

Supporting Information:
Thiolate ligands for synthesis of water-soluble gold clusters.
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Transmission electron micrographs and particle size analysis for clusters reported in **Table 1** are presented. The particle size distribution depends on both the ligand and the amount of NaBH₄ used. The size distributions presented here therefore underrepresent the size ranges that may be achieved.

Particle sizes were determined with a MATLAB algorithm devised for the purpose. The algorithm begins with a particle picker such as “boxer¹,” placing all particle images in boxes of uniform size. For each of the MPCs we selected on the order of 100 particles by choosing an area on a TEM micrograph and picking all the particles in that area. The algorithm centers each particle in its box by calculating the center of mass with a low signal filter. Centered particles were rotated 20 times (18° steps) to generate a rotational average, for the purpose of smoothing both the noise and the particle border. Rotational averages were fitted by trapezoidal templates to generate an envelope. The envelope and the original particle images were then multiplied pixel by pixel. The resulting images were thresholded, giving bitwise representations (each pixel was either 1 or 0). Similarities between the original and thresholded images were satisfactory at all scales (see **figure 1**). The total area of each particle was calculated as the sum of all the pixel values and the diameter was calculated assuming a round particle.

In addition to a trapezoidal template, we also tried a Gaussian template. The Gaussian envelope tended to increase the size of small particles and to decrease the size of larger particles. The problem was that the particle images were saturated in the neighborhood of the cluster core and so fit a trapezoid better than a Gaussian. The algorithm is apparently robust and general and is completely automated once particles are boxed, the entire process taking not longer than 10 minutes. The algorithm is available upon request.

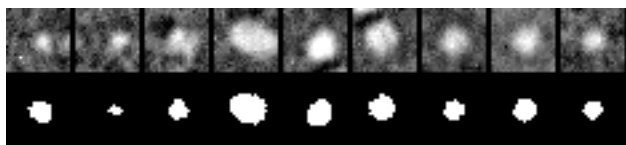
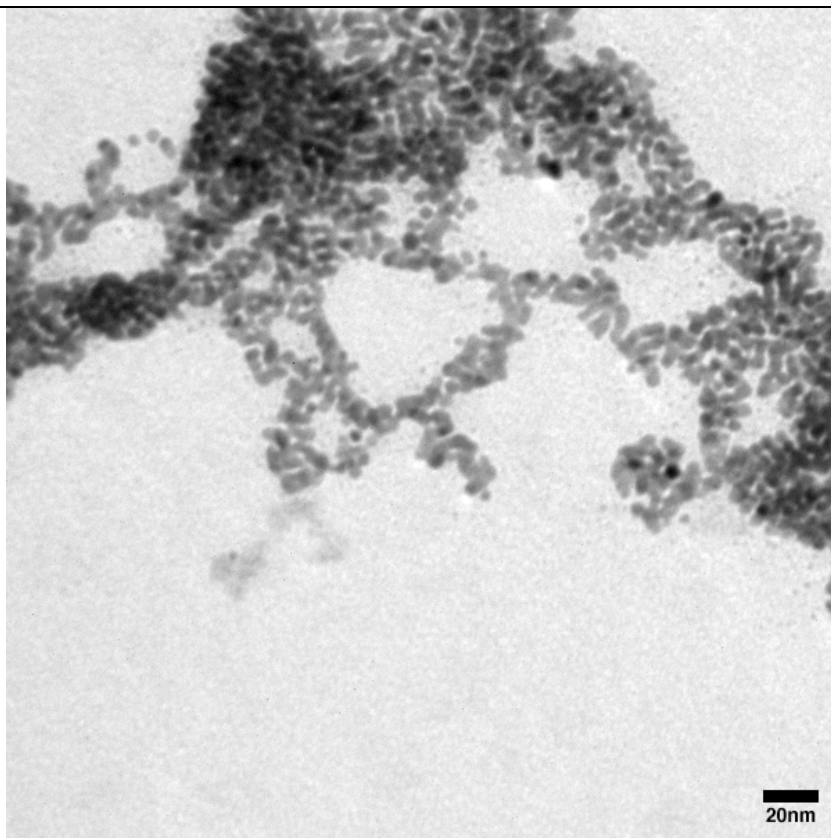


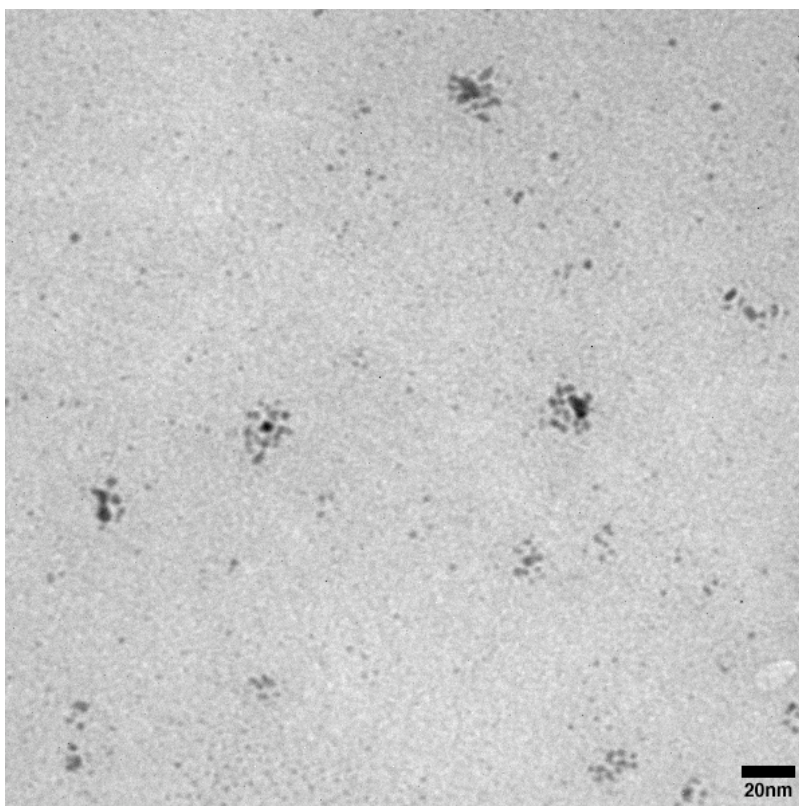
Figure 1. Comparison of boxed particle images to thresholded images made with our algorithm.

3-mercaptopropionic acid

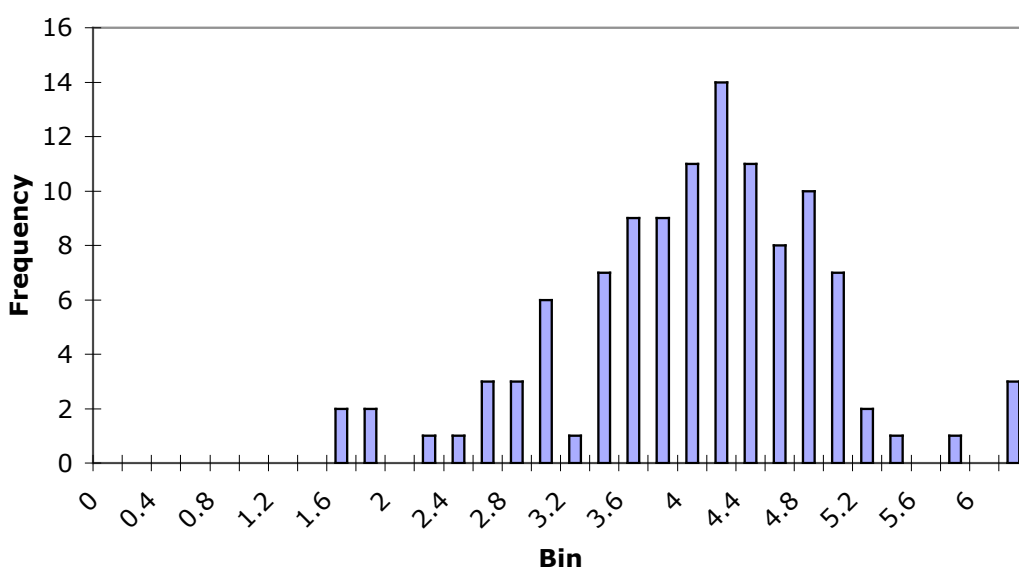


Particles not size analyzed due to aggregation.

