

SUPPLEMENTARY MATERIALS

Impact of Non-Covalent Interactions of Chiral Linked Systems in Solution on Photoinduced Electron Transfer Efficiency

Ilya M. Magin¹, Ivan A. Pushkin^{1,2}, Aleksandra A. Ageeva^{1,2}, Sofia O. Martianova^{1,2}, Nikolay E. Polyakov¹, Alexander B. Doktorov^{1*} and Tatyana V. Leshina¹

¹Voevodsky Institute of Chemical Kinetics and Combustion, 630090 Novosibirsk, Russia;

²Department of Natural Sciences, Novosibirsk State University, 630090 Novosibirsk, Russia

* Correspondence: doktorov@kinetics.nsc.ru

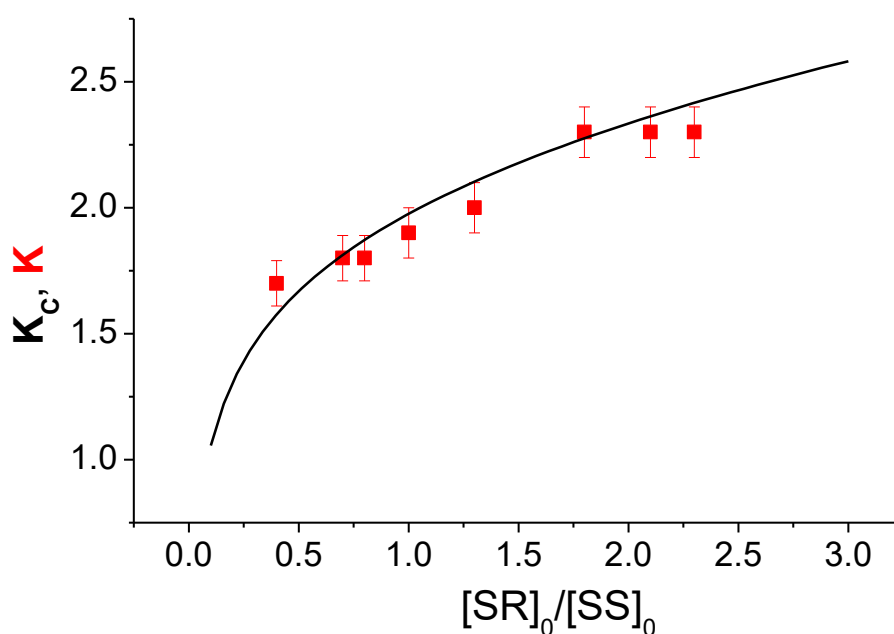


Figure S1. Experimental (K) and calculated (K_c) dependences of the CIDNP on the diastereomers (R,S)NPX-Pyr dyad concentrations ratio. Calculation parameters: $\alpha_{SR}=2$, $\alpha_{SS}=1$, $\beta_{SR}=0.1$, $\beta_{SS}=0.1$, $\gamma=0$; dimerization equilibrium constants: $K_{RS}=2\times 10^5$ M⁻¹, $K_{SS}=2\times 10^5$ M⁻¹, $K_{RS,SS}=1\times 10^5$ M⁻¹. Here, α , β and γ are the efficiencies of polarization formation in homo-, hetero-dimers and monomers.

