Supplementary Information

DNA threading intercalation of enantiopure [Ru(phen)$_2$bidppz]$^{2+}$ induced by hydrophobic catalysis

Bobo Feng[a], Elin Sundin[a], Per Lincoln[a] and Anna K. F. Mårtensson[a,b]*

[a]Department of Chemistry and Chemical Engineering, Chalmers University of Technology, Kemigården 4, SE-412 96 Gothenburg, Sweden.

[b]Wallenberg Laboratory for Cardiovascular and Metabolic Research, Institute of Medicine, University of Gothenburg, Sahlgrenska University Hospital, Bruna Stråket 16, SE-413 45 Gothenburg, Sweden.
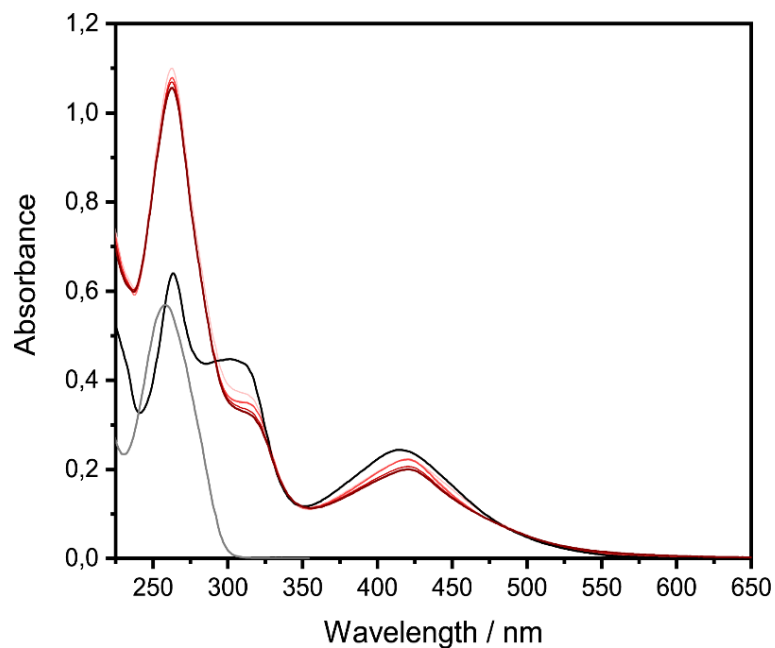
E-mail: anna.martensson@wlab.gu.se

Figure S1. Absorption spectra of Λ-**Ru-1** in the presence of ctDNA at [base pairs]/[complex] ratio 5 in 50 mM NaCl aqueous buffer solution with 20% (w/w) PEG-400. The color change from light to dark specify spectral change with time (0, 0.5, 1.5, 24 and 48 h; green) after 50°C incubation. The black line shows the complex without the addition of ctDNA. The gray line shows ctDNA alone. The concentration of ctDNA is 80 µM nucleotides.
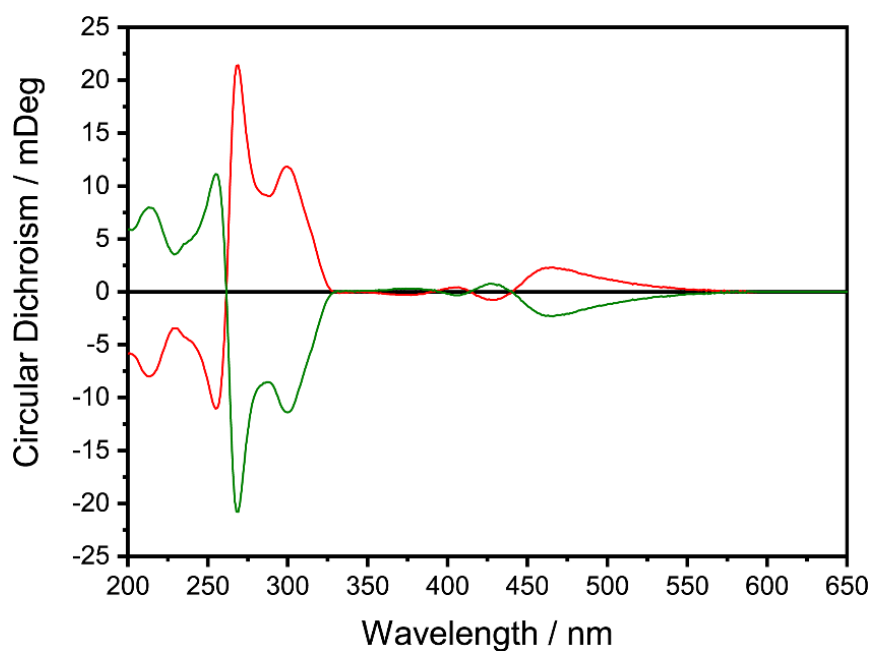

