Supplementary information

for

Induced CD of iron(II) clathrochelates: sensing of the structural and conformational alterations of serum albumins

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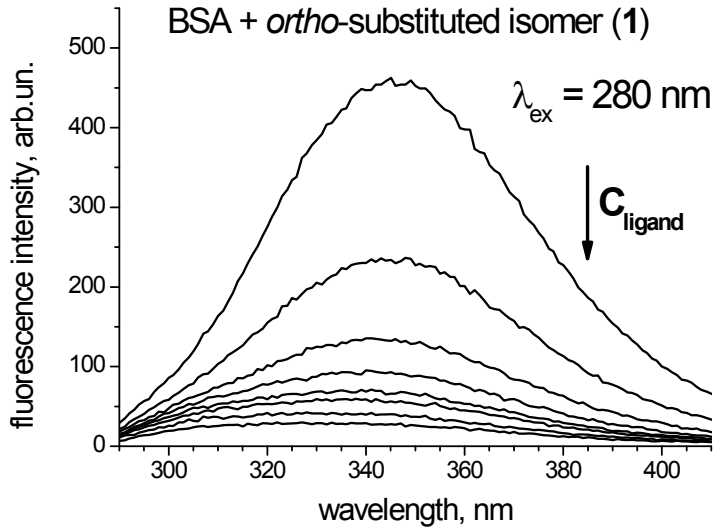

Figure S1a. Fluorescence spectra (non-corrected for inner filter effect) of 3μM BSA solution in the presence of 0, 1, 2, 2.5, 3, 4, 6 and 10 μM of *ortho*-substituted isomer (**1**) in 50mM Tris-HCl buffer, pH 7.9; λ_{ex} = 280 nm.

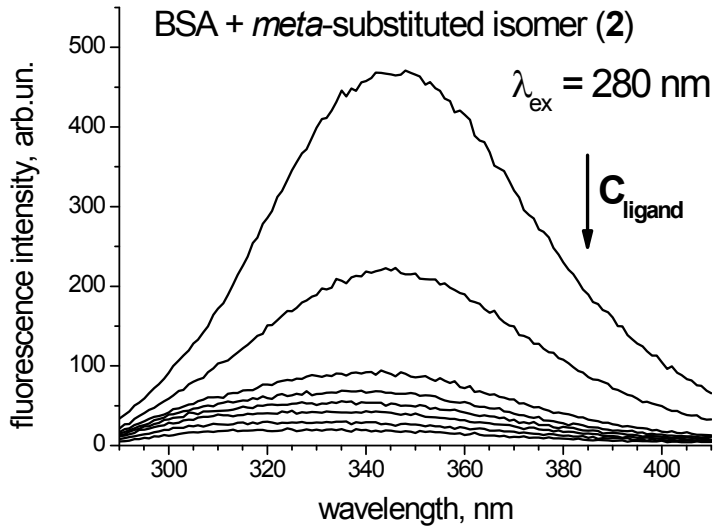

Figure S1b. Fluorescence spectra (non-corrected for inner filter effect) of 3μM BSA solution in the presence of 0, 1, 2, 2.5, 3, 4, 6 and 10 μM of *meta* -substituted isomer (**2**) in 50mM Tris-HCl buffer, pH 7.9; λ_{ex} = 280 nm.

