Conformational Changes of Anoplin, W-MreB1-9, and (KFF)3K Peptides near the Membranes

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Supplementary Materials

**Figure S1.** The model of anoplin bound to a DPC micelle visualized based on the solution NMR structure with PDB ID 2MJQ [26]. Anoplin forms a helix marked as pink ribbon, with the Lys side-chains shown in blue, Arg in orange, Thr in yellow, and Leu, Ile, and Gly in grey. The central Lys amine hydrogen bonds with the phosphate oxygen of the micelle. The figure was prepared with VMD (https://www.ks.uiuc.edu/Research/vmd/).
Figure S2. Mass spectrum and RP-HPLC chromatogram of anopiln after purification. For the HPLC method see section "Materials and Methods", subsection 4.1 in the main text "Peptide synthesis and purification".

Figure S3. Mass spectrum and RP-HPLC chromatogram of W-MreB 1-9 after purification. For the HPLC method see section "Materials and Methods", subsection 4.1 in the main text "Peptide synthesis and purification".
Figure S4. Mass spectrum and RP-HPLC chromatogram of (KFF)₃K after purification. For the HPLC method see section "Materials and Methods", subsection 4.1 in the main text "Peptide synthesis and purification".

Figure S5. CD spectra of anoplin in the presence of A) POPC:POPG (3:1) and B) POPC:POPE (3:1) SUVs with the legends showing the lipids concentrations in mM.
Figure S6. CD spectra of (KFF)₃K in the presence of A) DPC micelles, B) POPC:POPG (3:1) SUVs, C) POPC:POPE (3:1) SUVs, and D) E. coli BL21(DE3) cells. The legends show the membrane concentrations.
Anoplin  |  W-MreB<sub>Δ4</sub>  |  (KFF<sub>ΔK</sub>)

Figure S7. Secondary structure contents (in percent) in the peptide structures determined from the DichroWeb server using the CDSSTR algorithm and reference data set 4 [47,48]. The percentages of helices and strands are the sum of the contributions of the regular and distorted α-helices or the regular and distorted β-sheets, respectively. The percentages of turns and unordered structures were taken directly from the output data.
Figure S8. Optical density (OD) as a measure of E. coli K12 and BL21(DE3) growth shown after 20 h incubation with various concentrations of (KFF)3K, anoplin, and W-MreB1-9 peptides. Error bars represent the standard error of the mean. G.C. stands for growth control. The **** mark the MIC.

A) For the K12 strain, the OD differences between the G.C. and samples treated with different (KFF)3K concentrations were statistically highly significant (P < 0.001 for 0.5 µM and P < 0.0001 for all other (KFF)3K concentrations). For the BL21 strain, the OD differences between the G.C. and 0.5 µM – 8 µM (KFF)3K were not significant (P > 0.05), between G.C. and 16 µM (KFF)3K were marginally significant (P < 0.05), and between G.C. and 32 – 256 µM were highly significant (P < 0.0001).

B) For K12, the OD differences between the G.C. and samples treated with anoplin were statistically highly significant (P < 0.0001) except for anoplin concentration of 2 µM (P < 0.05). For BL21, the OD differences between the G.C. and 0.5 µM – 8 µM anoplin samples were not significant, and between G.C. and anoplin concentrations ≥ 16 µM were highly significant (P < 0.0001).

C) For K12, the OD differences between the G.C. and samples treated with W-MreB1-9 were statistically highly significant (P < 0.001). For BL21, the OD differences between the G.C. and MreB1-9 concentrations up to 64 µM were insignificant (P > 0.05), and for higher MreB1-9 concentrations they were highly statistically significant (P < 0.0001).
Figure S9. Optical density (OD) as a measure of *E. coli* K12 and BL21(DE3) growth shown after 20 h incubation with various concentrations of ampicillin or tetracycline. Error bars represent the standard error of the mean. G.C. stands for growth control. The **** mark the MIC concentrations.

A) For the K12 strain, the OD differences between the G.C. and samples with ampicillin concentrations starting from 4 µM were highly statistically significant (P < 0.0001). For BL21, the differences between the G.C. and samples for ampicillin concentrations ≥ 2 µM were highly significant (P < 0.0001).

B) For K12, the differences between the G.C. and samples treated with tetracycline concentrations up to 2 µM were statistically insignificant (P > 0.05) and for ≥ 4 µM were highly significant (P < 0.0001). For BL21, the differences between the G.C. and tetracycline concentrations up to 1 µM were statistically insignificant (P > 0.05), and for higher tetracycline concentrations they were highly significant.

