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

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Supporting Information Figures

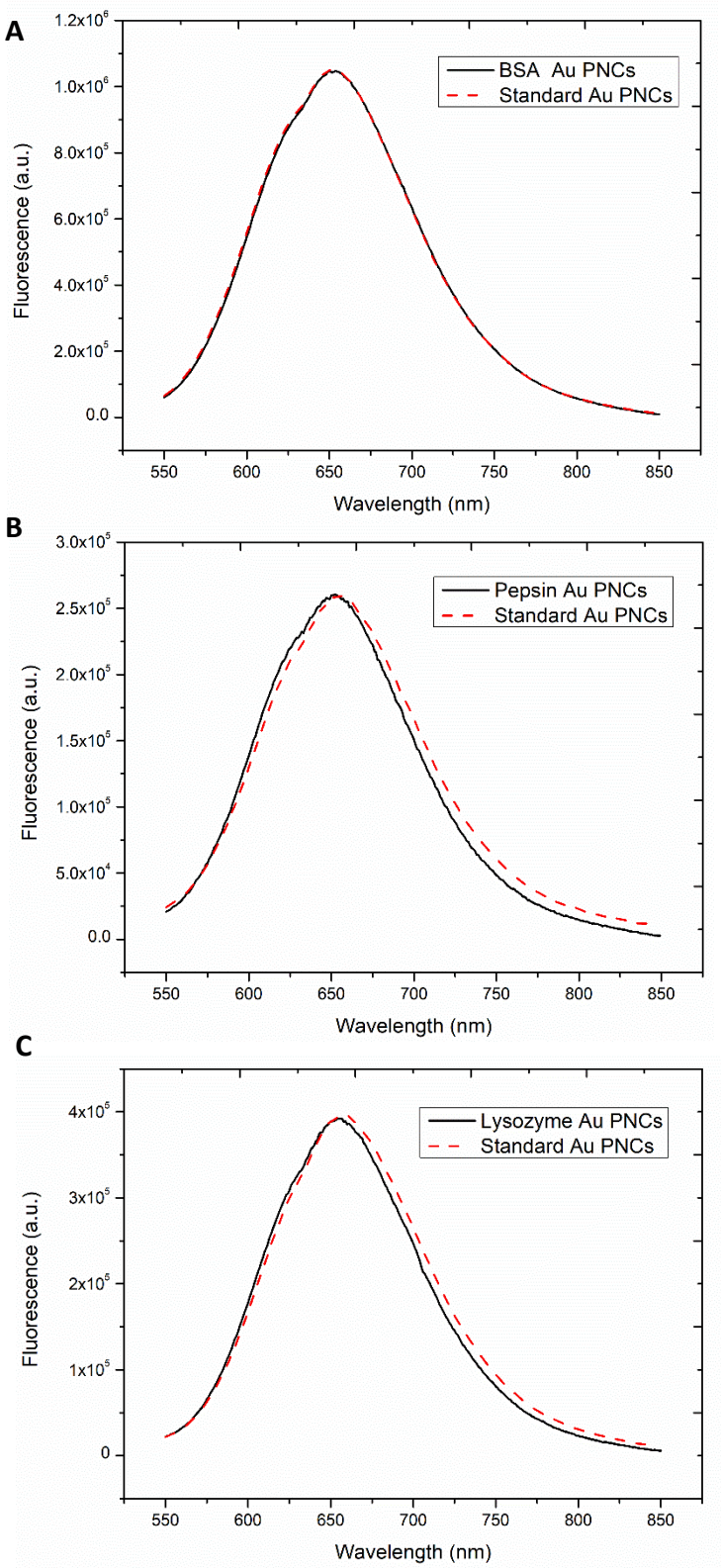

Figure S1. Fluorescence data for standard and microwave PNCs using A) BSA; B) Pepsin, and C) lysozyme as protein models.