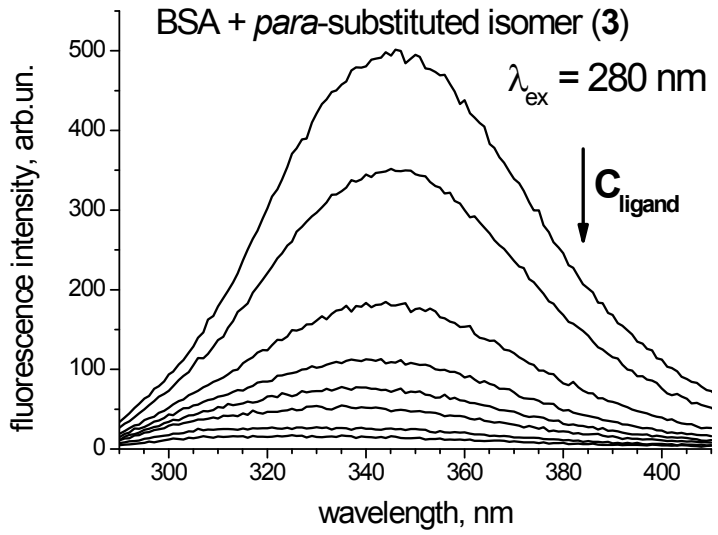

Figure S1c. Fluorescence spectra (non-corrected for inner filter effect) of 3μM BSA solution in the presence of 0, 1, 2, 2.5, 3, 4, 6 and 10 μM of *para*-substituted isomer (**3**) in 50mM Tris-HCl buffer, pH 7.9; λ_{ex} = 280 nm.

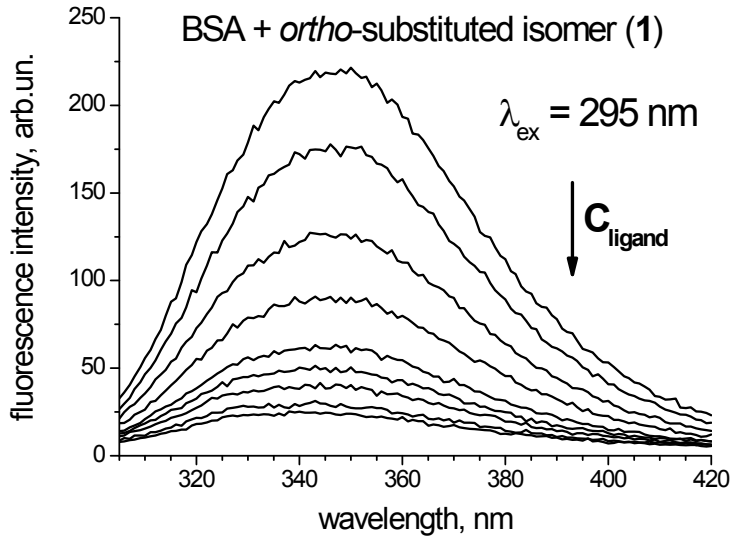

Figure S1d. Fluorescence spectra (non-corrected for inner filter effect) of 3μM BSA solution in the presence of 0, 0.5, 1, 1.5, 2, 2.5, 3, 4.5, and 6 μM of *ortho*-substituted isomer (**1**) in 50mM Tris-HCl buffer, pH 7.9; λ_{ex} = 295 nm.

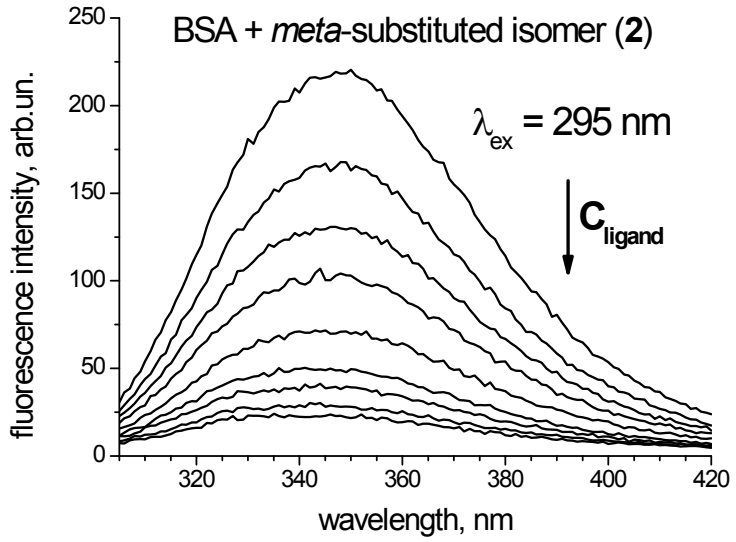

Figure S1e. Fluorescence spectra (non-corrected for inner filter effect) of 3μM BSA solution in the presence of 0, 1, 2, 2.5, 3, 4, 6 and 10 μM of *meta* -substituted isomer (**2**) in 50mM Tris-HCl buffer, pH 7.9; λ_{ex} = 295 nm.

