Supporting Information for:

Quantification of Ostwald Ripening in Emulsions via Coarse-Grained Simulations

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Additional Results

In Figure S1 we show that the Ostwald ripening rate does not change when we start from different initial configurations, as well as when we simulate different oil droplets sizes in water. In these simulations no surfactants are present.

In Figure S2 we show that the rate by which oil beads leave droplet 1 does not change when droplet 2 has either finite or infinite curvature. The infinite curvature droplet was simulated as a flat interface, as shown in the snapshot of Figure S3.

In Figure S4, the number of surfactant molecules attached to the surfaces of the droplets are shown as a function of time, when 2000 H1T2 molecules and 1300 H3T2 molecules are added to the emulsions. For these simulations, the initial configuration is the second of those shown in Figure 3 of the main text. From the plateaus in Figure S4, it is estimated that ~252 H1T2 surfactants are needed to cover droplet 1 and ~1728 to cover droplet 2. The correspondent values for H3T2 surfactants are ~168 and ~1026, respectively. In Figure S5 and S6 we report similar results for H1T2 and H3T2 surfactants, respectively, starting from 3 different initial configurations. The plateaus are independent of the initial configuration.

In Figure S7 and Figure S8, we report the number of oil beads in the two droplets as a function of simulation time, starting from different initial configurations, when 2000 H1T2 and 1300 H3T2 surfactants are present, respectively. The horizontal dashed lines indicate the sizes of the two droplets at the beginning of the simulations, provided for reference.

In Figure S9, we show the number of both oil beads within, and surfactant molecules on the surface of droplet 1 as a function of simulation time. The results are shown in the presence of H1T2 (top) and H3T2 (bottom) surfactants.

In Figure S10 we compare the cube of the mean radius of droplet 2 as a function of simulation time when H1T2 (top) or H3T2 (bottom) surfactants are present. In both cases, the results are shown for different amounts of surfactants adsorbed in droplet 1 (~252, ~125, and zero for H1T2 surfactants; ~168, ~88, and zero for H3T2 surfactants).

In Table S1, we report results for surface density, interfacial tension, Ostwald ripening rate from simulation results such as those of Figure S10, and Ostwald ripening rate from the LSW theory when simulation data are used as input. Direct simulations agree well with LSW predictions for both H1T2 and H3T2 surfactants at low surface coverage.

In Figure S11, we show a detailed analysis of the molecular exchange between the two droplets and the micelle in the presence of the micelle. We show in Figure S11 (a) the transfer of oil beads from the micelle to droplet 1 and droplet 2, and in Figure S11 (b) the transfer of H1T2 surfactant molecules from the micelle and droplet 1 to droplet 2.

