Supporting Information

Photoinduced dimerization of a photosensory DNA-binding protein EL222 and its LOV domain

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SI-1 Yield of photoinduced dimerization of EL222

In the main text, we concluded that the weak diffusion signal of EL222 is due to lower efficiency of the photoinduced dimerization in the adduct state. Therefore, two adduct species must exist in solution: reactive and nonreactive. We analyzed the TG signals of EL222 using eq. (SI-1):

$$I_{\mathrm{TG}}(t) = \alpha\{g_1 \delta n_{spe}^{reactive}(t) + g_2 \delta n_{spe}^{nonreactive}(t)\}^2 \qquad \text{(SI-1)}$$

where g_1 and g_2 are the fractions of the reactive and the nonreactive conformations, respectively ($g_1 + g_2 = 1$). The dimerization reaction of the reactive species is expressed by the scheme

$$\mathrm{R} \xrightarrow{h\nu} \mathrm{I} \xrightarrow{k} \mathrm{P}$$

and the temporal dependence is given by eq. (3). On the other hand, the photoexcitation of nonreactive species yields only the adduct species and no further reaction takes place. Under these conditions, the TG signal is written as:

$$I_{TG}(t) = \alpha\left[g_1\left\{-\delta n_{R1} exp\left(-D_{R1}q^2 t\right) + \left(\delta n_{I1} - \frac{k}{\left(D_{I1} - D_{P1}\right)q^2 + k}\delta n_{P1}\right)exp\{-\right.\right. \qquad \text{(SI-2)}$$

where D_{R1}, D_{I2}, D_{P1}, D_{R1}, D_{P2} and k are the D of the reactive conformation in the dark state, D of an intermediate during the reaction of the reactive conformation, D of the reaction product of the reactive conformation, D of the nonreactive conformation in the dark state, D of the product of the nonreactive conformation (i.e., adduct species) and the rate constant of the dimerization, respectively. We assumed that the refractive index change and the diffusion coefficient of two conformations in the dark are the same (

$\delta n_{R1} = \delta n_{R2}$ and $D_{R1} = D_{R2}$), and that D of the adduct species is the same as the reactant, ($D_{R2} = D_{P2}$), while it shows that the refractive index change is the same as the reactive conformation ($\delta n_{I1} = \delta n_{P2}$). Therefore, eq. (SI-2) is simplified to:

$$I_{TG}(t) = \alpha'\left\{ -\delta n_R' exp\left(-D_{R1}q^2t \right) + \left(\delta n_{I1} - \frac{k}{(D_{I1} - D_{P1})q^2 + k}\delta n_{P1} \right) exp\{ -(I \right.$$

(SI-3)

where $\alpha' = \alpha g_1$ and

$$\delta n_R' = \frac{\delta n_{R1} - (1 - g_1)\delta n_{I1}}{g_1} \quad \text{(SI-4).}$$

Eq. (SI-3) is the same as eq. (3) except for its coefficient. Because the origin of the difference between δn_{R1} and δn_{I1} in eq. (3) is the formation of the adduct species, the ratio of δn_{R1} and δn_{I1} should be the same to that of the EL-LOV case.

We fitted the diffusion signal of EL222 by eq. (3) (or (SI-3)), and the parameters are listed in Table SI-1. The fitting parameter of the apparent refractive index change $\delta n_R'$ was obtained as $\delta n_R' = 1.118$, when we normalized the values of refractive index changes as $\delta n_I = 1$. By using eq. (SI-4), we obtained g_1 from the $\delta n_R'$ and the intrinsic refractive index changes, δn_{R1} and δn_{I1}. From this calculation, we obtained $g_1 = 0.08$.

Table SI-1 Diffusion coefficients ($D/10^{-11}$ m^2s^{-1}), the refractive index changes (δn) relative to δn_{I1} and time constants of the reactions (k/ $M^{-1}s^{-1}$) obtained by the analysis of TG signals for EL-LOV and EL222. The fitting parameters were obtained by the analysis using eq. (5) (for EL-LOV) and eq. (3) (for EL222).

	D_{R1}	D_{I1}	D_{P1}	D_{R2}	D_{P2}	δn_{R1}	δn_{I1}	δn_{P1}	δn_{R2}	δn_{P2}	k
EL-LOV	9.2	9.2	7.3	7.3	7.3	1.009	1	0.976	0.986	0.976	1.4×10^5

	D_R	D_I	D_P	δn_R	δn_I	δn_P	k
EL222	8.8	8.5	6.6	1.118	1	1.025	8.6×10^3

SI-2 Temporal profile of the transient lens signal

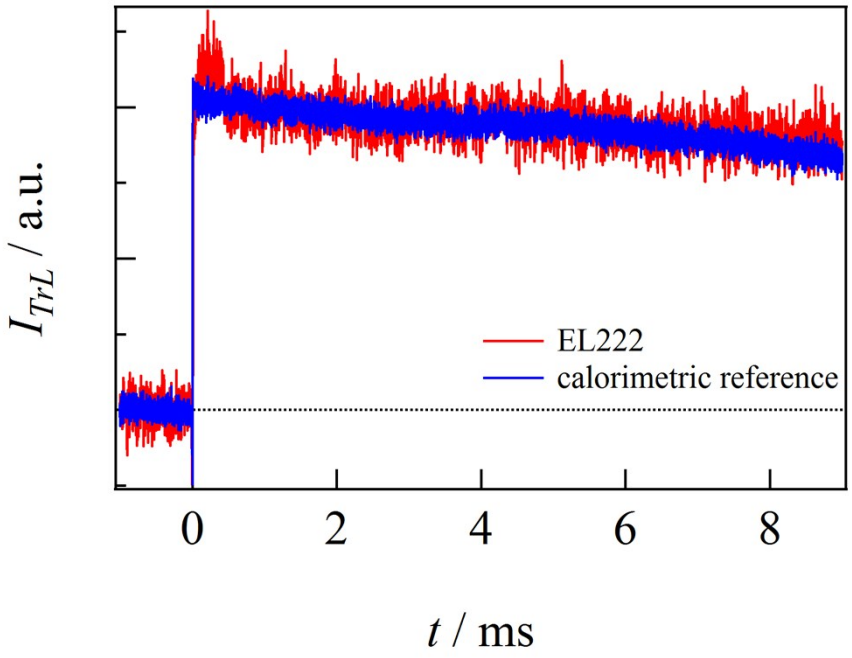

Fig. SI-1 A TrL signal of EL222 (red line) and the calorimetric reference sample (blue line) after photoexcitation.