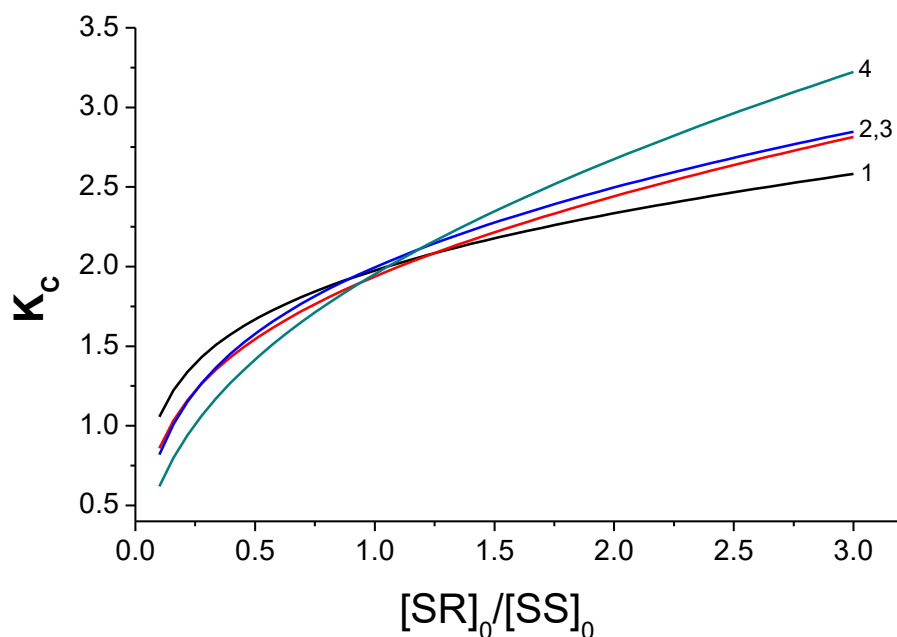


Figure S2. Calculated (K_c) dependences of the CIDNP on the diastereomers (R,S)NPX-Pyr dyad concentrations ratio with different dimerization equilibrium constants. Calculation parameters: $\alpha_{SR}=2$, $\alpha_{SR}=1$, $\beta_{SR}=0.1$, $\beta_{SS}=0.1$, $\gamma=0$. Dimerization equilibrium constants: 1) $K_{SR,SR}=2\times 10^5 \text{ M}^{-1}$, $K_{SS,SS}=2\times 10^5 \text{ M}^{-1}$, $K_{SR,SS}=1\times 10^5 \text{ M}^{-1}$; 2) $K_{SR,SR}=1\times 10^5 \text{ M}^{-1}$, $K_{SS,SS}=2\times 10^5 \text{ M}^{-1}$, $K_{SR,SS}=1\times 10^5 \text{ M}^{-1}$; 3) $K_{SR,SR}=2\times 10^5 \text{ M}^{-1}$, $K_{SS,SS}=1\times 10^5 \text{ M}^{-1}$, $K_{SR,SS}=1\times 10^5 \text{ M}^{-1}$; 4) $K_{SR,SR}=2\times 10^5 \text{ M}^{-1}$, $K_{SS,SS}=2\times 10^5 \text{ M}^{-1}$, $K_{SR,SS}=2\times 10^5 \text{ M}^{-1}$. Here, α , β and γ are the efficiencies of polarization formation in homo-, hetero-dimers and monomers.

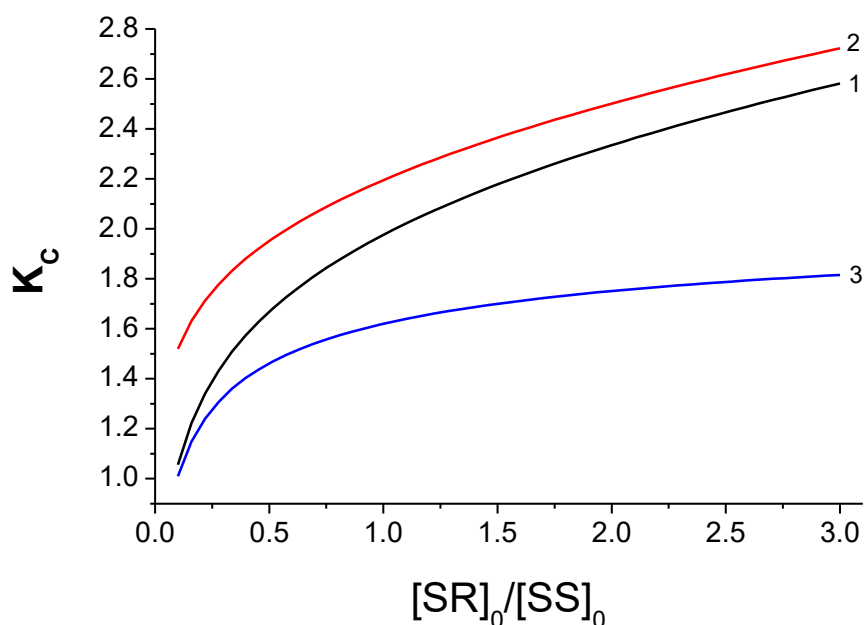


Figure S3. Calculated (K_c) dependences of the CIDNP on the diastereomers (R,S)NPX-Pyr dyad concentrations ratio with different β . Calculation parameters: $\alpha_{SR}=1.8$, $\alpha_{SS}=1$, $\gamma=0$; dimerization equilibrium constants: $K_{RS}=2\times 10^5 \text{ M}^{-1}$, $K_{SS}=2\times 10^5 \text{ M}^{-1}$, $K_{RS,SS} = 1\times 10^5 \text{ M}^{-1}$. 1) $\beta_{SR}=0.1$, $\beta_{SS}=1$; 2) $\beta_{SR}=0.1$, $\beta_{SS}=1$; 3) $\beta_{SR}=0.1$, $\beta_{SS}=1$; Here, α , β and γ are the efficiencies of polarization formation in homo-, hetero-dimers and monomers.

