

Design and Characterization of Myristoylated and Non-Myristoylated Peptides Effective against *Candida* spp. Clinical Isolates

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Table S1: MIC values (mg/L) of different myristoylated and non-myristoylated peptides against different isolates of *C. albicans*, *C. glabrata*, *C. parapsilosis*, *C. tropicalis* and *C. Auris*.

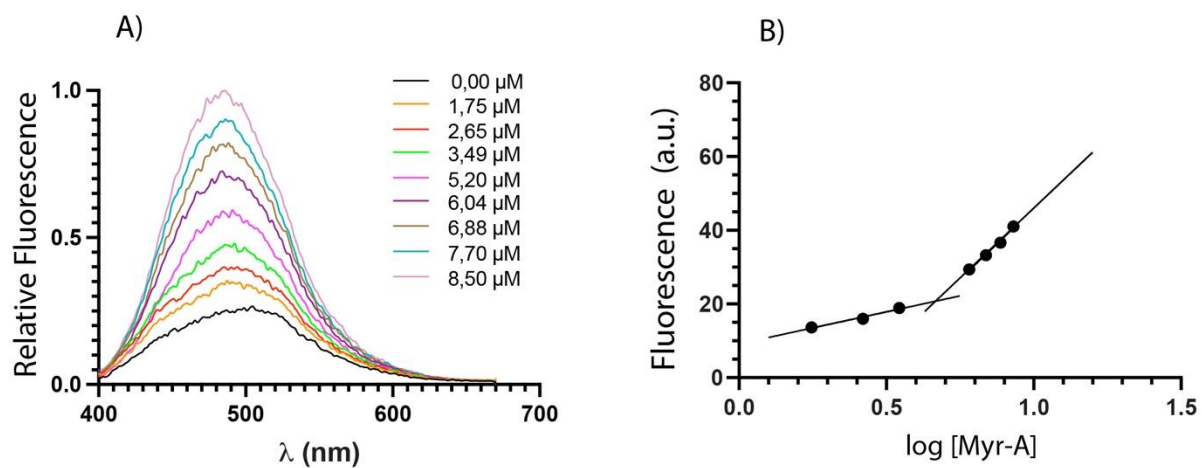


Figure S1. Determination of CMC. A) ANS fluorescence spectra of peptide Myr-A at increasing concentration. B) The plot of ANS fluorescence at 465 nm vs. logarithm of lipopeptide concentration. The intersection of the lines indicates the CMC.

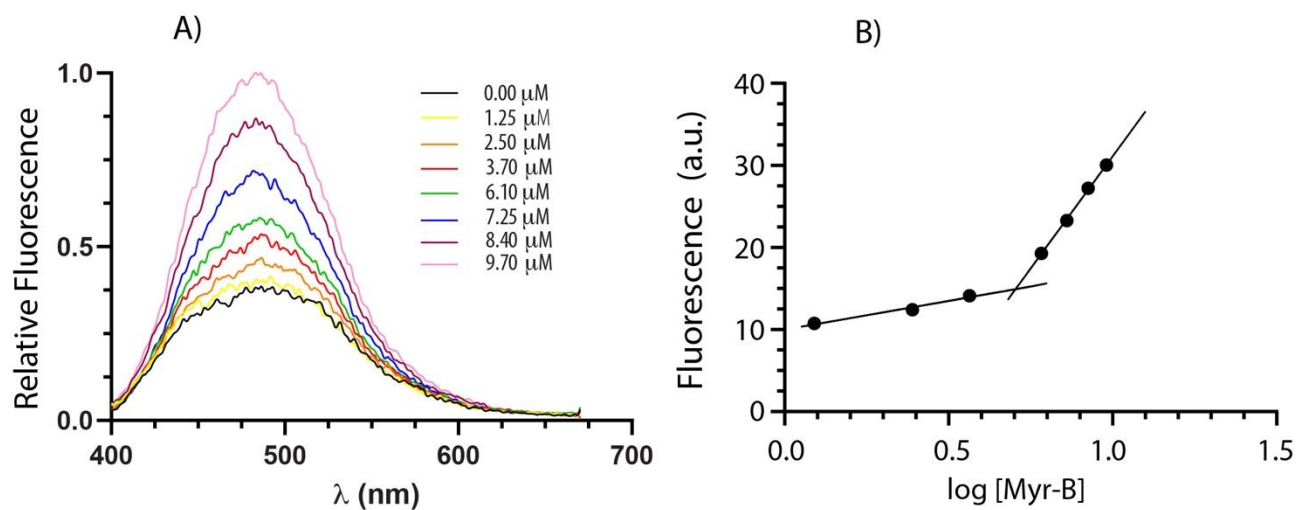


Figure S2. Determination of CMC. A) ANS fluorescence spectra of peptide Myr-B at increasing concentration. B) The plot of ANS fluorescence at 465 nm vs. logarithm of lipopeptide concentration. The intersection of the lines indicates the CMC.