Figure S2. Circular dichroism spectra of the Δ (green) and Λ (red) enantiomers of **Ru-1** at a concentration of 4 µM in 50 mM NaCl aqueous buffer solution.
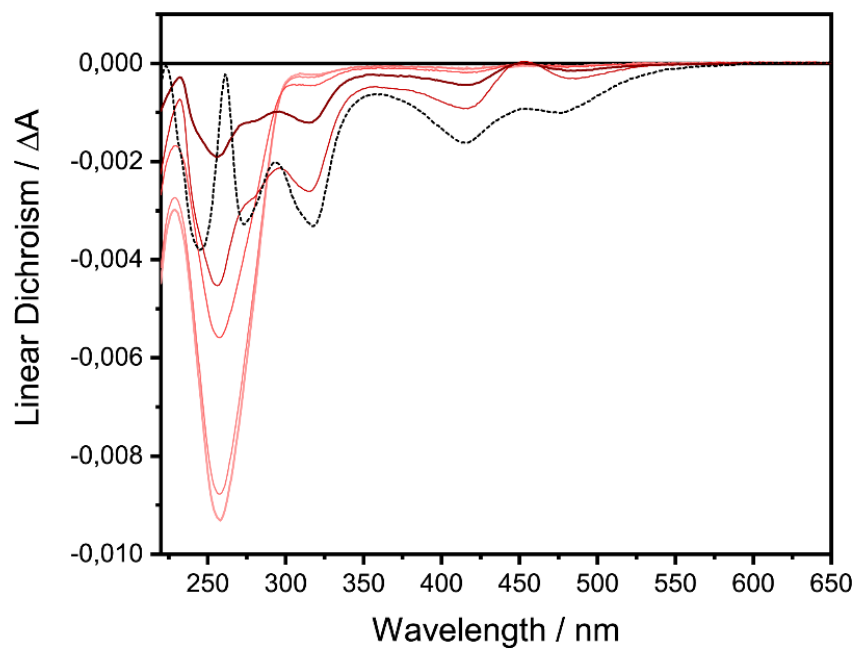
Figure S3. Linear dichroism spectra of Λ-**Ru-1** (red) and ΛΛ-**Ru-2** (dotted black, incubated 1 d at 50°C) in the presence of ctDNA at [base pairs]/[complex] ratio 5 in 50 mM NaCl aqueous buffer solution with 20% (w/w) PEG-400. The color change from light to dark specify spectral change for Λ-**Ru-1** with time (0.5 h, 1.5 h, 1 d, 2 d, and 7 d) after 50°C incubation. The concentration of ctDNA is 150 μM nucleotides.
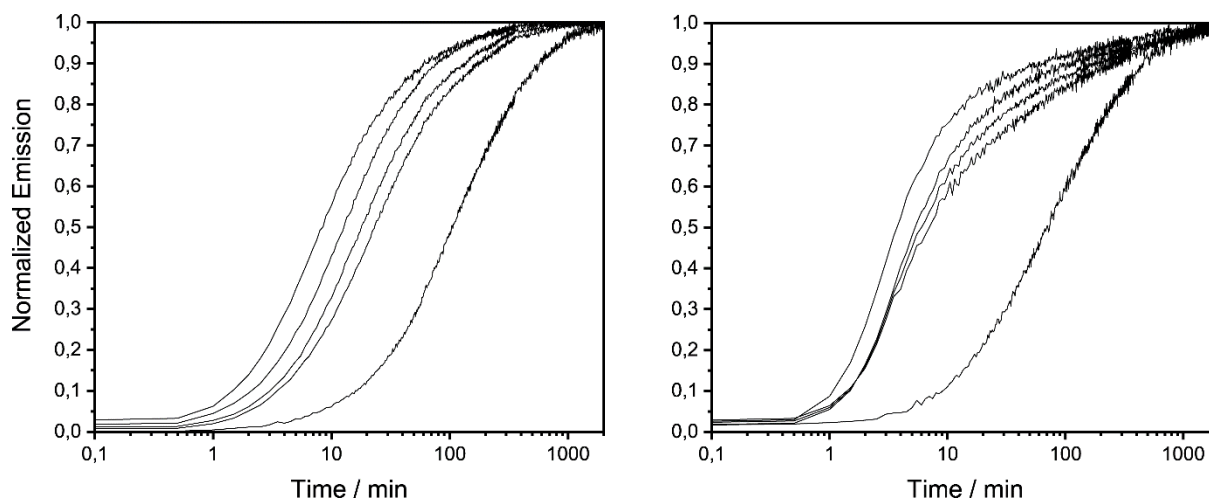

