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, $\Delta E$ means the transition energy, and $f$ stands for the oscillator strength.

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<th>TD-DFTB</th>
<th>B3LYP/6-31+G(d,p)</th>
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<tbody>
<tr>
<td></td>
<td>$\Delta E$ (eV)</td>
<td>$f$</td>
</tr>
<tr>
<td>$L_b$</td>
<td>4.13</td>
<td>0.073</td>
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<tr>
<td>$L_a$</td>
<td>4.59</td>
<td>0.033</td>
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Captions for figures

Fig. S1. Absorption spectra\textsuperscript{22} of (a) W198, (b) W250 and (c) W302 for differently substituted models.

Fig. S2. Absorption spectra\textsuperscript{22} 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 spectra\textsuperscript{22} of amino acids apart from tryptophan contained in UVR8.
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