Supplementary data for the article:

Zianna, A.; Ristović, M. Š.; Psomas, G.; Hatzidimitriou, A.; Coutouli-Argyropoulou, E.; Lalia-Kantouri, M. Cadmium(II) Complexes of 5-Bromo-Salicylaldehyde and α-Diimines: Synthesis, Structure and Interaction with Calf-Thymus DNA and Albumins. *Polyhedron* **2016**, *107*, 136–147. https://doi.org/10.1016/j.poly.2016.01.020

Cadmium(II) complexes of 5-bromo-salicylaldehyde and α-diimines: Synthesis, structure and interaction with calf-thymus DNA and albumins

Ariadni Zianna [a], Maja Šumar Ristović [a, b], George Psomas [a], Antonis Hatzidimitriou [a], Evdoxia Coutouli-Argyropoulou [c] and Maria Lalia-Kantouri [a *]

[a] *Department of General and Inorganic Chemistry, Faculty of Chemistry, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, GREECE*

[b] *Faculty of Chemistry, University of Belgrade, Studenski trg 12-16, Belgrade, SERBIA*

[c] *Department of Organic Chemistry and Biochemistry, Faculty of Chemistry, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, GREECE*

Supplementary information

S1. Interaction with CT DNA

The binding constant, K_b, can be obtained by monitoring the changes in the absorbance at the corresponding λ_{max} with increasing concentrations of CT DNA and it is given by the ratio of slope to the y intercept in plots $\frac{[DNA]}{(\varepsilon_A - \varepsilon_f)}$ versus [DNA], according to the Wolfe–Shimer equation: [1]

$$\frac{[DNA]}{(\varepsilon_A - \varepsilon_f)} = \frac{[DNA]}{(\varepsilon_b - \varepsilon_f)} + \frac{1}{K_b(\varepsilon_b - \varepsilon_f)} \qquad \text{(eq. S1)}$$

where [DNA] is the concentration of DNA in base pairs, $\varepsilon_A = A_{obsd}$/[compound], ε_f = the extinction coefficient for the free compound and ε_b = the extinction coefficient for the compound in the fully bound form.

S2. Competitive studies with EB

The Stern–Volmer constant K_{SV} is used to evaluate the quenching efficiency for each compound according to the Stern–Volmer equation:

$$\frac{Io}{I} = 1 + K_{SV}[Q] \qquad \text{(eq. S2)}$$

where Io and I are the emission intensities in the absence and the presence of the quencher, respectively, [Q] is the concentration of the quencher (i.e. complexes **1–5**); K_{SV} is obtained from the Stern–Volmer plots by the slope of the diagram $\frac{Io}{I}$ vs [Q].

[*] Corresponding author. Tel./fax: +30 2310 997844, E-mail address: lalia@chem.auth.gr

S3. Interaction with serum albumins

The extent of the inner–filter effect can be roughly estimated with the following formula:

$$I_{corr} = I_{meas} \times 10^{\frac{\varepsilon(\lambda_{exc})cd}{2}} \times 10^{\frac{\varepsilon(\lambda_{em})cd}{2}} \quad \text{(eq. S3)}$$

where I_{corr} = corrected intensity, I_{meas} = the measured intensity, c = the concentration of the quencher, d = the cuvette (1 cm), $\varepsilon(\lambda_{exc})$ and $\varepsilon(\lambda_{em})$ = the ε of the quencher at the excitation and the emission wavelength, respectively, as calculated from the UV–Vis spectra of the complexes [2].

The Stern–Volmer and Scatchard graphs are used in order to study the interaction of a quencher with serum albumins. According to Stern–Volmer quenching equation: [3]

$$\frac{Io}{I} = 1 + k_q \tau_0 [Q] = 1 + K_{SV}[Q] \quad \text{(eq. S4),}$$

where Io = the initial tryptophan fluorescence intensity of SA, I = the tryptophan fluorescence intensity of SA after the addition of the quencher, k_q = the quenching rate constants of SA, K_{SV} = the dynamic quenching constant, τ_o = the average lifetime of SA without the quencher, [Q] = the concentration of the quencher, the dynamic quenching constant (K_{SV}, M^{-1}) can be obtained by the slope of the diagram $\frac{Io}{I}$ vs [Q]. From the equation:

$$K_{SV} = k_q \tau_o \quad \text{(eq. S5)}$$

and taking $\tau_o = 10^{-8}$ s as fluorescence lifetime of tryptophan in SA, the approximate quenching constant (k_q, $M^{-1}s^{-1}$) is calculated.