Table S1. Fractions of secondary structures in anoplin in different surroundings calculated from DichroWeb [47,48]. The experimental CD spectra are shown in Figure 2 in the main text.

| Anoplin  | Method / Reference set. | α-helix regular | α-helix distorted | β-sheet regular | β-sheet distorted | Turns | Unordered | NRMSD^1 |
|----------|-------------------------|-----------------|------------------|----------------|-----------------|-------|-----------|---------|
| buffer   | CONTINLL/4              | 0.000           | 0.360            | 0.000          | 0.077           | 0.303 | 0.260     | 0.176   |
|          | CONTINLL/7              | 0.000           | 0.208            | 0.000          | 0.001           | 0.000 | 0.790     | 0.098   |
|          | CONTINLL/SP180          | 0.000           | 0.162            | 0.000          | 0.107           | 0.197 | 0.535     | 0.206   |
|          | CDSSTR/4               | 0.04            | 0.11             | 0.10           | 0.13            | 0.28  | 0.35      | 0.001   |
|          | CDSSTR/7               | 0.35            | 0.10             | 0.14           | 0.10            | 0.10  | 0.22      | 0.001   |
|          | CDSSTR/SP180           | 0.42            | 0.13             | 0.06           | 0.08            | 0.11  | 0.22      | 0.001   |
| 1        | CONTINLL/4              | 0.523           | 0.404            | 0.000          | 0.073           | 0.000 | 0.000     | 0.142   |
|          | CONTINLL/7              | 0.596           | 0.404            | 0.000          | 0.000           | 0.000 | 0.000     | 0.142   |
|          | CONTINLL/SP180          | 0.362           | 0.352            | 0.000          | 0.000           | 0.082 | 0.204     | 0.162   |
|          | CDSSTR/4               | 0.48            | 0.13             | 0.07           | 0.07            | 0.05  | 0.20      | 0.001   |
|          | CDSSTR/7               | 0.46            | 0.14             | 0.07           | 0.07            | 0.06  | 0.20      | 0.001   |
|          | CDSSTR/SP180           | 0.43            | 0.11             | 0.12           | 0.09            | 0.08  | 0.18      | 0.001   |
| SDS [mM] | 5                      | CONTINLL/4      | 0.490            | 0.510          | 0.000           | 0.000 | 0.000     | 0.107   |
|          | CONTINLL/7              | 0.591           | 0.409            | 0.000          | 0.000           | 0.000 | 0.000     | 0.107   |
|          | CONTINLL/SP180          | 0.473           | 0.527            | 0.000          | 0.000           | 0.000 | 0.000     | 0.114   |
|          | CDSSTR/4               | 0.52            | 0.15             | 0.06           | 0.06            | 0.04  | 0.17      | 0.000   |
|          | CDSSTR/7               | 0.50            | 0.16             | 0.06           | 0.06            | 0.05  | 0.18      | 0.000   |
|          | CDSSTR/SP180           | 0.45            | 0.11             | 0.13           | 0.09            | 0.08  | 0.15      | 0.000   |
|          | 10                     | CONTINLL/4      | 0.412            | 0.588          | 0.000           | 0.000 | 0.000     | 0.136   |
| DPC [mM] | CONTINLL/7 | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 | CONTINLL/4 | CONTINLL/7 | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 |
|-----------|------------|----------------|----------|----------|---------------|------------|------------|----------------|----------|----------|---------------|
| 0.5       | 0.537      | 0.463          | 0.000    | 0.000    | 0.000         | 0.000      | 0.000      | 0.000          | 0.136    |          |                |
|           | 0.000      | 0.671          | 0.000    | 0.000    | 0.152         | 0.178      | 0.146      |                |          |          |                |
|           | 0.48       | 0.13           | 0.07     | 0.07     | 0.05          | 0.20       | 0.000      |                |          |          |                |
|           | 0.47       | 0.13           | 0.09     | 0.08     | 0.05          | 0.20       | 0.000      |                |          |          |                |
|           | 0.41       | 0.10           | 0.14     | 0.10     | 0.08          | 0.19       | 0.000      |                |          |          |                |
| 30        | 0.509      | 0.491          | 0.000    | 0.000    | 0.000         | 0.000      | 0.103      |                |          |          |                |
|           | 0.604      | 0.396          | 0.000    | 0.000    | 0.000         | 0.000      | 0.103      |                |          |          |                |
|           | -          | -              | -        | -        | -             | -          | -          |                |          |          |                |
|           | 0.54       | 0.16           | 0.04     | 0.07     | 0.04          | 0.15       | 0.000      |                |          |          |                |
|           | 0.52       | 0.17           | 0.03     | 0.06     | 0.04          | 0.17       | 0.000      |                |          |          |                |
|           | 0.47       | 0.13           | 0.13     | 0.08     | 0.08          | 0.12       | 0.000      |                |          |          |                |
