Supporting Information:

Dissipative Particle Dynamics Simulation Study on the Mechanisms of Self-Assembly of Large Multimolecular Micelles from Amphiphilic Dendritic Multiarm Copolymers

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S1. The UM structures based on models b, c and d

![Figure S1](image)

**Figure S1.** The morphologies of unimolecular micelles formed after 500000-step DPD simulations from dendritic multiarm copolymers based on model b (a), model c (b) and model d (c). The concentration is 1%, $a_{BC}=20$, and water beads are omitted for clarity. Hydrophobic dendritic core: blue beads; hydrophilic linear arms: red beads.
S2. The UMA structures based on models a and c

(a1) (b1)

(c1) (d1)

(a2) (b2)

(c2) (d2)

Figure S2. The morphologies of the micelles formed after 500000-step DPD simulations from dendritic multiarm copolymers, the concentration is 1%, $a_{AC}=40$ and $a_{AB}=35$: (a1-d1) is for model a, (a2-d2) is for model c; (a1-a2) $a_{BC}=24$, (b1-b2) $a_{BC}=26$, (c1-c2) $a_{BC}=28$, and (d1-d2) $a_{BC}=30$. Water beads are omitted for clarity. The color codes are the same as those in Figure S1.
S3. The ms-SM structures based on models a and c

Figure S3. The morphologies of the micelles formed after 500000-step DPD simulations from dendritic multiarm copolymers, the concentration is 1%, $a_{BC}=27$ and $a_{AB}=45$: (a1-d1) is for model a, (a2-d2) is for model c. (a1-a2) $a_{AC}=60$, (b1-b2) $a_{AC}=90$, (c1-c2) $a_{AC}=150$, (d1-d2) $a_{AC}=200$. Water beads are omitted for clarity. The color codes are the same as those in Figure S1.