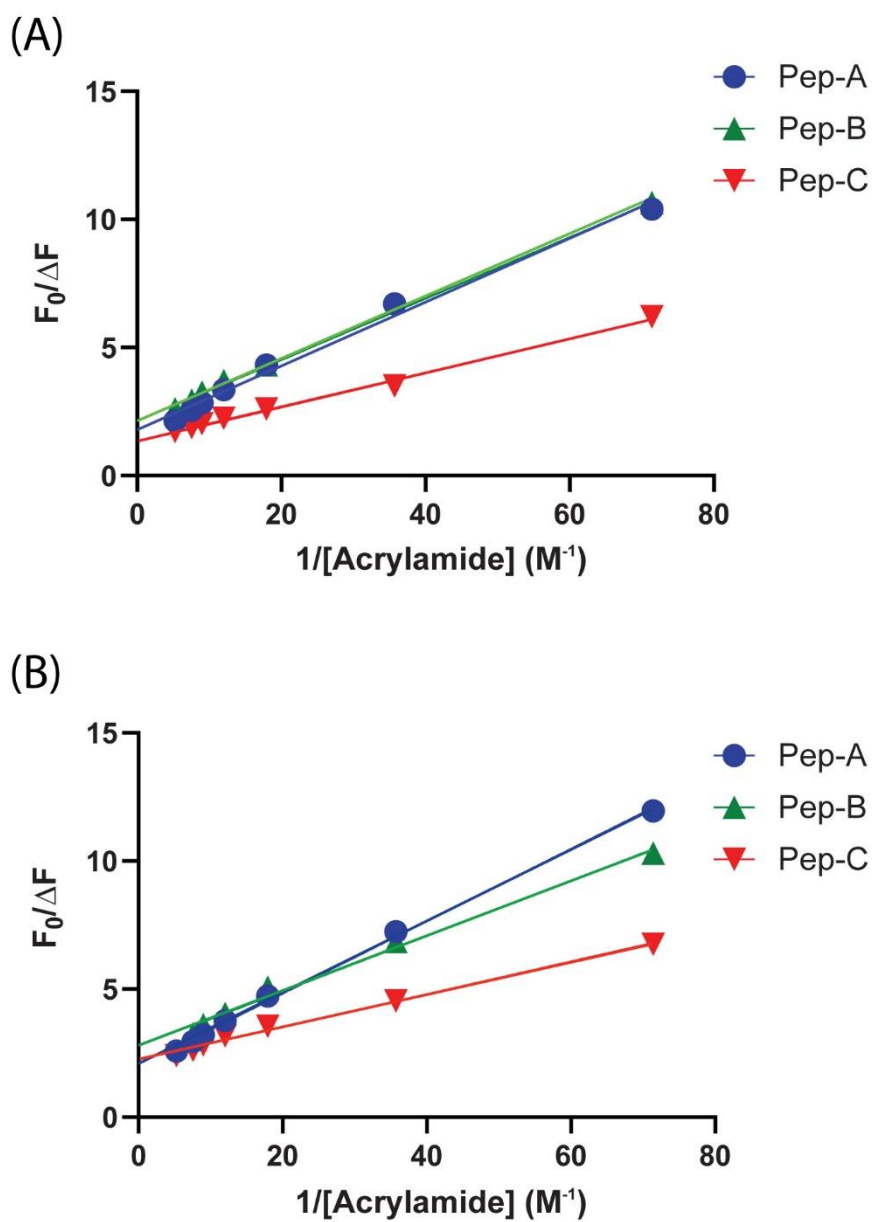


Figure S3. Stern Volmer Modified Plot for Acrylamide quenching of non-myristoylated peptides in presence of (A) POPC/POPG and (B) POPC vesicles.

