Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences

Supplemental data

Diffusion pathways of oxygen species in the phototoxic fluorescent protein KillerRed

Arijit Roy, Philippe Carpentier, Dominique Bourgeois* and Martin Field*

Rotation of Ile-163 during the molecular dynamics simulation of KillerRed

During the KillerRed molecular dynamics simulation we observed a rotation of the sidechain of Ile-163 away from His-62. The Rmsd values of Ile-163 in both monomers are shown in Figure S1. The rotation occurs after about 30 ps in monomer A, and at almost 700 ps in monomer B. The distances between C_δ of Ile-163 and C_γ of His-62 for both monomers along the simulation were also calculated and are presented in Figure S2.

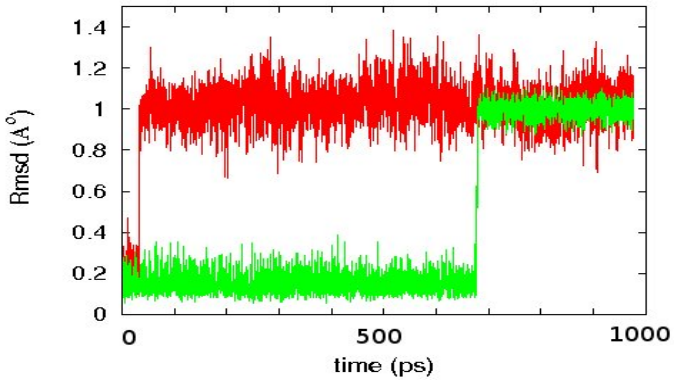

Figure S1: Rmsd values of Ile-163 during the molecular dynamics simulation with KillerRed prior to LES simulation. Red: monomer A; Green: monomer B.

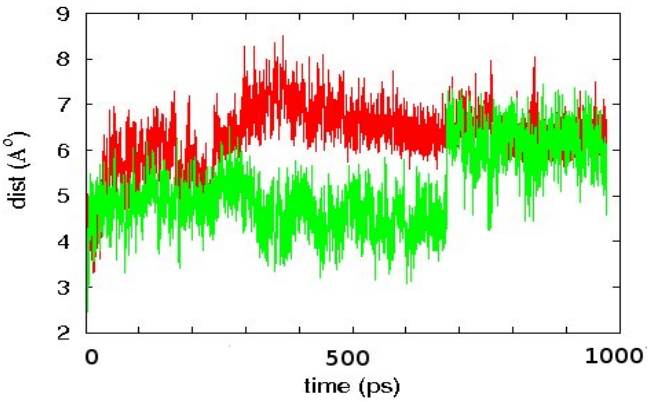

Figure S2: Distance between C_δ of Ile-163 and C_γ of His-62 in monomer A (red) and monomer B (green) during the MD simulation of KillerRed prior to LES simulation.

Rmsd and total energy along the LES simulation of KillerRed with molecular oxygen

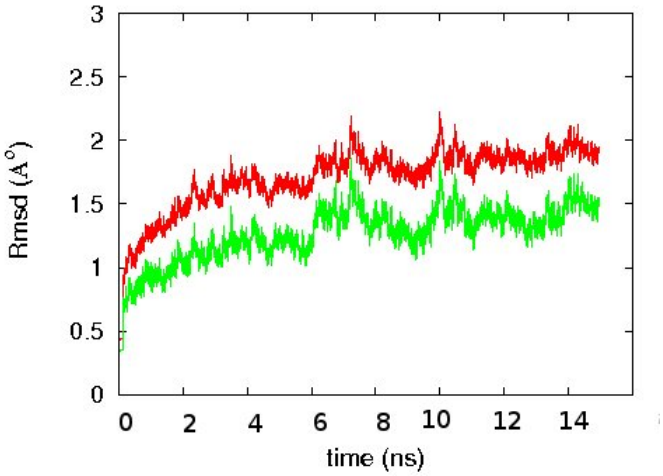

Figure S3: Rmsd values of non-hydrogen atoms of KillerRed along the LES simulation with molecular oxygen. Red: all atoms; green: backbone atoms only.

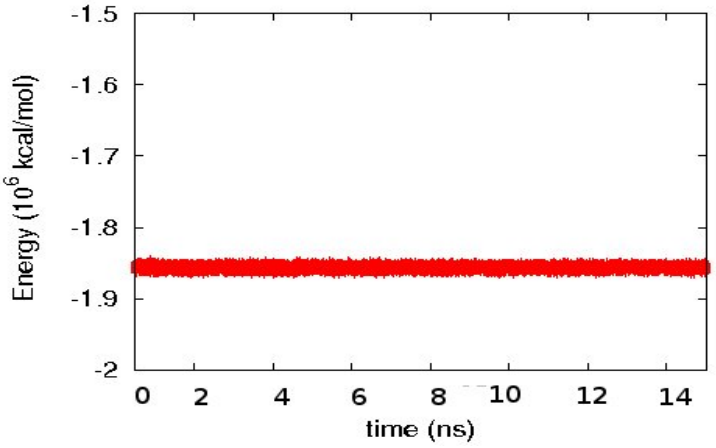

Figure S4: Total energy along the LES simulation of KillerRed with molecular oxygen.

A 180° rotation of Tyr-74 and His-80 allows oxygen diffusion in KillerRed

During the LES simulation with molecular oxygen in KillerRed, we observed that 7 oxygen molecules left monomer A between 3.8 ns and 5.7 ns (for details see Table 1 in the main manuscript). Conformational changes that may have helped trigger these events are 180° rotations of the side chains of Tyr-74 and of His-80, that occur after 4.7 ns and 3.1 ns of simulation, respectively. The Rmsd values for the side chains of these amino acids are displayed in Figure S5.

After flipping of His-80, 6 oxygen molecules left the protein either side of Pro-192 in quick succession starting at 3.8 ns, whereas only a single oxygen left the protein after flipping of Tyr-74, at 5.7 ns. Both Tyr-74 and His-80 remain in their 180° flipped states for the remainder of the simulation.

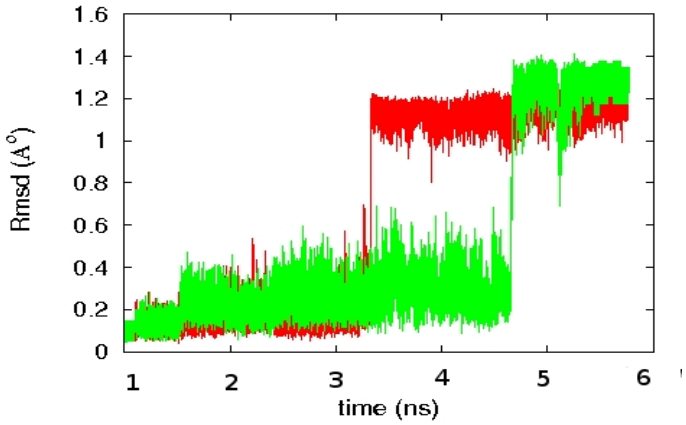

Figure S5: Rmsd values of Tyr-74 (green) and His-80 (red) during the LES simulation of KillerRed with molecular oxygen (between 1 and 6 ns).