Supplementary Information for

Impact of Chirality on the Photoinduced Charge Transfer in Linked Systems Containing Naproxen Enantiomers.

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Synthesis and Characterization of Dyads

Materials and solvents. (R)- and (S)-naproxen (NPX), (S)-N-methyl-2-pyrrolidinemethanol, N-(3-dimethylaminopropyl)-N-ethylcarbodiimide hydrochloride (EDCI), N-hydroxysuccinimide, 2,4,6-trichlorobenzoyl chloride, 4-aminobutyric acid, dicyclohexylcarbodiimide (DCC), 4-dimethylaminopyridine (DMAP), pyridine and triethylamine were purchased from Sigma-Aldrich; (1S,3R)-3-aminocyclopentane carboxylic acid was provided by Acros Organics. Tetrahydrofuran (THF), dimethylaminopyridine (DMAP), pyridine and triethylamine were purchased from Sigma-Aldrich; ethyl acetate, n-hexane, dichloromethane, methanol, benzene and sodium hydrogen carbonate were from Scharlab. Acetonitrile and benzene for optic measurements were from Cryochrom and Soyuzchemprom, respectively. Deuteroacetonitrile (D 99.9%) and deuterobenzene (D 99.8%) for CIDNP measurements were provided by Aldrich.

Synthesis of dyads. The synthetic strategy employed to prepare the dyads used in this study is outlined in Scheme 1.

Scheme 1. Synthesis of NPX-pyrrolidine dyads: (i) N-hydroxysuccinimide, DCC, THF, rt.; (ii) 4-aminobutyric acid, NaHCO₃, H₂O, THF, rt.; (iii) (1S,3R)-3-aminocyclopentane carboxylic acid, NaHCO₃, H₂O, THF, rt.; (iv) 2,4,6-trichlorobenzoyl chloride, Et₃N, (S)-N-methyl-2-pyrrolidinemethanol, DMAP, THF, rt.; (v) EDCi, pyridine, DMAP, (S)-N-methyl-2-pyrrolidinemethanol, N₂, rt.

Synthesis of (R/S)-NPX-amino acids 5(a,b) and 6(a,b). To a cold solution of (R)- or (S)-NPX (2.0 g, 8.7 mmol) in THF (60 mL), DCC (2.0 g, 9.6 mmol) was added portionwise, and the mixture was stirred at 0 °C for 20 min. Then, N-hydroxysuccinimide (1.0 g, 8.7 mmol) was added and the mixture was stirred overnight at room temperature. The resulting reaction mixture was filtered, and the filtrate was distilled under reduced pressure. The product (3.0 g, 9.0 mmol) was dissolved in THF (35 mL) and was added dropwise, under stirring, to a solution of 4-aminobutyric acid or (1S,3R)-3-aminocyclopentane carboxylic acid (9.0 mmol) and NaHCO₃ (1.5 g, 18 mmol) in distilled water (25 mL) and then stirred at room temperature for 2 days. Afterwards, the reaction was filtered, and the filtrate was concentrated to approximately 25 mL. Then, concentrated hydrochloric acid was added dropwise until pH 5, and the filtrate was extracted with AcOEt (3 x 25 mL). The combined organic layers were washed with brine, dried over anhydrous magnesium sulfate and concentrated. The crude was purified by column chromatography (CH₂Cl₂/CH₃OH, 97 : 3) to give (R)-NPX-AA (1.8 g, 62 %), (S)-NPX-AA (1.6 g, 54 %), (R)-NPX-CyAA (2.3 g, 69 %) or (S)-NPX-CyAA (2.4 g, 77 %), respectively, as white solids.

Synthesis of (R,S)- and (S,S)-NPX-amino acid–pyrrolidine ester dyads 2(a,b) and 3(a,b). 2,4,6-trichlorobenzoyl chloride (381 µL, 2.4 mmol) and Et₃N (621 µL, 4.4 mmol) were added dropwise to a solution of the corresponding NPX-amino acid (2.2 mmol) in anhydrous THF (10 mL) at room temperature under nitrogen. The resulting solution was stirred for 1 h and reacted with a solution of (S)-
N-methyl-2-pyrrolidinemethanol (343 µL, 2.9 mmol) in anhydrous THF (3 mL), in the presence of DMAP (353 mg, 2.9 mmol), overnight at room temperature. Then, the reaction was quenched with saturated aq. NaHCO₃ solution, and extracted with AcOEt. The combined organic layers were washed with aqueous acetic acid and brine, dried over anhydrous magnesium sulfate and evaporated under reduced pressure, to get a white solid, which was recrystallized from a mixture of n-hexane : AcOEt (2 : 3). Dyads 2a (0.7 g, 74 %), 2b (0.6 g, 62 %), 3a (0.7 g, 79 %) and 3b (0.8 g, 83 %) were obtained as white solids.

