Electronic Supplementary Material (ESI) for RSC Advances.

Identification of Modes of Interactions between 9-Aminoacridine Hydrochloride Hydrate and Serum Proteins by Low and High Resolution Spectroscopy and Molecular Modeling

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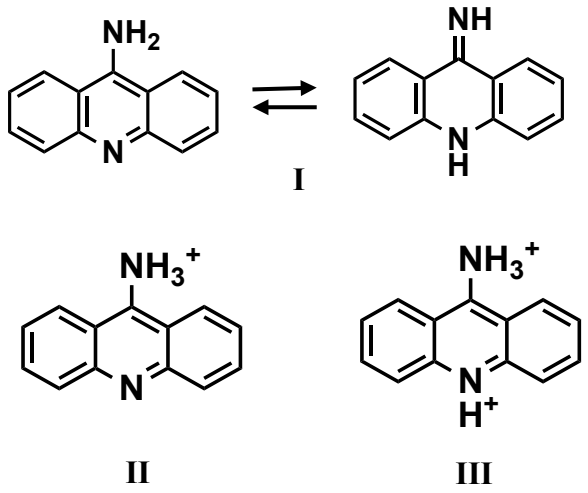

Figure S1: Different forms of 9-aminoacridine hydrochloride hydrate (9AA-HCl); (I) neutral 9AA-HCl (9AA), (II) protonated 9AA-HCl ($9AAH^+$) and (III) doubly protonated 9AA-HCl.

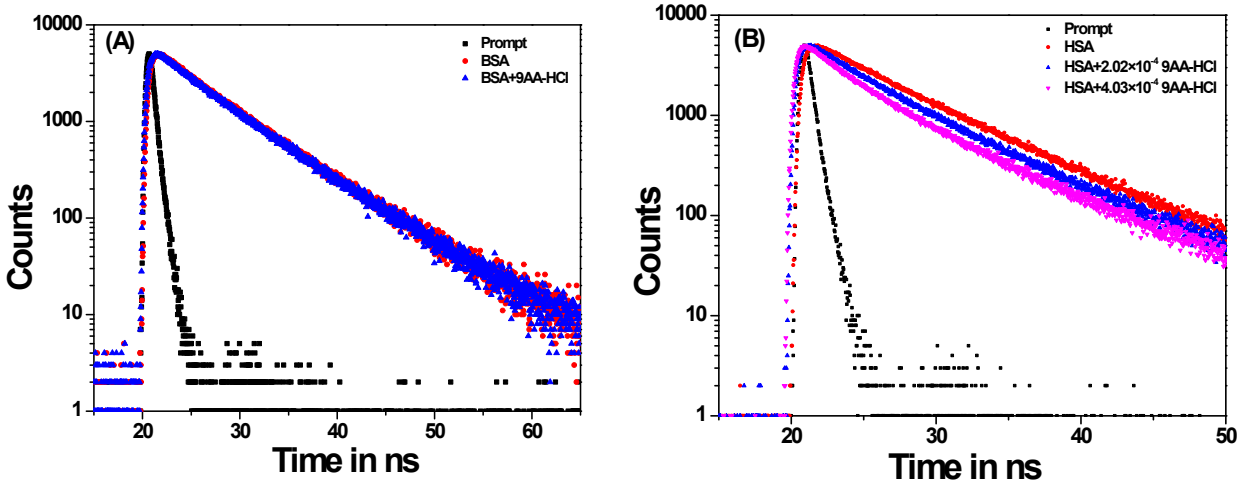

Figure S2: Time-resolved fluorescence intensity decays of (A) BSA and 9AA-HCl (B) HSA and 9AA-HCl in phosphate buffer (λ_{ex}=280 nm). The legends show the respective environments.

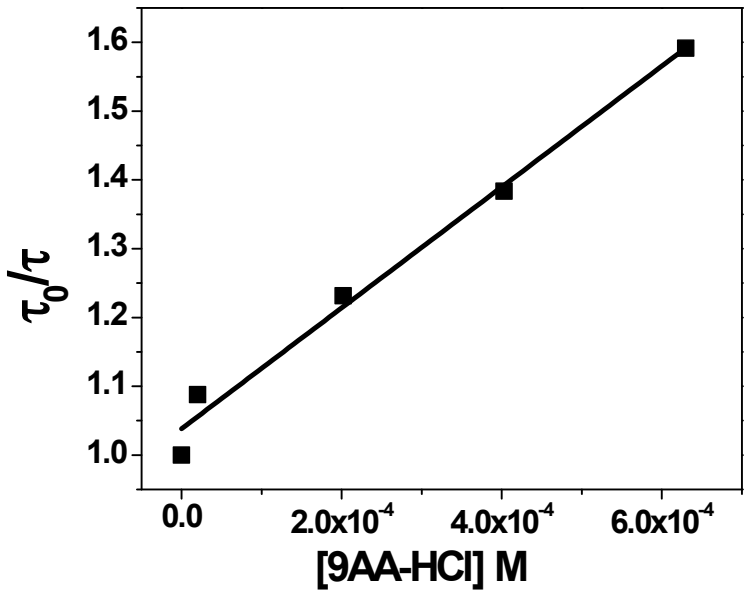

Figure S3: Time-resolved Stern-Volmer plot for quenching of HSA by 9AA-HCl where [HSA] = 1.5×10^{-5} M and [9AA-HCl] ranges from 0.0 to 6.30×10^{-4} M.