From the Scatchard equation: [3]

$$\frac{\Delta I / Io}{[Q]} = nK - K\frac{\Delta I}{Io} \quad \text{(eq. S6)}$$

where n is the number of binding sites per albumin and K is the association binding constant, K (in M^{-1}) is calculated from the slope in plots $\frac{\Delta I / Io}{[Q]}$ versus $\frac{\Delta I}{Io}$ and n is given by the ratio of y intercept to the slope [3].

References

[1] A. Wolfe, G. Shimer and T. Meehan, *Biochemistry*, 1987, **26**, 6392–6396.

[2] L. Stella, A.L. Capodilupo and M. Bietti, *Chem. Commun.*, 2008, 4744–4746.

[3] Y. Wang, H. Zhang, G. Zhang, W. Tao and S. Tang, *J. Luminescence*, 2007, **126**, 211–218.

Table S1. The HSA constants derived for complexes **1–5**.

Compound	**Ksv (M^{-1})**	**k_q (M^{-1} s^{-1})**	**K (M^{-1})**	**n**
[Cd(5–Br–salo)$_2$(CH_3OH)]$_2$, (**1**)	1.47(±0.12)×10^4	1.47(±0.12)×10^{12}	1.06(±0.08)×10^5	0.35
[Cd(5–Br–salo)$_2$(bipy)]$_2$,(**2**)	4.11(±0.26)×10^4	4.11(±0.26)×10^{12}	1.74(±0.15)×10^5	0.60
[Cd(5–Br–salo)$_2$(phen)]$_{2,}$ (**3**)	9.72(±0.29)×10^4	9.72(±0.29)×10^{12}	1.60(±0.07)×10^5	0.86
[Cd(5–Br–salo)(neoc)(NO_3)]$_{2,}$ (**4**)	1.03(±0.46)×10^5	1.03(±0.46)×10^{13}	1.35(±0.12)×10^5	0.90
[Cd(5–Br–salo)$_2$(dpamH)], (**5**)	5.40(±0.21)×10^4	5.40(±0.21)×10^{12}	9.10(±0.43)×10^4	0.79

Table S2. The BSA constants derived for complexes **1–5**.

Compound	**Ksv (M^{-1})**	**k_q (M^{-1} s^{-1})**	**K (M^{-1})**	**n**
[Cd(5–Br–salo)$_2$(CH_3OH)]$_2$, (**1**)	3.40(±0.21)×10^4	3.40(±0.21)×10^{12}	4.07(±0.32)×10^4	1.00
[Cd(5–Br–salo)$_2$(bipy)]$_2$,(**2**)	8.82(±0.35)×10^4	8.82(±0.35)×10^{12}	5.85(±0.35)×10^4	1.23
[Cd(5–Br–salo)$_2$(phen)]$_{2,}$ (**3**)	6.16(±0.34)×10^5	6.16(±0.34)×10^{13}	2.42(±0.12)×10^5	1.13
[Cd(5–Br–salo)(neoc)(NO_3)]$_{2,}$ (**4**)	2.46(±0.13)×10^5	2.46(±0.13)×10^{13}	1.17(±0.09)×10^5	1.29
[Cd(5–Br–salo)$_2$(dpamH)], (**5**)	9.37(±0.29)×10^4	9.37(±0.29)×10^{12}	1.10(±0.06)×10^5	0.94

