Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Ultrafast Nonequilibrium Dynamics of Short-Range Protein Electron Transfer in Flavodoxin

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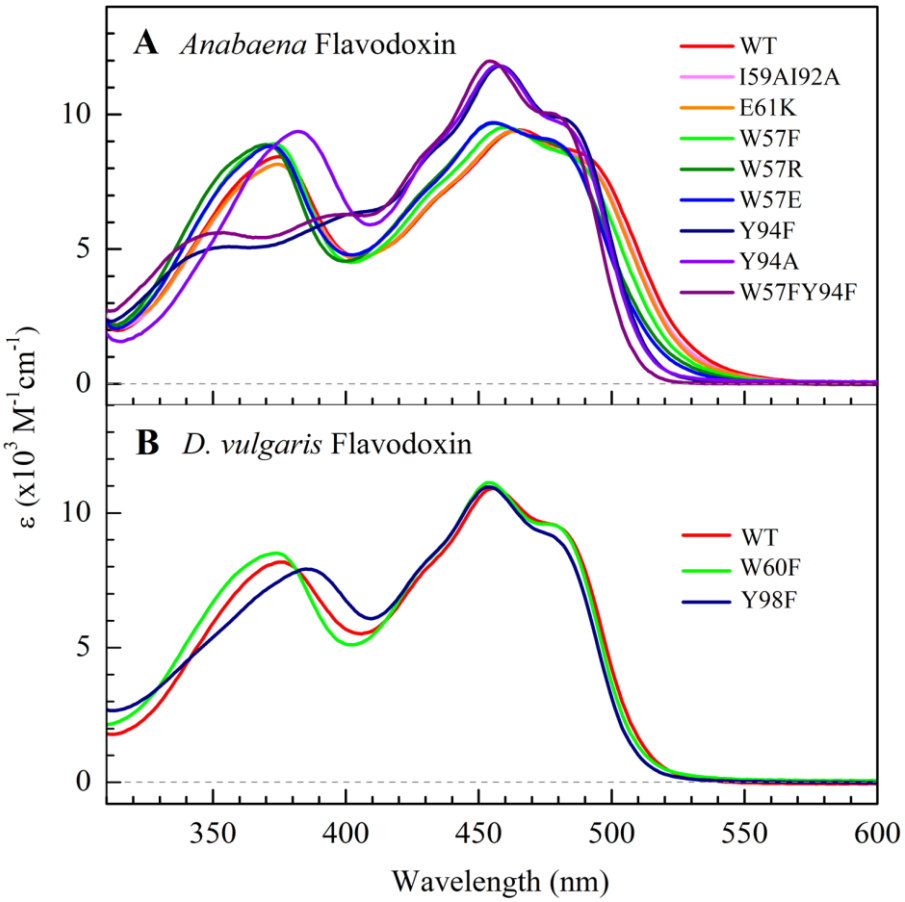

Figure S1. (**A**) Absorption spectra of *Anabaena* flavodoxin and (**B**) *D. vulgaris* flavodoxin.