Figure S4. Association kinetics of ΔΔ- (left) and ΛΛ-**Ru-2** (right) in the presence of ctDNA, measured at different concentrations of PEG-400. PEG-400 concentrations from left to right are 20, 15, 10, 5 and 0% (w/w). Measurements performed at 50°C in 50 mM NaCl. The concentrations of complex and ctDNA were 15 μM and 150 μM nucleotides, respectively.
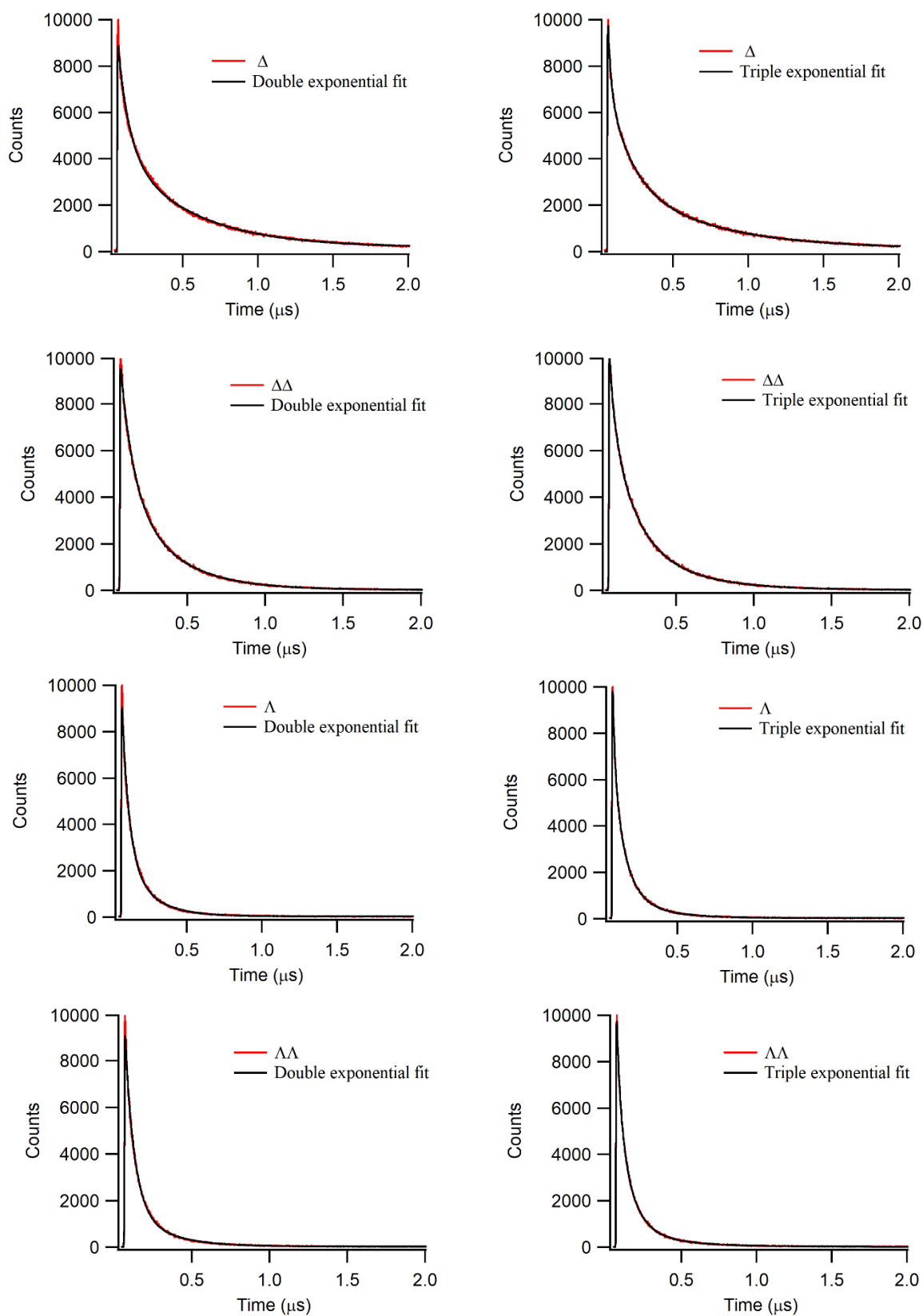
