ESI

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Enantioselective regulation of a metal complex in reversible binding to serum albumin: dynamic helicity inversion signalled by circularly polarised luminescence

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1. Experimental

Details of luminescence, CPL and MR instrumentation may be traced through references 11 and 12.
For (*SSS*)-)-Δ-[Tb.L^{1a}]$^{3+}$, at 545 nm the g_{lum} value is + 0.27 (Figure 2 ESI and main text, Figure 2); for (*SSS*)-Δ-[Eu.L^{1a}]$^{3+}$, the g_{lum} values at 589 and 595 nm are + 0.19 and – 0.16 respectively (Fig. 1 ESI and Fig. 3 main text). These allow calibration of the other transitions observed I these and related Figures. The scale used in each CPL figure in the ESI refers to (I_L- I_R) and is on a scale of x60 with respect to (I_L + I_R).

2. List of Supplementary Figures

Figure 1

Mirror image CPL spectra for (*SSS*)-Δ-[Eu.L^{1a}]$^{3+}$ and (*RRR*)-Λ-[Eu.L^{2a}]$^{3+}$; (red = (Δ), blue = (Λ); 295K, D_2O, 15μM)

Figure 2

Mirror image CPL spectra for (*SSS*)-Δ-[Tb.L^{1a}]$^{3+}$ and (*RRR*)-Λ-[Tb.L^{2a}]$^{3+}$; (red = (Δ), blue = (Λ); 295K, D_2O, 15μM)

Figure 3

CPL spectra for (*RRR*)-Λ-[Eu.L^{2a}]$^{3+}$; (295K, D_2O, 15μM) in the presence and absence of one equivalent of BSA (blue = without; green = with BSA)

Figure 4

CPL spectra for (*RRR*)-Λ-[Tb.L^{2a}]$^{3+}$; (295K, D_2O, 15μM) in the presence and absence of one equivalent of BSA (blue = without; green = with BSA)

Figure 5

CPL spectra for (*SSS*)-Δ-[Tb.L^{1b}]$^{3+}$; (295K, D_2O, 15μM) in the presence and absence of one equivalent of BSA (red = without; green = with BSA)

Figure 6

CPL spectra for (*SSS*)-Δ-[Eu.L^3]$^{3+}$; (295K, D_2O, 15μM) in the presence and absence of 10 equivalents of BSA (red = without; green = with BSA)

Figure 7

CPL spectra for (*RRR*)-Λ-[Tb.L^3]$^{3+}$; (295K, D_2O, 15μM) in the presence and absence of 10 equivalents of BSA (blue = without; green = with BSA)

Figure 8

CPL spectra for (*SSS*)-Δ-[Tb.L^5]$^{3+}$; (295K, D_2O, 15μM) in the presence and absence of 10 equivalents of BSA (red = without; green = with BSA); ligand L^5 replaces the dpqC chromophore in L^1(bidentate moiety) for a unidentate 2-methyl-aza-xanthone moiety, and in this complex the macrocyclic ligand is octadentate and one water molecule is bound in an axial site [13]

Figure 9

Variation of the observed dissymmetry factor, g_{em}, with added BSA for (*SSS*)-Δ-[Eu.L^{1a}]$^{3+}$; (295K, D_2O, 15μM) ; (blue triangles = 589 nm, red squares = 593 nm).

Figure 10

Variation of the measured relaxivity of (*SSS*)-Δ-[Gd.L^{1a}]$^{3+}$ and (*RRR*)-Λ-[Gd.L^{2a}]$^{3+}$; (310K, D_2O, 1.6 mM complex) as a function of added HSA (Red triangles = (Δ), blue squares = (Λ)).

Figure 11

Variation of the measured relaxivity of (*SSS*)-Δ-[Gd.L^{1a}]$^{3+}$ and (*RRR*)-Λ-[Gd.L^{2a}]$^{3+}$; (310K, D_2O, 1.6 mM complex) as a function of added warfarin (Red triangles = (Δ), blue squares = (Λ)).

Figure 12

Total emission spectra for (*SSS*)-Δ-[Eu.L^{1a}]$^{3+}$; (295K, D_2O, 15μM) in the presence (red; scaled x 3) and absence (blue) of 10 equivalents of BSA.