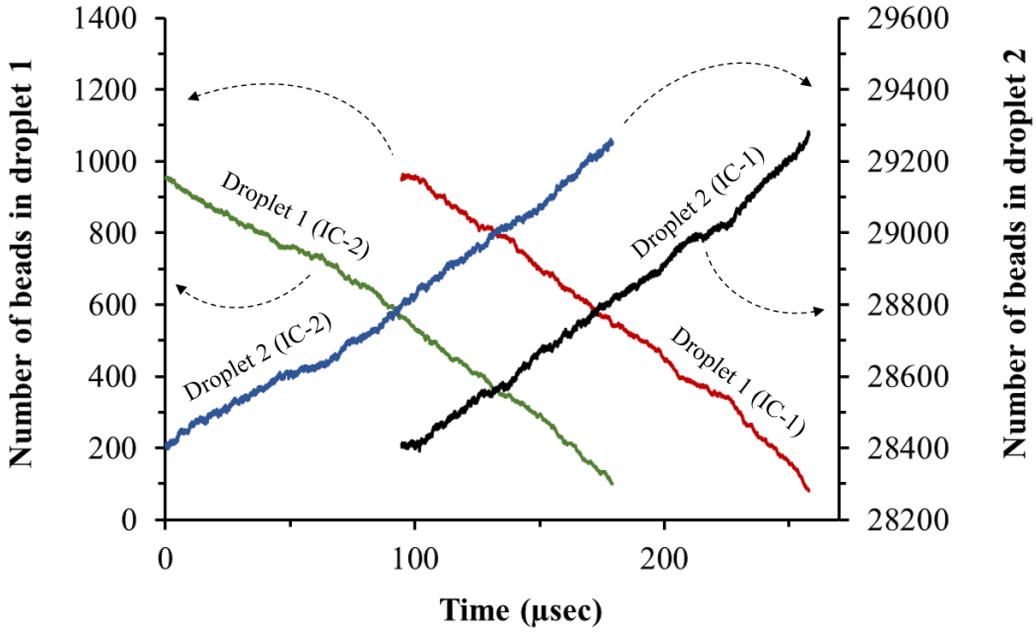


Figure S1. The molecular exchange between two droplets of different sizes in two simulations starting from different starting points.

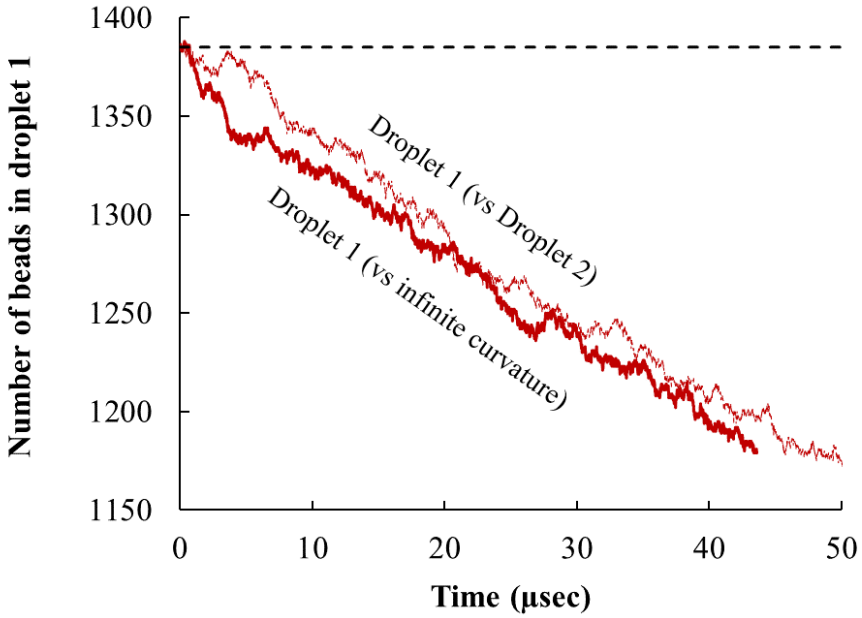


Figure S2. The molecular exchange between small and big droplets, varying the curvature of droplet 2 (see Figure S3 for a snapshot representing the system with a flat interface).

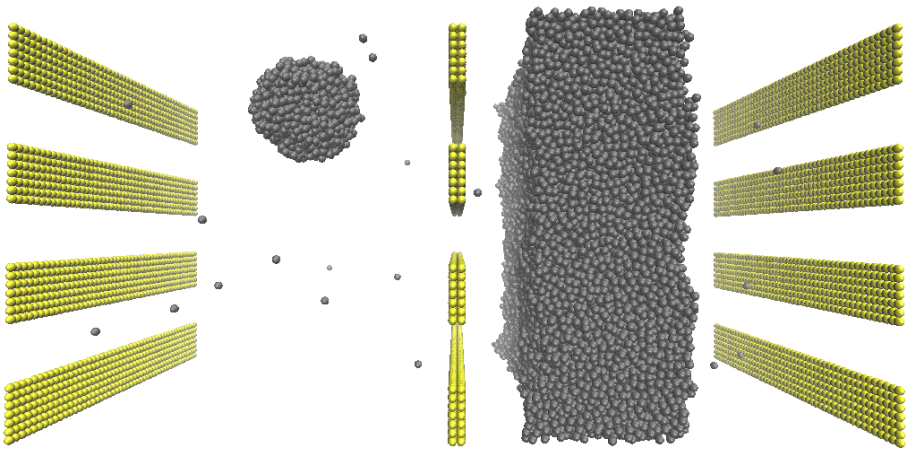


Figure S3. A snapshot of the oil-in-water emulsion when droplet 2 has infinite curvature.

