Supporting Information

Formation of nanoparticles and nanocrystals of mercury by α-lactalbumin[#]

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SI 01. MD studies of α-LA with 10 equiv of Hg^{2+}

The MD simulation of 10 equiv. of Hg^{2+} ions with α-LA resulted in binding of three Hg^{2+} ions to the surface of α-LA (Fig. S7). The Hg1 shows nine coordination geometry extended by both the carboxylate oxygens of Asp 82 and 87, amide oxygens of Lys79 and Asp 84, one of the carboxylate oxygens of Asp 84 and 88 and a water molecule. The binding site analysis reveals that the Hg1 takes the position of the native calcium site with few modifications. These modifications includes that the carboxylates of Asp 82 and 87 turned bidentate, additional binding takes place in case of Asp 84 through the carboxylate group, and removal of one of the water molecules from the metal ion coordination sphere. The Hg2 binds through the bidentate carboxylate of Asp 83 and a water molecule. The Hg3 binds to the initial α-helix region (residues 5 to 11) of core structural stabilizing unit of α-LA through monodentate carboxylates of Glu7 and Glu11.[a] Thus the observed binding pattern suggests that the mercury preferably binds to the side chain carboxylates and the binding pattern of Hg1 and Hg2 are similar to that observed in the primary and seconary calcium binding sites of the human holo α-LA.[b]

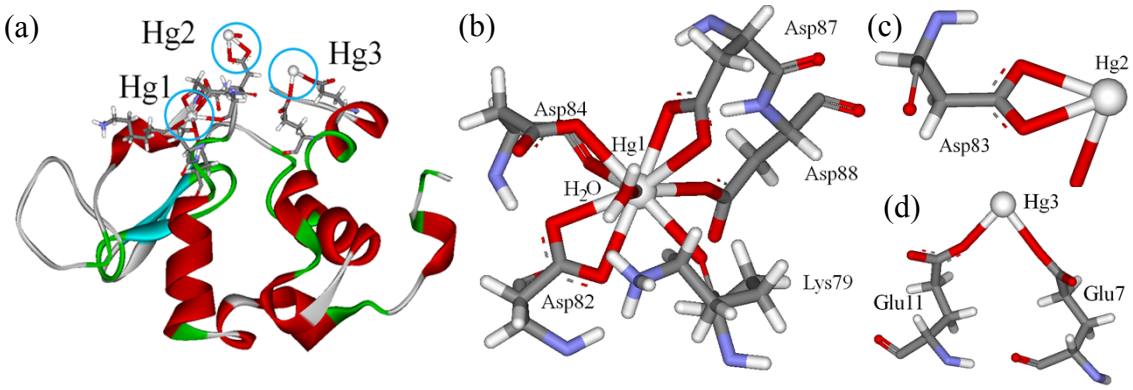

Fig.S7 (a) Snap shot taken after 25 ns simulation of MD simulations of 10 equiv. of Hg^{2+} model shows the interaction of three mecury ions with α-LA. The binding cores for Hg1, Hg2 and Hg3 are shown under (b), (c) and (d) respectively.

(a) E. D. Chrysina, K. Brew and K. R. Acharya, *J. Biol. Chem.* 2000, **47**, 37021–37029.

(b) N. Chandra, K. Brew and K. R. Acharya, *Biochemistry*, 1998, **37**, 4767–4772.

SI 01. TEM images of α-LA + 100 equiv Hg^{2+}

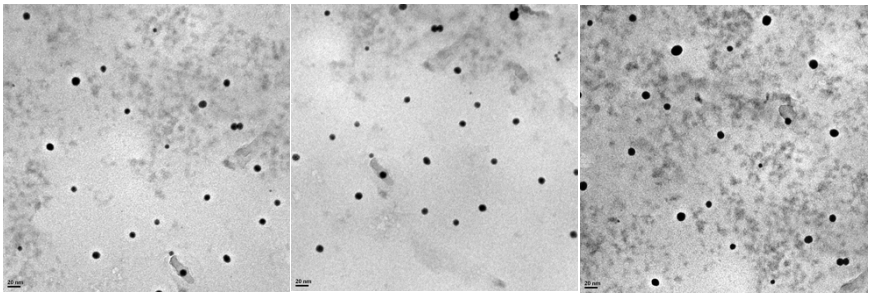

Fig. S1 TEM images of α-LA + 100 equiv Hg^{2+}

SI 02. TEM images of α-LA + Hg^{2+}after dialysis

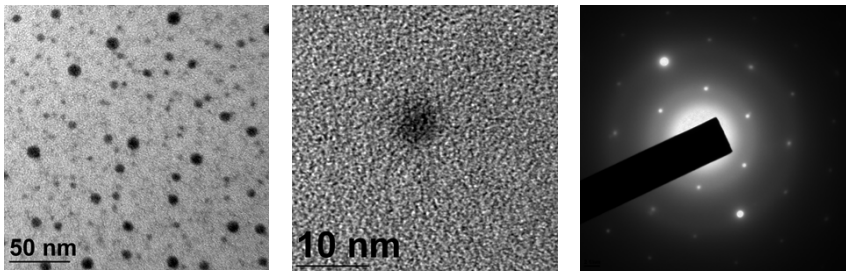

Fig. S2 TEM images of α-LA + 100 equiv Hg^{2+} after dialysis.