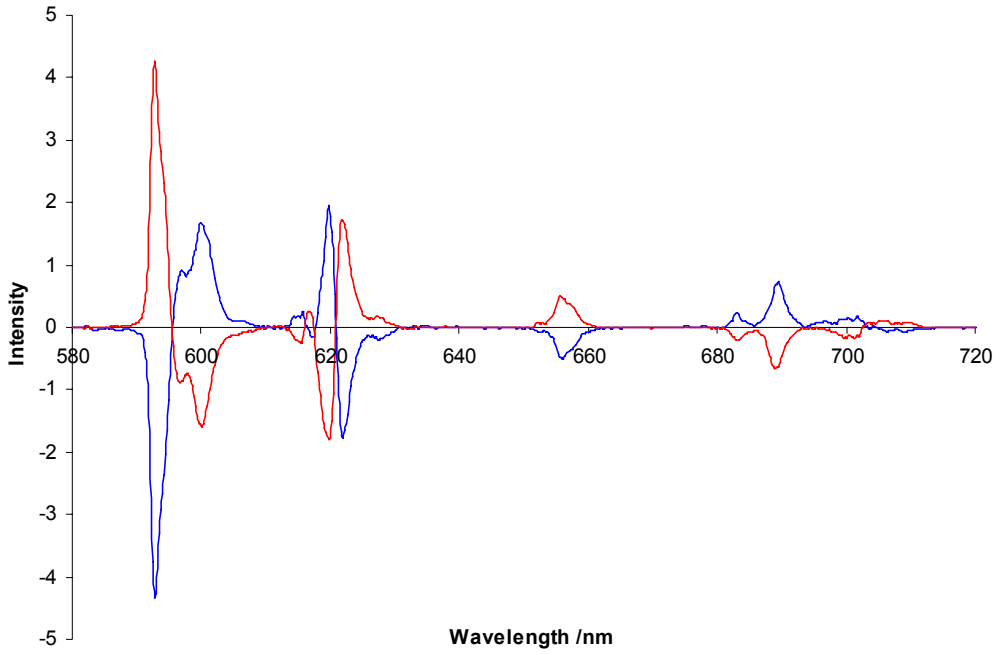


Figure 1 (above)
Mirror image CPL spectra for (*SSS*)-Δ-[Eu.L^{1a}]$^{3+}$ and (*RRR*)-Λ-[Eu.L^{2a}]$^{3+}$; (red = (Δ), blue = (Λ); 295K, D_2O, 15μM)