Figure S5. Excited state lifetime decay fittings curves for **Ru-1** and **Ru-2** enantiomers in the presence of ctDNA and 20% (w/w) PEG-400. The concentrations of complex and ctDNA were 15 μM and 150 μM nucleotides, respectively. Measurements were performed at room temperature in 50 mM NaCl.
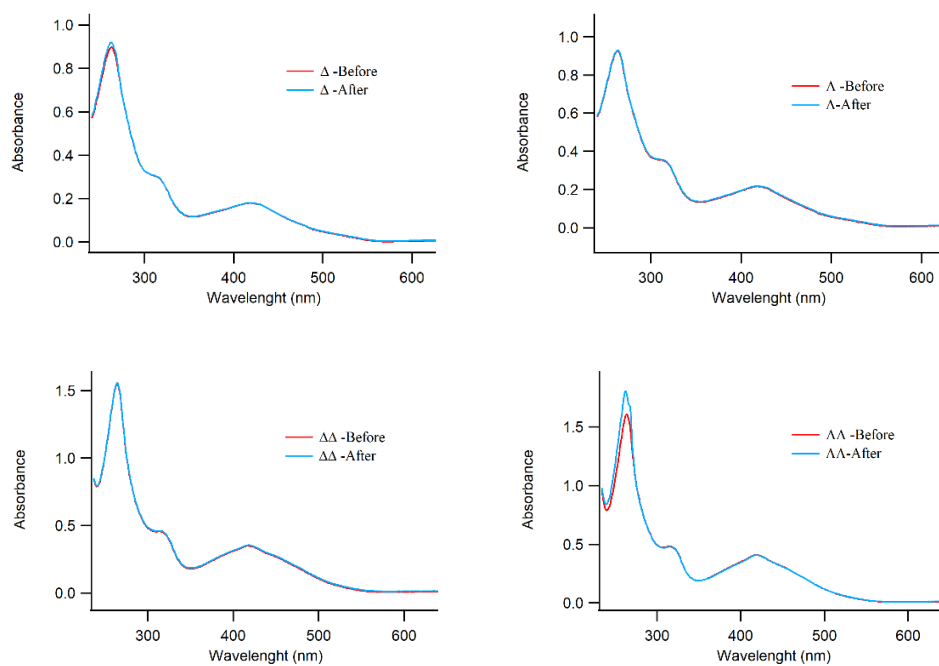
Figure S6. Absorption spectra of **Ru-1** and **Ru-2** enantiomers before (red) and after (blue) excited state lifetime measurements.

