

Electronic Supplementary Information

Molecular insights into the self-assembly of short amphiphilic peptides F_mD_n and F_mK_n

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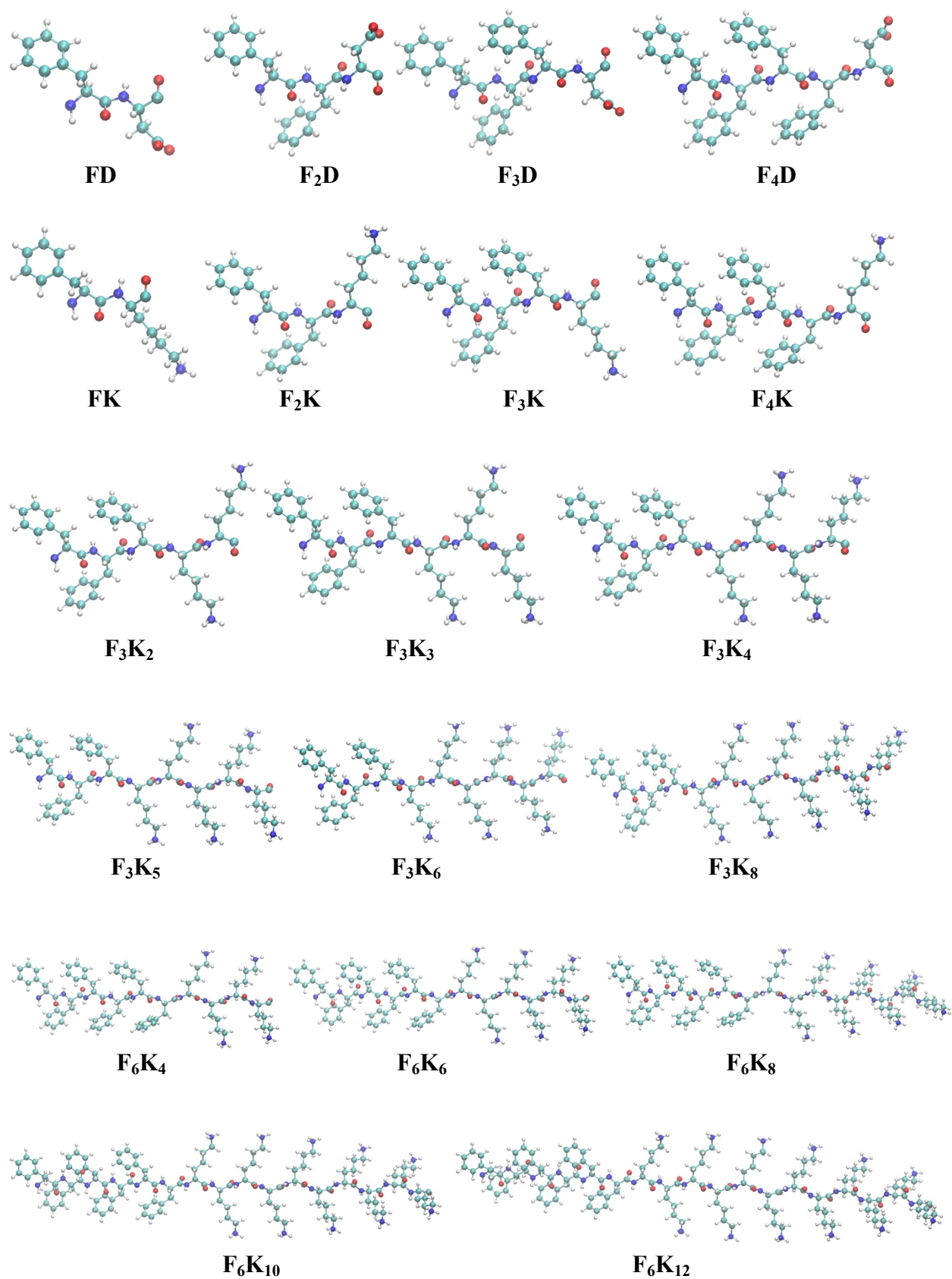


Fig. S1 Atomistic representations of peptides F_mD_n and F_mK_n .
N: blue, O: red, C: cyan, and H: white.