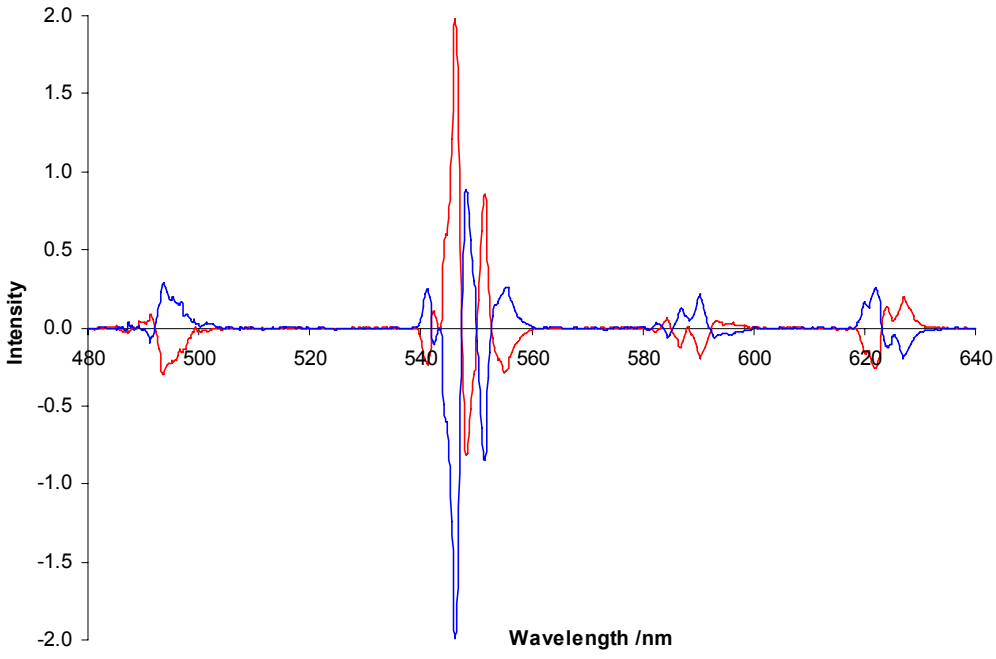
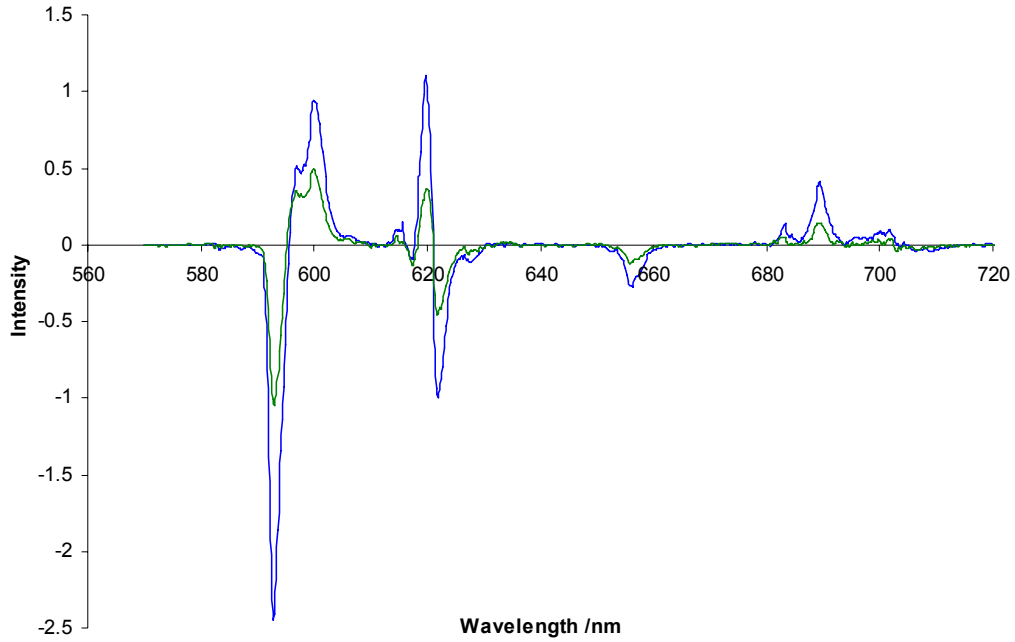


Figure 2

Mirror image CPL spectra for (*SSS*)-Δ-[Tb.L^{1a}]$^{3+}$ and (*RRR*)-Λ-[Tb.L^{2a}]$^{3+}$; (red = (Δ), blue = (Λ); 295K, D_2O, 15μM)



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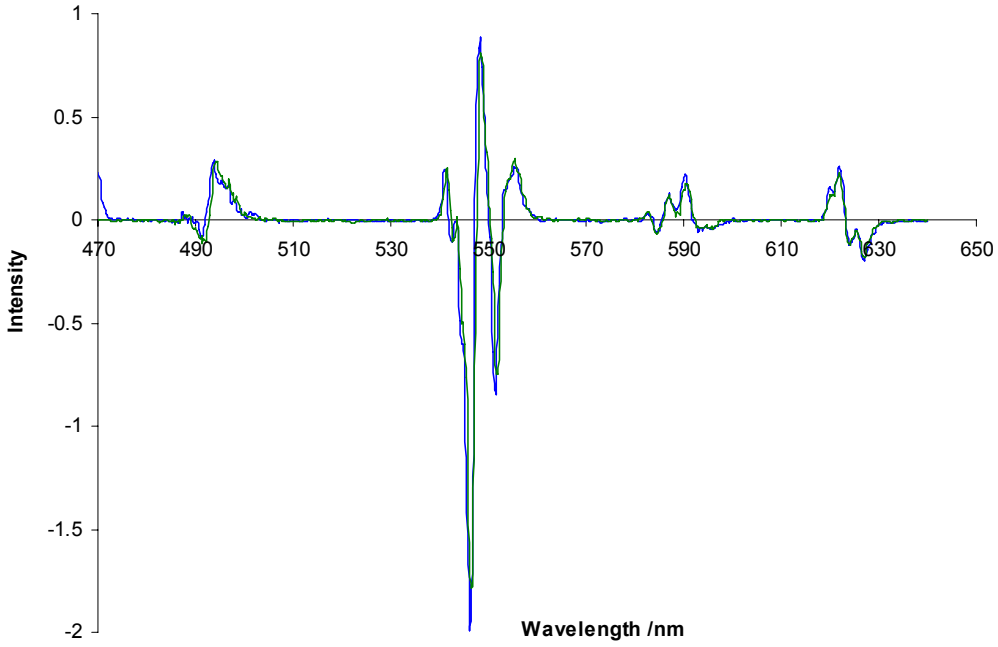
CPL spectra for (*RRR*)-Λ-[Eu.L^{2a}]$^{3+}$; (295K, D_2O, 15μM) in the presence and absence of one equivalent of BSA (blue = without; green = with BSA)