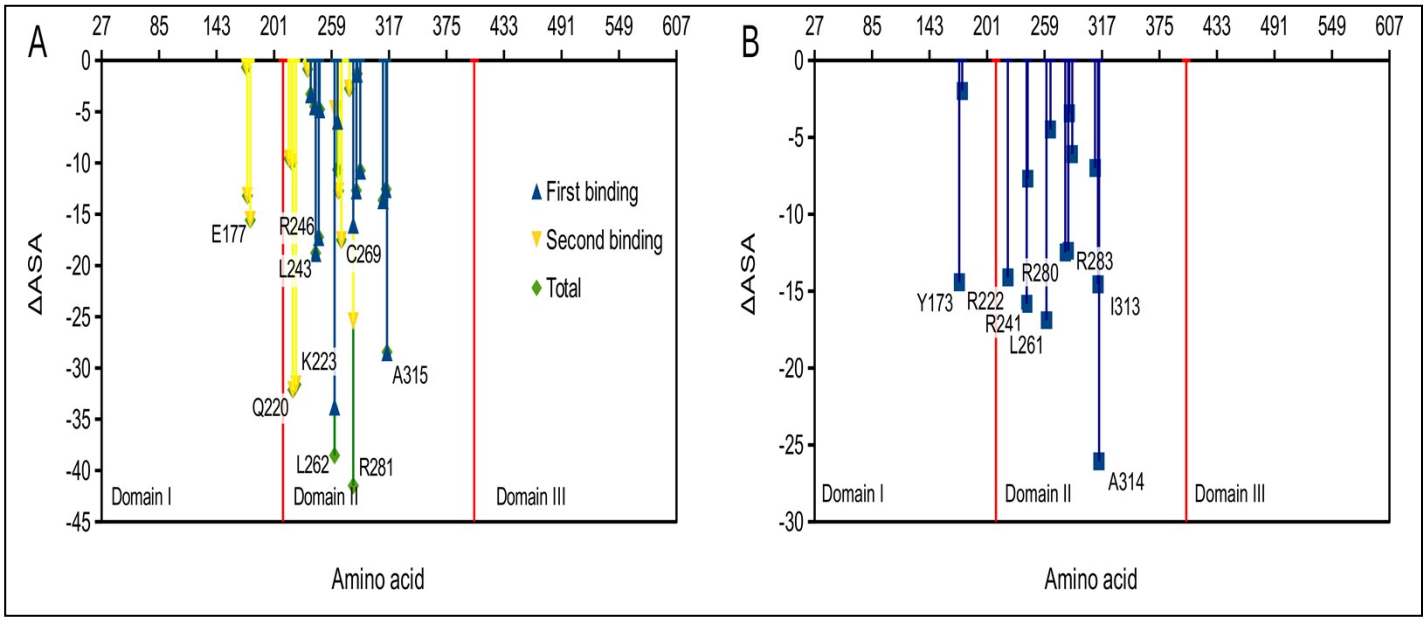

Figure S4. Per residue change in the accessible surface area plot for HSA (A) and BSA (B). Higher change indicates more involvement in ligand binding. Peaks are tagged with residue code and their position in peptide chain.