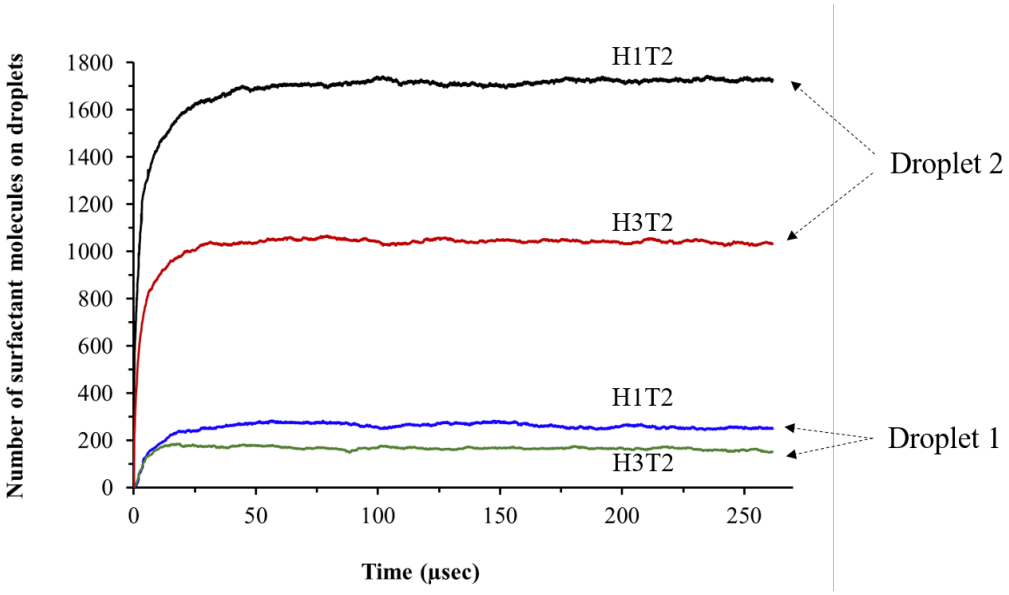


Figure S4. The number of surfactants molecules attached to each droplet when 2000 and 1300 molecules of H1T2 and H3T2 surfactants are added to the system, respectively, starting from the second of the initial configurations shown in Figure 3 of the main text.

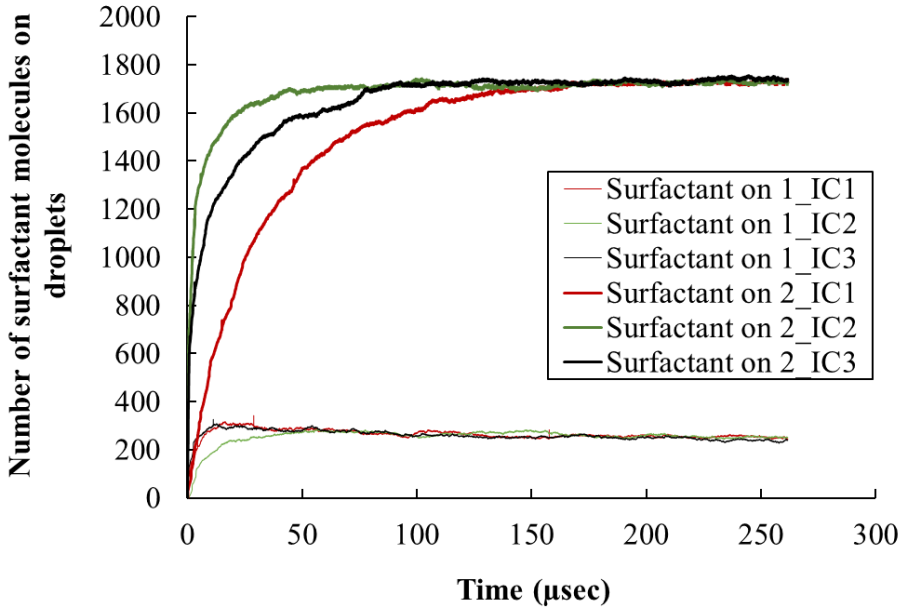


Figure S5. H1T2 surfactant molecules attached to the droplet surfaces as a function of simulation time, starting from three different initial configurations.