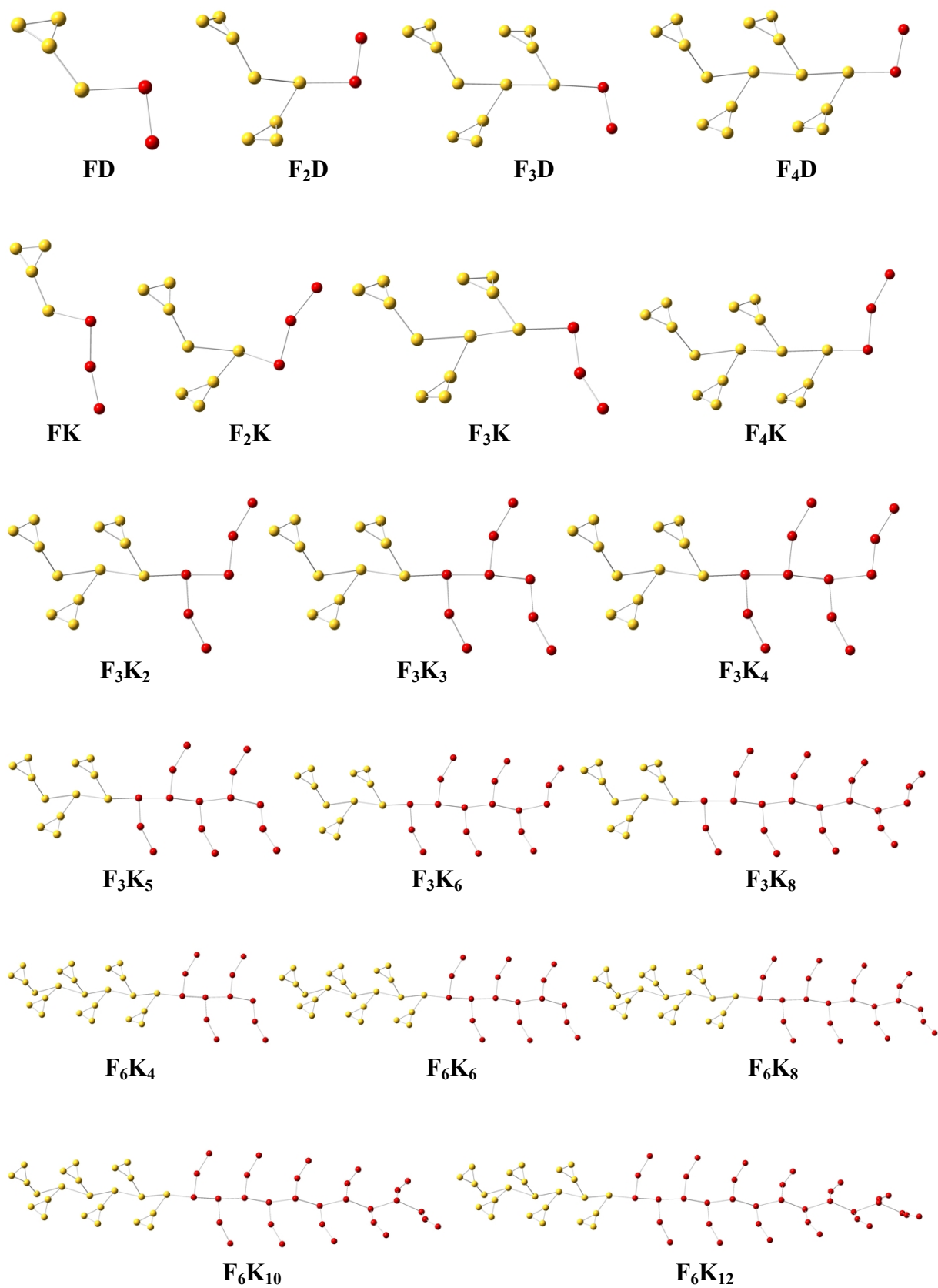


Fig. S2 CG representations of F_mD_n and F_mK_n peptides using the MARTINI model. F: yellow, D and K: red.

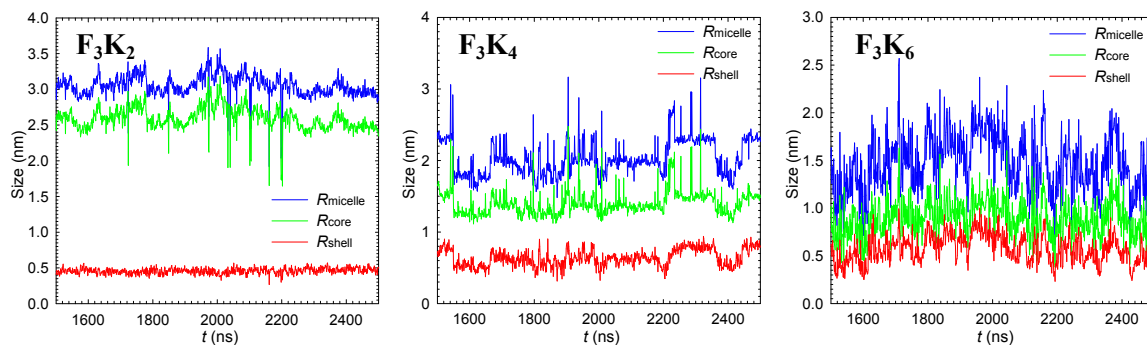


Fig. S3 Radii of micelle (R_{micelle}), core (R_{core}) and shell (R_{shell}) for F_3K_2 , F_3K_4 and F_3K_6 .