| 0.5       | 0.062      | 0.374          | 0.000    | 0.131    | 0.433         | 0.000      | 0.376      |                |          |          |                |
|           | 0.098      | 0.403          | 0.000    | 0.113    | 0.387         | 0.000      | 0.376      |                |          |          |                |
|           | 0.079      | 0.168          | 0.000    | 0.090    | 0.181         | 0.481      | 0.427      |                |          |          |                |
|           | 0.36       | 0.09           | 0.14     | 0.11     | 0.09          | 0.21       | 0.002      |                |          |          |                |
|           | 0.44       | 0.16           | 0.10     | 0.07     | 0.06          | 0.15       | 0.002      |                |          |          |                |
|           | 0.45       | 0.14           | 0.07     | 0.05     | 0.13          | 0.15       | 0.004      |                |          |          |                |
| 2         | 0.628      | 0.372          | 0.000    | 0.000    | 0.000         | 0.000      | 0.099      |                |          |          |                |
|           | 0.694      | 0.306          | 0.000    | 0.000    | 0.000         | 0.000      | 0.099      |                |          |          |                |
|           | 0.583      | 0.417          | 0.000    | 0.000    | 0.000         | 0.000      | 0.112      |                |          |          |                |
|           | 0.55       | 0.16           | 0.05     | 0.06     | 0.04          | 0.13       | 0.001      |                |          |          |                |
|           | 0.51       | 0.17           | 0.05     | 0.07     | 0.06          | 0.15       | 0.000      |                |          |          |                |
|           | 0.54       | 0.12           | 0.08     | 0.06     | 0.05          | 0.14       | 0.000      |                |          |          |                |
| 5         | 0.619      | 0.381          | 0.000    | 0.000    | 0.000         | 0.000      | 0.057      |                |          |          |                |
|           | 0.629      | 0.371          | 0.000    | 0.000    | 0.000         | 0.000      | 0.057      |                |          |          |                |
|           | 0.422      | 0.417          | 0.000    | 0.000    | 0.042         | 0.118      | 0.079      |                |          |          |                |
|           | 0.52       | 0.12           | 0.06     | 0.08     | 0.07          | 0.16       | 0.000      |                |          |          |                |
|           | 0.51       | 0.15           | 0.05     | 0.07     | 0.06          | 0.17       | 0.000      |                |          |          |                |
|           | 0.47       | 0.16           | 0.12     | 0.08     | 0.07          | 0.10       | 0.000      |                |          |          |                |
| 10        | 0.557      | 0.443          | 0.000    | 0.000    | 0.000         | 0.000      | 0.073      |                |          |          |                |
|           | 0.615      | 0.385          | 0.000    | 0.000    | 0.000         | 0.000      | 0.073      |                |          |          |                |
|           | 0.401      | 0.438          | 0.000    | 0.000    | 0.041         | 0.119      | 0.091      |                |          |          |                |
|           | 0.51       | 0.13           | 0.05     | 0.08     | 0.05          | 0.18       | 0.000      |                |          |          |                |
|           | 0.50       | 0.16           | 0.04     | 0.06     | 0.05          | 0.19       | 0.000      |                |          |          |                |
|           | 0.45       | 0.12           | 0.13     | 0.08     | 0.08          | 0.14       | 0.000      |                |          |          |                |
| POPC:POPG (3:1) [mM] | CONTINLL/4 | 0.000          | 0.365    | 0.000    | 0.057         | 0.386      | 0.192      |                |          |          |                |
|           | 0.000      | 0.219          | 0.000    | 0.000    | 0.000         | 0.781      | 0.121      |                |          |          |                |
|           | 0.000      | 0.321          | 0.000    | 0.040    | 0.169         | 0.470      | 0.196      |                |          |          |                |
|           | 0.23       | 0.09           | 0.16     | 0.11     | 0.17          | 0.24       | 0.001      |                |          |          |                |
|           | 0.44       | 0.17           | 0.05     | 0.06     | 0.07          | 0.20       | 0.001      |                |          |          |                |
|           | 0.43       | 0.13           | 0.06     | 0.08     | 0.09          | 0.20       | 0.001      |                |          |          |                |
| 0.5       | 0.339      | 0.324          | 0.000    | 0.037    | 0.190         | 0.111      | 0.097      |                |          |          |                |
|           | 0.348      | 0.331          | 0.000    | 0.079    | 0.242         | 0.000      | 0.097      |                |          |          |                |
