

Supporting Information

Role of Tryptophans in UV-B Absorption of UVR8 Photoreceptor – A Computational Study

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Table S1. Calculated transition energies and oscillator strengths for tryptophan dimer W285 and W337 in the gas phase, ΔE means the transition energy, and f stands for the oscillator strength.

	TD-DFTB		B3LYP/6-31+G(d,p)	
	ΔE (eV)	f	ΔE (eV)	f
L_b	4.13	0.073	4.29	0.040
L_a	4.59	0.033	4.74	0.021

Captions for figures

Fig. S1. Absorption spectra²² of (a) W198, (b) W250 and (c) W302 for differently substituted models.

Fig. S2. Absorption spectra²² of (a) M1, (b) M2, (c) M3, (d) M4, (e) M5, (f) M6, (g) M8 and (h) M9 for distal Trps, interfacial Trps, and interfacial Trps with neighboring residues included.

Fig. S3. Absorption spectra²² of amino acids apart from tryptophan contained in UVR8.

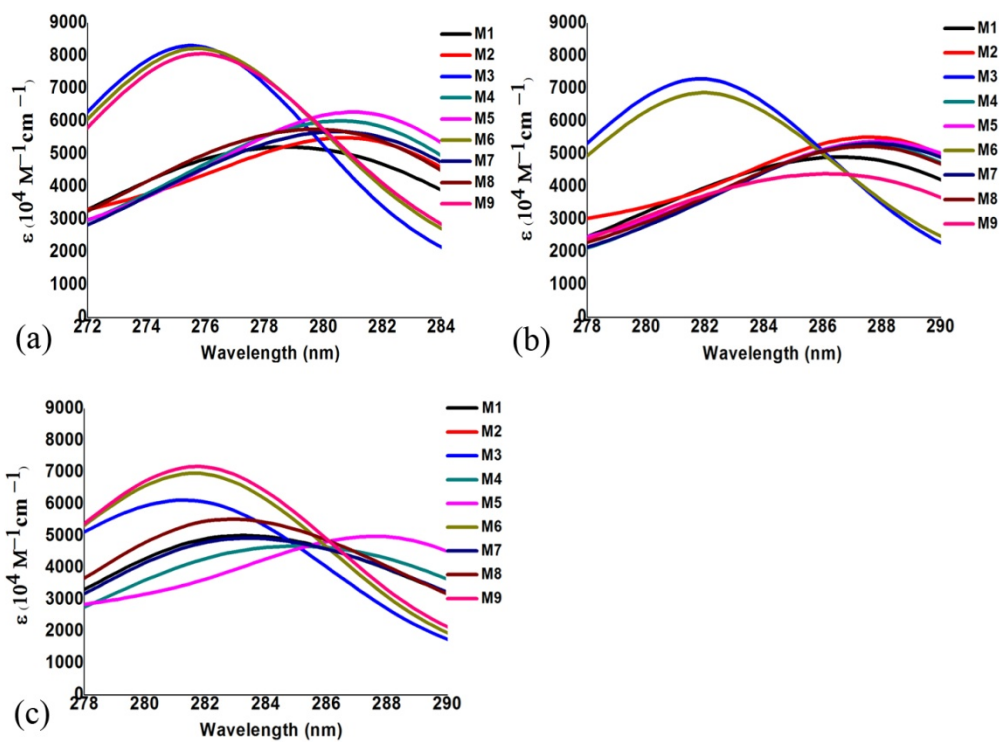
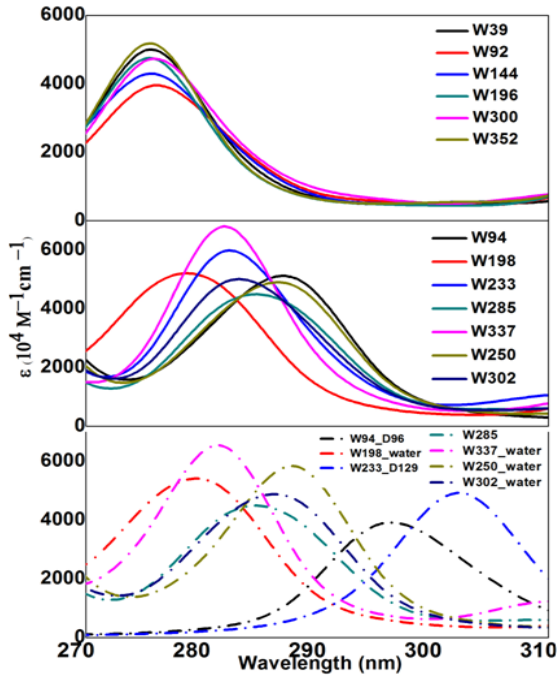
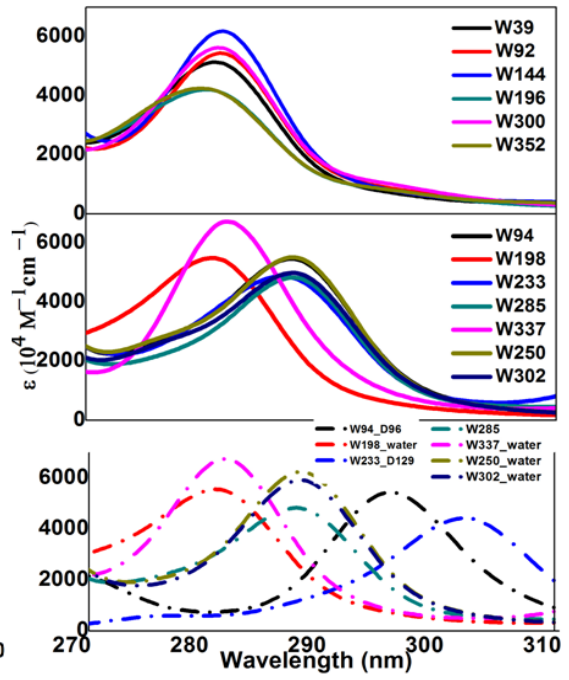