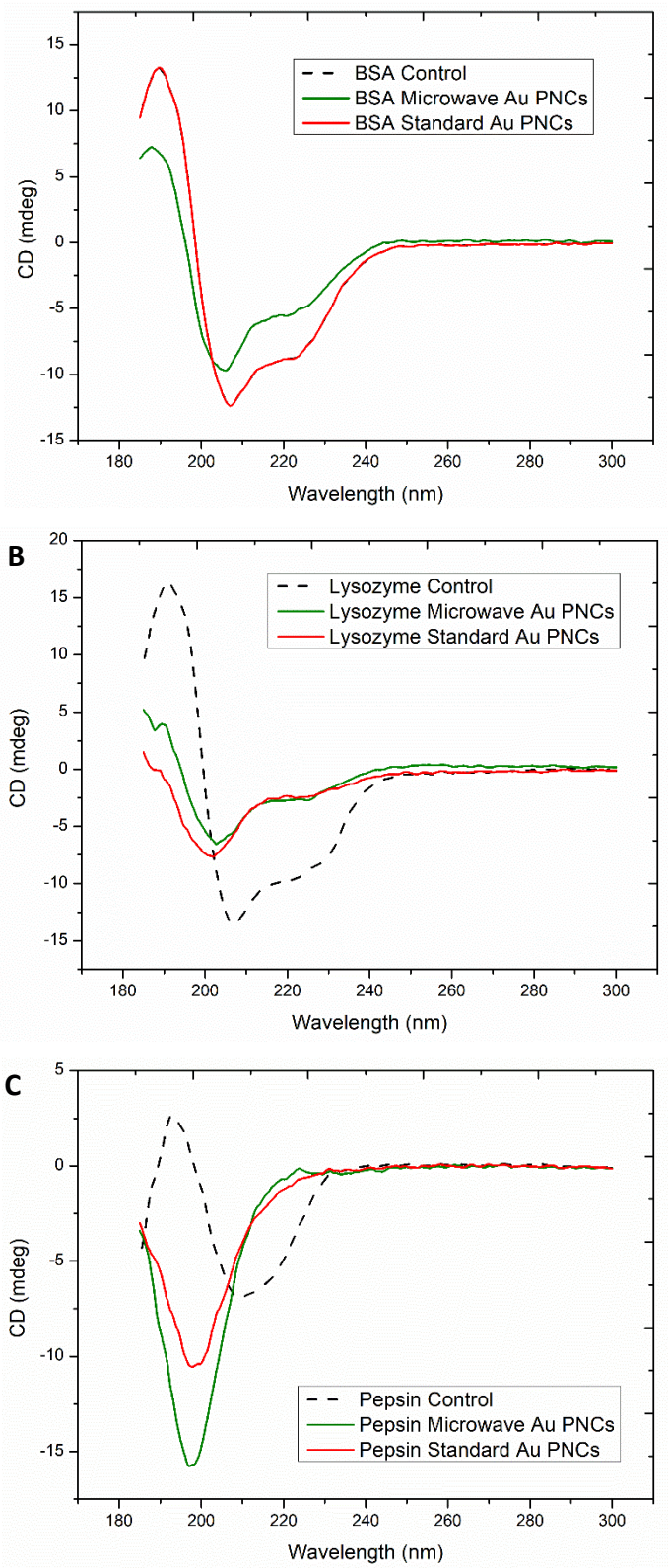

Figure S2. CD spectra for native proteins, standard and microwave PNCs using A) BSA; B) Pepsin, and C) lysozyme as protein models.