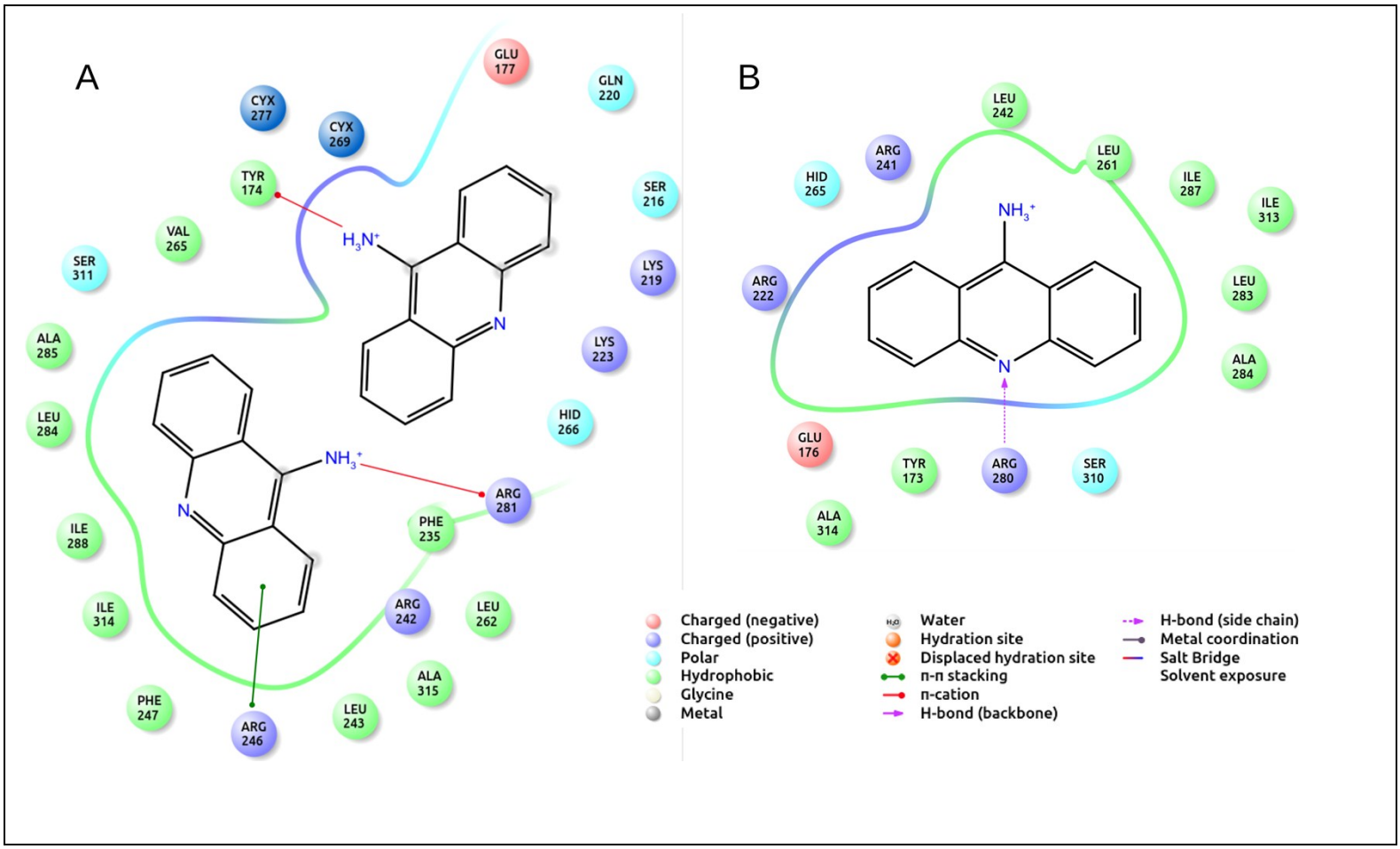

Figure S5: Detailed interaction diagram of 9AA-HCl with serum albumins. (A) Interactions of two 9AA-HCl molecules with the binding site residues of HSA. (B) Interactions of 9AA-HCl with the binding site residues of BSA.

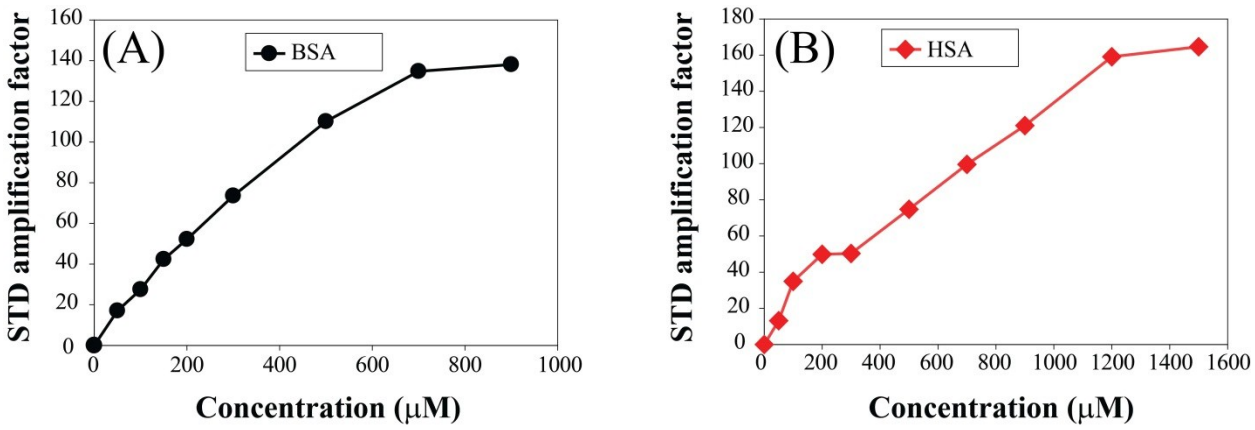

Figure S6. Plot displaying change in STD amplification factor vs concentration of 9AA-HCl used for (A) BSA and (B) HSA protein showing discrimination between binding affinities and modes for both proteins. Saturation time (t_{sat}) was kept at 2 sec.

Table S1. Properties of the binding site in domain II of serum albumins as analyzed by the POCASA program.

	Bindng site in BSA	Binding site in HSA	9AA-HCl
Volume ($Å^3$)	761	1267	338
Surface area ($Å^2$)	476	681	248
Sphericity, Ψ	0.85	0.83	0.95
Effective radius (Å)	4.79	5.58	4.09