PREDICTION OF AQUEOUS SOLUTION SURFACE TENSION OF SOME SURFACTANT MIXTURES AND COMPOSITION OF THEIR MONOLAYERS AT THE SOLUTION-AIR INTERFACE

BRONISŁAW JAŃCZUK [1,*], ANNA ZDZIENNICKA [1], KATARZYNA SZYMCZYK [1] and MARIA LUISA GONZÁLEZ MARTÍN [2,3]

1 *Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University in Lublin, Maria Curie-Skłodowska Sq. 3, 20-031 Lublin, Poland*

2 *Department of Applied Physics, Extremadura University, Avda. de Elvas, s/n, 06006 Badajoz, Spain*

3 *Networking Research Center on Bioengineering, Biomaterials and Nanomedicine (CIBER-BBN), 06006 Badajoz, Spain*

* Correspondence: bronislaw.janczuk@poczta.umcs.lublin.pl; Tel.: +48-81-537-56-49

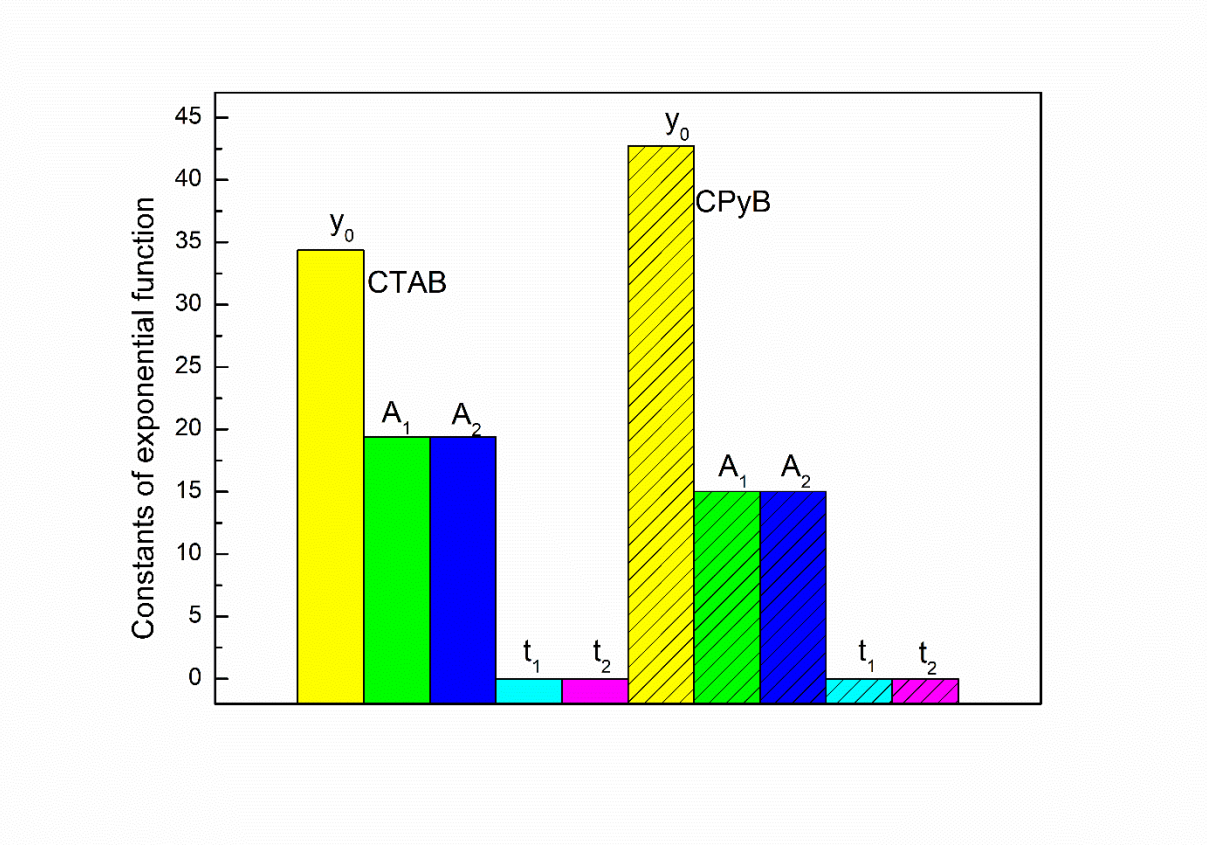

Figure S1. The values of the constants in the exponential function of the second order describing the changes of aqueous solutions of CTAB as well as CPyB surface tension.

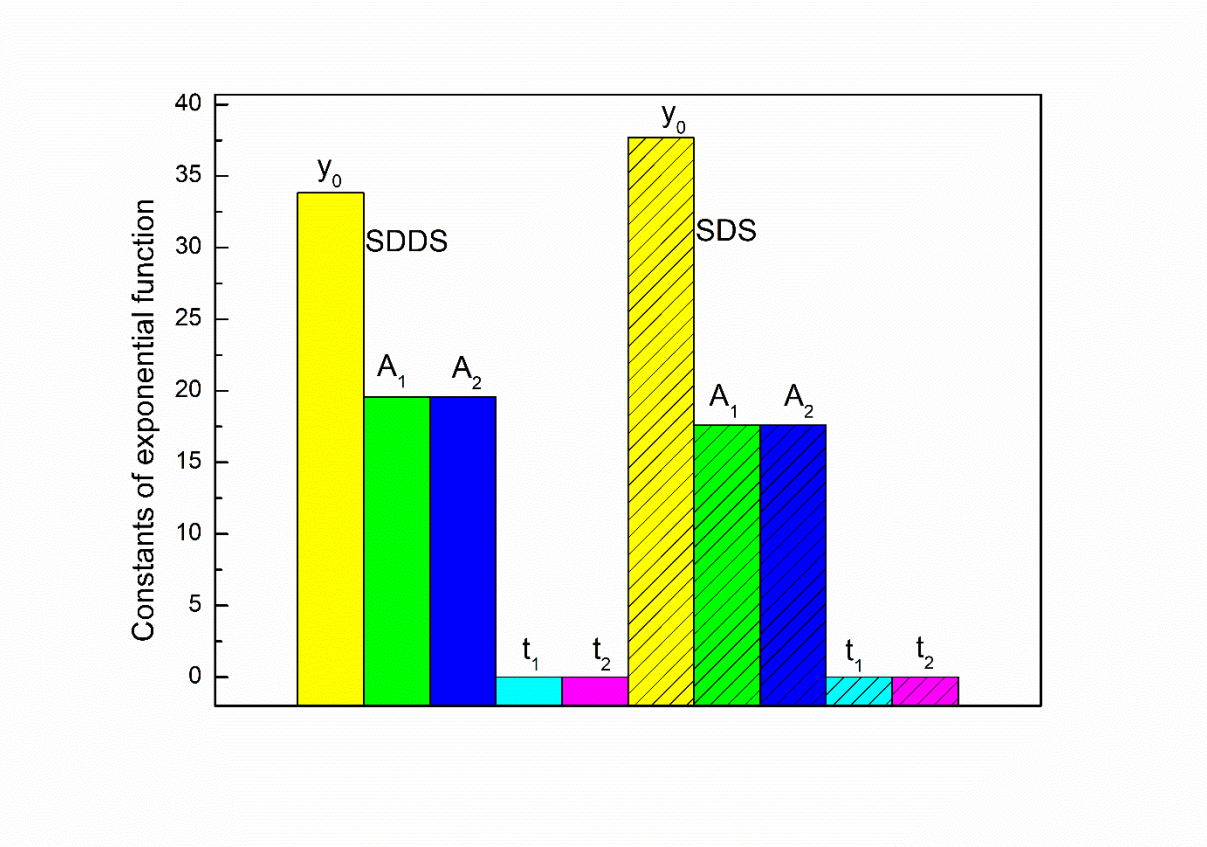

Figure S2. The values of the constants in the exponential function of the second order describing the changes of aqueous solutions of SDDS as well as SDS surface tension.

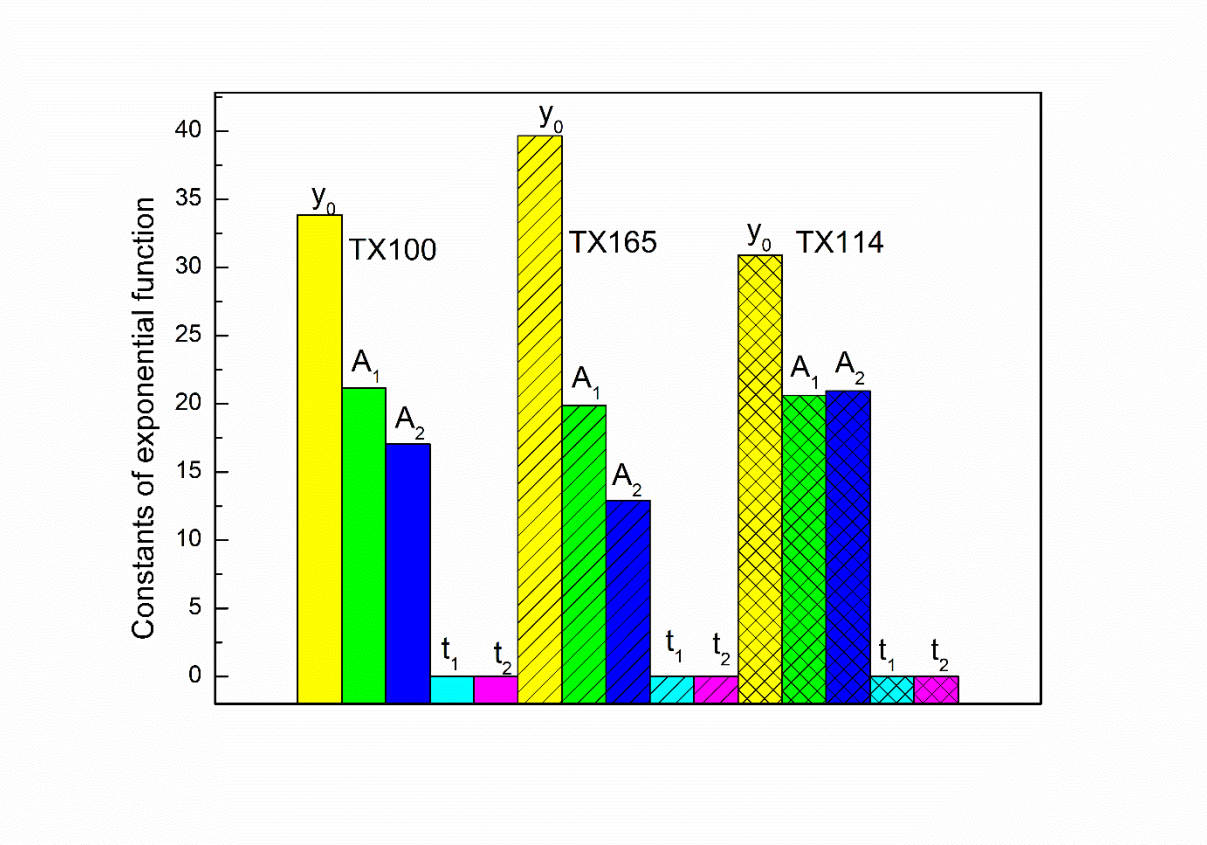

Figure S3. The values of the constants in the exponential function of the second order describing the changes of aqueous solutions of TX100, TX65 as well as TX114 surface tension.

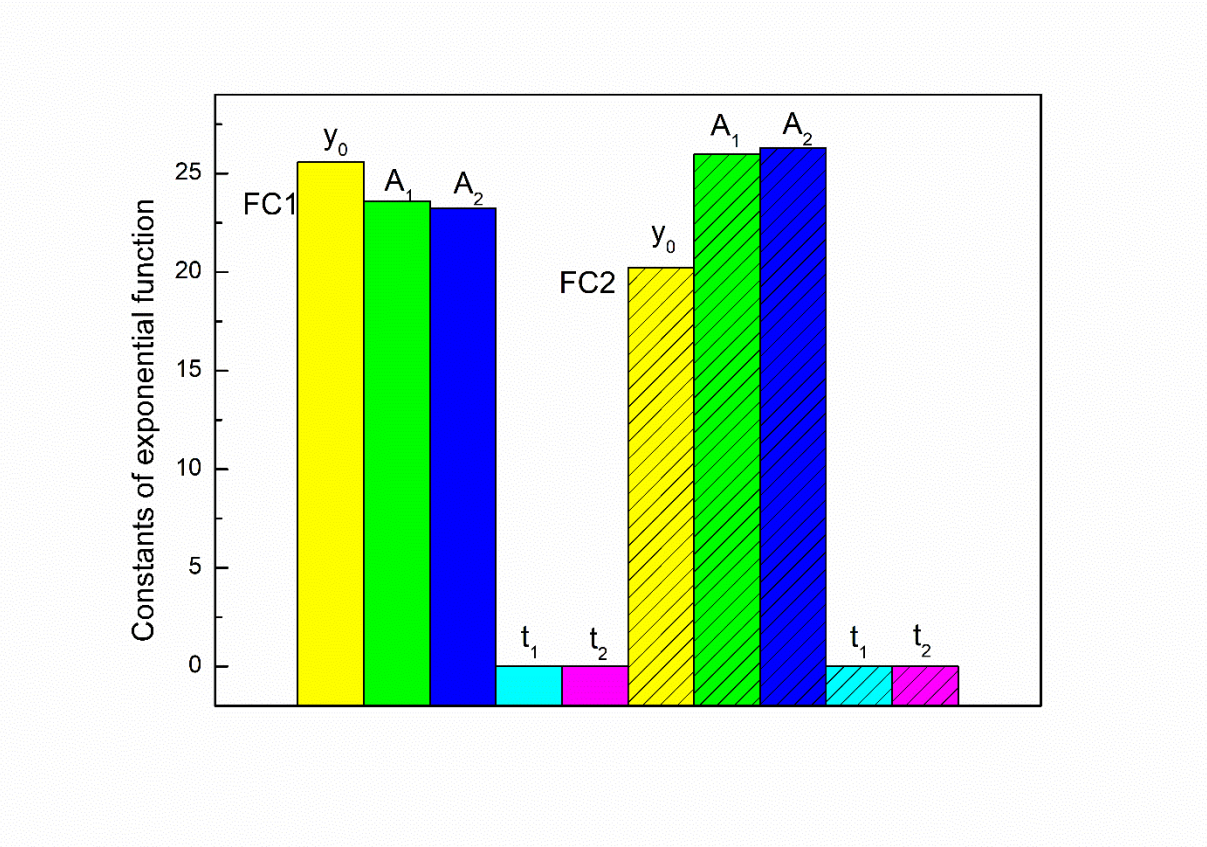

Figure S4. The values of the constants in the exponential function of the second order describing the changes of aqueous solutions of FC1 as well as FC2 surface tension.

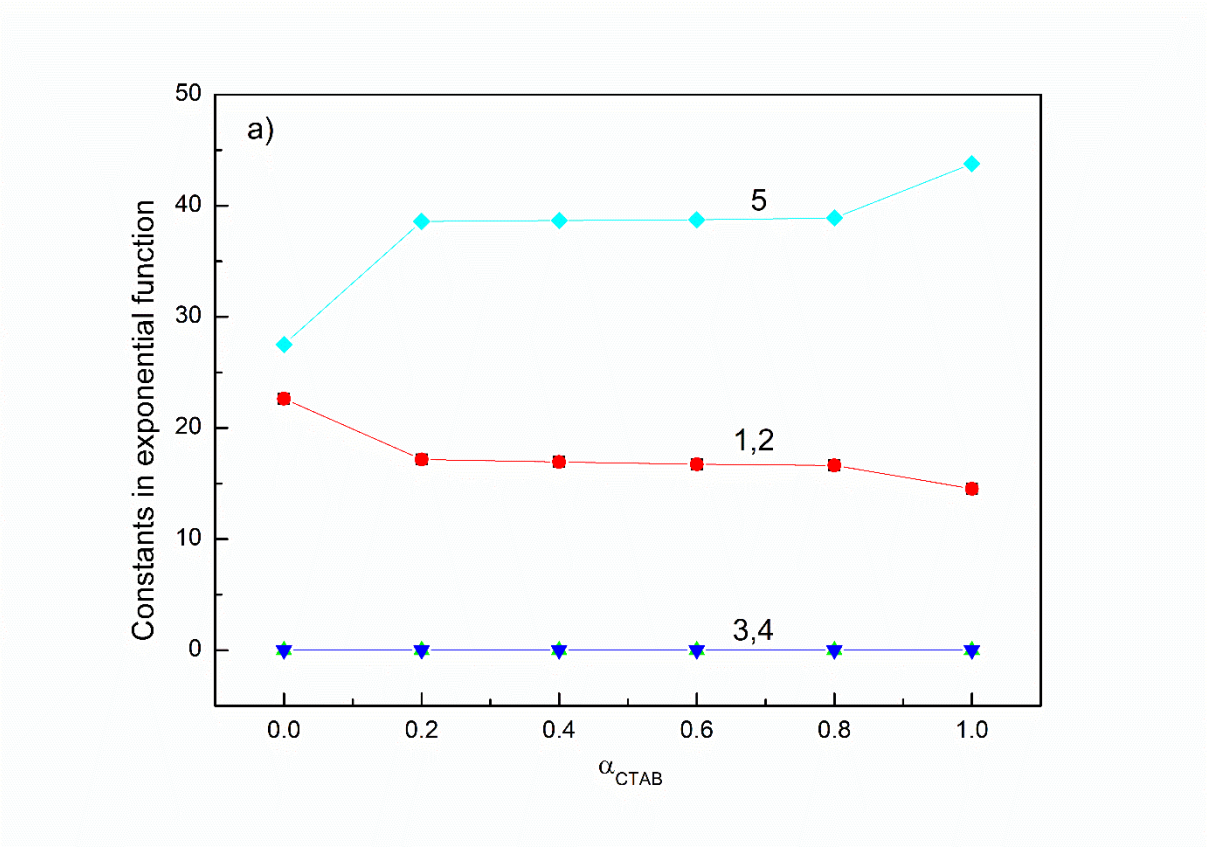

Figure S5a. A plot of the constants in the exponential function of the second order describing the changes of the surface tension of aqueous solutions of CTAB+CPyB mixtures vs. the mole fraction of CTAB in the bulk phase (α). Curve 1 corresponds to A_1, curve 2 to A_2, curve 3 to t_1, curve 4 to t_2 and curve 5 corresponds to y_0.

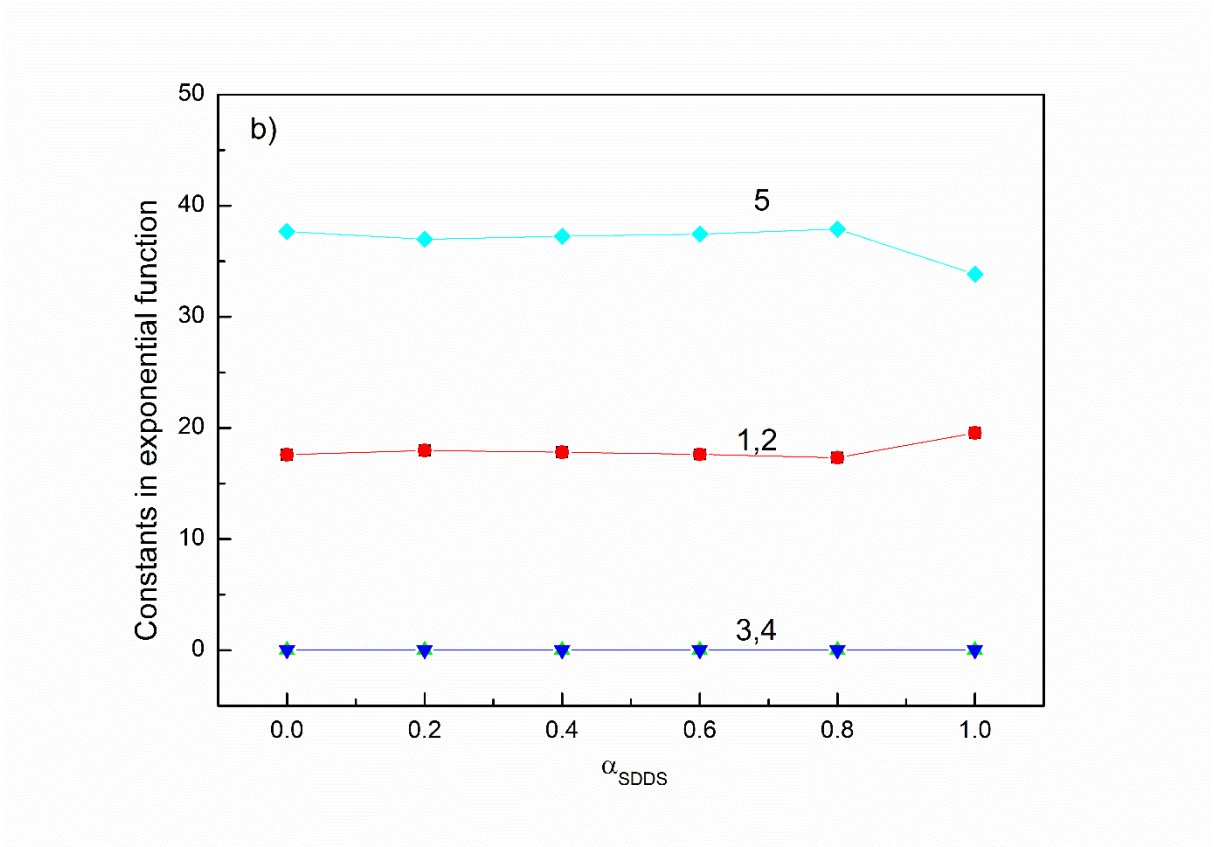

Figure S5b. A plot of the constants in the exponential function of the second order describing the changes of the surface tension of aqueous solutions of SDDS+SDS mixtures vs. the mole fraction of SDDS in the bulk phase (α). Curve 1 corresponds to A_1, curve 2 to A_2, curve 3 to t_1, curve 4 to t_2 and curve 5 corresponds to y_0.