Table S1. Luminescence decay parameters for **Ru-1 and Ru-2** enantiomers in the presence of ctDNA and 20% (w/w) PEG-400 using a triexponential fitting.

Sample[a]	τ_1(ns)	α_1	τ_2(ns)	α_2	τ_3(ns)	α_3	$\tau_{avg}{}^b$(ns)
Δ-**Ru-1**	587	0.29	145	0.38	19	0.33	232
Λ-**Ru-1**	227	0.12	77	0.50	16	0.38	72
ΔΔ-**Ru-2**	355	0.27	144	0.47	33	0.26	172
ΛΛ-**Ru-2**	303	0.08	90	0.52	26	0.40	81

[a]150 µM nucleotides and 15 µM complex in 50 mM NaCl after 50°C incubation.
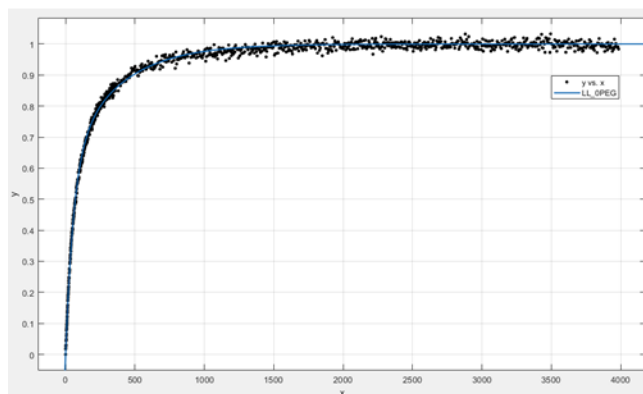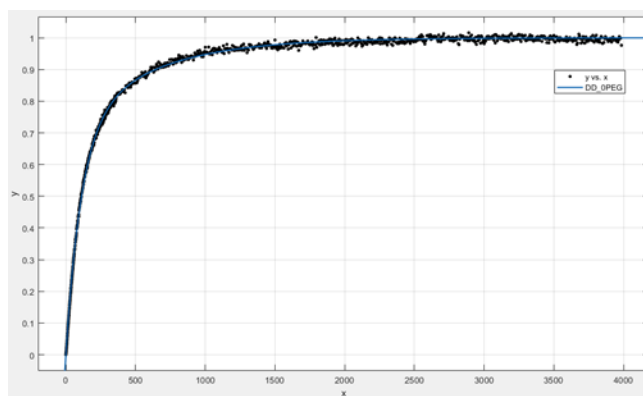[b]The average emission lifetime calculated as $\tau_{avg} = \alpha_1\tau_1 + \alpha_2\tau_2 + \alpha_3\tau_3$.

Figure S7. Fitting of biexponential model to association kinetic curves for ΔΔ- and ΛΛ-**Ru-2** at 0% (w/w) PEG-400 concentration (visualized in MATLAB 2017B).
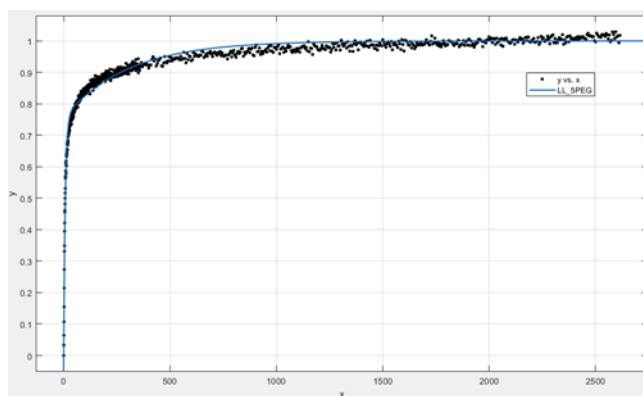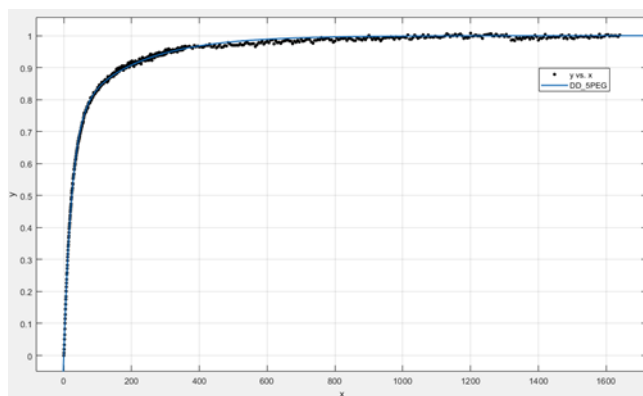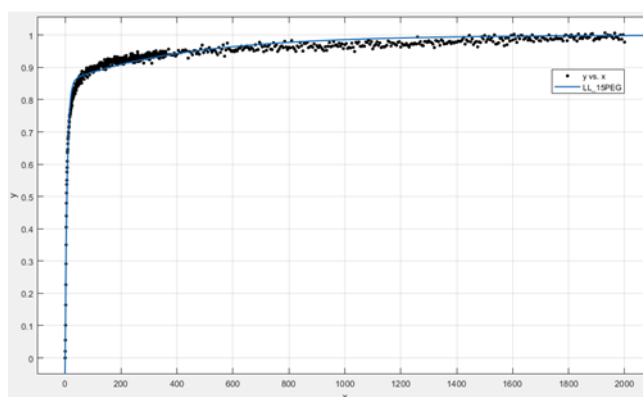

Figure S8. Fitting of biexponential model to association kinetic curves for ΔΔ- and ΛΛ-**Ru-2** at 5% (w/w) PEG-400 concentration (visualized in MATLAB 2017B).