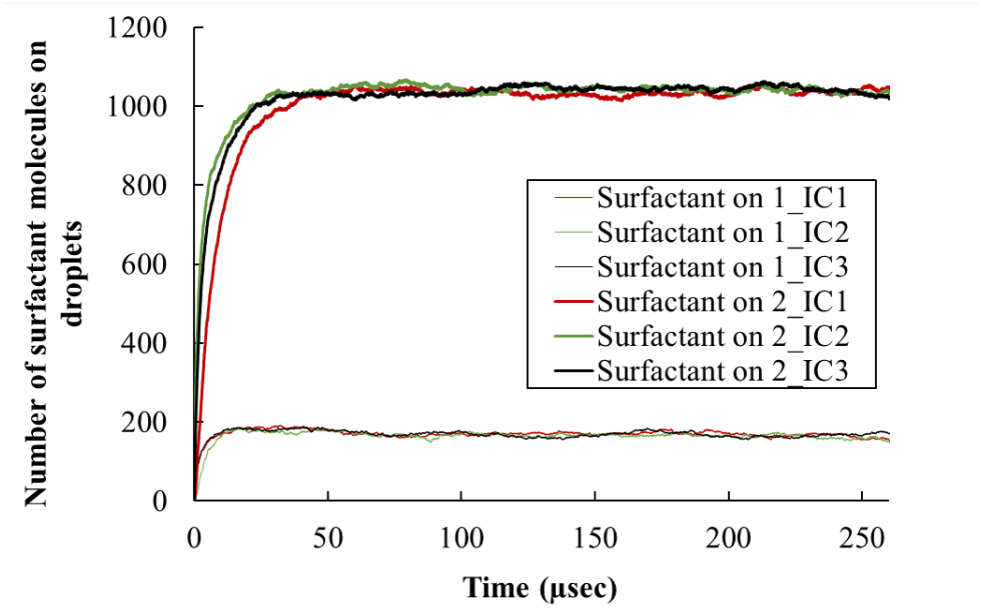


Figure S6. H3T2 surfactant molecules attached to the droplet surfaces as a function of simulation time, starting from three different initial configurations.

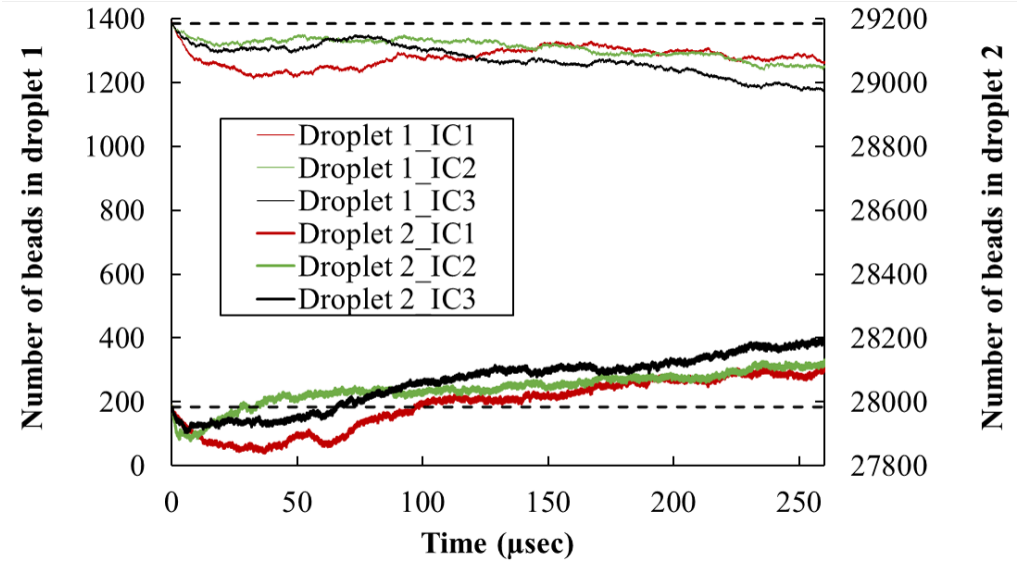


Figure S7. Number of oil beads in the two droplets, as a function of simulation time, in the presence of 2000 H1T2 molecules. The results obtained for three different initial configurations are shown in different colors.

