Supporting Information

Palmitic acid binding to conjugative traffic ATPases as a drug-target interaction to inhibit bacterial conjugation

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This document includes 2 figures (Figure 1S and Figure 2S) with their respective legends

Figure 1S

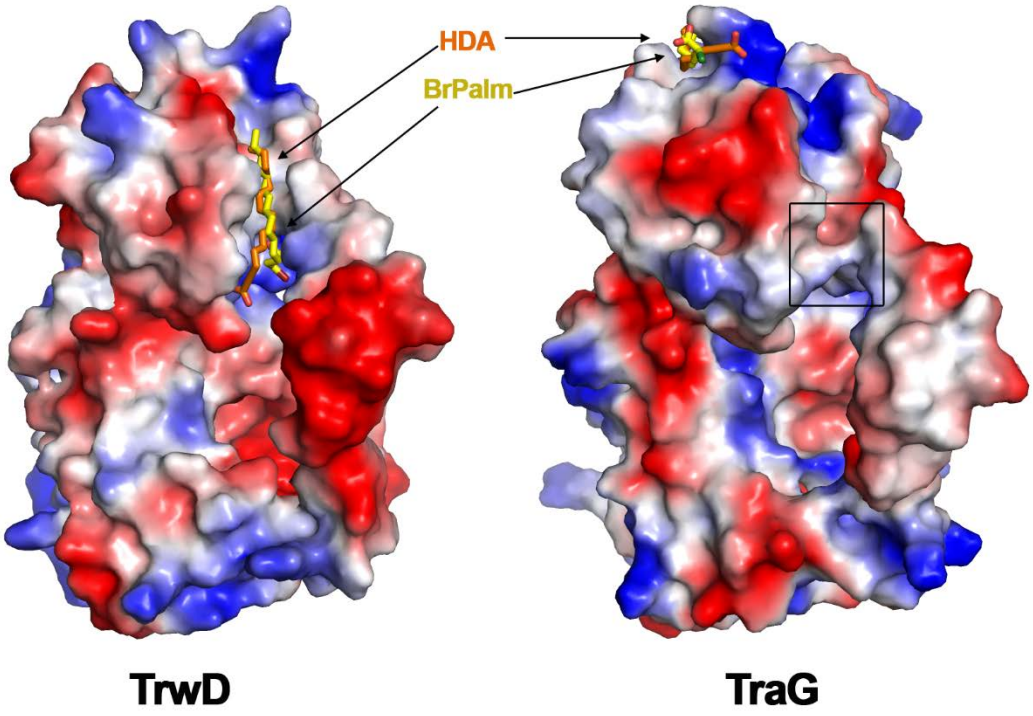

Figure 1S. Comparison of TrwD and TraG structures. Surface representation of VirB11 homologs from conjugative plasmids R388 and pKM101, respectively. The predicted binding site for 2-HDA (*orange*) and 2-bromopalmitic acid (*yellow*) in TrwD is located in a pocket formed by the N-terminus and the linker region of the protein. Such a pocket is occluded in TraG by two hydrophobic residues (boxed area). Moreover, the global charge balance is different, being much more electropositive in TrwD than in TraG.

Figure 2S

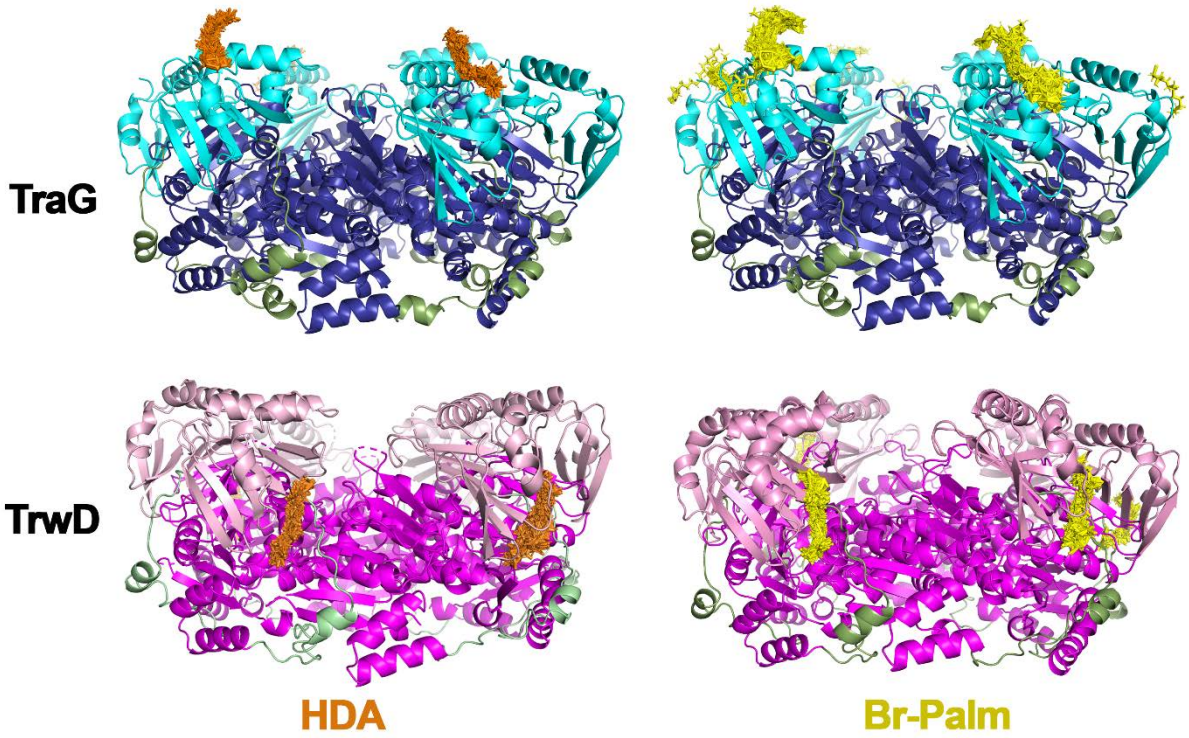

Figure 2S. Blind docking of fatty acids into the molecular models of TrwD and TraG. Blind docking predictions between both proteins and fatty acid ligands (2-HDA) and 2-bromopalmitic acid) were performed using the EADock dihedral spacing sampling engine of the Swiss-dock server (32). All predicted binding poses (250) are shown for both, TraG and TrwD, respectively. In TraG, all the binding poses locate at the upper side of the N-terminal domain (NTD, *cyan*), whereas in TrwD the fatty acids fit into a pocket located at the interface between the NTD (*pink*) and the linker region (*dark green*), which connects the NTD with the catalytic C-terminal domain (CTD, *magenta* in TrwD and *blue* in TraG). In the case of TrwD, binding of the fatty acids in that region will prevent the movement of the NTD over the CTD, whereas in TraG, such a movement will not be affected. This might explain the lack of inhibition of TraG by unsaturated fatty acids.