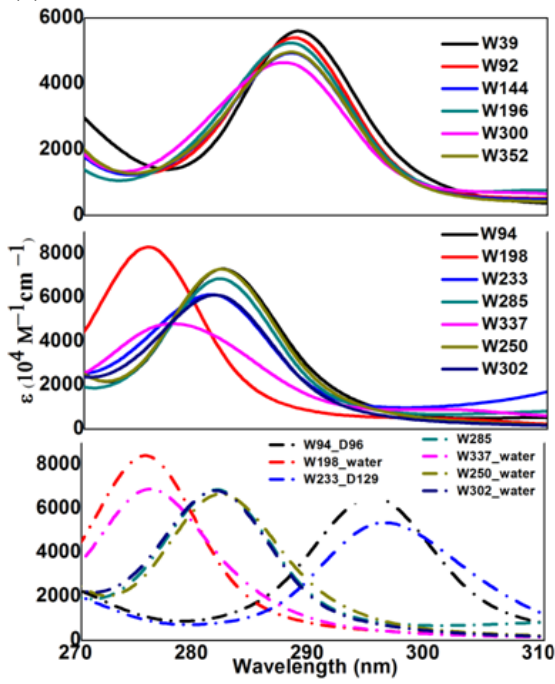
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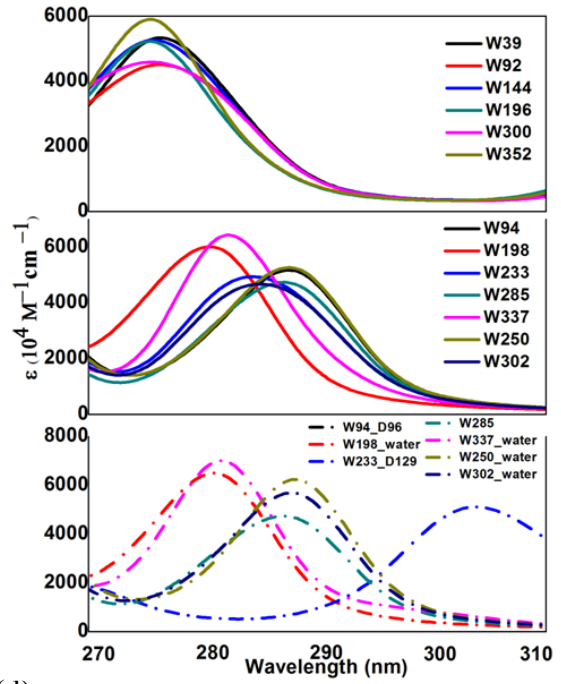
(a)



(b)



(c)



(d)

