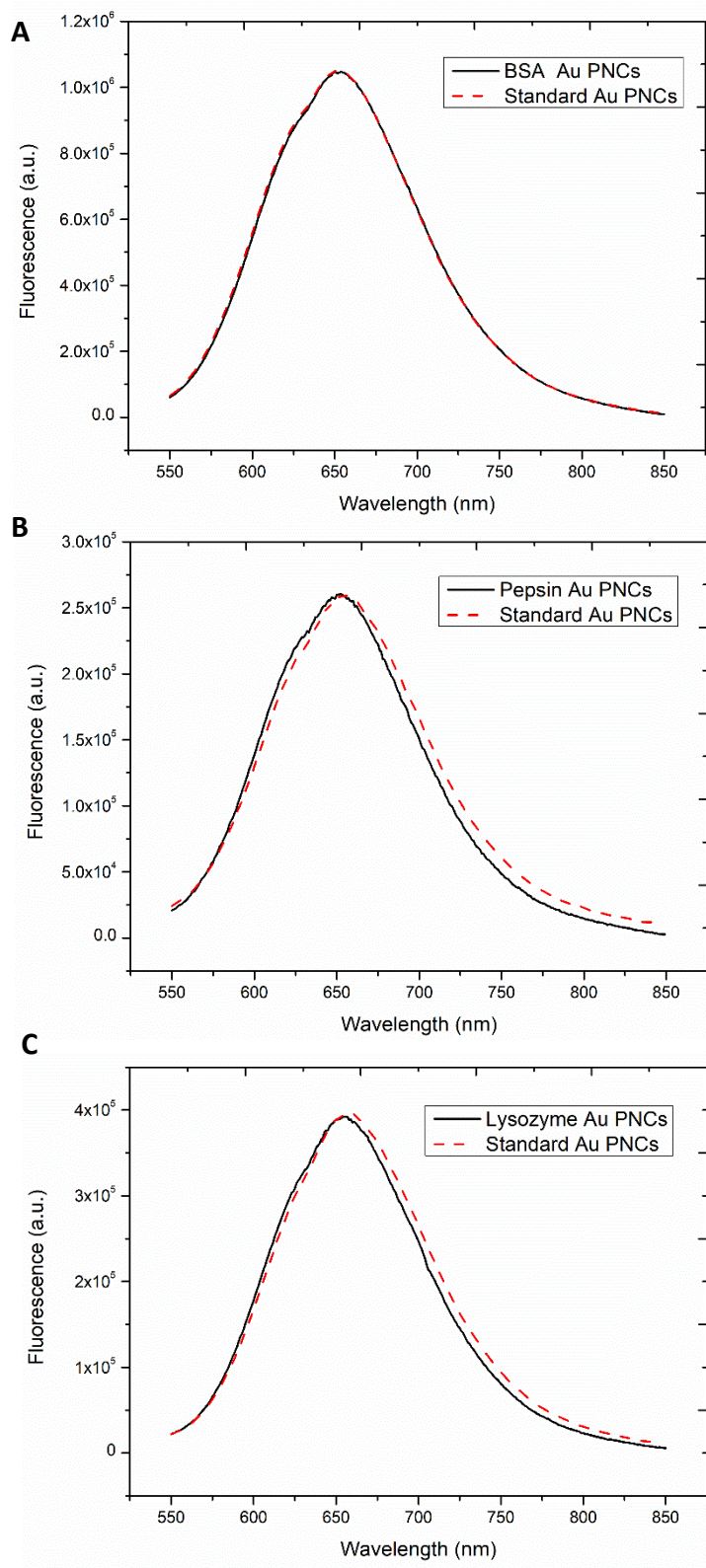


Figure S1. Fluorescence data for standard and microwave PNCs using A) BSA; B) Pepsin, and C) lysozyme as protein models.