**Synthesis of (R,S)- and (S,S)-NPX-pyrrolidine ester dyads 4(a,b).** To a solution of (R)- or (S)-NPX (2 g, 8.7 mmol) in anhydrous pyridine (20 mL), EDCi (1.6 g, 8.7 mmol) and DMAP (10 mg, 0.1 mmol) were added dropwise, at room temperature under nitrogen, and the resulting solution was stirred for 20 min. Then, (S)-N-methyl-2-pyrrolidinemethanol (1.1 mL, 8.9 mmol) was added, and the mixture was stirred 48 h at room temperature. Afterwards, the reaction mixture was distilled under reduced pressure, to get a residue, which was re-dissolved in AcOEt and washed with aqueous hydrochloric acid 1M and brine, dried over anhydrous magnesium sulfate and concentrated. The crude was purified by column chromatography (CH₂Cl₂ : CH₂OH, 97 : 3) to give 4a (1.4 g, 47 %) or 4b (1.5 g, 50 %) as orange oils. ¹H NMR and ¹³C NMR data were found to be coincident with those previously described. [1,2]

**Characterization.**

**(R)-NPX-AA-(S)-Pyr (2a).** ¹H NMR (300 MHz, CDCl₃): δ 1.45-1.53 (m, 1H), 1.55 (d, J = 7.2 Hz, 3H), 1.62-1.93 (m, 5H), 2.14-2.29 (m, 3H), 2.33 (s, 3H), 2.35-2.43 (m, 1H), 2.98-3.06 (m, 1H), 3.12-3.24 (m, 2H), 3.65 (q, J = 7.2 Hz, 1H), 3.88 (s, 3H), 3.97 (m, 2H), 5.83 (t, J = 5.4 Hz, 1H), 7.08-7.15 (m, 2H), 7.35 (dd, J = 8.4 and 1.8 Hz, 1H), 7.62-7.71 (m, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 18.4 (CH₃), 22.7 (CH₂), 24.4 (CH₃), 28.1 (CH₂), 31.4 (CH₂), 38.9 (CH₂), 41.3 (CH₃), 46.9 (CH), 55.2 (CH₂), 57.4 (CH₂), 63.7 (CH), 66.2 (CH₂), 105.5 (CH), 119.0 (CH), 125.9 (Ar-CH), 126.1 (CH), 127.4 (CH), 128.8 (C), 129.1 (CH), 133.6 (C), 136.4 (C), 157.6 (C), 173.1 (C), 174.4 (C). Exact mass: m/z found 413.2440, calculated for C₂₄H₃₃N₂O₄ (MH⁺) 413.2440.

**(S)-NPX-AA-(S)-Pyr (2b).** ¹H NMR (300 MHz, CDCl₃): δ 1.44-1.53 (m, 1H), 1.55 (d, J = 7.2 Hz, 3H), 1.62-1.91 (m, 5H), 2.14-2.27 (m, 3H), 2.33 (s, 3H), 2.34-2.40 (m, 1H), 2.97-3.05 (m, 1H), 3.19 (m, 2H), 3.64 (q, J = 7.2 Hz, 1H), 3.88 (s, 3H), 3.92 (dd, J = 11.1 and 5.1 Hz, 1H), 3.99 (dd, J = 10.8 and 5.1 Hz, 1H), 5.80 (br t, J = 5.4 Hz, 1H), 7.07-7.15 (m, 2H), 7.34 (dd, J = 8.4 and 1.8 Hz, 1H), 7.62-7.71 (m, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 18.4 (CH₃), 22.7 (CH₂), 24.4 (CH₂), 28.2 (CH₂), 31.4 (CH₂), 38.9 (CH₂), 41.3 (CH₃), 46.9 (CH), 55.2 (CH₂), 57.4 (CH₂), 63.7 (CH), 66.2 (CH₂), 105.5 (CH), 119.0 (CH), 125.9 (Ar-CH), 126.1 (CH), 127.4 (CH), 128.8 (C), 129.1 (CH), 133.6 (C), 136.4 (C), 157.6 (C), 173.1 (C), 174.4 (C). Exact mass: m/z found 413.2440, calculated for C₂₄H₃₃N₂O₄ (MH⁺) 413.2440.

**(R)-NPX-CyAA-(S)-Pyr (3a).** ¹H NMR (300 MHz, CDCl₃): δ 1.42-1.97 (m, 8H), 1.58 (d, J = 7.2 Hz, 3H), 2.01-2.27 (m, 3H), 2.29-2.40 (m, 1H), 2.34 (s, 3H), 2.74-2.92 (m, 1H), 2.99-3.09 (m, 1H), 3.64 (q, J = 7.2 Hz, 1H), 3.91 (br s, 5H), 4.26-4.38 (m, 1H), 6.10 (br d, J = 6.9 Hz, 1H), 7.09-7.17 (m, 2H), 7.39 (dd, J = 9.0 and 1.8 Hz, 1H), 7.66-7.74 (m, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 18.5 (CH₂), 22.8 (CH₂), 28.2 (CH₂), 33.0 (CH₂), 36.1 (CH₂), 41.4 (CH), 41.8 (CH), 47.1 (CH), 51.0 (CH), 55.3 (CH₃), 57.6 (CH₂), 63.8 (CH), 66.8 (CH₂), 105.6 (CH), 118.9 (CH), 126.0 (CH), 126.3 (CH), 127.3 (CH), 129.0 (C), 129.3 (CH), 133.6 (C), 136.6 (C), 157.6 (C), 173.7 (C), 177.3 (C). Exact mass: m/z found 439.2618, calculated for C₂₇H₃₅N₂O₄ (MH⁺) 439.2597.