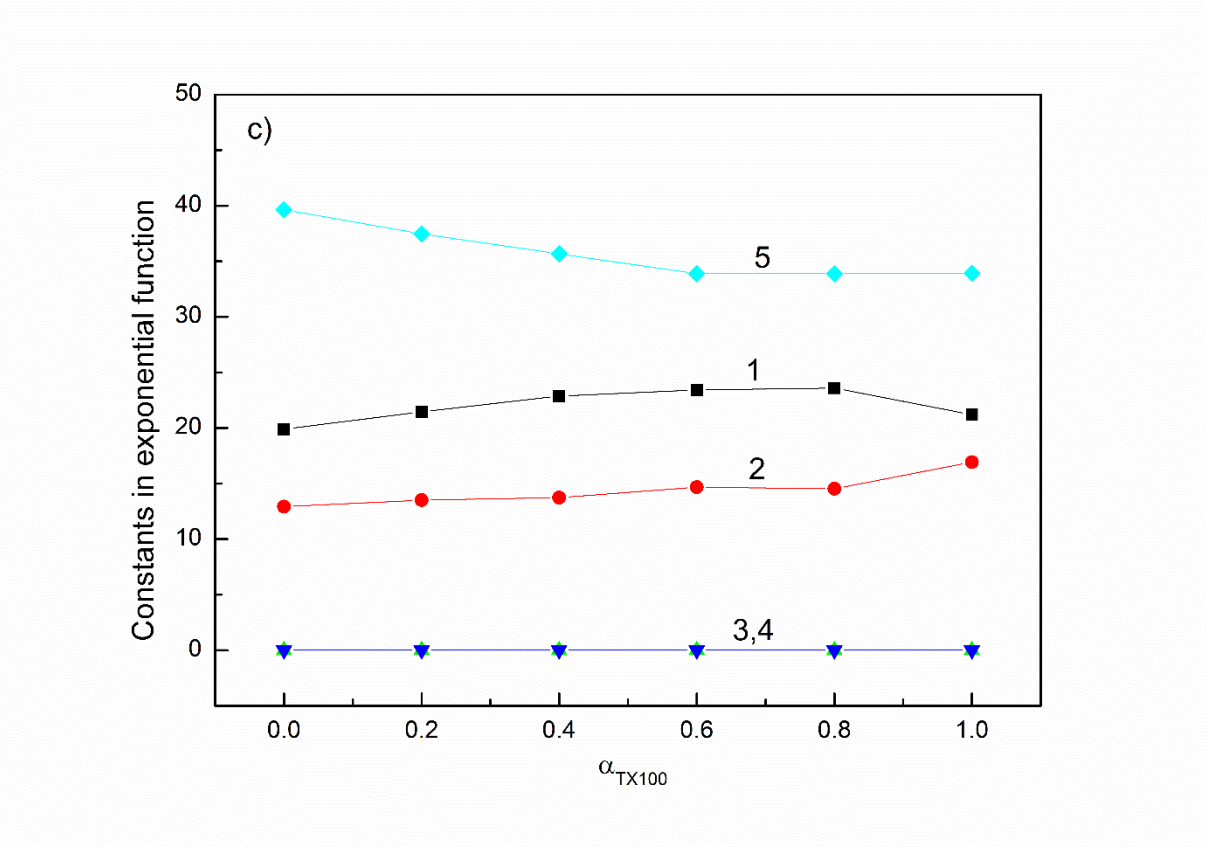

Figure S5c. A plot of the constants in the exponential function of the second order describing the changes of the surface tension of aqueous solutions of TX100+TX165 mixtures vs. the mole fraction of TX100 in the bulk phase (α). Curve 1 corresponds to A_1, curve 2 to A_2, curve 3 to t_1, curve 4 to t_2 and curve 5 corresponds to y_0.

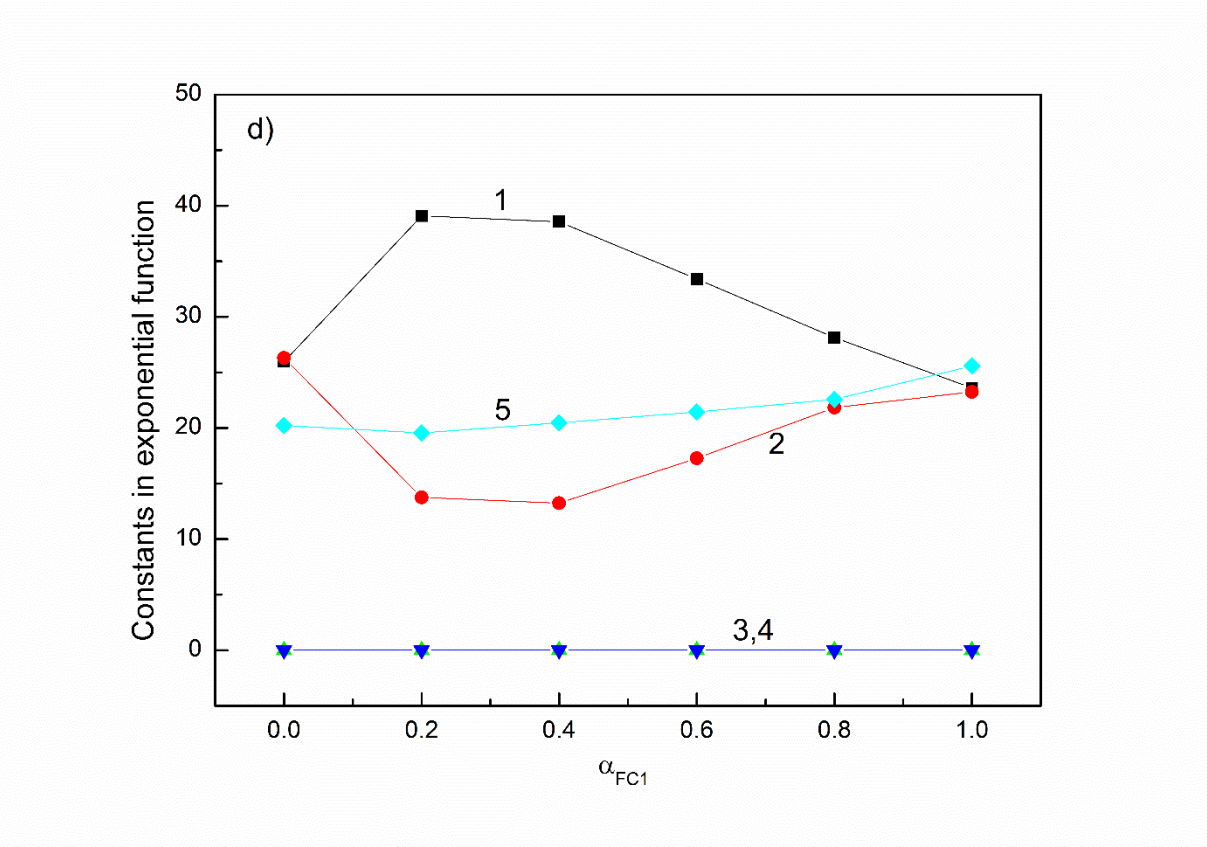

Figure S5d. A plot of the constants in the exponential function of the second order describing the changes of the surface tension of aqueous solutions of FC1+FC2 mixtures vs. the mole fraction of FC1 in the bulk phase (α). Curve 1 corresponds to A_1, curve 2 to A_2, curve 3 to t_1, curve 4 to t_2 and curve 5 corresponds to y_0.

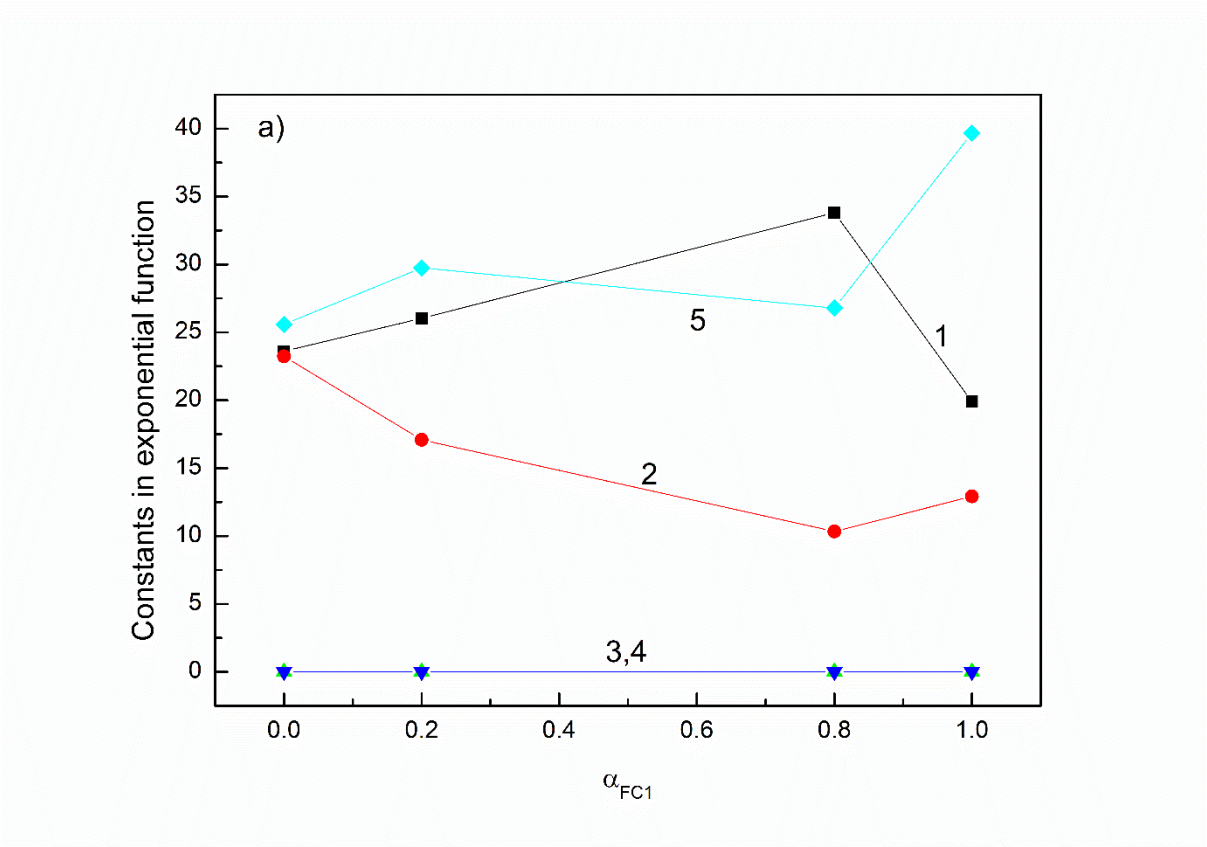

Figure S6a. The plot of the constants in the exponential function of the second order describing the changes of the surface tension of aqueous solutions of FC1+TX165 mixtures vs. the mole fraction of FC1 in the bulk phase (α). Curve 1 corresponds to A_1, curve 2 to A_2, curve 3 to t_1, curve 4 to t_2 and curve 5 corresponds to y_0.

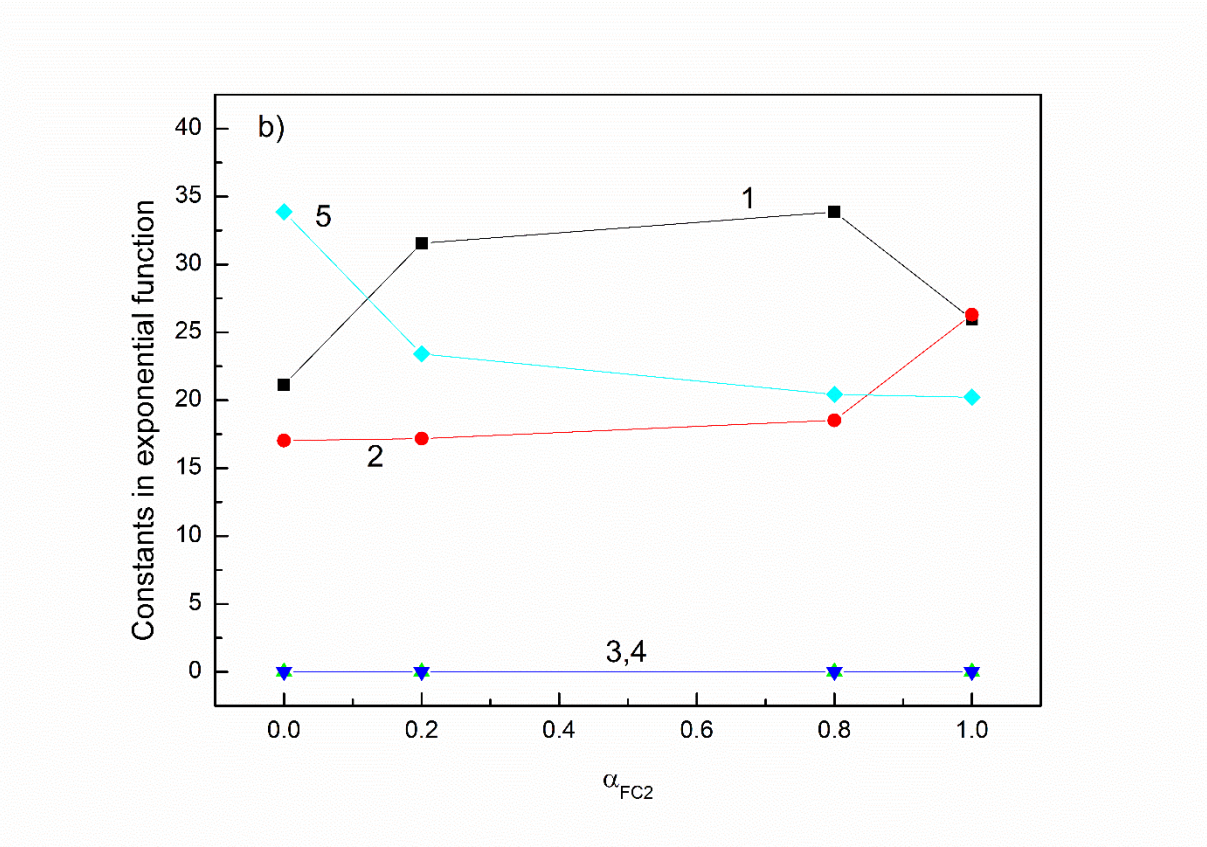

Figure S6b. The plot of the constants in the exponential function of the second order describing the changes of the surface tension of aqueous solutions of FC2+TX100 mixtures vs. the mole fraction of FC2 in the bulk phase (α). Curve 1 corresponds to A_1, curve 2 to A_2, curve 3 to t_1, curve 4 to t_2 and curve 5 corresponds to y_0.

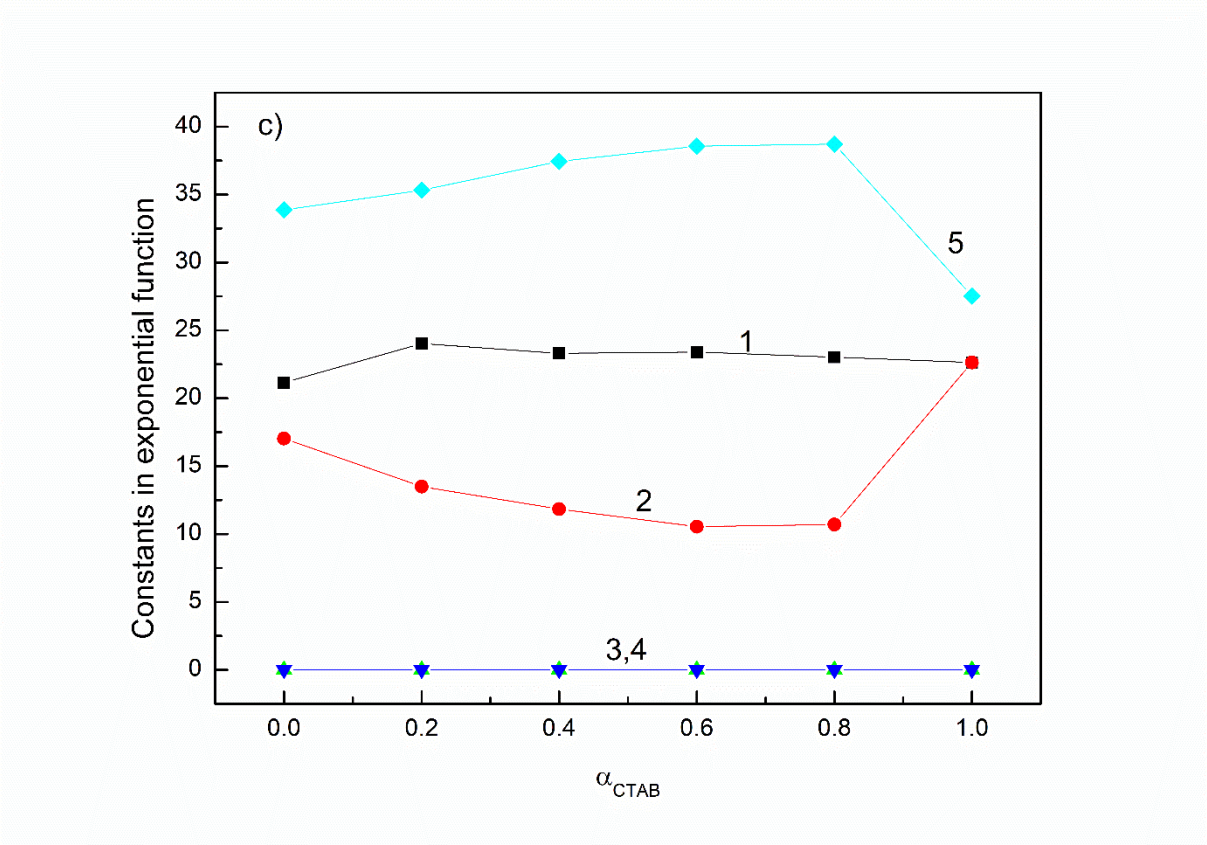

Figure S6c. The plot of the constants in the exponential function of the second order describing the changes of the surface tension of aqueous solutions of CTAB+TX100 mixtures vs. the mole fraction of CTAB in the bulk phase (α). Curve 1 corresponds to A_1, curve 2 to A_2, curve 3 to t_1, curve 4 to t_2 and curve 5 corresponds to y_0.

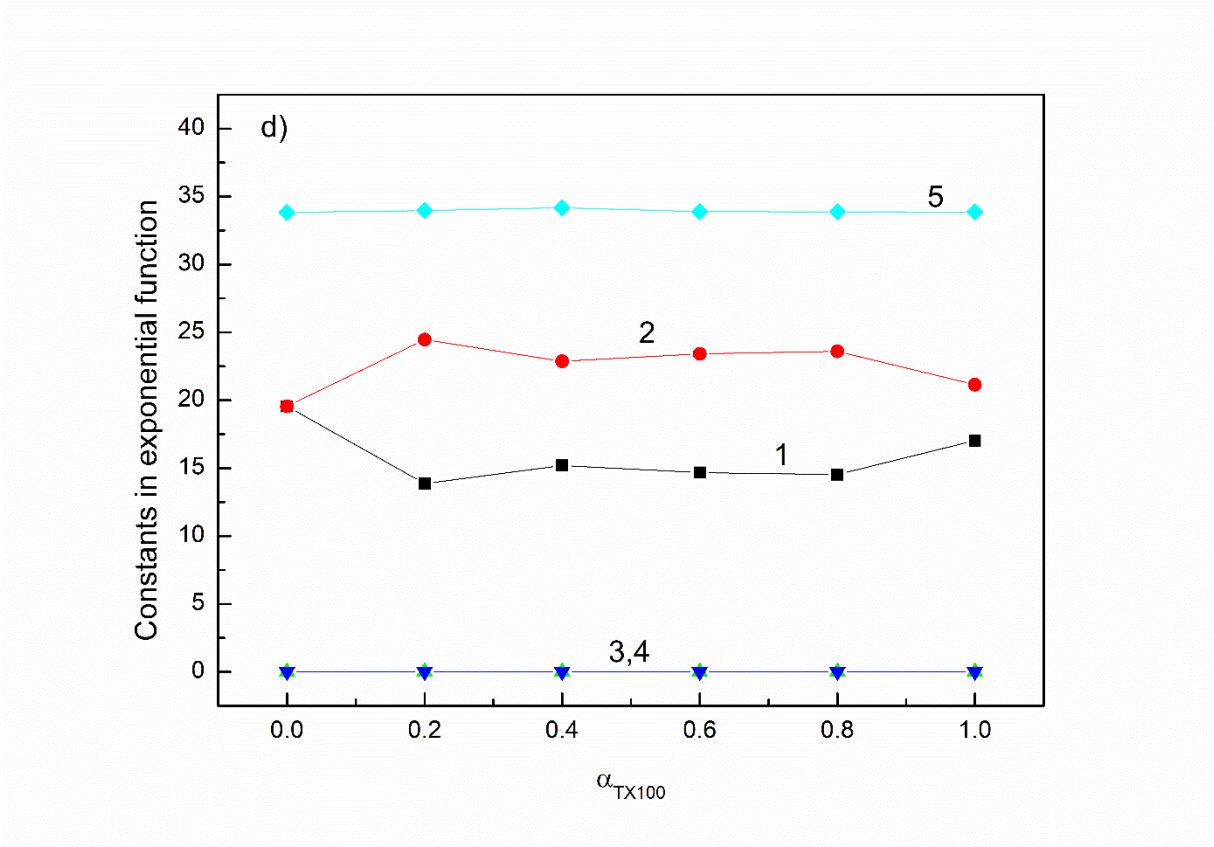

Figure S6d. The plot of the constants in the exponential function of the second order describing the changes of the surface tension of aqueous solutions of SDDS+TX100 mixtures vs. the mole fraction of TX100 in the bulk phase (α). Curve 1 corresponds to A_1, curve 2 to A_2, curve 3 to t_1, curve 4 to t_2 and curve 5 corresponds to y_0.