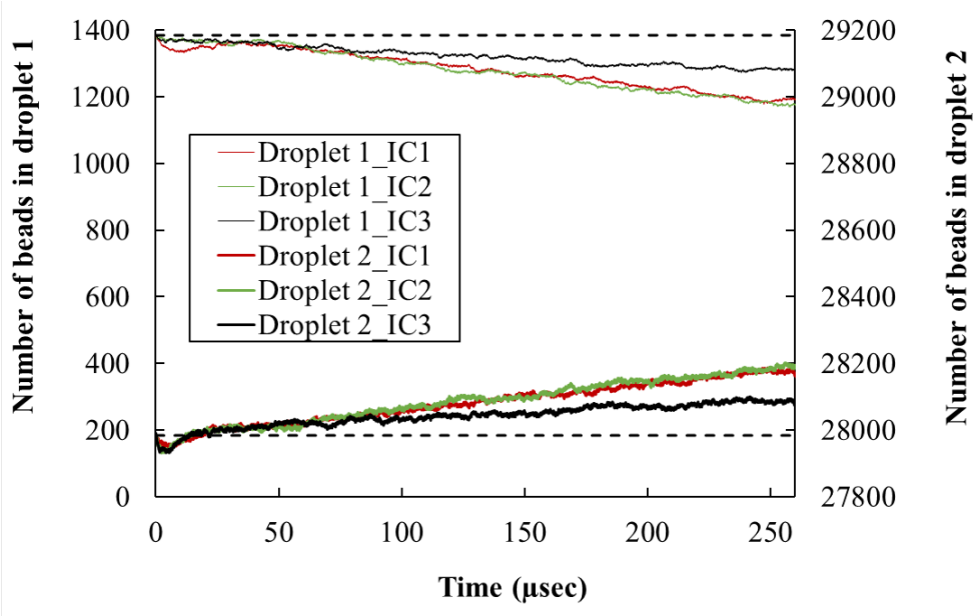


Figure S8. Number of oil beads in the two droplets, as a function of simulation time, in the presence of 1300 H3T2 molecules. The results obtained for three different initial configurations are shown in different colors.

