Figure S1: Time evolution of the number averaged aggregation number (N_N) for binary mixture simulations with 1:0.5 **(A)**, 1:1 **(B)**, 1:2 **(C)** and 1:4 **(D)** CA:Indo molar ratios.
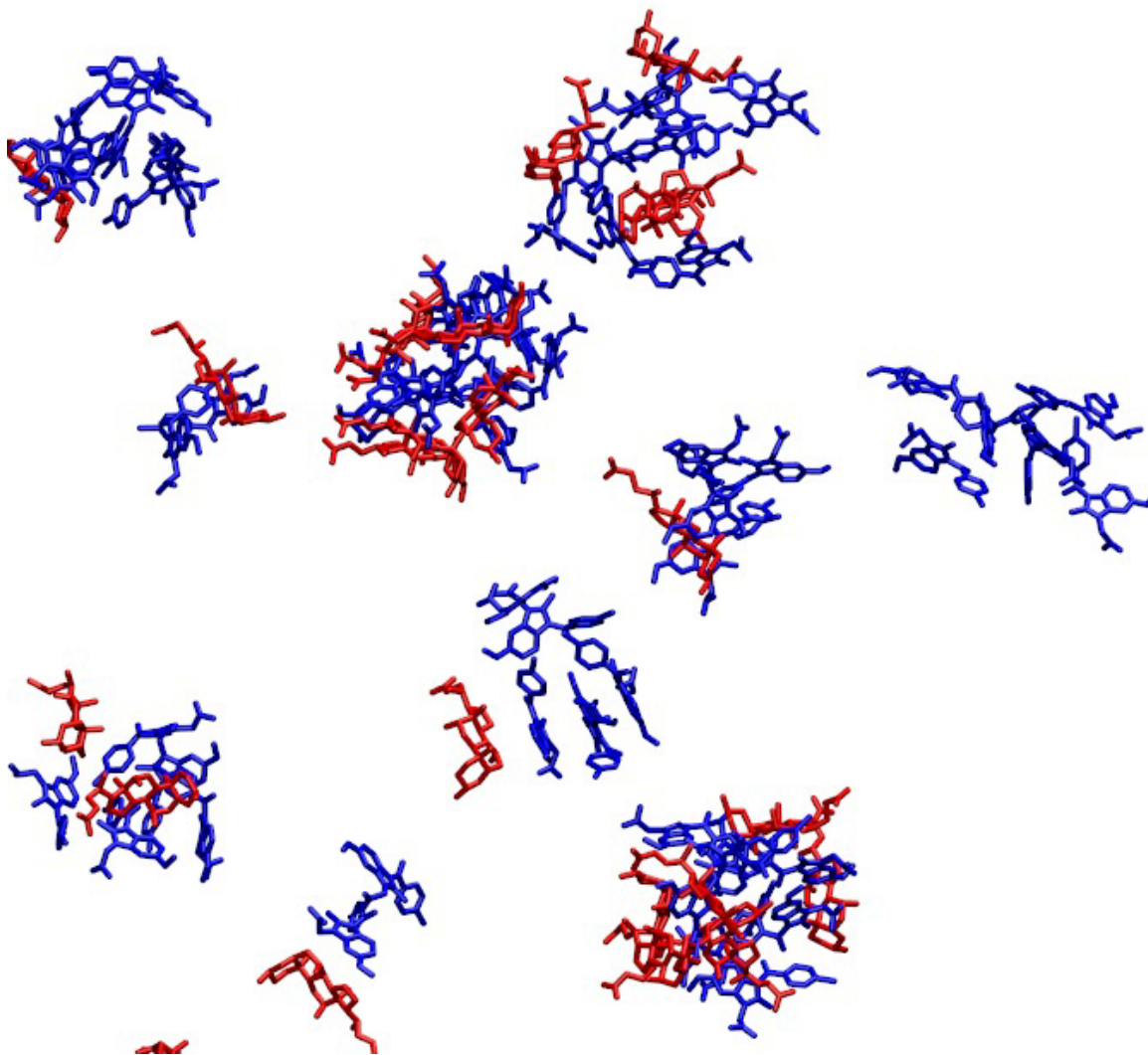
Figure S2: Snapshot of a typical CA-Indo mixed micelle formed at 100ns from simulation S_C. CA in red and Indo in blue.