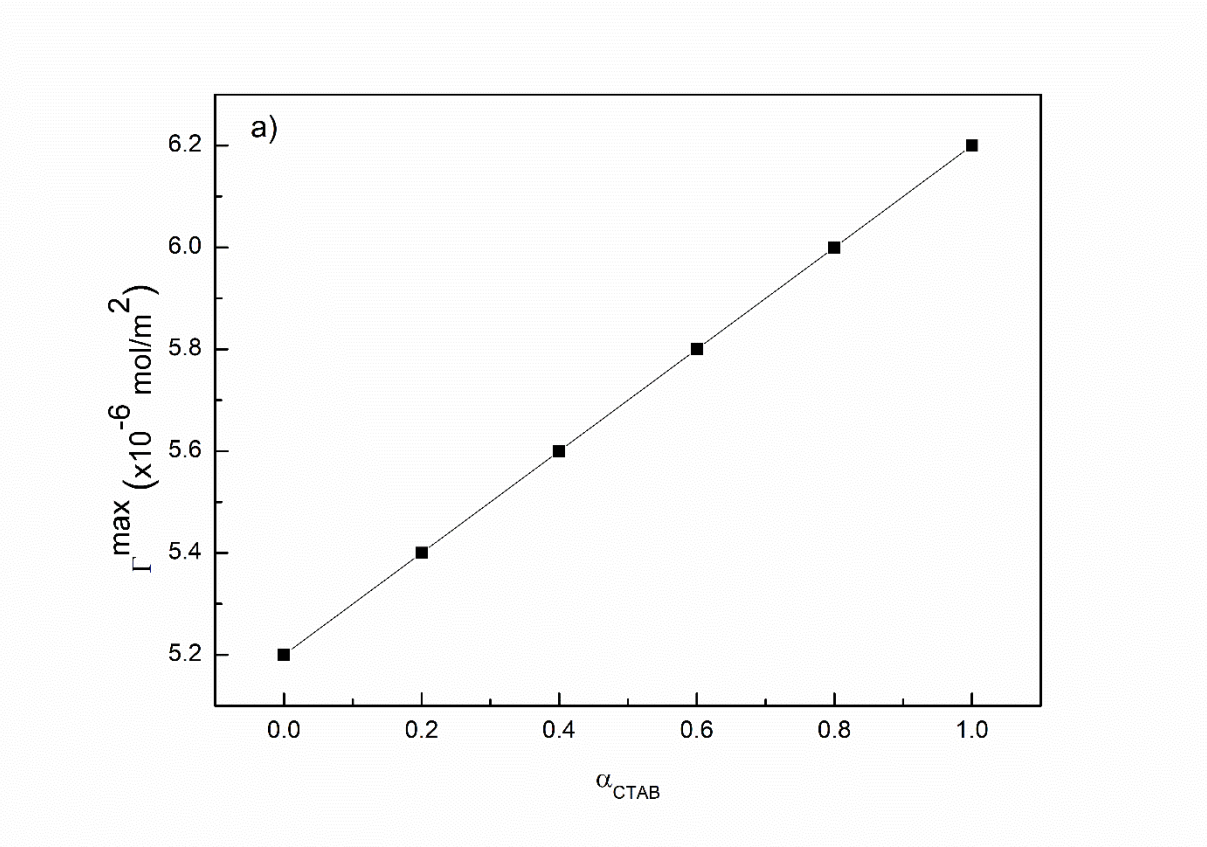

Figure S7a. The plot of the $k\Gamma^{max}$ values of CTAB+CPyB mixtures vs. the mole fraction of CTAB in the bulk phase (α).

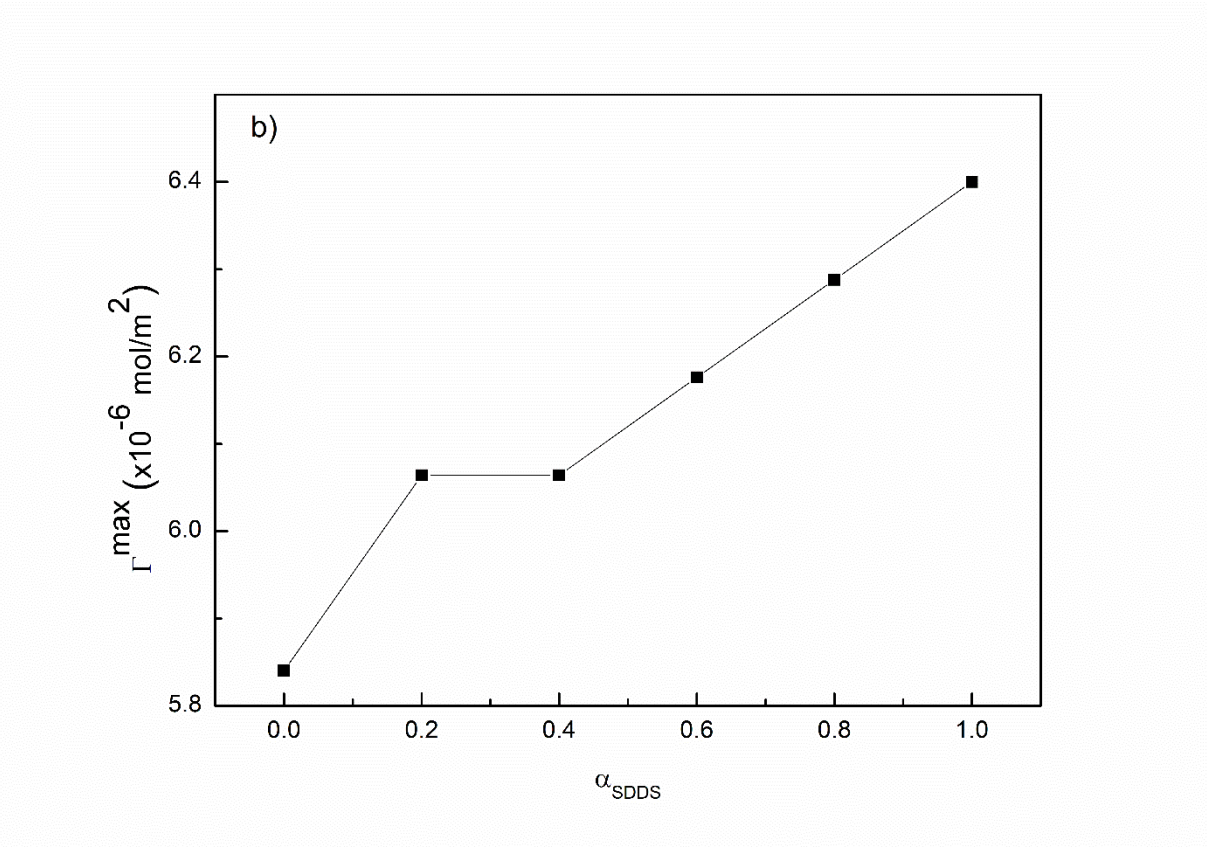

Figure S7b. The plot of the $k\Gamma^{max}$ values of SDDS+SDS mixtures vs. the mole fraction of SDDS in the bulk phase (α).

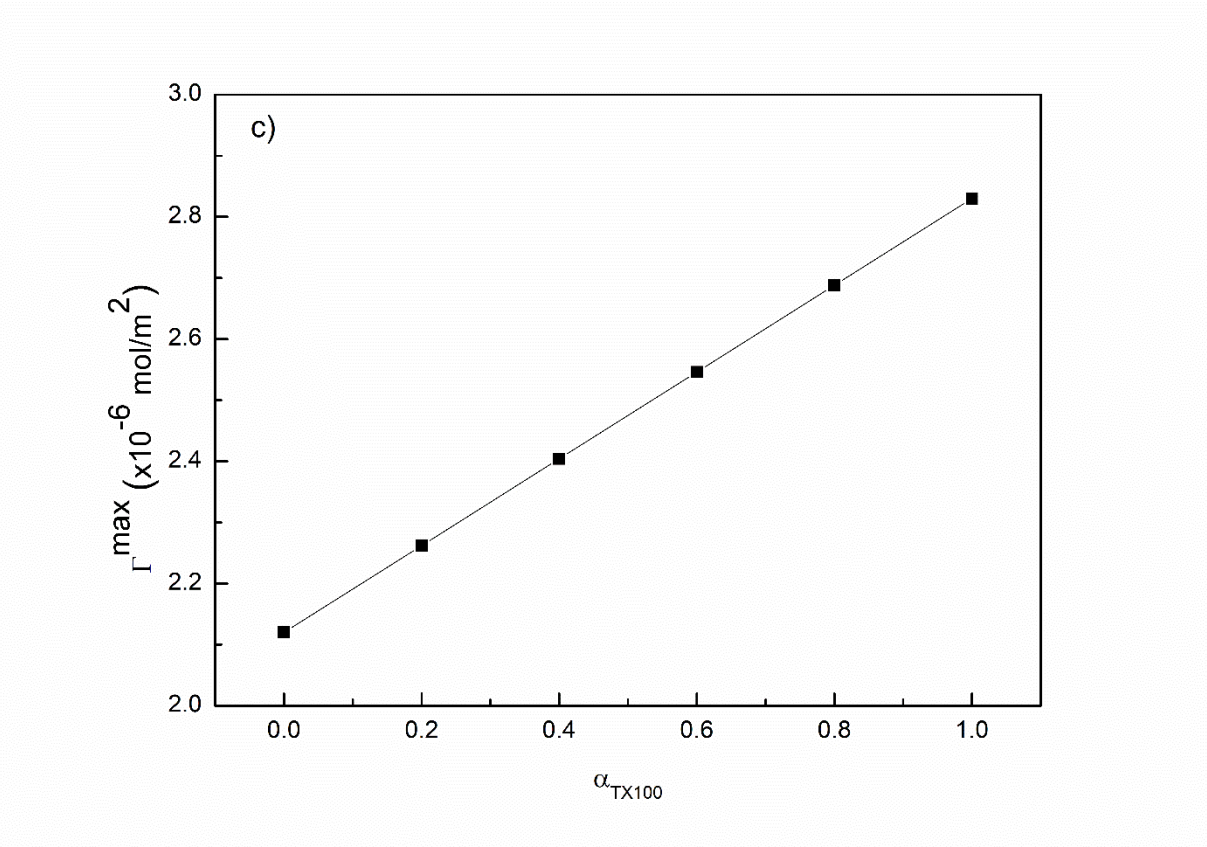

Figure S7c. The plot of the $k\Gamma^{max}$ values of TX00+TX165 (d) mixtures vs. the mole fraction of TX100 in the bulk phase (α).

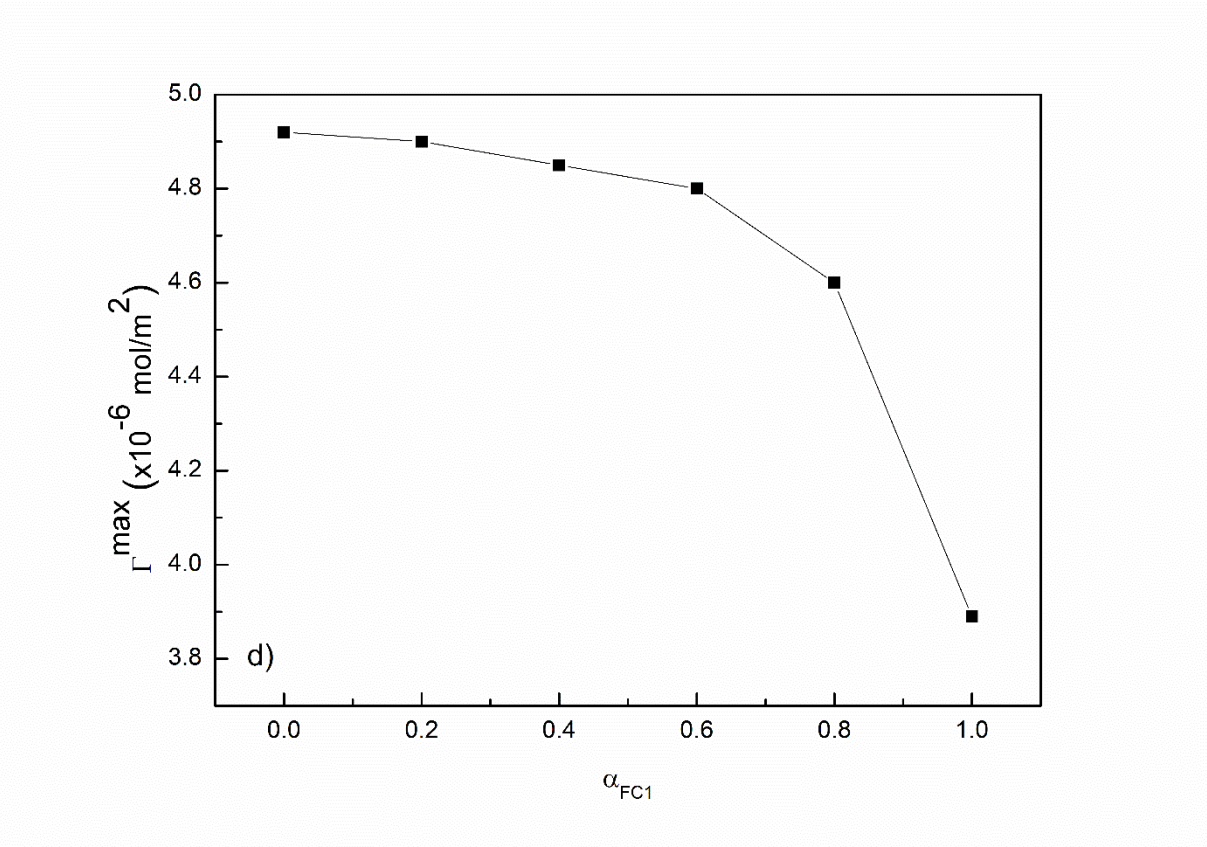

Figure S7d. The plot of the $k\Gamma^{max}$ values of FC1+FC2 mixtures vs. the mole fraction of FC1 in the bulk phase (α).

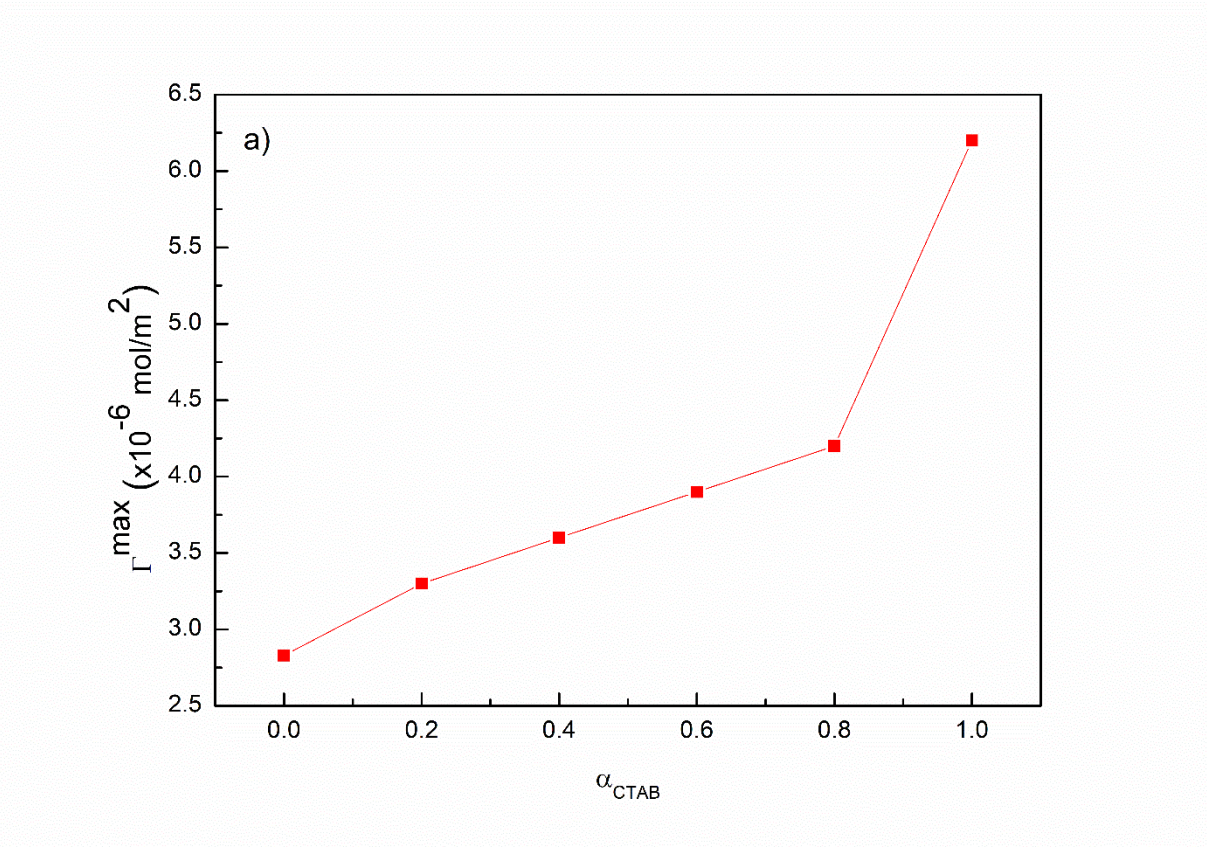

Figure S8a. The plot of the Γ^{max} values of CTAB+TX100 mixtures vs. the mole fraction of CTAB in the bulk phase (α).

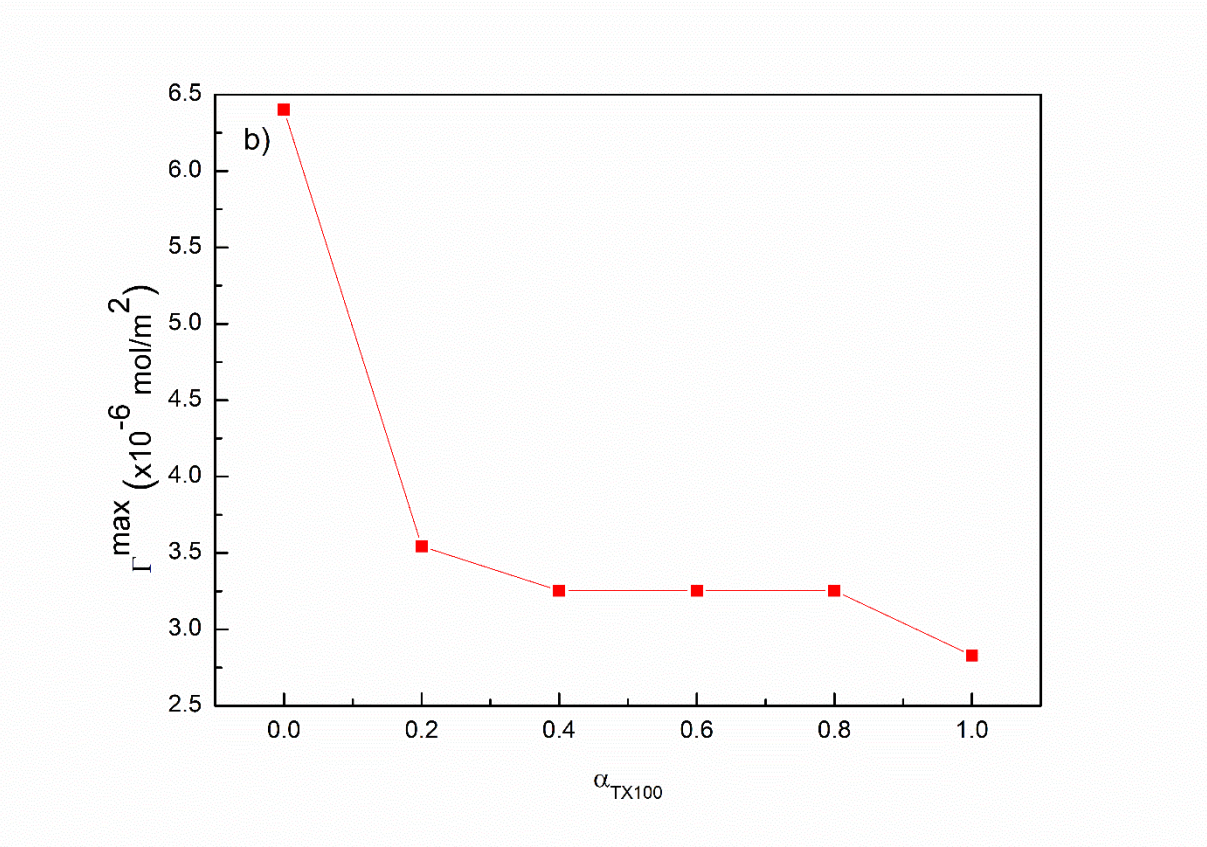

Figure S8b. The plot of the Γ^{max} values of SDDS+TX100 mixtures vs. the mole fraction of TX100 in the bulk phase (α).

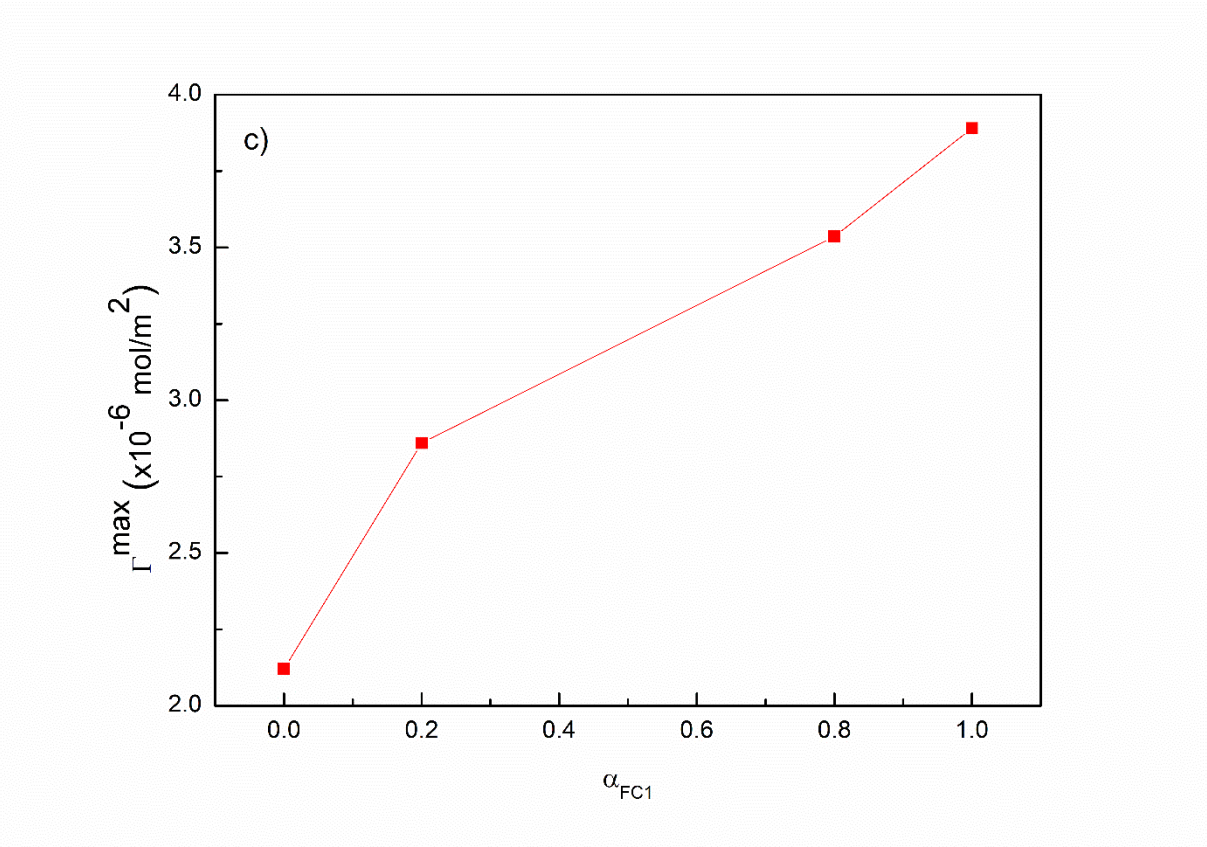

Figure S8c. The plot of the $k\Gamma^{max}$ values of FC1+TX165 mixtures vs. the mole fraction of FC1 in the bulk phase (α).