| LPS [µM] | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 | CONTINLL/4 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 |
|----------|----------------|-----------|-----------|---------------|-----------|-----------|-----------|---------------|
| 0.75     | 0.208          | 0.304     | 0.000     | 0.025         | 0.137     | 0.326     | 0.288     |
|          | 0.47           | 0.12      | 0.09      | 0.09          | 0.07      | 0.17      | 0.001     |
|          | 0.49           | 0.15      | 0.07      | 0.08          | 0.05      | 0.17      | 0.001     |
|          | 0.42           | 0.15      | 0.07      | 0.08          | 0.11      | 0.17      | 0.001     |
| 0.1      | 0.000          | 1.000     | 0.000     | 0.000         | 0.000     | 0.000     | 0.205     |
|          | 0.000          | 0.272     | 0.000     | 0.000         | 0.000     | 0.000     | 0.106     |
|          | 0.000          | 0.000     | 0.000     | 0.000         | 1.000     | 0.000     | 0.792     |
|          | 0.15           | 0.01      | 0.03      | 0.09          | 0.33      | 0.34      | 0.001     |
|          | 0.40           | 0.15      | 0.07      | 0.07          | 0.06      | 0.25      | 0.000     |
|          | 0.41           | 0.11      | 0.10      | 0.08          | 0.08      | 0.23      | 0.000     |
| 2        | 0.676          | 0.324     | 0.000     | 0.000         | 0.000     | 0.000     | 0.270     |
|          | 1.000          | 0.000     | 0.000     | 0.000         | 0.000     | 0.000     | 0.270     |
|          | 0.677          | 0.323     | 0.000     | 0.000         | 0.000     | 0.000     | 0.357     |
|          | 0.47           | 0.10      | 0.09      | 0.08          | 0.07      | 0.20      | 0.001     |
|          | 0.45           | 0.10      | 0.10      | 0.08          | 0.07      | 0.21      | 0.001     |
|          | 0.51           | 0.11      | 0.05      | 0.08          | 0.08      | 0.17      | 0.001     |
| 5        | 0.314          | 0.497     | 0.000     | 0.055         | 0.134     | 0.000     | 0.424     |
|          | 0.242          | 0.525     | 0.000     | 0.117         | 0.116     | 0.000     | 0.199     |
|          | 0.000          | 0.381     | 0.000     | 0.000         | 0.269     | 0.349     | 0.434     |
|          | 0.43           | 0.09      | 0.10      | 0.10          | 0.07      | 0.21      | 0.000     |
|          | 0.42           | 0.09      | 0.10      | 0.10          | 0.07      | 0.22      | 0.000     |
|          | 0.37           | 0.08      | 0.17      | 0.12          | 0.07      | 0.22      | 0.000     |
| 10       | 0.284          | 0.539     | 0.000     | 0.000         | 0.167     | 0.111     | 0.301     |
|          | 0.258          | 0.412     | 0.000     | 0.000         | 0.000     | 0.330     | 0.153     |
|          | 0.000          | 0.394     | 0.000     | 0.046         | 0.161     | 0.399     | 0.324     |
|          | 0.51           | 0.13      | 0.03      | 0.09          | 0.06      | 0.18      | 0.000     |
|          | 0.45           | 0.16      | 0.06      | 0.07          | 0.07      | 0.21      | 0.000     |
|          | 0.39           | 0.13      | 0.12      | 0.09          | 0.08      | 0.21      | 0.000     |
| 20       | 0.535          | 0.465     | 0.000     | 0.000         | 0.000     | 0.000     | 0.116     |
|          | 0.601          | 0.399     | 0.000     | 0.000         | 0.000     | 0.000     | 0.116     |
|          | 0.349          | 0.651     | 0.000     | 0.000         | 0.000     | 0.000     | 0.147     |
|          | 0.45           | 0.11      | 0.09      | 0.09          | 0.06      | 0.21      | 0.000     |
|          | 0.43           | 0.10      | 0.10      | 0.09          | 0.06      | 0.22      | 0.000     |
|          | 0.40           | 0.08      | 0.16      | 0.11          | 0.07      | 0.19      | 0.000     |
| 50       | 1.000          | 0.000     | 0.000     | 0.000         | 0.000     | 0.000     | 0.058     |
|          | 1.000          | 0.000     | 0.000     | 0.000         | 0.000     | 0.000     | 0.058     |
|          |                |           |           |               |           |           |           |
| POPC:POPE (3:1) [mM] | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 | CONTINLL/4 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 |
| 0.75     | 0.000          | 1.000     | 0.000     | 0.000         | 0.000     | 0.000     | 0.151     |
|          | 0.488          | 0.512     | 0.000     | 0.000         | 0.000     | 0.000     | 0.151     |
|          | 0.000          | 1.000     | 0.000     | 0.000         | 0.000     | 0.000     | 0.322     |
|          | 0.39           | 0.08      | 0.15      | 0.11          | 0.07      | 0.21      | 0.000     |
|          | 0.40           | 0.08      | 0.14      | 0.11          | 0.07      | 0.21      | 0.000     |
|          | 0.37           | 0.07      | 0.18      | 0.12          | 0.07      | 0.21      | 0.000     |
1 normalized root mean square deviation. The NRMSD value less than 0.1 suggests a good fit of anoplin CD spectrum to the reference set, and NRMSD above 0.5 suggests that the peptide CD spectrum does not fit well to the CD spectra of the reference set. But low NRMSD do not ensure that the analysis is accurate [47].