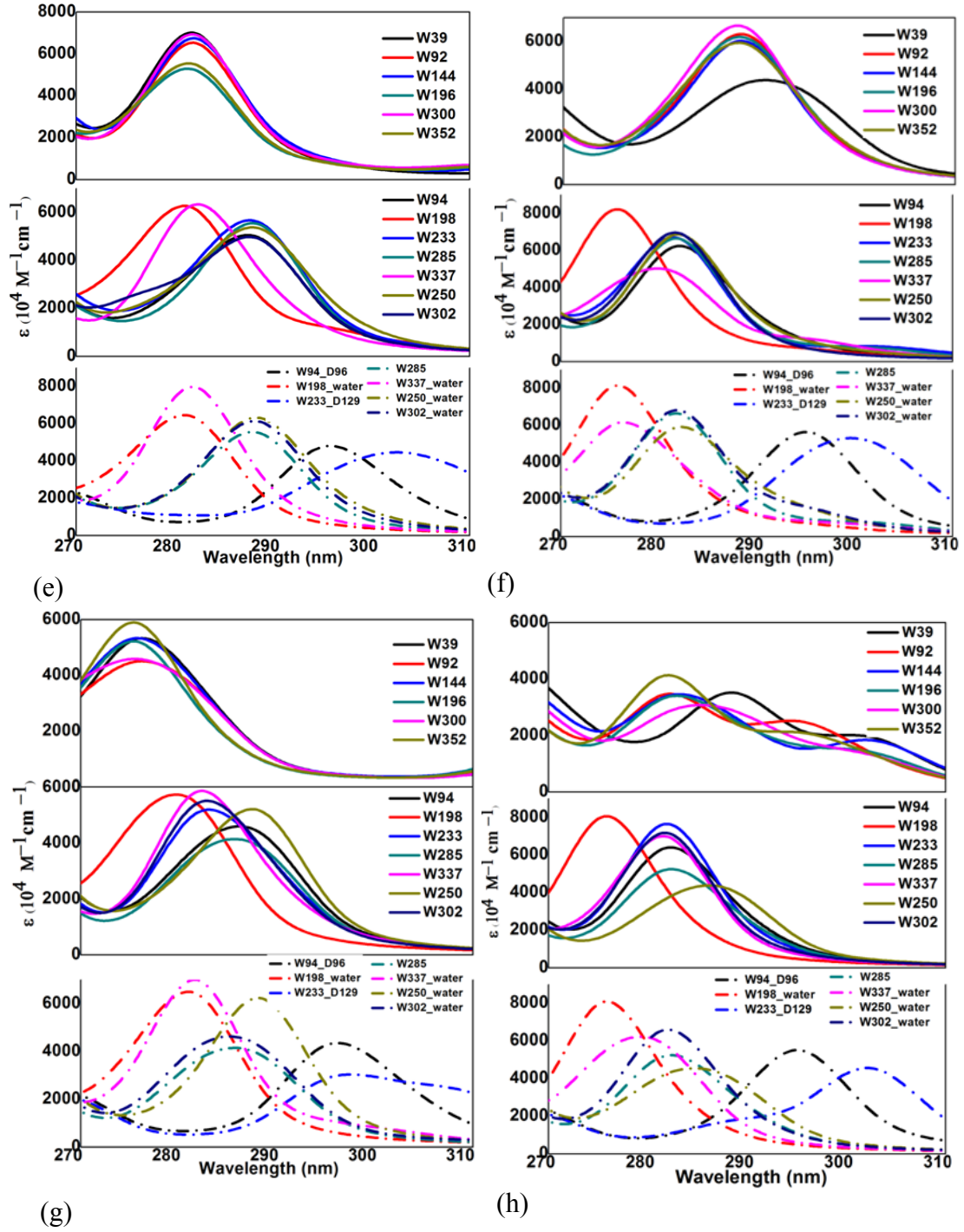


Fig. S2. Absorption spectra²² of (a) M1, (b) M2, (c) M3, (d) M4, (e) M5, (f) M6, (g) M8 and (h) M9 for distal Trps, interfacial Trps, and interfacial Trps with neighboring residues included.

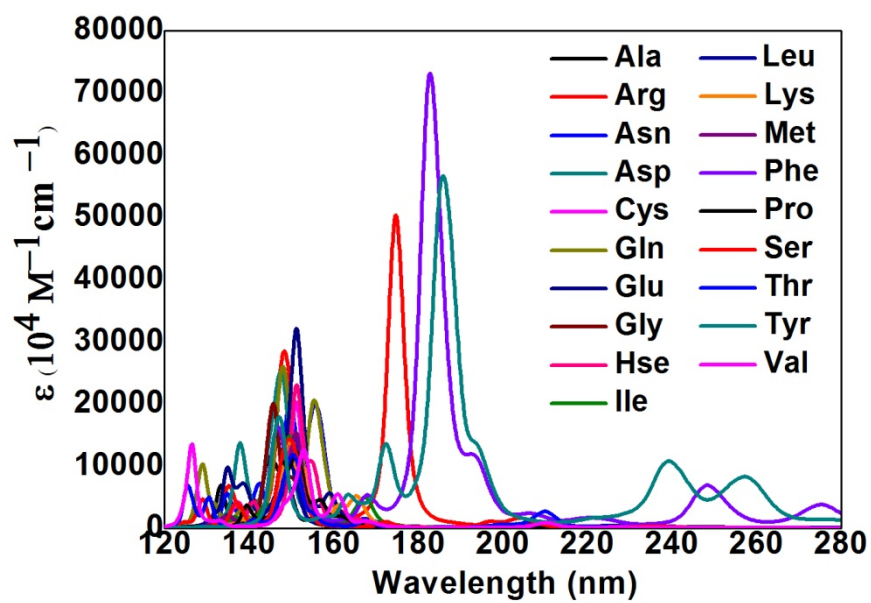


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