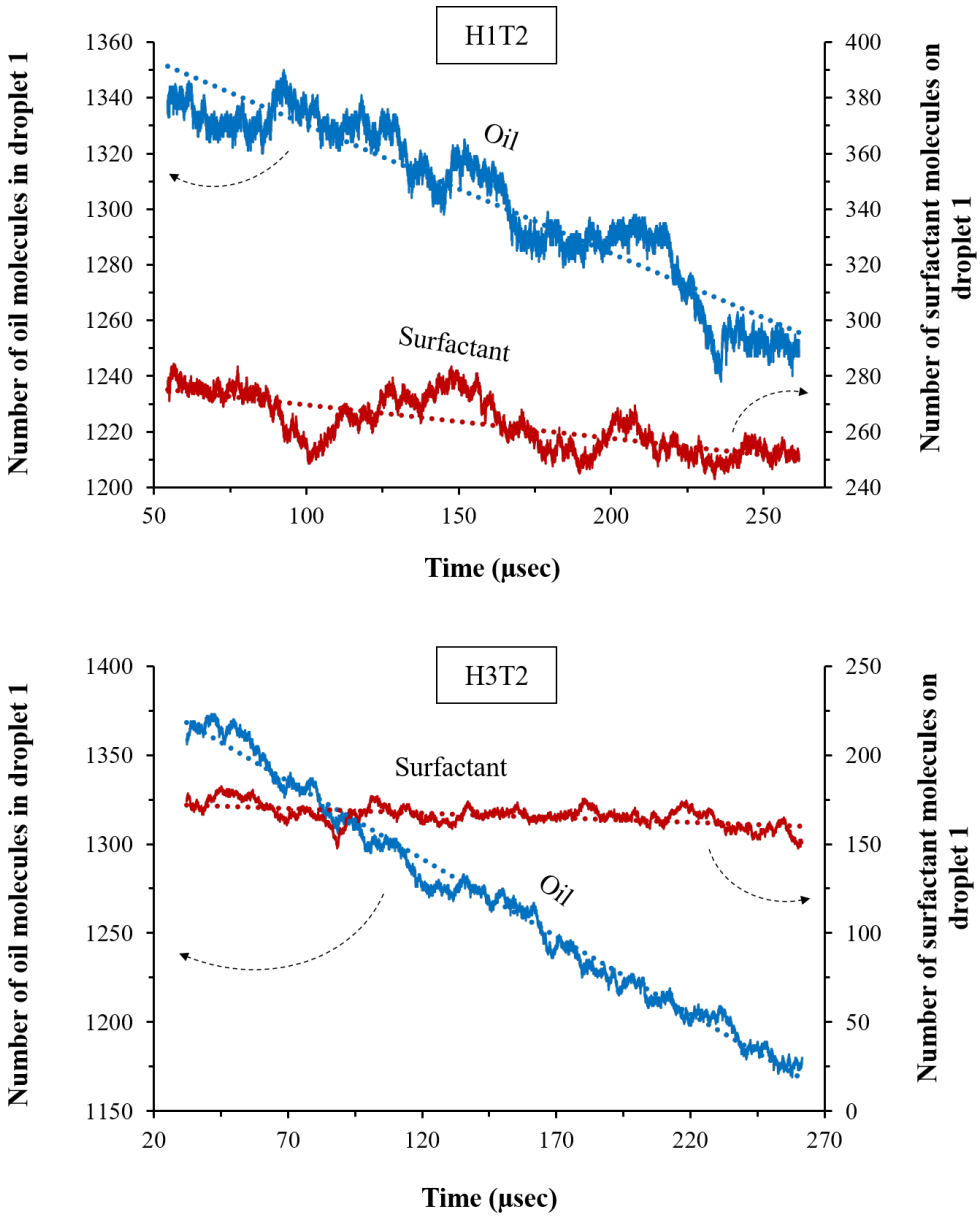
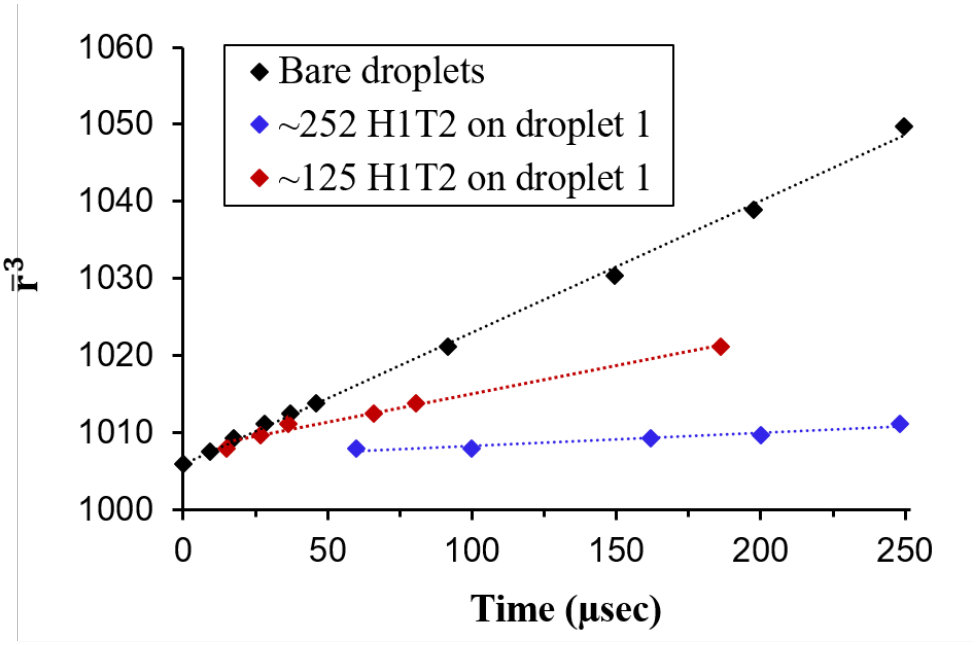