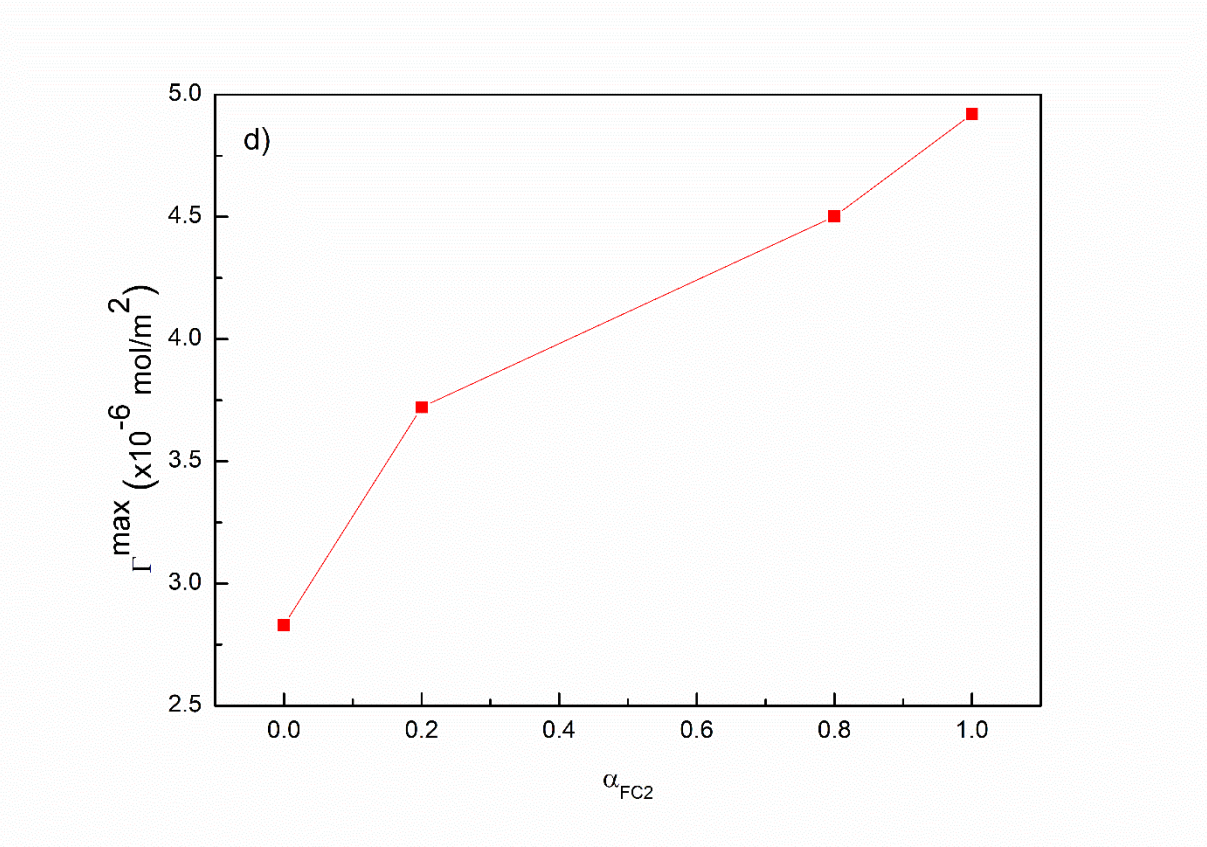

Figure S8d. The plot of the $k\Gamma^{max}$ values of FC2+TX100 mixtures vs. the mole fraction of FC2 in the bulk phase (α).

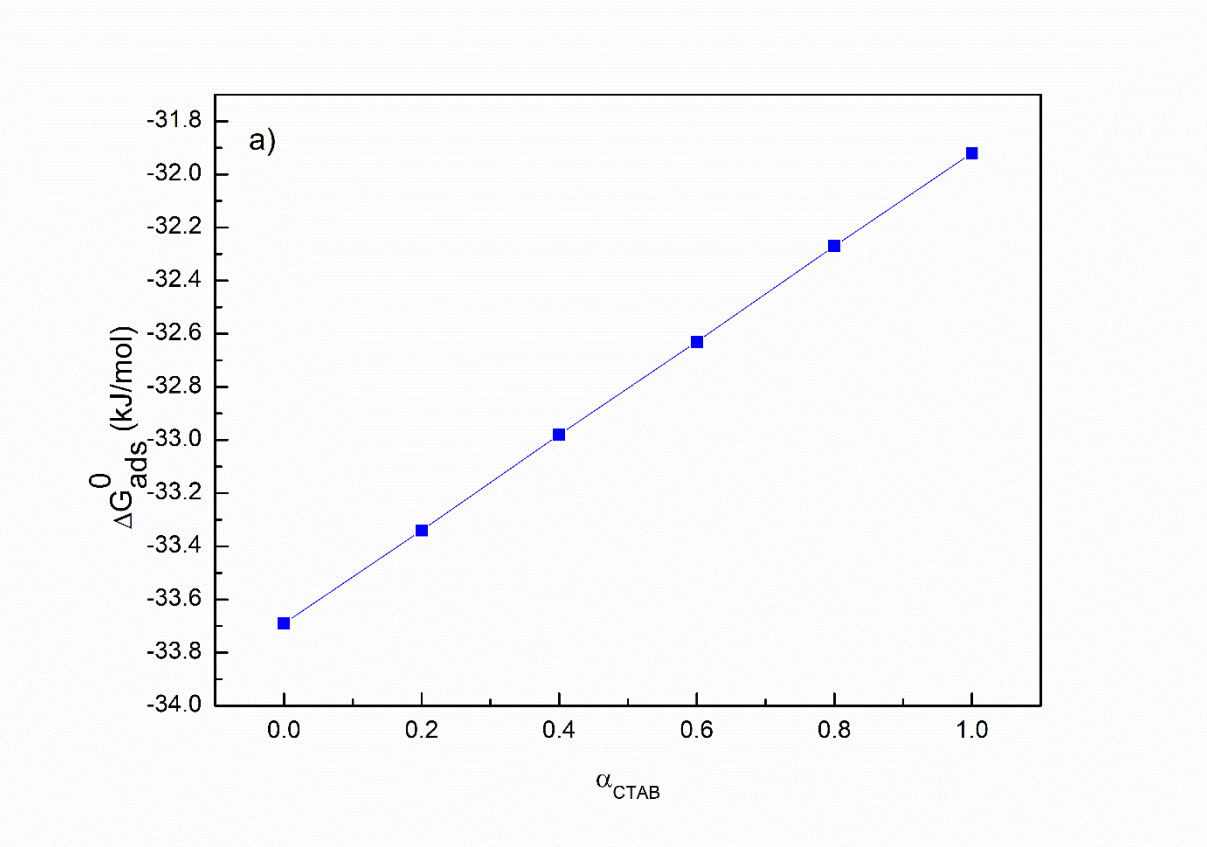

Figure S9a. The plot of the standard Gibbs free energy of adsorption (ΔG^0_{ads}) of CTAB +CPyB mixtures vs. the mole fraction of CTAB in the bulk phase (α).

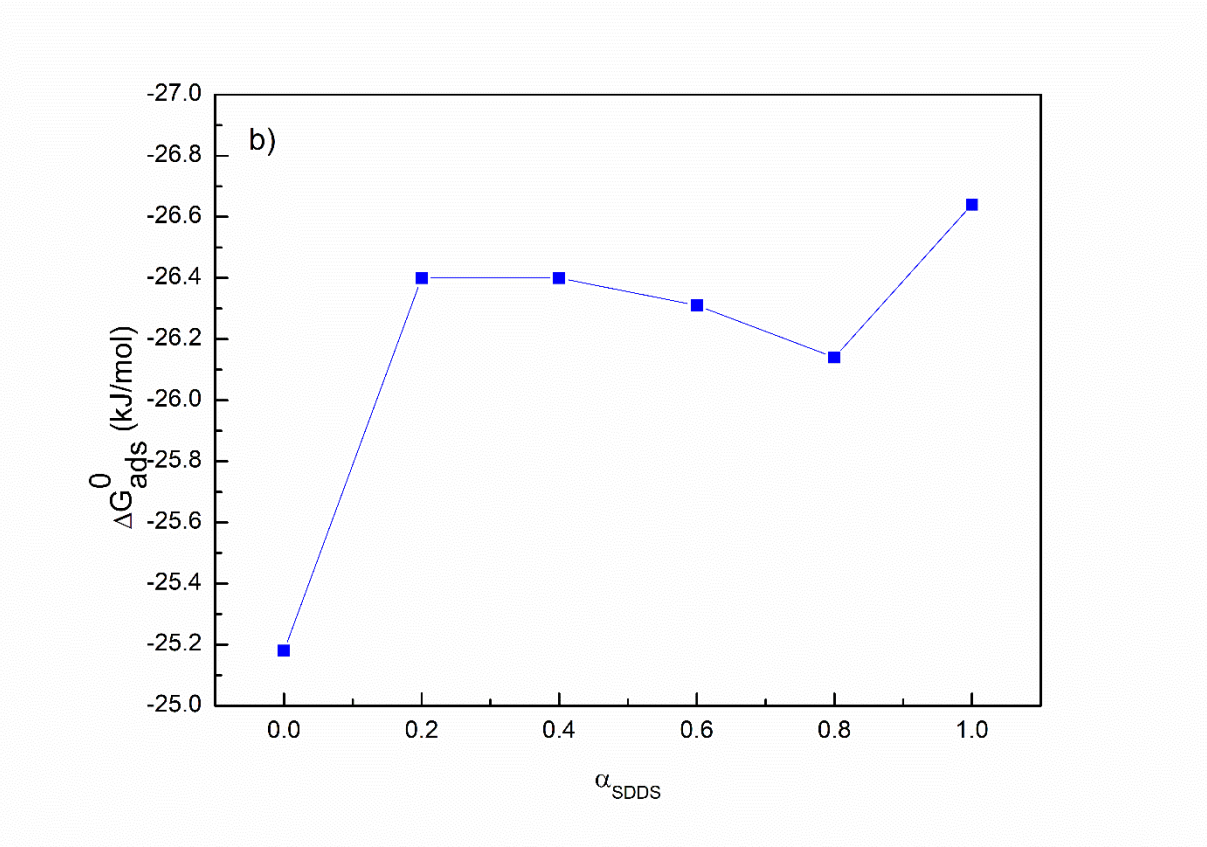

Figure S9b. The plot of the standard Gibbs free energy of adsorption (ΔG^0_{ads}) of SDDS+SDS mixtures vs. the mole fraction of SDDS in the bulk phase (α).

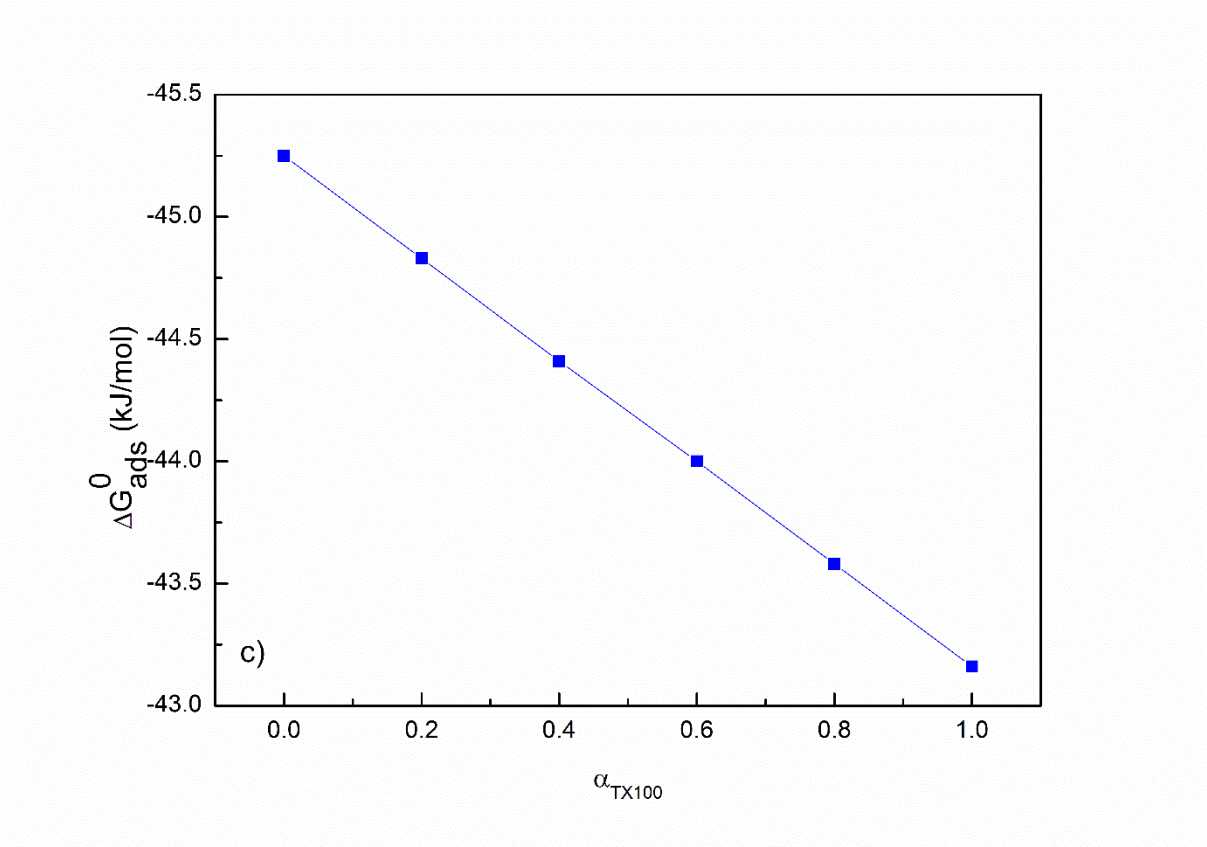

Figure S9c. The plot of the standard Gibbs free energy of adsorption (ΔG^0_{ads}) of TX100+TX165 mixtures vs. the mole fraction of TX100 in the bulk phase (α).

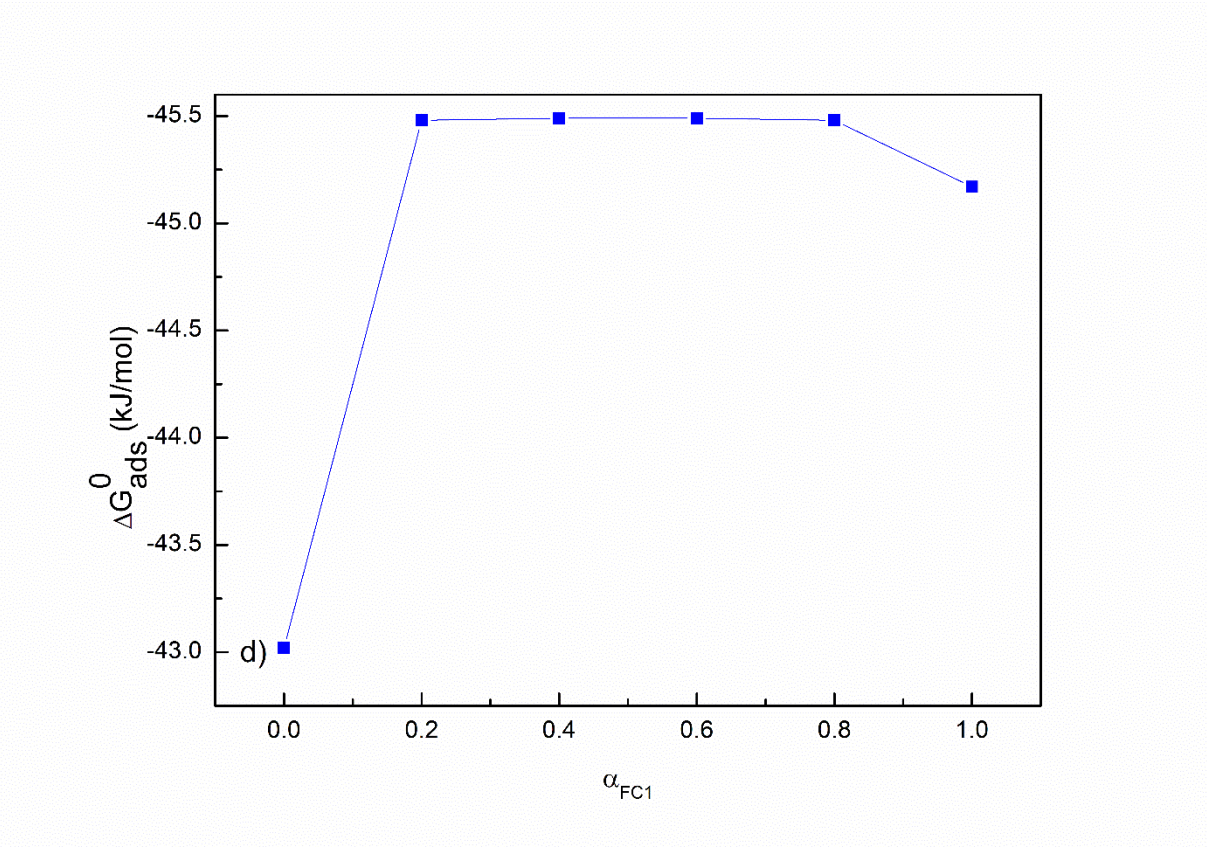

Figure S9d. The plot of the standard Gibbs free energy of adsorption (ΔG^0_{ads}) of FC1+FC2 mixtures vs. the mole fraction of FC1 in the bulk phase (α).

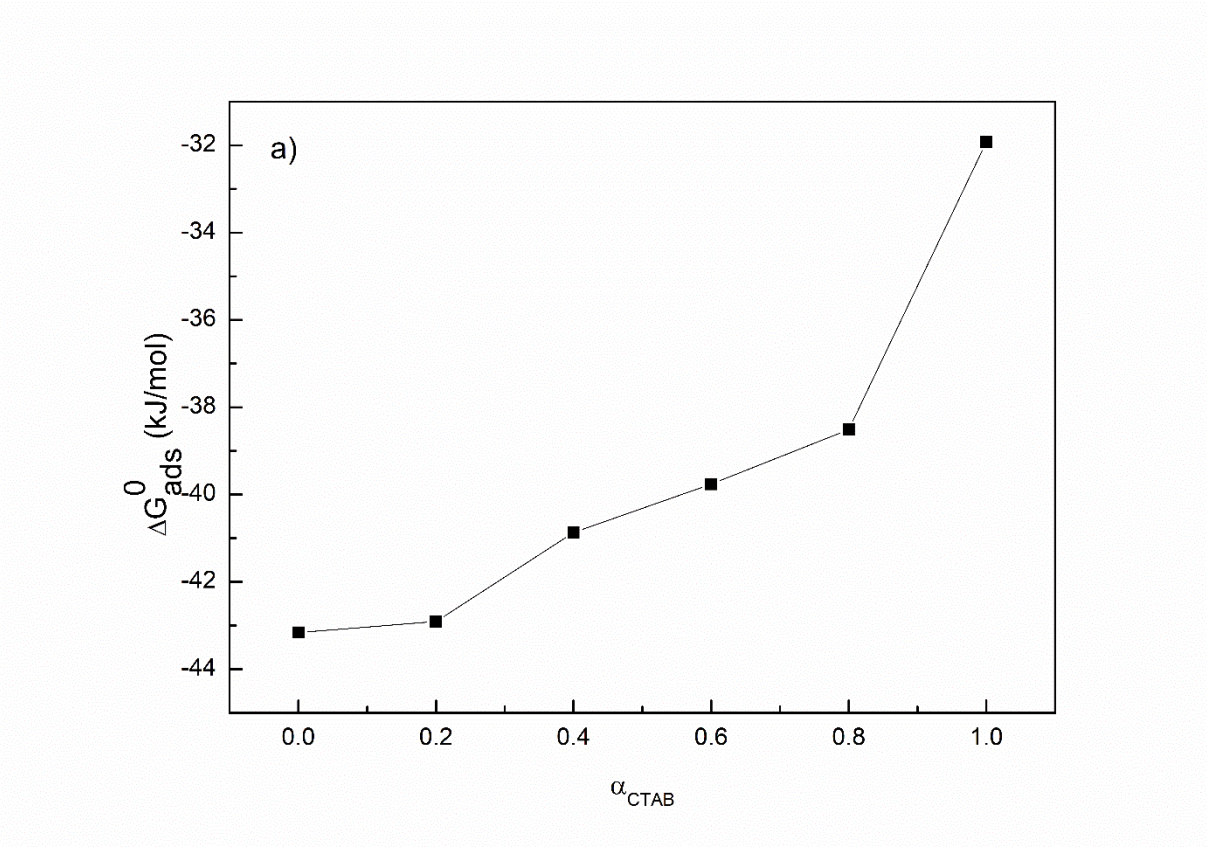

Figure S10a. The plot of the standard Gibbs free energy of adsorption (ΔG^0_{ads}) of CTAB+TX100 mixtures vs. the mole fraction of CTAB in the bulk phase (α).

