Electronic Supplementary Material (ESI) for Materials Horizons.

Supporting materials for "Cryogenic electron tomography to determine thermodynamic quantities for nanoparticle dispersions"

Quy Ong[1], Ting Mao[1], Neda Iranpour Anaraki[2,3,4], Łukasz Richter [1], Carla Malinverni[1], Xufeng Xu[1], Francesca Olgiati[1], Paulo Henrique Jacob Silva[1], Anna Murello[1], Antonia Neels[2,4], Davide Demurtas[5], Seishi Shimizu[6], and Francesco Stellacci[1,7]*

1. Institute of Materials, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland
2. Center for X-ray Analytics, Empa, Swiss Federal Laboratories for Materials Science and Technology, Lerchenfeldstrasse 5, St. Gallen, 9014, Switzerland
3. Laboratory of Particles-Biology Interactions, Empa, Swiss Federal Laboratories for Materials Science and Technology, Lerchenfeldstrasse 5, St. Gallen, 9014, Switzerland
4. Department of Chemistry, University of Fribourg, Chemin du Musée 9, Fribourg, 1700, Switzerland
5. Interdisciplinary Centre for Electron Microscopy (CIME), Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland
6. York Structural Biology Laboratory, Department of Chemistry, University of York, Heslington, York YO10 5DD, United Kingdom
7. Bioengineering Institute, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

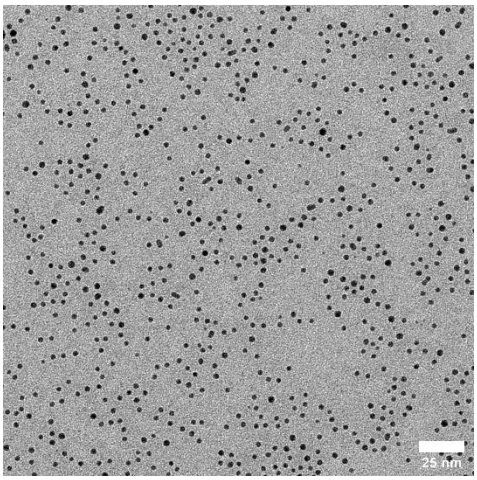

Figure SI1. Conventional TEM image of NP1.

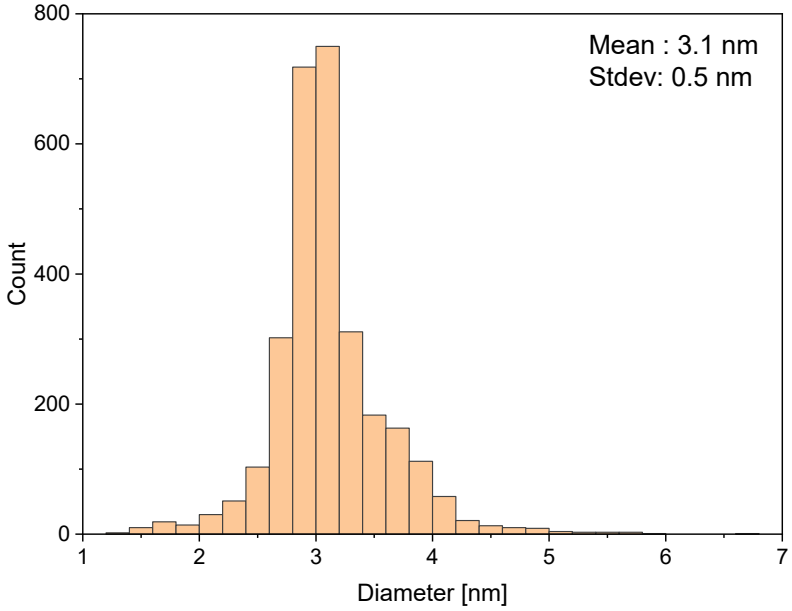

Figure SI2. Histogram of particle size (diameter) of NP1.

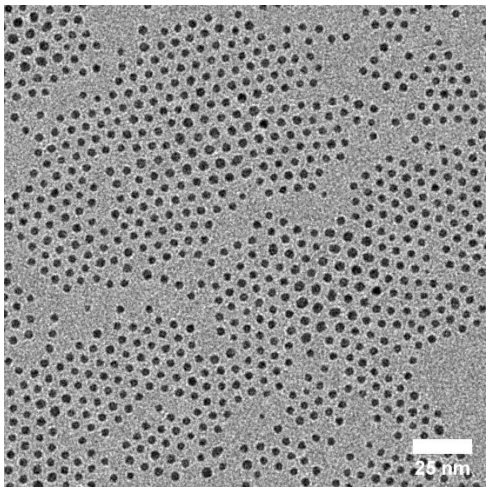

Figure SI3. Conventional TEM image of NP2.

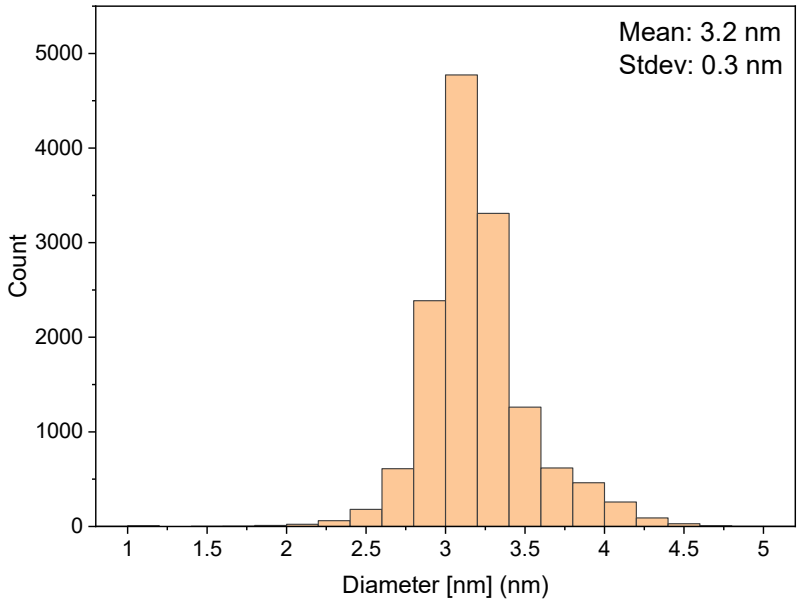

Figure SI4. Histogram of particle size (diameter) of NP2.

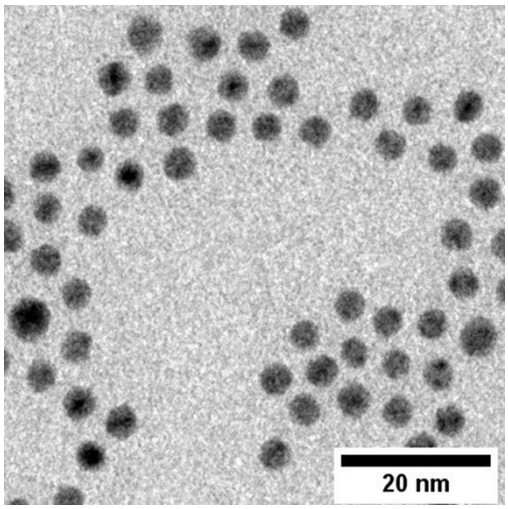

Figure SI5. Conventional TEM image of NP3.

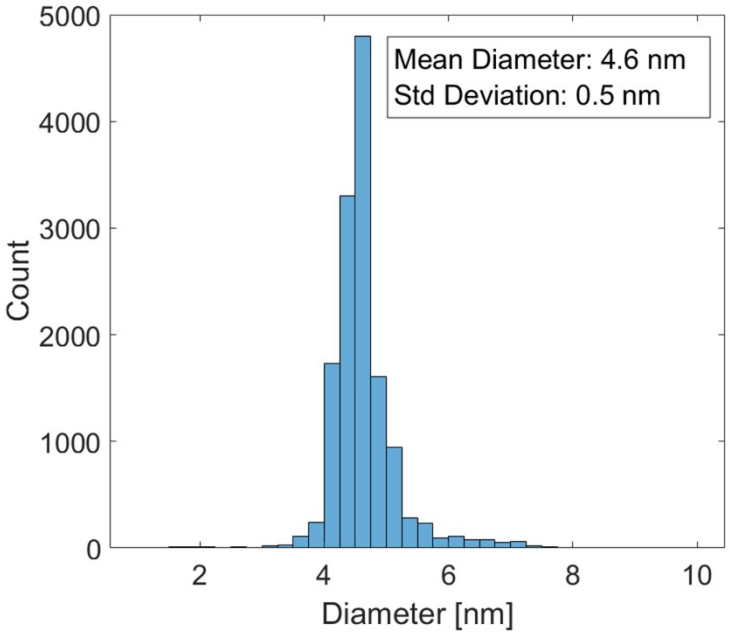

Figure SI6. Histogram of particle size (diameter) of NP3.

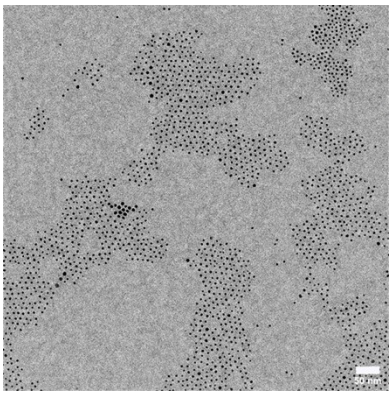

Figure SI7. Conventional TEM image of NP4.

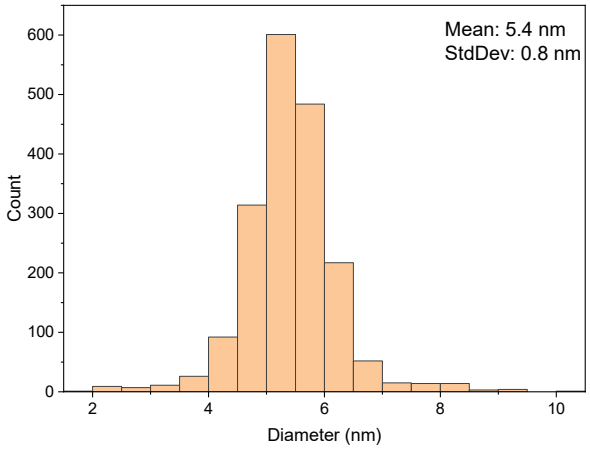

Figure SI8. Histogram of particle size (diameter) of NP4.

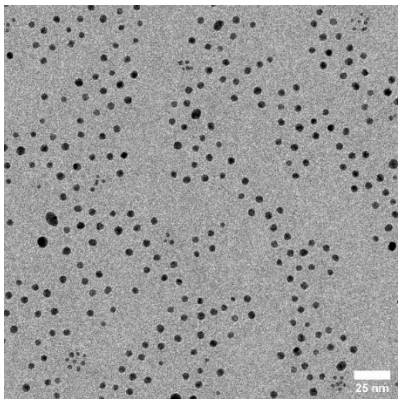

Figure SI9. Conventional TEM image of NP5.

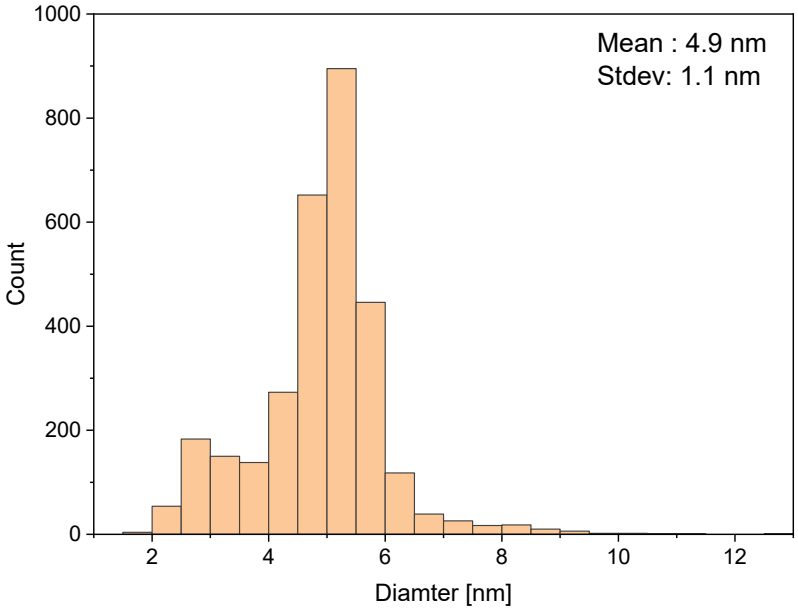

Figure SI10. Histogram of particle size (diameter) of NP5.