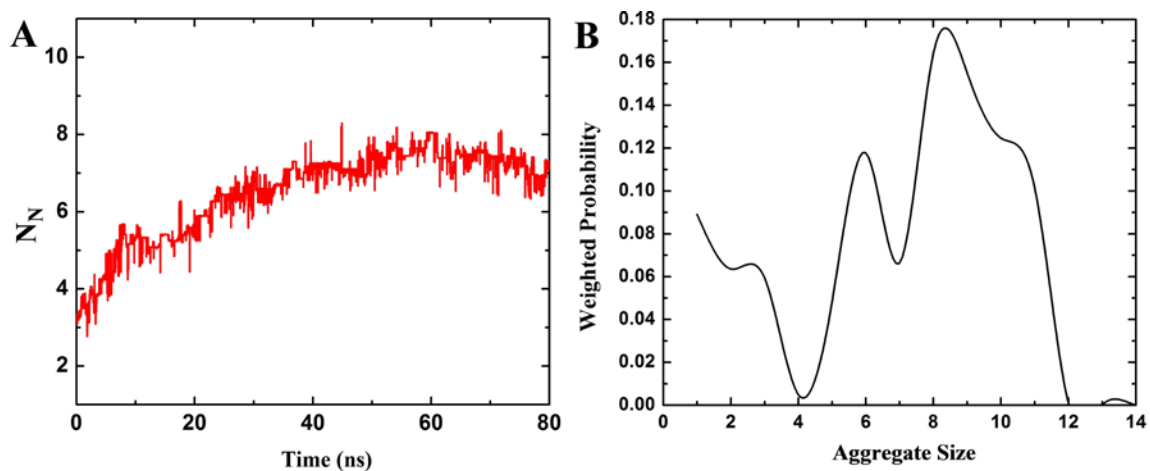
Figure S3: (A) Time evolution of the number averaged aggregation number (N_N) and **(B)** weighted probability distribution of Indo aggregates derived from a simulation of Indo in the pure phase.
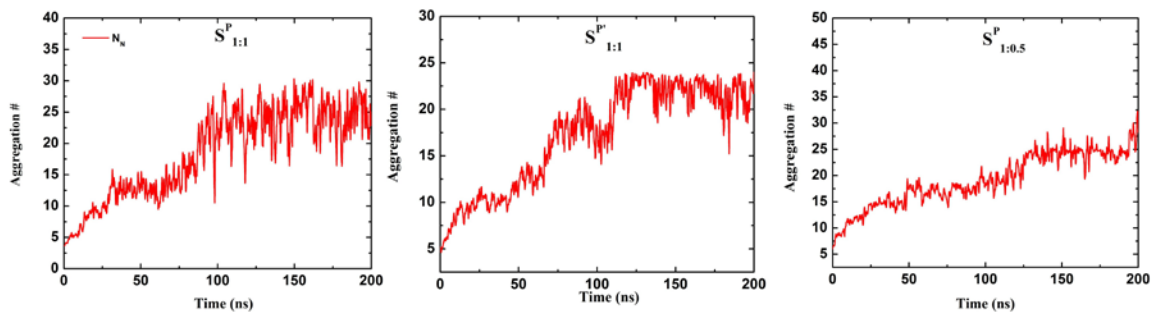

Figure S4: N_N of CA/Indo/POPC aggregates in ternary mixtures from simulations $S^P_{1:1}$, $S^{P'}_{1:1}$ and $S^P_{1:0.5}$.