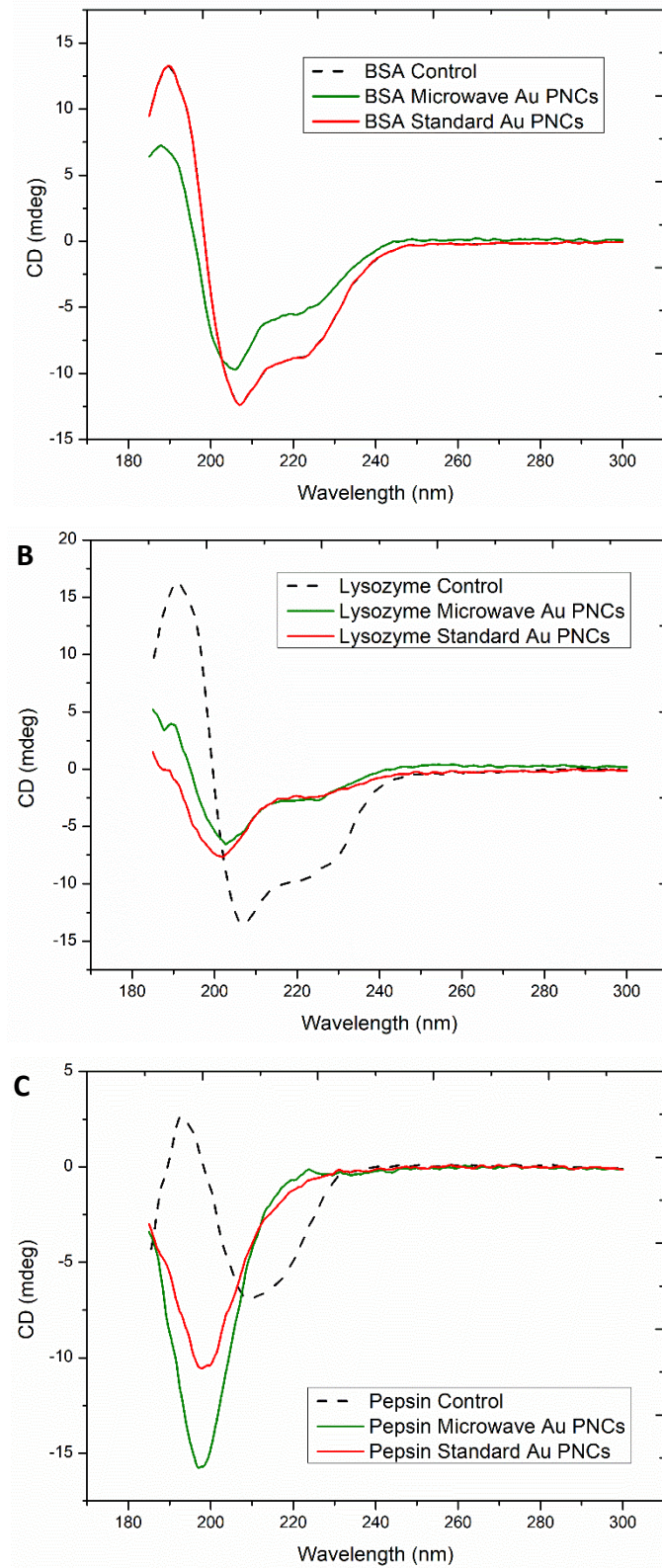


Figure S2. CD spectra for native proteins, standard and microwave PNCs using A) BSA; B) Pepsin, and C) lysozyme as protein models.