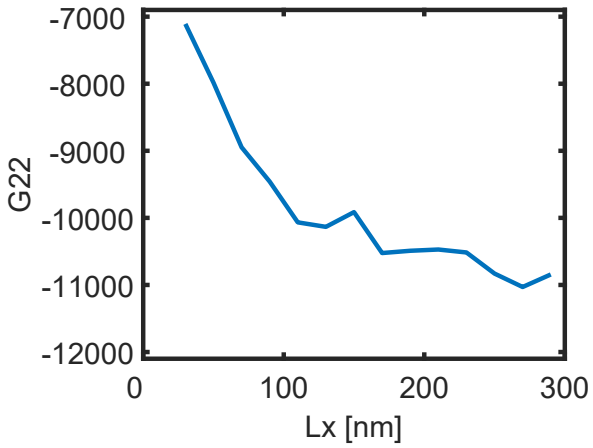

Figure SI11. Checking the calculation of G_{22} vs the box volume used to extract the number of particles. The box chosen to have the Lz = 80 nm, Lx and Ly were varied by the same value from 50 to 280 nm.

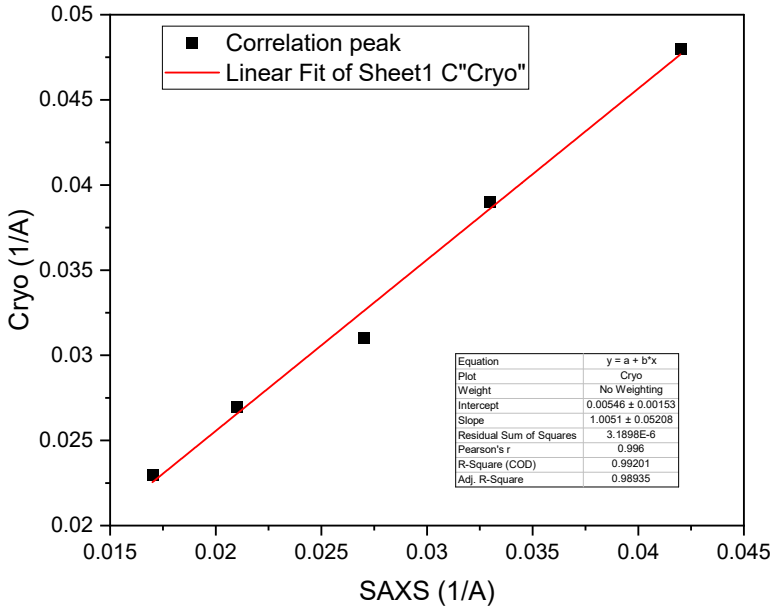

Figure S12. Plot of the correlation peaks (maxima obtained from *S(q)* vs *q*) from SAXS measurements against those calculated from cryoET data for NP1 dispersed in water by a concentration range from 5 mg/ml to 80 mg/ml. The data, represented as black squares, is fitted to a linear function. The slope found is close to 1. The small value of intercept at the y-axis is used as a constant to shift the S(q) calculated from CryoET for the whole range of concentration.

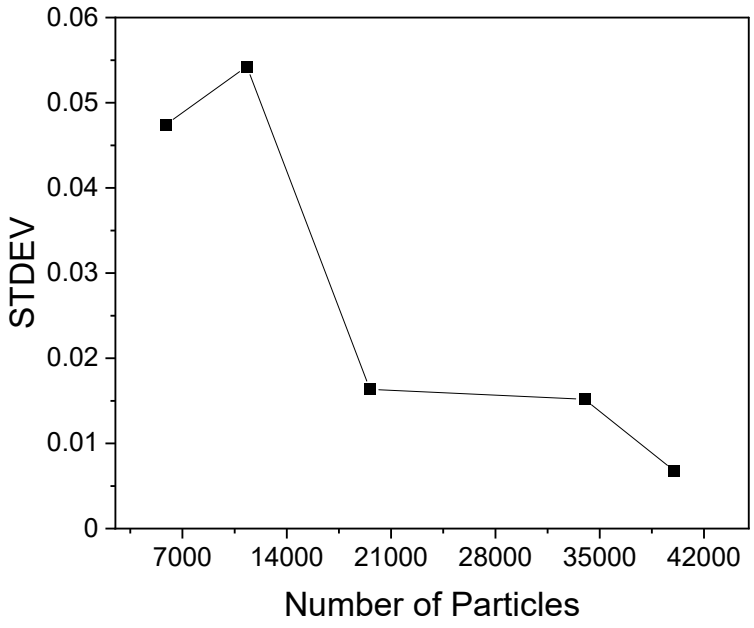

Figure SI13. Noise analysis on the g(r) for NP1 dispersed in water.

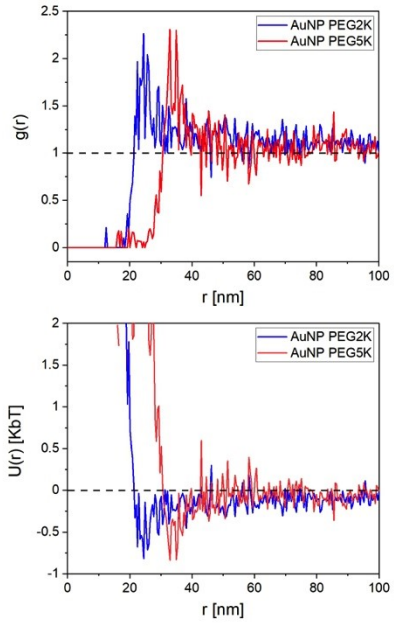

Figure SI14. g(r) and U(r) for NP4 and NP5 calculated for one tomogram for each particle.

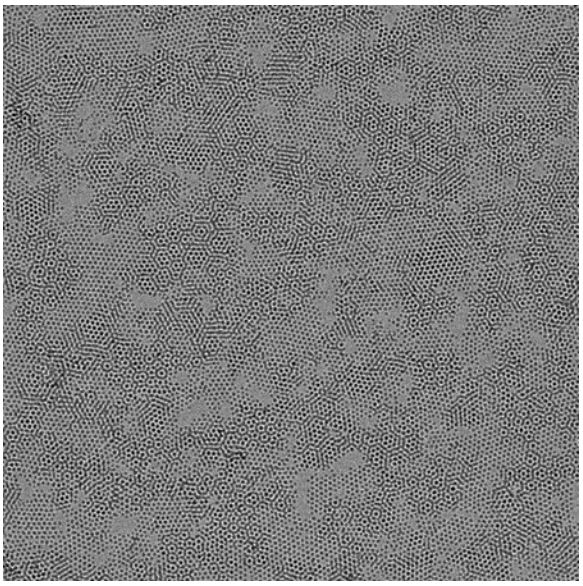

Figure SI15. 2D cryo-TEM image of NP2 at high salt concentration NaCl 150 mM showing extended aggregation.

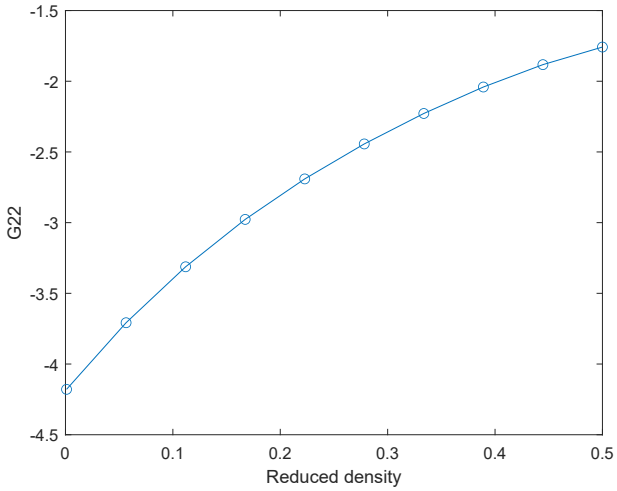

Figure SI16. Plot of theoretical G_{22} calculated as a function of density for hard spheres.

AUC analysis of NP3 particles for aggregation states						
S [Svd]	92	138	186	235	285	336
Normalized S	1	1.5	2.0	2.5	3	3.6
Agglomerate	Monomer	Dimer	Trimer	Tetramer	NA	NA

Figure SI17. Attribution of the aggregation states to the peaks observed in AUC -SV C(s).

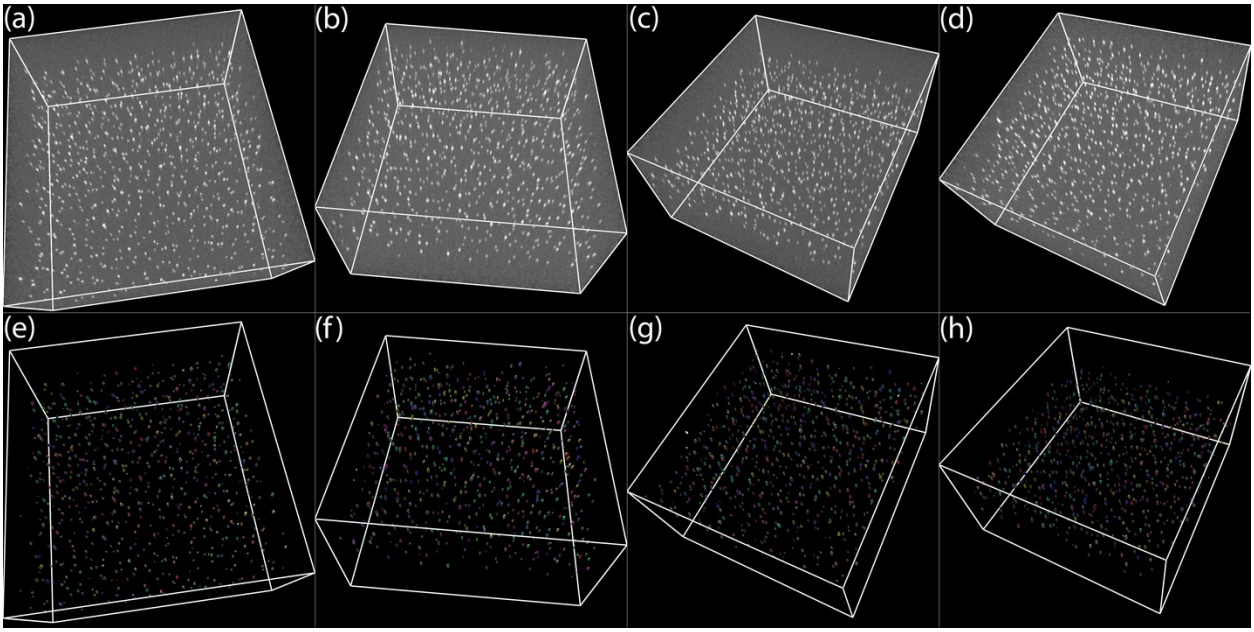

Figure SI18. (top row) examples of tomograms of sample NP2 at 5 mg/ml and (bottom row) the identification of particles from their tomograms.

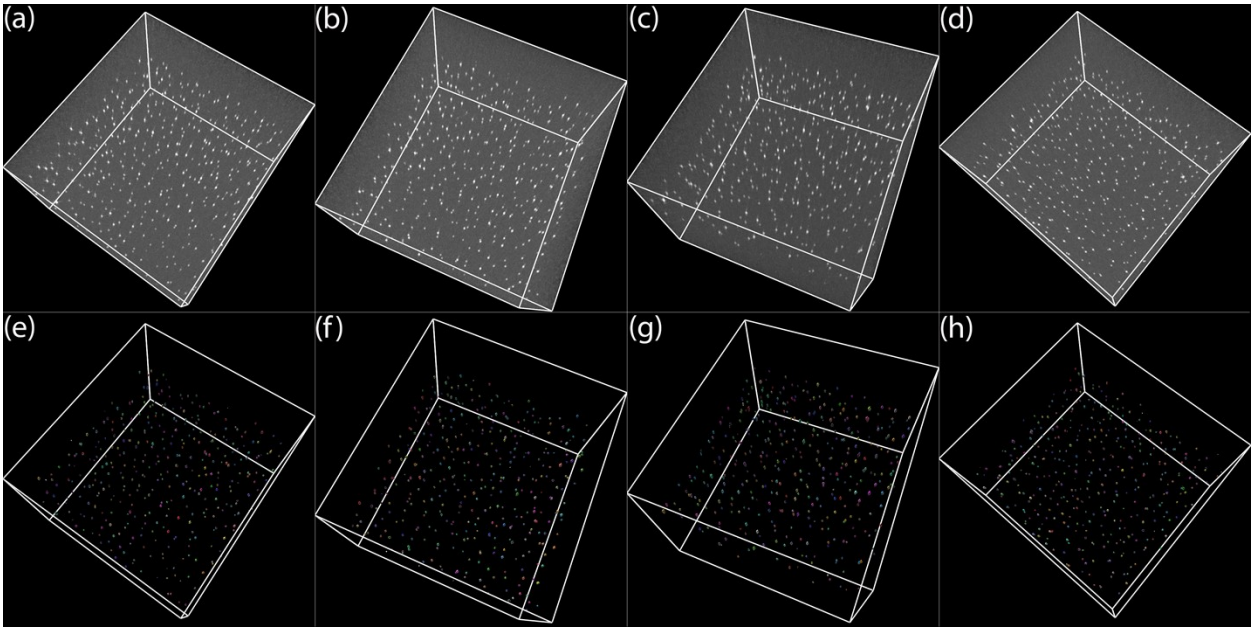

Figure SI19. (top row) examples of tomograms of sample NP2 at 5 mg/ml and (bottom row) the identification of particles from their tomograms.