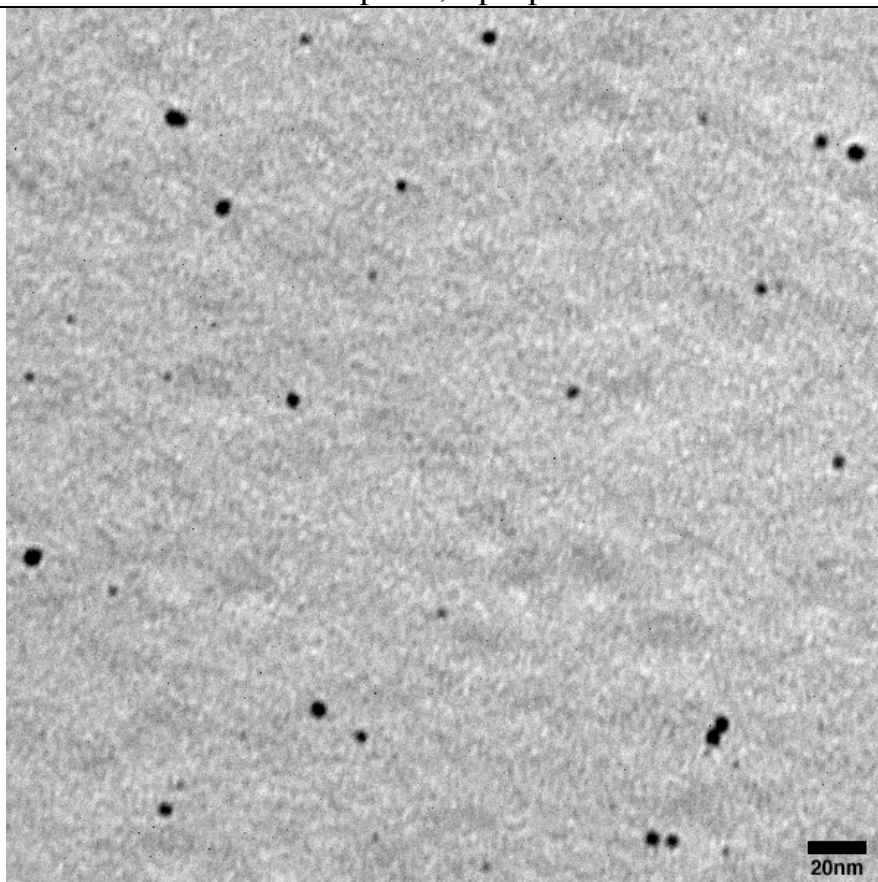
4-mercaptopbutyric acid MPC



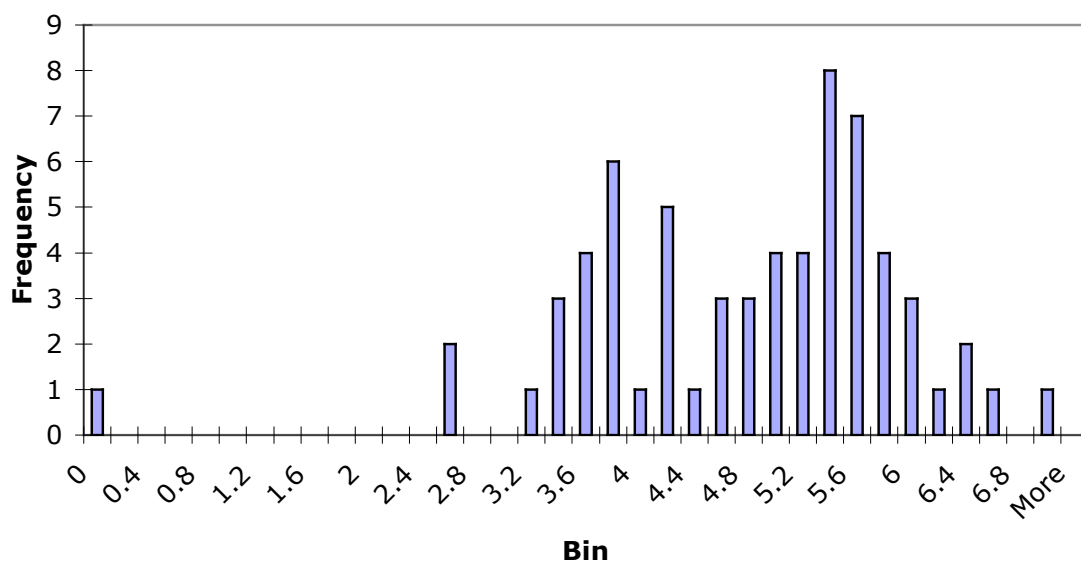
4-Mercaptobutyric Acid MPC Size Distribution



