Supporting Information for:

Improved Methods for Evaluating the Environmental Impact of Nanoparticle Synthesis

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Data table for metric analysis of Brust method. Synthesis of $Au_{286}(C_{12}H_{25}S)_{95}$. This is a Brust-type prep with additional experimental details reported by Murray.[1] This prep uses all the same amounts of reactants as the original Brust experiment but with a two-fold higher molar ratio of dodecanethiol to $HAuCl_4$ to achieve the desired size.

Brust-type Prep of Polydisperse Sample

Item	Reported Amount in Literature	Moles	Mass (grams)	Metric Value
Reagents				
Hydrogen tetrachloroaurate ($HAuCl_4$)	30 mL, 30 mmol/L	0.0009	0.306	
Tetraoctylammonium bromide (TOAB)	80 mL, 50 mmol/L	0.0040	2.187	
Dodecanethiol ($C_{12}H_{25}SH$)	170 mg in Brust paper. Thiol/$HAuCl_4$ = 2 molar ratio in Murray paper.	0.0018	0.364	
Sodium Borohydride ($NaBH_4$)	25 mL, .4 mol/L	0.0100	0.378	
Solvents/Work-up				
Toluene	90 mL	0.8450	77.858	
Ethanol	800 mL	13.7000	631.159	
Metrics (weighted average size 2.1 nm, $Au_{286}(C_{12}H_{25}S)_{95}$, full histogram)				
Yield	0.214 g	2.8218E-06	.214 g, 90%	
AE (%)				65.15
PMI				3328
ME (%)				1.94E-05
Metrics (weighted average size 2.1 nm, $Au_{286}(C_{12}H_{25}S)_{95}$, large window)				
Yield	0.214 g	2.7463E-06	.208 g, 87%	
AE (%)				65.15
PMI				3420
ME (%)				1.89E-05
Metrics (weighted average size 2.0 nm, $Au_{247}(C_{12}H_{25}S)_{86}$, medium window)				
Yield	0.214 g	2.3497E-06	.156 g, 65%	
AE (%)				65.47
PMI				4569
ME (%)				1.61E-05

Metrics (weighted average size 1.6 nm, $Au_{127}(C_{12}H_{25}S)_{56}$, small window)

Yield	0.214 g	1.2227E-06 .044 g, 17%	
AE (%)			66.43
PMI			16095
ME (%)			8.40E-06

Full Window	
E-factor	14
E-factor (solvent)	3327
RME (%)	32
ME (%)	1.69E-02
PMI	15
Big Window (1 – 4 nm)	
E-factor	15
E-factor (solvent)	3419
RME (%)	31
ME (%)	1.64E-02
PMI	16
Medium Window (1 – 3 nm)	
E-factor	20
E-factor (solvent)	4568
RME (%)	23
ME (%)	1.41E-02
PMI	21
Small Window (1 – 2 nm)	
E-factor	72
E-factor (solvent)	16094
RME (%)	7
ME (%)	7.32E-03
PMI	73

Data table for metric analysis of Jin method. Synthesis of $Au_{144}(PhC_2H_4S)_{60}$: This is a prep by Jin of monodisperse nanoparticles with Au144. It is assumed that the recovery of particles from the work-up was 50% to give a total of 25% yield.

Preparation of $Au_{144}(PhC_2H_4S)_{60}$

Item	Reported Amount in Literature	Moles	Mass (grams)	Metric Value
Reagents				
Hydrogen tetrachloroaurate ($HAuCl_4$)	.45 mmol, .1773 grams	0.0005	0.153	
Tetraoctylammonium bromide (TOAB)	.52 mmol, .284 grams	0.0005	0.284	
2-phenylethanethiol (C_8H_9SH)	.186 mL + .65 mL per 20 mg crude AUNP's	0.0152	2.105	
Sodium Borohydride ($NaBH_4$)	4.5 mmol, .171 grams	0.0045	0.170	
Solvents/Work-up				
Toluene	10 mL + 1 mL per 20 mg crude AUNP's	0.1207	11.118	
Methanol	20 mL per 20 mg crude AUNP's	1.407	45.080	
Metrics				
Yield	25%	7.8E-07	0.029	
AE (%)				63.96
PMI				2061
ME (%)				5.00E-05

E-factor	94
E-factor (solvent)	2060
RME (%)	1
ME (%)	3.77E-03
PMI	95

Data table for metric analysis of Murray method. Synthesis of $AuCl(PPh_3)_3$: Does not include amount of ethanol and methanol (these are not given in the literature).

