Electronic Supplementary Information

Computational predictions of interfacial tension, surface tension, and surfactant adsorption isotherms

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S1 Force field testing

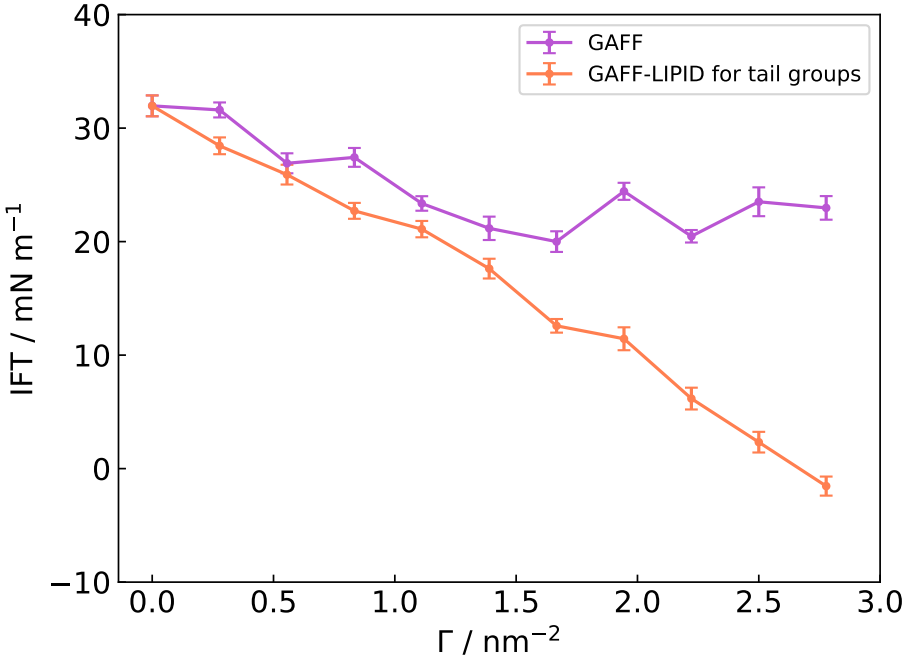

Figure S1: Simulated interfacial tensions (IFT) as a function of surface concentration (Γ) for SDS molecules at a water-triolein interface, with GAFF (purple) and GAFF-LIPID for tail groups (orange).

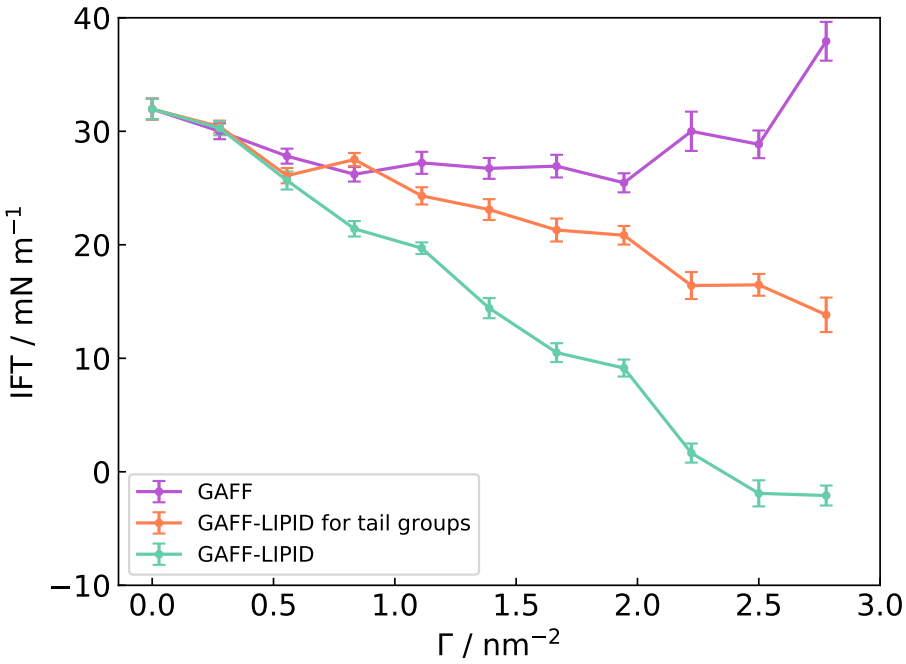

Figure S2: Simulated interfacial tensions (IFT) as a function of surface concentration (Γ) for C15E7 molecules at a water-triolein interface, with GAFF (purple), GAFF-LIPID for tail groups (orange) and GAFF-LIPID for both tail groups and head groups (green).