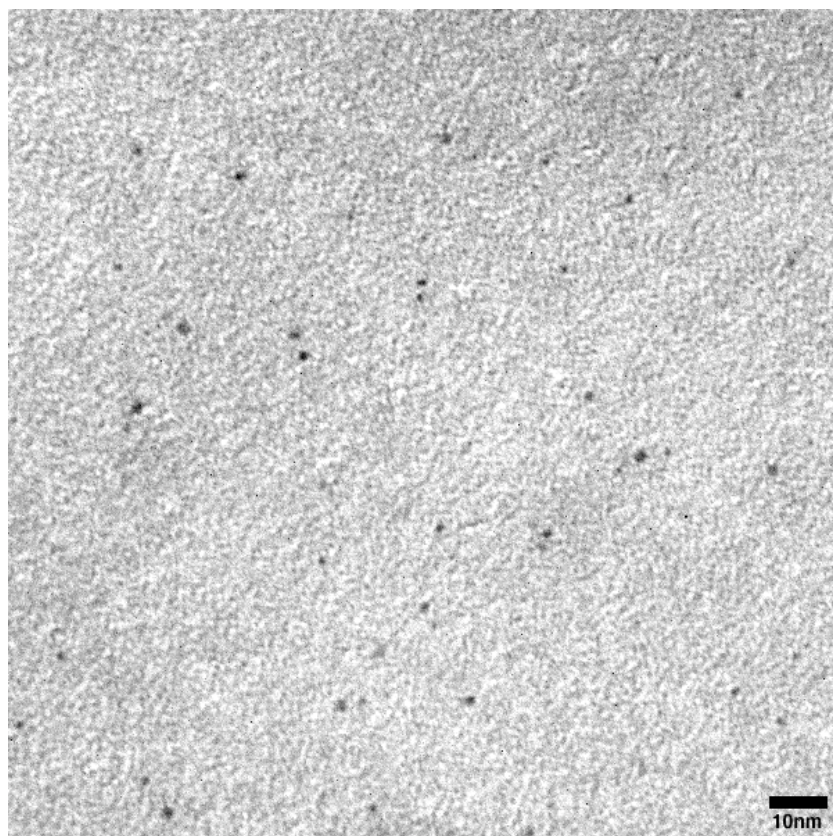
3-mercapto-1,2-propanediol



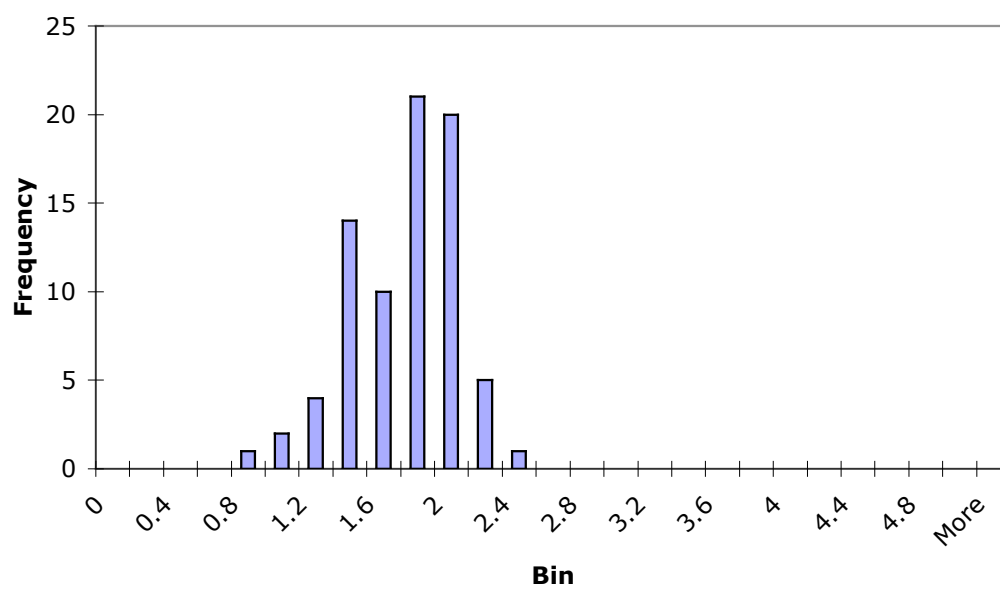
Mercaptopropanediol MPC Size Distribution