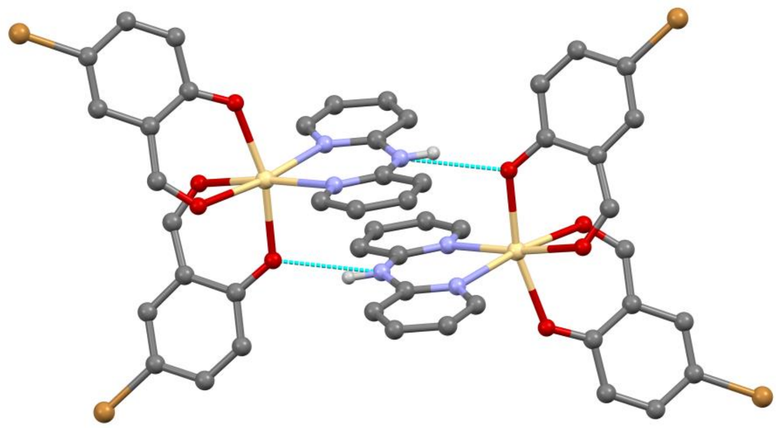

Figure S1. Hydrogen bonds between two adjacent molecules in **(5)** (symmetry 1-x, 1-y, 1-z). Cd atoms are in yellow, O atoms in red, N atoms in light blue, Br atoms in orange, C atoms in grey and H atoms in white.