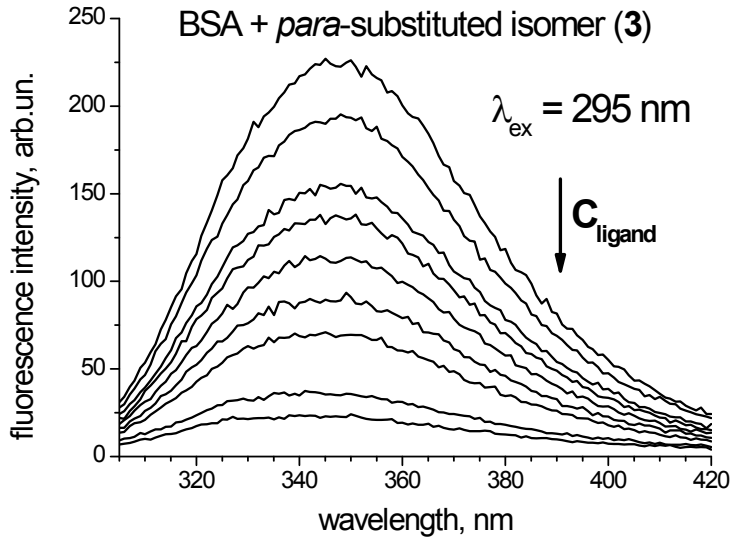

Figure S1f. Fluorescence spectra (non-corrected for inner filter effect) of 3μM BSA solution in the presence of 0, 0.5, 1, 1.5, 2, 2.5, 3, 4.5, and 6 μM of *para*-substituted isomer (**3**) in 50mM Tris-HCl buffer, pH 7.9; λ_{ex} = 295 nm.

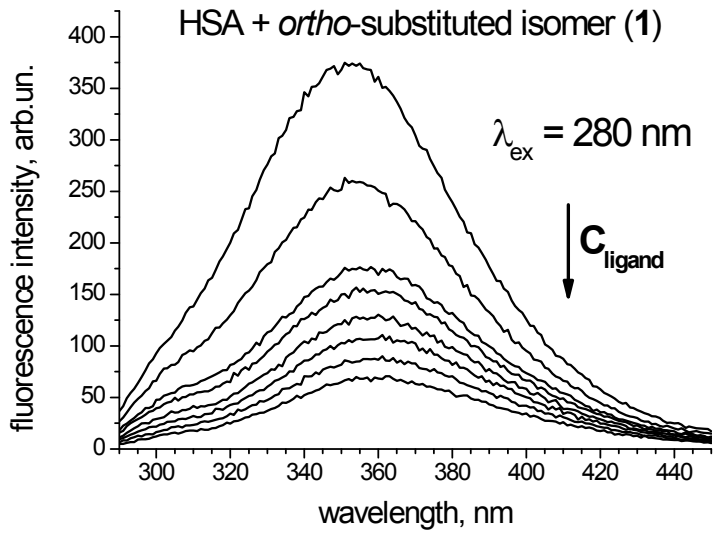

Figure S1g. Fluorescence spectra (non-corrected for inner filter effect) of 3μM HSA solution in the presence of 0, 1, 2, 2.5, 4, 6, 10 and 15 μM of *ortho*-substituted isomer (**1**) in 50mM Tris-HCl buffer, pH 7.9; λ_{ex} = 280 nm.