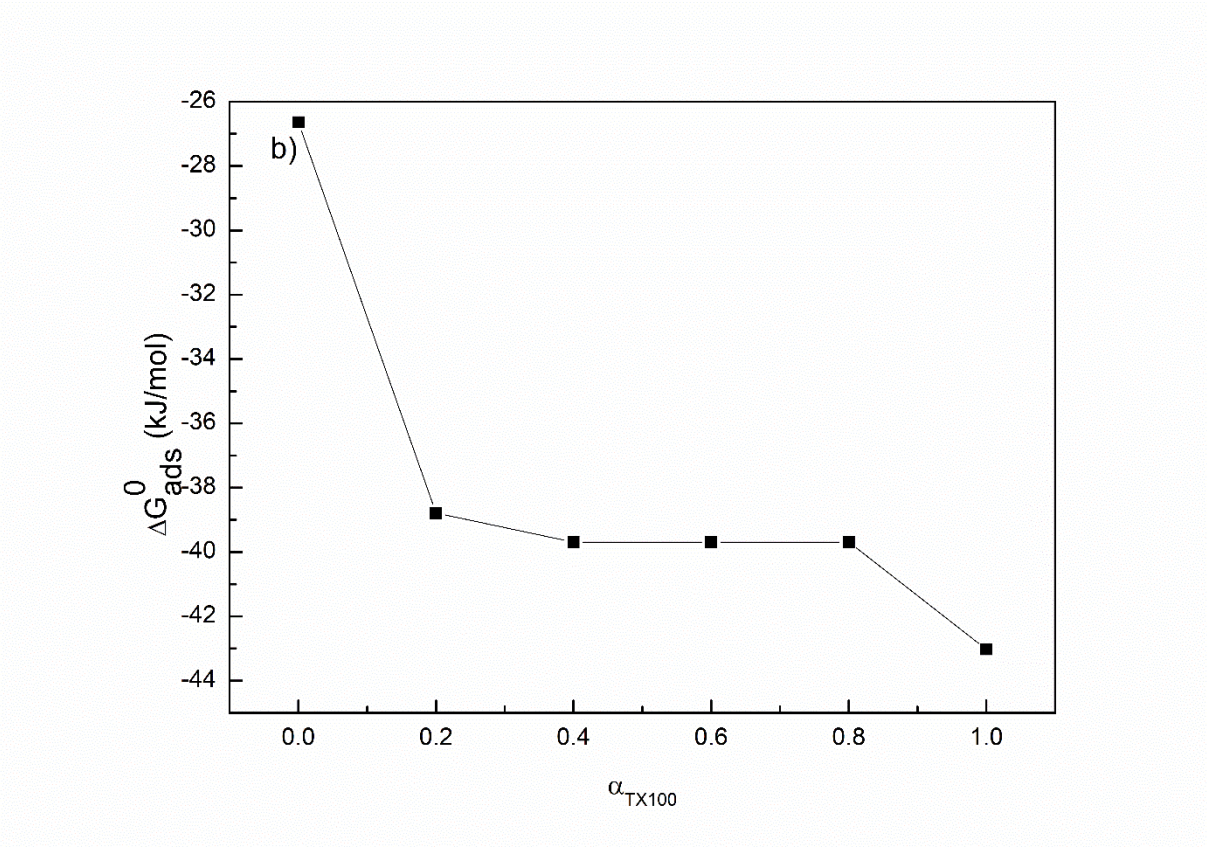

Figure S10b. The plot of the standard Gibbs free energy of adsorption (ΔG^0_{ads})of SDDS+TX100 mixtures vs. the mole fraction of TX100 in the bulk phase (α).

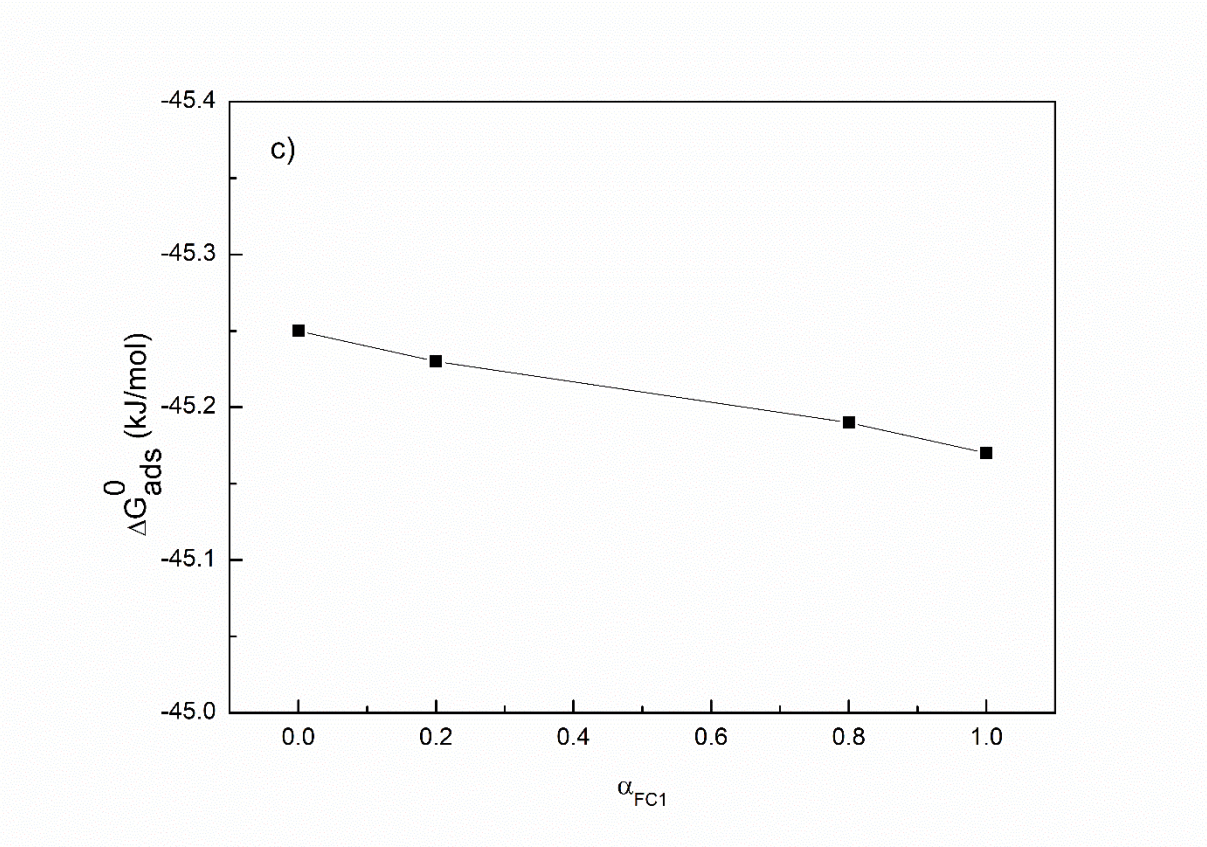

Figure S10c. The plot of the standard Gibbs free energy of adsorption (ΔG^0_{ads}) of FC1+TX165 mixtures vs. the mole fraction of FC1 in the bulk phase (α).

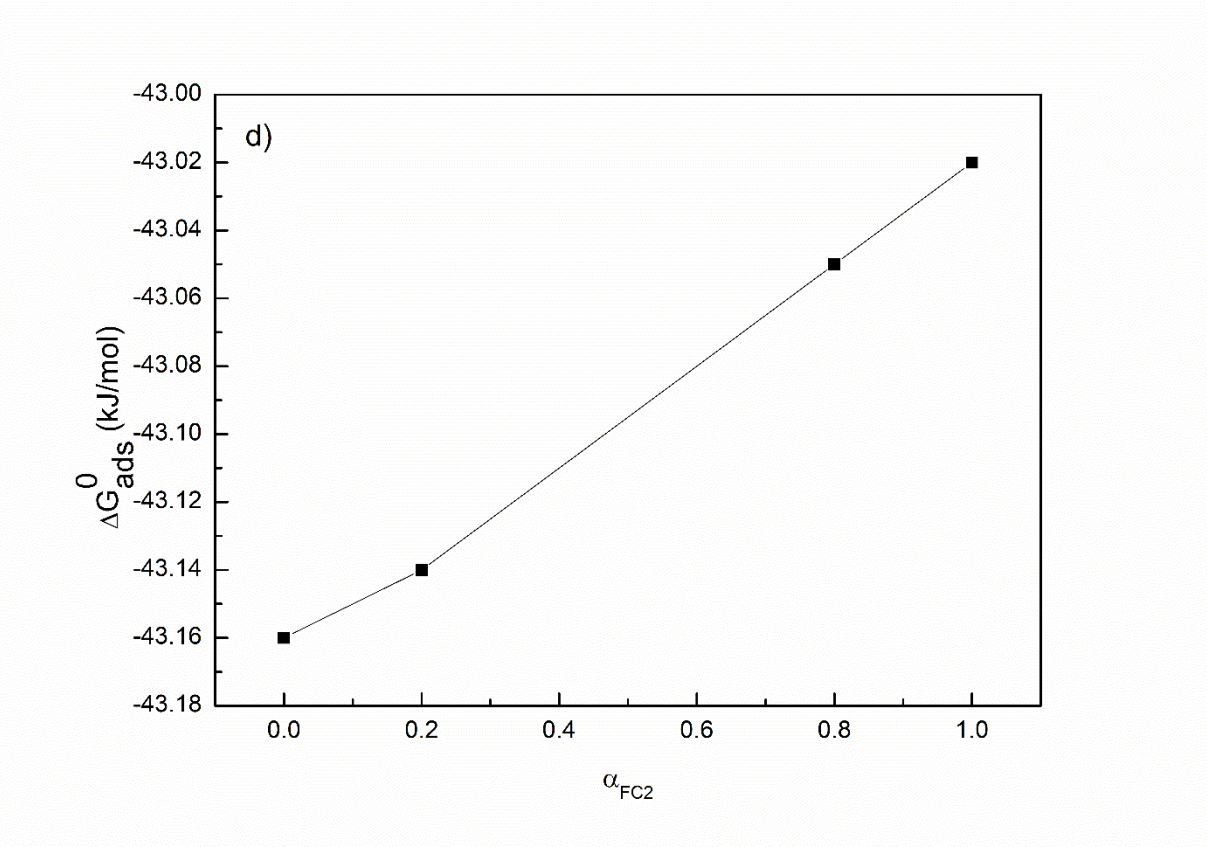

Figure S10d. The plot of the standard Gibbs free energy of adsorption (ΔG^0_{ads}) of FC2+TX100 mixtures vs. the mole fraction of FC2 in the bulk phase (α).

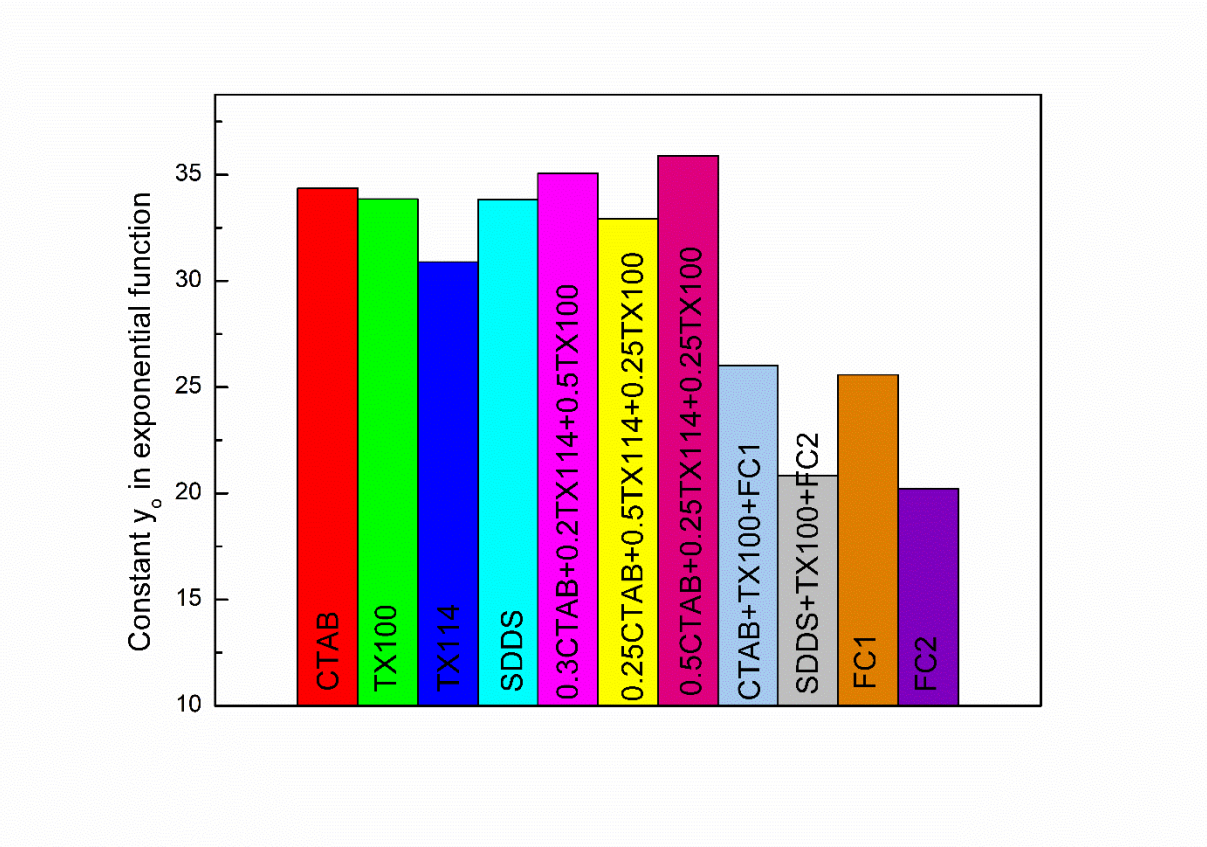

Figure S11. The values of the constant y_0 in the exponential function of the second order for CTAB, TX100, TX114, SDDS, CTAB+TX100+TX114, CTAB+TX100+FC1, SDDS+TX100+FC2, FC1 and FC2.

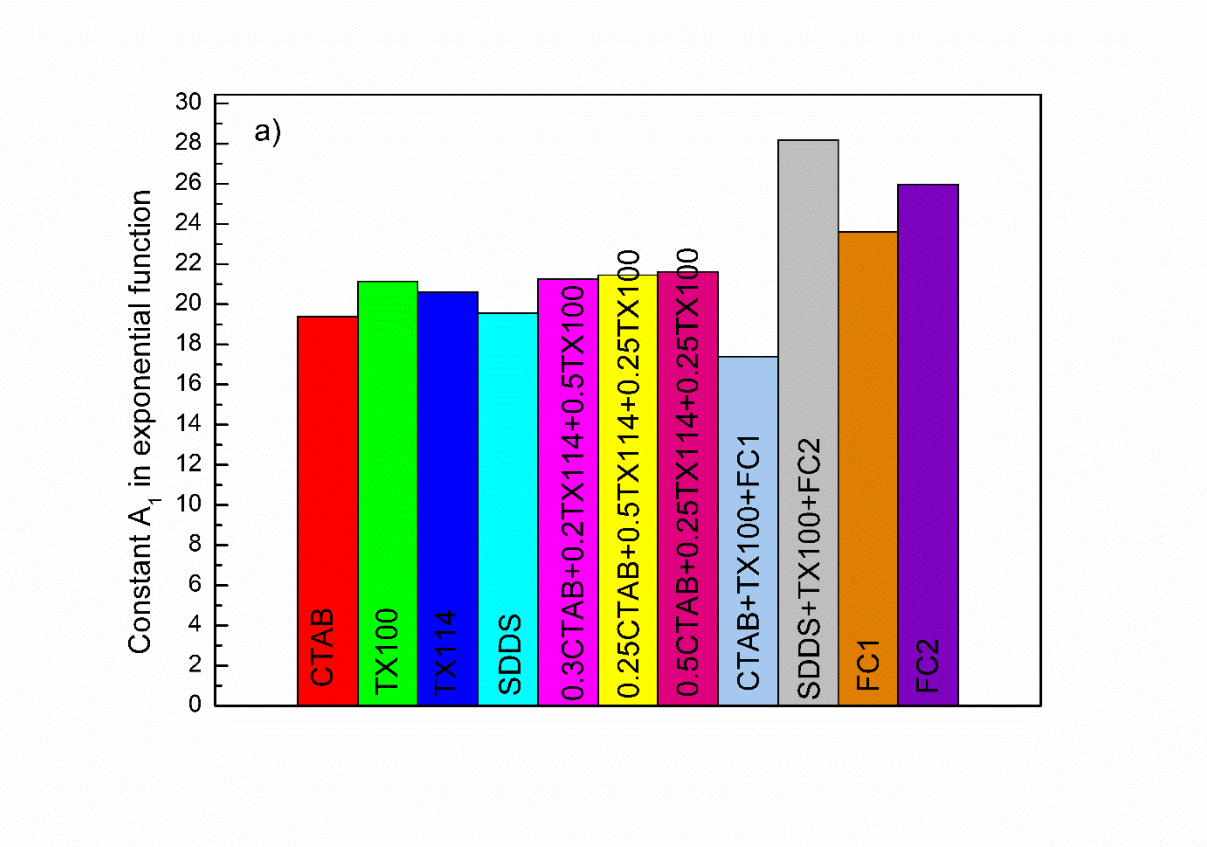

Figure S12a. The values of the constantA_1 in the exponential function of the second order for CTAB, TX100, TX114, SDDS, CTAB+TX100+TX114, CTAB+TX100+FC1, SDDS+TX100+FC2, FC1 and FC2.

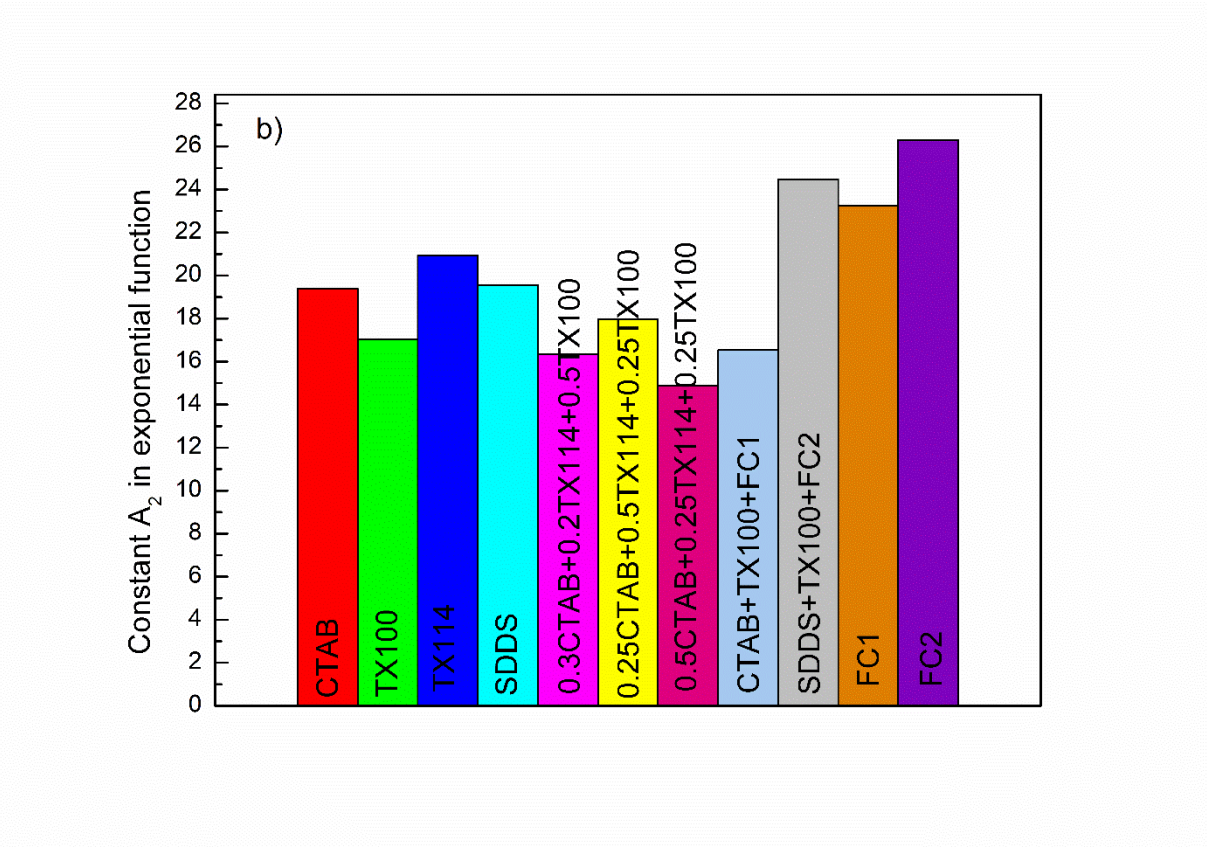

Figure S12b. The values of the constantA_2 in the exponential function of the second order for CTAB, TX100, TX114, SDDS, CTAB+TX100+TX114, CTAB+TX100+FC1, SDDS+TX100+FC2, FC1 and FC2.