SI 03. TEM images of mercury perchlorate (II)

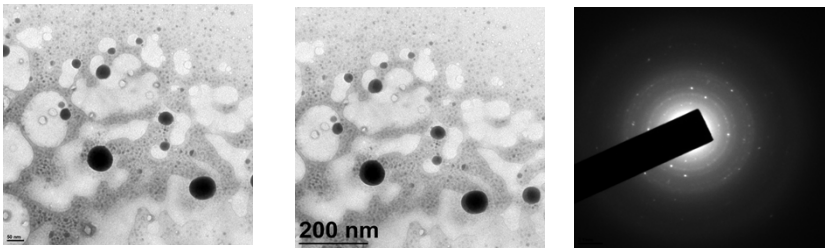

Fig. S3 TEM images of mercury (II) perchlorate.

SI 04. ANS binding studies of α-LA and {α-LA + Hg^{2+}}

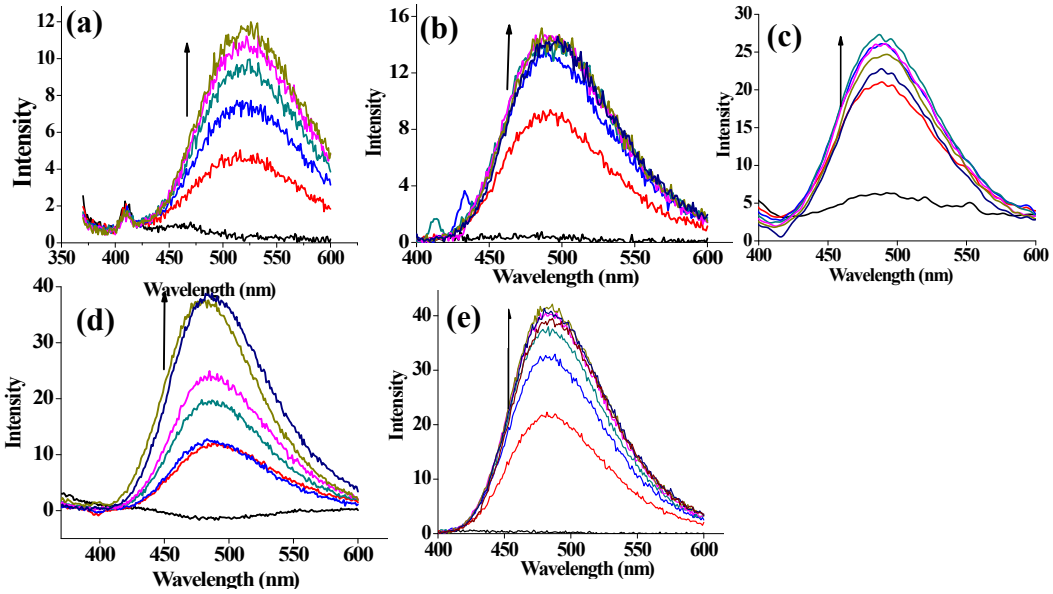

Fig. S4 ANS binding studies (2-10 µl of 2 mM ANS solution was added serially to a total volume of 1 ml cuvette) of α-LA + 'x' equiv Hg^{2+}: (a) x = 0, (b) x =1, (c) x = 5, (d) x = 10, (e) x = 100.

SI 05. XPS of α-LA with mercury

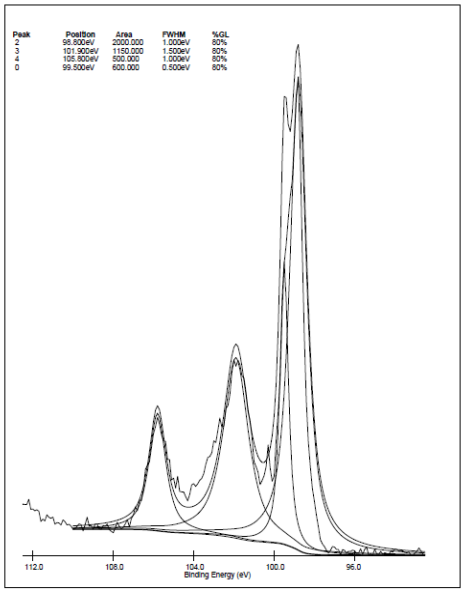

Fig. S6 XPS spectra of α-LA with 100 equiv. Hg^{2+}.