6
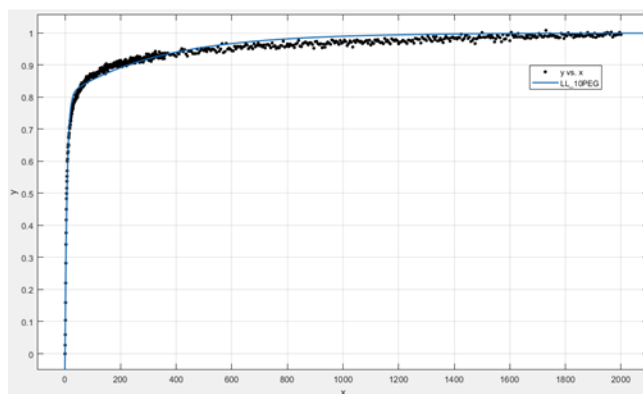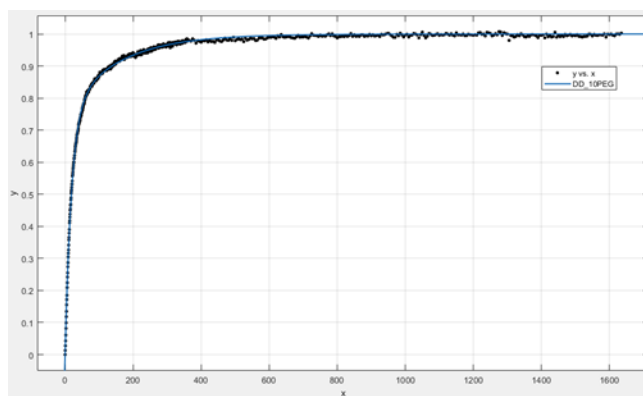
Figure S9. Fitting of biexponential model to association kinetic curves for ΔΔ- and ΛΛ-**Ru-2** at 10% (w/w) PEG-400 concentration (visualized in MATLAB 2017B).
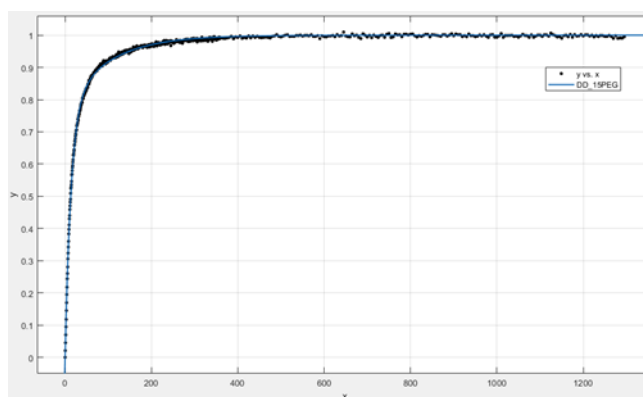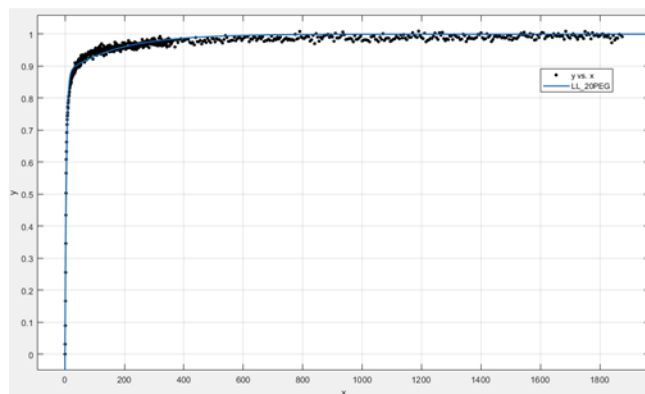

