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Supporting Information

# Spectroscopic and Molecular Docking Study of the Interaction between Neutral Re(I) Tetrazolate Complexes and Bovine Serum Albumin

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M.M. Conceptualization:Equal; Resources:Equal; Writing – review & editing:Equal
D.B. Funding acquisition:Lead; Project administration:Equal; Supervision:Equal; Writing – review & editing:Equal

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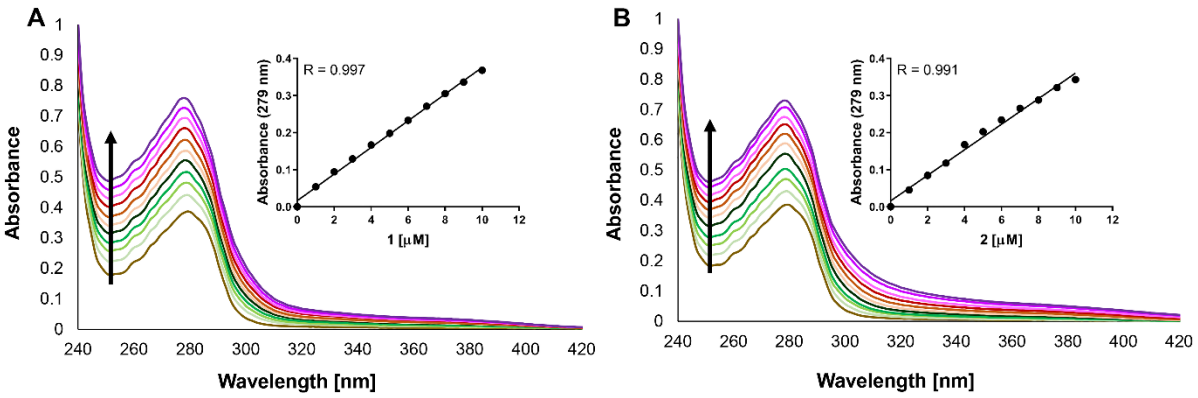


**Figure S1.** Changes in BSA absorbance upon increasing concentration (0–10 μM) of (A) complex **1** and (B) **2**. The concentration of BSA was maintained at 10 μM. Insets show changes in absorbance at 279 nm as a function of probe concentration.