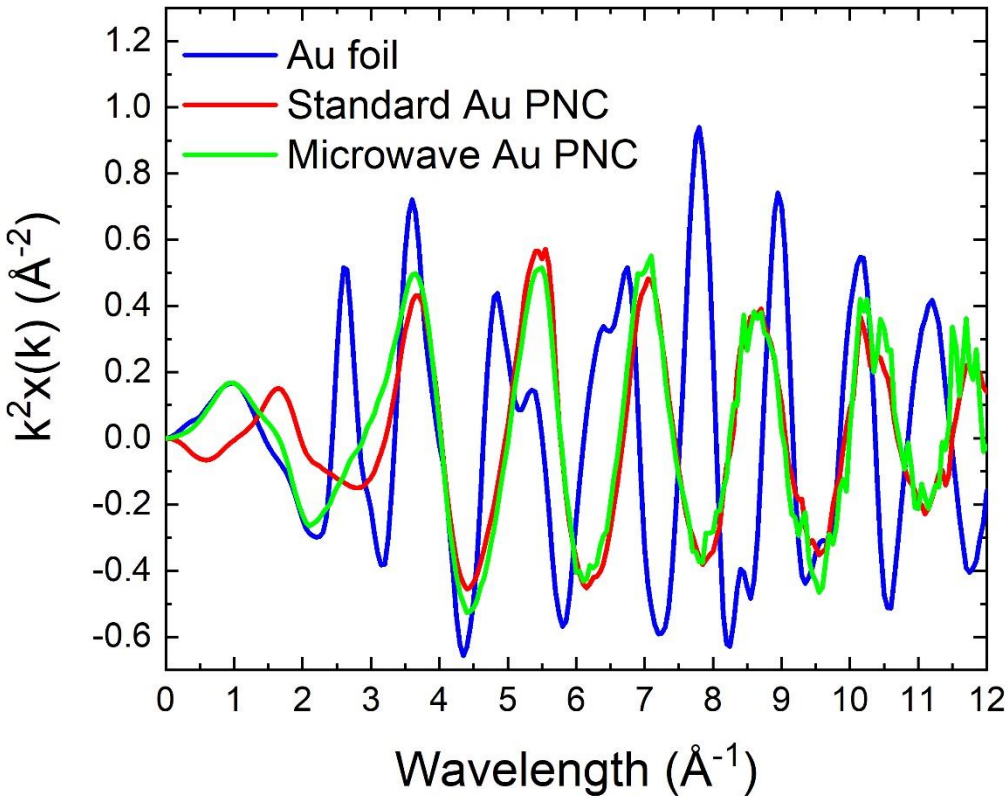

Figure S3. Au L_3-edge k^2-space EXAFS for a reference Au foil (blue line), standard trypsin Au PNC (red line) and microwave trypsin Au PNC

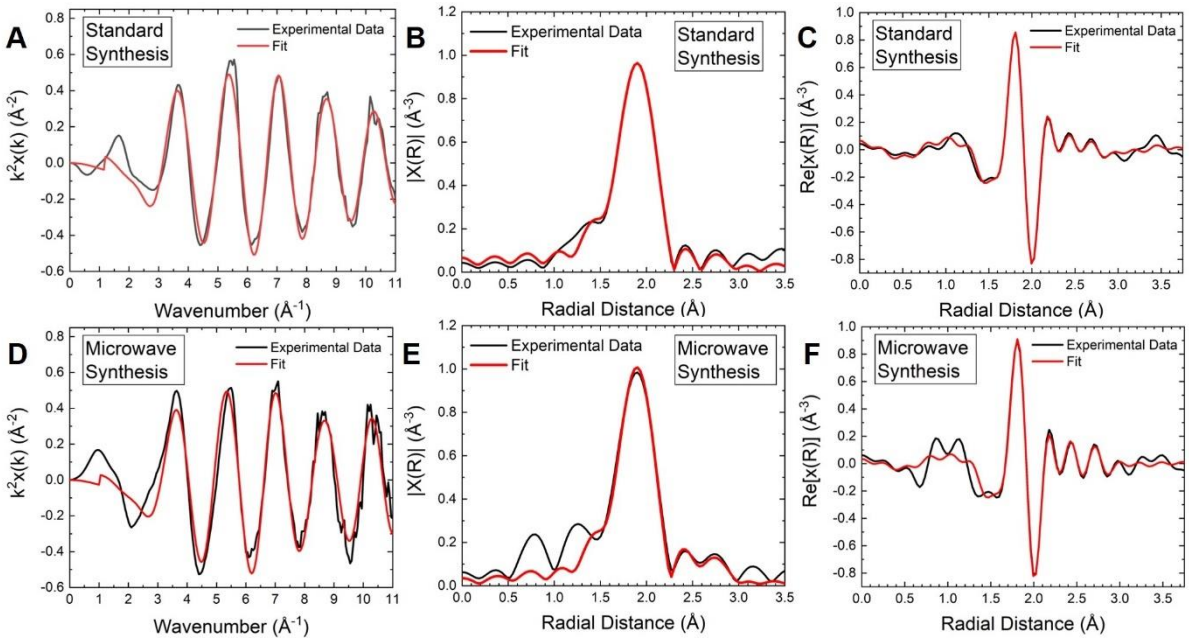

Figure S4. EXAFS fitting for standard trypsin Au PNCs in A) k^2-space, B) r-space and C) the real component of r-space and fitting for microwave-assisted Au PNCs in D) k^2-space, E) r-space and F) the real component of r-space.