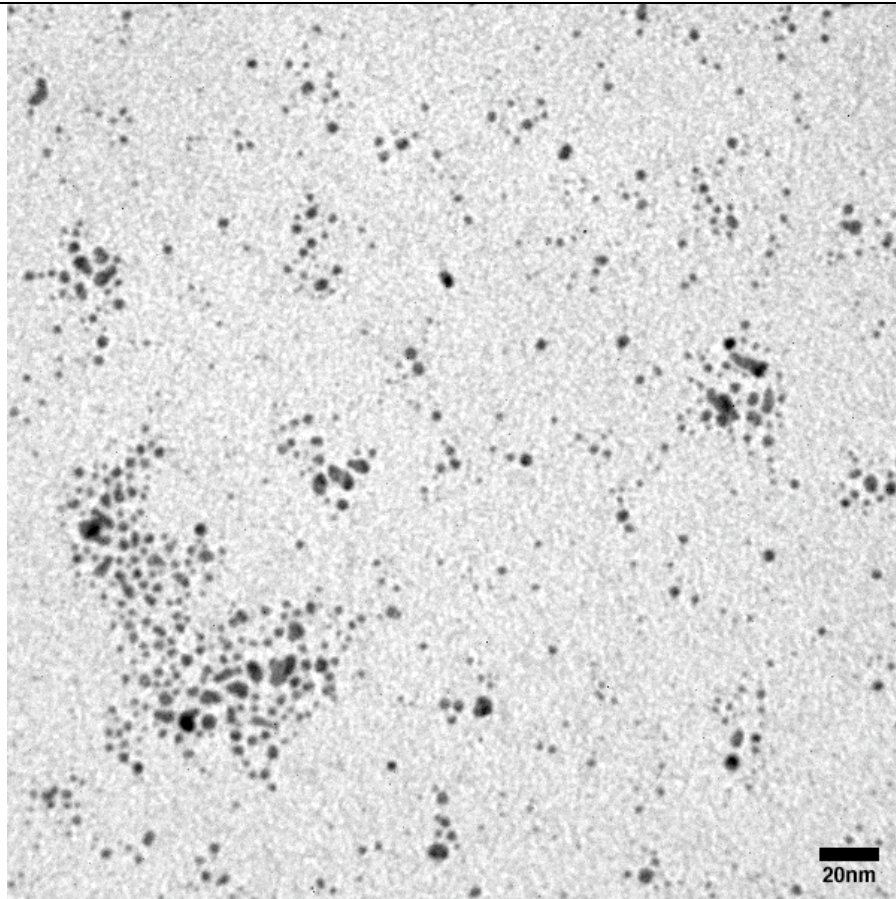
cysteine



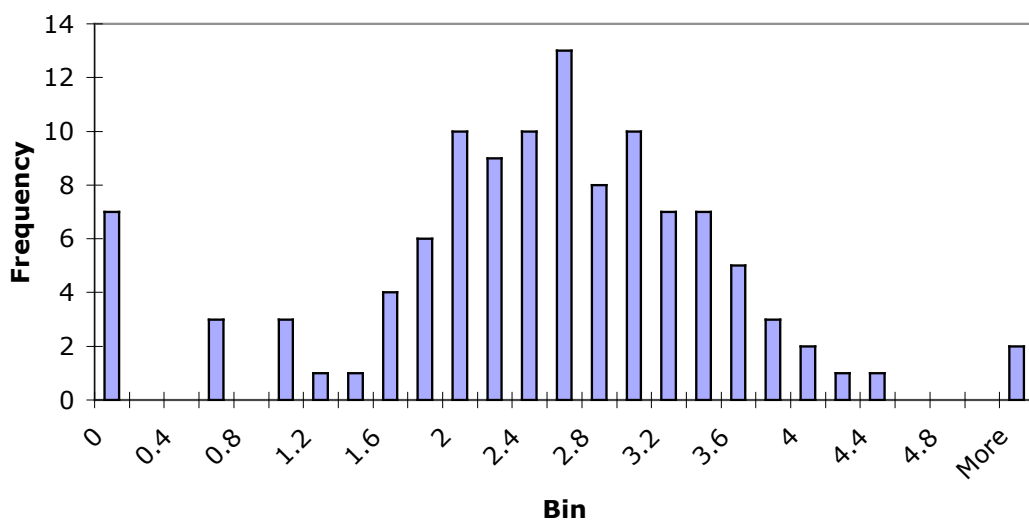
Cysteine MPC Size Distribution



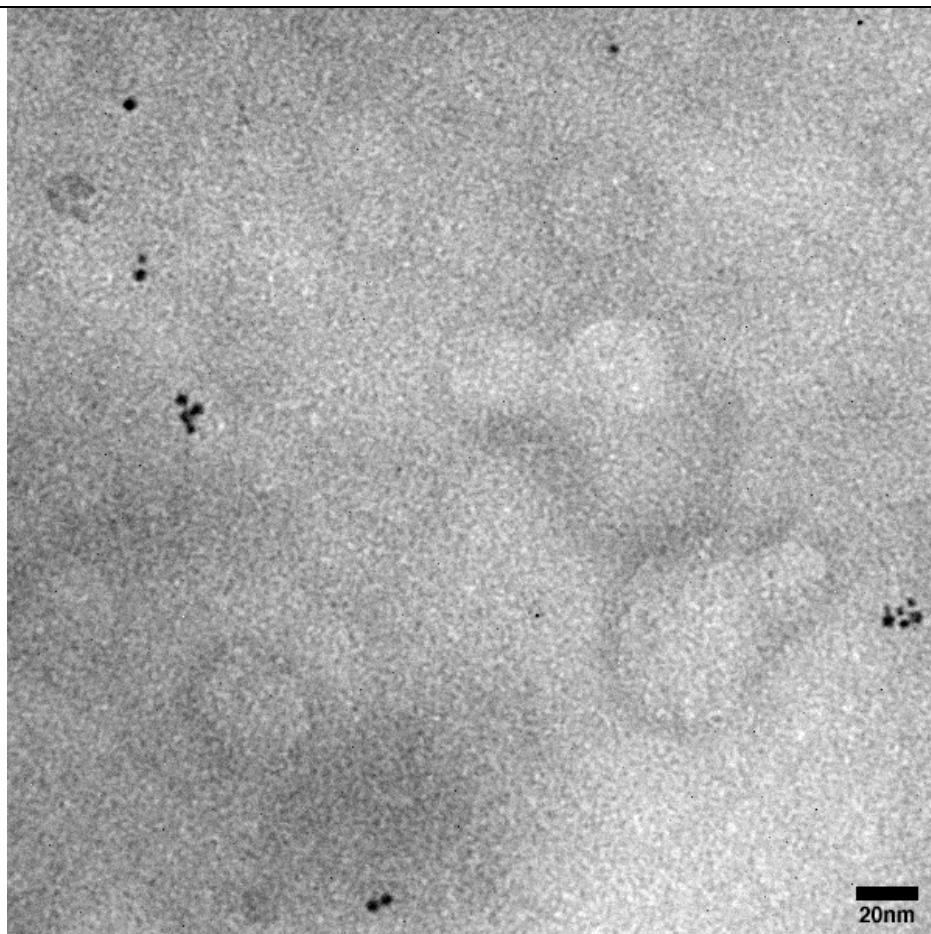
methionine



Methionine MPC Size Distribution

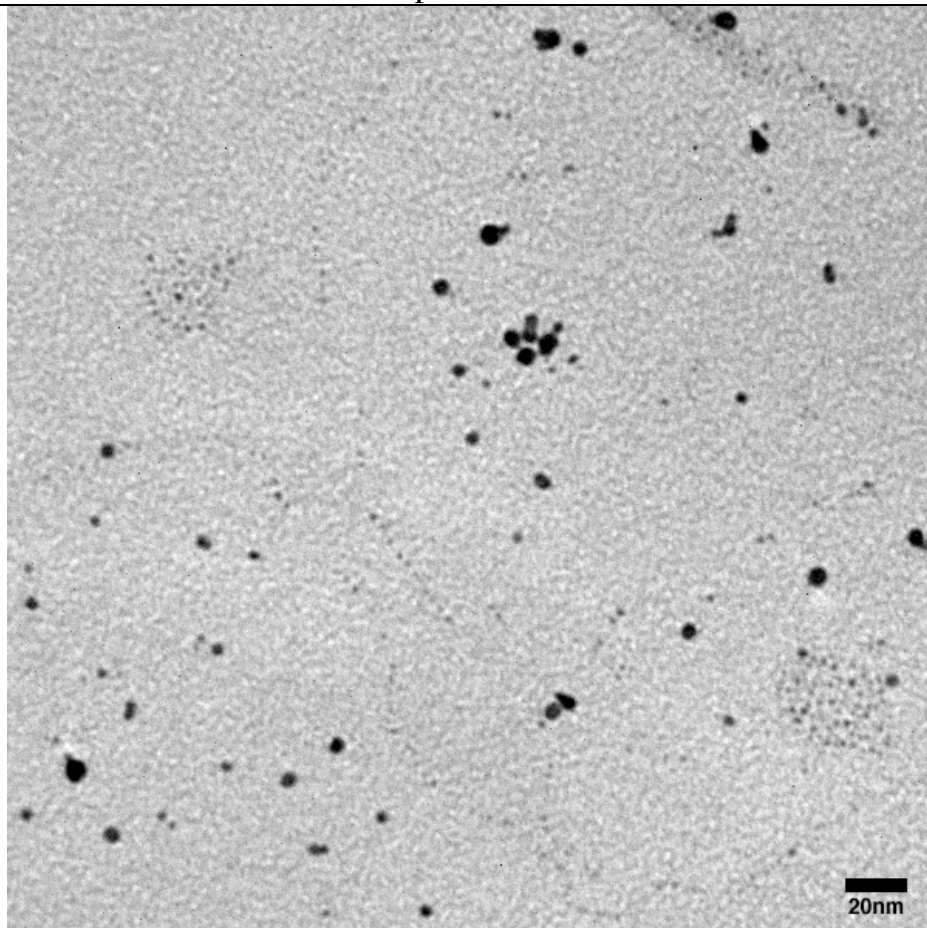


thiomalate

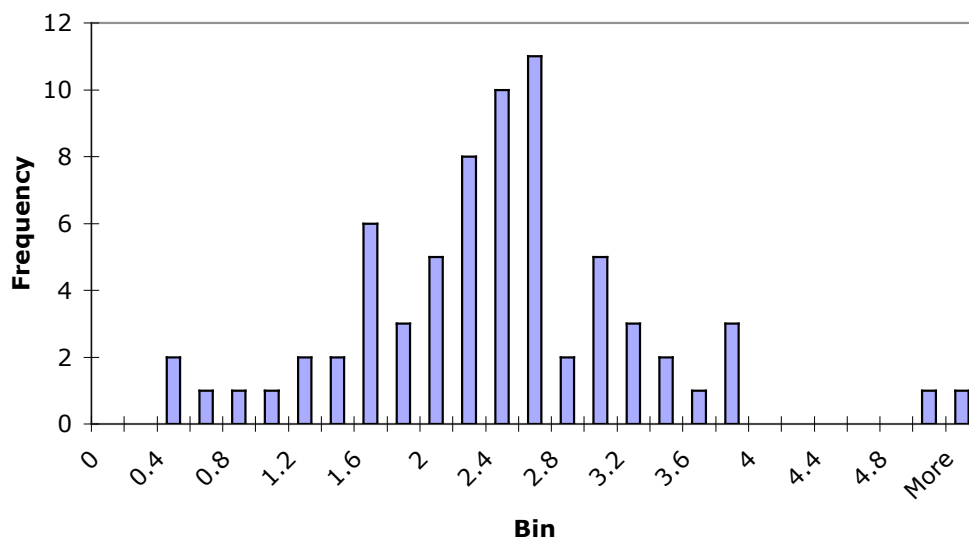


Particle aggregation makes automated size determination impossible.