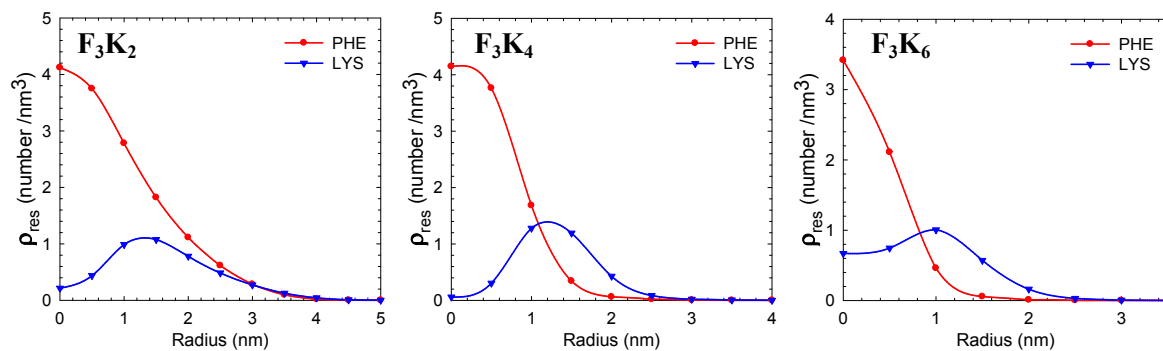


Fig. S4 Density profiles for F_3K_2 , F_3K_4 and F_3K_6 . The micelles contain 58, 10 and 5 peptides, respectively.

Table S1. Interaction energies (kJ/mol) at free and aggregated states.

| Peptide | Free State | | Aggregated State | |
|----------|---------------|----------|------------------|-----------|
| | Electrostatic | LJ | Electrostatic | LJ |
| F_3K | -112.82 | -4134.99 | -317.83 | -14048.97 |
| F_4K | -57.79 | -2137.47 | -260.06 | -15244.91 |
| F_3K_2 | -20.80 | -2425.49 | -94.08 | -12779.62 |

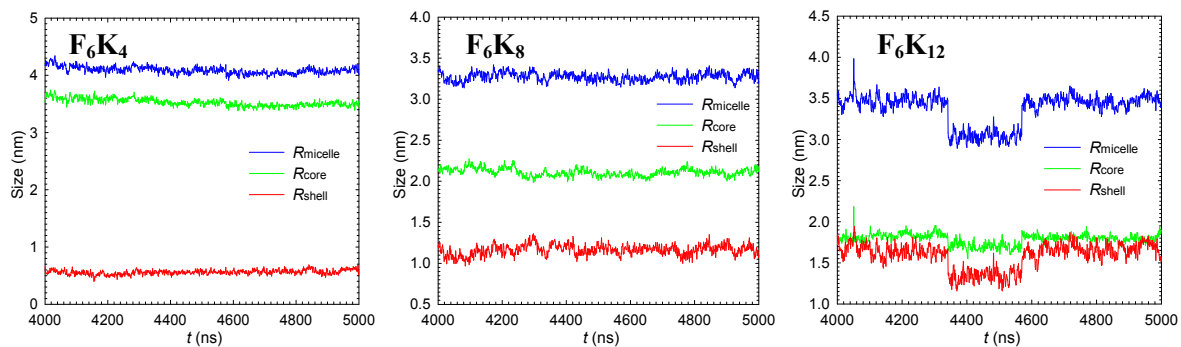


Fig. S5 Radii of micelle (R_{micelle}), core (R_{core}) and shell (R_{shell}) for F_6K_4 , F_6K_8 and F_6K_{12} .

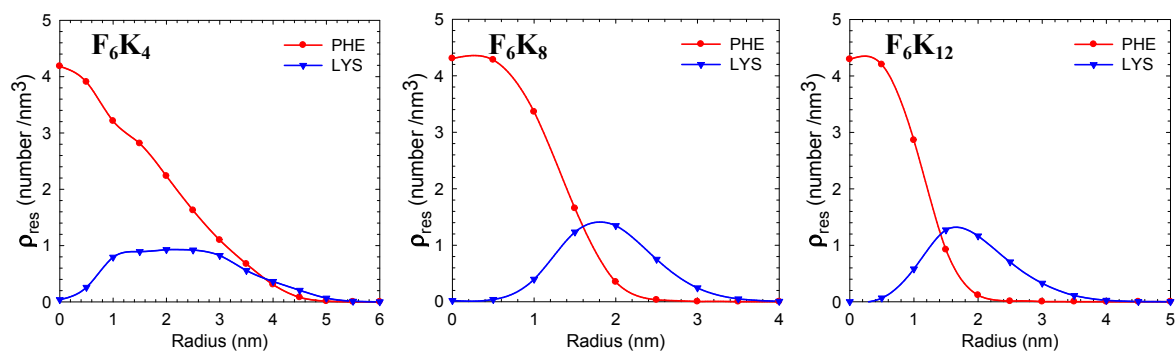


Fig. S6 Density profiles for F_6K_4 , F_6K_8 and F_6K_{12} . The micelles contain 72, 16 and 11 peptides, respectively.