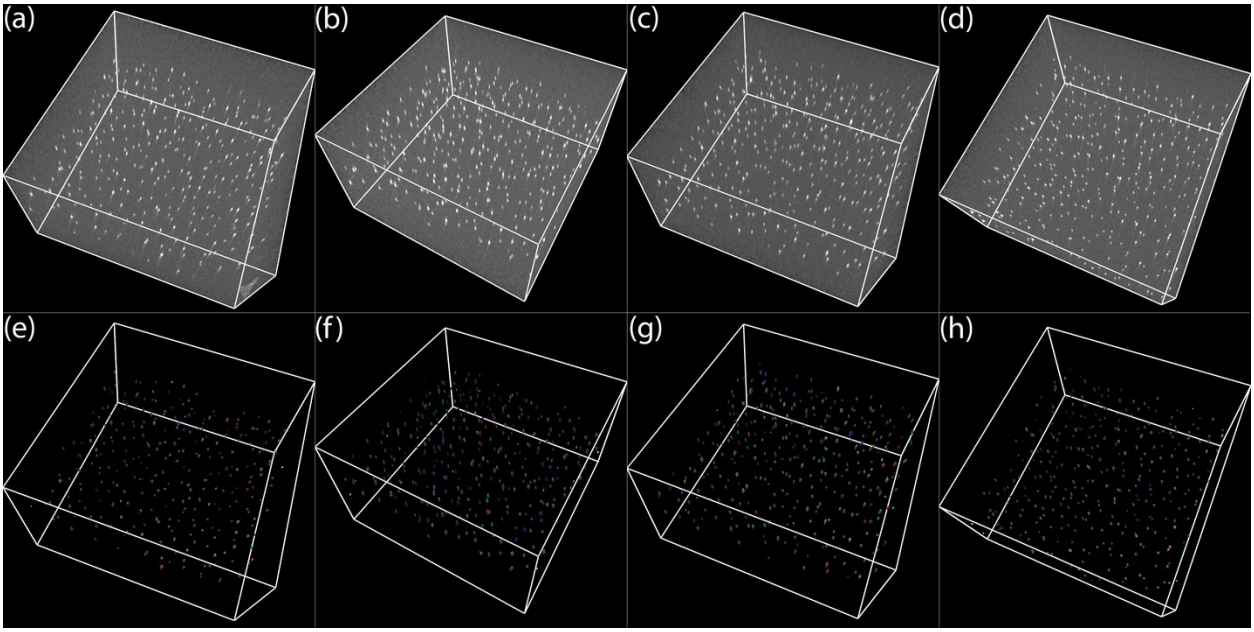

Figure SI20. (top row) examples of tomograms of sample NP2 at 5 mg/ml and (bottom row) the identification of particles from their tomograms.

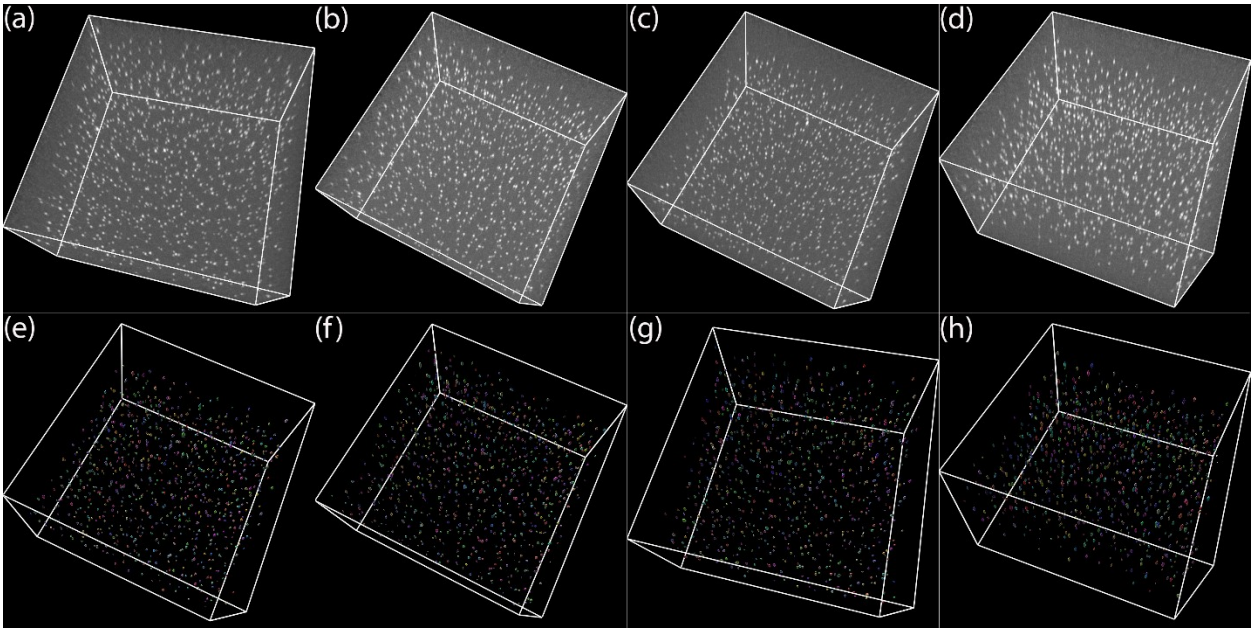

Figure SI21. (top row) examples of tomograms of sample NP2 at 10 mg/ml and (bottom row) the identification of particles from their tomograms.

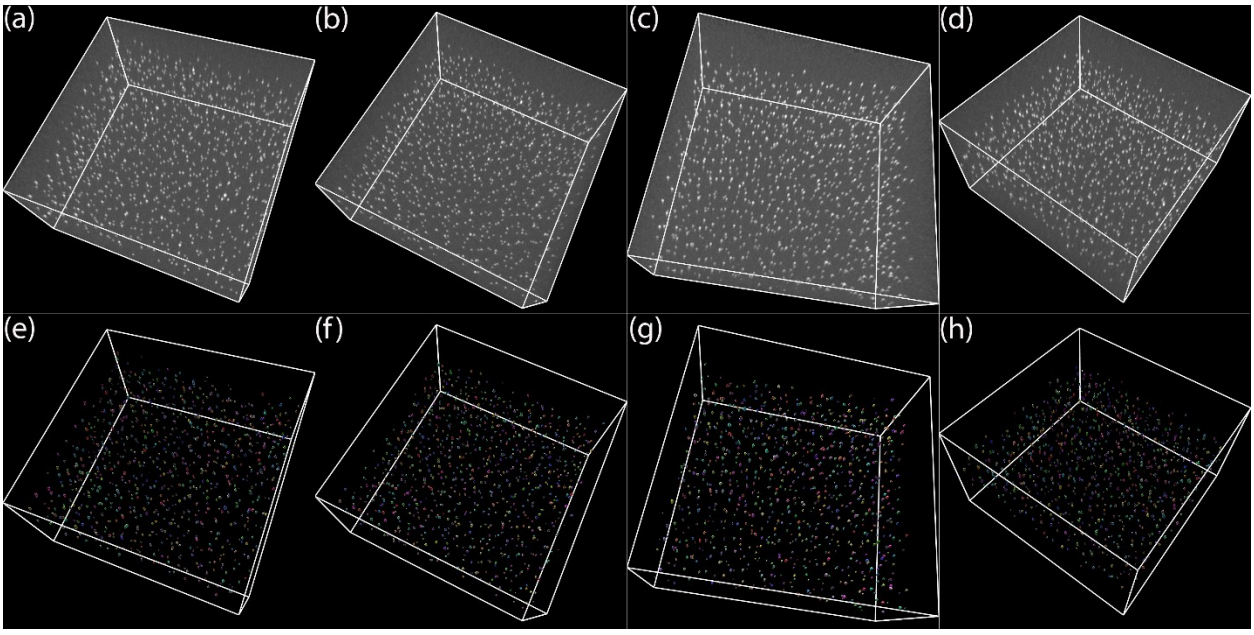

Figure SI22. (top row) examples of tomograms of sample NP2 at 10 mg/ml and (bottom row) the identification of particles from their tomograms.

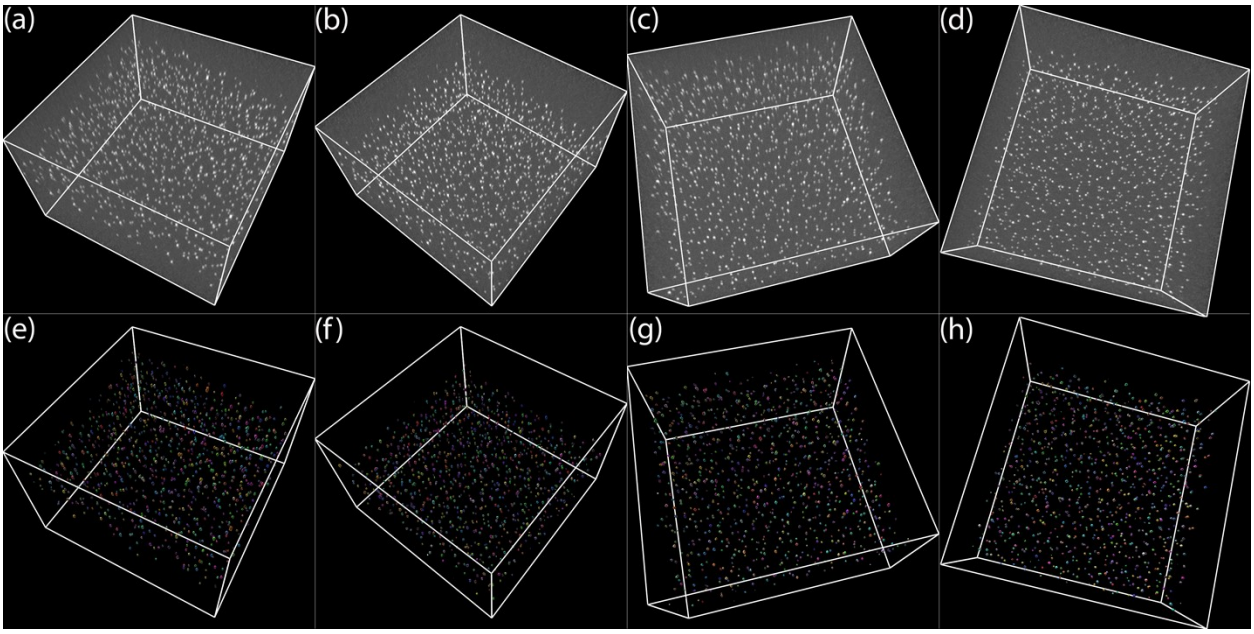

Figure SI23. (top row) examples of tomograms of sample NP2 at 10 mg/ml and (bottom row) the identification of particles from their tomograms.