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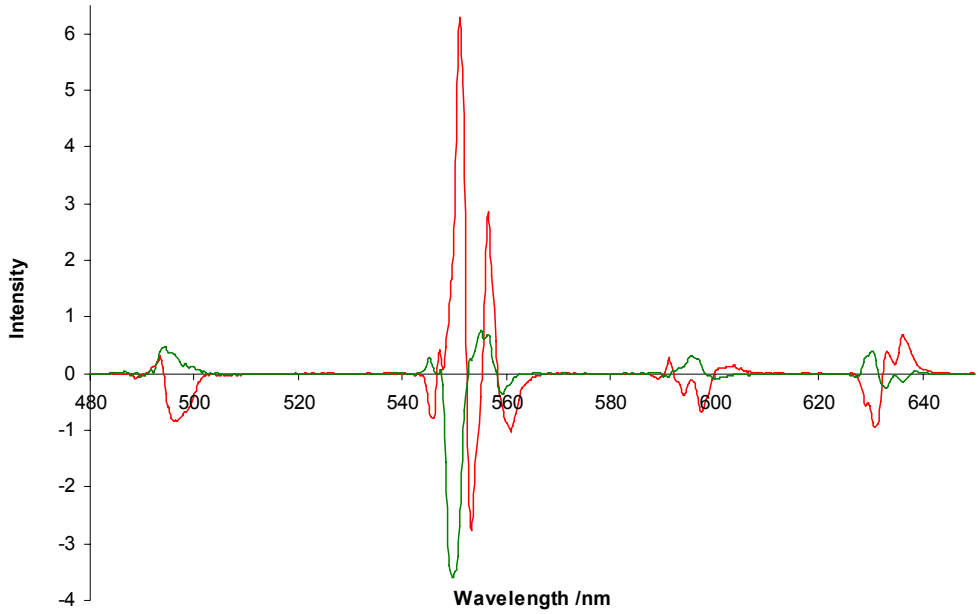


Figure 5
CPL spectra for (*SSS*)-Δ-[Tb.L^{1b}]$^{3+}$; (295K, D_2O, 15μM) in the presence and absence of one equivalent of BSA (red = without; green = with BSA)

