Electronic Supplementary Information

Elucidating the microscopic properties of a β-barrel protein and the solvent confined in and around it

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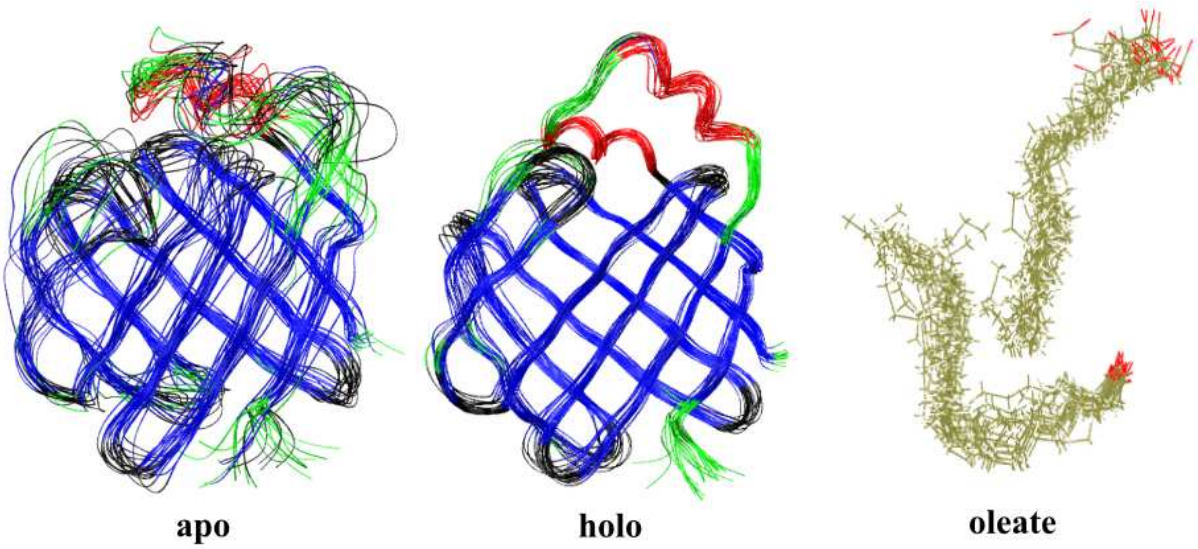

Fig. S1 Superposition of several simulated configurations of apo-rLFABP, holo-rLFABP, and the oleate ligands. These configurations were selected at regular intervals from equilibrated simulation trajectories. The hydrogen atoms are omitted to enhance visual clarity.

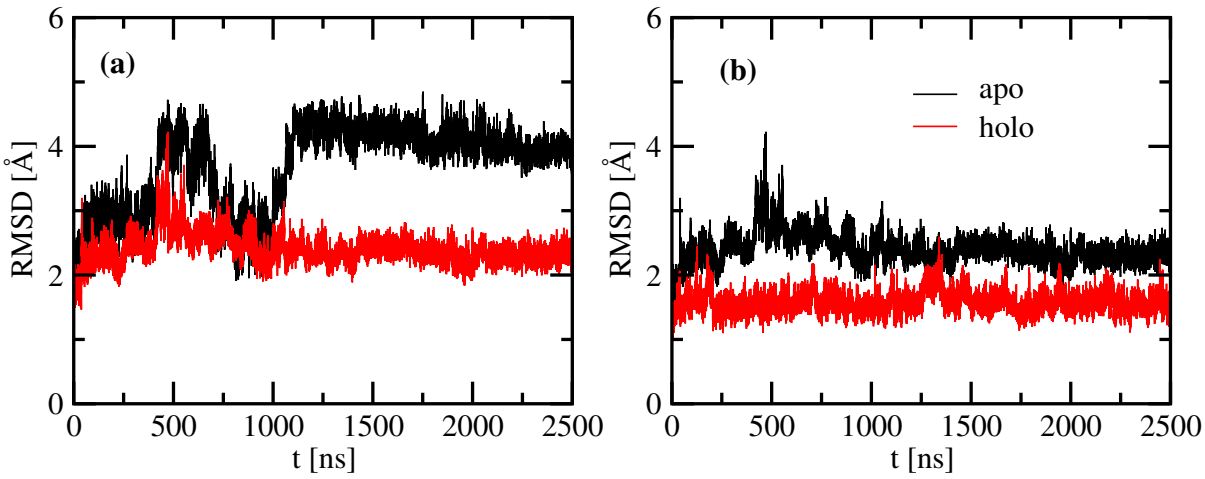

Fig. S2 Time evolutions of the root-mean-square deviations (RMSD) of the (a) β-E, F strands and their connecting loops and (b) the β-sheets except β-E and F strands compared to their crystal structures.