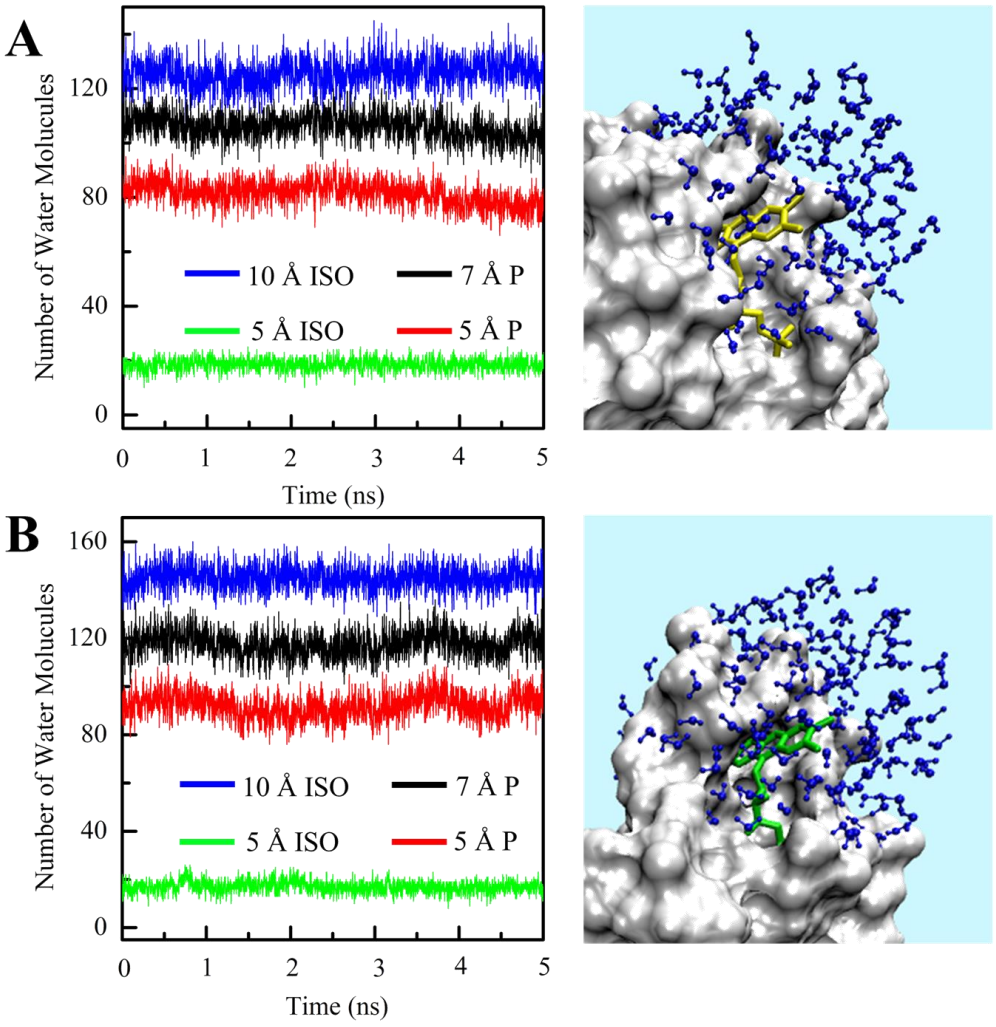

Figure S2. Comparison of water molecules from MD simulations and surface map structures of (**A**) *Anabaena* and (**B**) *D. vulgaris* flavodoxin.