**Table S2.** Fractions of secondary structures in W-MreB$_{1-9}$ in different surroundings calculated from DichroWeb [47,48]. The experimental CD spectra are shown in Figure 3 in the main text.
| Buffer | CONTINLL/4 | CONTINLL/7 | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 |
|--------|------------|------------|----------------|----------|----------|--------------|
|        | 0.178      | 0.425      | 0.000          | 0.000    | 0.220    | 0.177        |
|        | 0.456      | 0.544      | 0.000          | 0.000    | 0.000    | 0.000        |
|        | -          | -          | -              | -        | -        | -            |
| 1      | -          | -          | -              | -        | -        | -            |
|        | 0.22       | 0.10       | 0.18           | 0.10     | 0.18     | 0.21         |
|        | 0.41       | 0.17       | 0.08           | 0.07     | 0.05     | 0.20         |
|        | 0.43       | 0.14       | 0.06           | 0.07     | 0.10     | 0.20         |
|        | 0.00       | 0.620      | 0.000          | 0.084    | 0.296    | 0.000        |
|        | 0.00       | 0.404      | 0.000          | 0.000    | 0.000    | 0.596        |
|        | 0.00       | 0.326      | 0.000          | 0.000    | 0.330    | 0.344        |
|        | 0.38       | 0.08       | 0.15           | 0.10     | 0.08     | 0.21         |
|        | 0.39       | 0.13       | 0.09           | 0.08     | 0.08     | 0.23         |
|        | 0.43       | 0.12       | 0.07           | 0.07     | 0.11     | 0.21         |
| 5      | -          | -          | -              | -        | -        | -            |
|        | 0.00       | 1.000      | 0.000          | 0.000    | 0.000    | 0.000        |
|        | 0.00       | 0.616      | 0.000          | 0.000    | 0.000    | 0.245        |
|        | 0.00       | 0.489      | 0.000          | 0.029    | 0.085    | 0.396        |
|        | 0.41       | 0.11       | 0.12           | 0.09     | 0.06     | 0.21         |
|        | 0.39       | 0.13       | 0.11           | 0.09     | 0.06     | 0.21         |
|        | 0.39       | 0.08       | 0.14           | 0.11     | 0.09     | 0.21         |
| 10     | -          | -          | -              | -        | -        | -            |
|        | 0.00       | 0.000      | 0.000          | 0.000    | 1.000    | 0.000        |
|        | 0.00       | 0.616      | 0.000          | 0.000    | 0.000    | 0.384        |
|        | 0.00       | 0.489      | 0.000          | 0.029    | 0.085    | 0.396        |
|        | 0.35       | 0.07       | 0.17           | 0.11     | 0.09     | 0.21         |
|        | 0.38       | 0.14       | 0.12           | 0.09     | 0.07     | 0.20         |
|        | 0.40       | 0.10       | 0.12           | 0.10     | 0.09     | 0.21         |
| 30     | -          | -          | -              | -        | -        | -            |
|        | 0.017      | 0.499      | 0.000          | 0.000    | 0.277    | 0.207        |
|        | 0.036      | 0.411      | 0.000          | 0.000    | 0.099    | 0.455        |
|        | 0.000      | 0.316      | 0.000          | 0.098    | 0.143    | 0.443        |
|        | 0.37       | 0.08       | 0.15           | 0.11     | 0.08     | 0.22         |
|        | 0.40       | 0.16       | 0.05           | 0.05     | 0.07     | 0.27         |
|        | 0.42       | 0.13       | 0.08           | 0.07     | 0.09     | 0.22         |
| 0.5    | -          | -          | -              | -        | -        | -            |
|        | 0.00       | 0.271      | 0.000          | 0.084    | 0.191    | 0.454        |
|        | 0.00       | 0.136      | 0.000          | 0.028    | 0.000    | 0.836        |
|        | 0.00       | 0.105      | 0.000          | 0.098    | 0.118    | 0.679        |
|        | -          | -          | -              | -        | -        | -            |
|        | -          | -          | -              | -        | -        | -            |
|        | 0.34       | 0.06       | 0.17           | 0.12     | 0.07     | 0.25         |
| 2      | -          | -          | -              | -        | -        | -            |
|        | 0.229      | 0.536      | 0.000          | 0.005    | 0.230    | 0.000        |
|        | 0.386      | 0.513      | 0.000          | 0.101    | 0.000    | 0.000        |
|        | 0.00       | 0.001      | 0.733          | 0.266    | 0.000    | 0.000        |
|        | 0.51       | 0.06       | 0.000          | 0.06     | 0.07     | 0.33         |
|        | 0.39       | 0.09       | 0.14           | 0.10     | 0.07     | 0.20         |
|        | 0.40       | 0.09       | 0.15           | 0.10     | 0.08     | 0.19         |
| 5      | 0.537      | 0.463      | 0.000          | 0.000    | 0.000    | 0.000        |