**(S)-NPX-CyAA-(S)-Pyr (3b).** ¹H NMR (300 MHz, CDCl₃): δ 1.44-1.94 (m, 8H), 1.55 (d, J = 7.2 Hz, 3H), 2.03-2.28 (m, 3H), 2.29-2.45 (m, 1H), 2.34 (s, 3H), 2.77-2.89 (m, 1H), 3.00-3.09 (m, 1H), 3.64 (q, J = 7.2 Hz, 1H), 3.85-4.00 (m, 2H), 3.90 (s, 3H), 4.25-4.37 (m, 1H), 6.20 (br d, J = 7.5 Hz, 1H), 7.08-7.16 (m, 2H), 7.37 (dd, J = 8.7 and 1.8 Hz, 1H), 7.65-7.72 (m, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 18.4 (CH₂), 22.8 (CH₂), 28.1 (CH₂), 28.2 (CH₂), 32.9 (CH₂), 35.8 (CH₂), 41.4 (CH), 41.7 (CH), 47.0 (CH), 51.0 (CH), 55.2 (CH₃), 57.5 (CH₂), 63.8 (CH), 66.7 (CH₂), 105.5 (CH), 118.9 (CH), 126.0 (CH), 126.2
(CH), 127.3 (CH), 129.0 (C), 129.2 (CH), 133.6 (C), 136.8 (C), 157.5 (C), 173.6 (C), 177.3 (C). Exact mass: m/z found 439.2607, calculated for C_{26}H_{35}N_{2}O_{4} (MH\^+) 439.2597.

**(R)-NPX-AA.** \(^1\)H NMR (300 MHz, CDCl\(_3\)): δ 1.57 (d, J = 7.2 Hz, 3H), 1.64-1.76 (m, 2H), 2.26 (t, J = 7.2 Hz, 2H), 3.14-3.29 (m, 2H), 3.69 (q, J = 7.2 Hz, 1H), 3.89 (s, 3H), 5.88 (t, J = 5.7 Hz, 1H), 7.09-7.16 (m, 2H), 7.35 (dd, J = 8.7 and 1.8 Hz, 1H), 7.62-7.73 (m, 3H), 11.00 (s, 1H); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)): δ 18.3 (CH\(_3\)), 24.5 (CH\(_2\)), 31.2 (CH\(_2\)), 38.9 (CH\(_2\)), 46.8 (CH), 55.3 (CH\(_3\)), 105.6 (CH), 119.1 (CH), 126.1 (CH), 126.2 (CH), 127.5 (CH), 128.9 (C), 129.2 (CH), 133.7 (C), 136.1 (C), 157.7 (C), 175.2 (C), 177.5 (C). Exact mass: m/z found 316.1552, calculated for C\(_{18}\)H\(_{22}\)NO\(_4\) (MH\(^+\)) 316.1549.

**(S)-NPX-AA.** \(^1\)H NMR (300 MHz, CDCl\(_3\)): δ 1.57 (d, J = 7.2 Hz, 3H), 1.64-1.76 (m, 2H), 2.25 (m, 2H), 3.14-3.28 (m, 2H), 3.69 (q, J = 7.2 Hz, 1H), 3.88 (s, 3H), 6.00 (t, J = 5.7 Hz, 1H), 7.06-7.15 (m, 2H), 7.35 (dd, J = 8.4 and 1.8 Hz, 1H), 7.62-7.73 (m, 3H), 11.00 (s, 1H); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)): δ 18.3 (CH\(_3\)), 24.4 (CH\(_2\)), 31.2 (CH\(_2\)), 38.9 (CH\(_2\)), 46.8 (CH), 55.2 (CH\(_3\)), 105.6 (CH), 119.1 (CH), 126.0 (CH), 126.1 (CH), 127.5 (CH), 128.9 (C), 129.1 (CH), 133.7 (C), 136.1 (C), 157.6 (C), 175.2 (C), 177.4 (C). Exact mass: m/z found 316.1561, calculated for C\(_{18}\)H\(_{22}\)NO\(_4\) (MH\(^+\)) 316.1549.

**(R)-NPX-CyAA.** \(^1\)H NMR (300 MHz, CDCl\(_3\)): δ 1.56 (d, J = 7.2 Hz, 3H), 1.58-1.65 (m, 2H), 1.79-2.15 (m, 4H), 2.76-2.88 (m, 1H), 3.66 (q, J = 7.2 Hz, 1H), 3.88 (s, 3H), 4.25-4.38 (m, 1H), 6.25 (d, J = 7.8 Hz, 1H), 7.06-7.14 (m, 2H), 7.36 (dd, J = 8.4 and 1.8 Hz, 1H), 7.62-7.71 (m, 3H), 10.65 (s, 1H); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)): δ 18.3 (CH\(_3\)), 28.2 (CH\(_2\)), 32.9 (CH\(_2\)), 35.7 (CH\(_2\)), 41.6 (CH), 46.9 (CH), 51.1 (CH), 55.2 (CH\(_3\)), 105.6 (CH), 118.9 (CH), 125.9 (CH), 126.1 (CH), 127.3 (CH), 128.9 (C), 129.2 (CH), 133.6 (C), 136.2 (C), 157.5 (C), 174.3 (C), 181.6 (C). Exact mass: m/z found 342.1706, calculated for C\(_{20}\)H\(_{24}\)NO\(_4\) (MH\(^+\)) 342.1705.