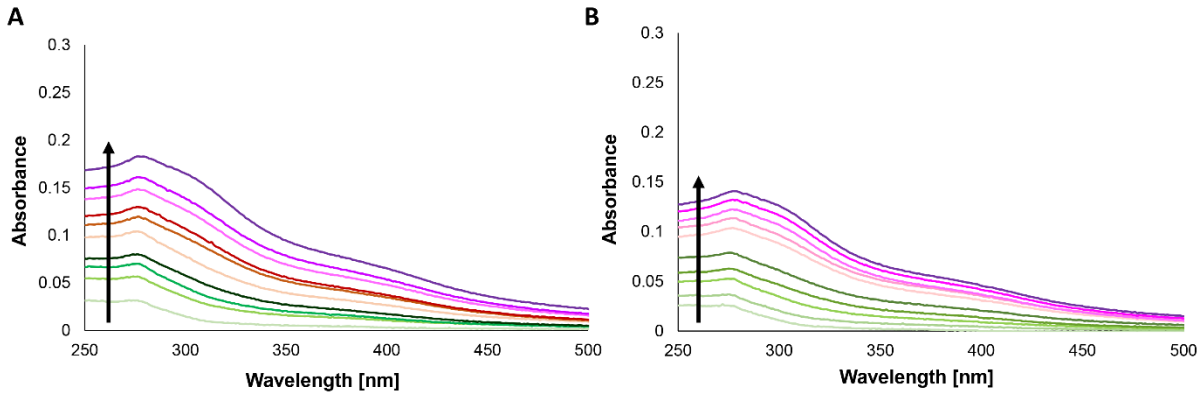


**Figure S2.** Absorption spectra of increasing concentration (0–10 μM) of Re(I) complex (A) **1** and (B) **2** in PBS.

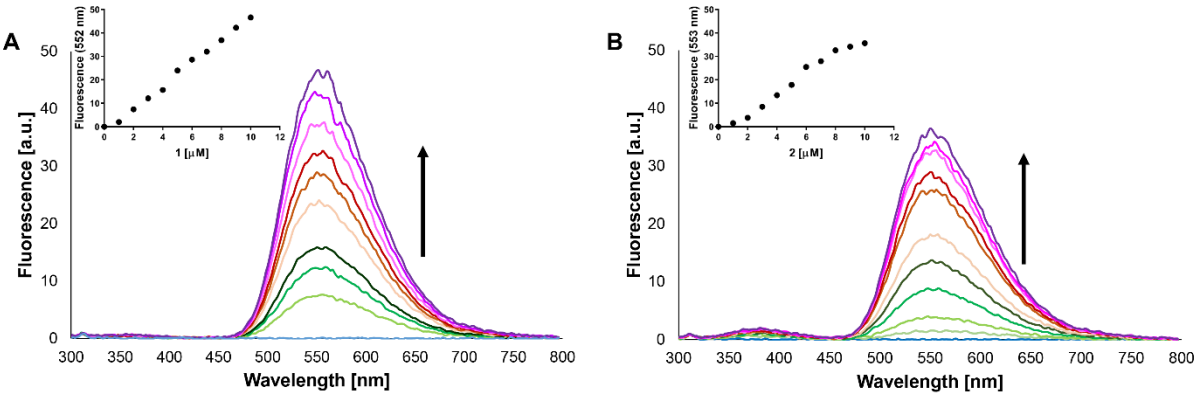


**Figure S3.** Emission spectra of increasing concentration (0–10 μM) of (A) complex **1** and (B) **2** in PBS. Excitation 280 nm. Insets show changes in fluorescence intensity at ~550 nm as a function of probe concentration.

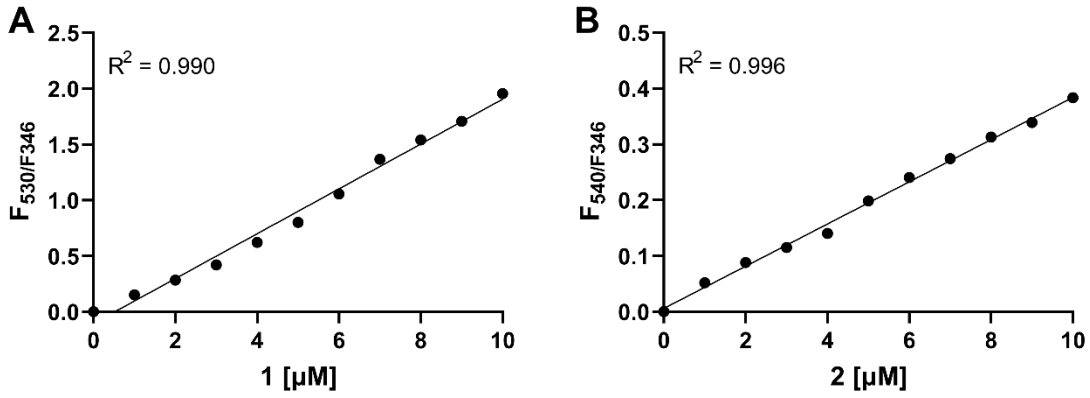


**Figure S4.** Linear correlation between (A) $F_{530}/F_{346}$ and complex **1** concentration and (B) between $F_{540}/F_{346}$ and complex **2** concentration.