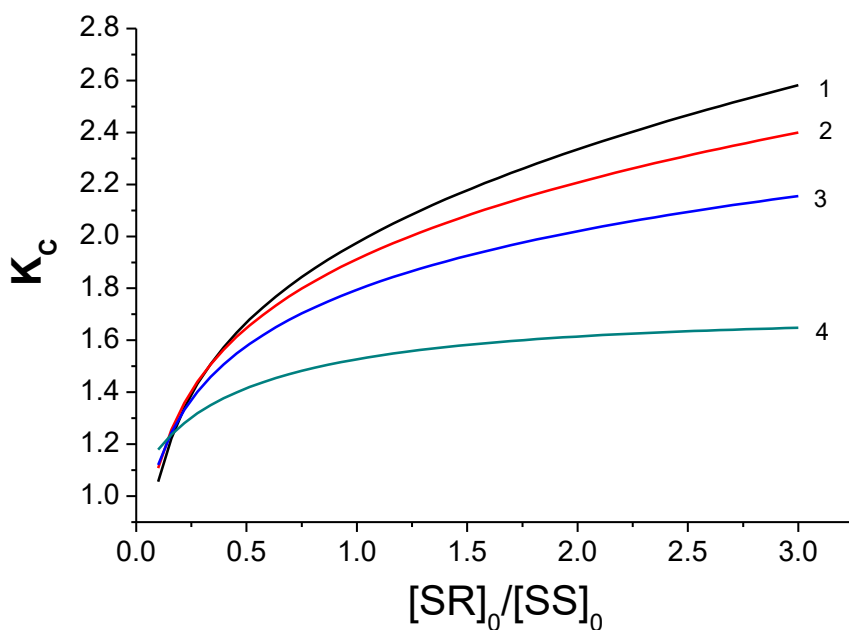


Figure S4. Calculated (K_c) dependences of the CIDNP on the diastereomers (R,S)NPX-Pyr dyad concentrations ratio with different dimerization equilibrium constants, taking into account γ . Calculation parameters: $\alpha_{SR}=2$, $\alpha_{SR}=1$, $\beta_{SR}=0.1$, $\beta_{SS}=0.1$. Dimerization equilibrium constants: 1) $\gamma=0$, $K_{SR,SR}=2\times 10^5$, $K_{SS,SS}=2\times 10^5$, $K_{SR,SS}=1\times 10^5 \text{ M}^{-1}$; 2) $\gamma=1$, $K_{SR,SR}=2\times 10^5 \text{ M}^{-1}$, $K_{SS,SS}=2\times 10^5 \text{ M}^{-1}$, $K_{SR,SS}=1\times 10^5 \text{ M}^{-1}$; 3) $\gamma=1$, $K_{SR,SR}=2\times 10^4 \text{ M}^{-1}$, $K_{SS,SS}=2\times 10^4 \text{ M}^{-1}$, $K_{SR,SS}=1\times 10^4 \text{ M}^{-1}$; 4) $\gamma=1$, $K_{SR,SR}=2\times 10^3 \text{ M}^{-1}$, $K_{SS,SS}=2\times 10^3 \text{ M}^{-1}$, $K_{SR,SS}=1\times 10^3 \text{ M}^{-1}$. Here, α , β and γ are the efficiencies of polarization formation in homo-, hetero-dimers and monomers.