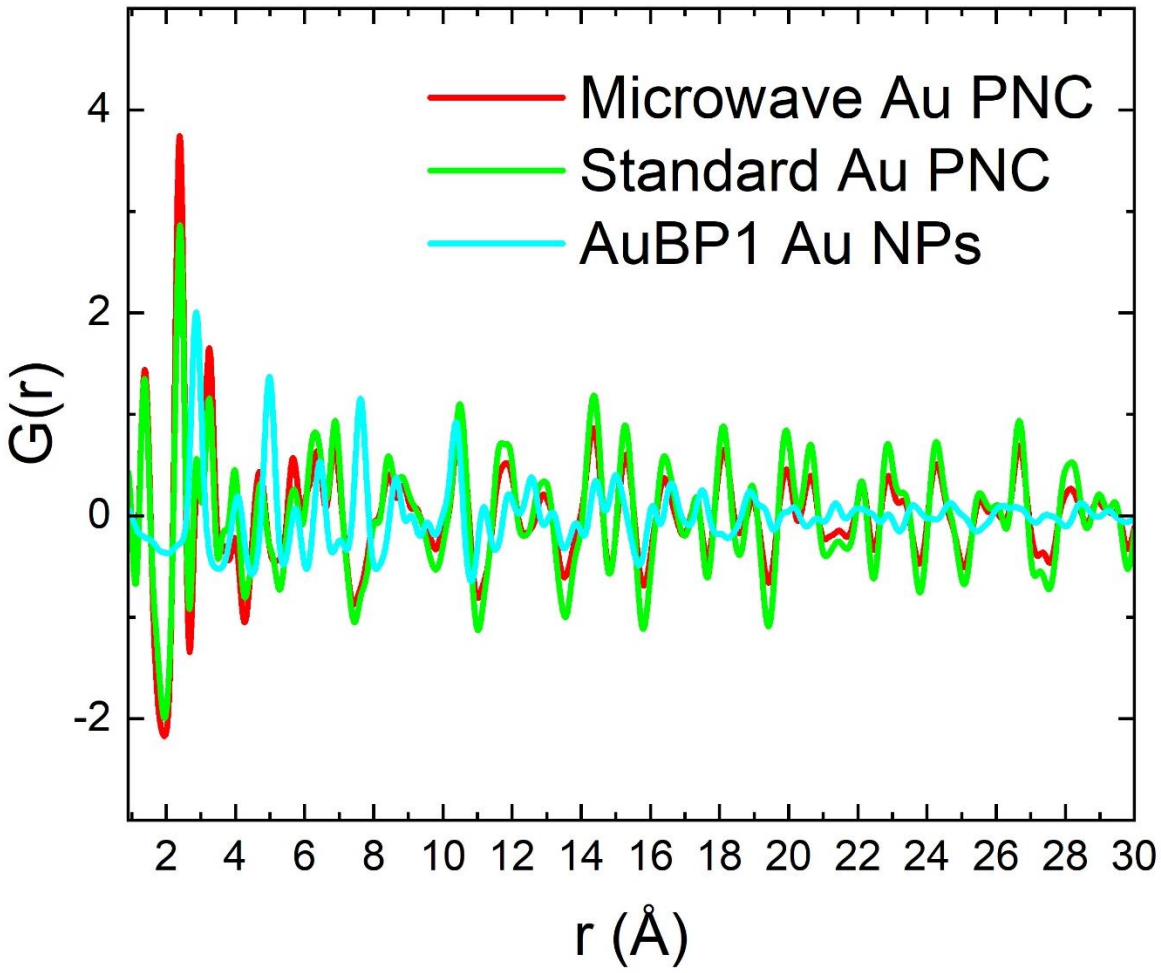

Figure S5. Atomic PDFs for Au PNCs and Au NP up to 30 Å.