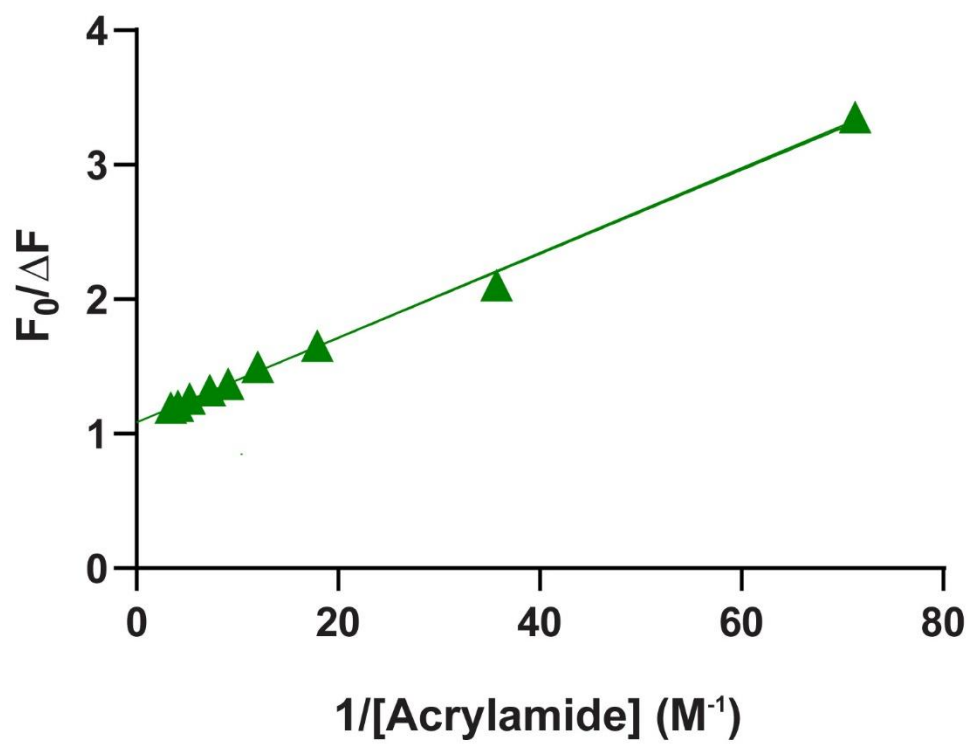


Figure S4. Stern Volmer Modified Plot for Acrylamide quenching of Myr-B in buffer.