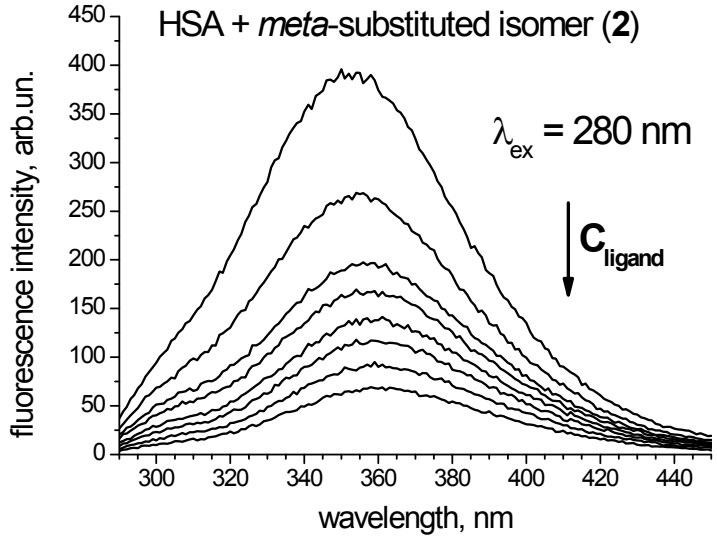

Figure S1h. Fluorescence spectra (non-corrected for inner filter effect) of 3μM HSA solution in the presence of 0, 1, 2, 2.5, 4, 6, 10 and 15 μM of *meta*-substituted isomer (**2**) in 50mM Tris-HCl buffer, pH 7.9; λ_{ex} = 280 nm.

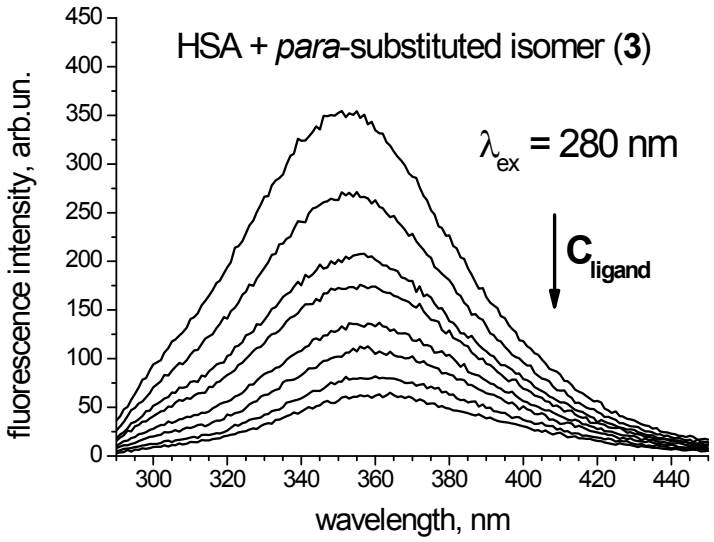

Figure S1i. Fluorescence spectra (non-corrected for inner filter effect) of 3μM HSA solution in the presence of 0, 1, 2, 2.5, 4, 6, 10 and 15 μM of *para*-substituted isomer (**3**) in 50mM Tris-HCl buffer, pH 7.9; λ_{ex} = 280 nm.

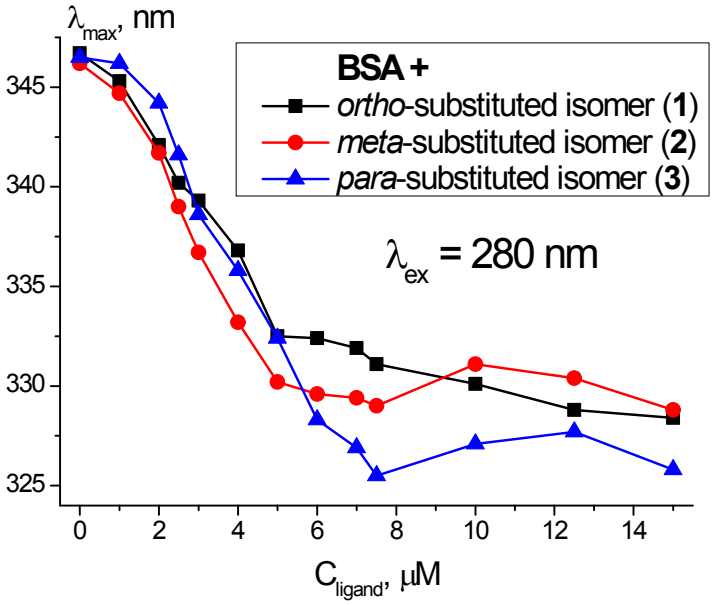

Figure S2a. Dependence of maximum wavelength (λ_{max}) of BSA fluorescence (λ_{ex} = 280 nm) for 3μM BSA solution in the presence of 0-15 μM of *ortho*-substituted isomer (**1**), *meta*-substituted isomer (**2**) and *para*-substituted isomer (**3**) in 50mM Tris-HCl buffer, pH 7.9.

