Supporting Information

Excited state interactions between flurbiprofen and tryptophan in drug/protein complexes and in model dyads. Fluorescence studies from the femtosecond to the nanosecond time domains

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S1. This page.

S2. Figure SI-1. UV-vis absorption spectra of (*S*)-FBP (black), (*S*)-TrpMe (green), (*S*,*S*)-FBP-TrpMe (red) and (*R*,*S*)-FBP-TrpMe (blue) at λ_{exc} = 267 nm in acetonitrile/air (2.5×10^{-5} M).

S3. Figure SI-2. Steady-state emission of (*S*)-FBP (black), (*S*)-TrpMe (green), (*S*,*S*)-FBP-TrpMe (red) and (*R*,*S*)-FBP-TrpMe (blue) at λ_{exc} = 267 nm in acetonitrile/air. A) The relative intensities are representative of the quantum yields. B) Normalised spectra.

S4. Figure SI-3. FU anisotropy decays of (*S*)-FBP (black), (*S*,*S*)-FBP-TrpMe (red), (*R*,*S*)-FBP-TrpMe (blue) and (*S*)-TrpMe (green) at λ_{exc} = 267 nm in acetonitrile/air at A) λ_{em} = 310 nm and B) λ_{em} = 340 nm.

S5. Figure SI-4. Normalised TCSPC decays of (*S*,*S*)-FBP-TrpMe (red) and (*R*,*S*)-FBP-TrpMe (blue) at λ_{exc} = 267 nm and λ_{em} = 310 nm (solid lines) and λ_{em} = 340 nm (open circles) in acetonitrile/air.

S6. Figure SI-5. Normalised TCSPC decays of HSA at λ_{exc} = 267 nm and λ_{em} = 380 nm in PBS solution. Best fit (in red) obtained using A) second order exponential fit and B) third order exponential fit. Inset: residual of the corresponding fit.

S7. Figure SI-6. Normalised TCSPC decays of (*S*)-FBP@HSA at λ_{exc} = 267 nm and λ_{em} = 380 nm in PBS solution. Best fit (in red) obtained using A) second order exponential fit and B) third order exponential fit. Inset: residual of the corresponding fit.

S8. Figure SI-7. Normalised TCSPC decays of (*R*)-FBP@HSA at λ_{exc} = 267 nm and λ_{em} = 380 nm in PBS solution. Best fit (in red) obtained using A) second order exponential fit and B) third order exponential fit. Inset: residual of the corresponding fit.

S9. Figure SI-8. Geometry optimised (HyperChem Release 8.0.3 for Windows Molecular Model System, PM3) structure for (*S*,*S*)-FBP-TrpMe (A) and (*S*,*R*)-FBP-TrpMe (B).

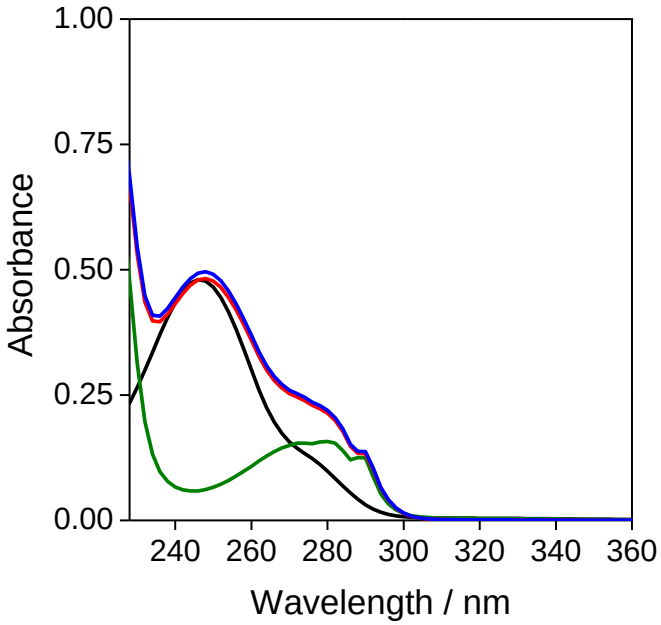

Figure SI-1. UV-vis absorption spectra of (*S*)-FBP (black), (*S*)-TrpMe (green), (*S*,*S*)-FBP-TrpMe (red) and (*R*,*S*)-FBP-TrpMe (blue) in acetonitrile/air (2.5×10^{-5} M).