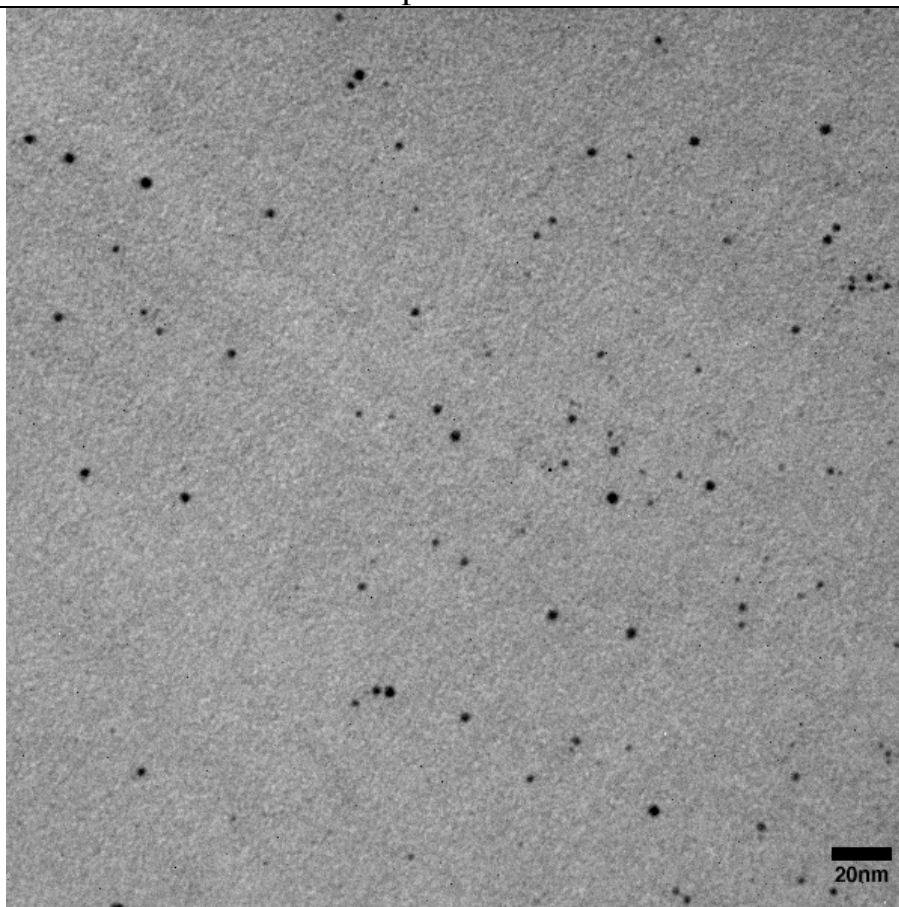
2-mercaptobenzoic acid



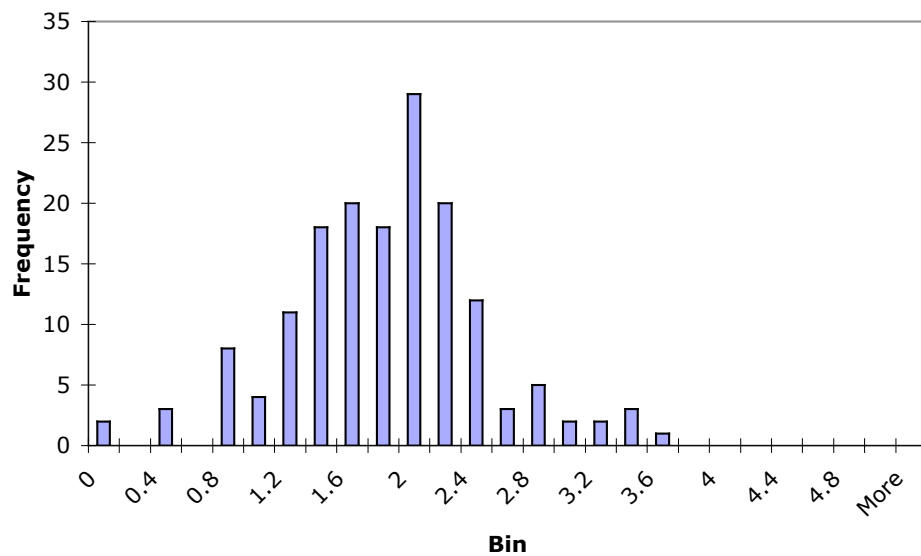
2-Mercaptobenzoic acid MPC Size Distribution



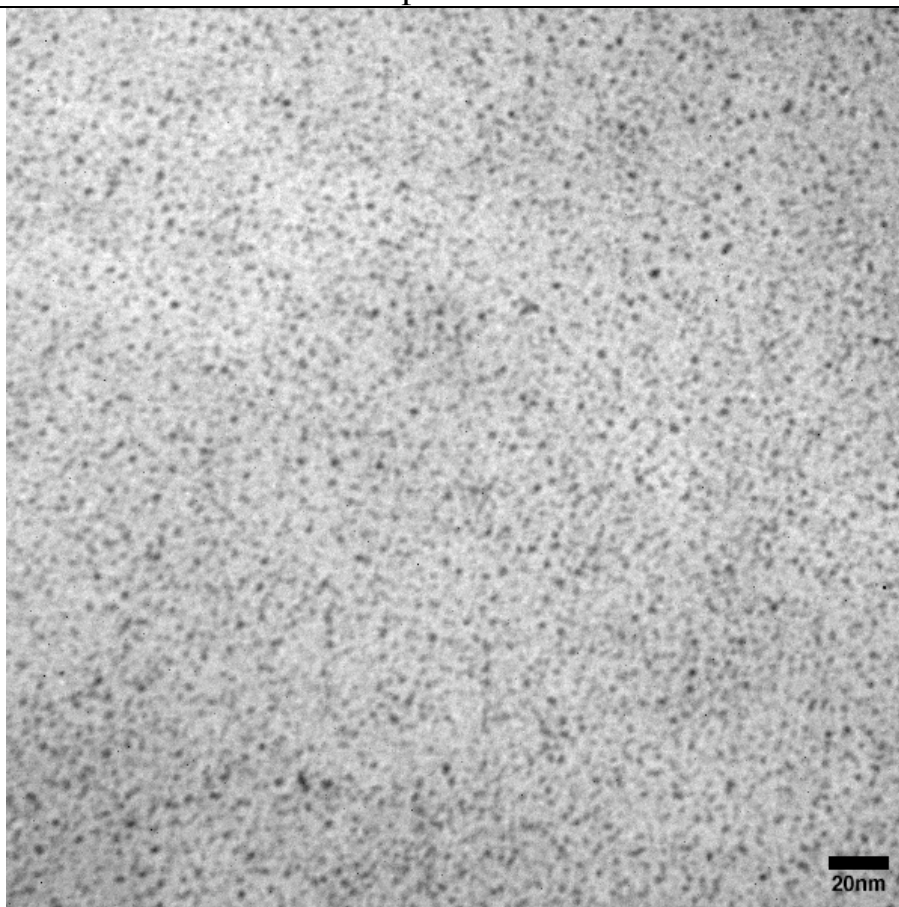
3-mercaptopbenzoic acid



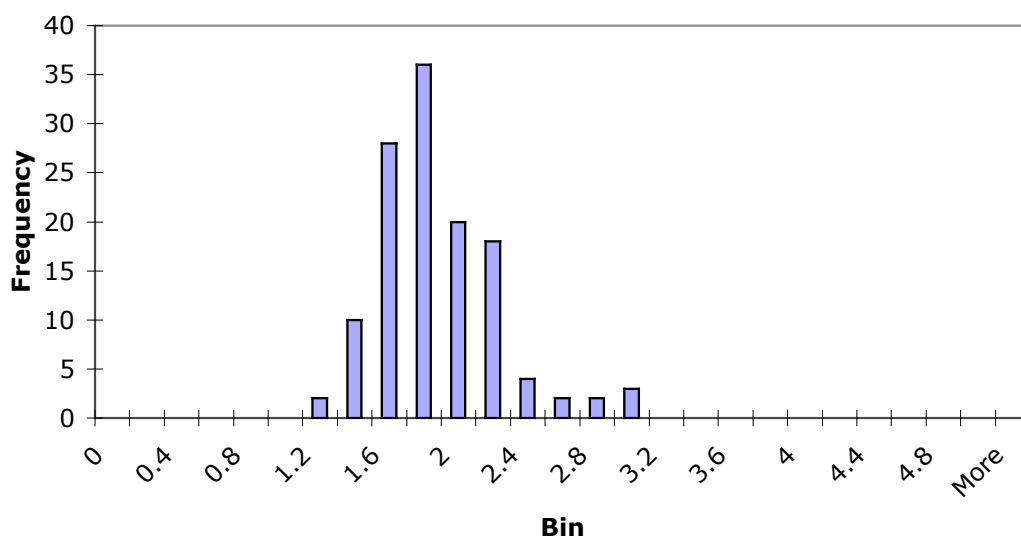
3-Mercaptopbenzoic acid MPC Size Distribution