**(S)-NPX-CyAA.** \(^1\)H NMR (300 MHz, CDCl\(_3\)): δ 1.44-2.00 (m, 5H), 1.56 (d, J = 7.2 Hz, 3H), 2.07-2.22 (m, 1H), 2.78-2.89 (m, 1H), 3.65 (q, J = 7.2 Hz, 1H), 3.90 (s, 3H), 4.27-4.38 (m, 1H), 5.99 (d, J = 7.5 Hz, 1H), 7.09-7.16 (m, 2H), 7.35 (dd, J = 8.4 and 1.8 Hz, 1H), 7.62-7.72 (m, 3H); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)): δ 18.4 (CH\(_3\)), 28.2 (CH\(_2\)), 32.9 (CH\(_2\)), 35.8 (CH\(_2\)), 41.5 (CH), 47.0 (CH), 51.1 (CH), 55.3 (CH\(_3\)), 105.6 (CH), 119.0 (CH), 126.0 (CH), 126.1 (CH), 127.4 (CH), 129.0 (C), 129.2 (CH), 133.7 (C), 136.5 (C), 157.6 (C), 174.0 (C), 181.5 (C). Exact mass: m/z found 342.1714, calculated for C\(_{20}\)H\(_{24}\)NO\(_4\) (MH\(^+\)) 342.1705.
Photochemical Properties of Studied Compounds.

Table 1. Emission Quantum Yields and Lifetimes of the Local Excited State of 2 (a,b) and 3 (a,b) Dyads (LE) ($\lambda_{\text{max}} = 351 \text{ nm}$) and Exciplex in the Process of photoirradiation of Dyad Isomers in Solvents with different Dielectric Constants.

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<th>LE</th>
<th>Exciplex</th>
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<td>(R)-NPX-AA-(S)-Pyr, 2a</td>
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<td>(S)-NPX-CyAA-(S)-Pyr, 3b</td>
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Experimental Details

Preparation of solutions. Stock solutions were prepared in two solvents: acetonitrile (ε = 36.8) [3] or benzene (ε = 2.28) [4] for optic measurements and deuteroacetonitrile (D 99.9%) and deuterobenzene (D 99.8%) for CIDNP measurements. Solvent permittivity values are shown for 293 K. The solvent permittivities for the mixtures were taken from the literature. [5] There is no room for doubt that the linear correlation between solvent polarity and its dielectric coefficient, and so we use both term hereafter. Concentrations of dyads in stock solutions for optic measurements were kept about 1.0 x 10^{-4} M or 5.0 x 10^{-3} M for CIDNP experiments to exclude all potential bimolecular reactions.

Fluorescence Measurements. All spectroscopic measurements were performed using a quartz cuvette of 1 cm optical length. Spectra and kinetic curves of luminescence were recorded with an Edinburgh Instruments FLSP-920 spectrofluorometer with either a Xenon lamp or a laser diode EPLED-320 (λ_{ex} = 320 nm, pulse duration 0.6 ns) as excitation sources. The kinetic traces were fitted by biexponential decay (or formation and decay) functions using a reconvolution procedure. For the correct selection of the weak band of exciplex luminescence the spectrum was recorded twice: without a filter and with the step 395 nm filter. The using of step filter allows removing the luminescence of NPX baseband (350 nm) which appears in the second order in the long-wavelength part of the spectrum (700 nm) and distorts the exciplex band. The absorbance at the excitation wavelength was kept ca. 0.1. UV/Visible absorption spectra were recorded using an Agilent 8453 spectrophotometer (Agilent Technologies).

Luminescence quantum yields were measured relative to that of NPX, using the value for the fluorescence quantum yield of naproxen in acetonitrile (0.47, [6]), as it has been previously shown that quantum yield of naproxen fluorescence is basically solvent-independent. All samples were bubbled with argon for 15 min to remove dissolved oxygen just before the experiments. After every experimental series a control fluorescence spectrum was recorded for checking the absence of oxygen in samples. All experiments were performed at room temperature 296 K.

CIDNP Measurements. ^1H pseudo steady state (PSS) CIDNP experiments [7] were performed on DPX-200 NMR spectrometer (Bruker, 200 MHz ^1H operating frequency, τ(90) = 3.0 μs). The samples in standard 5 mm Pyrex NMR tubes were irradiated directly in the probe of the NMR spectrometer. EMG 101 MSC excimer laser was used as a light source (Lambda Physik, 308 nm, 100 mJ at output window, 20 mJ per pulse in sample volume, with pulse duration 15 ns).
Calculation Details

Computational Methods. In numeric kinetic simulations the differential equations were solved using proprietary software (SPARK) based on the fourth-order Runge-Kutta method. The program allows calculations and fitting to experimental kinetic curves simultaneously at many wavelengths.

CIDNP simulations. To describe the dependence of CIDNP on solvent permittivity theoretically we used method of the calculation based on the Radical pair (RP) theory. This method includes the solution of the master-equation of spin chemistry using Liouvill representation. [8,9]

\[
\frac{\partial \rho(\vec{r},t)}{\partial t} = \hat{L} \rho(\vec{r},t) + \mathcal{L}(\vec{r})\rho(\vec{r},t) - (\hat{K}(\vec{r}) + \hat{J}(\vec{r}))\rho(\vec{r},t)
\]

(S1)

\[
\rho(\vec{r},t) = \begin{pmatrix} \rho_{SS} \\ \rho_{ST} \\ \rho_{TS} \\ \rho_{TT} \\ \rho_{exc} \\ \rho_\star \end{pmatrix}, \quad \text{where } \rho_{SS}, \rho_{ST}, \rho_{TS}, \rho_{TT}
\]

are matrix elements for the dyad’s RP (in the \(S \rightarrow T_0\) approximation), and \(\rho_{exc}\) and \(\rho_\star\) are populations of exciplex and excited states, respectively; \(\hat{L}\) – the Liouvillian describing the RP spin evolution; \(\hat{L}(\vec{r})\) - the operator of RP motion; \(\hat{K}(\vec{r})\) – reaction’s operator corresponding to the suggested scheme of reaction, \(\hat{J}(\vec{r})\) – the operator of exchange interaction.

