Electronic Supplementary Material (ESI) for Soft Matter

Cite this: DOI: 10.1039/c0xx00000x

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ARTICLE TYPE

Surporting materials:

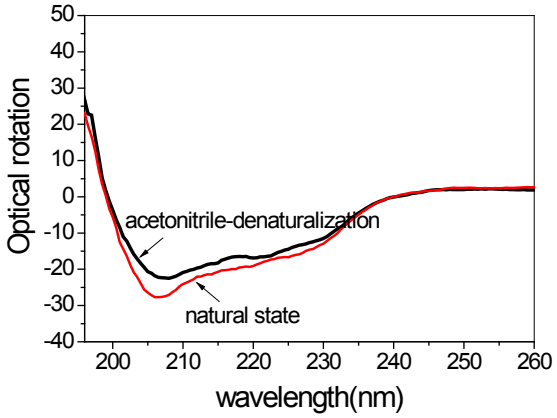

Fig.S1 Determination of secondary structure by circular dichroism specta. The spectum of acetonitrile denatruaed lysozyme shows a considerable amount of secondary structure remained. Protein concerntration= 0.5mg/ml, acetonitrile solution= 80% (V/V)

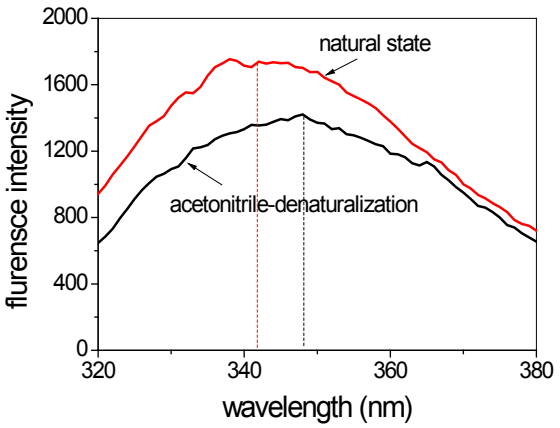

Fig.S2 Determination of tertiary structure by fluorescence spectra. The shift of fluorescence maximum shows a blue shift of fluorescence emission maximum from natural state to acetonitrile denatruaed state. It indicates that tryptophan residues of lysozyme denatruaed by acetonitrile are in a more exposed environment of nonpolar solvent and lost some tertiary structure. Protein concerntration= 0.3mg/ml, acetonitrile solution= 80% (V/V), at 280 nm.

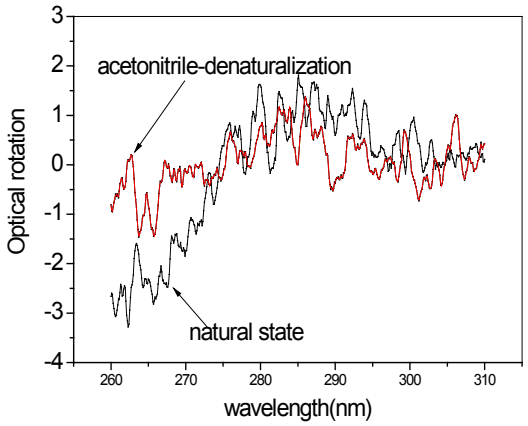

Fig.S3 Determination of tertiary structure by fluorescence spectra circular dichroism specta. The spectum of acetonitrile denatruaed lysozyme shows a considerable loss of ordered tertiary structure. Protein concerntration= 2mg/ml, acetonitrile solution= 80% (V/V).