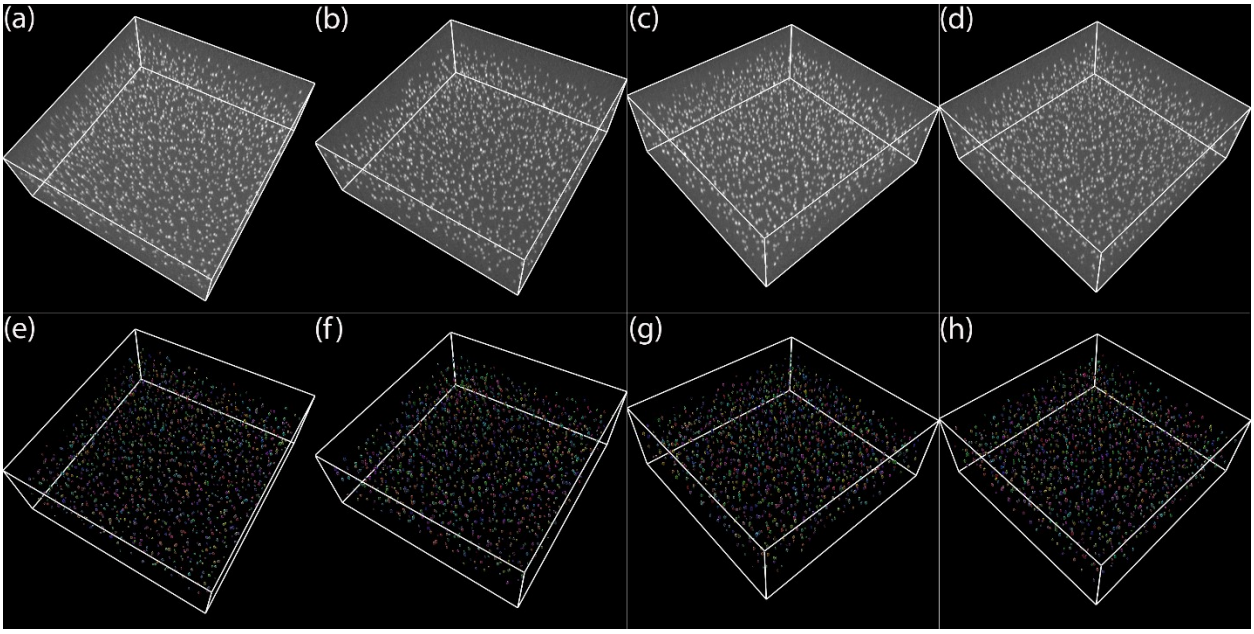

Figure SI24. (top row) examples of tomograms of sample NP2 at 20 mg/ml and (bottom row) the identification of particles from their tomograms.

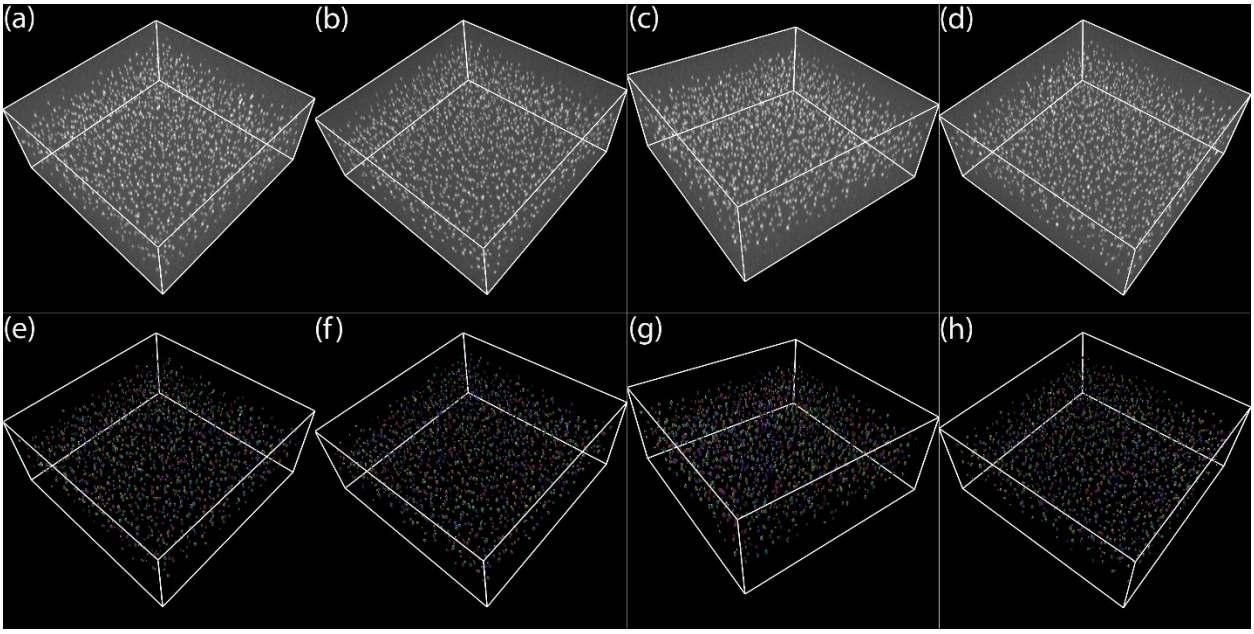

Figure SI25. (top row) examples of tomograms of sample NP2 at 20 mg/ml and (bottom row) the identification of particles from their tomograms.

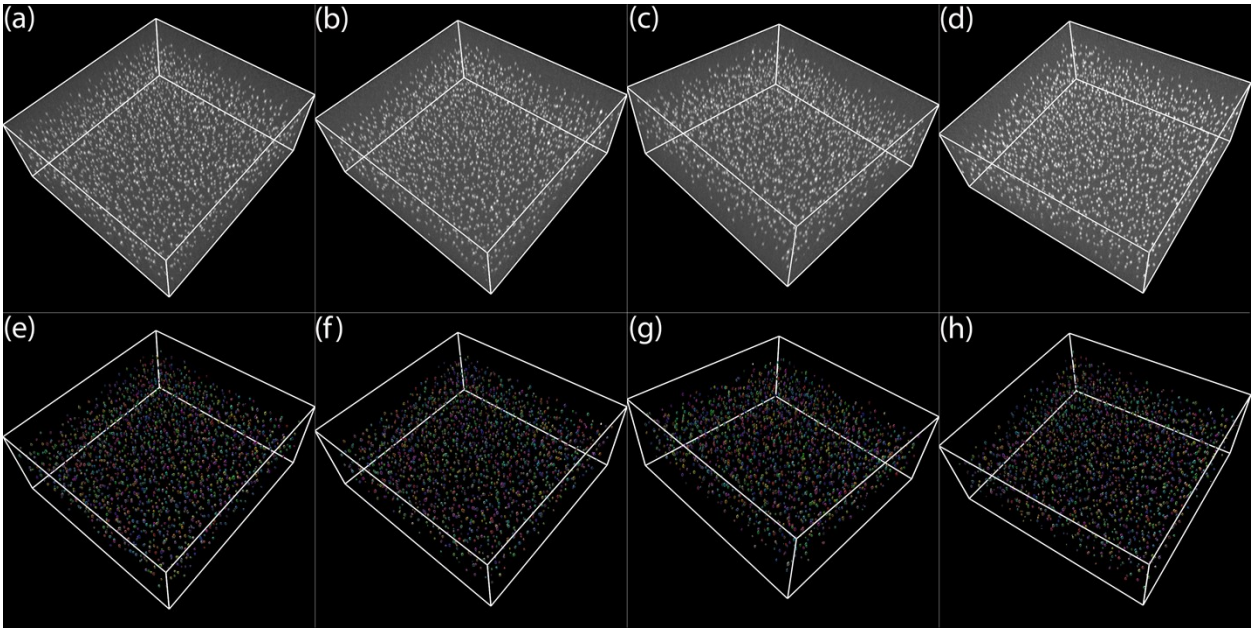

Figure SI26. (top row) examples of tomograms of sample NP2 at 20 mg/ml and (bottom row) the identification of particles from their tomograms.

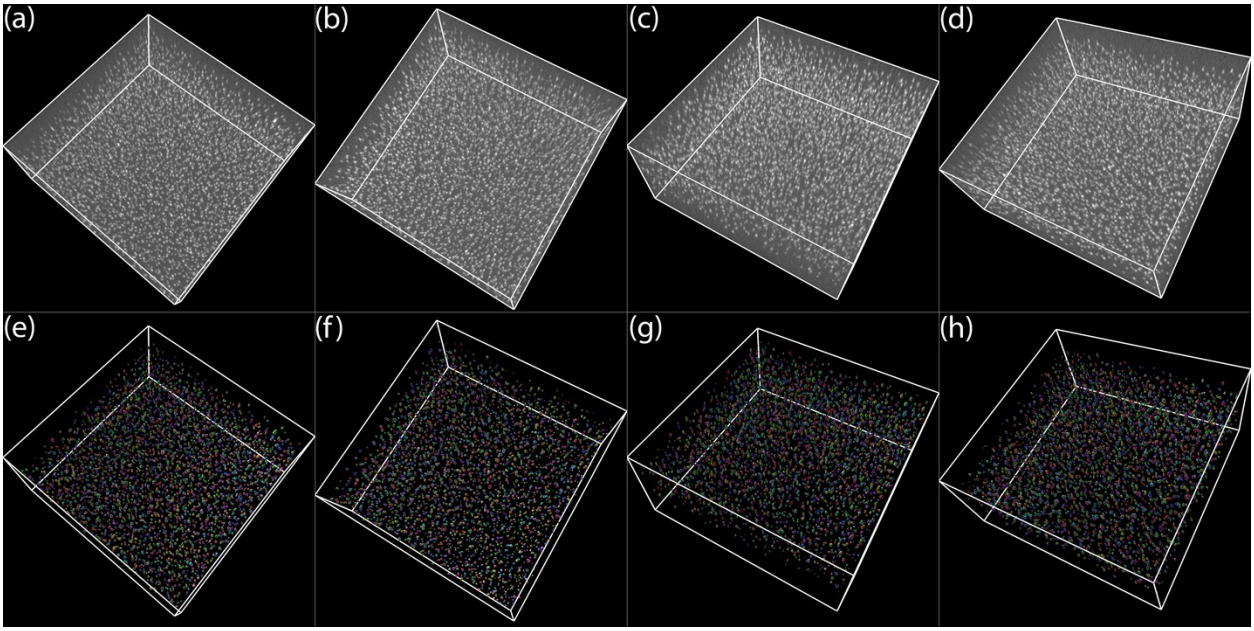

Figure SI27. (top row) examples of tomograms of sample NP2 at 40 mg/ml and (bottom row) the identification of particles from their tomograms.

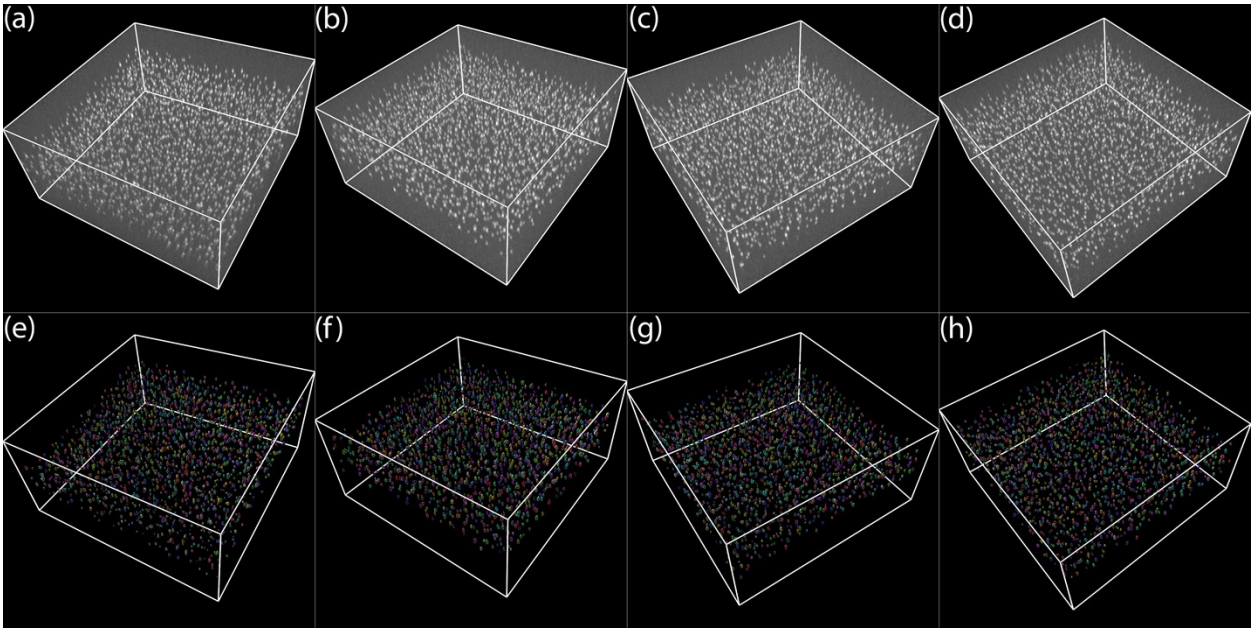

Figure SI28. (top row) examples of tomograms of sample NP2 at 40 mg/ml and (bottom row) the identification of particles from their tomograms.