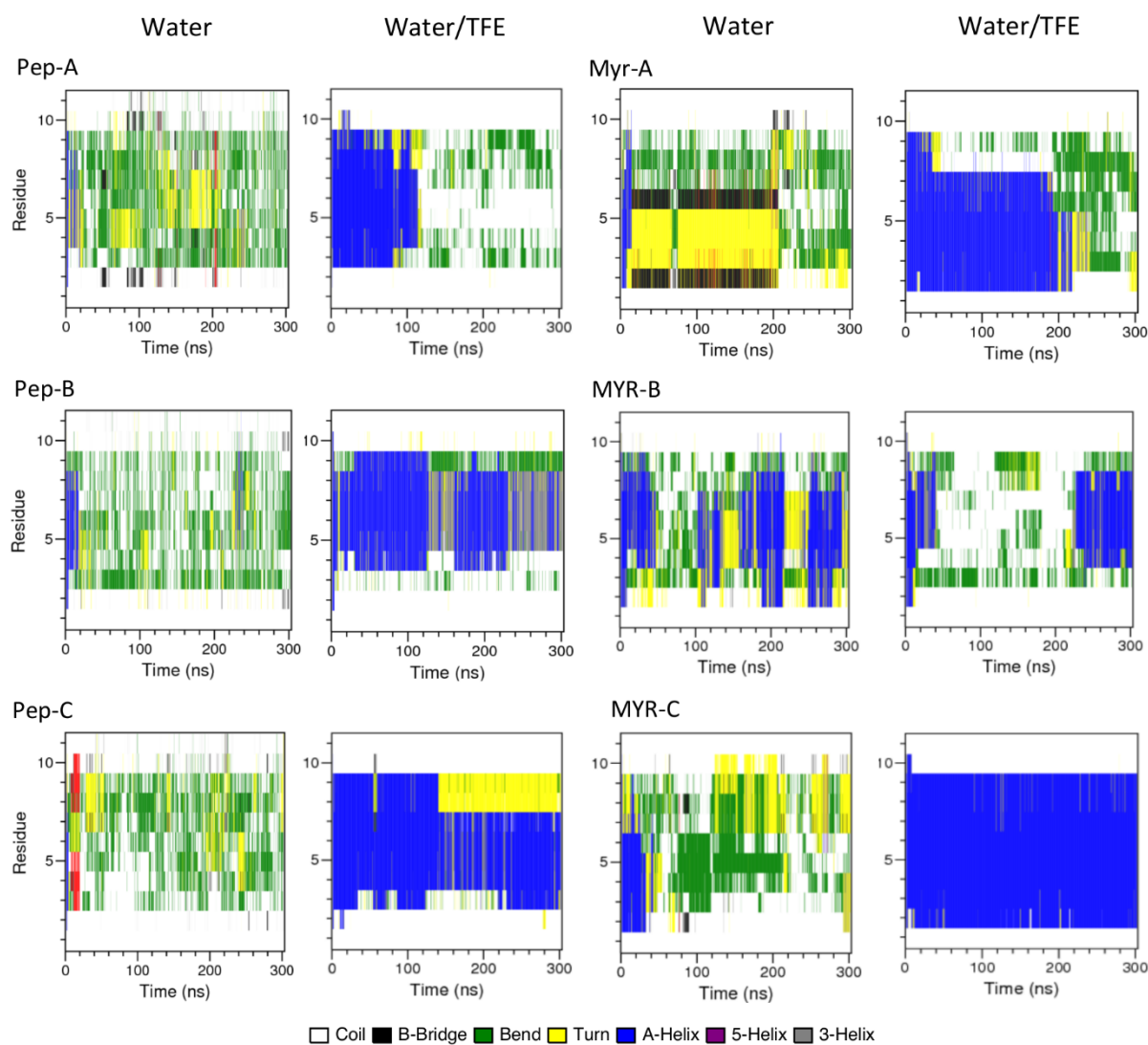


Figure S5. Time evolution of secondary structure of non-myristoylated and myristoylated peptides in water and TFE/water (50 % v/v).