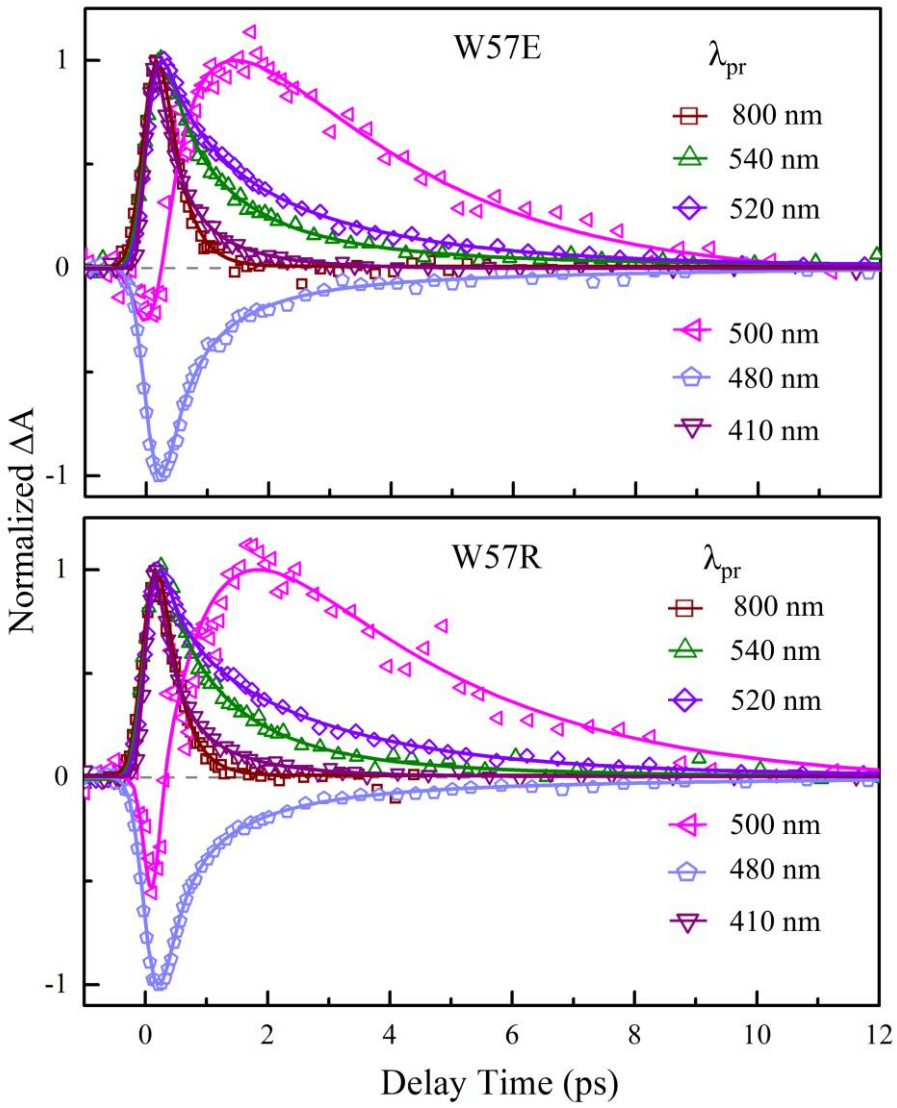

Figure S3. Normalized transient absorption of *Anabaena* flavodoxin W57E and W57R probed from 800 to 410 nm for the ET reactions with the donor Y94.

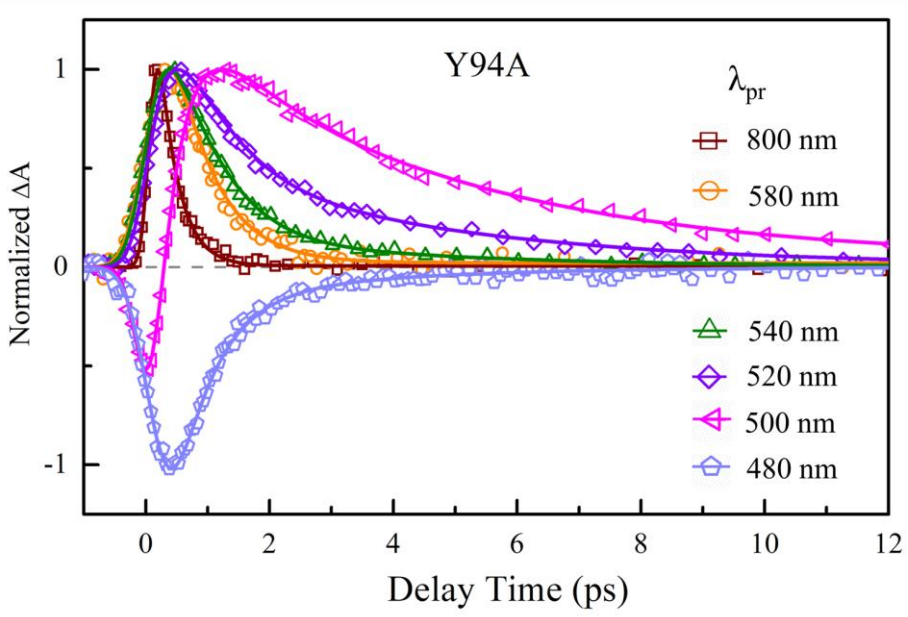

Figure S4. Normalized transient absorption of *Anabaena* flavodoxin Y94A probed from 800 to 410 nm for the ET reaction with the donor W57.

