



Figure S2: (A) ^{31}P -NMR spectra of the titration of lipid II with NAI-107. The solution contained 2.65 mM lipid II in DPC-d38. The phosphate group in DPC yields a strong signal at -3.4 ppm, an impurity in commercially available DPC yields two weak signals at -14.0 and -15.1 ppm (see Fig. S1). The pyrophosphate group of lipid II yields two signals at -14.0 and -16.3 ppm, respectively. Impurities/buffer components are marked with an “*”. Signals of free lipid II disappear up to a molar ratio of 1:1.2 (3 mM NAI-107), whereafter new signals appear. All spectra are scaled to the DPC peak at -3.4 ppm, different noise levels reflect different numbers of scans recorded. Spectra were processed with 2 Hz exponential line broadening. Fig. S2 shows spectra of the titration end points together with buffer background spectra. **(B)** ^1H -NMR spectra of the titration of lipid II with NAI-107. The solution contained 2.65 mM lipid II in DPC-d38. Only signals with higher shifts than water are shown (aromatic, olefinic and amide signals). The signals at approx. 5 ppm come from the olefinic and anomeric hydrogen atoms of lipid II. their intensity drops up to a peptide-lipid II ratio of 1:1. Peptide signals, e.g. the characteristic indole NH of 5-chlorotryptophane at 10.8 ppm, only start to appear at peptide-lipid II ratios >1:1.