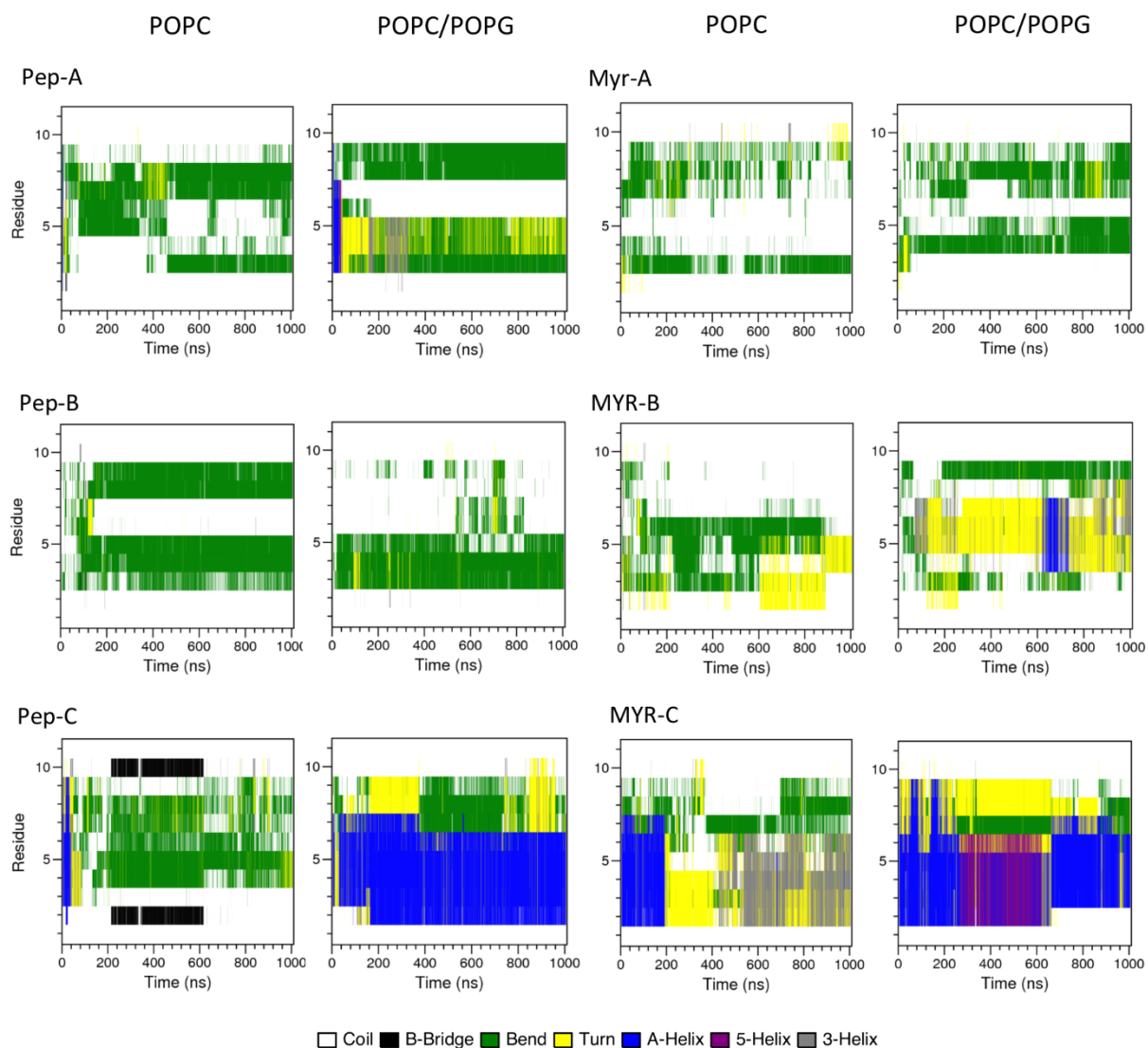


Figure S6. Time evolution of secondary structure of non-myristoylated and and myristoylated peptides in POPC and POPC/POPG (70/30 w/w) lipid membranes.