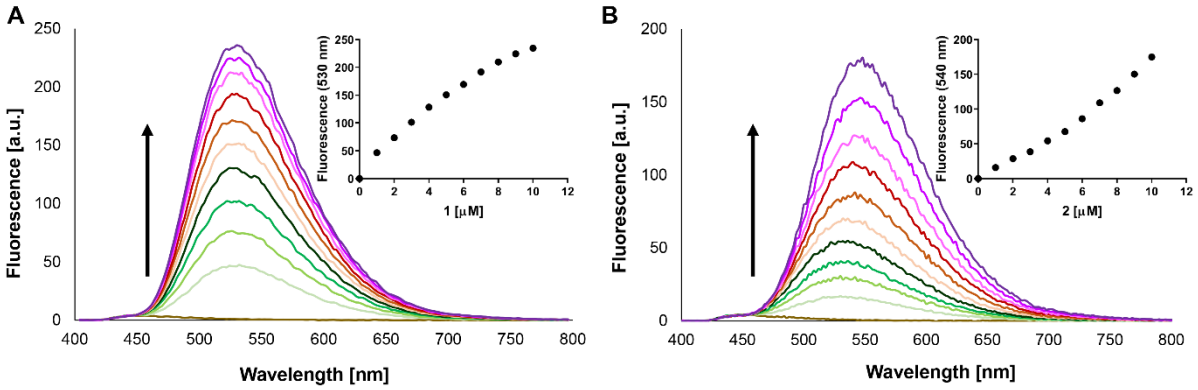


**Figure S5.** Emission spectra changes observed upon increasing concentration (0–10 µM) of (A) complex **1** and (B) **2.** Excitation 350 nm. The BSA concentration was kept constant at 10 µM. Insets show changes in fluorescence intensity at 530 and 540 nm as a function of concentration of probe **1** and **2**, respectively.

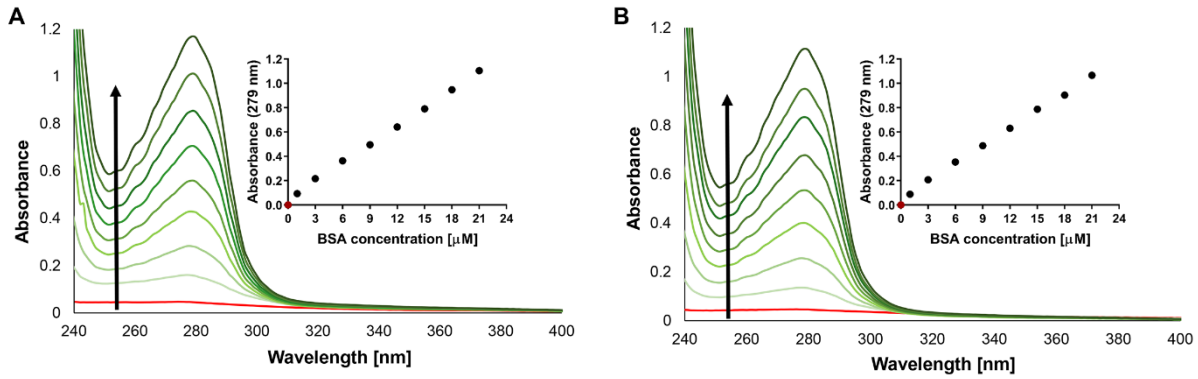


**Figure S6.** Changes in absorbance upon increasing concentration of BSA (0–21 µM) added to complex (A) **1** and (B) **2**. The concentration of probes was maintained at 3 µM. Insets show changes in absorbance at 279 nm as a function of BSA concentration.

$$\frac{F_S - F_0}{F - F_0} = \frac{1}{K_b[\mathrm{Q}]} \quad \text{(S1)}$$

where $F_s$, $F_0$ and F are BSA fluorescence intensities at Re(I) compound concentration where the system is saturated, in the absence of the Re(I) complex, and at an intermediate Re(I) complex concentration, respectively. $K_b$ is the binding constant and [Q] is the concentration of the quencher.