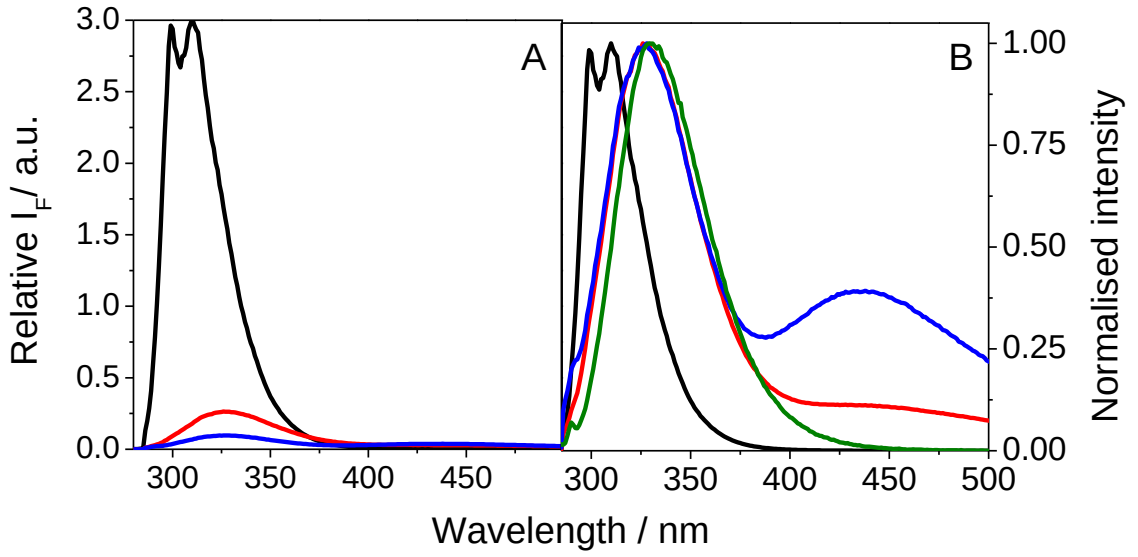

Figure SI-2. Steady-state emission of (*S*)-FBP (black), (*S*)-TrpMe (green), (*S*,*S*)-FBP-TrpMe (red) and (*R*,*S*)-FBP-TrpMe (blue) at λ_{exc} = 267 nm in acetonitrile/air. A) The relative intensities are representative of the quantum yields. B) Normalised spectra.

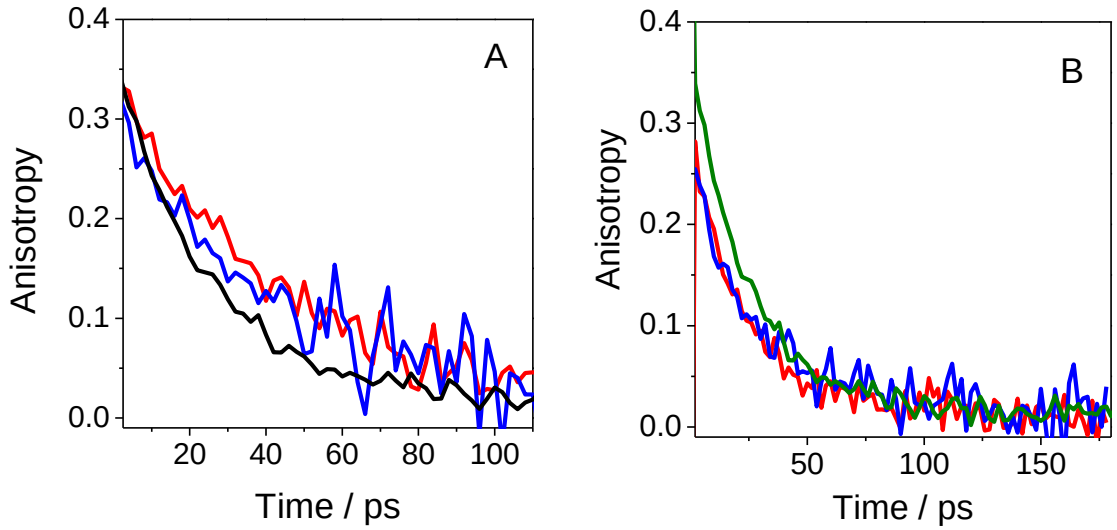

Figure SI-3. FU anisotropy decays of (*S*)-FBP (black), (*S*,*S*)-FBP-TrpMe (red), (*R*,*S*)-FBP-TrpMe (blue) and (*S*)-TrpMe (green) at λ_{exc} = 267 nm in acetonitrile/air at A) λ_{em} = 310 nm and B) λ_{em} = 340 nm.