1 Tunneling pathway calculation

The dynamic behavior of tunnels was examined using CAVER WEB V2.0. Tunnels were reviewed in each trajectory snapshot utilizing a probe radius of 0.9 Å, a shell radius of 4 Å, a shell depth of 3 Å, and a clustering threshold of 3.5 Å. In summary, each run produced 500 pdb files, equivalent to 5000 frames. We have only considered the first three tunnels, which are visible in more than 80% of frames for each case. The tunneling pathway results have been shown in the Fig S3.

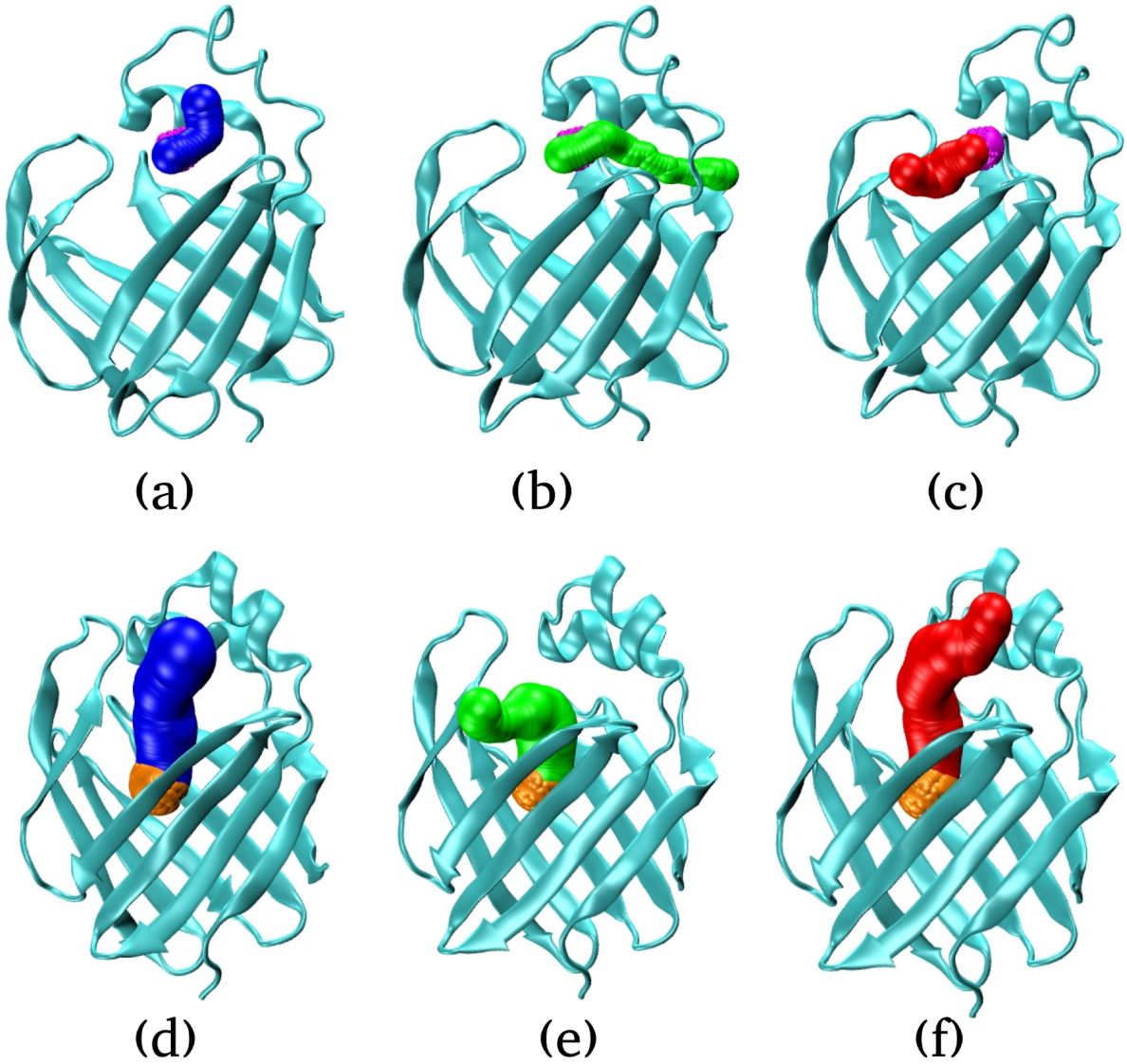

Fig. S3 Depiction of the tunnel networks examined in the study for oleate1 and oleate2 in the holo-rLFABP system. The Tunnel 1 (blue), Tunnel 2 (green) and Tunnel (red) are shown for both cases. (a), (b) and (c) illustrates the three tunneling pathways for the oleate1. The starting point of the simulation for oleate1 is shown by magenta colored sphere. Similarly, (d), (e) and (f) illustrates the three tunneling pathways for the oleate2. The starting point of the simulation for oleate1 is shown by orange colored sphere