The CIDNP effect is determined by the following equation

\[
P = \langle I_z \rangle = \langle I_z \rangle_S + \langle I_z \rangle_T. \quad (2S)
\]

Here,

\[
\langle I_z \rangle_S = \text{Tr} \left( I_z \cdot k_S \int_0^t \hat{P}_S \rho(t) dt \right), \quad \langle I_z \rangle_T = \text{Tr} \left( I_z \cdot k_T \int_0^t \hat{P}_T \rho(t) dt \right)
\]

\(\hat{P}_S\) and \(\hat{P}_T\) are the projection operators of singlet and triplet states, correspondingly; \(\rho(t)\) is the average value of \(\rho(\vec{r},t)\) in the reaction zone.

To simplify the theoretical analysis we have used the Laplace transformation and the Green functions technique. [10] We have obtained the integral equation:

\[
\tilde{\rho}(\vec{r},s) = \int \tilde{G}(\vec{r},\vec{x};s)\rho_0(\vec{x})d\vec{x} - \int \tilde{G}(\vec{r},\vec{x};s)(\hat{K}(\vec{x}) + \hat{J}(\vec{x}))\rho(\vec{x},s)d\vec{x} \quad (3S)
\]

Here,

\[
\tilde{G}(\vec{r},\vec{x};s) = \int_0^\infty \exp(i\lambda t)\varphi(\vec{r},\vec{x};t)\exp(-st)dt
\]

In the continuous–medium approximation we suppose the diffusional motion with the Coulomb interaction of RP centers. In this case, the distribution function \(\varphi(\vec{r},\vec{x};t)\) obeys the following equation:

\[
\frac{\partial \varphi(\vec{r},\vec{x};t)}{\partial t} + \nabla \left( \nabla \cdot \varphi(\vec{r},\vec{x};t) + \varphi(\vec{r},\vec{x};t) \frac{\nabla U(\vec{r})}{k_B T} \right) = -\frac{\delta(\vec{r} - \vec{x})}{D}. \quad (4S)
\]

Here, \(\vec{x}\) indicates at the initial distance between RP: \(\vec{x} = \vec{r}(t = 0)\), \(D\) – diffusivity of the RP relative motion. The method of solution of the equation (4S) is known. [10]

The solution can be derived analytically under the following approximations:

1. Reaction occurs in a thin spherical layer of thickness \((\Delta \ll r)\) where \(r\) is the distance between radical centers of biradical-zwitterion.


2. In the coordinate system of one of the radicals the initial location of the other radical is in the reaction zone. The moving radical mostly remains located in the reaction zone.

3. Spin evolution and motion occurs at sufficiently strong Coulomb interaction:
\[
\frac{4s^4}{D\alpha^2} \ll 1
\]
where \( s \) is the parameter of Laplace transformation and \( \alpha = \frac{e^2}{k_BT^r} \) Onsager radius.

4. CIDNP was calculated for long times, where \( s \) is small enough; therefore we use Taylor series for the Green function.

After averaging \( \rho(\vec{r},t) \) in the reaction zone we obtain
\[
s\rho(s) = (1 + \hat{g}(s)(\hat{U}_0 \hat{J}_0))^{-1}\hat{g}(s)\rho_0
\]
Here, \( \hat{g}(s), \hat{U}_0, \hat{J}_0 \), are the average value of \( \hat{v}(\vec{r},x,s), \hat{k}(\vec{x}), \hat{j}(\vec{x}) \) in the reaction zone, \( \rho_0 = (k,\rho,0,0,0,0,0) \).

All calculations were done with using original Mathematica code and a standard desktop computer (Intel core i5 at 3.5 GHz).

To simplify all analytical and numerical calculations we have used the next approximations:

1. Electron-electron exchange interaction in the reaction zone equals infinity: \( J \to \infty \).
2. Rates of the singlet recombination and triplet recombination were constant during the calculation; they were given by \( k_S = 2k_T \). The rates of all chemical reactions are independent of permittivity (the mean values of rates are used in the calculation).
3. Only one magnetic nucleus of spin \( \frac{1}{2} \) on the pyrrolidine fragment interacts with the unpaired electron.
4. There is no spin-spin interaction between electrons and nuclei on the naproxen fragment.

The following parameters were used in the calculations: \( \alpha = 20 \text{ G} \) for the isotropic HFI constant for both optical isomers on the pyrrolidine fragment; \( \omega = 10^{10} \text{ s}^{-1} \) – rate of singlet-triplet interconversion; \( k_S = 2k_T = 2 \cdot 10^9 \text{ s}^{-1} \) – rate of recombination; \( k_e = 0.1k_S \), \( k_{exc} = k_{exc}^+ = k_S \), \( \tau = 10^{-7} \text{ s} \) RP lifetime; the rates \( k_{esc} \) and \( k^* \), and the boundary distances \( R_1 \) and \( R_2 \) were taken from the photochemical experiments; the Onsager radius \( \alpha \), the diffusivity \( D \) and the thickness of the reaction zone \( \Delta \) were free variable parameters. The Onsager radius changes from dyad to dyad because the distribution of electron density and the electric interaction change. Diffusivity in our model is an abstract parameter that occurs on going from microscopic to macroscopic motion.
Quantum-Chemical Calculations.