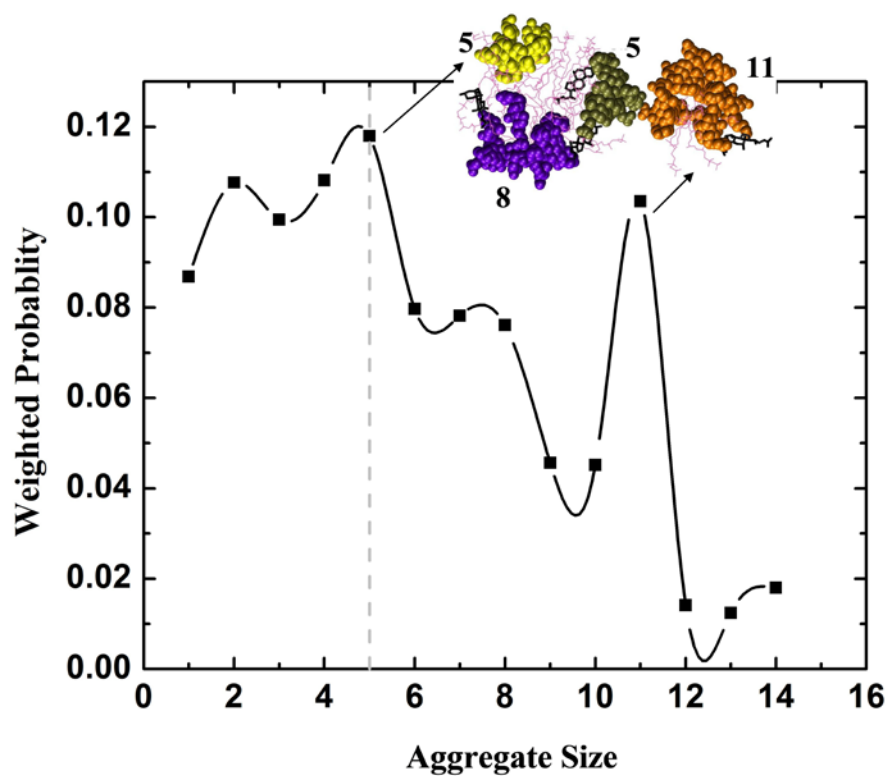
Figure S5: Weighted probability distribution of pure-CA micelles from CA/POPC 2:1 binary simulation. Last 30ns of the data was used for this analysis. Small pure-CA aggregates of size 5 (ochre and yellow) and 8 (purple) are observed. The aggregate of size 11 (orange) contains very few POPC molecules which may eventually fuse with the larger CA/POPC mixed micelle. The POPC is shown in magenta lines. The gray dotted line shows the maximum pure-CA aggregate size.
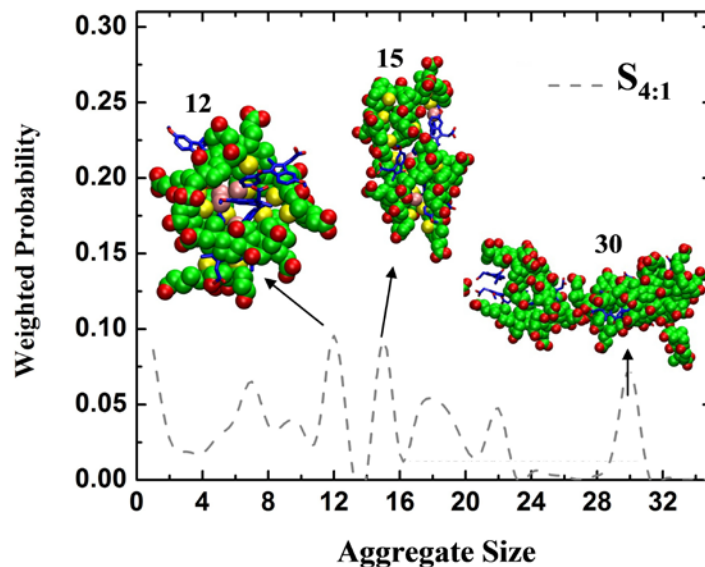
Figure S6: Weighted probability distribution of the number of CA/Indo micelles (grey dotted lines) from simulation $S_{4:1}$. The color scheme is the same as in Figure 5 (main text). Here the concentration of CA was four-times that of Indo. This simulation yielded $N_W = 14.6 \pm 2.1$, a value very similar to that in which the concentration of Indo was higher (ca. simulations $S_{1:2}$ and $S_{1:4}$). The smaller aggregates are unstable (< 10 % occurrence). Also, the appearance of a secondary micelle made up of two primary micelles of size 15 is a unique feature of simulation $S_{4:1}$.