Figure S9. Number of surfactant molecules adsorbed on, and of oil beads within droplet 1 as a function of simulation time (starting from the second initial configuration in Figure 3, main text). Top and bottom plots are for simulations conducted in the presence of 2000 H1T2 or 1300 H3T2 surfactants, respectively.



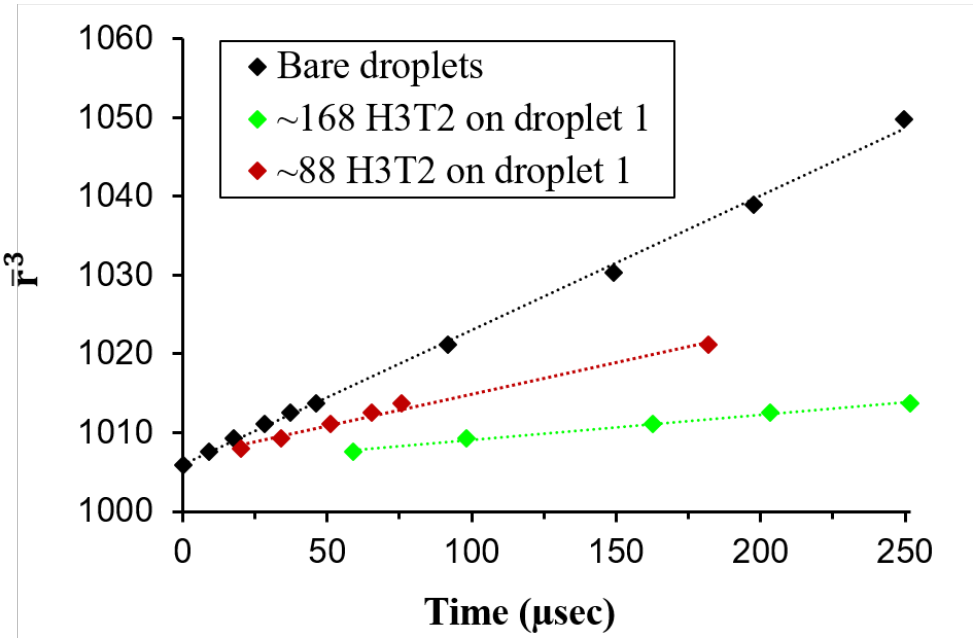


Figure S10. The cube of the mean radius of droplet 2 as a function of simulation time when droplet 1 is covered with ~252, ~125, and zero H1T2 surfactants (top), and ~168, ~88, and zero H3T2 surfactants (bottom).

Table S1. The interfacial tension at different surface densities of H1T2 and H3T2 surfactants; Ostwald ripening rate from simulation (Figure S10); Ostwald ripening rate estimated from the LSW theory when simulation data are used as input.

Surfactant Type	**Surface Density $\mathbf{molecule/nm^2}$**	**Interfacial Tension mN/m**	**Ostwald ripening rate Simulated $\mathbf{nm^3/\mu sec}$**	**Ostwald ripening rate LSW prediction $\mathbf{nm^3/\mu sec}$**
None	NA	30 ± 8	0.17 ± 0.01	0.12 ± 0.06
H1T2	1.5	17.4 ± 8.5	0.02 ± 0.01	0.07 ± 0.04
H1T2	0.7	19.7 ± 8	0.074 ± 0.01	0.077 ± 0.04
H3T2	1	16.3 ± 10	0.03 ± 0.01	0.06 ± 0.04
H3T2	0.5	20.98 ± 9	0.081 ± 0.01	0.082 ± 0.05

