Supplementary Materials for

Unraveling the fibrillation mechanism of ovalbumin in the presence of mercury at its isoelectric pH

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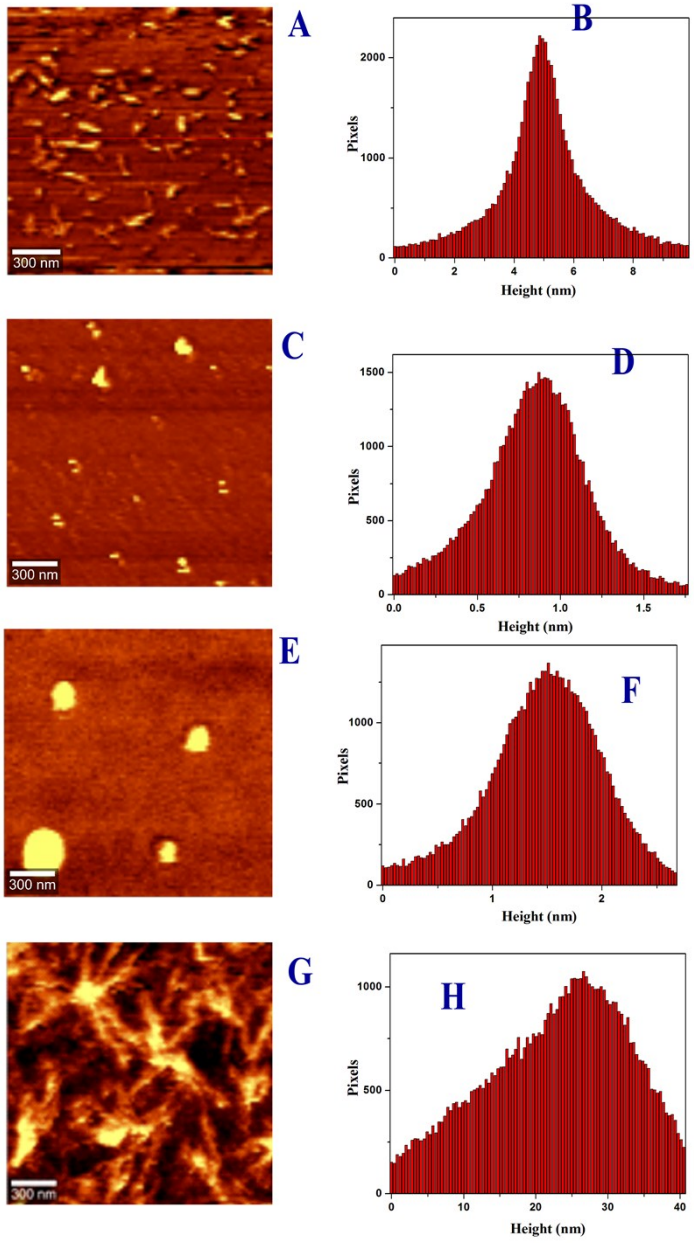

Figure S1. 2D Topographical features of OVA and OVA-$HgCl_2$ complex at pI; (A) AFM images of OVA (pH 4.5) prior to exposure of $HgCl_2$, showing WL fibrils and the corresponding (B) height; (C) formation of 'hillock' like oligomer after introducing the chemical stress (1.5 μM $HgCl_2$) and the corresponding (D) height; (E) Globule structure of oligomer with the increment

of $HgCl_2$ to 2.5 µM and the corresponding (F) height; (G) 'hydra' like oligomer with the increment of $HgCl_2$ to 6.25 µM and the corresponding (H) height

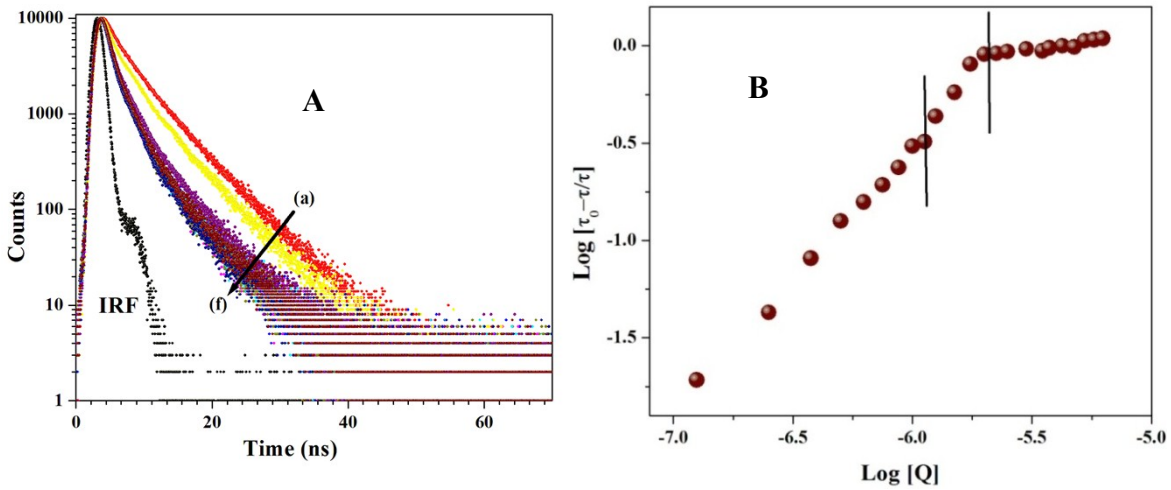

Figure S2. The time-resolved fluorescence decay plot of OVA– $HgCl_2$ systems at pI. Stern-Volmer plot using life time data