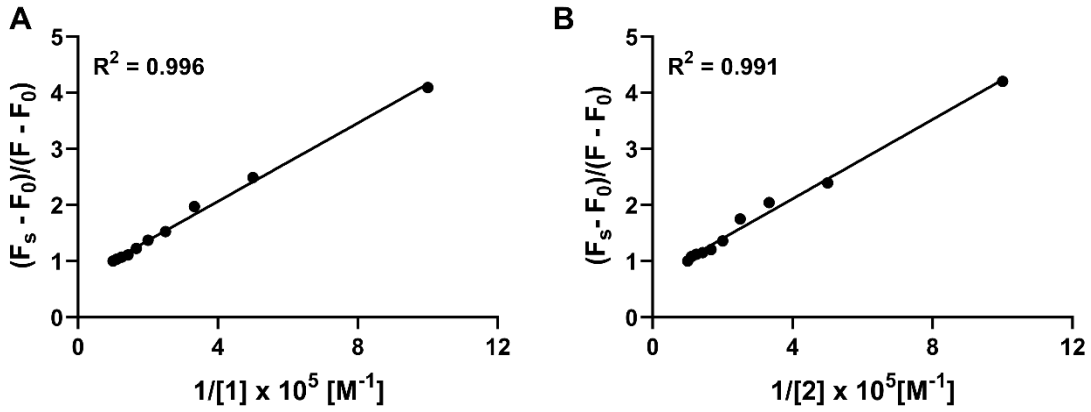


**Figure S7.** Linear Benesi−Hildebrand plots indicating 1:1 complex formation between BSA and compound (A) **1** and (B) **2**.

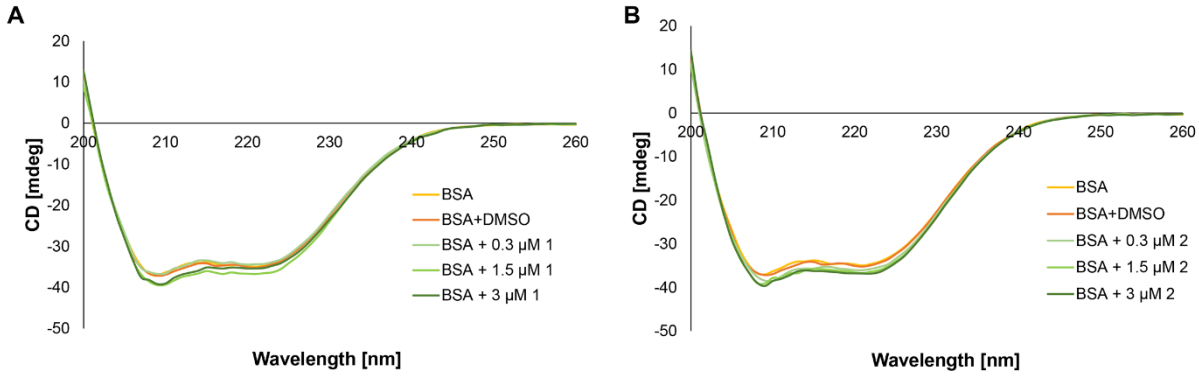


**Figure S8**. Circular dichroism spectra of BSA in the presence and absence of (A) complex **1** and (B) **2**.

**Table S1**. Residues comprising the three sites used in induced-fit docking.[a]

| **Site Ia**[b] | **Site Ib**[c] | **Trp134 site**[d] |
|---|---|---|
| Tyr149 | Arg194 | Glu17 |
| Arg198 | Leu197 | His18 |
| Trp213 | Arg198 | Glu130 |
| Arg217 | Ser201 | Lys131 |
| Leu218 | Lys204 | Trp134 |
| Lys221 | Trp213 | Asn158 |
| Leu237 | Arg217 | Asn161 |
| Val240 | Val342 | Gln165 |
| His241 | Ser343 | |
| Arg256 | Leu346 | |
| Ile289 | Asp450 | |
| Ala290 | Ser453 | |
| | Leu454 | |
| | Leu480 | |
| | Val481 | |

[a] For each site, the centre of the docking box is defined as the centroid of the listed residues. [b] Comprises residues within 4.0 Å of ketoprofen in the BSA-ketoprofen complex, including Trp213. [c] Comprises residues within 4.0 Å of naproxen in the BSA-naproxen complex, including Trp213. [d] Comprises Trp134 and nearby residues visibly contributing to a surface pocket near this residue.