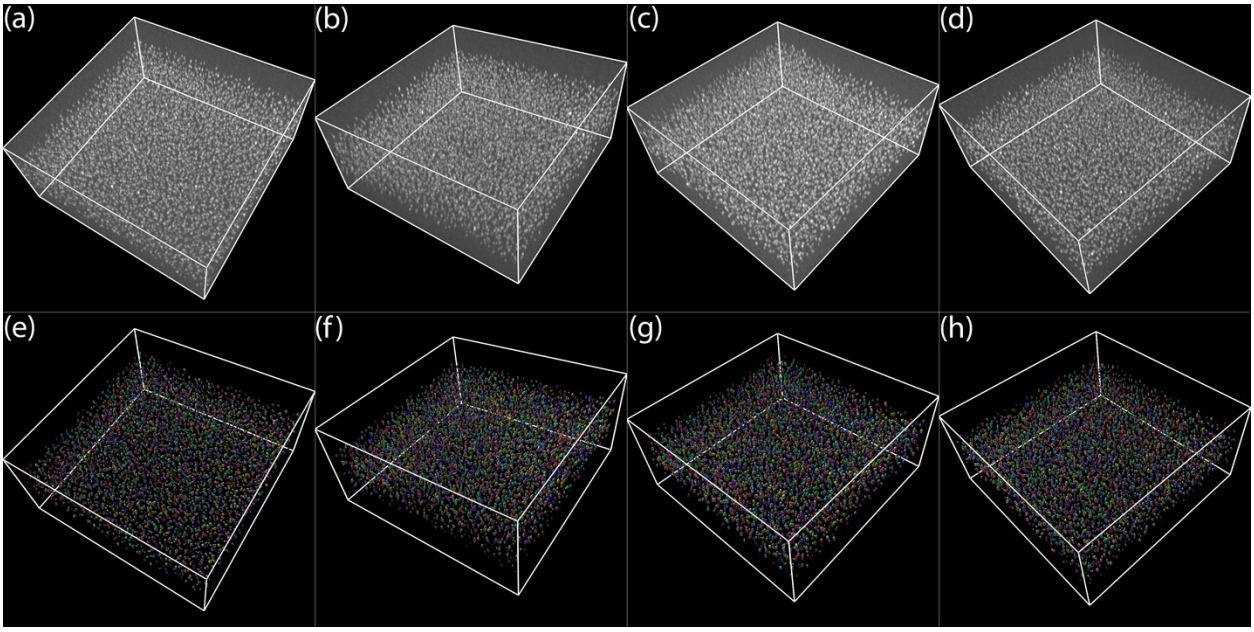

Figure SI29. (top row) examples of tomograms of sample NP2 at 80 mg/ml and (bottom row) the identification of particles from their tomograms.

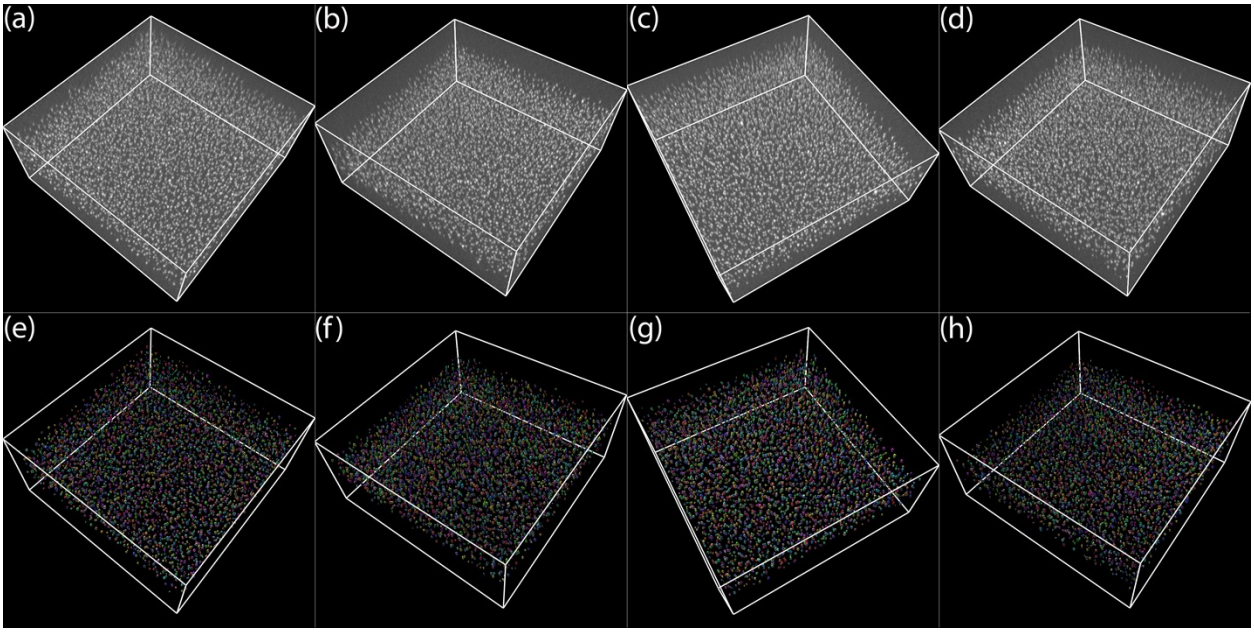

Figure SI30. (top row) examples of tomograms of sample NP2 at 80 mg/ml and (bottom row) the identification of particles from their tomograms.

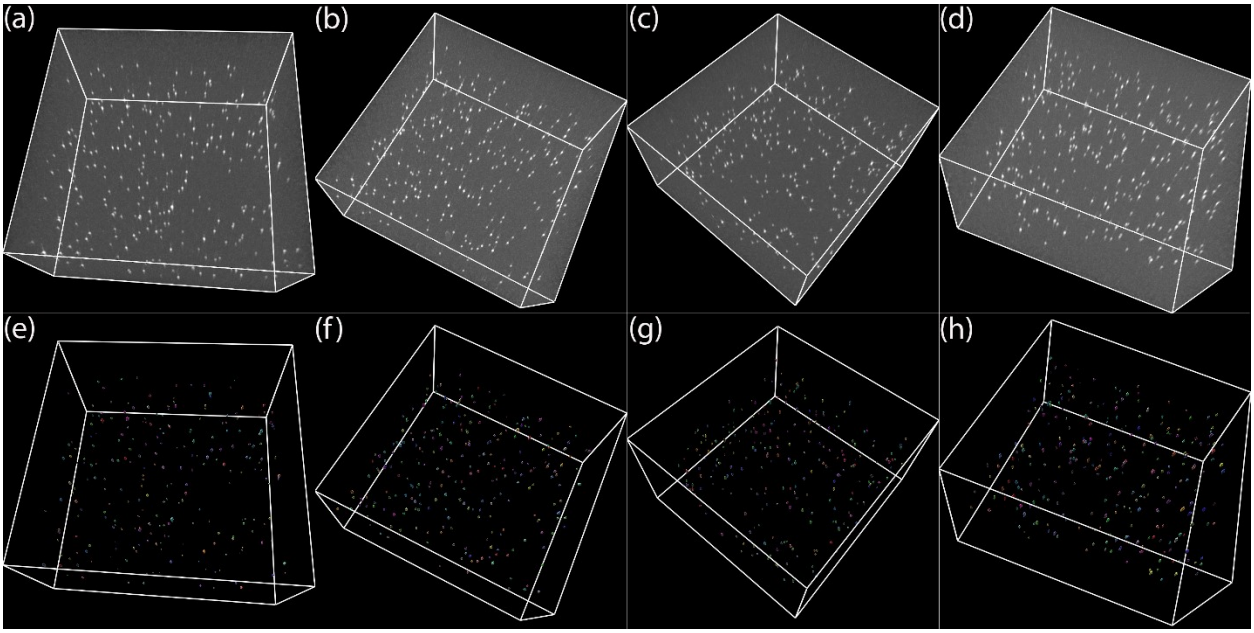

Figure SI31. (top row) examples of tomograms of sample NP2 at 10 mg/ml in NaCl 30mM and (bottom row) the identification of particles from their tomograms.

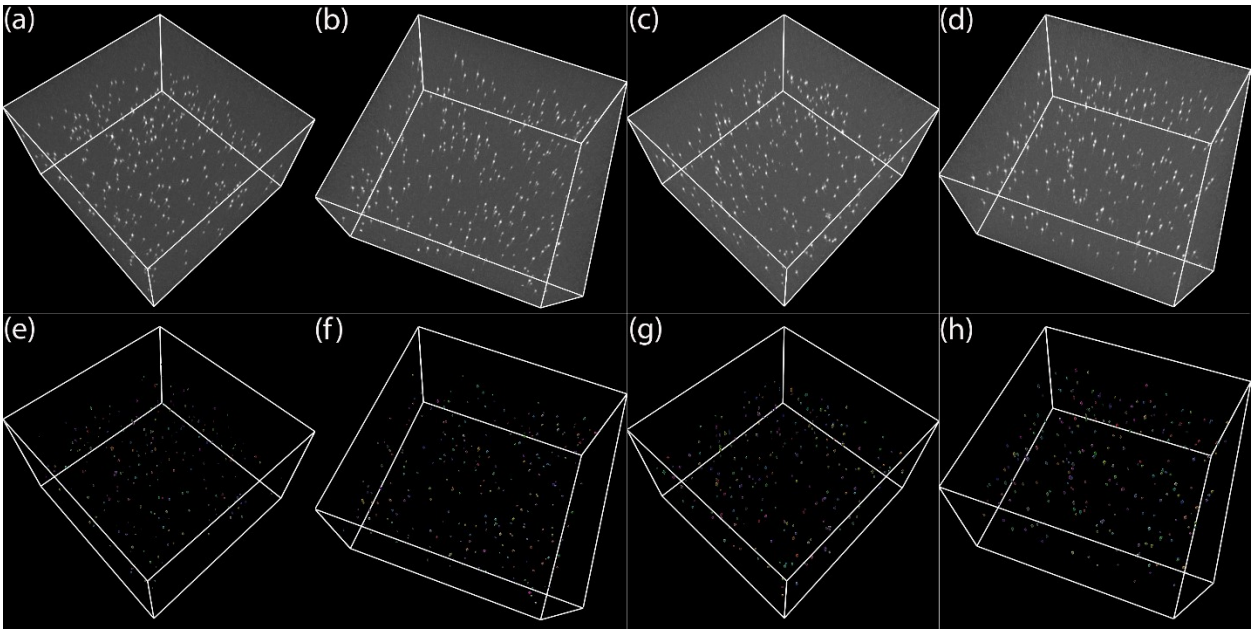

Figure SI32. (top row) examples of tomograms of sample NP2 at 10 mg/ml in NaCl 30mM and (bottom row) the identification of particles from their tomograms.

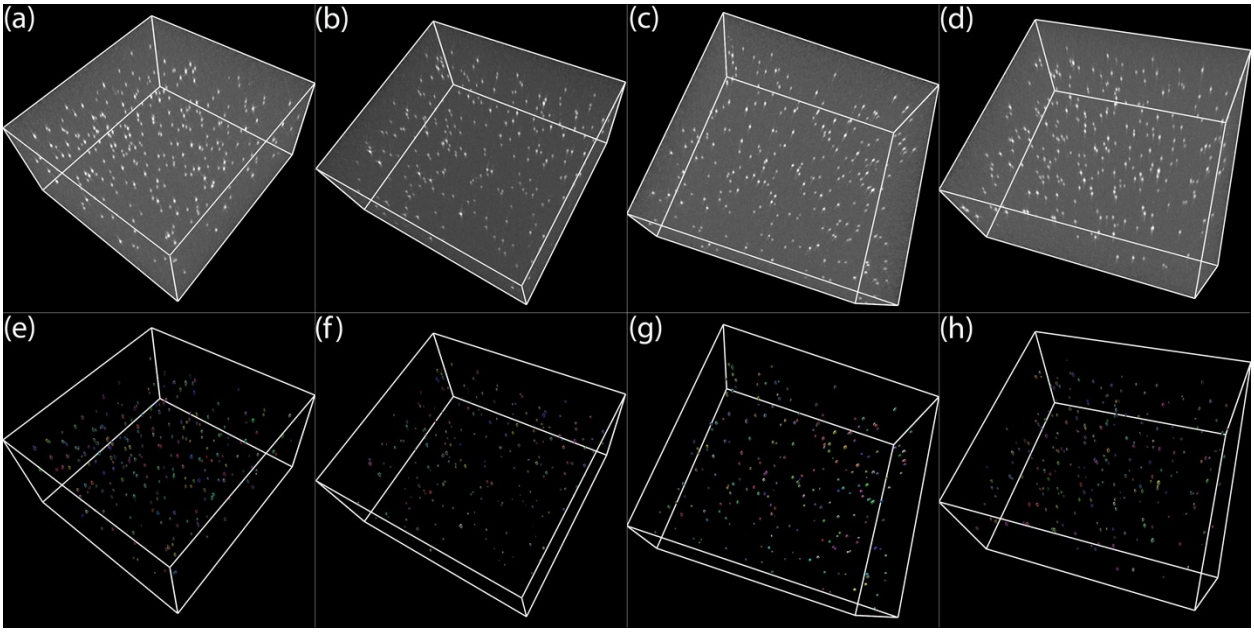

Figure SI33. (top row) examples of tomograms of sample NP2 at 10 mg/ml in NaCl 30mM and (bottom row) the identification of particles from their tomograms.