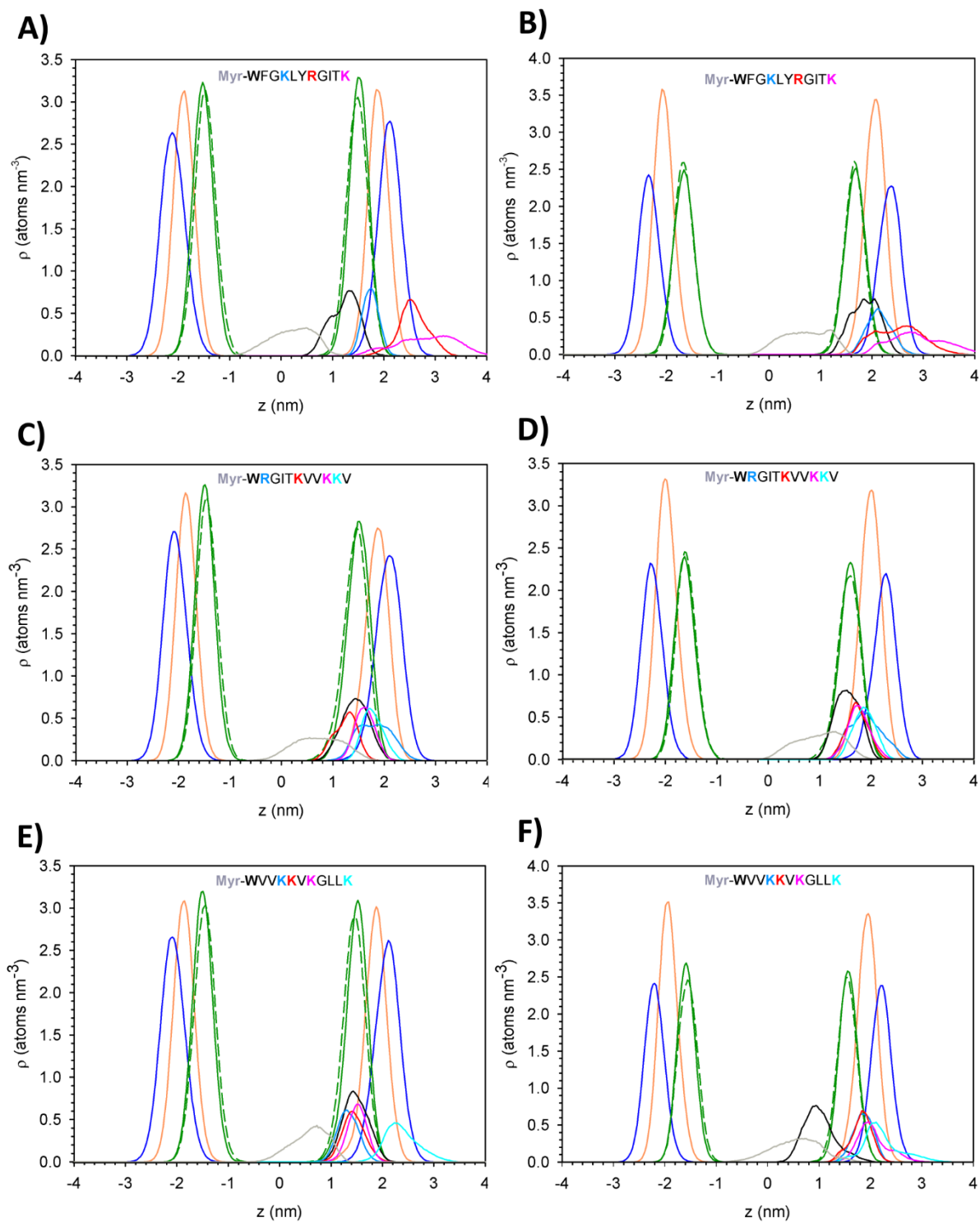


Figure S7. Average density profiles across lipid bilayer of phosphate (orange), nitrogen atoms of choline (blue), carbonyl atoms (green) of lipid molecules and myristoyl chain, Trp-1 and charged aminoacids (Lys and Arg) of (A) Myr-A in POPC, (B) Myr-A in POPC/POPG, (C) Myr-B in POPC, (D) Myr-B in POPC/POPG, (E) Myr-C in POPC and (F) Myr-C in POPC/POPG. The density is calculated with respect to the lipid bilayer center ($z = 0$).

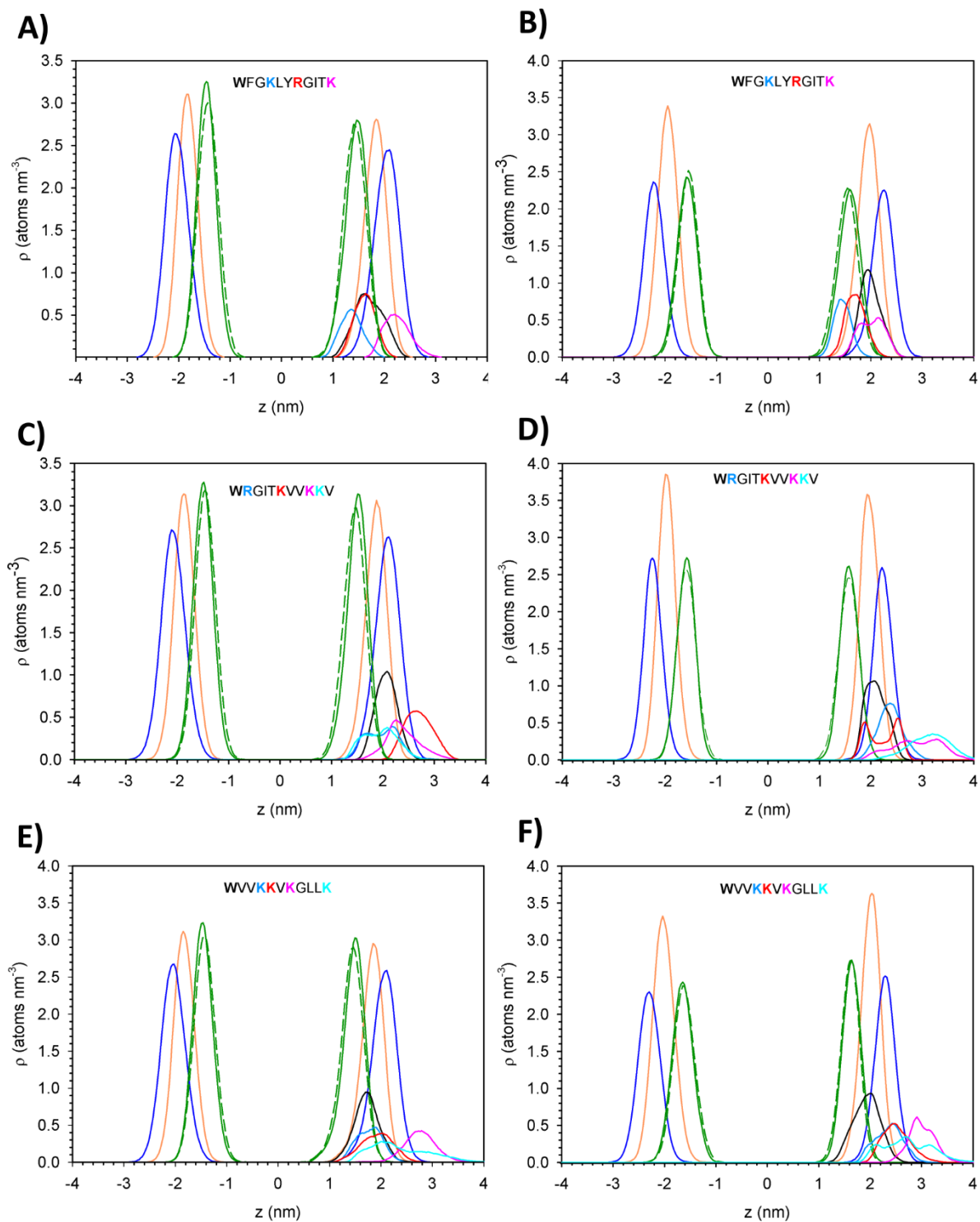


Figure S8. Average density profiles across lipid bilayer of phosphate (orange), nitrogen atoms of choline (blue), carbonyl atoms (green) of lipid molecules, Trp-1 and charged amino acids (Lys and Arg) of (A) Pep-A in POPC, (B) Pep-A in POPC/POPG, (C) Pep-B in POPC, (D) Pep-B in POPC/POPG, (E) Pep-C in POPC and (F) Pep-C in POPC/POPG. The density is calculated with respect to the lipid bilayer center ($z = 0$).