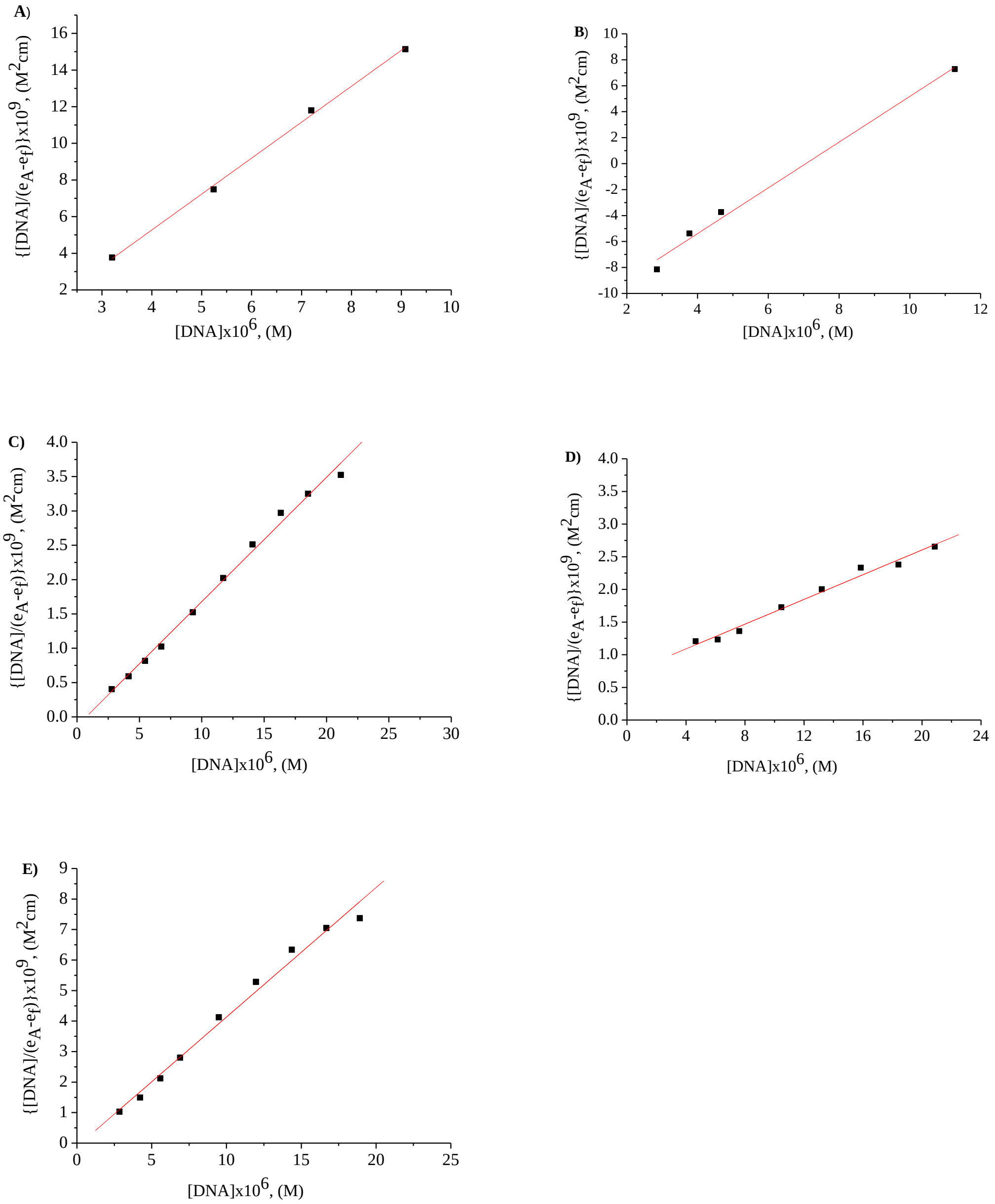

Figure S2. (A) – (E) Plot of $\frac{[\mathrm{DNA}]}{(\varepsilon_A - \varepsilon_f)}$ vs [DNA] for complexes **1–5**, respectively.

