

Supporting Information

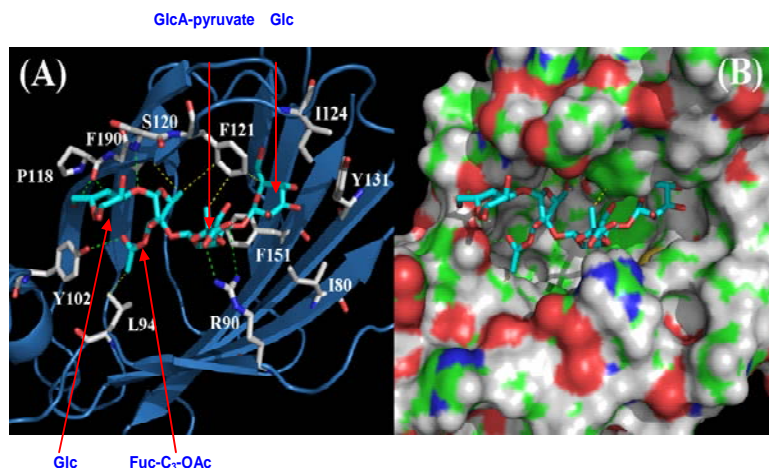
Structure and immunological characterization of the capsular polysaccharide of a pyrogenic liver abscess *Klebsiella pneumoniae*: activation of macrophages through Toll-like receptor 4

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Running title: PLA *K. pneumoniae* CPS activates macrophages via TLR4

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Supporting data. Computational molecular models of the PLA *K. pneumoniae* CPS in the active site of TLR4 are shown in panels (A) and (B). In panel (A), carbon atoms in the PLA *K. pneumoniae* CPS are colored as cyan. The carbon atoms of TLR4 are shown in gray. Nitrogen and oxygen are colored as blue and red, respectively. The TLR4 backbone structure is shown as a blue tube. Side-chains of TLR4 residues within a 7Å radius centered on the PLA *K. pneumoniae* CPS are shown explicitly. Secondary structure elements are shown as a ribbon drawing and important residues involved in PLA *K. pneumoniae* CPS binding are labeled. The green and yellow dotted lines represent, respectively, tentative hydrogen bonding donor-acceptor pairs or hydrophobic interactions of the PLA *K. pneumoniae* CPS with TLR4. In panel (B), the carbon atoms of TLR4 are shown in green, while nitrogen, oxygen, and hydrogen are colored blue, red, or gray, respectively. The molecular models were generated using PyMOL software.