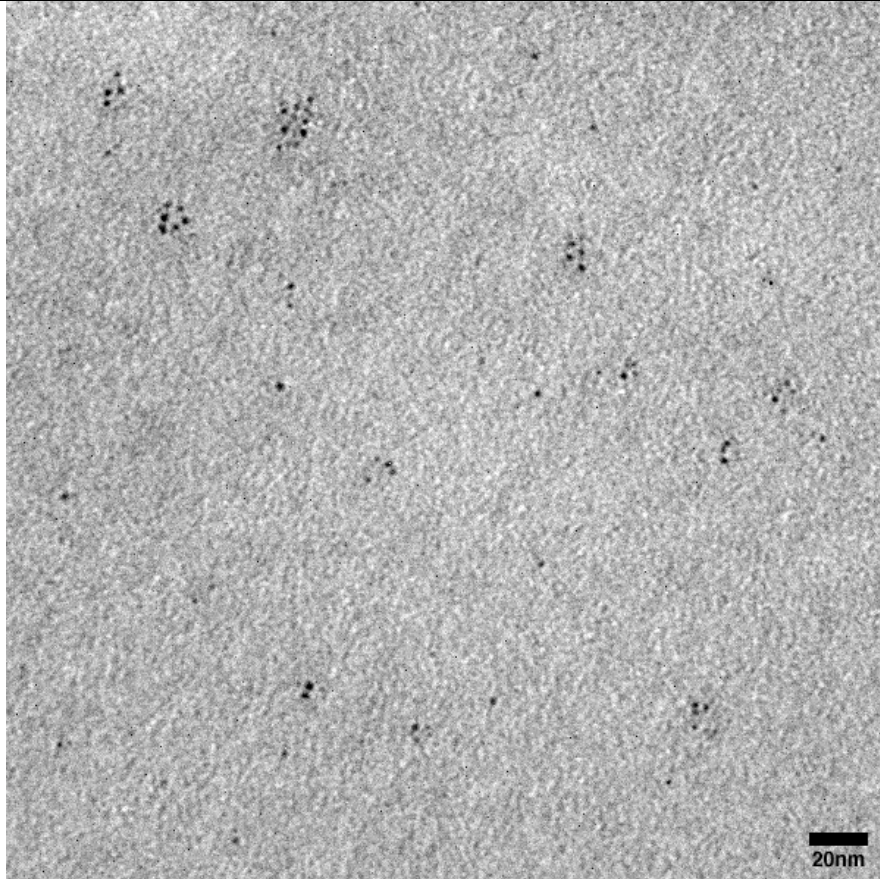
4-mercaptobenzoic acid



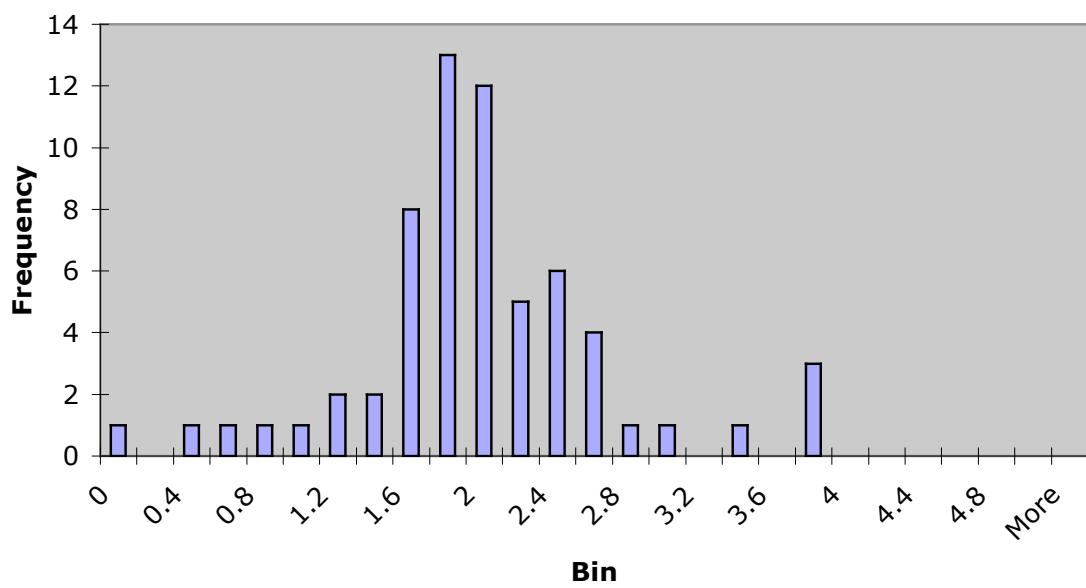
4-Mercaptobenzoic Acid MPC Sizer Distribution