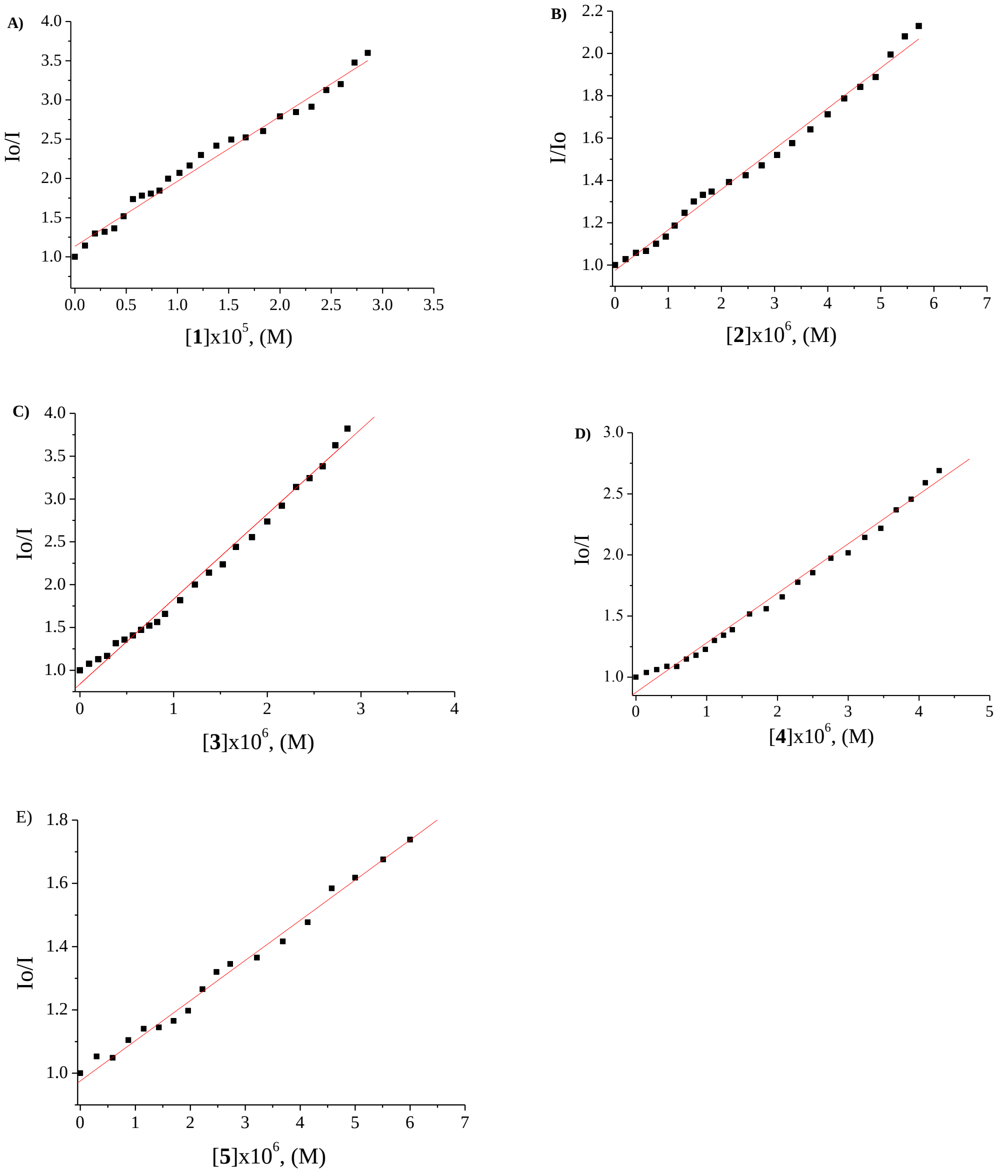

Figure S3. (A) – (E) Stern–Volmer quenching plot of EB bound to CT DNA for complexes **1–5**, respectively.

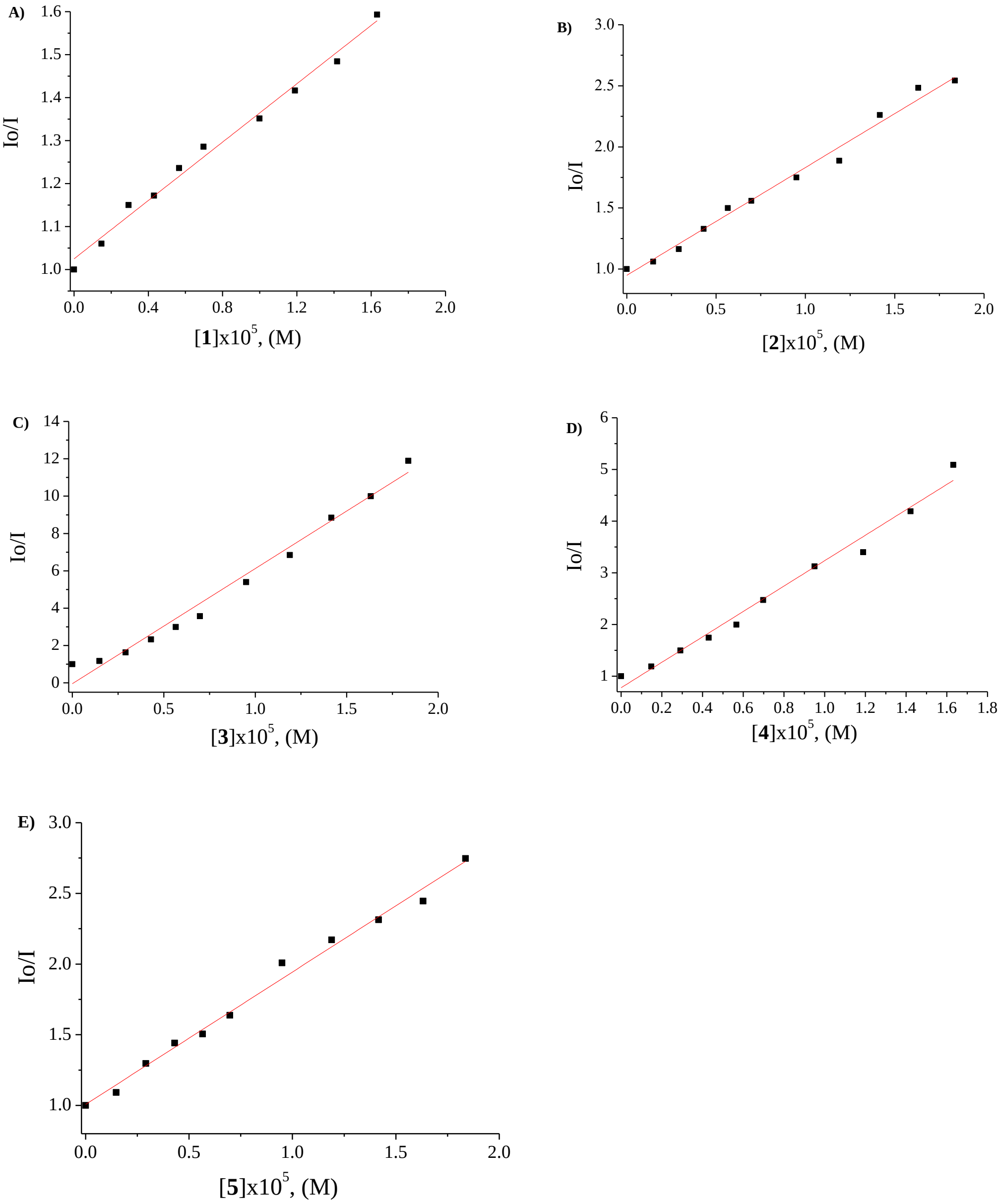

Figure S4. (A) – (E) Stern–Volmer quenching plot of BSA for complexes **1–5**, respectively.