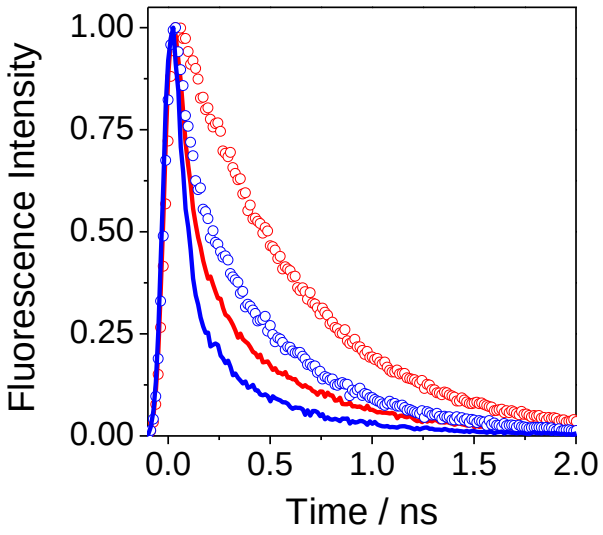

Figure SI-4. Normalised TCSPC decays of (*S*,*S*)-FBP-TrpMe (red) and (*R*,*S*)-FBP-TrpMe (blue) at λ_{exc} = 267 nm and λ_{em} = 310 nm (solid lines) and λ_{em} = 340 nm (open circles) in acetonitrile/air.

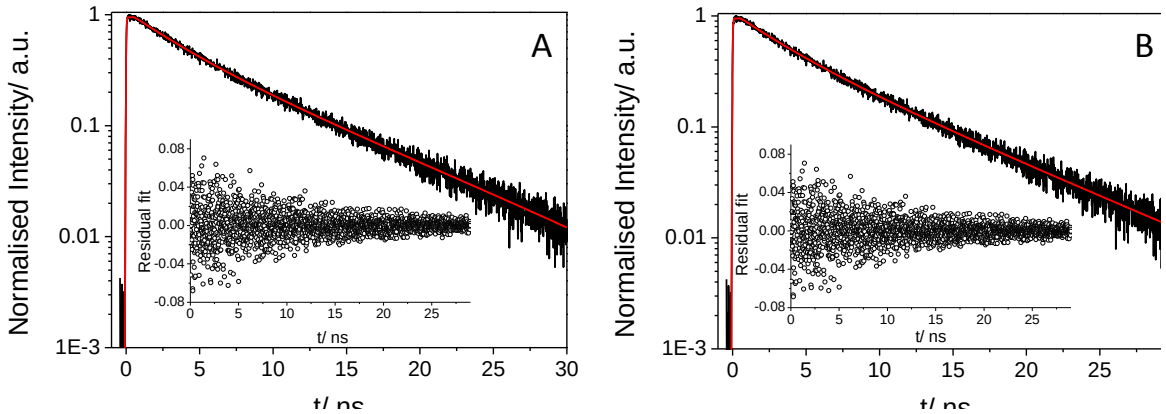

Figure SI-5. Normalised TCSPC decays of HSA at λ_{exc} = 267 nm and λ_{em} = 380 nm in PBS solution. Best fit (in red) obtained using A) second order exponential fit and B) third order exponential fit. Inset: residual of the corresponding fit.

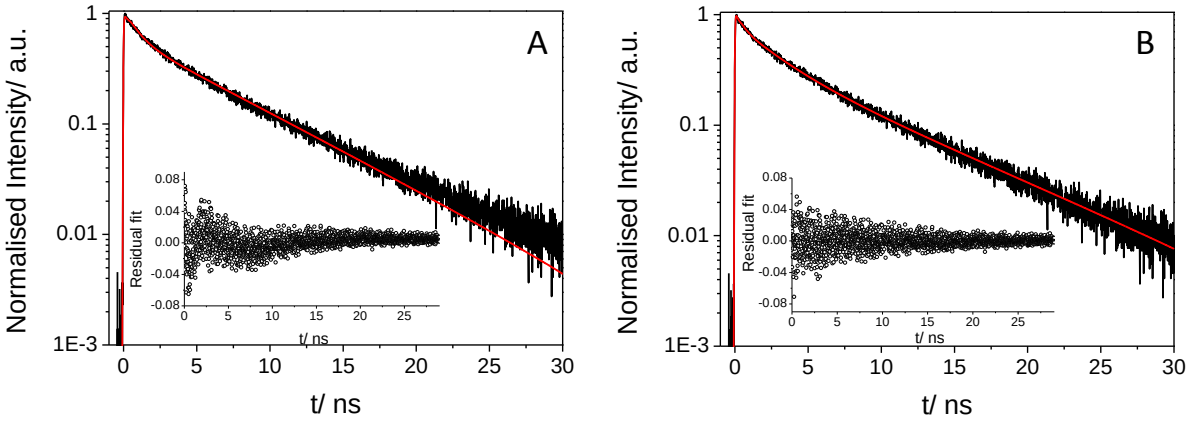

Figure SI-6. Normalised TCSPC decays of (*S*)-FBP@HSA at λ_{exc} = 267 nm and λ_{em} = 380 nm in PBS solution. Best fit (in red) obtained using A) second order exponential fit and B) third order exponential fit. Inset: residual of the corresponding fit.