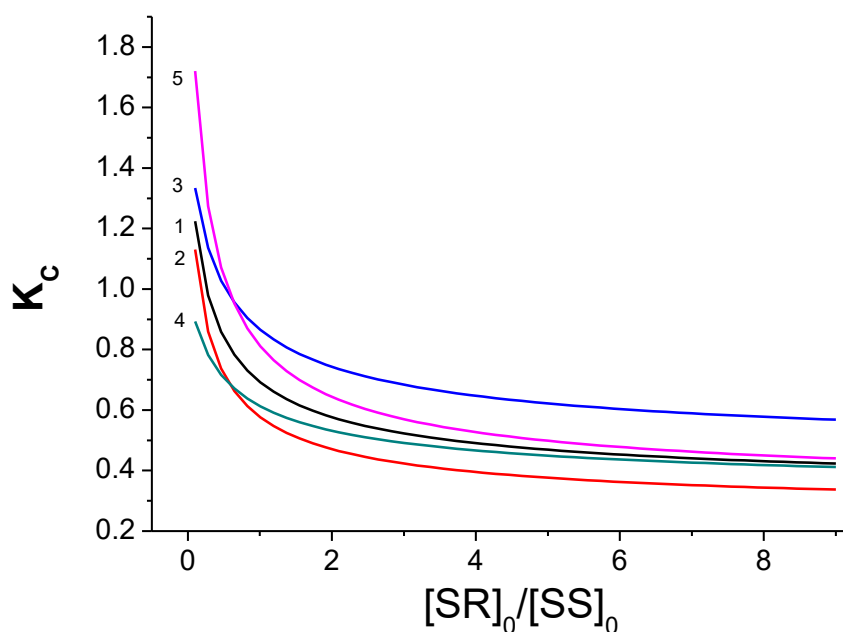


Figure S5. Calculated (K_c) dependences of the CIDNP on the diastereomers (R,S)NPX-Trp dyad concentrations ratio with different β . Calculation parameters: $\alpha_{SR}=1.8$, $\alpha_{SS}=1$, $\gamma=0$; dimerization equilibrium constants: $K_{RS} = 2 \times 10^5 \text{ M}^{-1}$, $K_{SS} = 2 \times 10^5 \text{ M}^{-1}$, $K_{RS,SS} = 2 \times 10^5 \text{ M}^{-1}$. 1) $\beta_{SR}=1.6$, $\beta_{SS}=5.5$; 2) $\beta_{SR}=1.6$, $\beta_{SS}=7$; 3) $\beta_{SR}=1.6$, $\beta_{SS}=4$; 4) $\beta_{SR}=1$, $\beta_{SS}=5.5$; 5) $\beta_{SR}=2.5$, $\beta_{SS}=5.5$. Here, α , β and γ are the efficiencies of polarization formation in homo-, hetero-dimers and monomers.

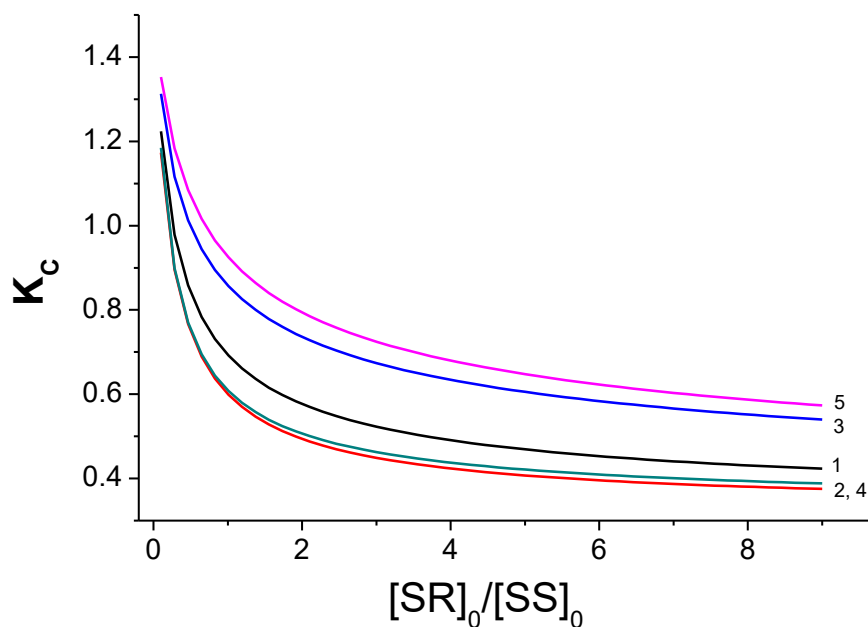


Figure S6. Calculated (K_c) dependences of the CIDNP on the diastereomers (R,S)NPX-Trp dyad concentrations ratio with different dimerization equilibrium constants. Calculation parameters: $\alpha_{SR}=1.8$, $\alpha_{SR}=1$, $\beta_{SR}=1.6$, $\beta_{SS}=5.5$, $\gamma=0$.