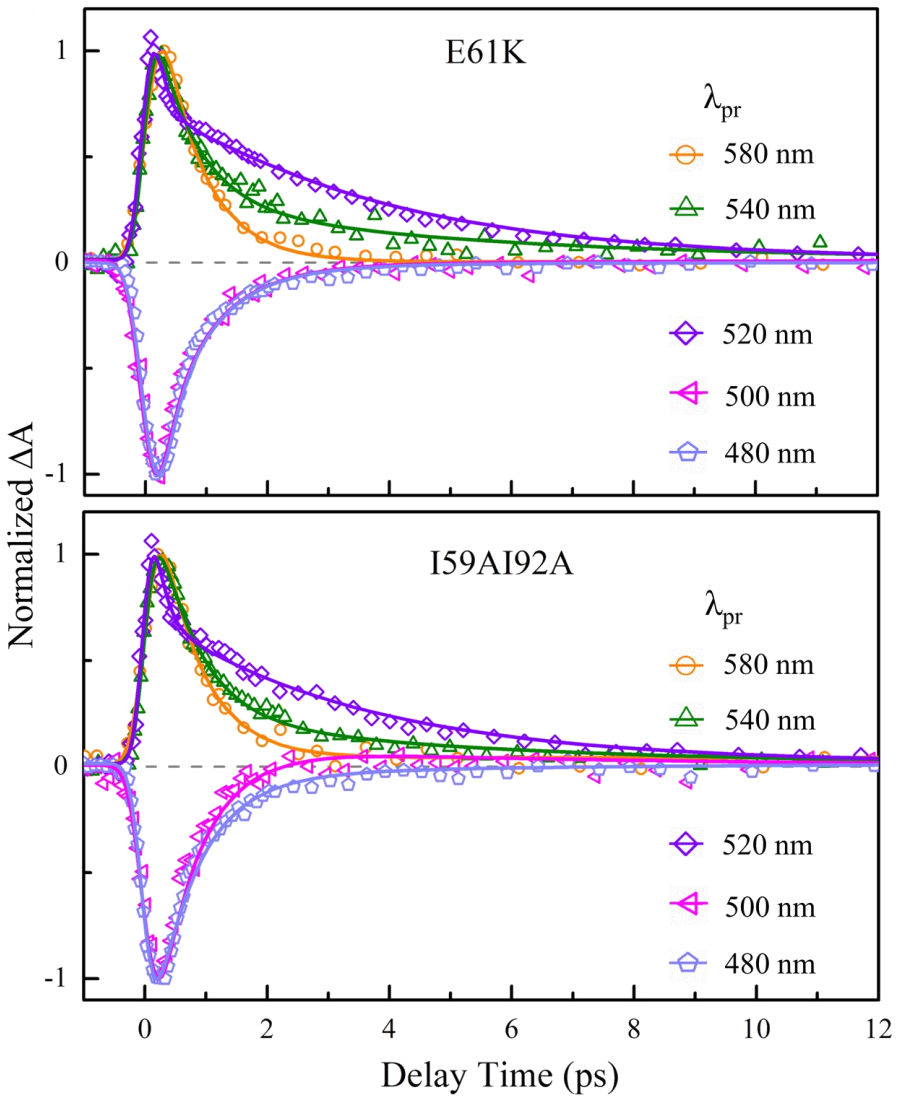

Figure S5. Normalized transient absorption of *Anabaena* E61K and I59AI92A probed from 580 to 480 nm for the ET reactions with dual donors Y94 and W57.

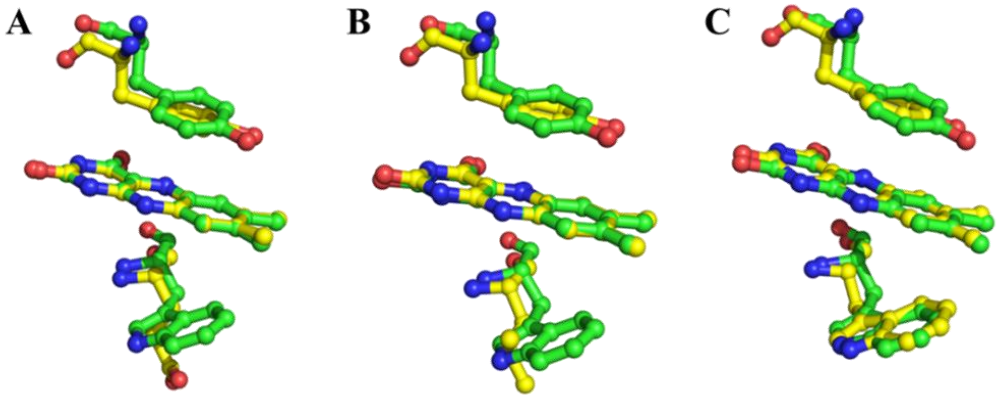

Figure S6. Structure alignment of *Anabaena* mutants (yellow) with *D. vulgaris* WT (green，PDB: 2FX2) flavodoxin. From the left to right, A-C represent W57E, W57L and I92A (PDB: 2V5V, 1OBO, 2V5U).

