

Supporting Materials: Computational Approaches to Toll-Like Receptor 4 Modulation

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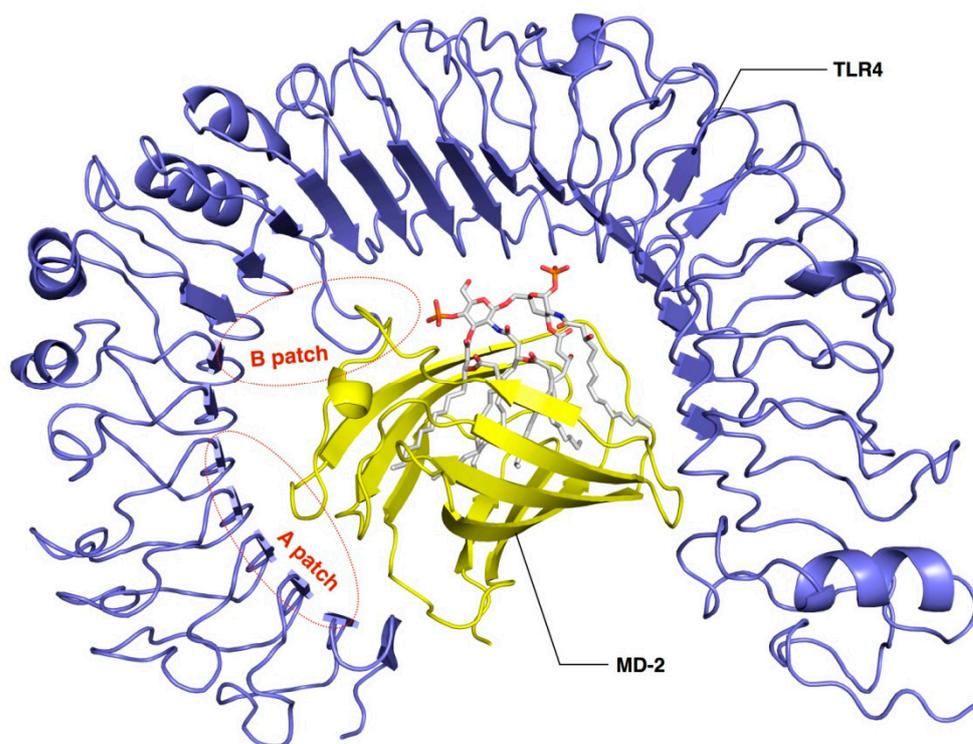


Figure S1. Detailed representation of the TLR4/MD-2 complex from the X-ray crystallographic structure for the extracellular domain (PDB ID 3FXI) in complex with *E. coli* LPS. Only the lipid A is shown for the sake of clarity. The TLR4 extracellular domain is shown in purple, MD-2 in yellow, and lipid A in green. Protein-protein interacting regions are highlighted: patch A (at the N-terminal domain of TLR4) and patch B (central domain of TLR4).