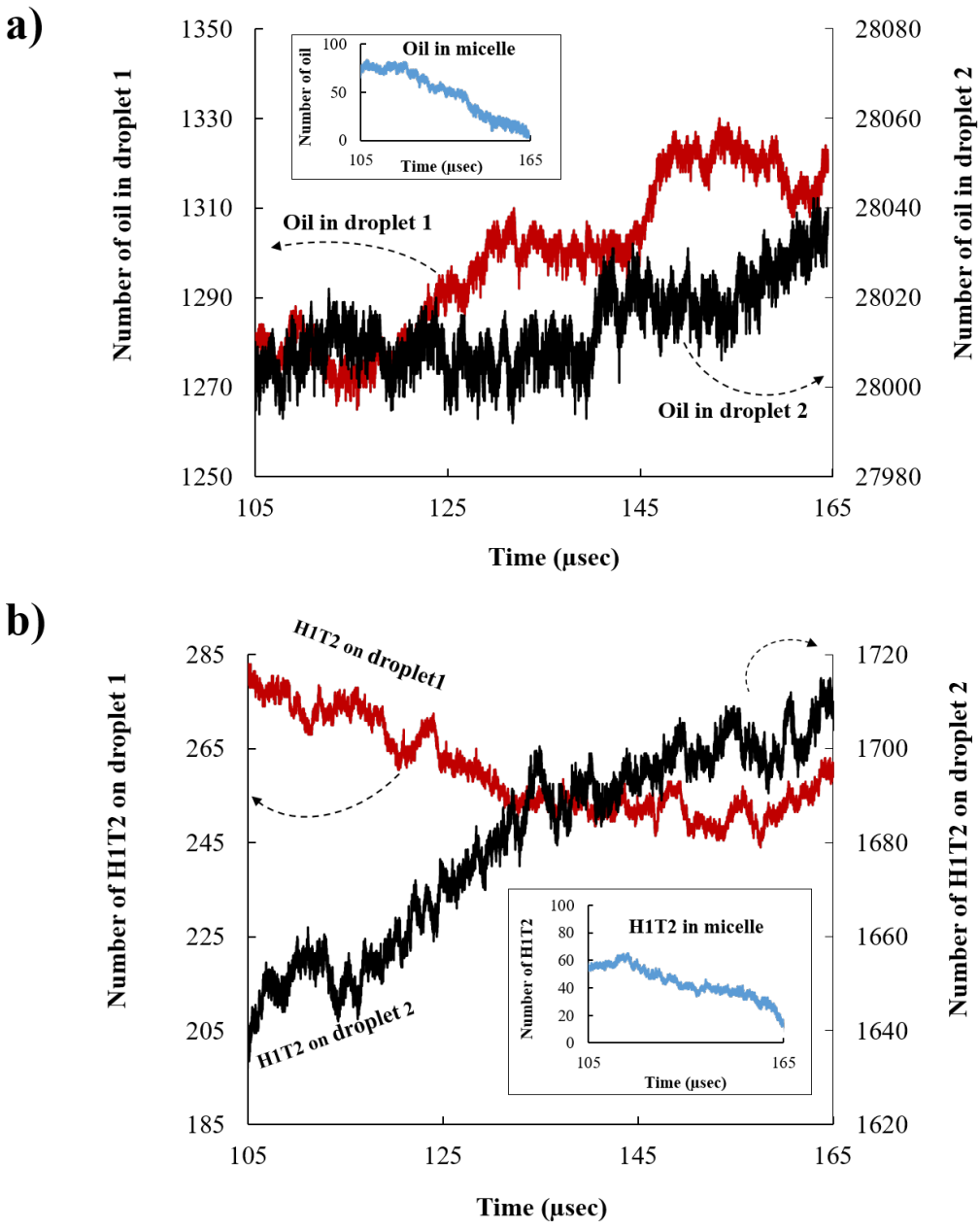


Figure S11. Molecular exchange occurring in presence of a micelle and two droplets. Panel (a) illustrates the transfer of oil molecules from the micelle (top) to droplet 1 and droplet 2. Panel (b) shows the transfer of H1T2 molecules from droplet 1 and the micelle (bottom) to droplet 2.