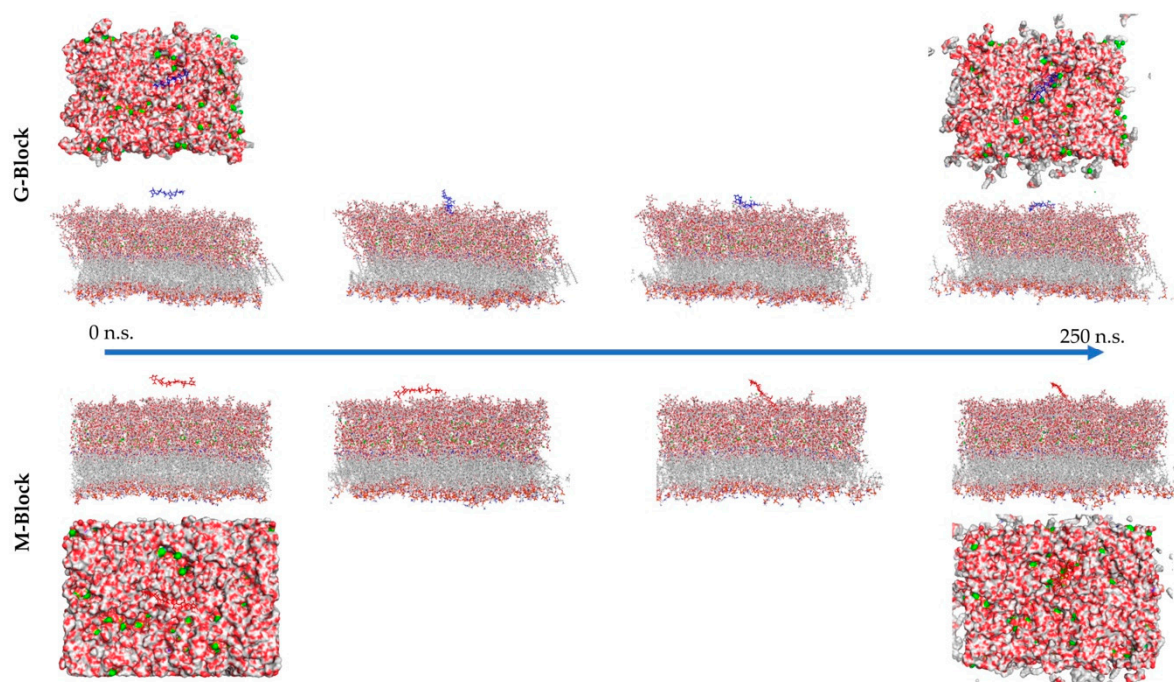


Supplementary Figure S1: schematic representation of potential LPS binding sites during MD simulations



Supplementary Figure S2: representative (side-view) images of the G-block and M-block simulations taken at equal intervals between 0 and 250 ns (Ca^{2+} ions are shown in orange), with arial view images at the start and end of the simulation also shown.