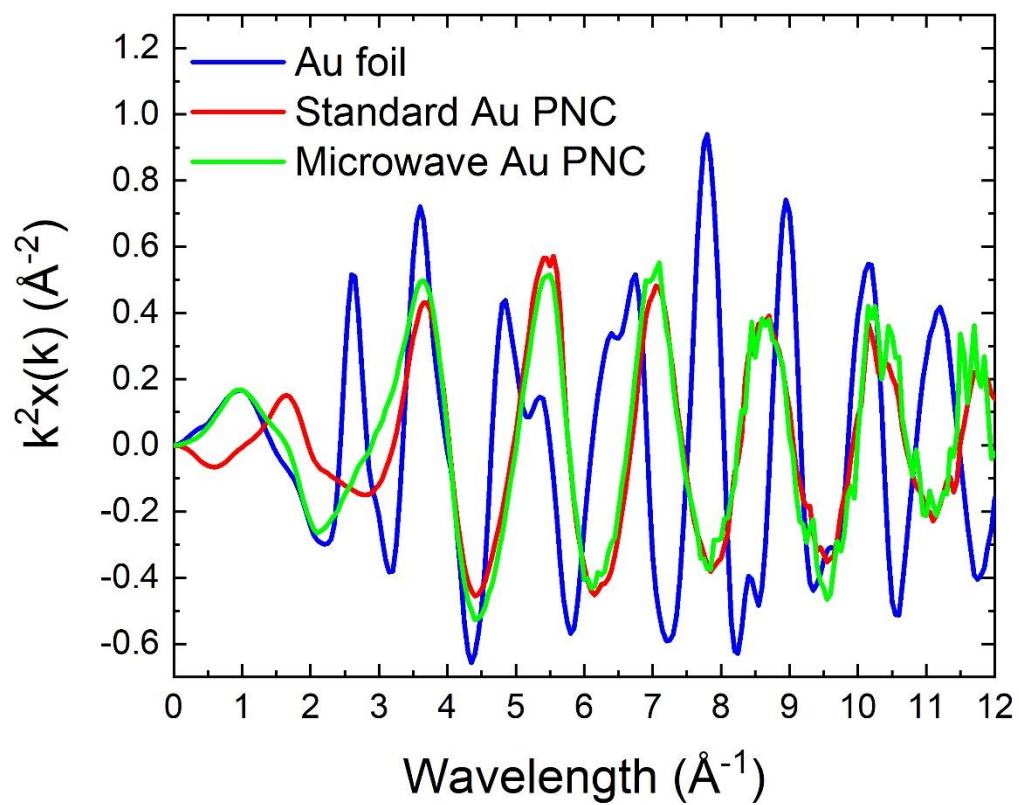


Figure S3. Au L₃-edge k^2 -space EXAFS for a reference Au foil (blue line), standard trypsin Au PNC (red line) and microwave trypsin Au PNC (green line)

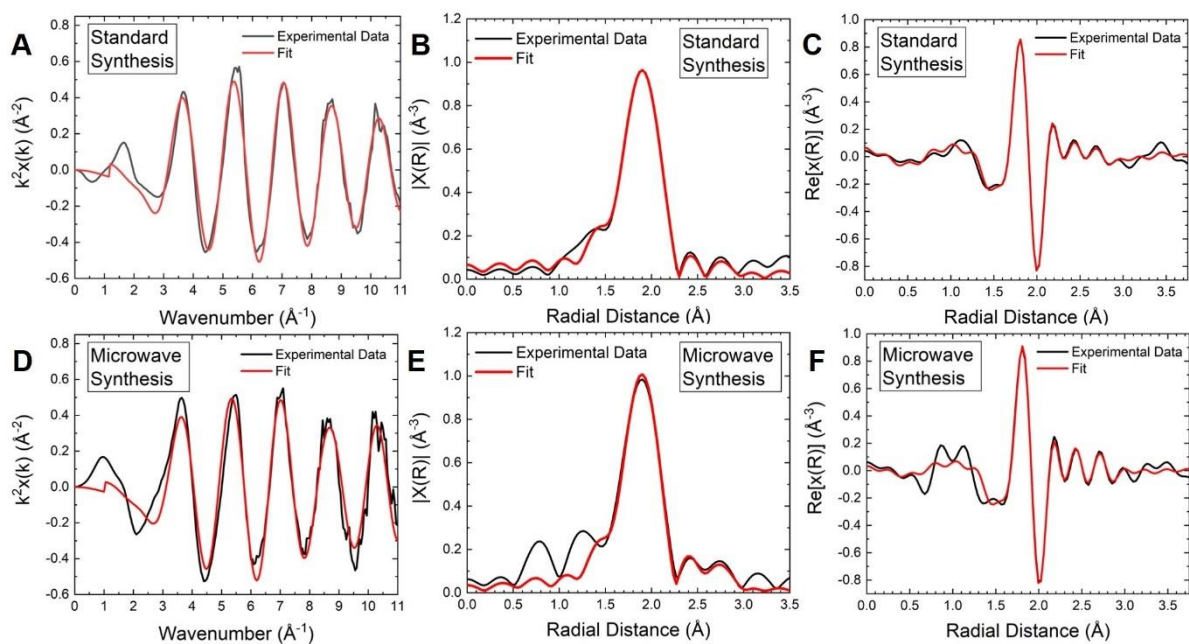


Figure S4. EXAFS fitting for standard trypsin Au PNCs in A) k^2 -space, B) r-space and C) the real component of r-space and fitting for microwave-assisted Au PNCs in D) k^2 -space, E) r-space and F) the real component of r-space.