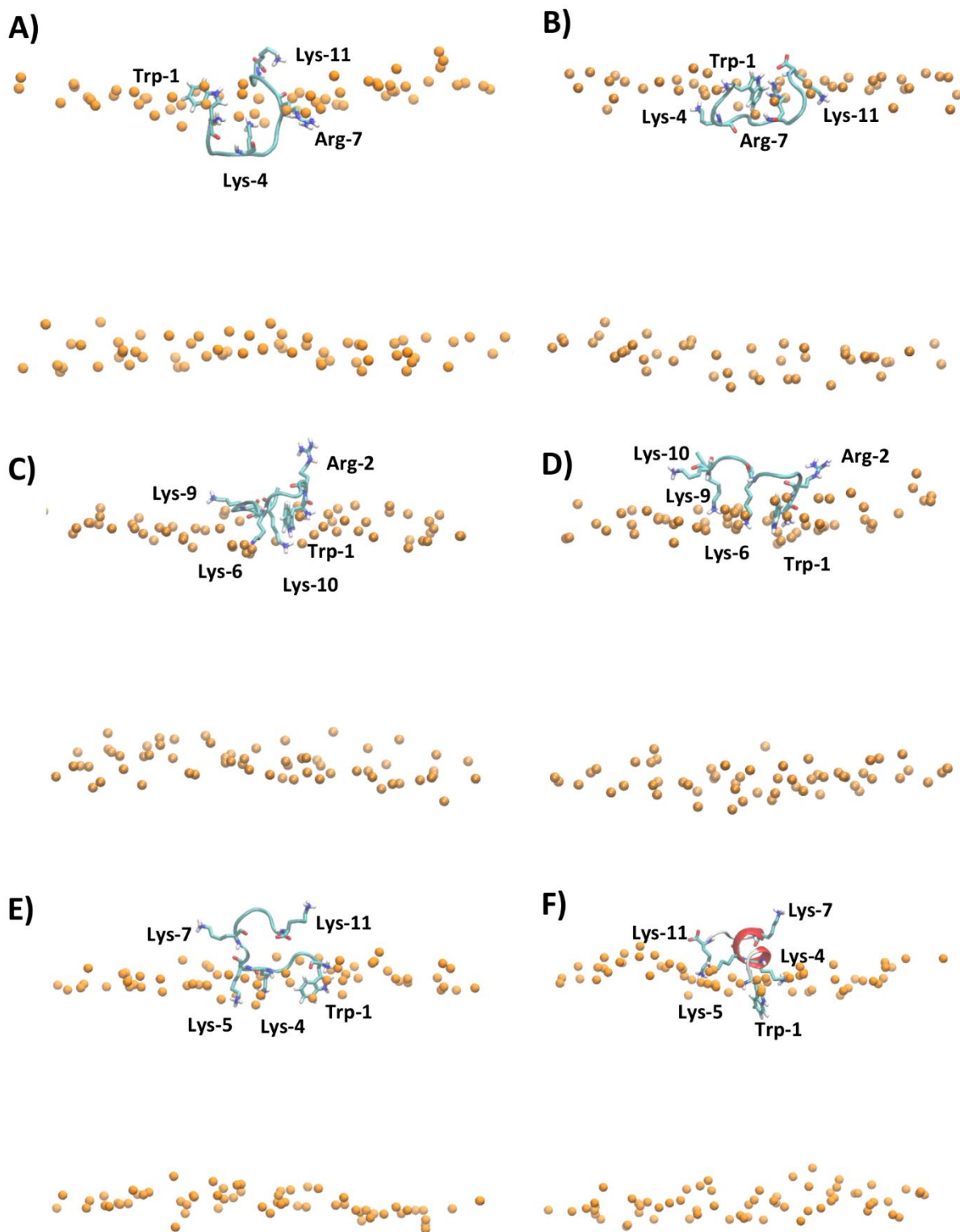


Figure S9. Snapshot of MD simulations at 1 μ s of (A) Pep-A in POPC, (B) Pep-A in POPC/POPG, (C) Pep-B in POPC, (D) Pep-B in POPC/POPG, (E) Pep-C in POPC and (F) Pep-C in POPC/POPG. The phosphorous atoms of lipids are represented as orange dots. The residue of lysine, arginine and tryptophan are represented in stick whereas the hydrophobic amino acids are represented as orange stick. The water and counterions are omitted for clarity

Table S1. MIC values (mg/L) of different myristoylated and non-myristoylated peptides against 10 different isolates of *Candida albicans*, *Candida glabrata*, *Candida parapsilosis*, *Candida tropicalis* and *Candida Auris*.