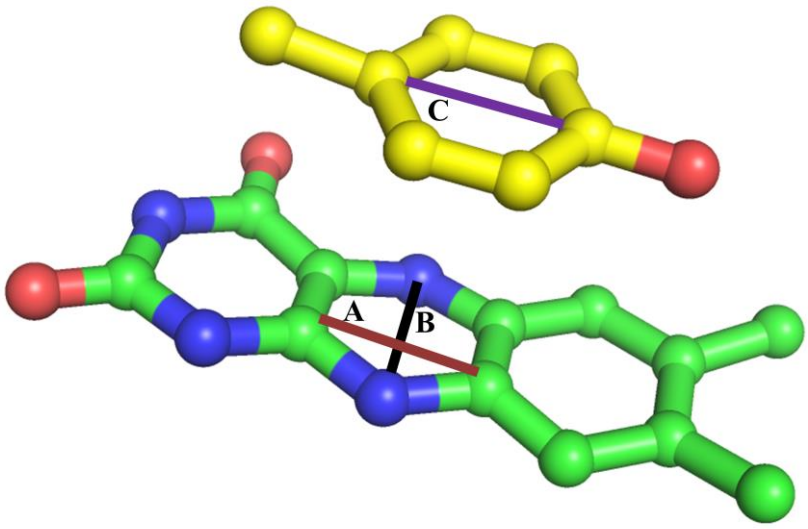

Figure S7. The several lines are used to calculate the angles between Tyr and ISO ring which are shown in Table S1.

Table S1. Angles between Tyr and ISO ring in two species.

	mutants	angle-AC (°)	angle-BC(°)
Anabaena	WT	2.3	88.4
	W57E	5.3	85.0
	W57L	9.6	80.3
	I92A	3.6	86.3
	K2AK3A	6.6	96.3
D. vulgaris	WT	21.7	68.6
	G61V	10.8	79.6
	D95E	18.3	71.3
	D95A	17.1	74.2
	S64C	18.7	72.7

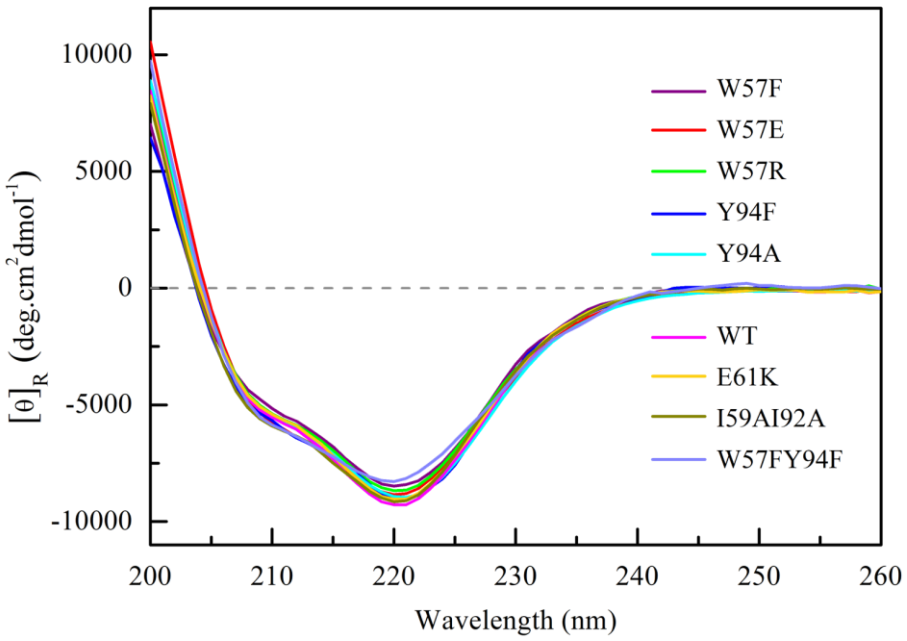

Figure S8. CD spectra of WT and mutant *Anabaena* flavodoxins.