Conformational Analysis.

B3LYP/6-31G(d)

Fig.1. the structures (4a) correspond to a minimum on the potential energy surface (red points in the graph of scan1).
Fig. 2. The structure (4a) corresponds to a minimum on the potential energy surface (red points in the graph of scan2).
Fig. 3. The structure (4a) corresponds to a minimum on the potential energy surface (red point in the graph of scan3).
Fig.4. The structures (4a) correspond to a minimum on the potential energy surface (red points in the graph of scan4).
Fig. 5. The structures (4a) correspond to a minimum on the potential energy surface (red points in the graph of scan5).
Fig. 6. The structures (4b) correspond to a minimum on the potential energy surface (red points in the graph of scan 1).
Fig. 7. The structure (4b) corresponds to a minimum on the potential energy surface (red point in the graph of scan2).
Fig. 8. the structure (4b) corresponds to a minimum on the potential energy surface (red point in the graph of scan3).
Fig. 9. The structures (4b) correspond to a minimum on the potential energy surface (red points in the graph of scan4).
Fig. 10. The structures (4b) correspond to a minimum on the potential energy surface (red points in the graph of scan5)
Re-optimization of Stable Conformers B3LYP/6-31G(d,p)

4a scan 4 and scan 5 (fig. 4-5)

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R-NPX-AA-8_Pyr

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R-NPK-AA-8_Pyr Acetonitrile

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Full point group C1 NOp 1

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R-NPK-AA-8_Pyr Benzene

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'S-NPX-AA-S_Pyr'

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Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.527932 (Hartree/Particle)
Thermal correction to Energy= 0.558127
Thermal correction to Enthalpy= 0.559071
Thermal correction to Gibbs Free Energy= 0.461026
Sum of electronic and zero-point Energies= -1344.073532
Sum of electronic and thermal Energies= -1344.043337
Sum of electronic and thermal Enthalpies= -1344.042392
Sum of electronic and thermal Free Energies= -1344.140437

Charge = 0 Multiplicity = 1

Stoichiometry C24H32N2O4
Framework group C1[X(C24H32N2O4)]
Deg. of freedom 180
Full point group C1 NoOp 1
RotChk: IX=2 Diff= 3.10D-15
Largest Abelian subgroup C1 NoOp 1
Largest concise Abelian subgroup C1 NoOp 1
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Normal termination of Gaussian 09 at Thu Mar 3 12:37:12 2016.
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S-NP-X-A-AA-S_Pyr Acetonitrile

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.527646 (Hartree/Particle)
Thermal correction to Energy= 0.557582
Thermal correction to Enthalpy= 0.558726
Thermal correction to Gibbs Free Energy= 0.461041
Sum of electronic and zero-point Energies= -1344.092630
Sum of electronic and thermal Energies= -1344.062495
Sum of electronic and thermal Enthalpies= -1344.061550
Sum of electronic and thermal Free Energies= -1344.159235

Charge = 0 Multiplicity = 1

Stoichiometry C24H32N2O4
Framework group Cl[X(C24H32N2O4)]
Deg. of freedom 180
Full point group Cl NOp 1
RotChk: TX=0 Diff= 3.95D-16
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- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.527830 (Hartree/Particle)
Thermal correction to Energy= 0.557997
Thermal correction to Enthalpy= 0.558941
Thermal correction to Gibbs Free Energy= 0.461044
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Sum of electronic and thermal Free Energies= -1344.148360

Charge = 0 Multiplicity = 1

Stoichiometry C24H32N2O4
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**R-NFX-RS-CyAA-S_Pyr**

- **Thermocemistry** -

---

**Temperature** 298.150 Kelvin, **Pressure** 1.00000 Atm.

- Zero-point correction = 0.565045 (Hartree/Particle)
- Thermal correction to Energy = 0.595601
- Thermal correction to Enthalpy = 0.596545
- Thermal correction to Gibbs Free Energy = 0.498917
- Sum of electronic and zero-point Energies = -1421.481215
- Sum of electronic and thermal Energies = -1421.450659
- Sum of electronic and thermal Enthalpies = -1421.449715
- Sum of electronic and thermal Free Energies = -1421.547314

**Charge** = 0, **Multiplicity** = 1

**Stoichiometry** C26H34N2O4

**Framework group** C1[X(C26H34N2O4)]

**Deg. of freedom** 192

- Full point group C1
- NOP 1

**RotChk:** IX=0 Diff = 8.35D-15

**Largest Abelian subgroup** C1

**Largest concise Abelian subgroup** C1

**Job cpu time:** 1 days 23 hours 37 minutes 51.7 seconds.

**File lengths (MBytes):** RHF = 3517 Int = 0 D2E = 0 Chk = 50 Scr = 1

**Normal termination of Gaussian 09 at Wed Mar 2 18:48:11 2016.**
#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-311G(d,p) Freq