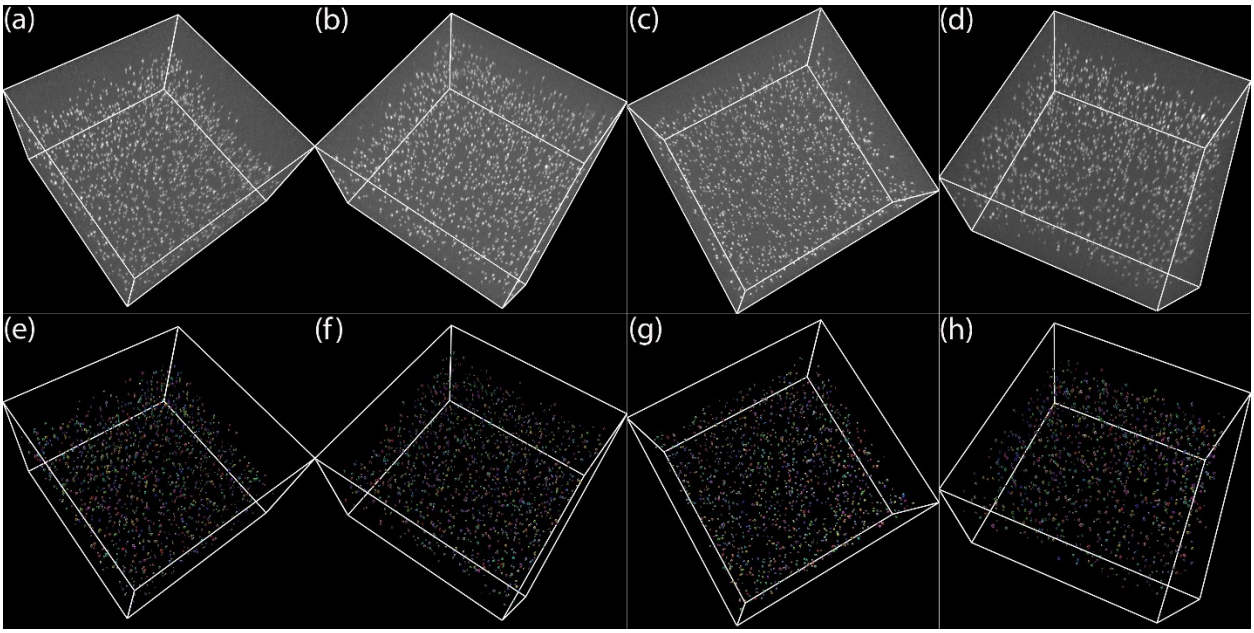

Figure SI34. (top row) examples of tomograms of sample NP2 at 20 mg/ml in NaCl 30mM and (bottom row) the identification of particles from their tomograms.

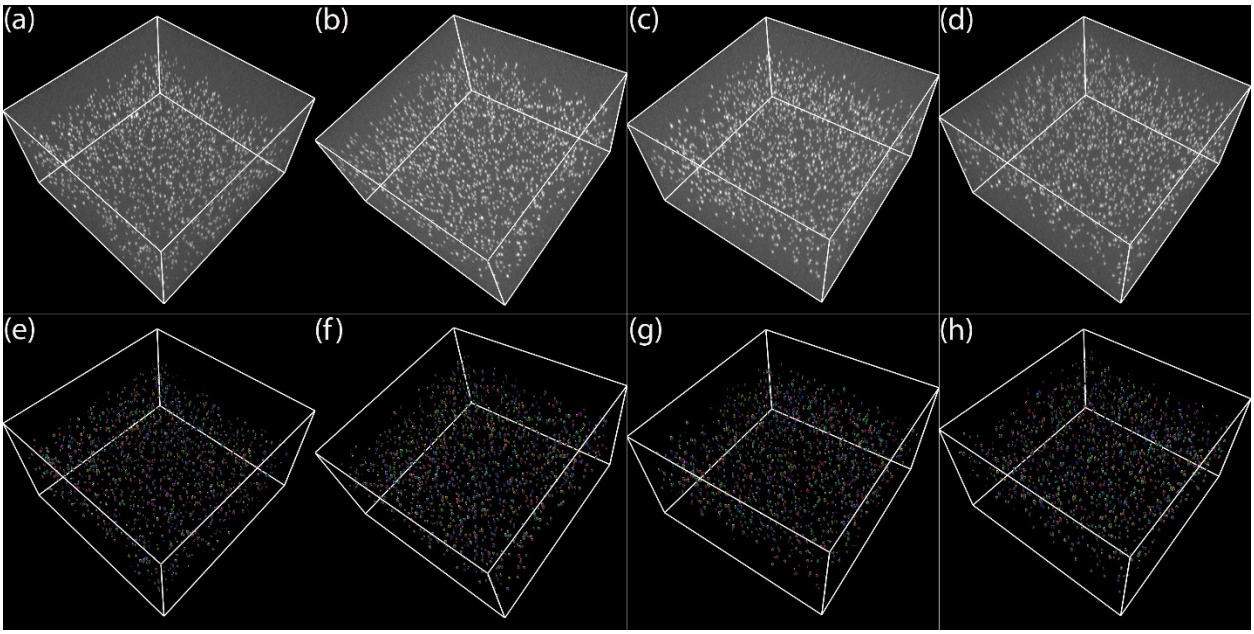

Figure SI35. (top row) examples of tomograms of sample NP2 at 20 mg/ml in NaCl 30mM and (bottom row) the identification of particles from their tomograms.

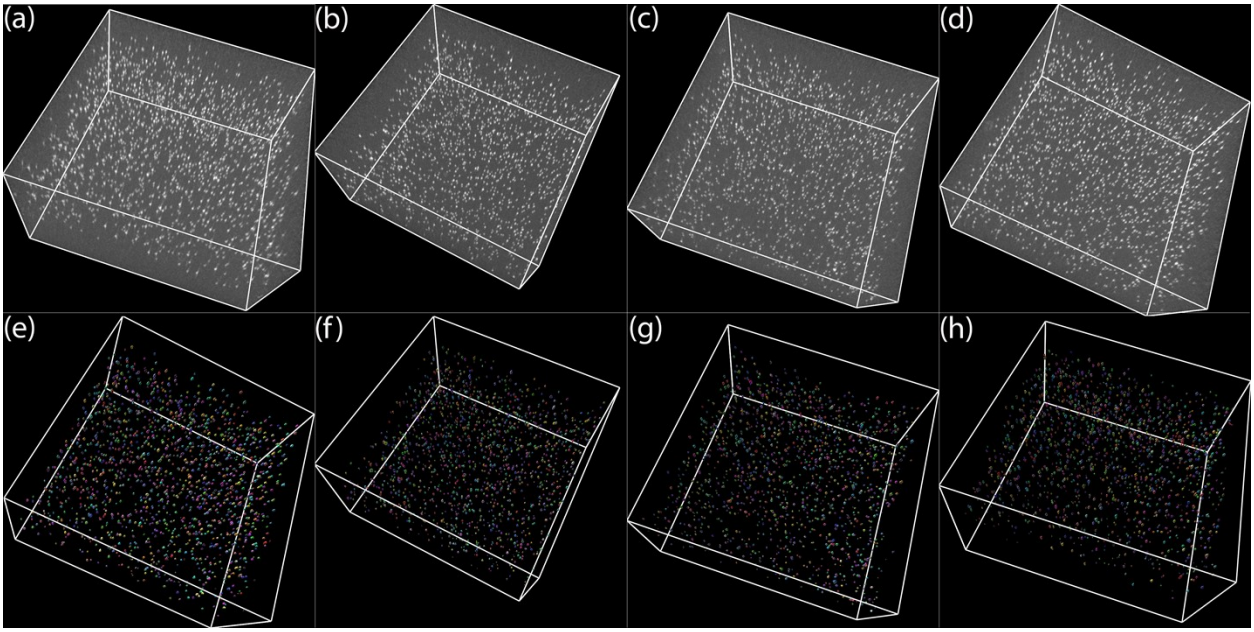

Figure SI36. (top row) examples of tomograms of sample NP2 at 20 mg/ml in NaCl 30mM and (bottom row) the identification of particles from their tomograms.

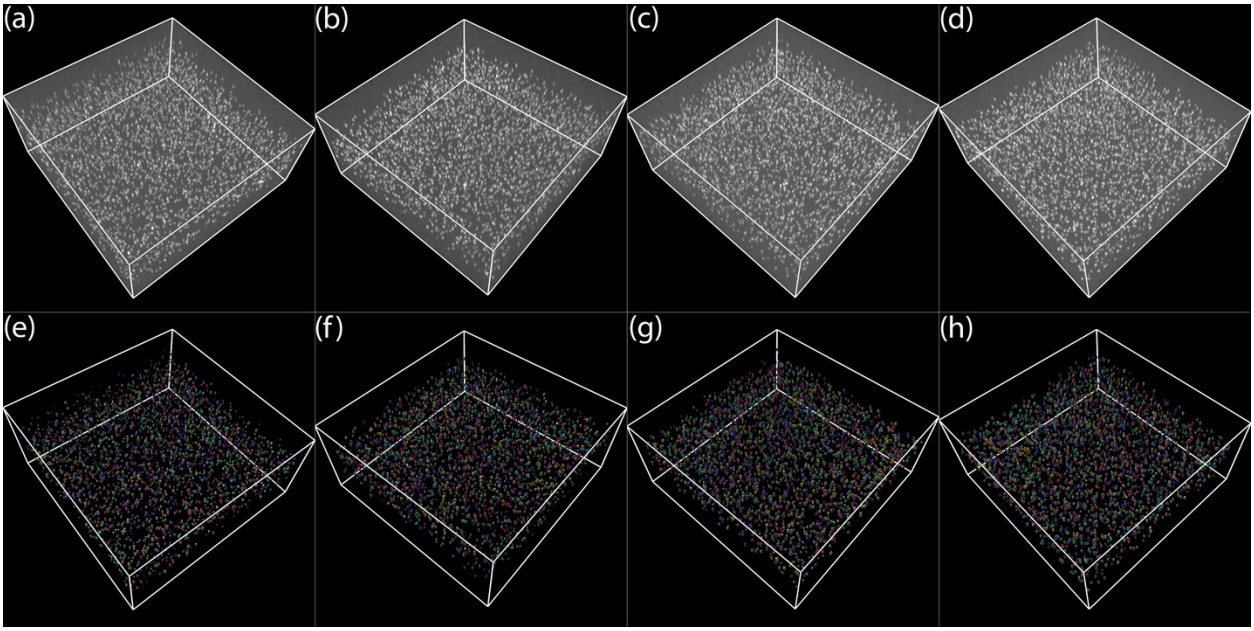

Figure SI37. (top row) examples of tomograms of sample NP2 at 40 mg/ml in NaCl 30mM and (bottom row) the identification of particles from their tomograms.