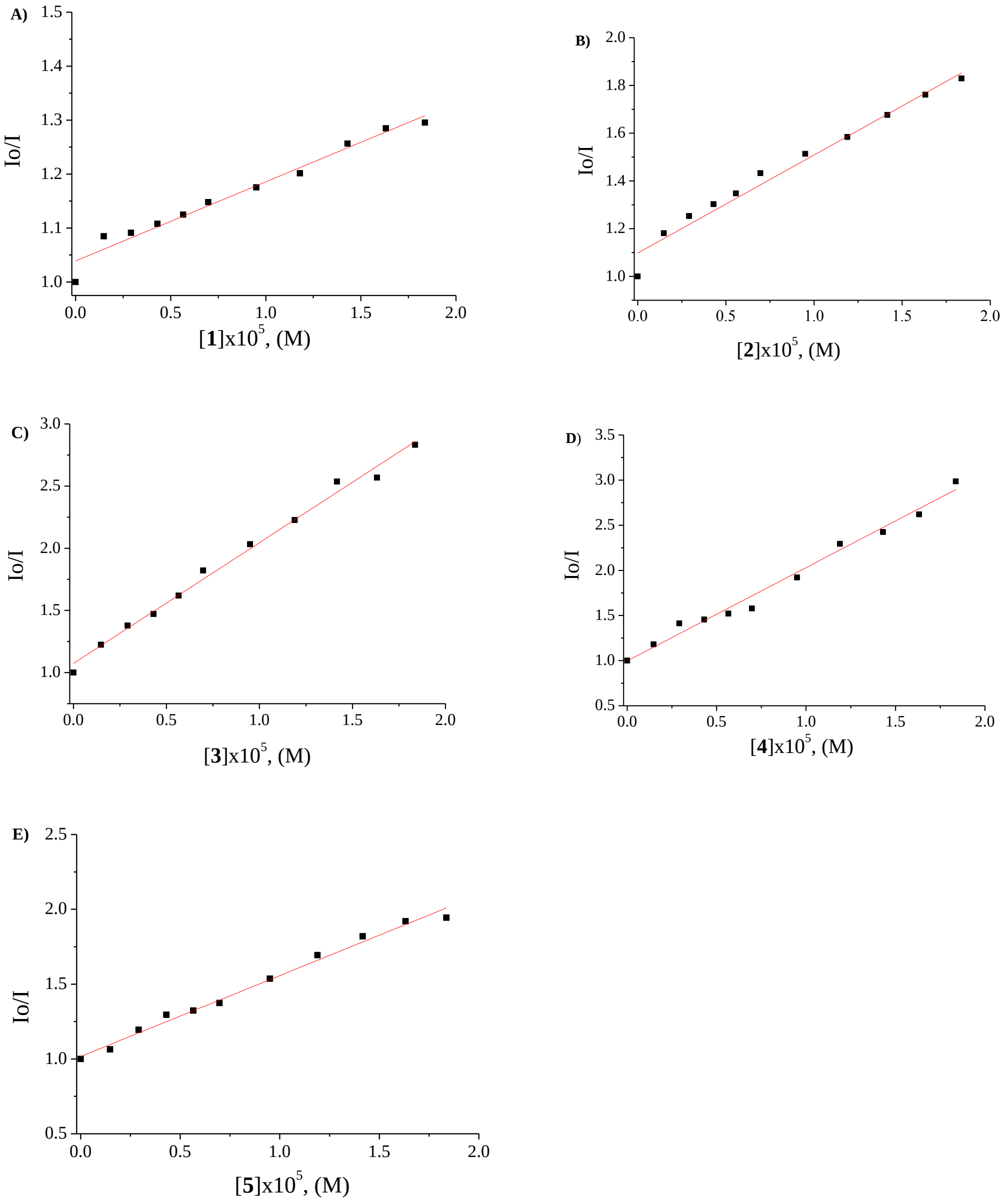

Figure S5. (A) – (E) Stern–Volmer quenching plot of HSA for complexes **1–5**, respectively.