| SDS [mM] | CONTINLL/4 | CONTINLL/7 | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 |
|----------|------------|------------|----------------|----------|----------|--------------|
| 0.5      | 0.229      | 0.536      | 0.000          | 0.005    | 0.230    | 0.000        |
| 2        | 0.386      | 0.513      | 0.000          | 0.101    | 0.000    | 0.000        |
| 5        | 0.537      | 0.463      | 0.000          | 0.000    | 0.000    | 0.000        |

| DPC [mM] | CONTINLL/4 | CONTINLL/7 | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 |
|----------|------------|------------|----------------|----------|----------|--------------|
| 0.5      | 0.229      | 0.536      | 0.000          | 0.005    | 0.230    | 0.000        |
| 2        | 0.386      | 0.513      | 0.000          | 0.101    | 0.000    | 0.000        |
| 5        | 0.537      | 0.463      | 0.000          | 0.000    | 0.000    | 0.000        |
|          | CONTINLL/4 | CONTINLL/7 | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 |
|----------|------------|------------|----------------|----------|----------|--------------|
| POPC:POPG (3:1) [mM] 1 | 0.579 | 0.421 | 0.000 | 0.000 | 0.000 | 0.000 | 0.158 |
| CONTINLL/4 | 0.44 | 0.10 | 0.12 | 0.09 | 0.06 | 0.19 | 0.000 |
| CONTINLL/7 | 0.44 | 0.12 | 0.10 | 0.08 | 0.07 | 0.19 | 0.000 |
| CONTINLL/SP180 | 0.46 | 0.09 | 0.12 | 0.09 | 0.07 | 0.18 | 0.000 |
| POPC:POPG (3:1) [mM] 2 | 0.408 | 0.592 | 0.000 | 0.000 | 0.000 | 0.000 | 0.121 |
| CONTINLL/4 | 1.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.121 |
| CONTINLL/7 | 0.000 | 1.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.170 |
| CONTINLL/SP180 | 0.39 | 0.07 | 0.16 | 0.11 | 0.07 | 0.21 | 0.000 |
| CDSSTR/4 | 0.39 | 0.09 | 0.15 | 0.11 | 0.07 | 0.20 | 0.000 |
| CDSSTR/7 | 0.39 | 0.08 | 0.17 | 0.11 | 0.07 | 0.19 | 0.000 |
| CDSSTR/SP180 | 0.579 | 0.246 | 0.19 | 0.000 | 0.000 | 0.000 | 0.269 |
| POPC:POPG (3:1) [mM] 3 | 0.093 | 0.246 | 0.19 | 0.000 | 0.000 | 0.211 | 0.432 |
| CONTINLL/4 | 0.000 | 0.378 | 0.622 | 0.000 | 0.000 | 0.000 | 0.136 |
| CONTINLL/7 | 0.000 | 0.324 | 0.000 | 0.107 | 0.069 | 0.501 | 0.374 |
| CONTINLL/SP180 | 0.26 | 0.09 | 0.16 | 0.09 | 0.15 | 0.24 | 0.001 |
| CDSSTR/4 | 0.40 | 0.15 | 0.10 | 0.08 | 0.08 | 0.19 | 0.001 |
| CDSSTR/7 | 0.41 | 0.13 | 0.08 | 0.07 | 0.09 | 0.22 | 0.001 |
| CDSSTR/SP180 | 0.47 | 0.08 | 0.10 | 0.08 | 0.17 | 0.11 | 0.000 |
| POPC:POPE (3:1) [mM] 4 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 1.000 | 0.208 |
| CONTINLL/4 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 1.000 | 0.208 |
| CONTINLL/7 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| CONTINLL/SP180 | 0.342 | 0.507 | 0.000 | 0.151 | 0.000 | 0.000 | 0.000 |
| CDSSTR/4 | 0.47 | 0.12 | 0.11 | 0.08 | 0.04 | 0.19 | 0.001 |
| CDSSTR/7 | 0.45 | 0.13 | 0.10 | 0.08 | 0.05 | 0.17 | 0.001 |
| CDSSTR/SP180 | 0.47 | 0.11 | 0.10 | 0.07 | 0.11 | 0.15 | 0.000 |
| POPC:POPE (3:1) [mM] 5 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 1.000 | 0.205 |
| CONTINLL/4 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 1.000 | 0.205 |
| CONTINLL/7 | 0.000 | 0.000 | 1.000 | 0.000 | 0.000 | 0.000 | 0.205 |
| LPS [µM] | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 |
|----------|----------------|----------|----------|---------------|
| 10       | 0.000          | 0.779    | 0.000    | 0.000         |
|          | 0.000          | 0.000    | 0.360    | 0.640         |
|          | 0.000          | 0.000    | 0.119    | 0.21          |
| 20       | 0.000          | 0.629    | 0.000    | 0.000         |
|          | 0.000          | 0.000    | 0.119    | 0.326         |
|          | 0.000          | 0.000    | 0.119    | 0.23          |
| 50       | 0.000          | 0.629    | 0.000    | 0.000         |
|          | 0.000          | 0.000    | 0.119    | 0.362         |
|          | 0.000          | 0.000    | 0.119    | 0.20          |
| 100      | 0.000          | 0.155    | 0.000    | 0.154         |
|          | 0.000          | 0.194    | 0.000    | 0.477         |
|          | 0.000          | 0.154    | 0.000    | 0.271         |

| E. coli | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 |
|---------|----------------|----------|----------|---------------|
| OD=1 [µl] | 0.000          | 0.425    | 0.000    | 0.185         |
|         | 0.000          | 0.185    | 0.000    | 0.390         |
|         | 0.000          | 0.185    | 0.000    | 0.237         |
|         | 0.000          | 0.185    | 0.000    | 0.237         |
The NRMSD value less than 0.1 suggests a good fit of anoplin CD spectrum to the reference set, and NRSMD above 0.5 suggests that the peptide CD spectrum does not fit well to the CD spectra of the reference set. But low NRMSD do not ensure that the analysis is accurate [47].

Table S3. Fractions of secondary structures in (KFF)₃K in different surroundings calculated from DichroWeb [47, 48]. The experimental CD spectra are shown in Figure 4 in the main text and Figure S6.