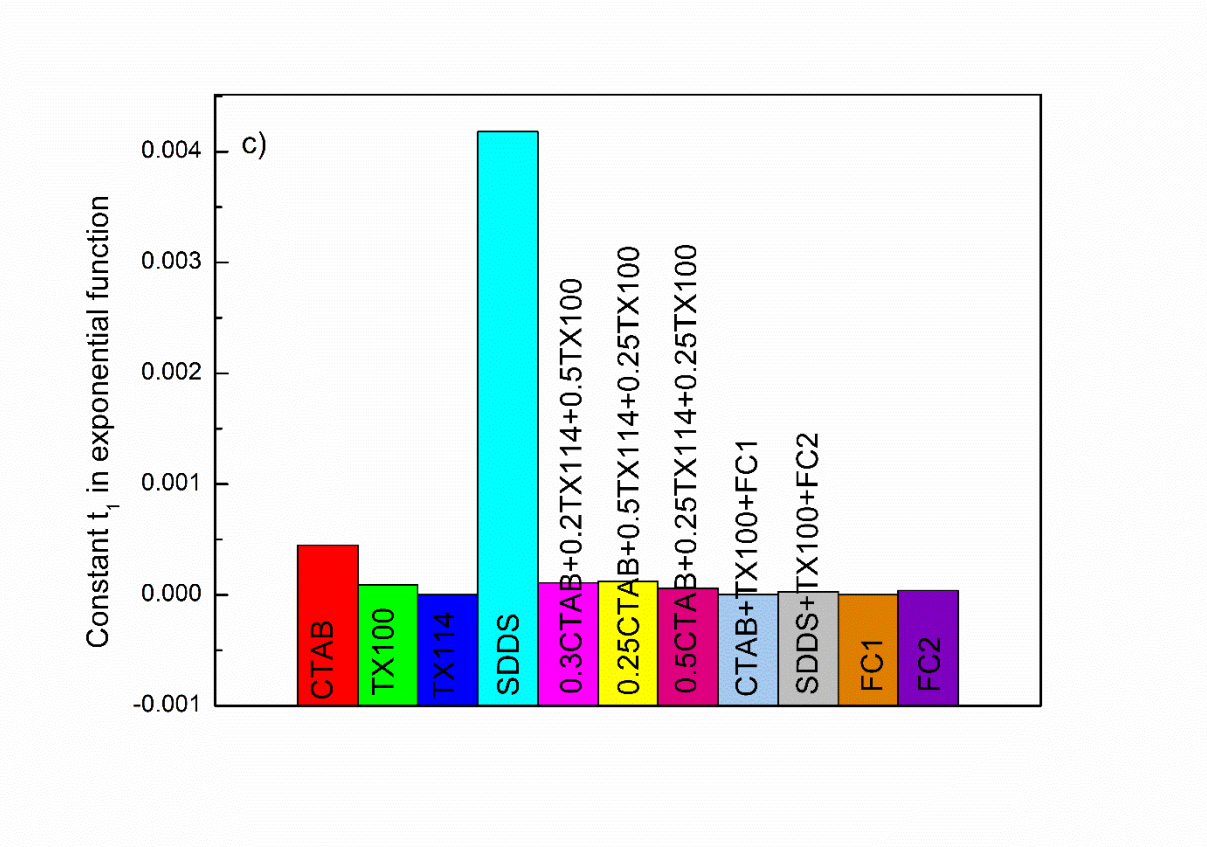

Figure S12c. The values of the constant t_1 in the exponential function of the second order for CTAB, TX100, TX114, SDDS, CTAB+TX100+TX114, CTAB+TX100+FC1, SDDS+TX100+FC2, FC1 and FC2.

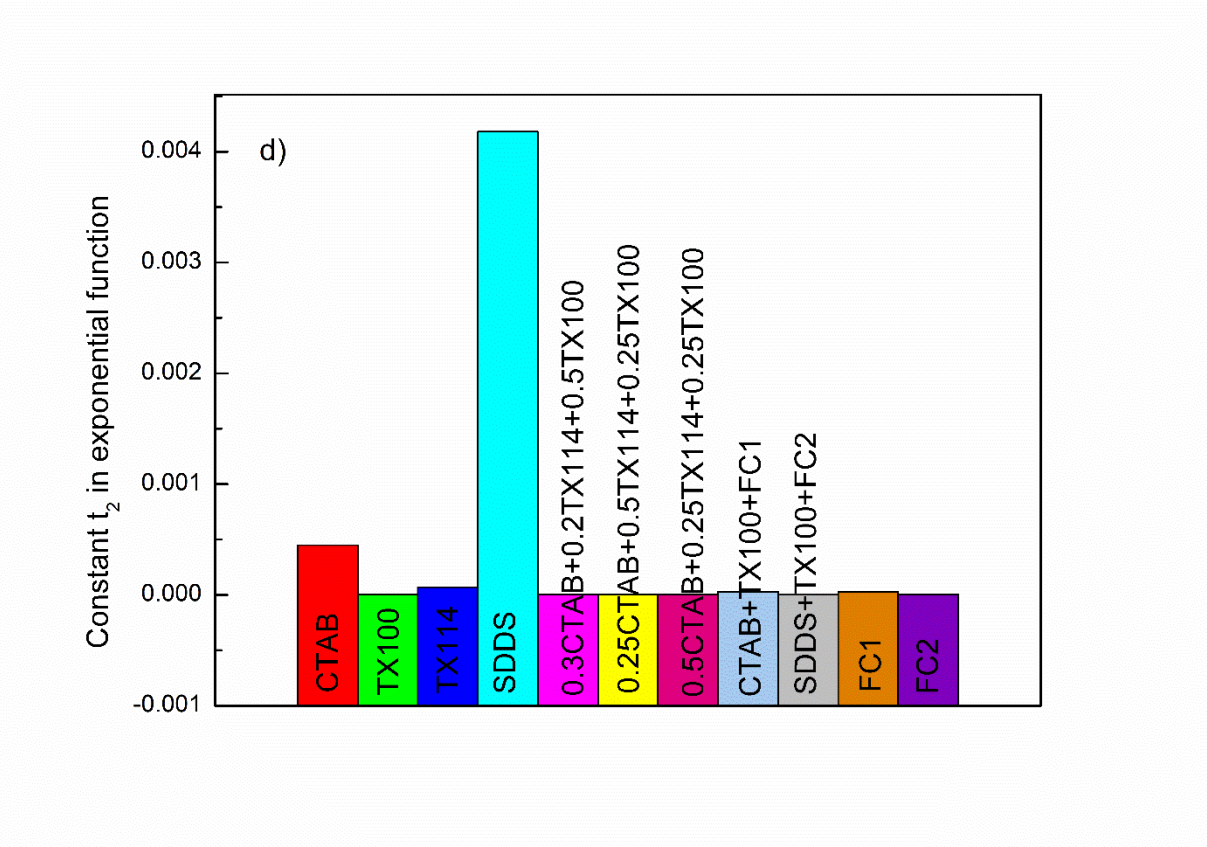

Figure S12d. The values of the constant t_2 in the exponential function of the second order for CTAB, TX100, TX114, SDDS, CTAB+TX100+TX114, CTAB+TX100+FC1, SDDS+TX100+FC2, FC1 and FC2.

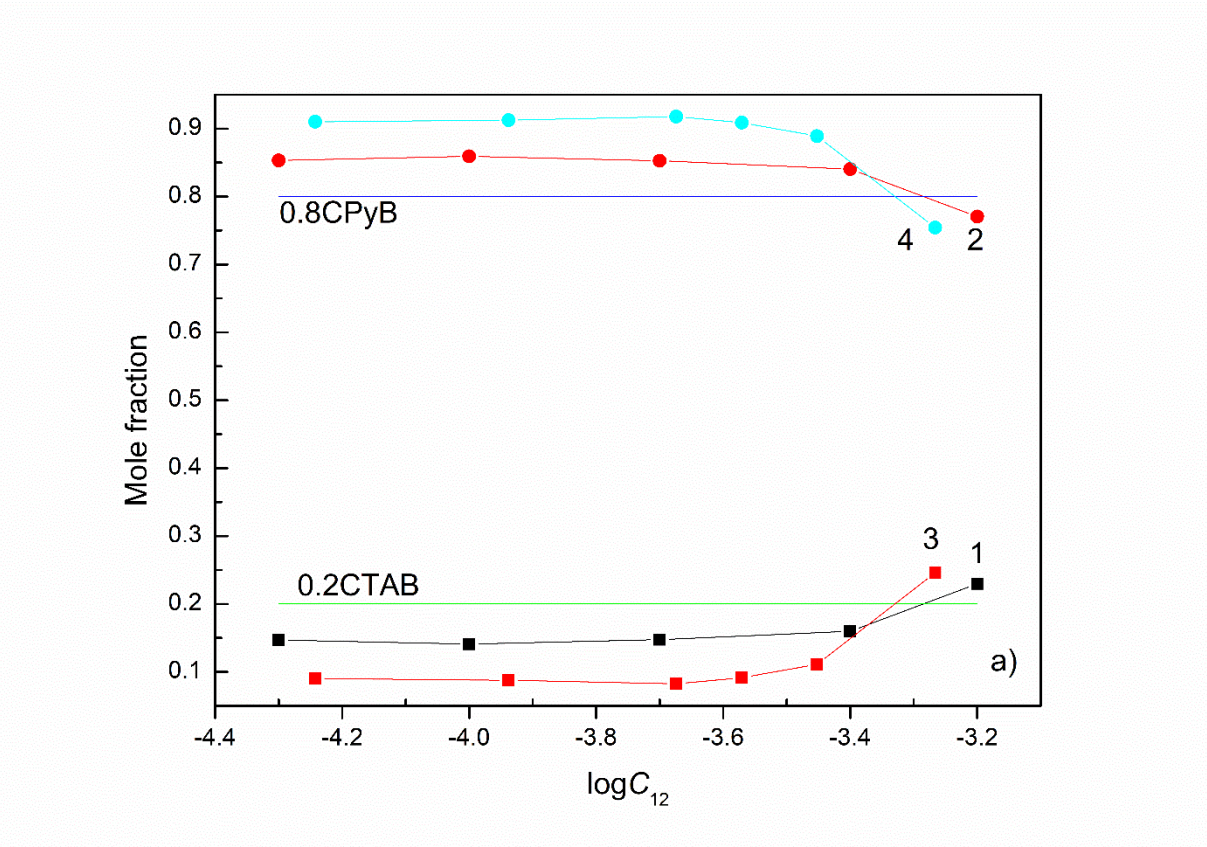

Figure S13a. The comparison of the mole fraction of the mixed surface layer formed by CTAB+CPyB at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

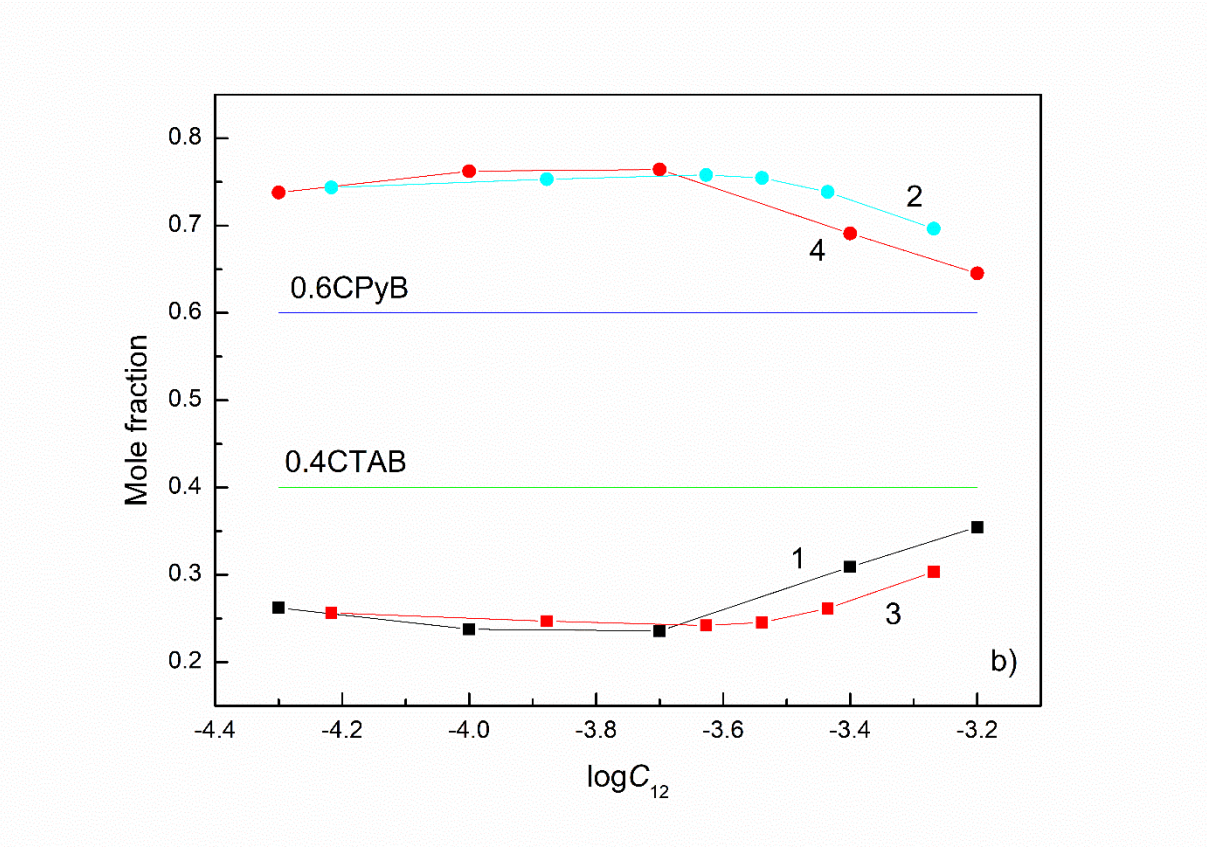

Figure S13b. The comparison of the mole fraction of the mixed surface layer formed by CTAB+CPyB at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

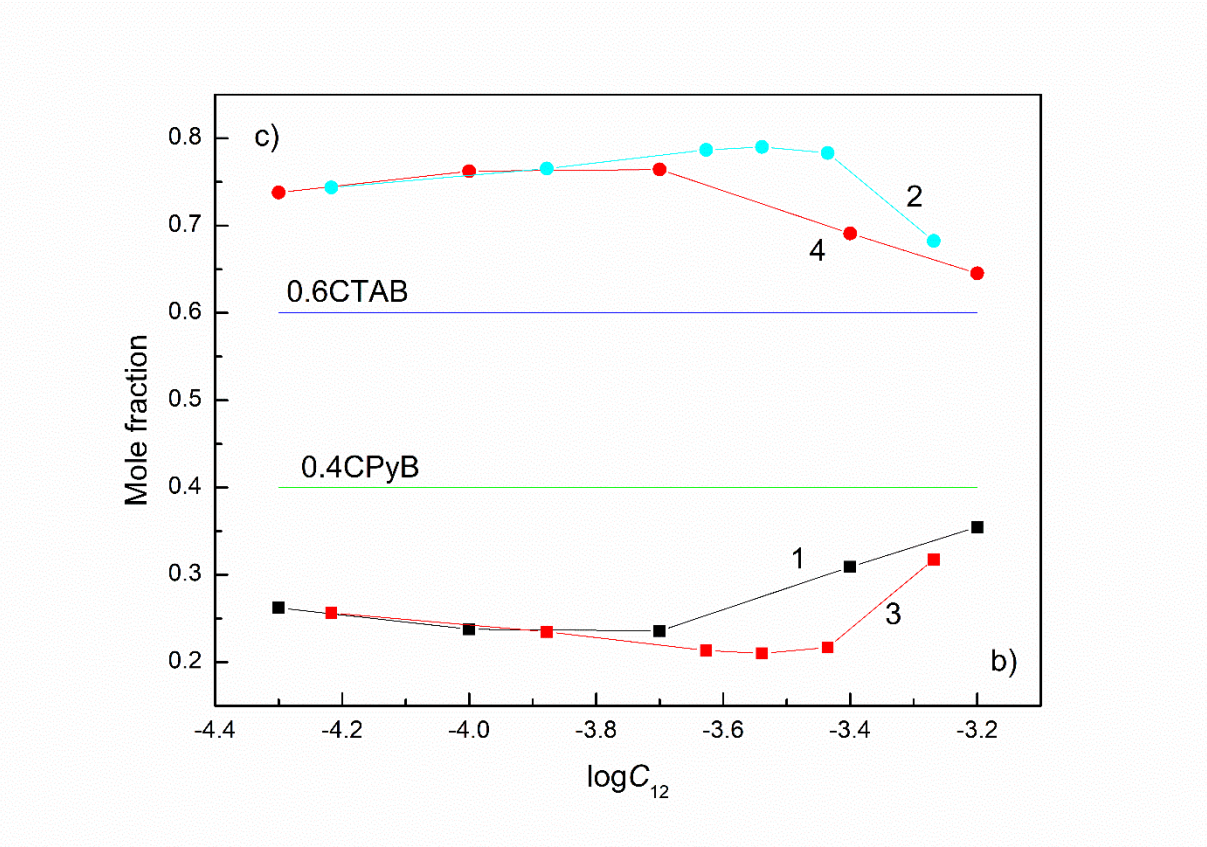

Figure S13c. The comparison of the mole fraction of the mixed surface layer formed by CTAB+CPyB at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

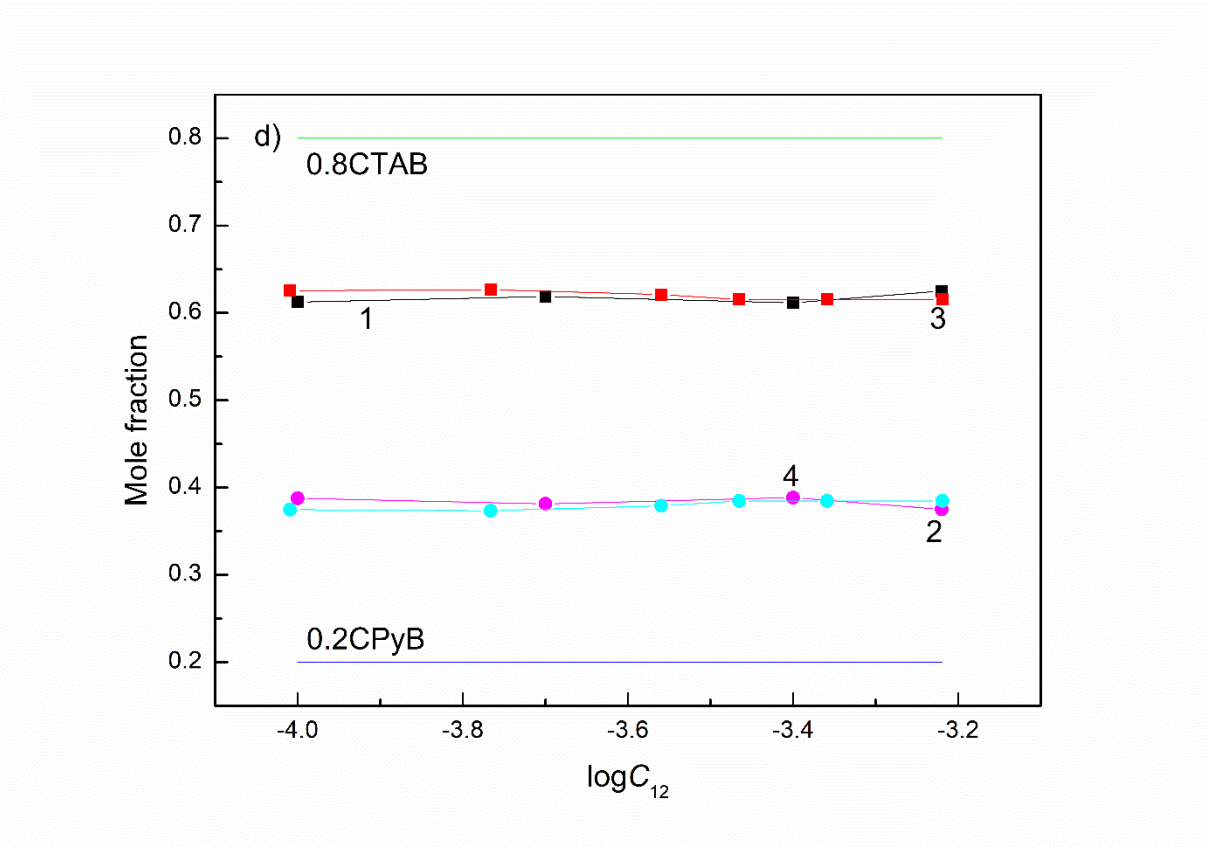

Figure S13d. The comparison of the mole fraction of the mixed surface layer formed by CTAB+CPyB at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

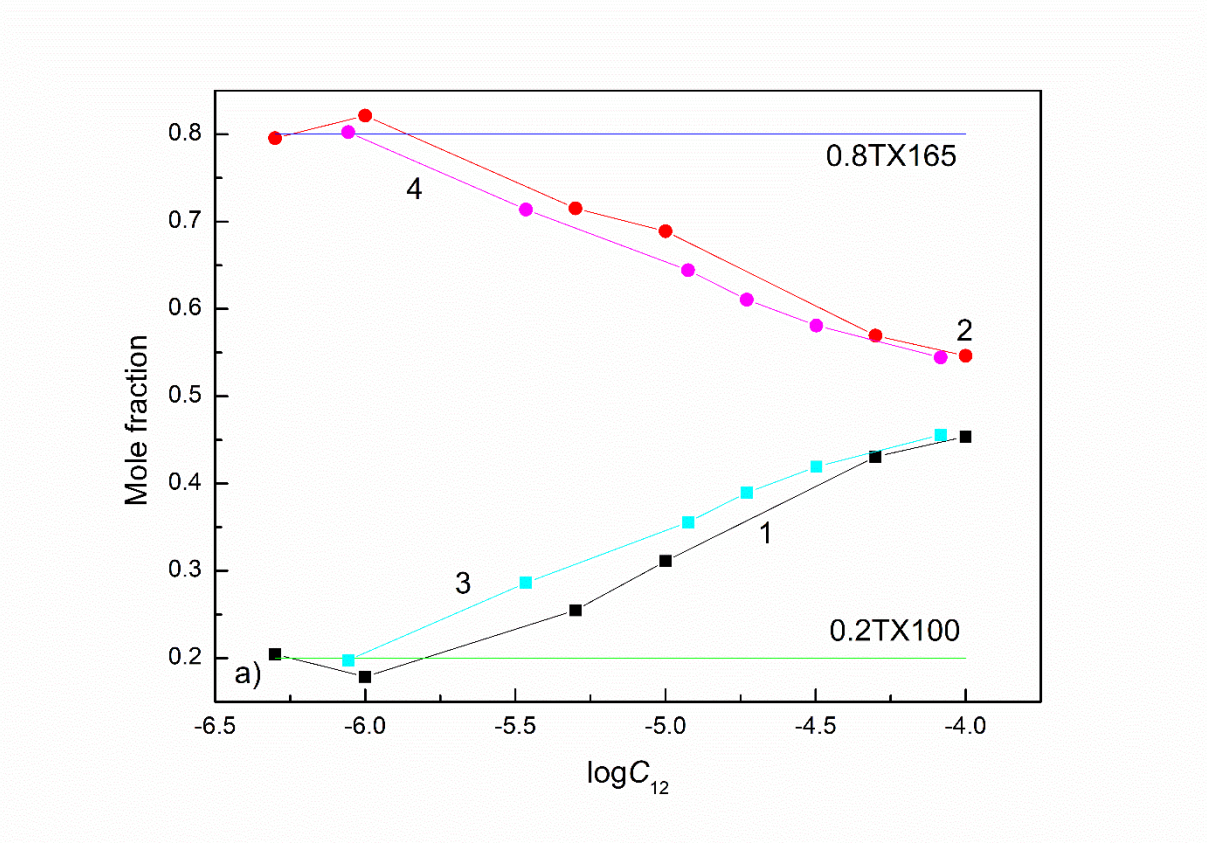

Figure S14a. The comparison of the mole fraction of the mixed surface layer formed by TX100+TX165 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