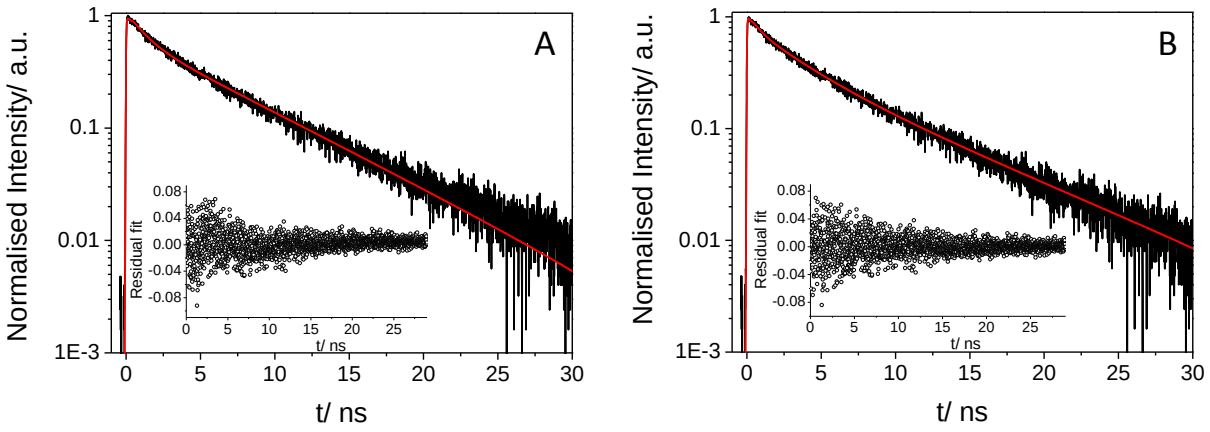

Figure SI-7. Normalised TCSPC decays of (*R*)-FBP@HSA at λ_{exc} = 267 nm and λ_{em} = 380 nm in PBS solution. Best fit (in red) obtained using A) second order exponential fit and B) third order exponential fit. Inset: residual of the corresponding fit.

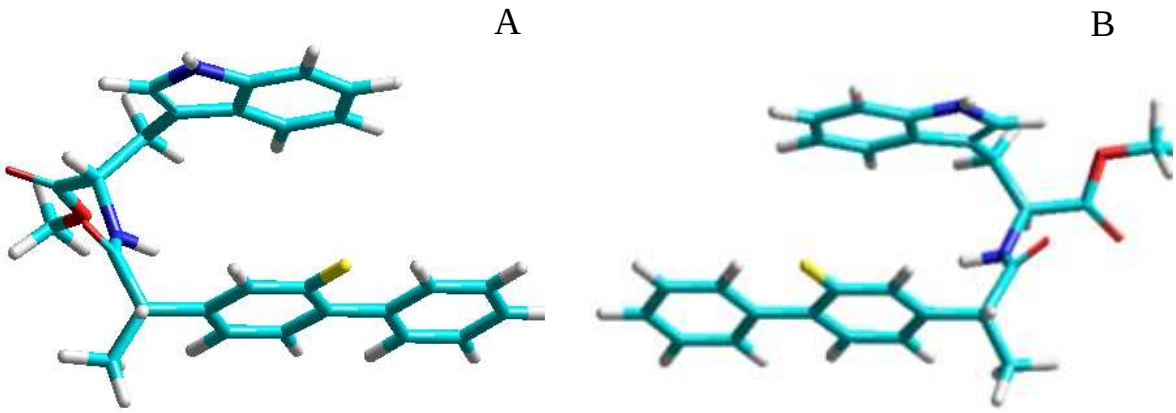

Figure SI-8. Geometry optimised (HyperChem Release 8.0.3 for Windows Molecular Model System, PM3) structure for (*S*,*S*)-FBP-TrpMe (A) and (*S*,*R*)-FBP-TrpMe (B).