



Figure S1. The largest aggregation number defined as the number of helices in the (a) 3HM, (b) 3&4 mixture micelle, and (c) 4HM as a function of time. The results are obtained from DPD CG simulations, including 3 different trials for each case and with 100 subunits for each system.

| | R_g Radial (Å) | R_g Tangential (Å) | R_g Total (Å) | R_{ee} (Å) | |
|-------------------------------------|------------------|----------------------|-----------------|--------------|----------|
| Free PEG | 8.4±3.4 | 13.0±3.5 | 14.8±2.9 | 37.3±14.8 | |
| PEG in 3-helix single bundle | 9.5±2.8 | 11.3±2.3 | 15.2±1.7 | 32.3±8.0 | |
| In micelle | 3HM | 9.6±0.8 | 13.5±0.8 | 17.0±0.6 | 42.6±2.6 |
| | 4HM | 9.0±0.6 | 13.8±0.6 | 17.2±0.5 | 43.9±2.5 |

Table S1. Average conformational size of PEG polymer chains, including radius of gyration R_g , R_g in the radial direction (along the helix bundle), R_g on the tangential direction (vertical to the helix bundle), R_g in total and end-to-end distance R_{ee} in CG DPD simulations. The results are given by the present DPD CG simulations for PEG in 3HM, 4HM and 3&4 mixture micelles, and PEG on the isolated triple helix bundle and free polymer chains in water with standard deviations included. All the data presented here studied the same PEG chains with molecular weight 2000 Da in DPD simulations.