R-NPX-RS-cyAA-8_Pyr Acetonitrile

- Thermochemistry -
---------------------
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.564373 (Hartree/Particle)
Thermal correction to Energy= 0.591981
Thermal correction to Enthalpy= 0.595305
Thermal correction to Gibbs Free Energy= 0.498517
Sum of electronic and zero-point Energies= -1421.497342
Sum of electronic and thermal Energies= -1421.466755
Sum of electronic and thermal Enthalpies= -1421.465811
Sum of electronic and thermal Free Energies= -1421.563199

Charge = 0 Multiplicity = 1

Stoichiometry C26H34N2O4
Framework group C1[x(C26H34N2O4)]
Deg. of freedom 192
Full point group C1 NoP 1
RotChk: IX=0 Diff= 9.59D-16
Largest Abelian subgroup C1 NoP 1
Largest concise Abelian subgroup C1 NoP 1
Job cpu time: 1 days 17 hours 49 minutes 16.0 seconds.
File lengths (MBytes): RWF= 3751 Int= 0 D2E= 0 Chk= 61 Scr= 1

#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-311G(d,p) Freq

R-NPX-RS-cyAA-8_Pyr Benzene

- Thermochemistry -
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Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.564873 (Hartree/Particle)
Thermal correction to Energy= 0.595391
Thermal correction to Enthalpy= 0.596336
Thermal correction to Gibbs Free Energy= 0.499360
Sum of electronic and zero-point Energies= -1421.487984
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Sum of electronic and thermal Free Energies= -1421.553458

Charge = 0 Multiplicity = 1

Stoichiometry C26H34N2O4
Framework group C1[x(C26H34N2O4)]
Deg. of freedom 192
Full point group C1 NoP 1
RotChk: IX=0 Diff= 6.36D-16
Largest Abelian subgroup C1 NoP 1
Largest concise Abelian subgroup C1 NoP 1
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SC-NPX-RS-Cy2A-S_Py

---

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction=       0.565039 (Hartree/Particle)
Thermal correction to Energy=    0.595604
Thermal correction to Enthalpy=    0.595604
Thermal correction to Gibbs Free Energy=    0.499432
Sum of electronic and zero-point Energies=    -1421.481871
Sum of electronic and thermal Energies=    -1421.451306
Sum of electronic and thermal Enthalpies=    -1421.450361
Sum of electronic and thermal Free Energies=    -1421.547478

Charge = 0 Multiplicity = 1

Stoichiometry C26H34N2O4
Framework group C1[X(C26H34N2O4)]
Deg. of freedom 192
Full point group C1 NOp 1
RotChk: IX=1 Diff= 1.59D-15
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Job cpu time:       2 days 2 hours 50 minutes 31.1 seconds.
File lengths (NBytes):   HWF=   3817 Int=     0 D2E=     0 chk=  50 Scr=     1
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S-NPX-3S-cyAA-S_Pyr Acetonitrile

- Thermochemistry -

Temperature 298.150 Kelvin, Pressure 1.00000 Atm.

Zero-point correction= 0.564380 (Hartree/Particle)
Thermal correction to Energy= 0.594983
Thermal correction to Enthalpy= 0.595527
Thermal correction to Gibbs Free Energy= 0.498759
Sum of electronic and zero-point Energies= -1421.497337
Sum of electronic and thermal Energies= -1421.466734
Sum of electronic and thermal Enthalpies= -1421.465790
Sum of electronic and thermal Free Energies= -1421.562957

Charge = 0 Multiplicity = 1

Stoichiometry C26H34N2O4
Framework group C1[X(C26H34N2O4)]
Deg. of freedom 192
Full point group C1 NoOp 1
RotChk: IX=1 Diff= 1.19D-16
Largest Abelian subgroup C1 NoOp 1
Largest concise Abelian subgroup C1 NoOp 1
Job cpu time: 0 days 19 hours 10 minutes 33.8 seconds.
File lengths (MBytes): RWF= 3786 Int= 0 D2E= 0 Chk= 61 Scr= 1
Normal termination of Gaussian 09 at Fri Mar 4 00:00:36 2016.

$P$ Geometry=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-311G(d,p) Freq

S-NPX-3S-cyAA-S_Pyr Benzene

- Thermochemistry -

Temperature 298.150 Kelvin, Pressure 1.00000 Atm.

Zero-point correction= 0.564696 (Hartree/Particle)
Thermal correction to Energy= 0.595333
Thermal correction to Enthalpy= 0.596277
Thermal correction to Gibbs Free Energy= 0.498437
Sum of electronic and zero-point Energies= -1421.488334
Sum of electronic and thermal Energies= -1421.457967
Sum of electronic and thermal Enthalpies= -1421.456753
Sum of electronic and thermal Free Energies= -1421.554593

Charge = 0 Multiplicity = 1

Stoichiometry C26H34N2O4
Framework group C1[X(C26H34N2O4)]
Deg. of freedom 192
Full point group C1 NoOp 1
RotChk: IX=1 Diff= 1.12D-15
Largest Abelian subgroup C1 NoOp 1
Largest concise Abelian subgroup C1 NoOp 1
Job cpu time: 0 days 13 hours 49 minutes 46.1 seconds.
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Structure 4a (geometrical parameters see higher)

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R-NPX-S-Pyr

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.415612 (Hartree/Particle)
Thermal correction to Energy= 0.438561
Thermal correction to Enthalpy= 0.439505
Thermal correction to Gibbs Free Energy= 0.360440

Sum of electronic and zero-point Energies= -1057.466313
Sum of electronic and thermal Energies= -1057.443365
Sum of electronic and thermal Enthalpies= -1057.442420
Sum of electronic and thermal Free Energies= -1057.521486