| (KFF)₃K | Calculated secondary structure fractions | NRMSD¹ |
|---------|----------------------------------------|--------|
|         | Method / Reference set. | α-helix regular | α-helix distorted | β-sheet regular | β-sheet distorted | Turns | Unordered |          |
| buffer  | CONTINLL/4 | 0.000 | 0.421 | 0.000 | 0.044 | 0.349 | 0.187 | 0.209 |
|         | CONTINLL/7 | 0.000 | 0.364 | 0.000 | 0.009 | 0.000 | 0.627 | 0.105 |
|         | CONTINLL/SP180 | 0.000 | 0.221 | 0.000 | 0.051 | 0.140 | 0.589 | 0.496 |
|         | CDSSTR/4 | - | - | - | - | - | - | - |
|         | CDSSTR/7 | 0.14 | -0.0 | 0.28 | 0.13 | 0.20 | 0.23 | 0.001 |
|         | CDSSTR/SP180 | 0.41 | 0.14 | 0.06 | 0.08 | 0.10 | 0.21 | 0.001 |

| 1      | CONTINLL/4 | 0.000 | 0.508 | 0.000 | 0.029 | 0.000 | 0.463 | 0.497 |
|        | CONTINLL/7 | 0.000 | 0.343 | 0.000 | 0.000 | 0.000 | 0.657 | 0.317 |
|        | CONTINLL/SP180 | 0.000 | 0.222 | 0.000 | 0.129 | 0.254 | 0.396 | 0.459 |
|        | CDSSTR/4 | 0.23 | 0.07 | 0.19 | 0.12 | 0.11 | 0.25 | 0.000 |
|        | CDSSTR/7 | 0.41 | 0.12 | 0.11 | 0.09 | 0.04 | 0.24 | 0.000 |
|        | CDSSTR/SP180 | 0.36 | 0.06 | 0.16 | 0.12 | 0.07 | 0.22 | 0.000 |

| 5      | CONTINLL/4 | 0.000 | 0.000 | 0.000 | 1.000 | 0.000 | 0.000 | 0.000 |
|        | CONTINLL/7 | 0.000 | 0.589 | 0.000 | 0.317 | 0.000 | 0.000 | 0.094 |
|        | CONTINLL/SP180 | 0.000 | 0.000 | 0.000 | 0.000 | 0.623 | 0.377 | 0.588 |
|        | CDSSTR/4 | 0.36 | 0.07 | 0.16 | 0.12 | 0.08 | 0.21 | 0.000 |
|        | CDSSTR/7 | 0.38 | 0.09 | 0.13 | 0.10 | 0.06 | 0.24 | 0.000 |
|        | CDSSTR/SP180 | 0.43 | 0.10 | 0.07 | 0.08 | 0.10 | 0.21 | 0.000 |

| 10     | CONTINLL/4 | 0.000 | 0.591 | 0.000 | 0.409 | 0.000 | 0.000 | 0.493 |
|        | CONTINLL/7 | 0.000 | 0.624 | 0.000 | 0.376 | 0.000 | 0.000 | 0.421 |
|        | CONTINLL/SP180 | 0.000 | 0.000 | 0.000 | 0.000 | 1.000 | 0.000 | 0.000 |
|        | CDSSTR/4 | 0.38 | 0.07 | 0.15 | 0.11 | 0.08 | 0.21 | 0.000 |
|        | CDSSTR/7 | 0.38 | 0.08 | 0.13 | 0.10 | 0.06 | 0.24 | 0.000 |
|        | CDSSTR/SP180 | 0.38 | 0.08 | 0.13 | 0.11 | 0.08 | 0.22 | 0.000 |

| 30     | CONTINLL/4 | 0.000 | 0.613 | 0.000 | 0.387 | 0.000 | 0.000 | 0.627 |
|        | CONTINLL/7 | 0.000 | 0.617 | 0.000 | 0.383 | 0.000 | 0.000 | 0.467 |

¹ normalized root mean square deviation. The NRMSD value less than 0.1 suggests a good fit of anoplin CD spectrum to the reference set, and NRSMD above 0.5 suggests that the peptide CD spectrum does not fit well to the CD spectra of the reference set. But low NRMSD do not ensure that the analysis is accurate [47].
| DPC [mM] | CONTINLL/4 | CONTINLL/7 | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 |
|----------|------------|------------|----------------|----------|----------|-------------|
| 0.5      | CONTINLL/4 0.050 0.697 0.000 0.253 0.000 0.000 | CONTINLL/7 0.162 0.619 0.000 0.219 0.000 0.000 | CONTINLL/SP180 0.000 0.349 0.000 0.000 0.214 0.437 | CDSSTR/4 0.39 0.08 0.14 0.10 0.07 0.21 | CDSSTR/7 0.40 0.10 0.10 0.08 0.07 0.24 | CDSSTR/SP180 0.41 0.10 0.10 0.09 0.10 0.22 |
| 2        | CONTINLL/4 0.000 0.078 0.922 0.000 0.000 0.000 | CONTINLL/7 0.000 0.000 1.000 0.000 0.000 0.000 | CONTINLL/SP180 0.000 0.323 0.000 0.050 0.131 0.497 | CDSSTR/4 0.37 0.07 0.17 0.11 0.07 0.21 | CDSSTR/7 0.40 0.10 0.12 0.09 0.06 0.23 | CDSSTR/SP180 0.41 0.13 0.07 0.08 0.10 0.21 |
| 5        | CONTINLL/4 0.000 0.000 1.000 0.000 0.000 0.000 | CONTINLL/7 0.000 0.000 0.000 0.000 0.000 0.000 | CONTINLL/SP180 0.000 0.508 0.000 0.306 0.186 0.342 | CDSSTR/4 0.22 0.11 0.11 0.11 0.16 0.29 | CDSSTR/7 0.38 0.17 0.11 0.09 0.06 0.16 | CDSSTR/SP180 0.43 0.11 0.08 0.08 0.10 0.21 |
| 10       | CONTINLL/4 0.000 0.000 0.000 0.000 1.000 0.000 | CONTINLL/7 0.000 0.000 1.000 0.000 0.000 0.000 | CONTINLL/SP180 0.000 0.000 0.000 0.069 0.931 0.000 | CDSSTR/4 0.25 0.02 0.28 0.14 0.12 0.20 | CDSSTR/7 0.40 0.14 0.10 0.07 0.10 0.19 | CDSSTR/SP180 0.39 0.10 0.16 0.11 0.07 0.17 |
| 0.1      | POPC:POPG (3:1) [mM] |
| 0.5      | POPC:POPG (3:1) [mM] |
| 0.1      | POPC:POPE (3:1) [mM] |