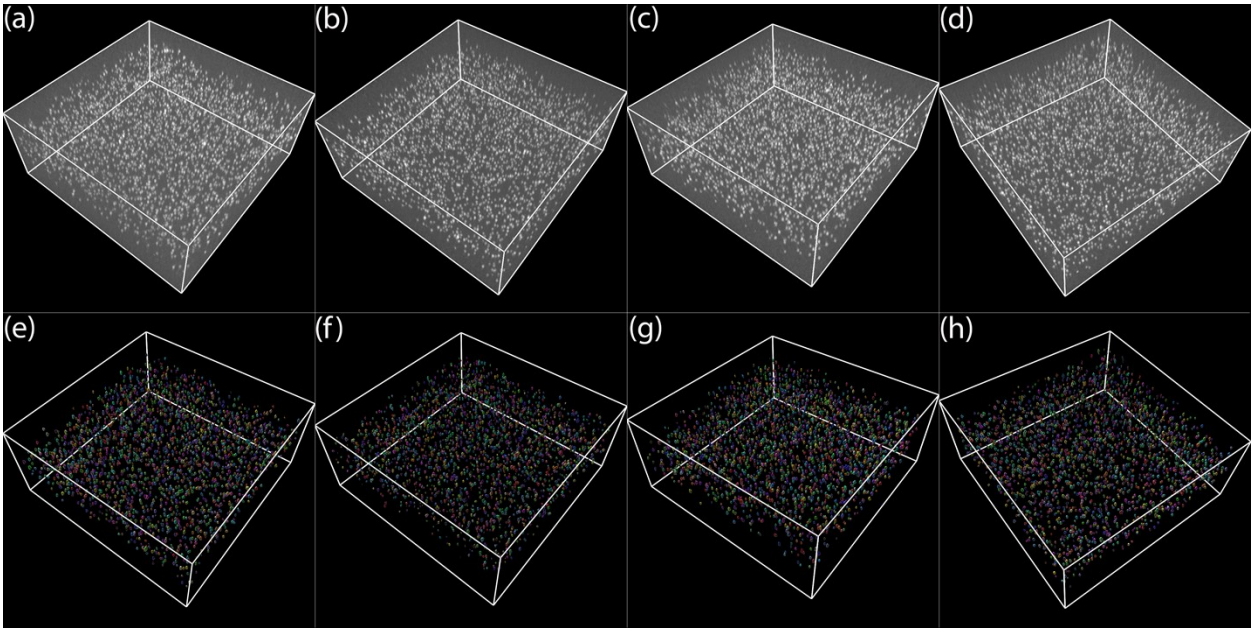

Figure SI38. (top row) examples of tomograms of sample NP2 at 40 mg/ml in NaCl 30mM and (bottom row) the identification of particles from their tomograms.

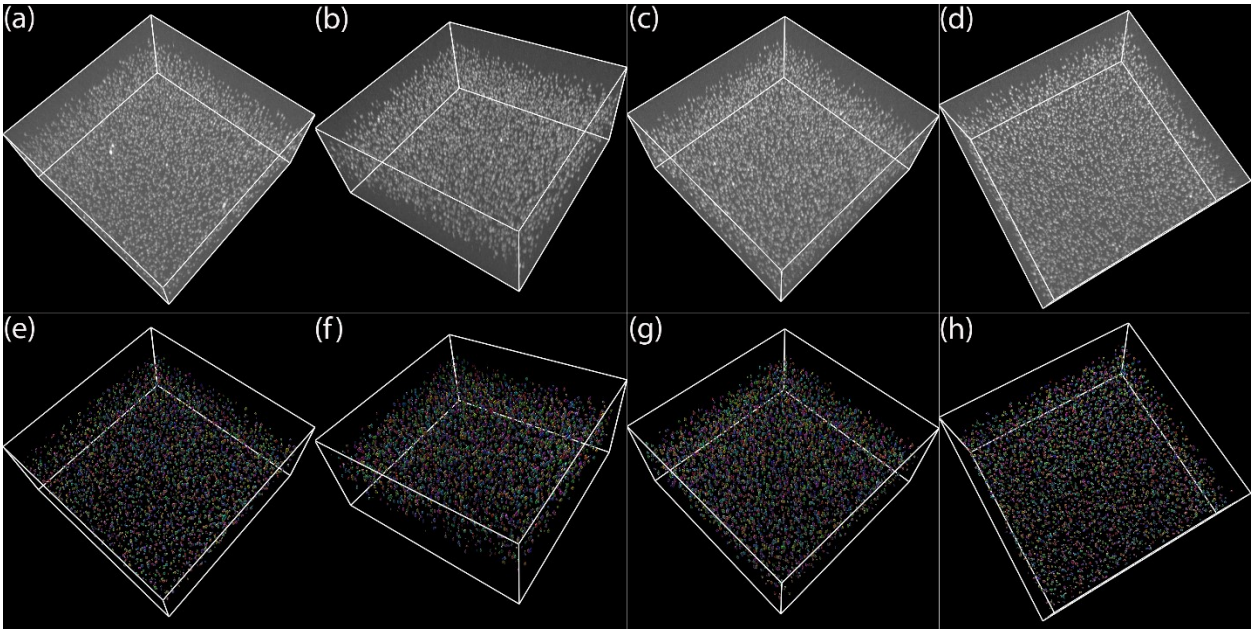

Figure SI39. (top row) examples of tomograms of sample NP2 at 80 mg/ml in NaCl 30mM and (bottom row) the identification of particles from their tomograms.

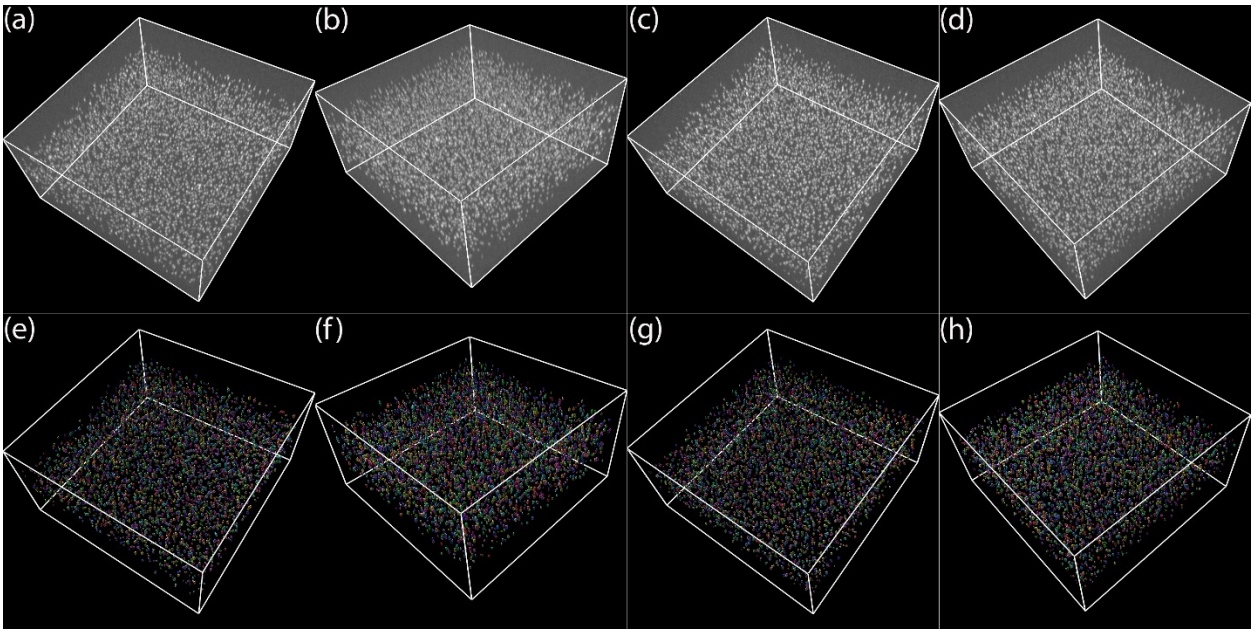

Figure SI40. (top row) examples of tomograms of sample NP2 at 80 mg/ml in NaCl 30mM and (bottom row) the identification of particles from their tomograms.

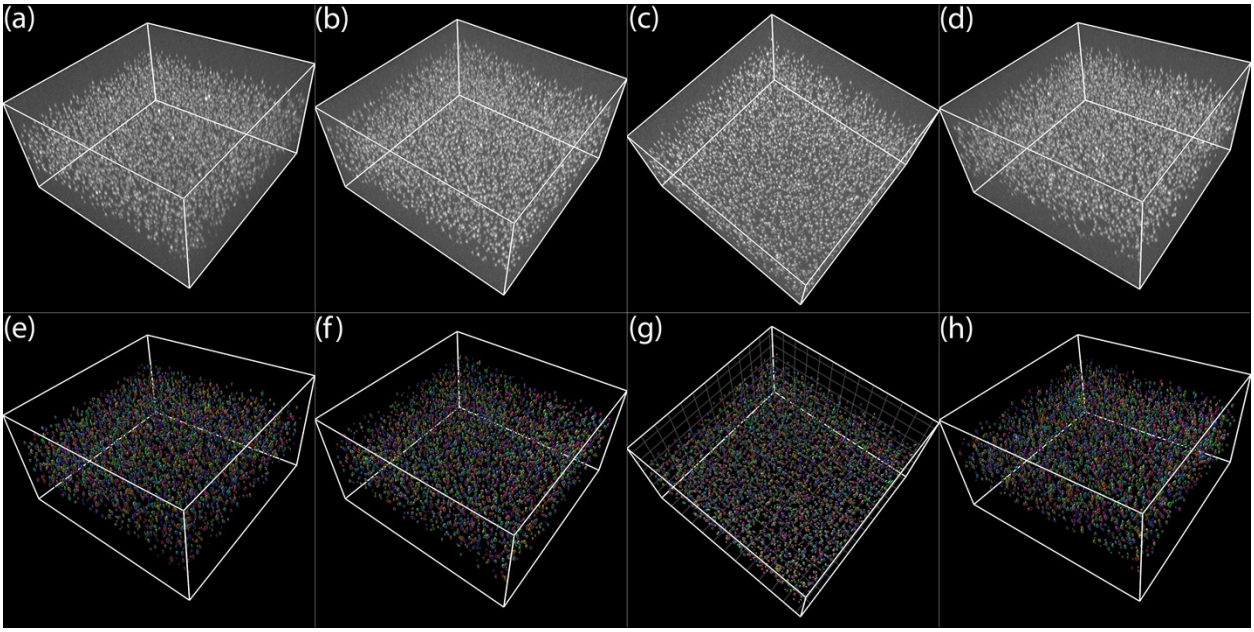

Figure SI41. (top row) examples of tomograms of sample NP2 at 80 mg/ml in NaCl 30mM and (bottom row) the identification of particles from their tomograms.

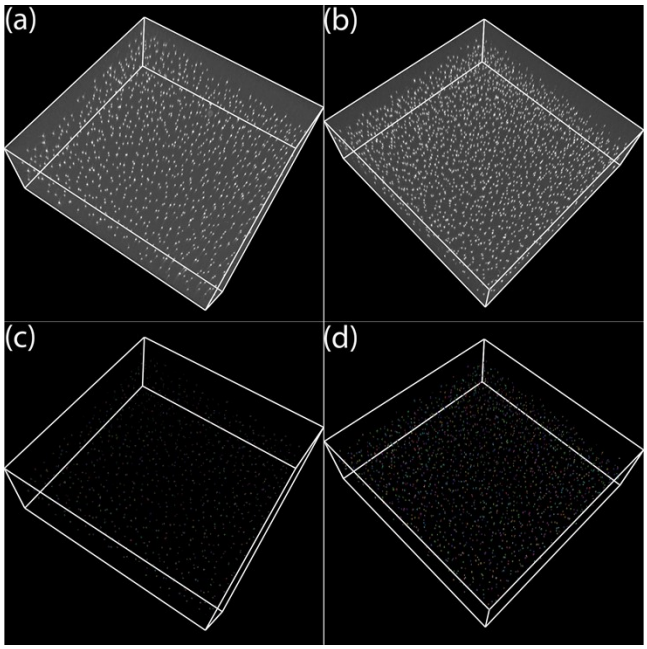

Figure SI42. (top row) examples of tomograms of sample NP1 at 10 mg/ml in water and (bottom row) the identification of particles from their tomograms.