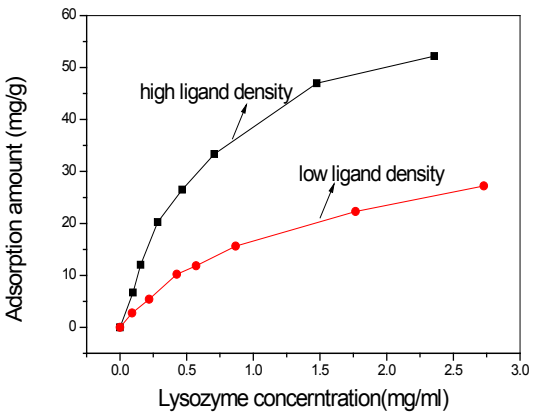

Fig.S4 Adsorption isotherm of lysozyme on two phenyl-Sepharose 6FF media. High ligand density = 80 pmol phenyl/cm^2 medium, and low ligand density = 50 pmol phenyl/cm^2 medium.

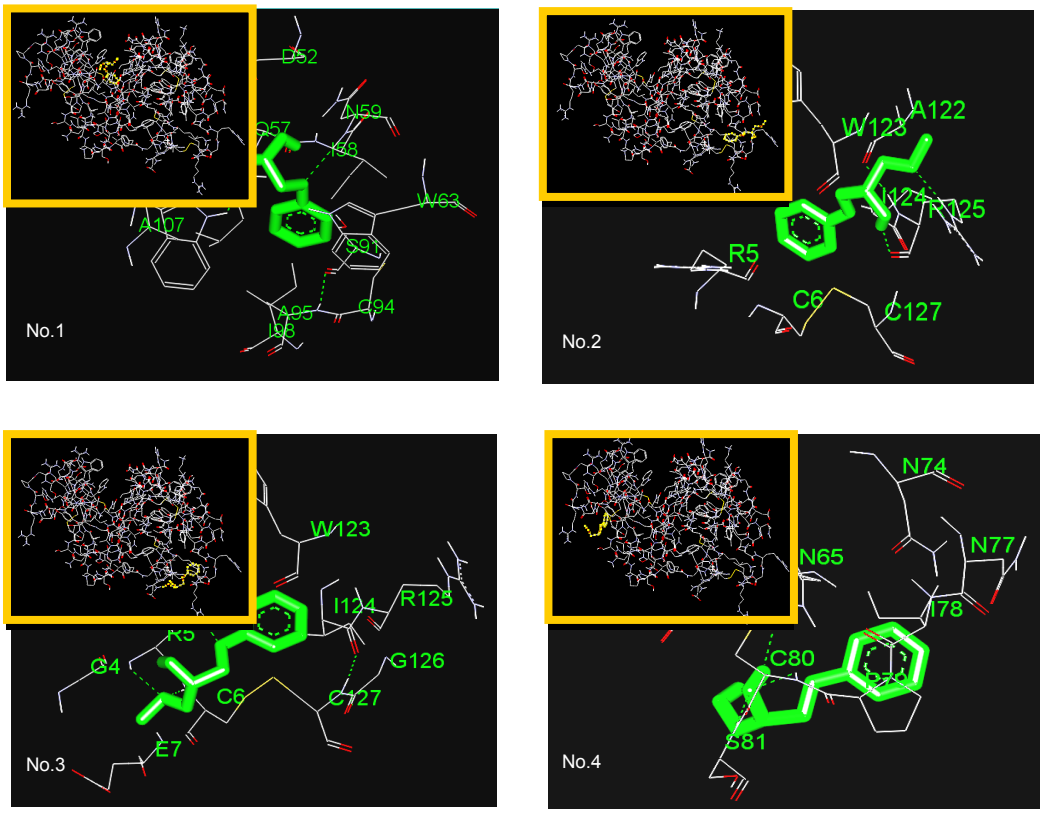

Fig.S5 The top 4 lysozyme-ligand complexes with the minimum binding energy. The left upper figure plots the ligand distribution on lysozyme. According to the reported selection criterion that hydrophobic patches located at convex zones are more accessible to the hydrophobic ligand[1], the conformation of complex ranked at No.1 is discarded due to its location at concave zone of active cleft.

[1] A. Mahn, G. Zapata-Torres, J.A. Asenjo, a theory of protein-resin interaction in hydrophobic interaction chromatography, Journal of Chromatography A, 1066, 2005, 81-88