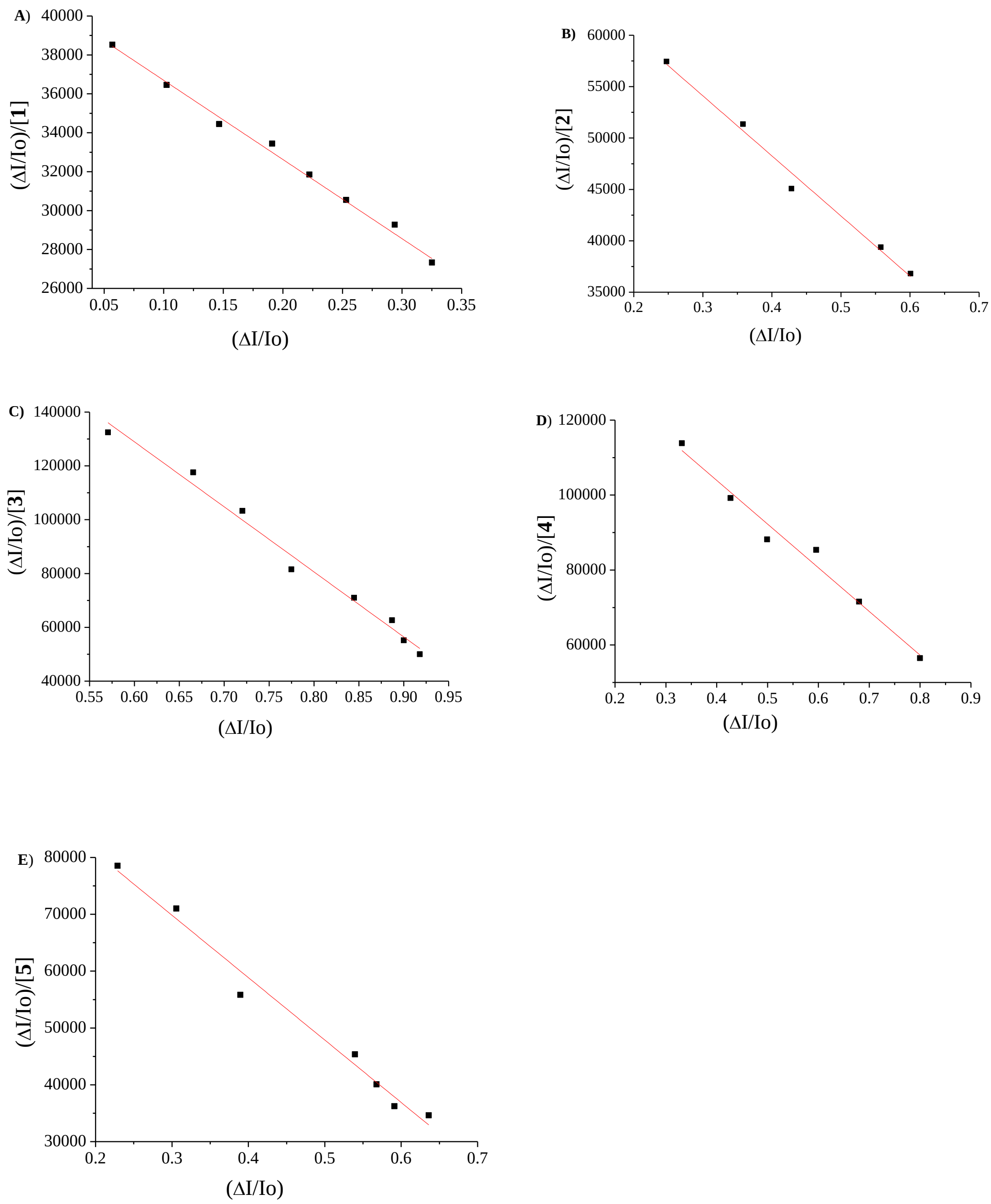

Figure S6. (A) – (E) Scatchard plot of BSA for complexes **1–5**, respectively.