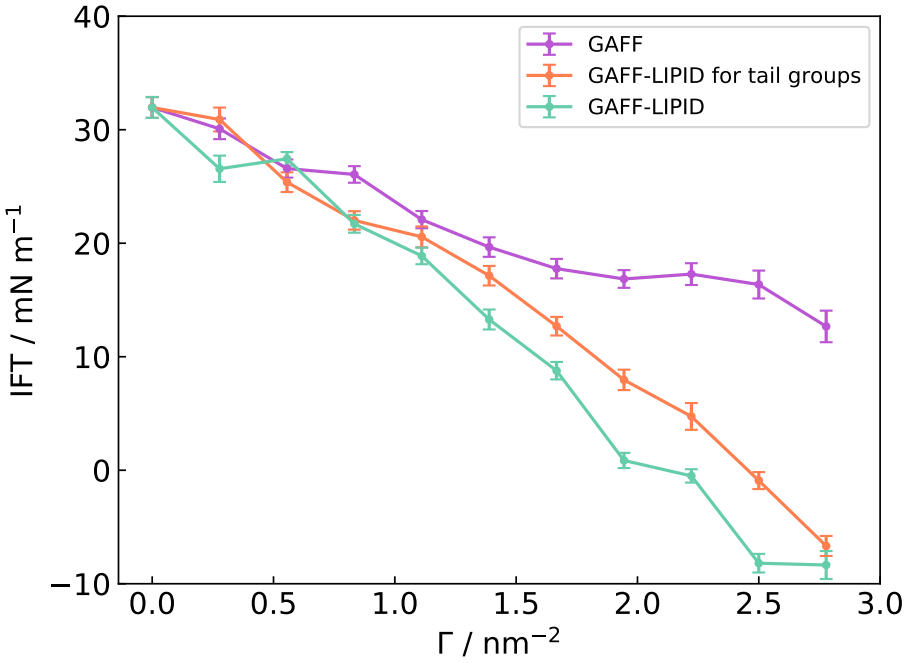

Figure S3: Simulated interfacial tensions (IFT) as a function of surface concentration (Γ) for SLE3S molecules at a water-triolein interface, with GAFF (purple), GAFF-LIPID for tail groups (orange) and GAFF-LIPID for both tail groups and head groups (green).