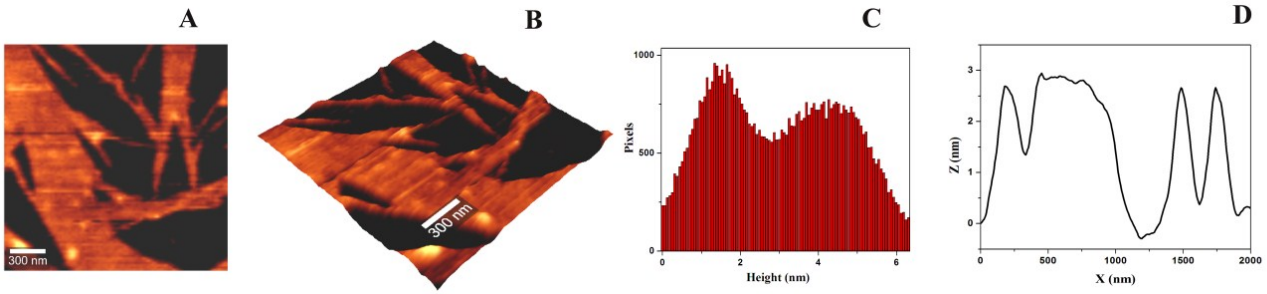

Figure S3. Topographical features of OVA-$HgCl_2$ complex after the incubation of 25 days at pI: (A): Appearance of long straight fibrils from Hydra like structure after the incubation and the corresponding (B): 3D representation (C): height (D): width profile.

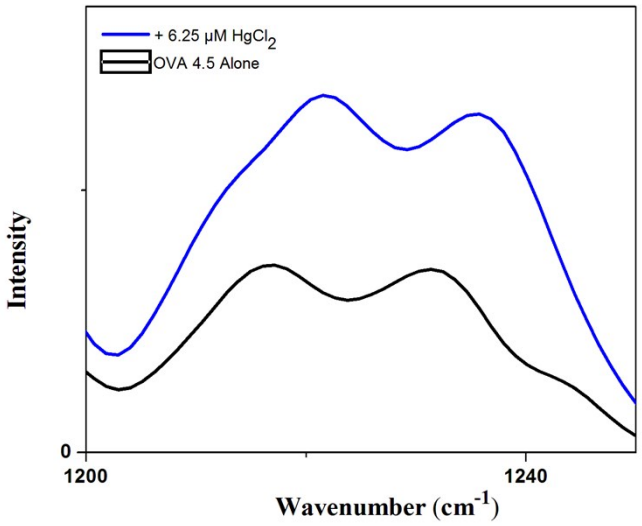

Figure S4. Increase in intensity of Amide III peak of OVA and OVA-HgCl2 at pI indicating the removal of water from protein

Table S1. Fluorescence decay time constant and amplitudes of OVA at pI in the absence and presence of $HgCl_2$.

OVA + $HgCl_2$ (pH 4.5)								
$HgCl_2$ (μM)	τ_1(ns)	τ_2 (ns)	τ_3 (ns)	α_1	α_2	α_3	τ_m(ns)	χ^2
0	2.60	0.48	5.89	35.52	10.85	53.63	4.13	1.1
0.25	2.3	0.43	5.75	34.82	11.49	53.69	4.05	1.19
0.5	2.29	0.45	5.69	36.91	14.57	48.53	3.96	1.18
0.75	2.2	0.43	5.69	39.26	16.25	44.49	3.67	1.15
1	2.17	0.43	5.76	42.6	19.94	37.46	3.34	1.14
1.25	1.97	0.38	5.61	44.34	21.4	34.26	3.16	1.15
1.5	1.98	0.43	5.58	47.04	24.65	28.32	3.13	1.15
1.75	1.72	0.33	5.50	51.6	24.35	24.06	2.88	1.16
2	1.72	0.35	5.56	52.45	26.34	21.21	2.17	1.09

2.5	1.74	0.35	5.67	52.06	27.97	19.97	2.14	1.12
3	1.66	0.29	5.44	50.71	27.58	21.72	2.11	1.21
3.5	1.78	0.36	5.63	50.62	29.46	19.92	2.13	1.18
3.75	1.72	0.35	5.58	50.62	29.35	20.03	2.09	1.15
4.75	1.73	0.35	5.49	49.54	30.05	20.41	2.08	1.14
5.25	1.64	0.28	5.38	50.74	28.91	20.35	2.01	1.13
5.75	1.71	0.31	5.59	50.49	30.99	18.52	1.99	1.15
6.25	1.75	0.35	5.62	49.39	32.84	17.77	1.98	1.15

Table S2. Secondary structural estimation of different elements obtained after deconvolution of the amide III (1200-1300 cm^{-1}) region of ovalbumin at pI alone and with the addition of $HgCl_2$.

	OVA 4.5	+ 1.5 µM $HgCl_2$	+ 2.5 µM $HgCl_2$	+ 6.25 µM $HgCl_2$
Unordered	34.59	35.32	42.01	52.75
β-sheet	51.57	47.35	31.06	40.57
α-helix	4.74	3.38	3.34	2.27
Coils/extended	9.07	13.93	23.56	4.39