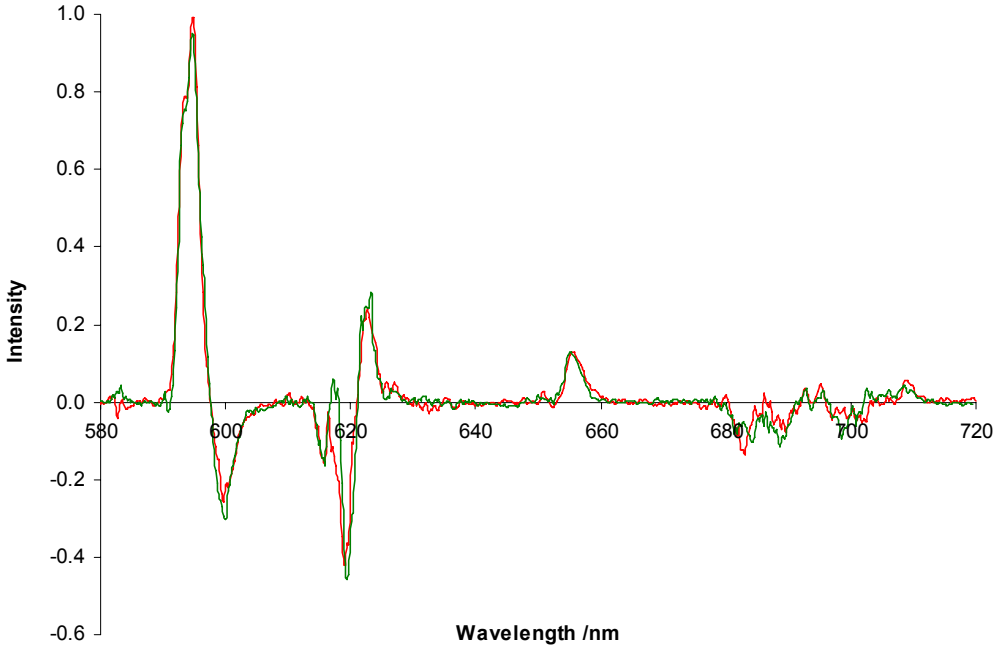
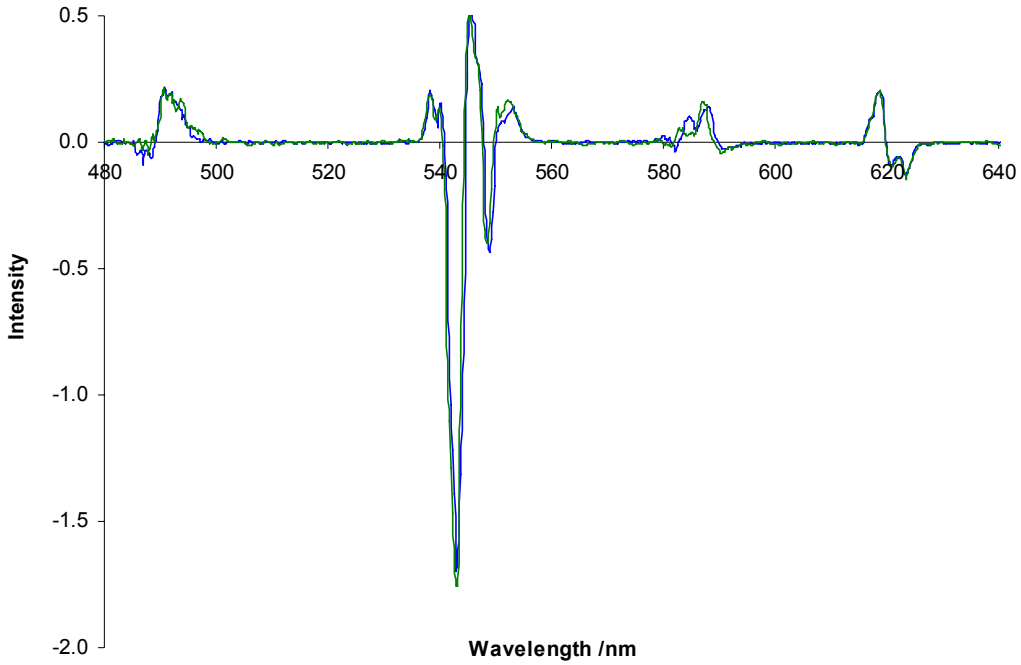


Figure 6
CPL spectra for (*SSS*)-Δ-[Eu.L^{3}]$^{3+}$; (295K, D_2O, 15μM) in the presence and absence of 10 equivalents of BSA (red = without; green = with BSA); note the absence of any quenching of emission following protein addition.



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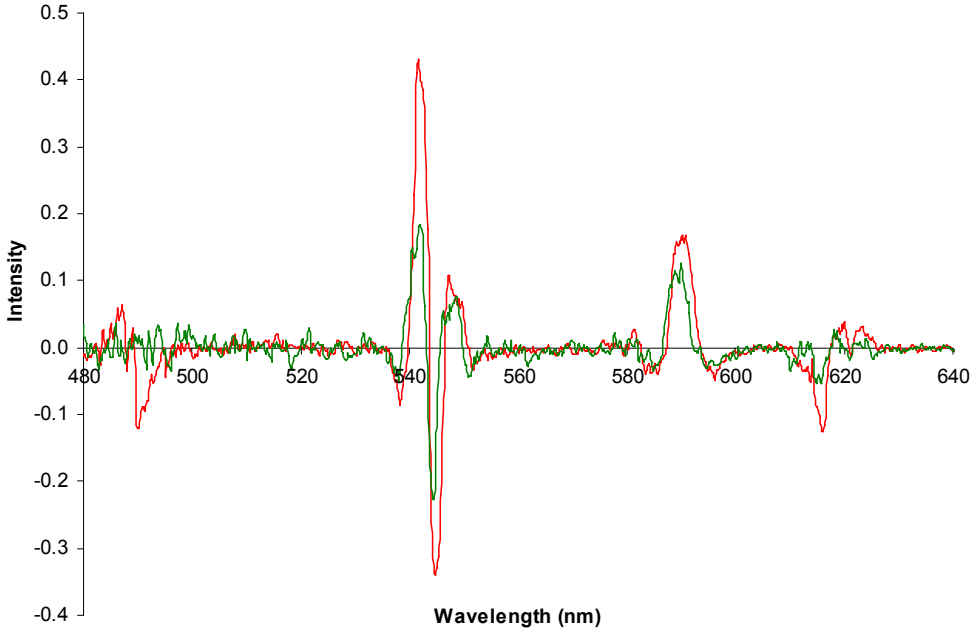
CPL spectra for (*RRR*)-Λ-[Tb.L^3]$^{3+}$; (295K, D_2O, 15μM) in the presence and absence of 10 equivalents of BSA (blue = without; green = with BSA)