S2 Force field modifications

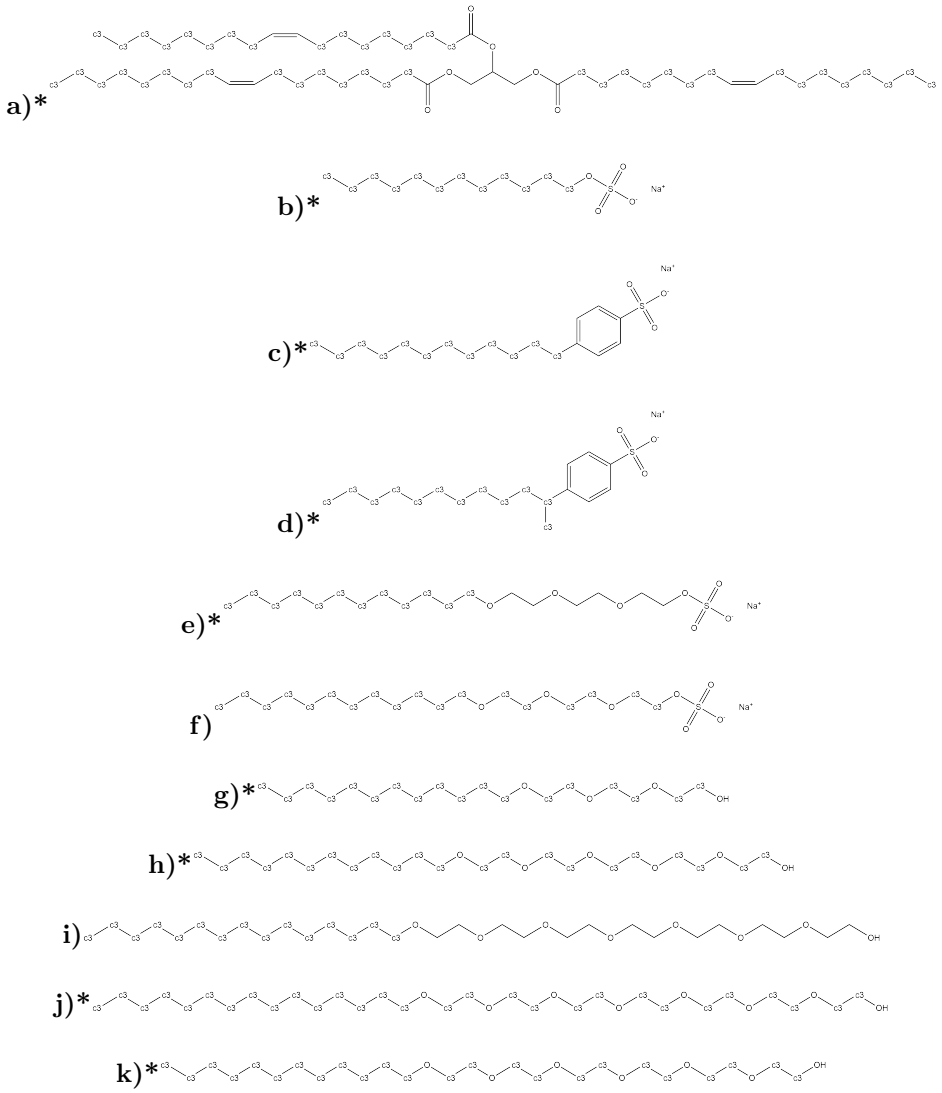

Figure S4: Molecular structures used in this study. A * symbol marks those structures where force field modifications were employed: (a) triolein, (b) SDS, (c) SDBS, (d) SD2BS, (e) SLE3S (GAFF-LIPID for tail groups), (f) SLE3S (GAFF-LIPID), (g) C12E3, (h) C12E5, (i) C15E7 (GAFF-LIPID for tail groups), (j) C15E7 (GAFF-LIPID) and (k) C12E6.

We used the Lennard-Jones σ and ϵ parameters for the "atomtype c3" from the GAFF-LIPID force field for the c3 atoms of the labelled molecules in figure S4. In addition, Lennard-Jones σ and ϵ parameters for "atomtype hc" from GAFF-LIPID are utilised in force field modifications for hc atoms in the above molecules. We have also used dihedral angle parameters from GAFF-LIPID for all c3-c3-c3-c3 torsions in these molecules.[1]

S3 IFT results

Table S1: Simulated interfacial tensions (IFT, with the unit of mN m^{-1}) of water-surfactants-triolein interfaces, with GAFF/GAFF-LIPID parameters and TIP3P water model.

Γ/nm^{-2}	SDS	SDBS	SD2BS	SLE3S
0	31.96 ± 0.92	31.96 ± 0.92	31.96 ± 0.92	31.96 ± 0.92
0.28	28.44 ± 0.74	30.94 ± 0.63	30.46 ± 1.09	30.90 ± 1.05
0.56	25.90 ± 0.87	31.93 ± 0.71	27.73 ± 0.70	25.38 ± 0.87
0.83	22.71 ± 0.70	28.40 ± 0.68	28.79 ± 0.79	22.01 ± 0.81
1.11	21.10 ± 0.72	25.79 ± 0.56	25.26 ± 0.73	20.56 ± 0.92
1.39	17.62 ± 0.87	22.56 ± 0.84	19.14 ± 0.79	17.14 ± 0.86
1.67	12.58 ± 0.60	17.42 ± 0.84	13.56 ± 0.88	12.69 ± 0.82
1.94	11.44 ± 1.01	17.51 ± 0.92	11.70 ± 0.88	7.96 ± 0.90
2.22	6.17 ± 0.96	15.89 ± 0.88	3.69 ± 1.61	4.74 ± 1.18
2.50	2.33 ± 0.91	14.06 ± 0.99	-0.74 ± 0.96	-0.91 ± 0.75
2.78	-1.54 ± 0.84	10.06 ± 1.45	-6.80 ± 0.97	-6.67 ± 0.88

Table S2: Simulated interfacial tensions (IFT, with the unit of mN m^{-1}) of water-surfactants-triolein interfaces, with GAFF/GAFF-LIPID parameters and TIP3P water model.