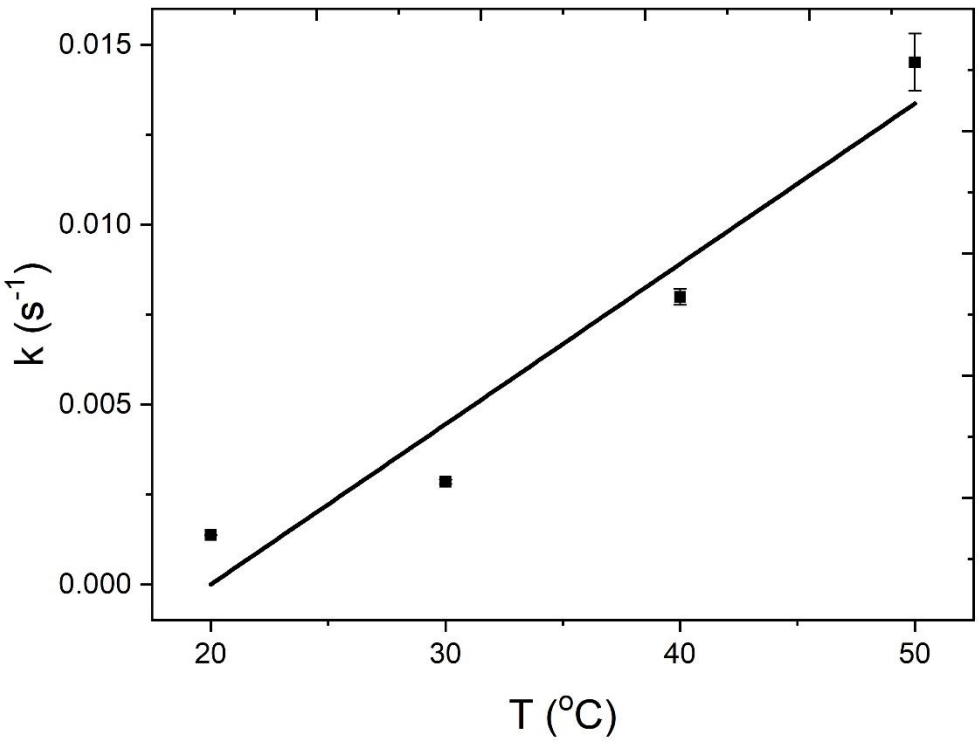

Figure S6. 4-NP reduction rate constant vs temperature for the standard trypsin Au PNCs.

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

Cluster Size	**Stabilizing Agent**	**Form**	**Temperature (K)**	**Au-ligand CN**	**Au-ligand NND (Å)**	**1st Au-Au CN**	**1st 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_2H_4SH	Solid	RT	1.0	2.32	1.0	2.82	28
25	PhC_2H_4SH	Solid	10	1.0	2.32	1.0	2.80	28
25	PhC_2H_4SH	Toluene	RT	1.0	2.33	1.0	2.79	28
25	PhC_2H_4SH	ACN	RT	1.0	2.32	1.0	2.79	28
25	SC_2H_4Ph	Solid	8	1.6 (2)	2.319 (4)	1.5 (4)	2.700 (4)	34
38	SC_2H_4Ph	Solid	8	1.2 (2)	2.315 (4)	2.8 (4)	2.788 (1)	34
144	SC_2H_4Ph	Solid	8	0.9 (2)	2.326 (8)	1.2 (5)	2.733 (9)	34
25	SC_8H_9	Solid (on Al_2O_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_2H_4Ph	Solid	RT	2.340 (3)	0.83 (6)	2.831 (2)	7.0 (4)	27
30	SC_2H_4Ph	Solid	90	1.2	2.32 (1)	2.07	2.77 (3)	36
30	SC_2H_4Ph	Solid	RT	1.2	2.311 (4)	2.07	2.69 (2)	36
30	SC_2H_4Ph	Aqueous	RT	1.2	2.297 (7)	2.07	2.69 (2)	36