Dimerization equilibrium constants: 1) $K_{SR,SR}=2\times 10^5\text{ M}^{-1}$, $K_{SS,SS}=2\times 10^5\text{ M}^{-1}$, $K_{SR,SS}=2\times 10^5\text{ M}^{-1}$; 2) $K_{SR,SR}=1\times 10^5$, $K_{SS,SS}=2\times 10^5\text{ M}^{-1}$, $K_{SR,SS}=2\times 10^5\text{ M}^{-1}$; 3) $K_{SR,SR}=5\times 10^5\text{ M}^{-1}$, $K_{SS,SS}=2\times 10^5\text{ M}^{-1}$, $K_{SR,SS}=2\times 10^5\text{ M}^{-1}$; 4) $K_{SR,SR}=2\times 10^5\text{ M}^{-1}$, $K_{SS,SS}=1\times 10^5\text{ M}^{-1}$, $K_{SR,SS}=2\times 10^5\text{ M}^{-1}$; 5) $K_{SR,SR}=2\times 10^5\text{ M}^{-1}$, $K_{SS,SS}=2\times 10^5\text{ M}^{-1}$, $K_{SR,SS}=1\times 10^5\text{ M}^{-1}$. Here, α , β and γ are the efficiencies of polarization formation in homo-, hetero-dimers and monomers.

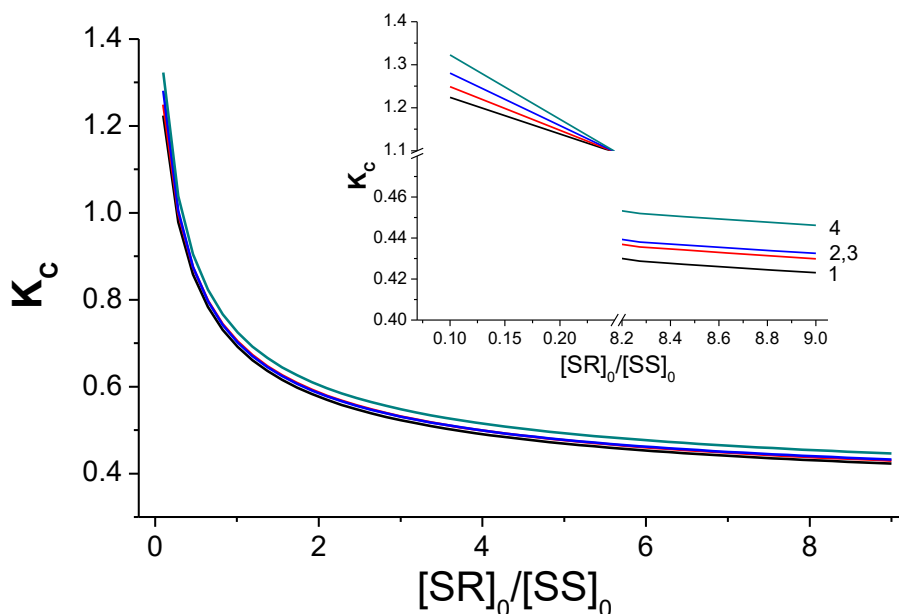


Figure S7. Calculated (K_c) dependences of the CIDNP on the diastereomers (R,S)NPX-Trp dyad concentrations ratio with different γ at height dimerization equilibrium constants. Calculation parameters: $\alpha_{SR}=1.8$, $\alpha_{SR}=1$, $\beta_{SR}=1.6$, $\beta_{SS}=5.5$. Dimerization equilibrium constants γ . $K_{SR,SR}=2\times 10^5\text{ M}^{-1}$, $K_{SS,SS}=2\times 10^5\text{ M}^{-1}$, $K_{SR,SS}=2\times 10^5\text{ M}^{-1}$ 1) $\gamma=0$; 2) $\gamma=2$; 3) $\gamma=5$; 4) $\gamma=5$. Here, α , β and γ are the efficiencies of polarization formation in homo-, hetero-dimers and monomers