Figure S10. Fitting of biexponential model to association kinetic curves for ΔΔ- and ΛΛ-**Ru-2** at 15% (w/w) PEG-400 concentration (visualized in MATLAB 2017B).
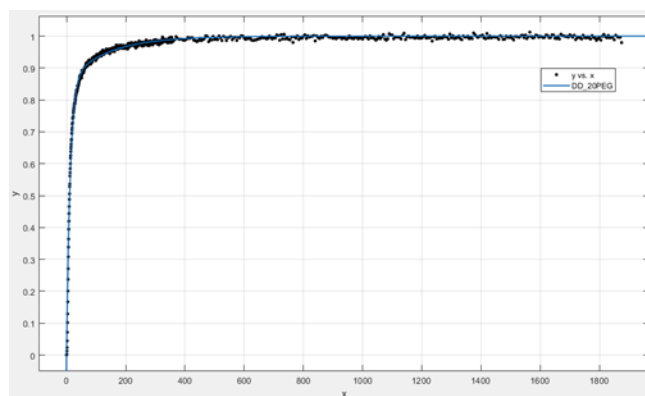
Figure S11. Fitting of biexponential model to association kinetic curves for ΔΔ- and ΛΛ-**Ru-2** at 20% (w/w) PEG-400 concentration (visualized in MATLAB 2017B).
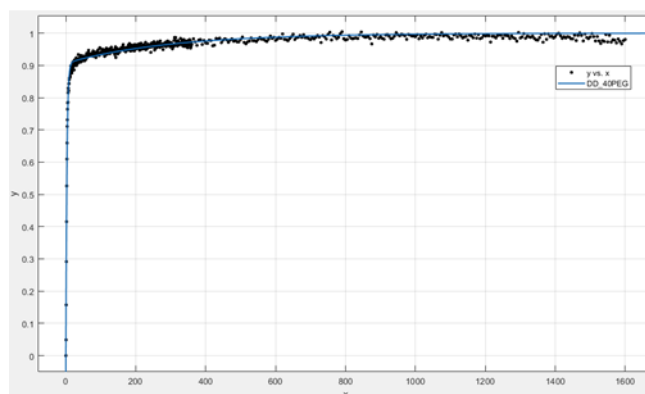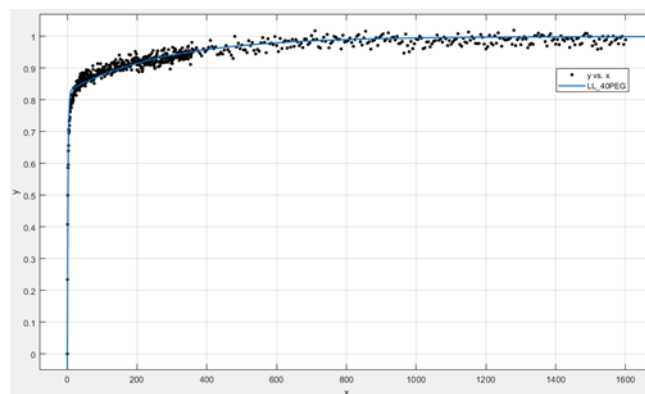