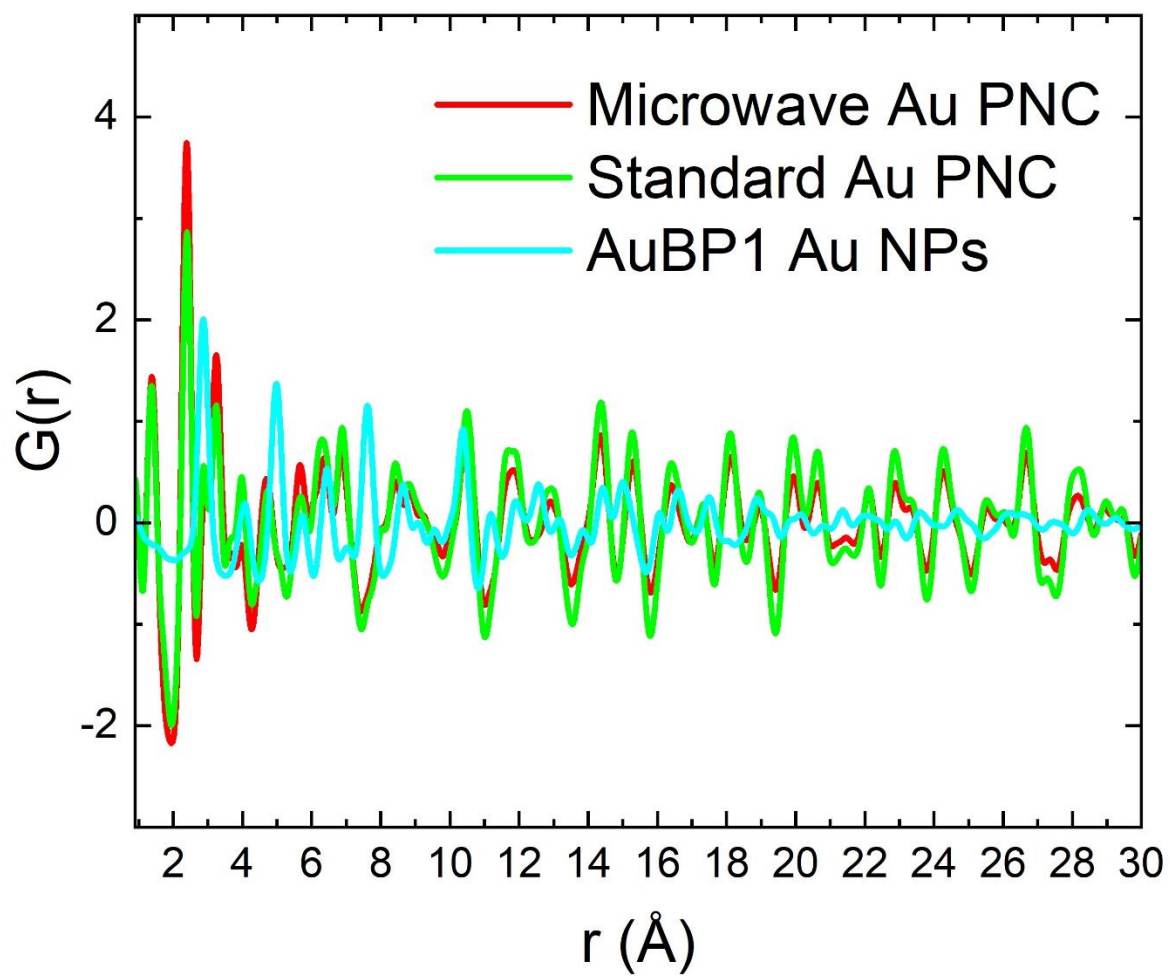


Figure S5. Atomic PDFs for Au PNCs and Au NP up to 30 \AA .