<i>Candida spp.</i>	Pep-A	Myr-A	Pep-B	Myr-B	Pep-C	Myr-C
<i>Candida albicans</i> 1	>256	16	>256	16	>256	32
<i>Candida albicans</i> 2	>256	16	>256	16	>256	32
<i>Candida albicans</i> 3	>256	16	>256	16	>256	32
<i>Candida albicans</i> 4	>256	16	>256	16	>256	32
<i>Candida albicans</i> 5	>256	8	>256	16	>256	32
<i>Candida albicans</i> 6	>256	16	>256	16	>256	32
<i>Candida albicans</i> 7	>256	16	>256	16	>256	32
<i>Candida albicans</i> 8	>256	16	>256	16	>256	32
<i>Candida albicans</i> 9	>256	16	>256	16	>256	32
<i>Candida albicans</i> 10	>256	16	>256	16	>256	32
<i>Candida glabrata</i> 1	>256	16	>256	32	>256	32
<i>Candida glabrata</i> 2	>256	16	>256	32	>256	32
<i>Candida glabrata</i> 3	>256	16	>256	32	>256	32
<i>Candida glabrata</i> 4	>256	16	>256	32	>256	32
<i>Candida glabrata</i> 5	>256	16	>256	16	>256	32
<i>Candida glabrata</i> 6	>256	16	>256	32	>256	32
<i>Candida glabrata</i> 7	>256	16	>256	32	>256	32
<i>Candida glabrata</i> 8	>256	16	>256	32	>256	32
<i>Candida glabrata</i> 9	>256	16	>256	32	>256	32
<i>Candida glabrata</i> 10	>256	16	>256	32	>256	32
<i>Candida parapsilosis</i> 1	>256	16	>256	32	>256	32
<i>Candida parapsilosis</i> 2	>256	16	>256	32	>256	32
<i>Candida parapsilosis</i> 3	>256	16	>256	32	>256	32
<i>Candida parapsilosis</i> 4	>256	16	>256	32	>256	32
<i>Candida parapsilosis</i> 5	>256	16	>256	32	>256	32
<i>Candida parapsilosis</i> 6	>256	16	>256	32	>256	32
<i>Candida parapsilosis</i> 7	>256	16	>256	32	>256	32

<i>Candida parapsilosis</i> 8	>256	16	>256	32	>256	32
<i>Candida parapsilosis</i> 9	>256	16	>256	32	>256	32
<i>Candida parapsilosis</i> 10	>256	16	>256	32	>256	32
<i>Candida tropicalis</i> 1	>256	16	>256	8	>256	16
<i>Candida tropicalis</i> 2	>256	16	>256	8	>256	16
<i>Candida tropicalis</i> 3	>256	16	>256	8	>256	16
<i>Candida tropicalis</i> 4	>256	16	>256	8	>256	16
<i>Candida tropicalis</i> 5	>256	16	>256	8	>256	16
<i>Candida tropicalis</i> 6	>256	16	>256	8	>256	16
<i>Candida tropicalis</i> 7	>256	16	>256	8	>256	16
<i>Candida tropicalis</i> 8	>256	16	>256	8	>256	16
<i>Candida tropicalis</i> 9	>256	16	>256	8	>256	16
<i>Candida tropicalis</i> 10	>256	16	>256	8	>256	16
<i>Candida Auris</i> 1	>256	>256	>256	8	>256	16
<i>Candida Auris</i> 2	>256	>256	>256	8	>256	16
<i>Candida Auris</i> 3	>256	>256	>256	16	>256	32
<i>Candida Auris</i> 4	>256	>256	>256	32	>256	32
<i>Candida Auris</i> 5	>256	>256	>256	32	>256	64
<i>Candida Auris</i> 6	>256	>256	>256	16	>256	32
<i>Candida Auris</i> 7	>256	>256	>256	16	>256	32
<i>Candida Auris</i> 8	>256	>256	>256	16	>256	32
<i>Candida Auris</i> 9	>256	>256	>256	32	>256	16
<i>Candida Auris</i> 10	>256	>256	>256	32	>256	32