Figure S12. Fitting of biexponential model to association kinetic curves for ΔΔ- and ΛΛ-**Ru-2** at 40% (w/w) PEG-400 concentration (visualized in MATLAB 2017B).
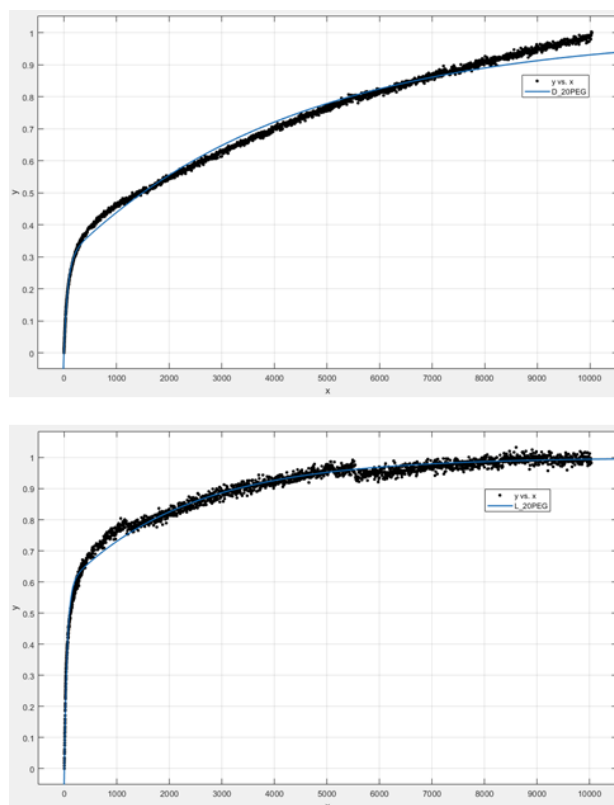
Figure S13. Fitting of biexponential model to association kinetic curves for Δ- and Λ-**Ru-1** at 20% (w/w) PEG-400 concentration (visualized in MATLAB 2017B).
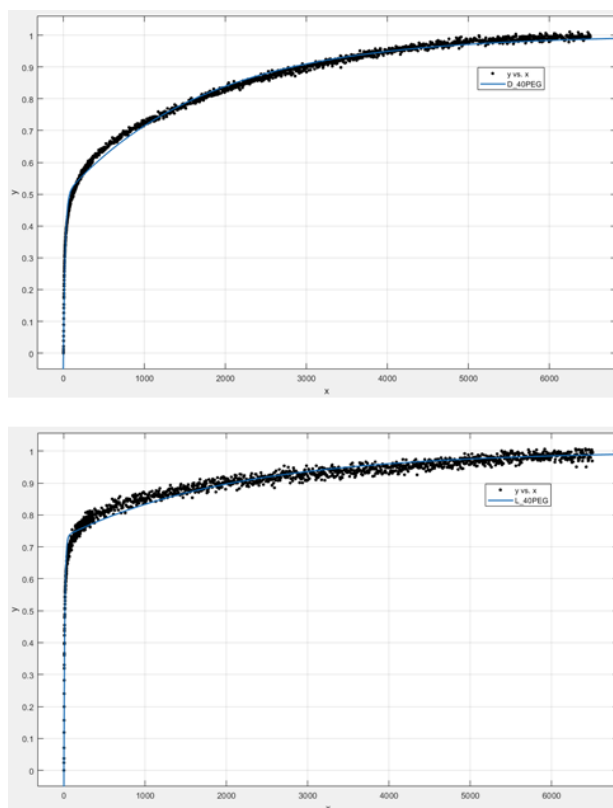

Figure S14. Fitting of biexponential model to association kinetic curves for Δ- and Λ-**Ru-1** at 40% (w/w) PEG-400 concentration (visualized in MATLAB 2017B).
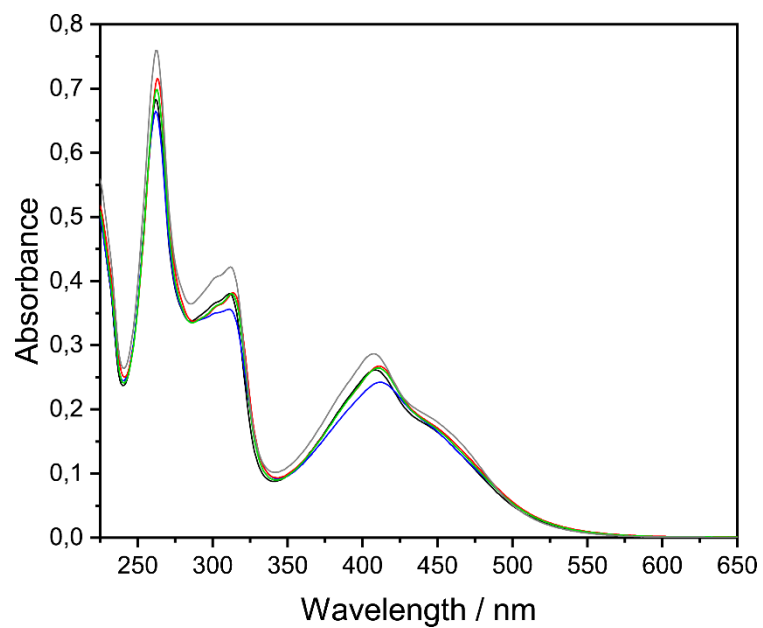
Figure S15. Absorption spectra of ΔΔ-**Ru-2** (~4 µM) in different solvents: MeOH/H2O (1:1) (gray), 40% (w/w) PEG-400 + 50 mM NaCl buffer (red), MilliQ-pure water (black), 15% (w/w) PEG-400 + 50 mM NaCl buffer (green), 50 mM NaCl buffer (blue). All measurements were performed in room-temperature.