Γ/nm^{-2}	C12E3	C12E5	C15E7
0	31.96 ± 0.92	31.96 ± 0.92	31.96 ± 0.92
0.28	30.92 ± 0.66	32.68 ± 0.95	30.27 ± 0.62
0.56	31.19 ± 0.78	28.22 ± 0.79	25.66 ± 0.79
0.83	24.87 ± 0.45	24.57 ± 0.73	21.41 ± 0.68
1.11	23.34 ± 0.66	19.81 ± 0.83	19.70 ± 0.51
1.39	21.65 ± 0.97	19.47 ± 0.78	14.42 ± 0.89
1.67	18.33 ± 0.94	14.88 ± 0.90	10.50 ± 0.83
1.94	17.23 ± 0.62	11.29 ± 0.63	9.14 ± 0.75
2.22	16.05 ± 0.78	8.23 ± 0.48	1.65 ± 0.84
2.50	12.59 ± 1.11	2.70 ± 0.75	-1.90 ± 1.15
2.78	7.74 ± 0.93	-2.12 ± 1.12	-2.09 ± 0.88

S4 ST results

Table S3: Simulated surface tensions (ST, with the unit of mN m^{-1}) of water-surfactants-vacuum interfaces, with GAFF/GAFF-LIPID parameters and OPC4 water model.

Γ/nm^{-2}	SDS	SDBS	SD2BS	SLE3S
0	70.66 ± 0.20	70.66 ± 0.20	70.66 ± 0.20	70.66 ± 0.20
0.28	68.83 ± 0.18	69.66 ± 0.19	69.35 ± 0.20	69.90 ± 0.15
0.56	67.63 ± 0.19	68.38 ± 0.22	68.46 ± 0.21	68.73 ± 0.23
0.83	65.36 ± 0.17	67.58 ± 0.18	66.79 ± 0.23	67.11 ± 0.31
1.11	63.36 ± 0.23	65.70 ± 0.25	65.23 ± 0.36	64.05 ± 0.23
1.39	59.83 ± 0.27	63.18 ± 0.27	62.15 ± 0.24	60.01 ± 0.21
1.67	55.97 ± 0.24	59.60 ± 0.23	56.74 ± 0.17	53.37 ± 0.27
1.94	51.50 ± 0.35	54.12 ± 0.28	49.28 ± 0.30	45.12 ± 0.37
2.22	45.44 ± 0.42	49.19 ± 0.39	40.05 ± 0.35	36.47 ± 0.43
2.50	40.43 ± 0.41	43.51 ± 0.34	31.70 ± 0.50	28.15 ± 0.57
2.78	34.51 ± 0.43	38.92 ± 0.44	23.43 ± 0.58	20.17 ± 0.68
Γ_{MAX} (Exp)	1.94 nm^{-2} [2]	-	-	-
ST_{CMC} (Exp)	39.5 mN m^{-1} [2]	-	-	-
CMC (Exp)	8.2×10^{-3} M [3]	-	-	-

Table S4: Simulated surface tensions (ST, with the unit of mN m^{-1}) of water-surfactants-vacuum interfaces, with GAFF/GAFF-LIPID parameters and OPC4 water model.

Γ/nm^{-2}	C12E3	C12E5	C12E6	C15E7
0	70.66 ± 0.20	70.66 ± 0.20	70.66 ± 0.20	70.66 ± 0.20
0.28	69.51 ± 0.16	69.38 ± 0.21	69.36 ± 0.19	69.29 ± 0.16
0.56	69.01 ± 0.16	66.79 ± 0.21	65.59 ± 0.22	64.46 ± 0.24
0.83	66.92 ± 0.20	61.70 ± 0.25	59.30 ± 0.15	57.64 ± 0.27
1.11	63.56 ± 0.28	56.37 ± 0.24	54.41 ± 0.17	52.12 ± 0.28
1.39	59.75 ± 0.25	51.84 ± 0.30	48.60 ± 0.34	47.82 ± 0.33
1.67	55.31 ± 0.29	47.15 ± 0.26	44.29 ± 0.37	42.93 ± 0.39
1.94	50.27 ± 0.33	41.64 ± 0.35	38.70 ± 0.26	37.40 ± 0.49
2.22	45.88 ± 0.33	35.68 ± 0.48	32.18 ± 0.44	31.95 ± 0.43
2.50	40.13 ± 0.21	28.63 ± 0.38	25.69 ± 0.48	27.07 ± 0.50
2.78	33.32 ± 0.37	21.63 ± 0.55	17.15 ± 0.90	27.13 ± 0.94
Γ_{MAX} (Exp)	2.50 nm^{-2} [4]	2.22 nm^{-2} [5]	2.22 nm^{-2} [6]	2.22 nm^{-2} [7]
ST_{CMC} (Exp)	27.9 mN m^{-1} [4]	30.5 mN m^{-1} [5]	32.1 mN m^{-1} [6]	34.6 mN m^{-1} [7]
CMC (Exp)	5.2×10^{-5} M [5]	6.4×10^{-5} M [5]	8.7×10^{-5} M [8]	3.5×10^{-6} M [9]

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