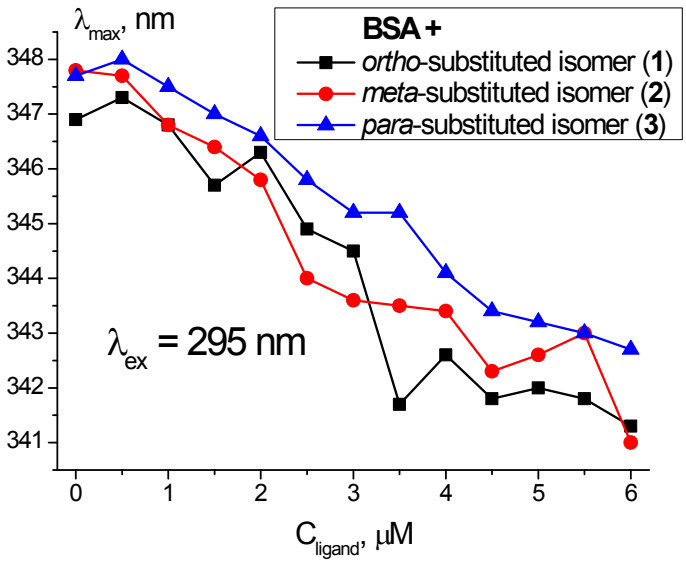

Figure S2b. Dependence of maximum wavelength (λ_{max}) of BSA fluorescence (λ_{ex} = 295 nm) for 3μM BSA solution in the presence of 0-6 μM of *ortho*-substituted isomer (**1**), *meta*-substituted isomer (**2**) and *para*-substituted isomer (**3**) in 50mM Tris-HCl buffer, pH 7.9.

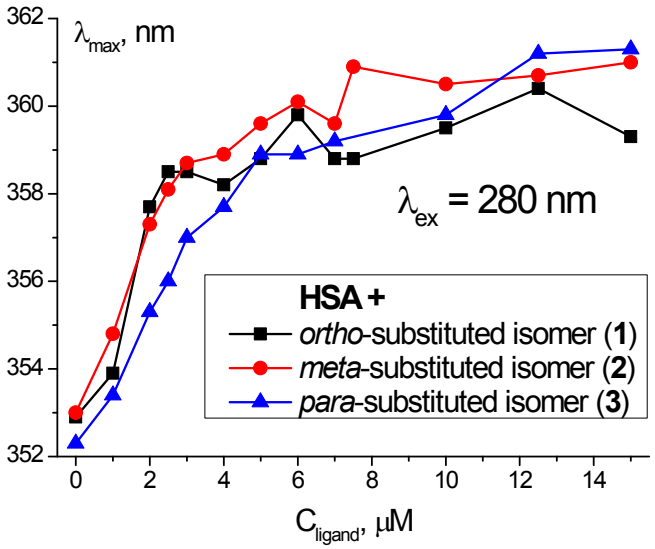

Figure S2c. Dependence of maximum wavelength (λ_{max}) of HSA fluorescence (λ_{ex} = 280 nm) for 3μM BSA solution in the presence of 0-15 μM of *ortho*-substituted isomer (**1**), *meta*-substituted isomer (**2**) and *para*-substituted isomer (**3**) in 50mM Tris-HCl buffer, pH 7.9.

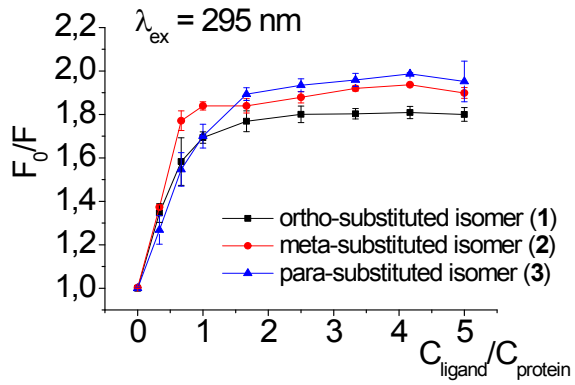

Figure S3. Stern–Volmer plots of HSA fluorescence quenching at and 295 nm by studied clathrochelates; F_0 and F are the protein fluorescence intensities in absence and in presence of clathrochelates.

