Supplementary Information

Computational prediction of the critical micelle concentration (CMC) of surfactants using the non-Bornian solvation model

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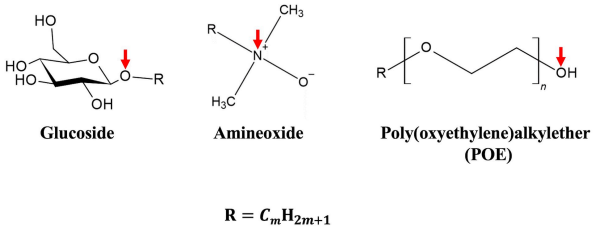

Fig S1 The respective red arrow shows an arbitrarily chosen atom for three different types of non-ionic surfactants, *i.e.*, glucoside, amineoxide, and poly(oxyethylene)alkylether (POE).

Table S1 Theoretical parameters representing the adsorption states of anionic and cationic surfactants at the NB/W interface (25 °C)

Surfactant	d (Å)	θ (°)	ω (°)
Anionic			
$C_8H_{17}SO_4^-Na^+$	−1.8	164	0
$C_9H_{19}SO_4^-Na^+$	−1.8	163	118
$C_{10}H_{21}SO_4^-Na^+$	−1.8	162	0
$C_{12}H_{25}SO_4^-Na^+$	−1.8	160	0
$C_6H_{13}SO_3^-Na^+$	−1.4	152	0
$C_8H_{17}SO_3^-Na^+$	−1.4	154	1
$C_{11}H_{23}SO_3^-H^+$	−1.4	157	0
$C_7H_{15}COO^-K^+$	−1.0	154	0
$C_8H_{17}COO^-K^+$	−1.0	154	180
$C_9H_{19}COO^-K^+$	−1.0	155	0
$C_{10}H_{21}COO^-K^+$	−1.0	156	1
$C_{11}H_{23}COO^-K^+$	−0.8	150	0
$C_{12}H_{25}COO^-K^+$	−0.8	153	20
$C_{13}H_{27}COO^-K^+$	−0.8	153	19
Cationic			
$C_8H_{17}NH_3^+Cl^-$	−0.8	158	180
$C_8H_{17}N(CH_3)_3^+Br^-$	2.0	136	180
$C_{10}H_{21}N(CH_3)_3^+Br^-$	2.2	136	179
$C_{12}H_{25}NH_3^+Cl^-$	−0.8	158	1
$C_{12}H_{25}N(CH_3)_3^+Cl^-$ [a]	2.2	137	180
$C_{12}H_{25}N(CH_3)_3^+Br^-$ [a]	2.2	137	180
$C_{14}H_{29}NH_3^+Cl^-$	−0.8	158	0
$C_{14}H_{29}N(CH_3)_3^+Cl^-$	2.2	133	180
$C_{18}H_{37}N(CH_3)_3^+Cl^-$	2.0	136	180

[a] Possible effects of hydrophilic counterions were not taken into account in the present theoretical simulation.

Table S2 Theoretical parameters representing the adsorption states of non-ionic surfactants at the NB/W interface (25 °C)

Surfactant	*d* (Å)	*θ* (°)	*ω* (°)
Non-ionic			
$C_8H_{17}(OC_2H_4)OH$	2.8	29	180
$C_8H_{17}(OC_2H_4)_3OH$	9.0	26	1
$C_8H_{17}(OC_2H_4)_6OH$	17.6	36	181
$C_8H_{17}(OC_2H_4)_9OH$	27.2	27	0
$C_{10}H_{21}(OC_2H_4)_3OH$	9.0	25	187
$C_{10}H_{21}(OC_2H_4)_6OH$	17.6	36	45
$C_{10}H_{21}(OC_2H_4)_9OH$	14.8	179	152
$C_{12}H_{25}(OC_2H_4)_6OH$	17.4	37	0
$C_{13}H_{27}(OC_2H_4)_5OH$	14.8	29	4
$C_{14}H_{29}(OC_2H_4)_6OH$	18.0	34	5
n-octyl-β-D-glucoside	1.8	102	124
n-decyl-β-D-glucoside	1.8	63	99
n-dodecyl-β-D-glucoside	1.6	69	89
$C_9H_{19}N(CH_3)_2$-O	0.6	67	106
$C_{10}H_{21}(OC_2H_4)N(CH_3)_2$-O	0.6	68	138
$C_{12}H_{25}(OC_2H_4)N(CH_3)_2$-O	0.6	68	302
$C_{14}H_{29}(OC_2H_4)N(CH_3)_2$-O	0.6	68	299
$C_{16}H_{33}(OC_2H_4)N(CH_3)_2$-O	0.4	65	304
$C_{18}H_{37}(OC_2H_4)N(CH_3)_2$-O	0.4	65	304