Charge = 0 Multiplicity = 1

Stoichiometry C20H25NO3
Framework group C1[X(C20H25NO3)]
Deg. of freedom 141
Full point group C1 NOp 1
RotChk: IX=0 Diff= 2.45D-15
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
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R-NPX-S-Pyr Acetonitrile

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.415062 (Hartree/Particle)
Thermal correction to Energy= 0.438065
Thermal correction to Enthalpy= 0.439010
Thermal correction to Gibbs Free Energy= 0.359734

Sum of electronic and zero-point Energies= -1057.477478
Sum of electronic and thermal Energies= -1057.454474
Sum of electronic and thermal Enthalpies= -1057.453530
Sum of electronic and thermal Free Energies= -1057.532806

Charge = 0 Multiplicity = 1

Stoichiometry C20H25NO3
Framework group C1[X(C20H25NO3)]
Deg. of freedom 141
Full point group C1 NOp 1
RotChk: IX=0 Diff= 2.27D-16
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Job cpu time: 0 days 23 hours 51 minutes 24.7 seconds.
File lengths (MBytes): RHF= 1749 Int= 0 D2E= 0 Chk= 39 Scr= 1
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R-NFX-S-Pyr Benzene

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.000000 Atm.

Zero-point correction = 0.415546 (Hartree/Particle)
Thermal correction to Energy = 0.438407
Thermal correction to Enthalpy = 0.439351
Thermal correction to Gibbs Free Energy = 0.360282
Sum of electronic and zero-point Energies = -1057.470987
Sum of electronic and thermal Energies = -1057.448046
Sum of electronic and thermal Enthalpies = -1057.447102
Sum of electronic and thermal Free Energies = -1057.526171

Charge = 0 Multiplicity = 1

Stoichiometry C20H25NO3
Framework group C1[X(C20H25NO3)]
Deg. of freedom 141
Full point group C1 NOp 1
RotChk: IX=0 Diff= 1.29D-15
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Job cpu time: 0 days 15 hours 14 minutes 7.4 seconds.
File lengths (MBytes): RWF= 1747 Int= 0 D2E= 0 Chk= 40 Scr= 1
Normal termination of Gaussian 09 at Thu Mar 3 21:45:07 2016.

Structure 4b (geometrical parameters see higher)

#P Geom=AllCheck Guess=TCheck SCRF=Check Genchk RB3LYP/6-311G(d,p) Freq

S-NFX-S-Pyr

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.000000 Atm.

Zero-point correction = 0.415546 (Hartree/Particle)
Thermal correction to Energy = 0.438518
Thermal correction to Enthalpy = 0.439463
Thermal correction to Gibbs Free Energy = 0.360284
Sum of electronic and zero-point Energies = -1057.466403
Sum of electronic and thermal Energies = -1057.443430
Sum of electronic and thermal Enthalpies = -1057.442486
Sum of electronic and thermal Free Energies = -1057.521655

Charge = 0 Multiplicity = 1

Stoichiometry C20H25NO3
Framework group C1[X(C20H25NO3)]
Deg. of freedom 141
Full point group C1 NOp 1
RotChk: IX=0 Diff= 1.32D-15
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Job cpu time: 1 days 0 hours 49 minutes 6.3 seconds.
File lengths (MBytes): RWF= 1554 Int= 0 D2E= 0 Chk= 29 Scr= 1
$P$ Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-311G(d,p) Freq

S-NPX-S-Pyr Acetonitrile

- Thermochemistry -
----------------------
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.415250 (Hartree/Particle)
Thermal correction to Energy= 0.438195
Thermal correction to Enthalpy= 0.439399
Thermal correction to Gibbs Free Energy= 0.360187
Sum of electronic and zero-point Energies= -1057.477280
Sum of electronic and thermal Energies= -1057.454335
Sum of electronic and thermal Enthalpies= -1057.453391
Sum of electronic and thermal Free Energies= -1057.532343

Charge = 0 Multiplicity = 1

Stoichiometry C20H25N03
Framework group C1[X(C20H25N03)]
Deg. of freedom 141
Full point group C1 NOp 1
RotChk: IX=0 Diff= 5.81D-16
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Job cpu time: 0 days 10 hours 48 minutes 44.6 seconds.
File lengths (MBytes): RWF= 1747 Int= 0 D2E= 0 Chk= 38 Scr= 1

$P$ Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-311G(d,p) Freq

S-NPX-S-Pyr Benzene

- Thermochemistry -
----------------------
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.415444 (Hartree/Particle)
Thermal correction to Energy= 0.438400
Thermal correction to Enthalpy= 0.439345
Thermal correction to Gibbs Free Energy= 0.360296
Sum of electronic and zero-point Energies= -1057.471048
Sum of electronic and thermal Energies= -1057.448092
Sum of electronic and thermal Enthalpies= -1057.447147
Sum of electronic and thermal Free Energies= -1057.526156

Charge = 0 Multiplicity = 1

Stoichiometry C20H25N03
Framework group C1[X(C20H25N03)]
Deg. of freedom 141
Full point group C1 NOp 1
RotChk: IX=0 Diff= 7.57D-16
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Job cpu time: 0 days 7 hours 0 minutes 29.2 seconds.
File lengths (MBytes): RWF= 1746 Int= 0 D2E= 0 Chk= 38 Scr= 1
References