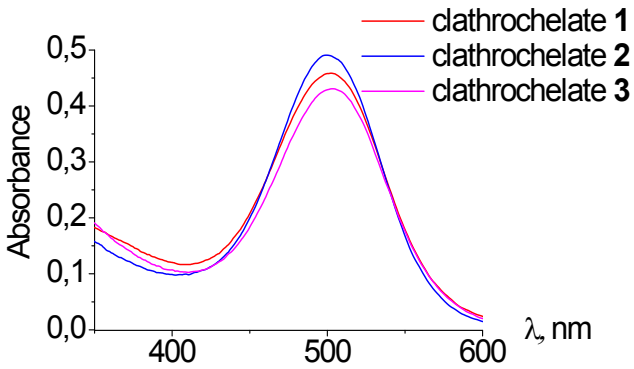

Figure S4. Absorption spectra of the clathrochelates **1** – **3**.

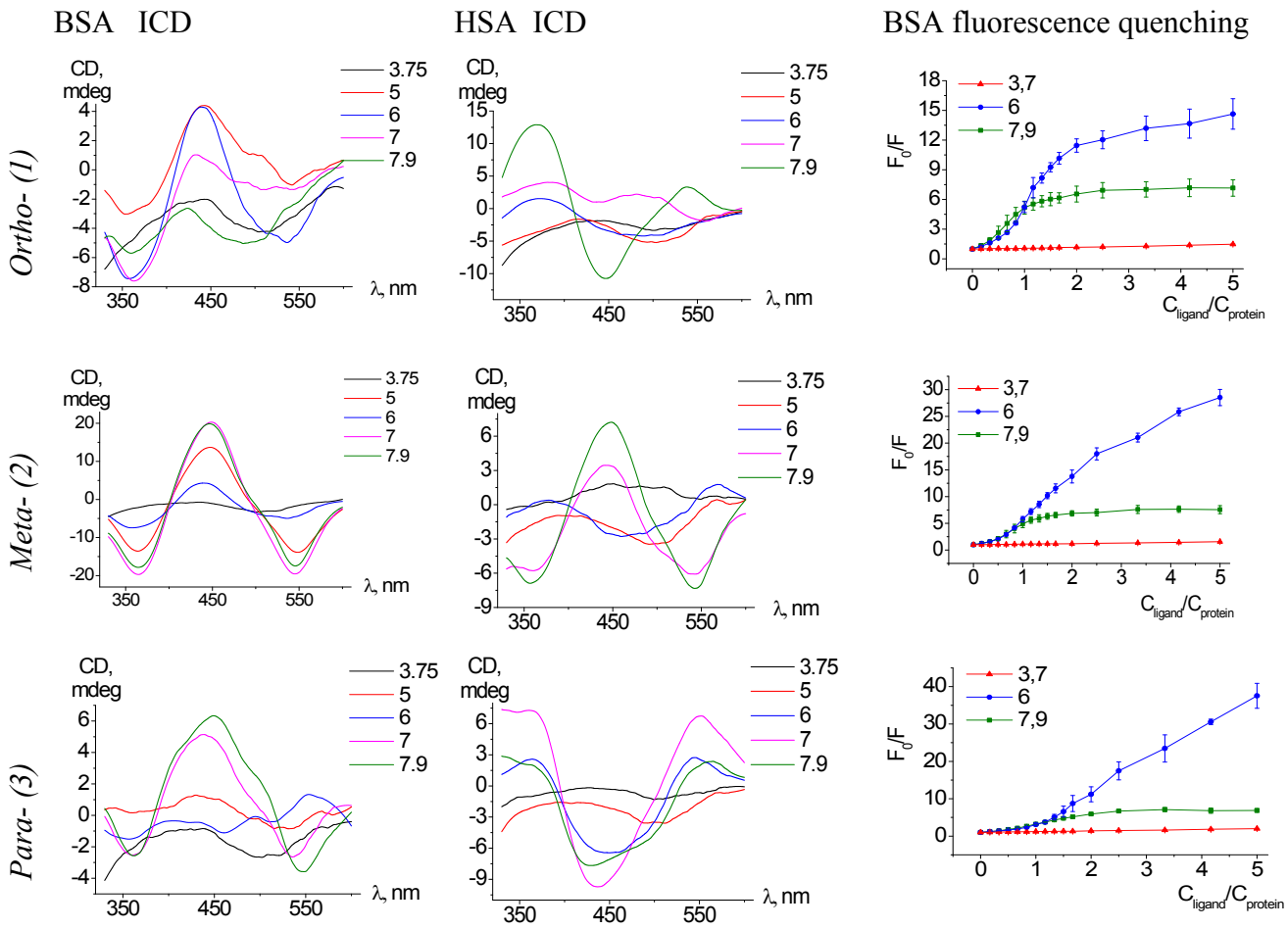

Figure S5. ICD spectra of iron(II) clathrochelates in the presence of