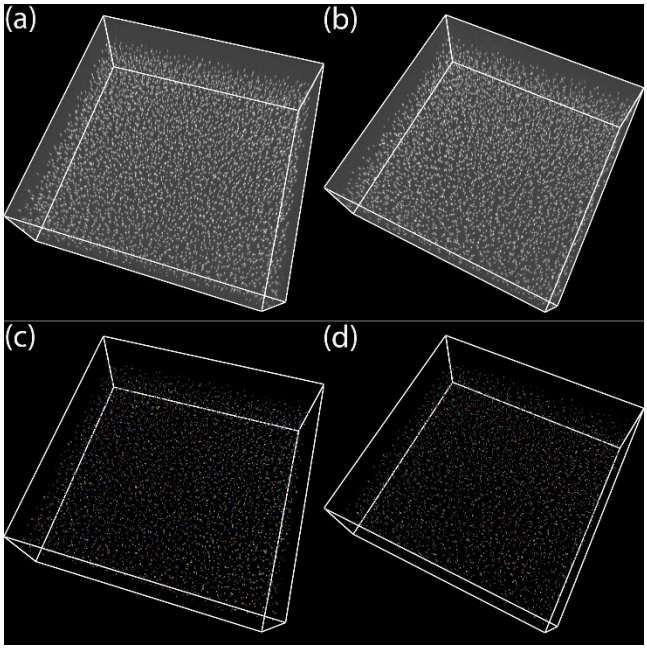

Figure SI43. (top row) examples of tomograms of sample NP1 at 20 mg/ml in water and (bottom row) the identification of particles from their tomograms.

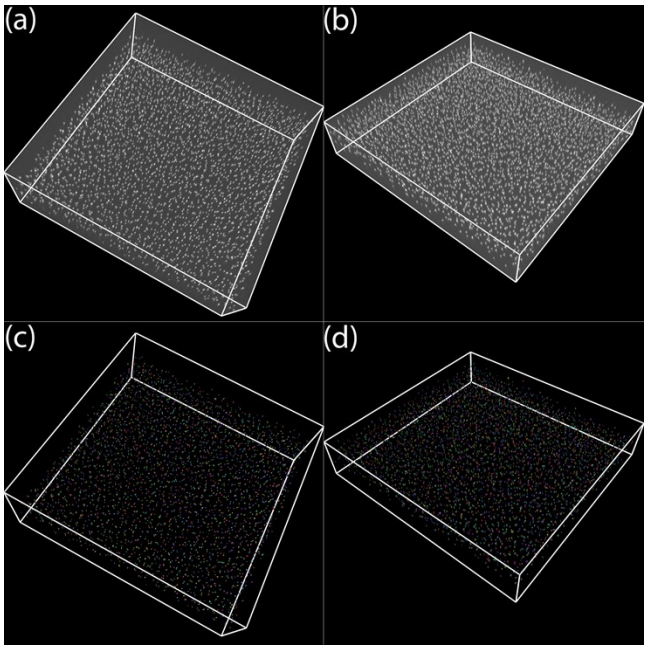

Figure SI44. (top row) examples of tomograms of sample NP1 at 40 mg/ml in water and (bottom row) the identification of particles from their tomograms.

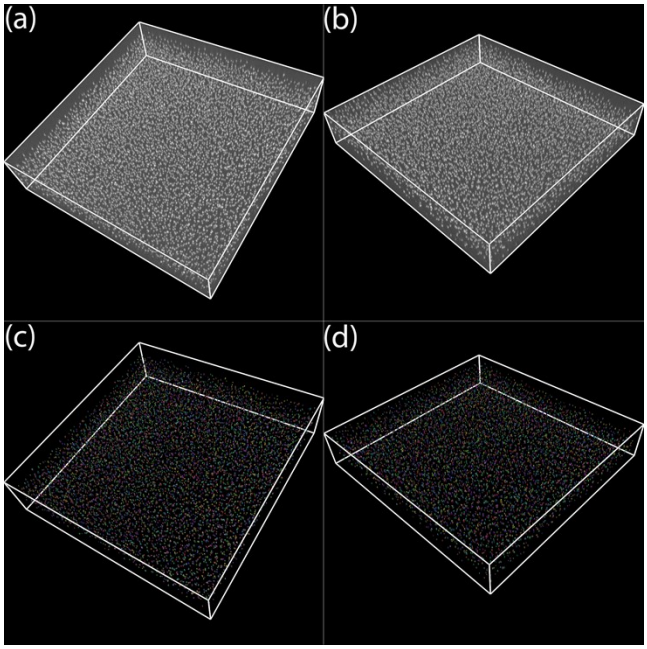

Figure SI45. (top row) examples of tomograms of sample NP1 at 80 mg/ml in water and (bottom row) the identification of particles from their tomograms.

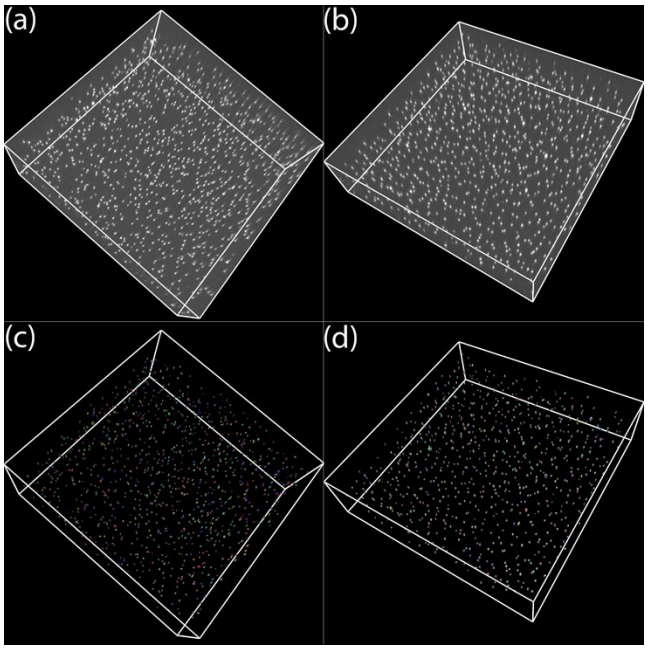

Figure SI46. (a and b) examples of tomograms of sample NP4 and NP5 in water in water, respectively and (bottom row) the identification of particles from their tomograms.

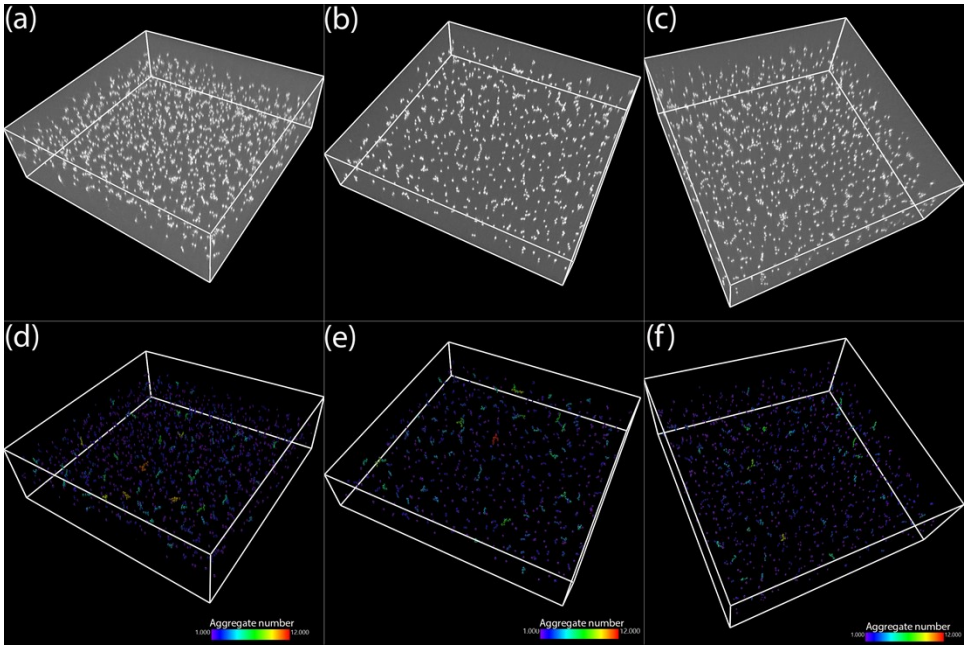

Figure SI47. (top row) examples of tomograms of sample NP3 at 20 mg/ml in water and (bottom row) the identification of particles from their tomograms. The particles are assigned a color based on their aggregate numbers.

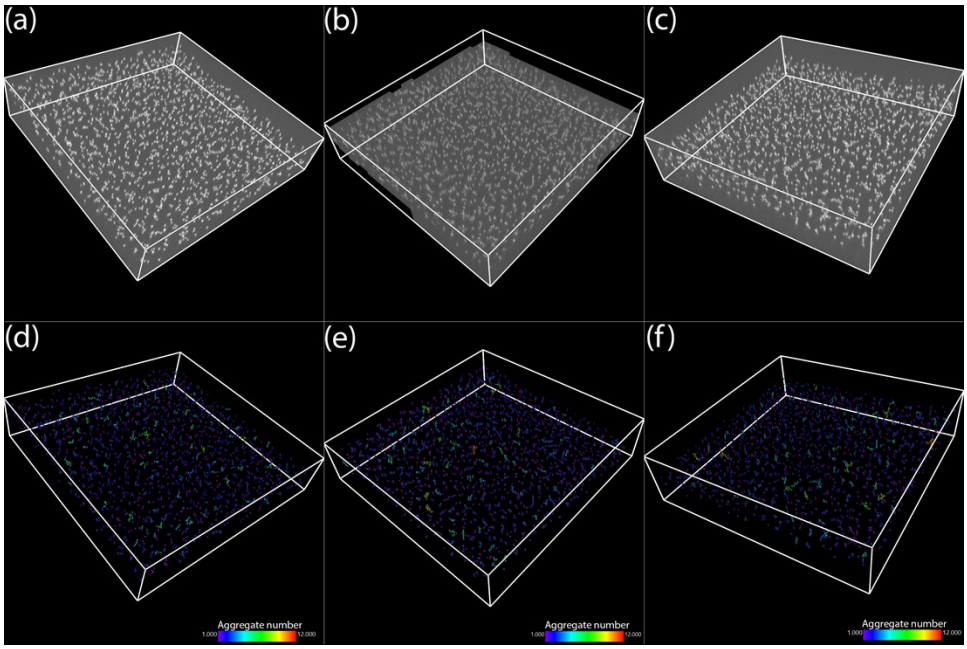

Figure SI48. (top row) examples of tomograms of sample NP3 at 40 mg/ml in water and (bottom row) the identification of particles from their tomograms. The particles are assigned a color based on their aggregate numbers.

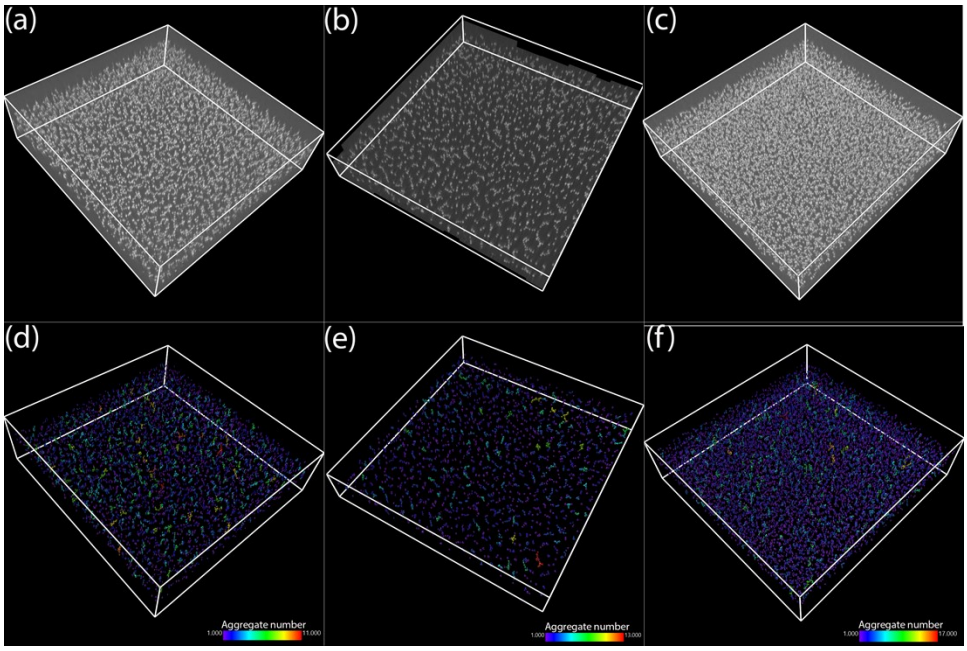

Figure SI49. (top row) examples of tomograms of sample NP3 at 80 mg/ml in water and (bottom row) the identification of particles from their tomograms. The particles are assigned a color based on their aggregate numbers.