**Notes:**
- The table compares the effects of different DPC concentrations (0.5, 2, 5, 10 mM) on various lipid composition variables.
- The numbers represent statistical significance levels (p-values) for the differences observed.
- The table includes lipid composition ratios such as CONTINLL/SP180 and CDSSTR/SP180.
- The significance levels range from 0.000 to 1.000, indicating the level of significance for the observed differences.
| LPS [µM] | CONTINLL/4 | CONTINLL/7 | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 |
|-----------|------------|------------|----------------|----------|----------|--------------|
| 0.5       | 0.000      | 0.366      | 0.000          | 0.000    | 0.124    | 0.000        |
| 10        | 0.000      | 0.366      | 0.000          | 0.000    | 0.124    | 0.000        |
| 20        | 0.000      | 0.366      | 0.000          | 0.573    | 0.371    | 0.000        |
| 50        | 0.000      | 0.366      | 0.000          | 0.147    | 0.000    | 0.000        |
| 100       | 0.000      | 0.366      | 0.000          | 0.147    | 0.000    | 0.000        |

**E. coli OD=1 [µl]**

| E. coli OD=1 [µl] | CONTINLL/4 | CONTINLL/7 | CONTINLL/SP180 | CDSSTR/4 | CDSSTR/7 | CDSSTR/SP180 |
|-------------------|------------|------------|----------------|----------|----------|--------------|
| 2                 | 0.000      | 0.366      | 0.000          | 0.000    | 0.124    | 0.000        |
| 4                 | 0.000      | 0.366      | 0.000          | 0.000    | 0.124    | 0.000        |
|                  | CDSSTR/7 | 0.40 | 0.10 | 0.13 | 0.10 | 0.08 | 0.18 | 0.001 |
|------------------|----------|------|------|------|------|------|------|-------|
|                  | CDSSTR/SP180 | 0.43 | 0.13 | 0.04 | 0.08 | 0.12 | 0.19 | 0.001 |
|                  | CONTINLL/4 | 0.179 | 0.545 | 0.000 | 0.005 | 0.271 | 0.000 | 0.380 |
|                  | CONTINLL/7 | 0.184 | 0.459 | 0.000 | 0.000 | 0.000 | 0.358 | 0.343 |
|                  | CONTINLL/SP180 | 0.000 | 0.234 | 0.000 | 0.000 | 0.197 | 0.569 | 0.578 |
|                  | CDSSTR/4 | 0.41 | 0.08 | 0.14 | 0.10 | 0.07 | 0.19 | 0.001 |
|                  | CDSSTR/7 | 0.42 | 0.11 | 0.11 | 0.09 | 0.08 | 0.20 | 0.000 |
|                  | CDSSTR/SP180 | 0.43 | 0.12 | 0.06 | 0.07 | 0.12 | 0.20 | 0.001 |

|                  | CDSSTR/7 | 0.33 | 0.05 | 0.18 | 0.11 | 0.09 | 0.24 | 0.000 |
|                  | CDSSTR/SP180 | 0.39 | 0.10 | 0.10 | 0.09 | 0.10 | 0.22 | 0.000 |

|                  | CONTINLL/4 | 0.000 | 0.503 | 0.497 | 0.000 | 0.000 | 0.000 | 0.285 |
|                  | CONTINLL/7 | 0.000 | 0.439 | 0.561 | 0.000 | 0.000 | 0.000 | 0.200 |
|                  | CONTINLL/SP180 | 0.000 | 0.276 | 0.000 | 0.054 | 0.133 | 0.537 | 0.361 |
|                  | CDSSTR/4 | -     | -     | -     | -     | -     | -     | -     |
|                  | CDSSTR/7 | 0.33 | 0.05 | 0.18 | 0.11 | 0.09 | 0.24 | 0.000 |
|                  | CDSSTR/SP180 | 0.39 | 0.10 | 0.10 | 0.09 | 0.10 | 0.22 | 0.000 |

1 normalized root mean square deviation. The NRMSD value less than 0.1 suggests a good fit of anoplin CD spectrum to the reference set, and NRMSD above 0.5 suggests that the peptide CD spectrum does not fit well to the CD spectra of the reference set. But low NRMSD do not ensure that the analysis is accurate [47].