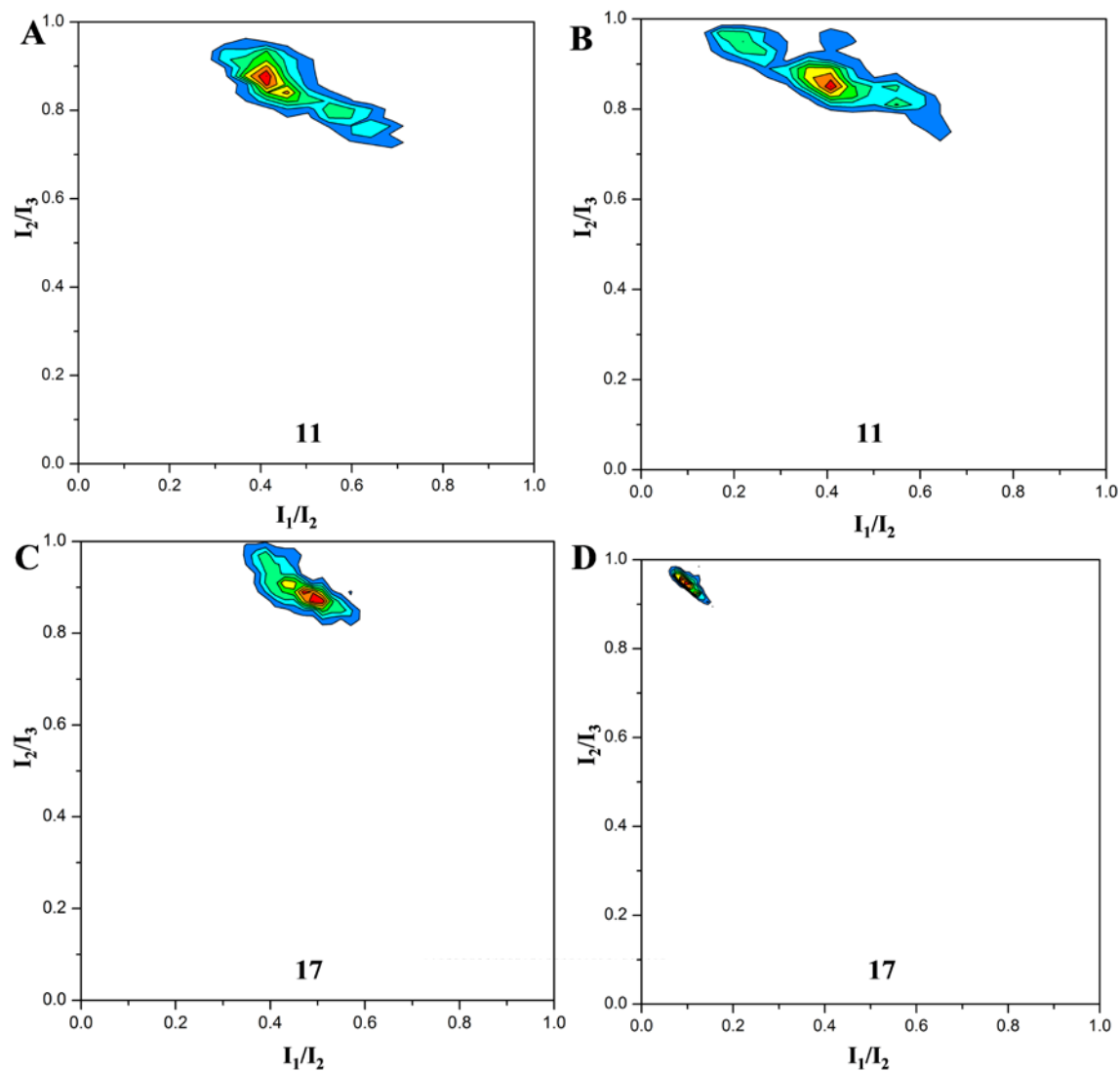
Figure S7: Bivariate distributions of the ratio of principal moments of inertia for aggregate size 11 and 17 from simulation $S_{1:2}$ **(A)** and **(C),** and $S_{1:4}$ **(B)** and **(D)**. The distribution is calculated from the last 10ns of the simulation when the reorganization of