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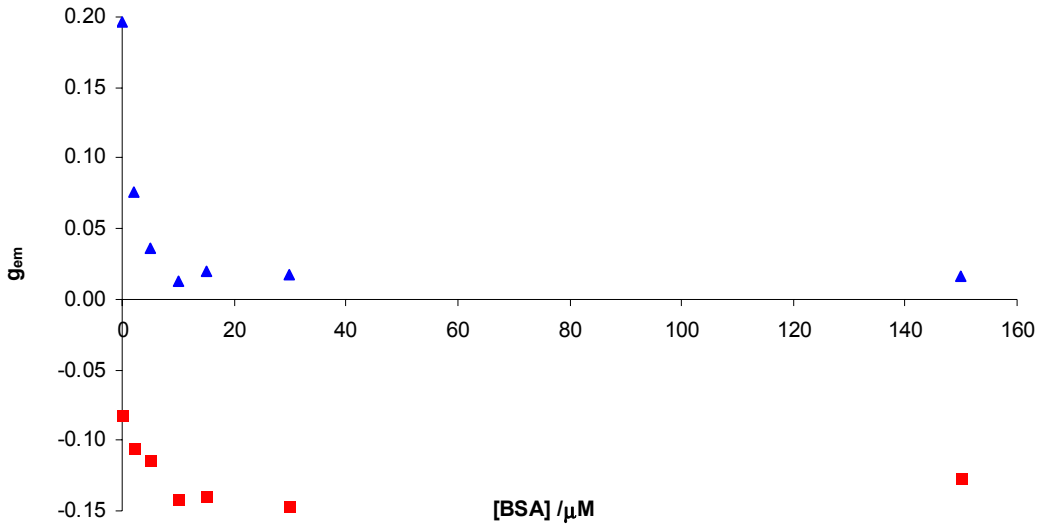
CPL spectra for (*SSS*)-Δ-[Tb.L^5]$^{3+}$; (295K, D_2O, 15μM) in the presence and absence of 10 equivalents of BSA (red = without; green = with BSA); ligand L^5 replaces the dpqC chromophore in L^1(bidentate moiety) for a unidentate 2-methyl-aza-xanthone moiety, and in this complex the ligand is octadentate and one water molecule is bound in an axial site [13]