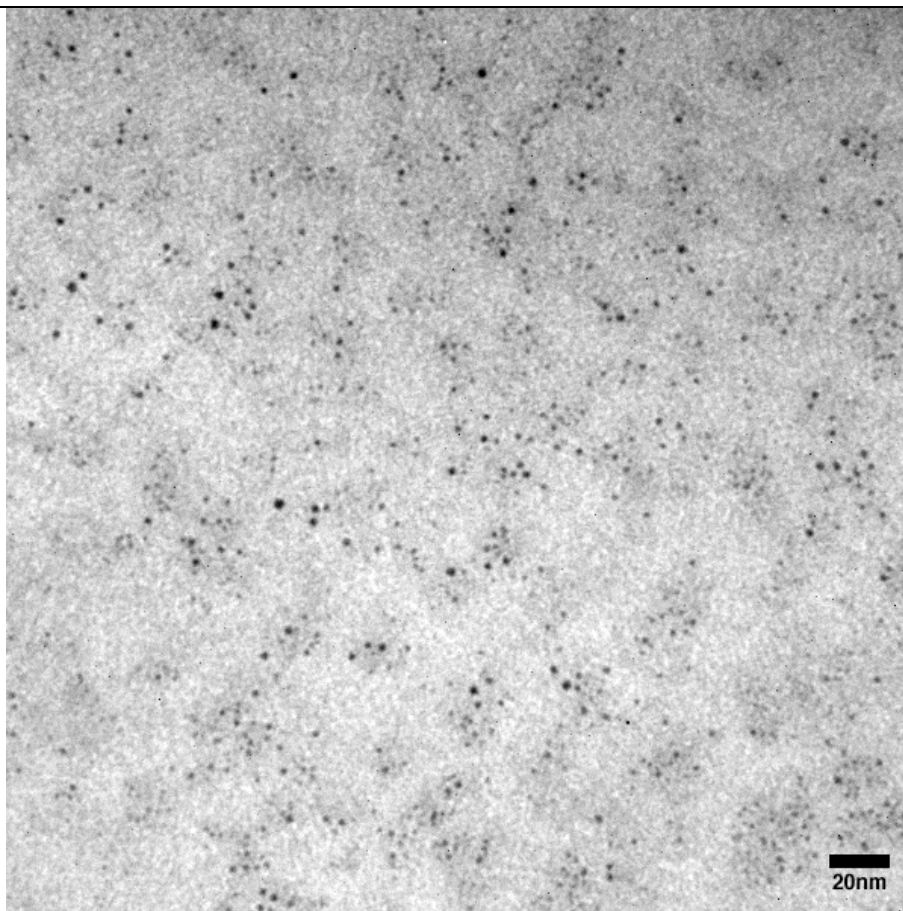
tiopronin



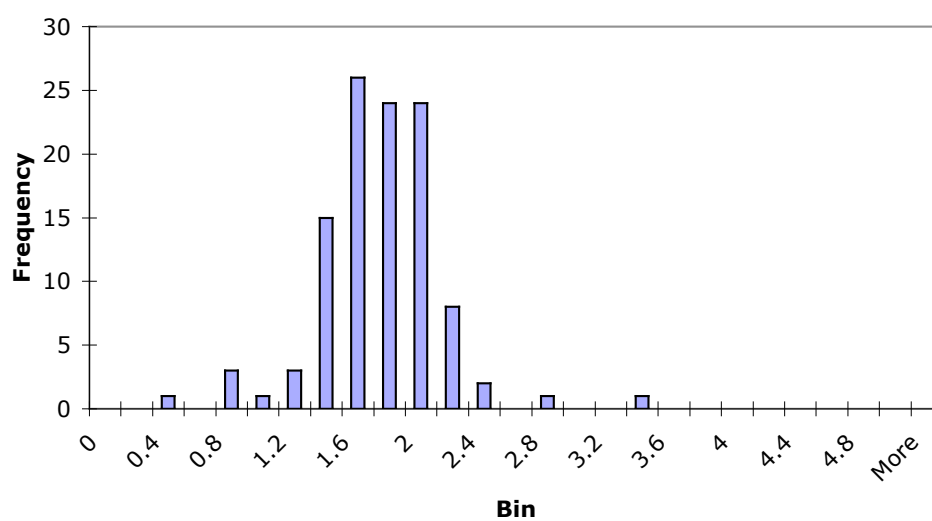
Tiopronin MPC Size Distribution



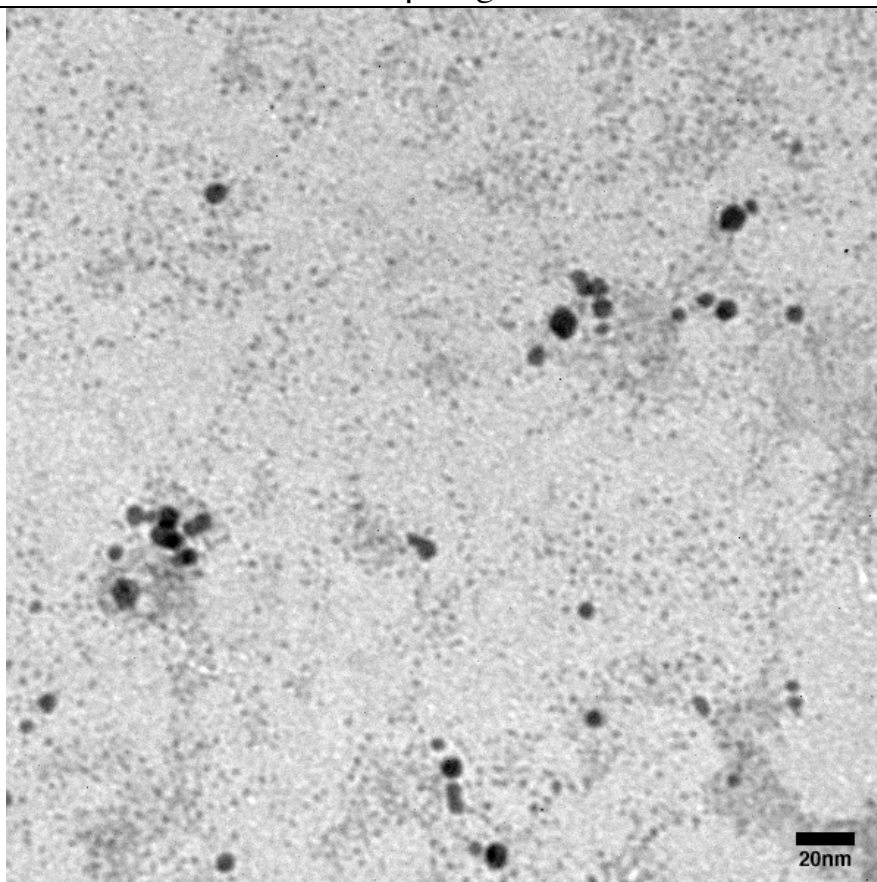
selenomethionine



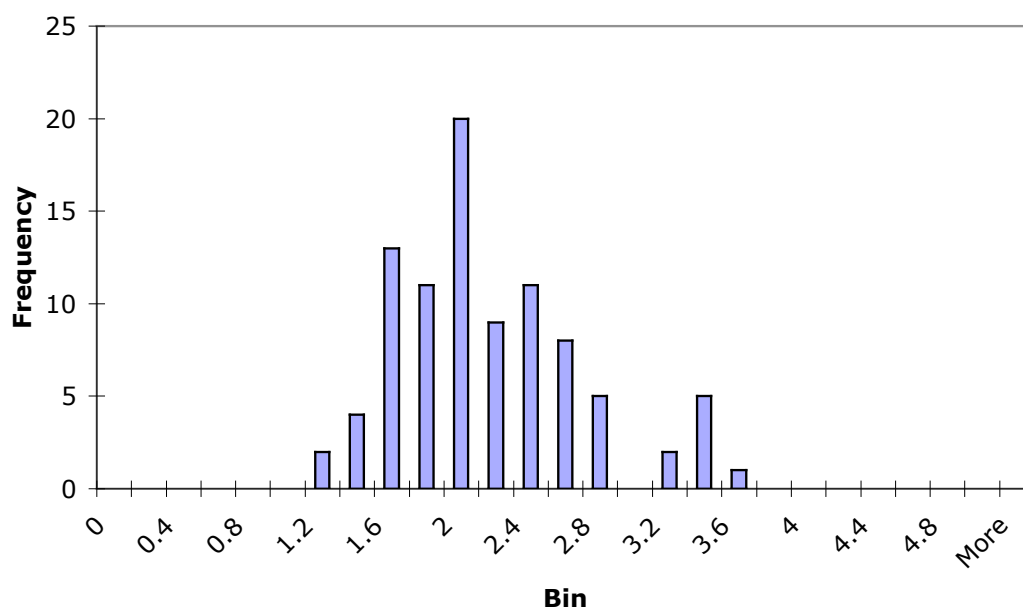
Selenomethionine MPC Size Distribution



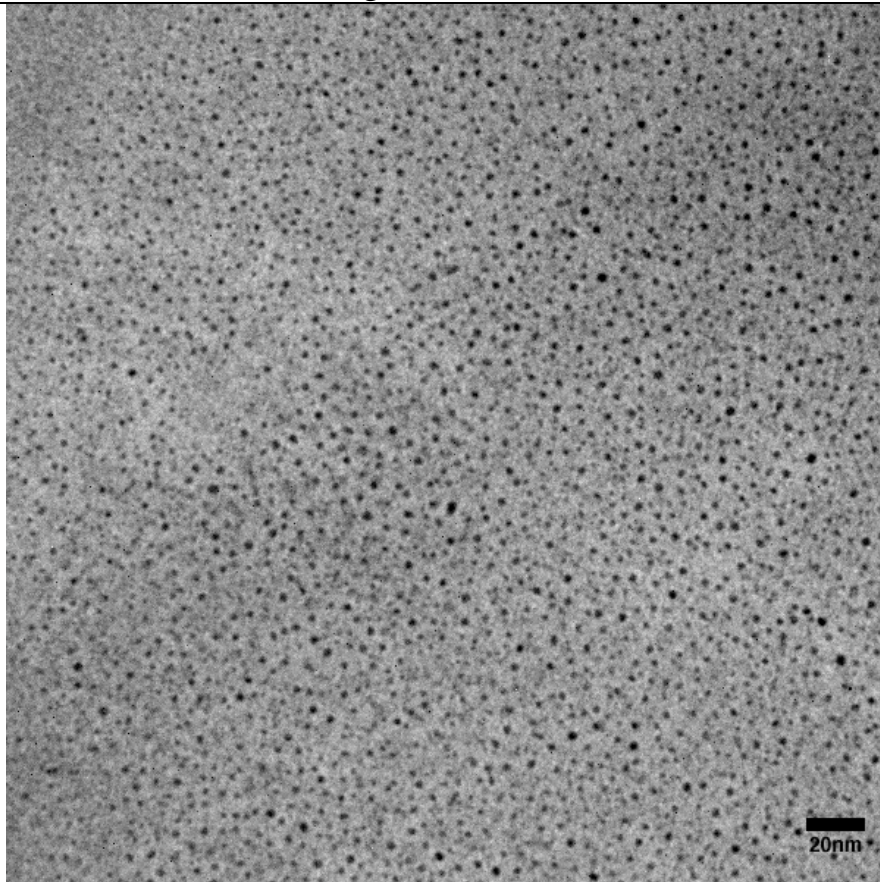
1-thio- β -D-glucose



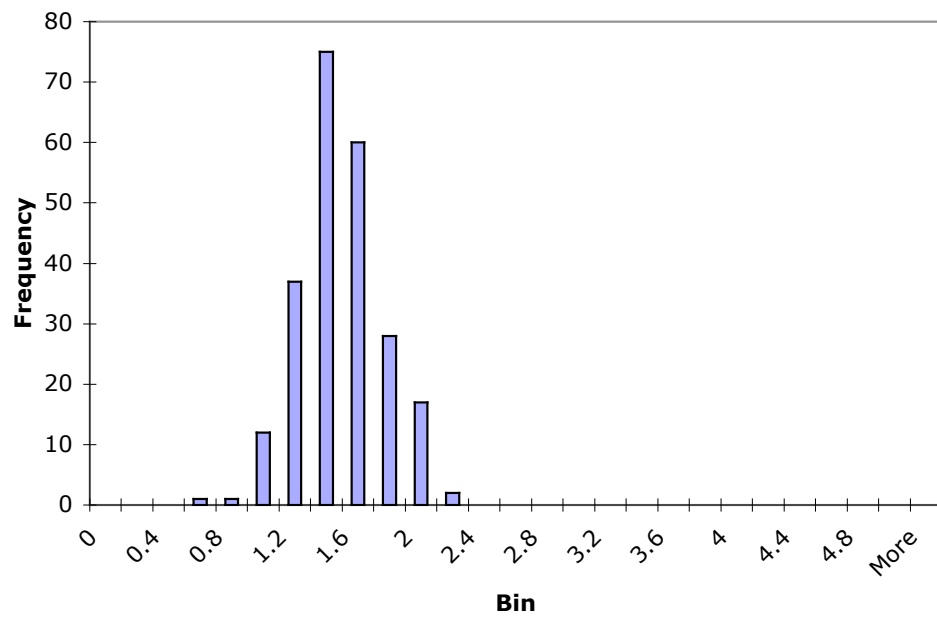