Preparation of $Au_{75}(C_6H_{13}S)_{40}$

Item	Reported Amount in Literature	Moles	Mass (grams)	Metric Value
Reagents				
Sodium tetrachloroaurate ($NaAuCl_4$)	1 mmol	0.0095	3.437	
Triphenylphosphine (PPh_3)	1 mmol	0.0095	2.492	
BF_3 - Ether	100 mL	0.8103	115.006	
Sodium Borohydride ($NaBH_4$)	20 grams	0.5287	20.001	
Hexanethiol	6 µL	0.0026	0.307	
Solvents/Work-up				
2, 2' - thiodiethanol	3 mmol	0.0284	3.470	
1, 2 - dimethoxyethane	100 mL	0.9621	86.704	
Benzene	150 mL	1.6899	131.998	
Dichloromethane	5.5 mL	5.1500	437.390	
Metrics				
Yield	70% (ligand exchange), 55% purity	1.1935E-05	0.232	
AE (%)				61.08
PMI (solvent)				3448
ME (%, solvent)				1.30E-04

E-factor	607
E-factor (solvent)	3447
RME (%)	4
ME (%)	8.77E-04
PMI	608

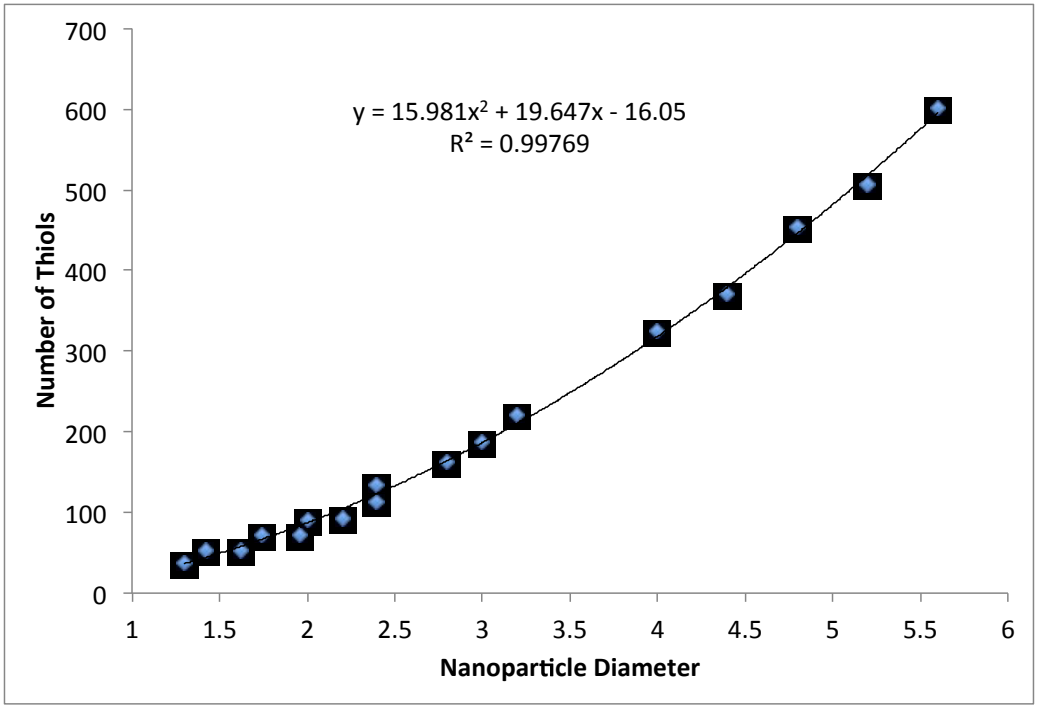
To calculate the molecular weight for a given gold nanoparticle, first the number of gold atoms (N_{Au}) was estimated using the method of Liu,[1] with the equation:

$$N_{Au} = (\pi/6) * (\sigma D^3/M) \qquad \text{(Eq. S1)}$$

where σ is the density for gold with fcc cystal packing (19.3 g/cm^3), M is the atomic weight of gold (197 g/mol) and D is the nanoparticle core diameter.

Thermogravimetric analysis data on different size nanoparticles, originally reported by Murray,[2] were used to determine the number of alkanethiols present on a each size nanoparticle. A plot of the number of thiols per particle determined by TGA versus the nanoparticle diameter was fit to a second order polynomial (Figure S1) resulting in an equation that was used to estimate the number of thiols (N_s) for other size nanoparticles:

$$N_s = 15.981D^2 + 19.647D - 16.05 \qquad \text{(Eq. S2)}$$



Finally the molecular weight of the nanoparticle was calculated using:

$$MW_{NP} = (N_{Au} * 197) + (N_s * MW_T) \qquad \text{(Eq. S3)}$$

where MW_T is the molecular weight of the thiol used in that preparation.

1) Michael J. Hostetler, J. E. W., Chuan-Jian Zhong, Jay E. Harris, Richard W. Vachet, Michael R. Clark, J. David Londono, Stephen J. Green, Jennifer J. Stokes, George D. Wignall, Gary L. Glish, Marc D. Porter, Neal D. Evans, and Royce W. Murray *Langmuir* **1997**, *14*, 17-30.

2) Liu, X. O.; Atwater, M.; Wang, J. H.; Huo, Q. Extinction Coefficient of Gold Nanoparticles with Different Sizes and Different Capping Ligands *Colloid Surface B* **2007**, *58*, 3-7.