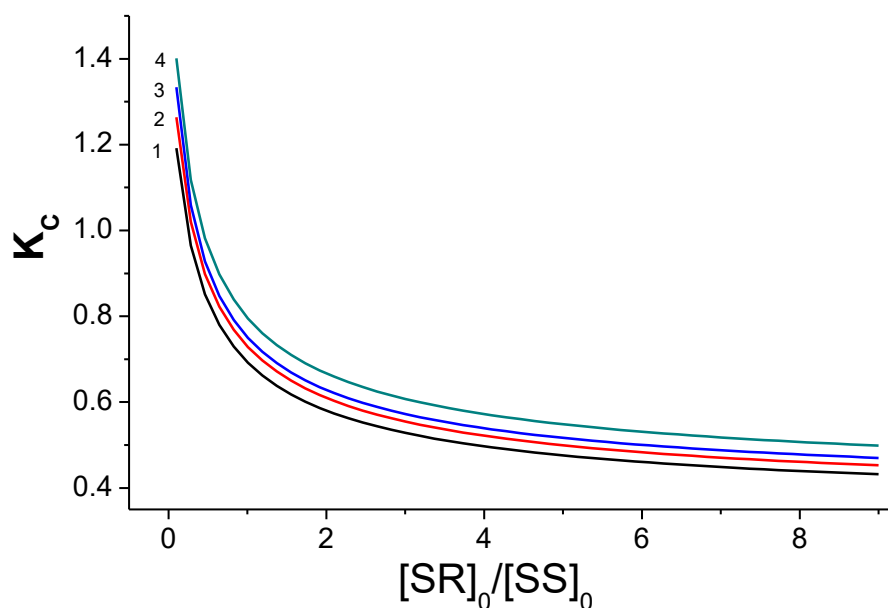


Figure S8. Calculated (K_c) dependences of the CIDNP on the diastereomers (R,S)NPX-Trp dyad concentrations ratio with different γ at medium dimerization equilibrium constants. Calculation parameters: $\alpha_{SR}=1.8$, $\alpha_{SR}=1$, $\beta_{SR}=1.6$, $\beta_{SS}=5.5$. Dimerization equilibrium constants γ . $K_{SR,SR}=2 \times 10^4 \text{ M}^{-1}$, $K_{SS,SS}=2 \times 10^4 \text{ M}^{-1}$, $K_{SR,SS}=2 \times 10^4 \text{ M}^{-1}$ 1) $\gamma=0$; 2) $\gamma=2$; 3) $\gamma=5$; 4) $\gamma=10$. Here, α , β and γ are the efficiencies of polarization formation in homo-, hetero-dimers and monomers.

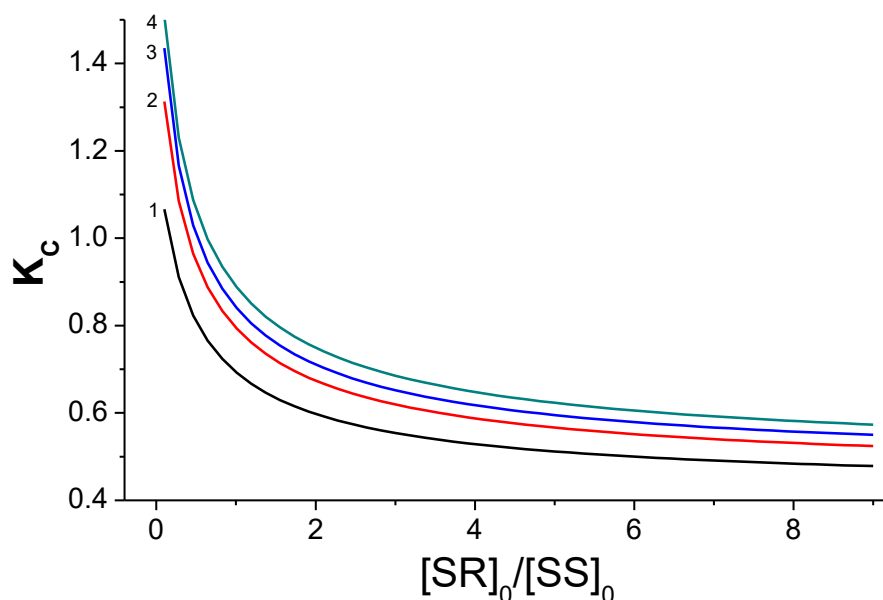


Figure S9. Calculated (K_c) dependences of the CIDNP on the diastereomers (R,S)NPX-Trp dyad concentrations ratio with different γ at low dimerization equilibrium constants. Calculation parameters: $\alpha_{SR}=1.8$, $\alpha_{SR}=1$, $\beta_{SR}=1.6$, $\beta_{SS}=5.5$.

Dimerization equilibrium constants γ . $K_{SR,SR}=2\times 10^3$, $K_{SS,SS}=2\times 10^3$, $K_{SR,SS}=2\times 10^3$. 1) $\gamma=0$; 2) $\gamma=2$; 3) $\gamma=5$; 4) $\gamma=10$. Here, α , β and γ are the efficiencies of polarization formation in homo-, hetero-dimers and monomers.