Thiogluucose MPC Size Distribution



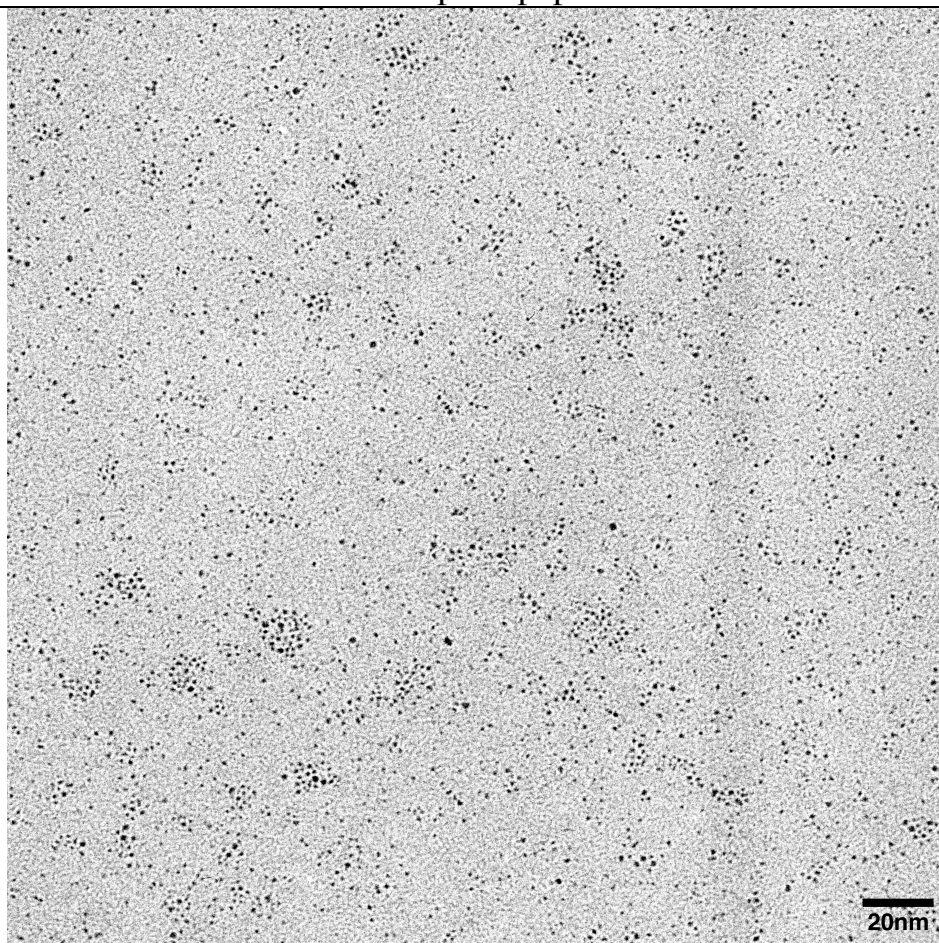
glutathione



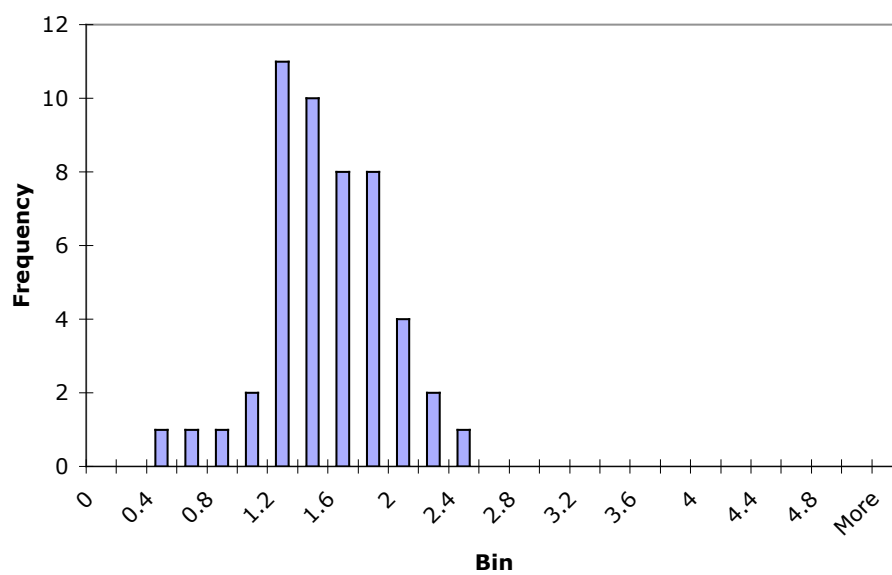
Glutathione MPC Size Distribution



ITCAE pentapeptide^g



ITCAE MPC Size Distrubtion



(1) Ludtke, S. J.; Baldwin, P. R.; Chiu, W. EMAN: semiautomated software for high-resolution single-particle reconstructions. *J Struct Biol* **1999**, *128*, 82-97.