BSA or HSA and plots of their quenching of BSA emission at different pH.

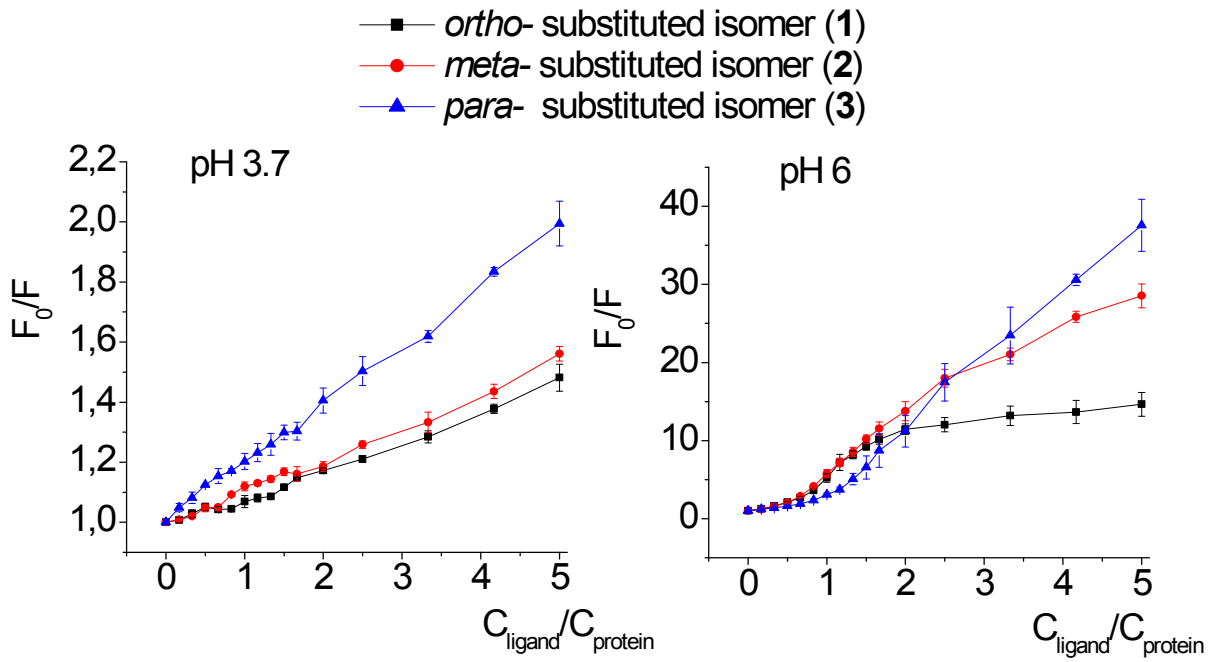

Figure S6. Stern–Volmer plots of BSA fluorescence quenching by the iron(II) clathrochelates at pH 3.7 and 6.