



Supplemental Figure 1. RMSD matrices relating the simulations with acyl-ACP starting in solvent exposed (x-axis) and solvent-shielded (y-axis) conformations. A) The RMSD of the protein backbone atoms (res. 3-75) of hexanoyl-ACP (upper) and hexadecanoyl-ACP (lower). B) The RMSD of the phosphopantetheine group and the attached acyl chain of hexanoyl-ACP (upper) and hexadecanoyl-ACP (lower). In both (A) and (B), the RMSDs between the trajectories start off high but converge very well as the simulation progresses.