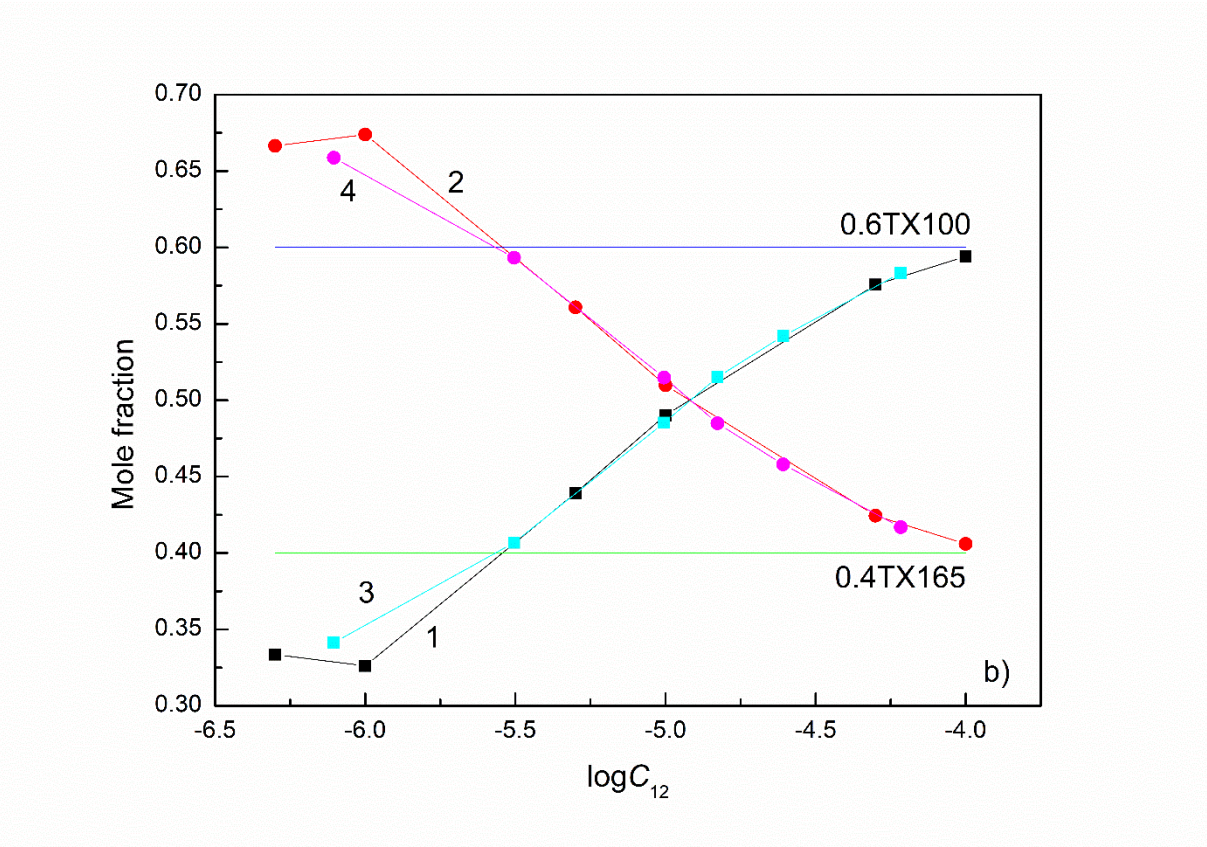

Figure S14b. The comparison of the mole fraction of the mixed surface layer formed by TX100+TX165 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

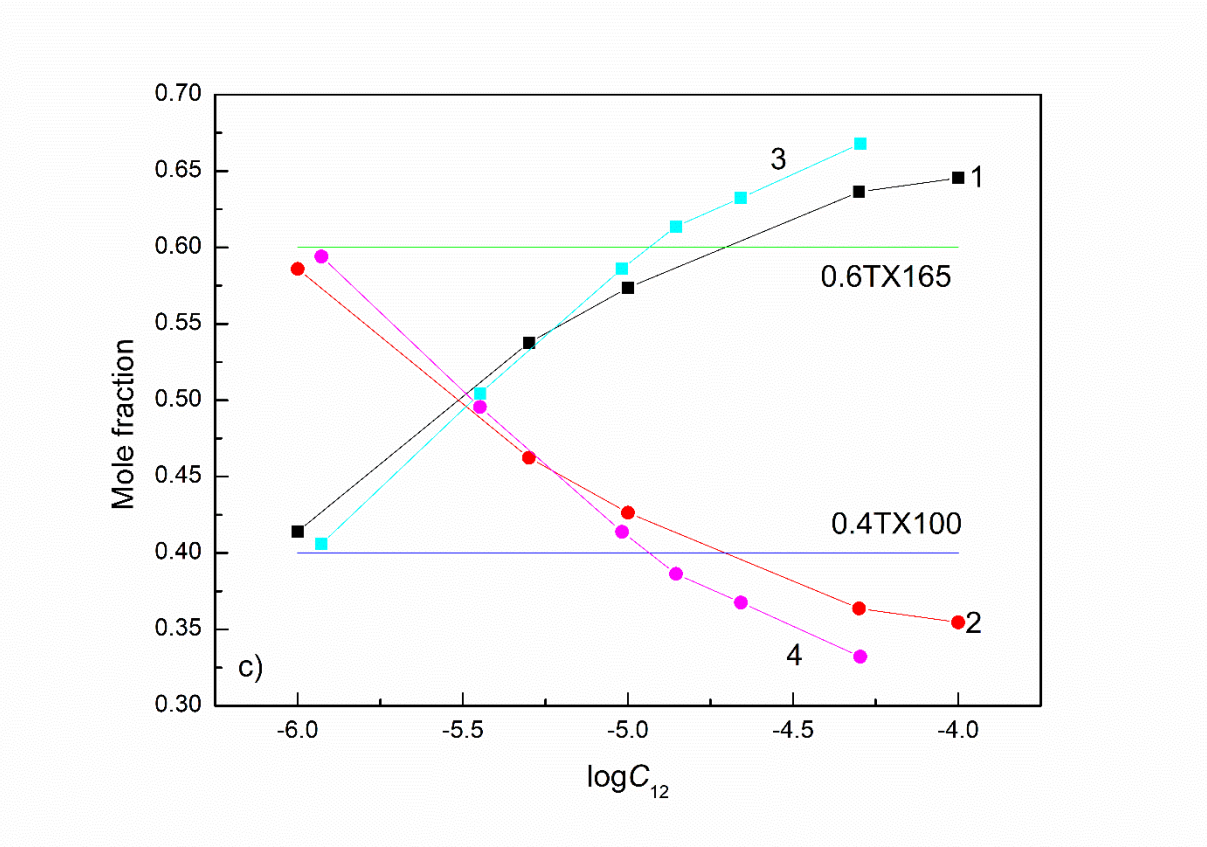

Figure S14c. The comparison of the mole fraction of the mixed surface layer formed by TX100+TX165 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

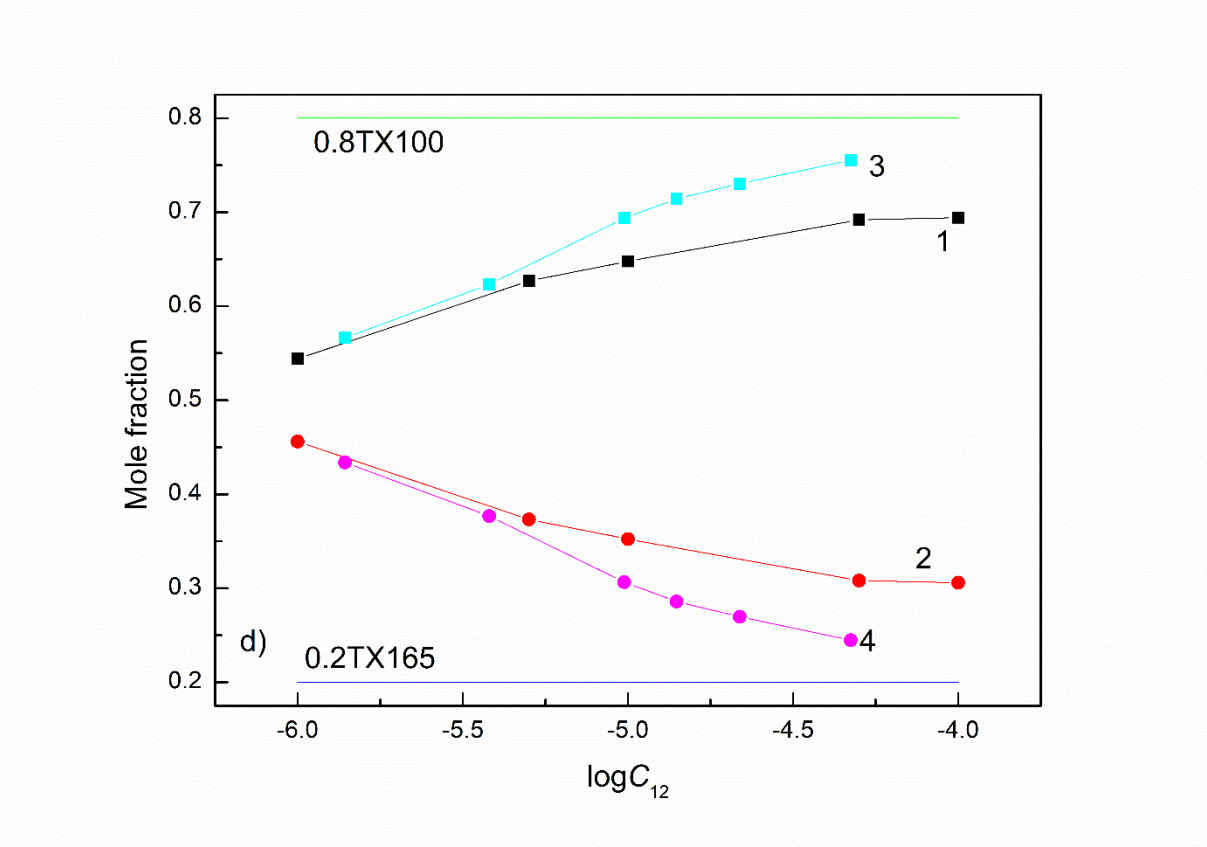

Figure S14d. The comparison of the mole fraction of the mixed surface layer formed by TX100+TX165 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

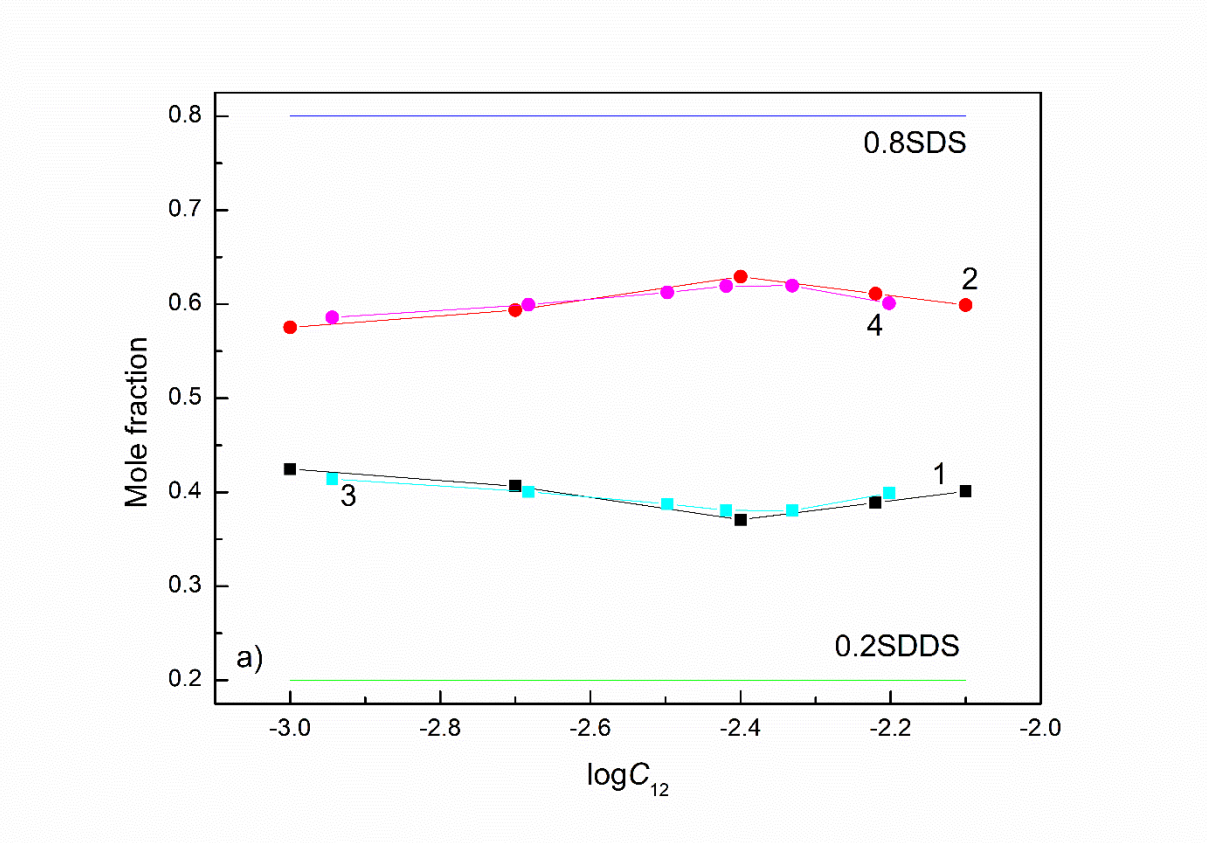

Figure S15a. The comparison of the mole fraction of the mixed surface layer formed by SDDS+SDS at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

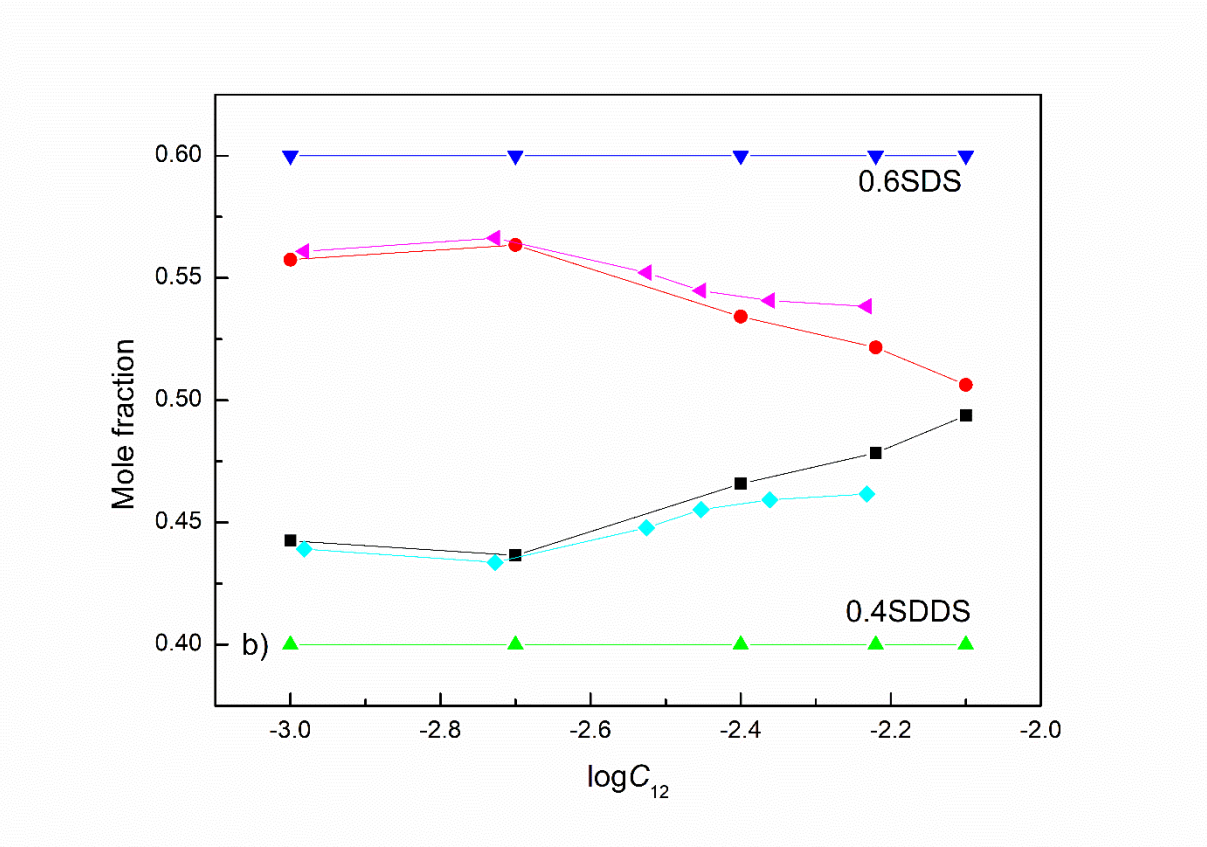

Figure S15b. The comparison of the mole fraction of the mixed surface layer formed by SDDS+SDS at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

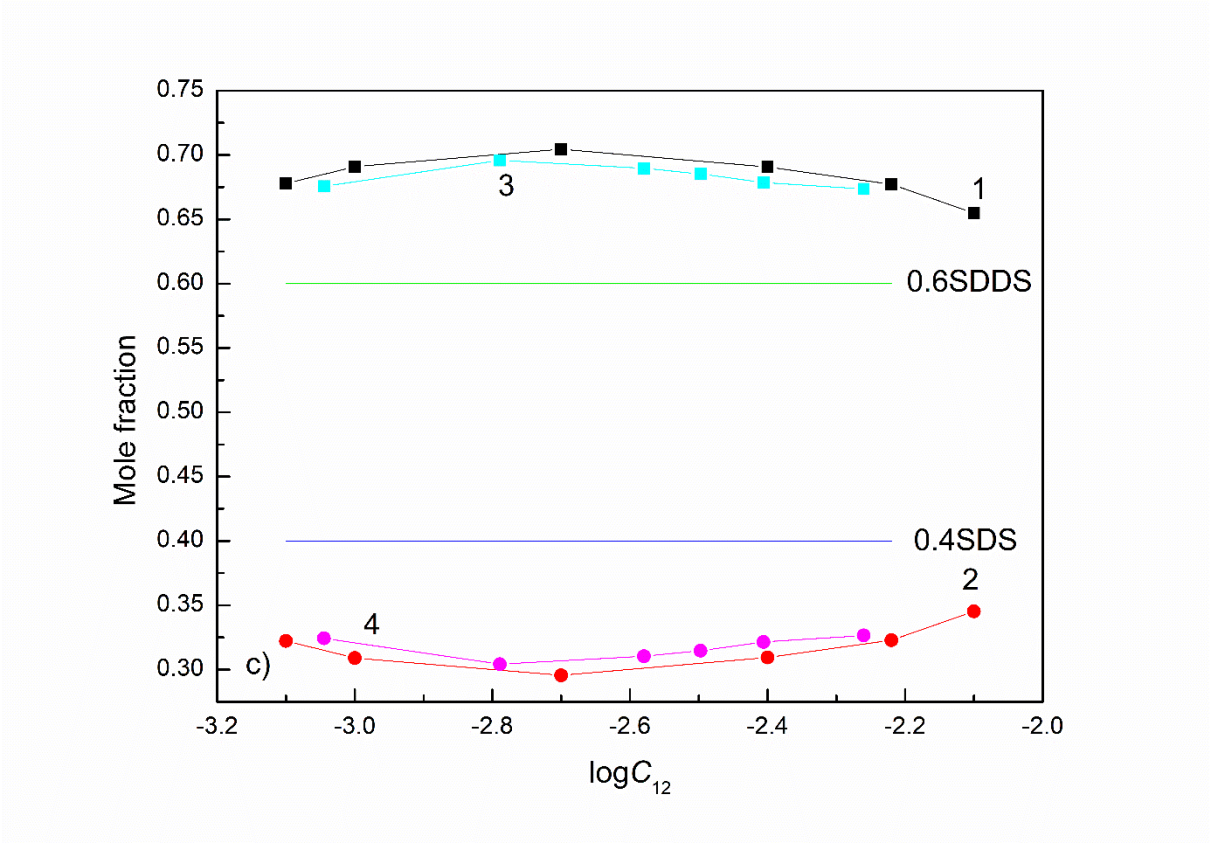

Figure S15c. The comparison of the mole fraction of the mixed surface layer formed by SDDS+SDS at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