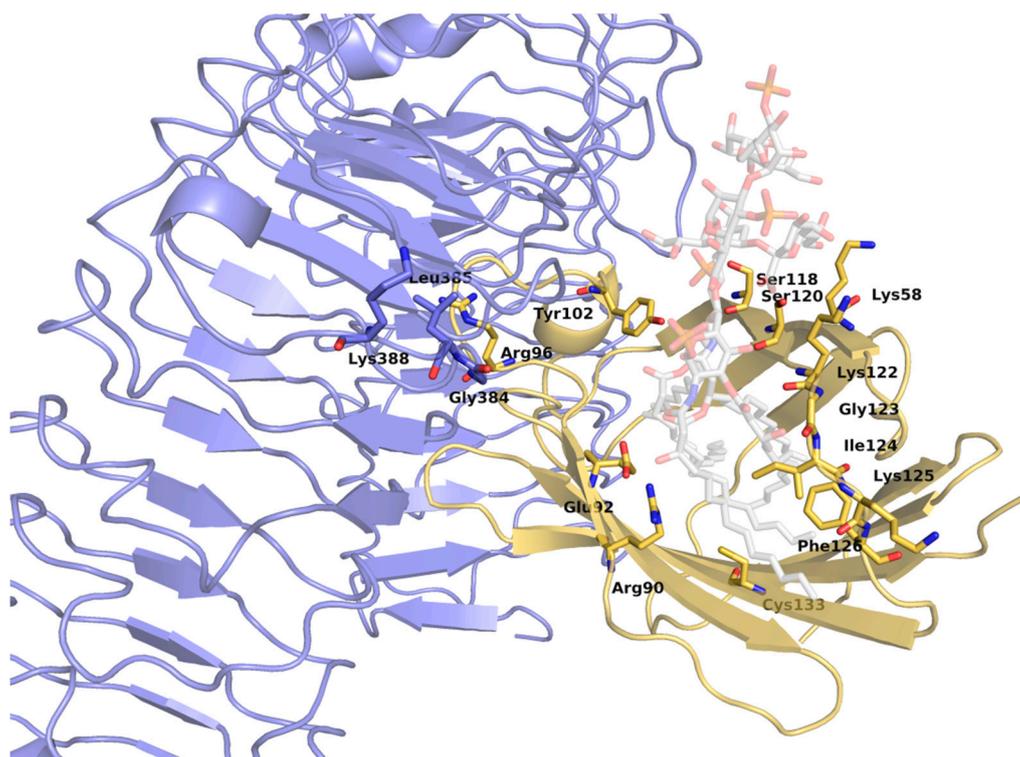


Figure S2. Detailed representation of the TLR4/MD-2 complex from the X-ray crystallographic structure for the extracellular domain (PDB ID 3FXI) in complex with *E. coli* LPS (CPK colors, partially shaded). Relevant residues discussed in this review are displayed. The TLR4 extracellular domain is shown in purple, MD-2 in yellow.

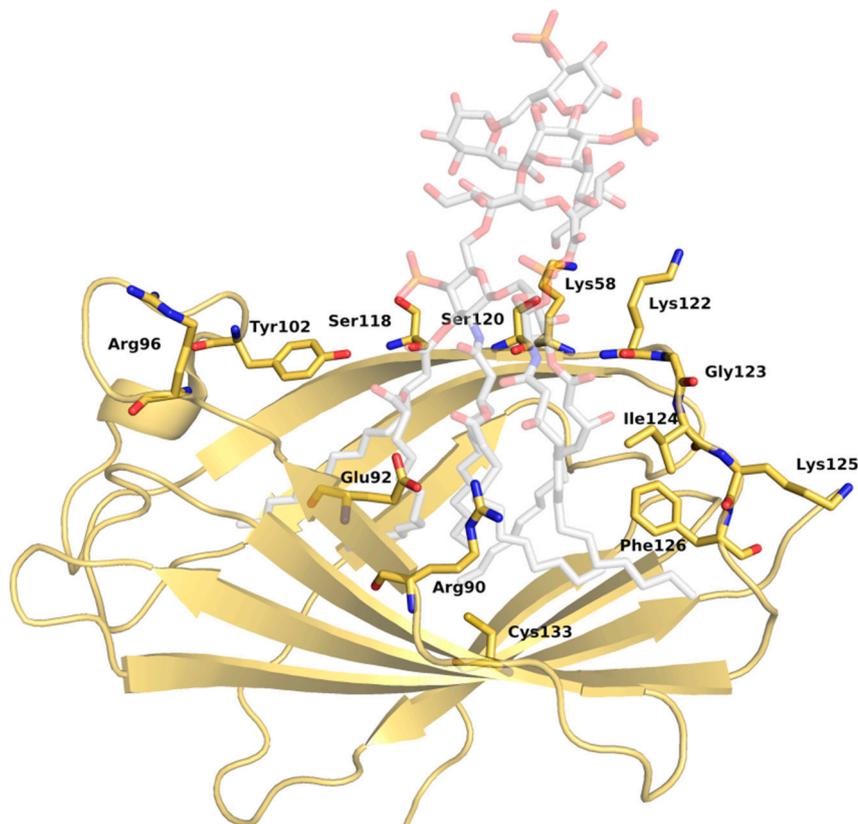


Figure S3. Detailed representation of the MD-2 complex from the X-ray crystallographic structure for the TLR4/MD-2 extracellular domain (PDB ID 3FXI) in complex with *E. coli* LPS (CPK colors, partially shaded). Relevant residues discussed in this review are displayed. MD-2 is shown in yellow. TLR4 is not displayed for the sake of clarity.