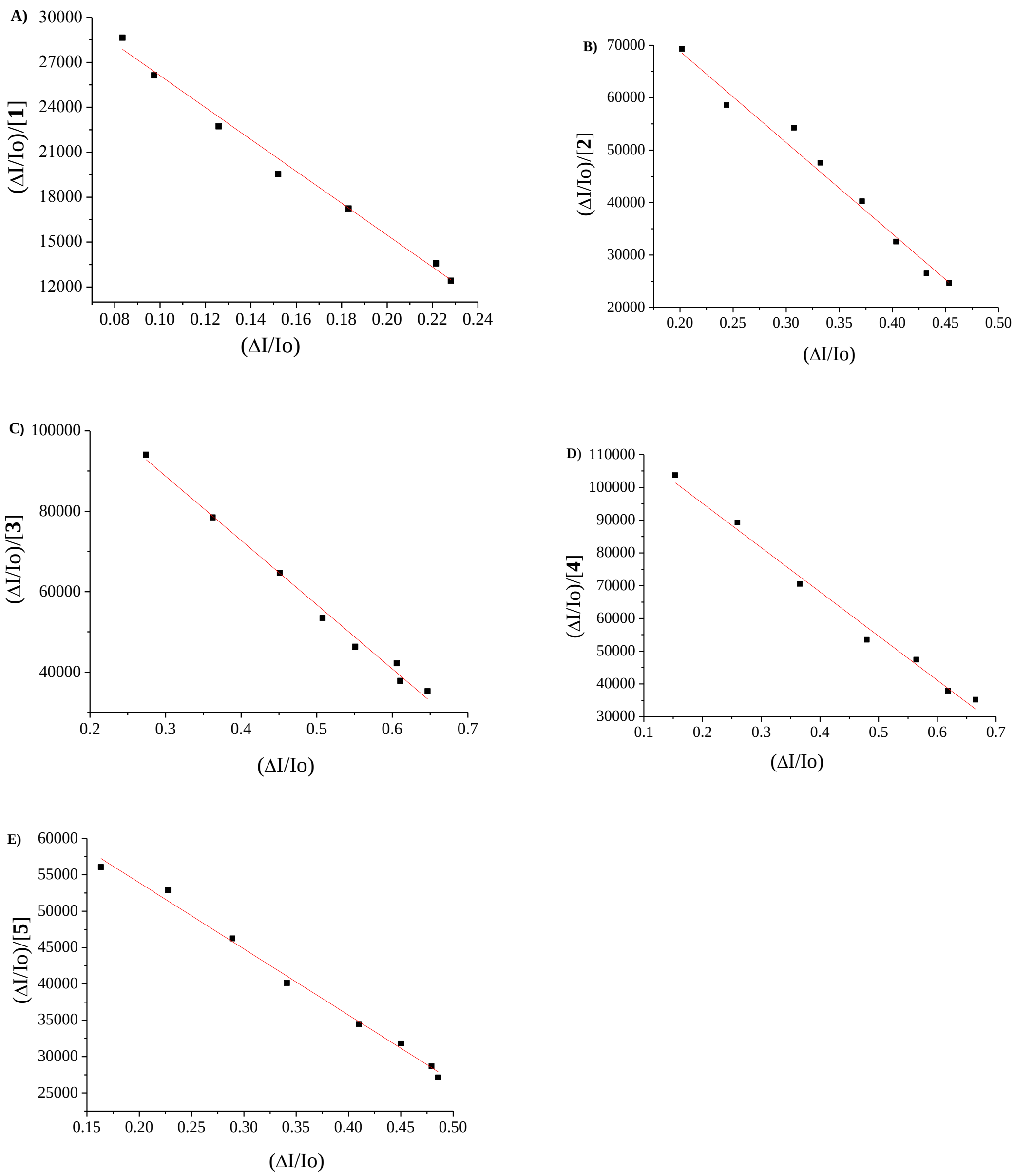

Figure S7. (A) – (E) Scatchard plot of HSA for complexes **1–5**, respectively.