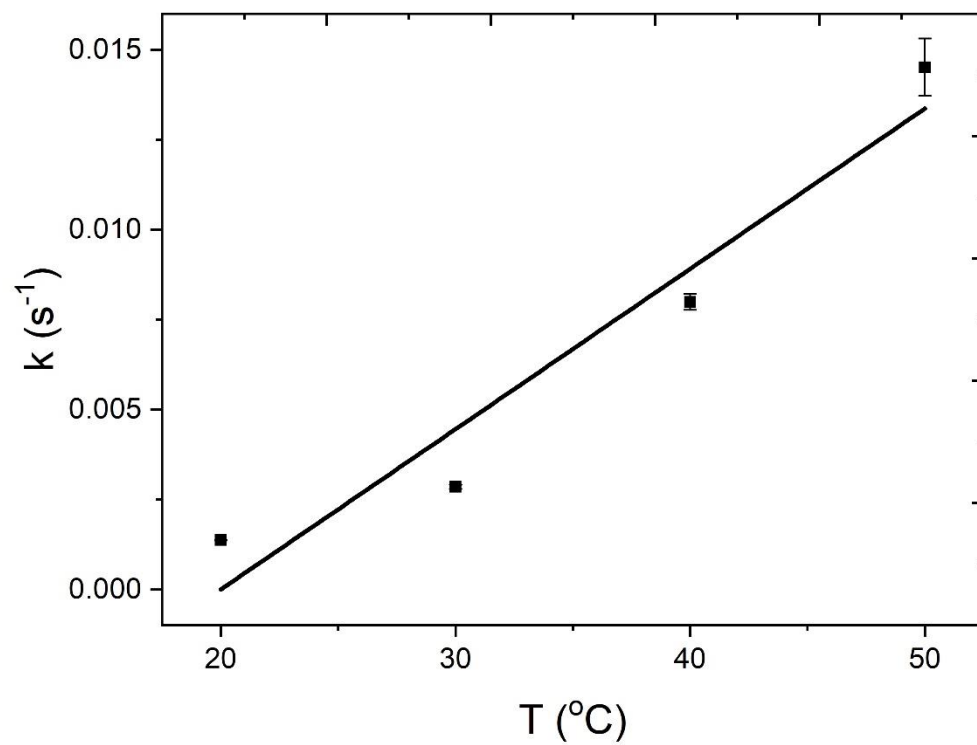


Figure S6. 4-NP reduction rate constant vs temperature for the standard trypsin Au PNCs.

Table S1. A summary of Au NC EXAFS data reported in the literature as compared to those reported in this work.

Cluster Size	Stabilizing Agent	Form	Temperature (K)	Au-ligand CN	Au-ligand NND (Å)	1 st Au-Au CN	1 st Au-Au NND (Å)	Reference
25 (est)	Trypsin (traditional synthesis)	Aqueous	RT	2.04 ± 0.28	2.317 ± 0.005	1.15 ± 0.42	2.79 ± 0.05	This work
25 (est)	Trypsin (microwave synthesis)	Aqueous	RT	1.92 ± 0.14	2.309 ± 0.005	1.46 ± 0.36	2.78 ± 0.03	This work
25	PhC ₂ H ₄ SH	Solid	RT	1.0	2.32	1.0	2.82	28
25	PhC ₂ H ₄ SH	Solid	10	1.0	2.32	1.0	2.80	28
25	PhC ₂ H ₄ SH	Toluene	RT	1.0	2.33	1.0	2.79	28
25	PhC ₂ H ₄ SH	ACN	RT	1.0	2.32	1.0	2.79	28
25	SC ₂ H ₄ Ph	Solid	8	1.6 (2)	2.319 (4)	1.5 (4)	2.700 (4)	34
38	SC ₂ H ₄ Ph	Solid	8	1.2 (2)	2.315 (4)	2.8 (4)	2.788 (1)	34
144	SC ₂ H ₄ Ph	Solid	8	0.9 (2)	2.326 (8)	1.2 (5)	2.733 (9)	34
25	SC ₈ H ₉	Solid (on Al ₂ O ₃)	RT	1.34 (0.1)	2.313 (5)	1.44	2.75 (2)	35
25 (est)	BSA	Solid	RT	1.2 (1)	2.30 (1)	3.0 (4)	2.81 (1)	29
144	SC ₂ H ₄ Ph	Solid	RT	2.340 (3)	0.83 (6)	2.831 (2)	7.0 (4)	27
30	SC ₂ H ₄ Ph	Solid	90	1.2	2.32 (1)	2.07	2.77 (3)	36
30	SC ₂ H ₄ Ph	Solid	RT	1.2	2.311 (4)	2.07	2.69 (2)	36
30	SC ₂ H ₄ Ph	Aqueous	RT	1.2	2.297 (7)	2.07	2.69 (2)	36