mixed micelles is considered to be complete. Red is most populated.
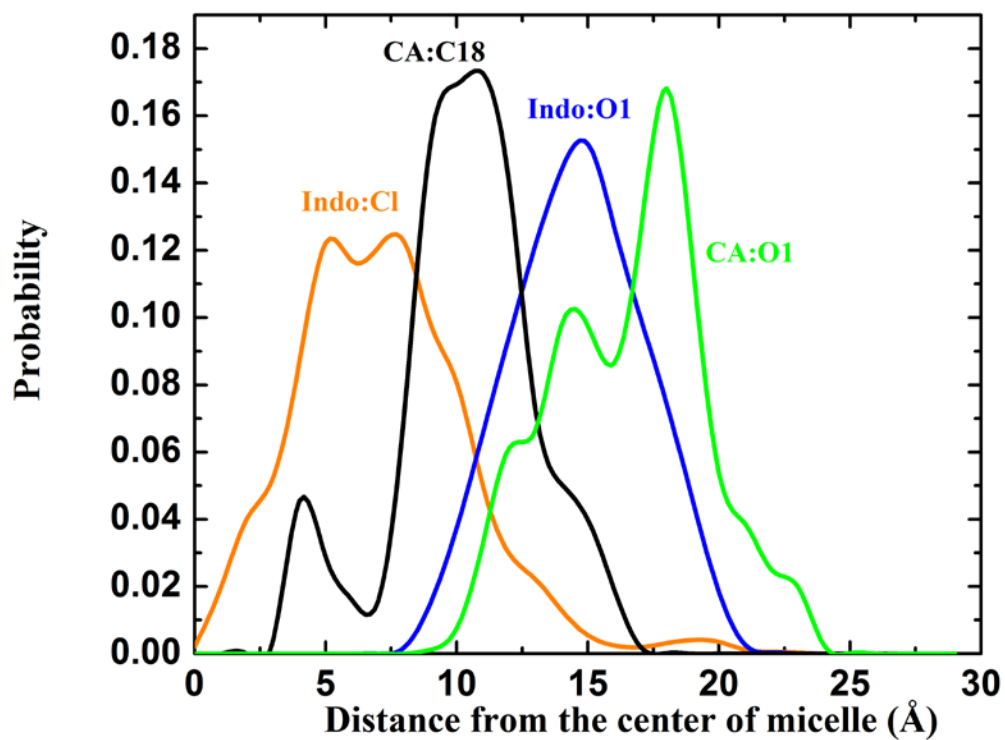
Figure S8: Distribution of selected atoms from the center of mass of a mixed micelle of size 25 from simulation $S_{1:4}$. The distribution is calculated for the last 10ns. Refer to Figure 1 (main text) for atom numbering.