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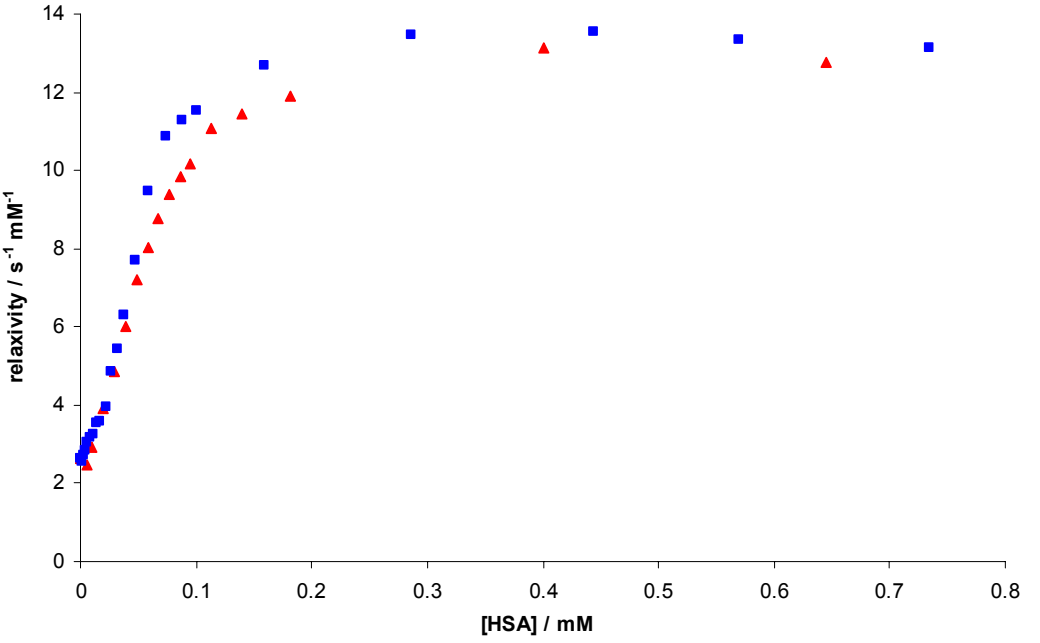
Variation of the observed dissymmetry factor, g_{em}, with added BSA for (*SSS*)-Δ-[Eu.L^{1a}]$^{3+}$; (295K, D_2O, 15μM) (blue triangles = 589 nm, red squares = 593 nm).



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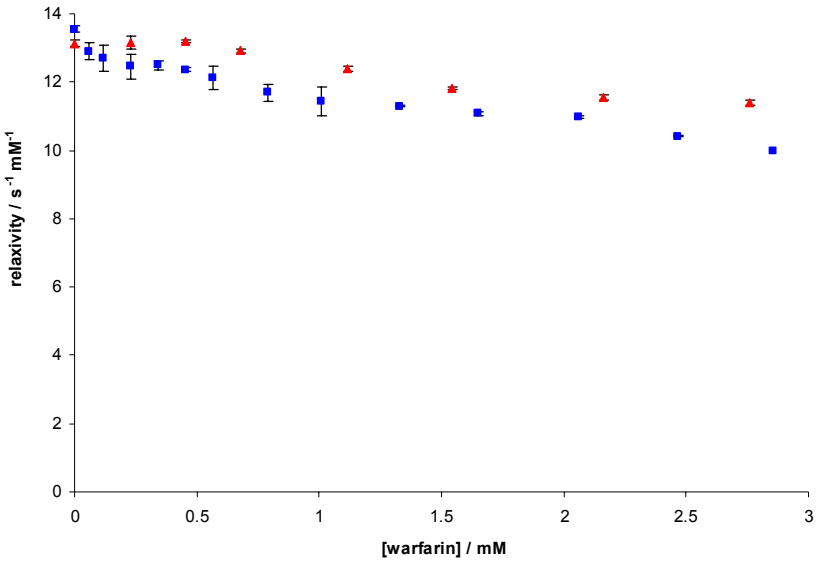

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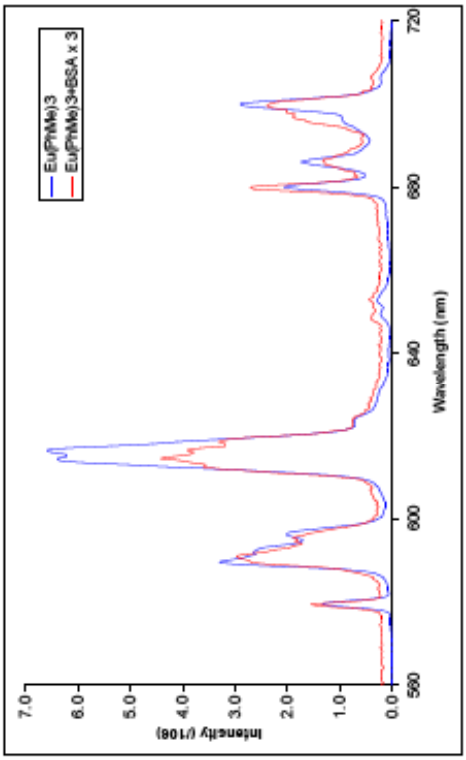

Figure 12
Total emission spectra for (*SSS*)-Δ-[Eu.L^{1a}]$^{3+}$; (295K, D_2O, 15μM) in the presence (red; scaled x 3) and absence (blue) of 10 equivalents of BSA, showing changes in spectral form in the ΔJ = 1 and ΔJ = 2 and 4 manifolds.