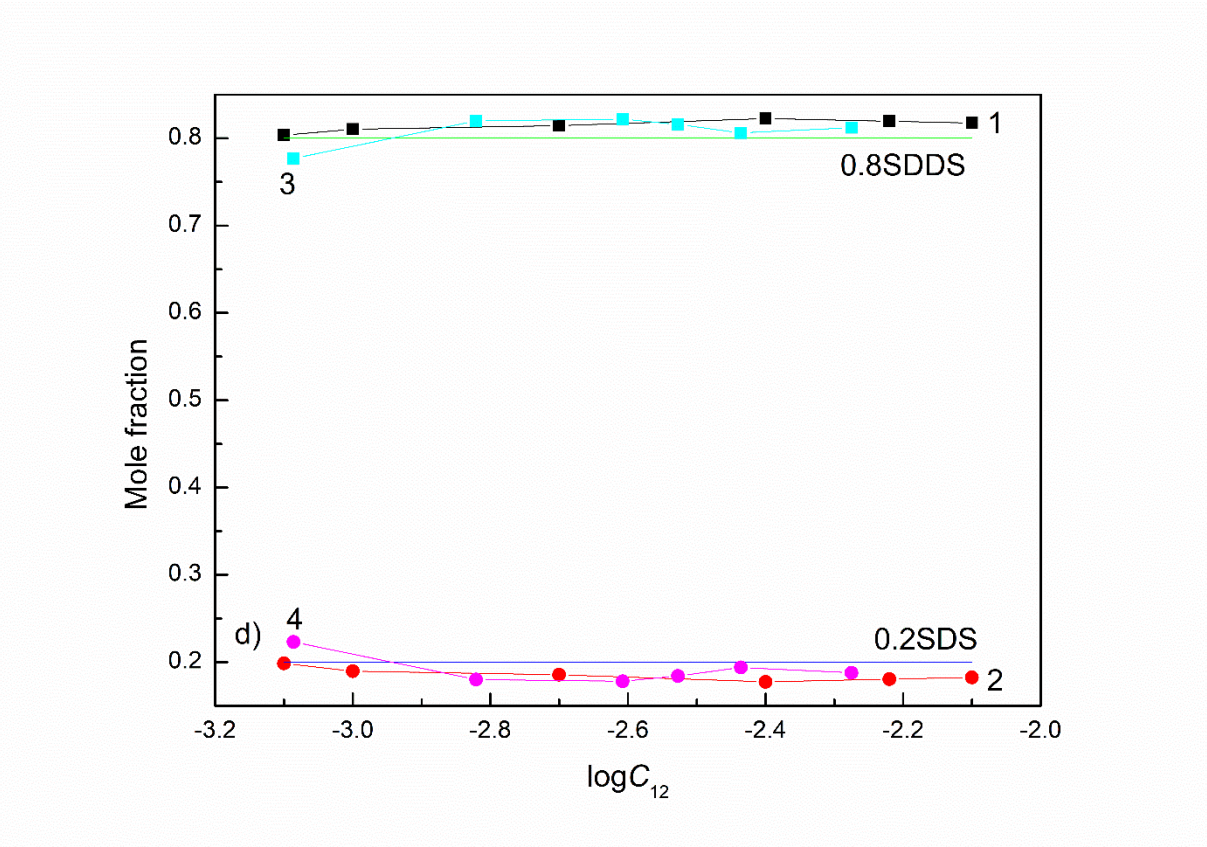

Figure S15d. The comparison of the mole fraction of the mixed surface layer formed by SDDS+SDS at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

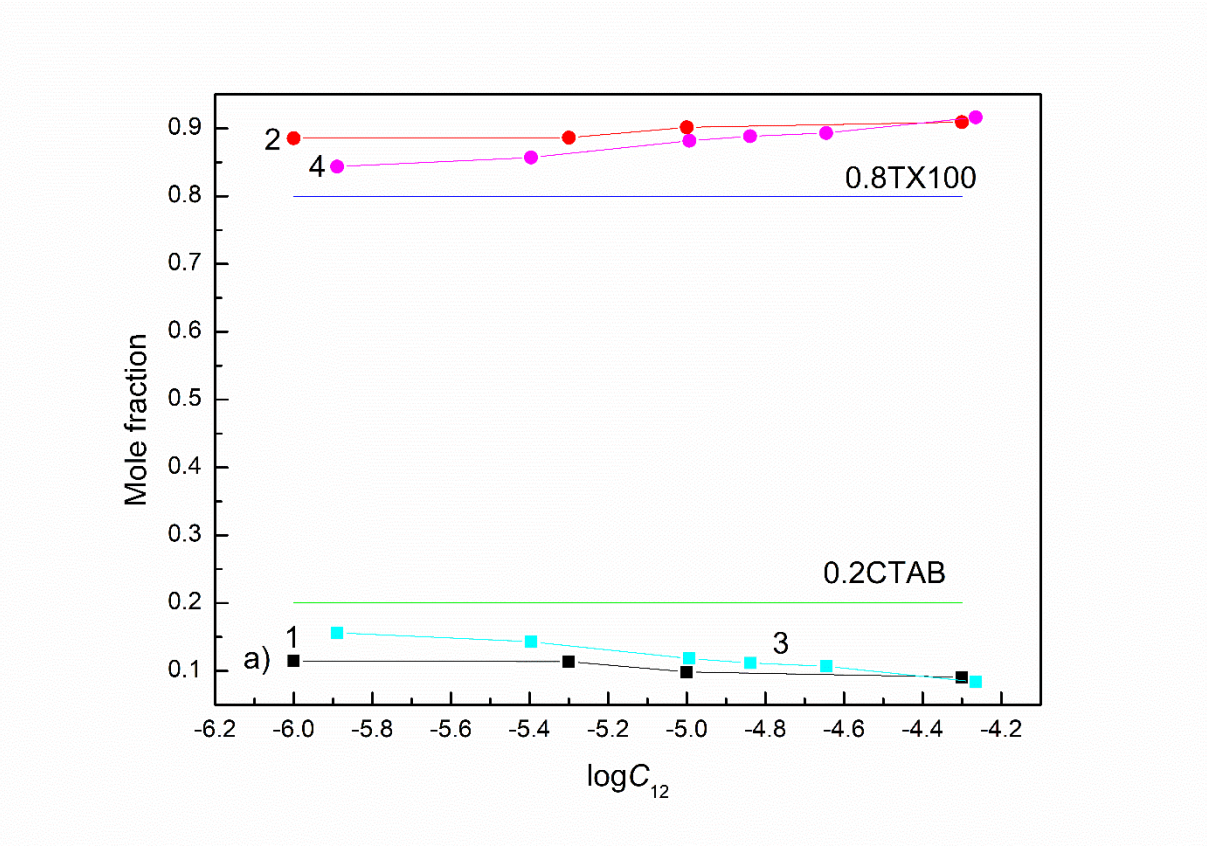

Figure S16a. The comparison of the mole fraction of the mixed surface layer formed by CTAB+TX100 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

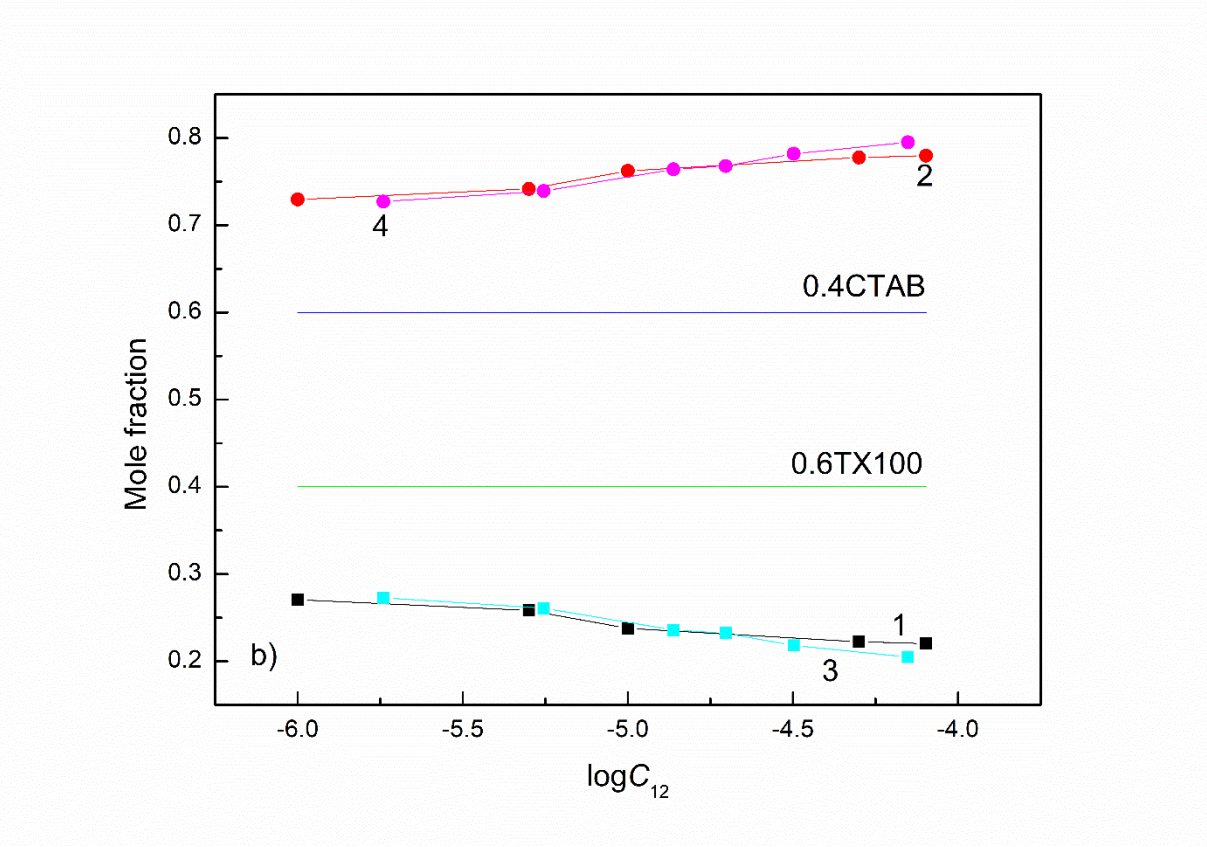

Figure S16b. The comparison of the mole fraction of the mixed surface layer formed by CTAB+TX100 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

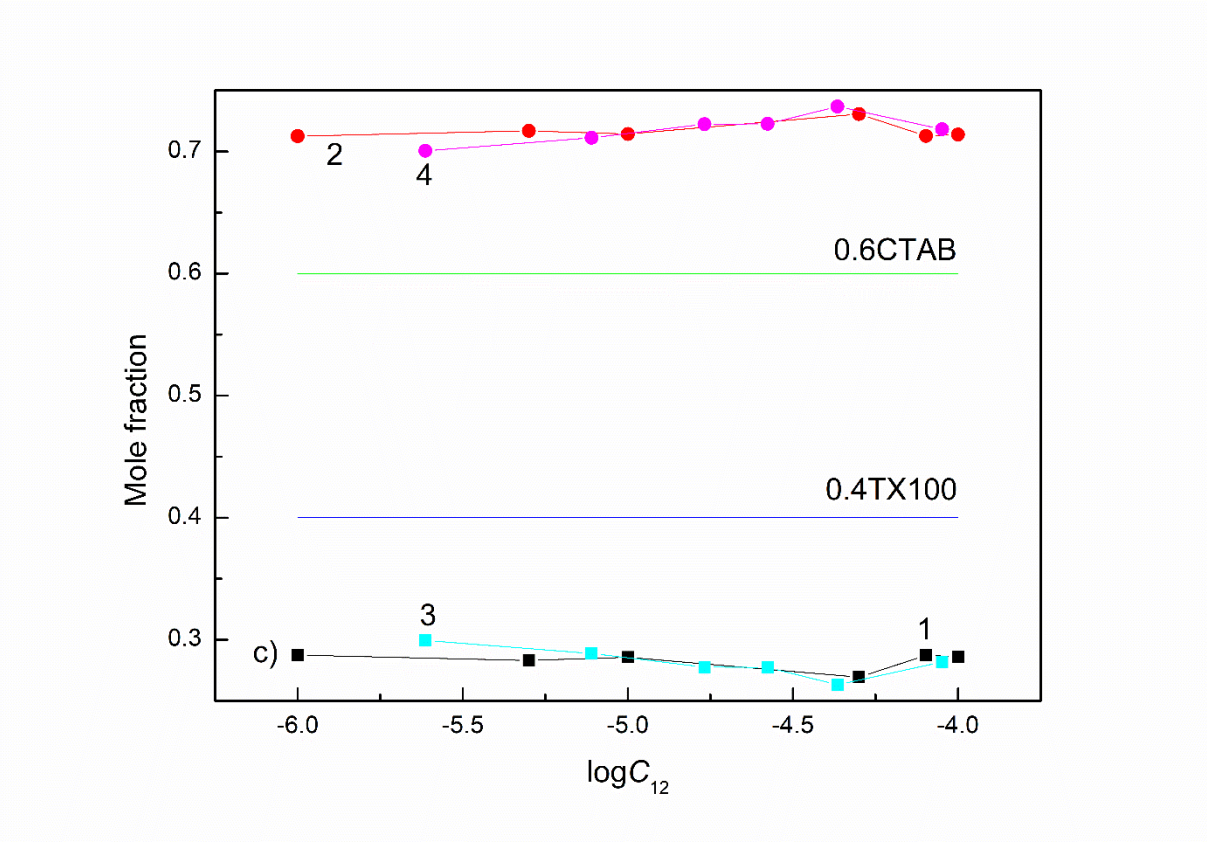

Figure S16c. The comparison of the mole fraction of the mixed surface layer formed by CTAB+TX100 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

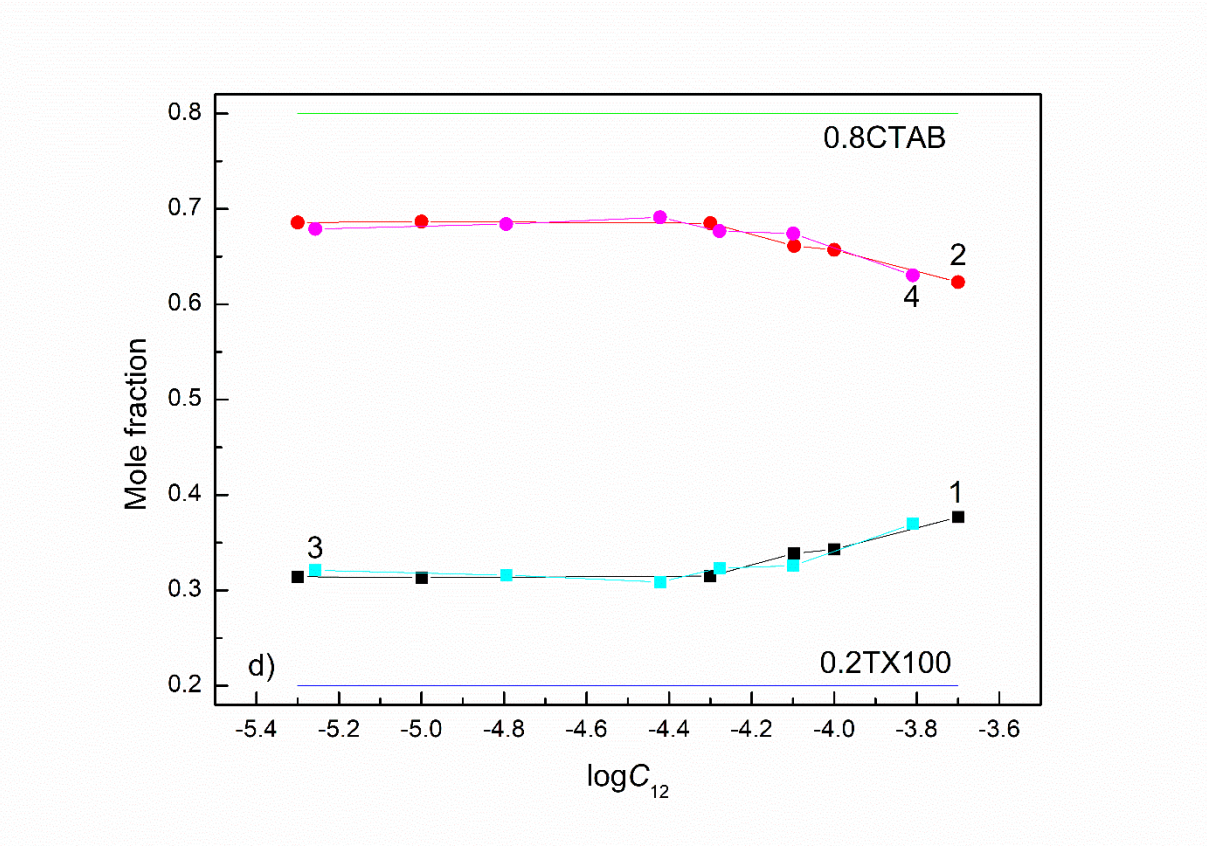

Figure S16d. The comparison of the mole fraction of the mixed surface layer formed by CTAB+TX100 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

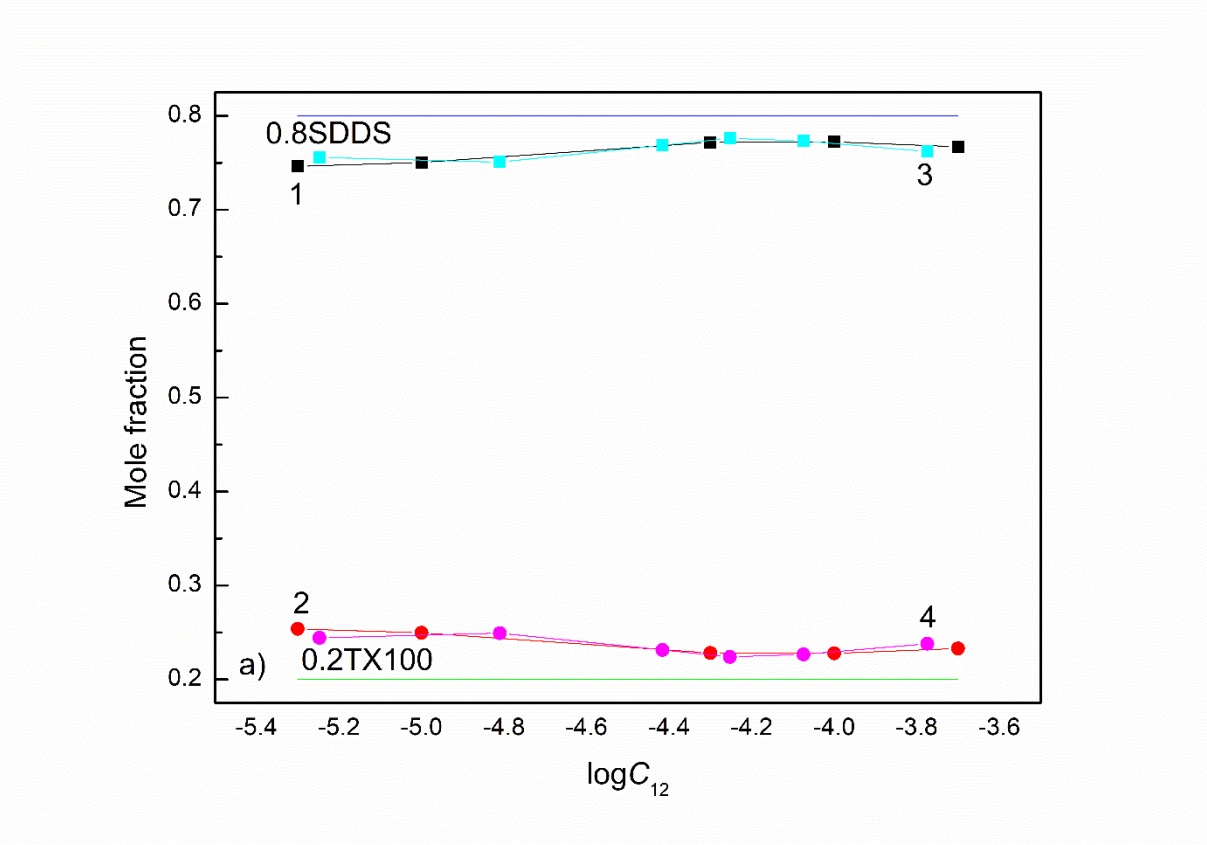

Figure S17a. The comparison of the mole fraction of the mixed surface layer formed by SDS+TX100 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

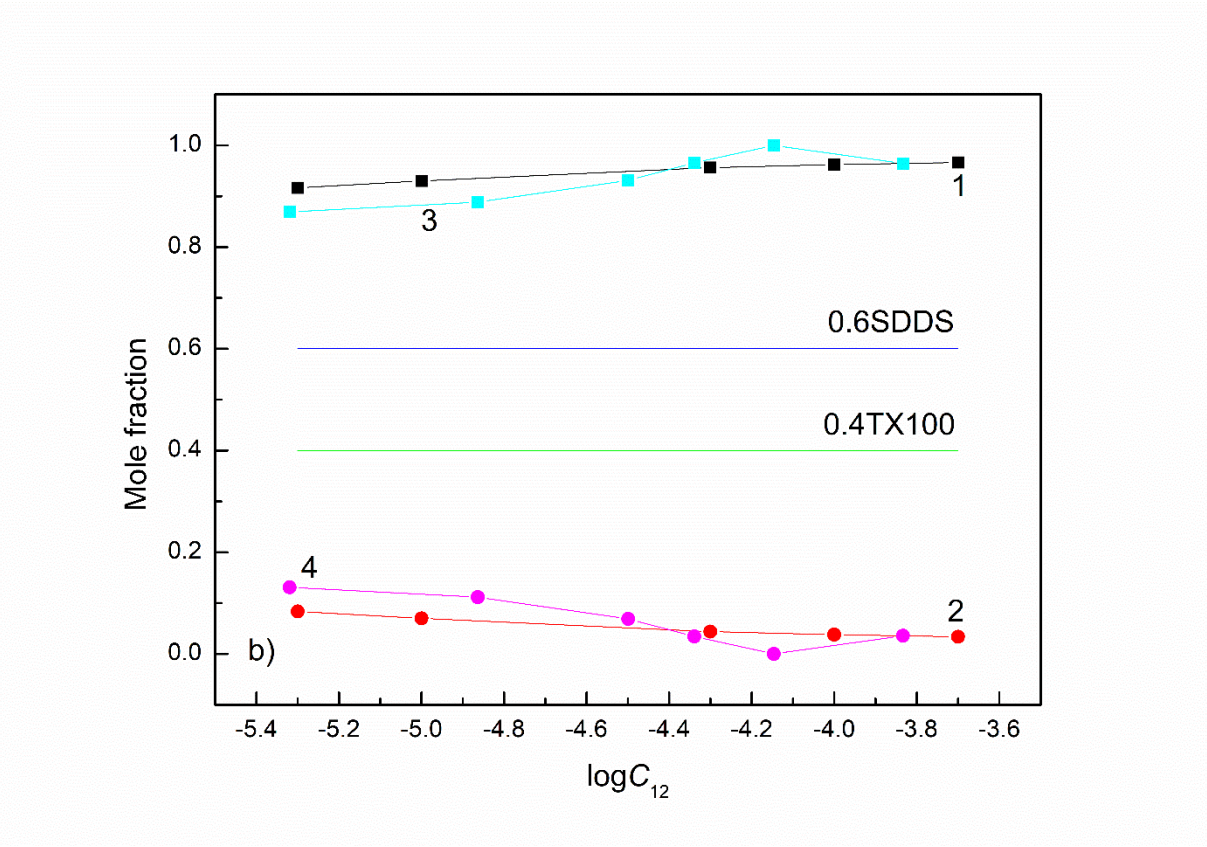

Figure S17b. The comparison of the mole fraction of the mixed surface layer formed by SDS+TX100 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

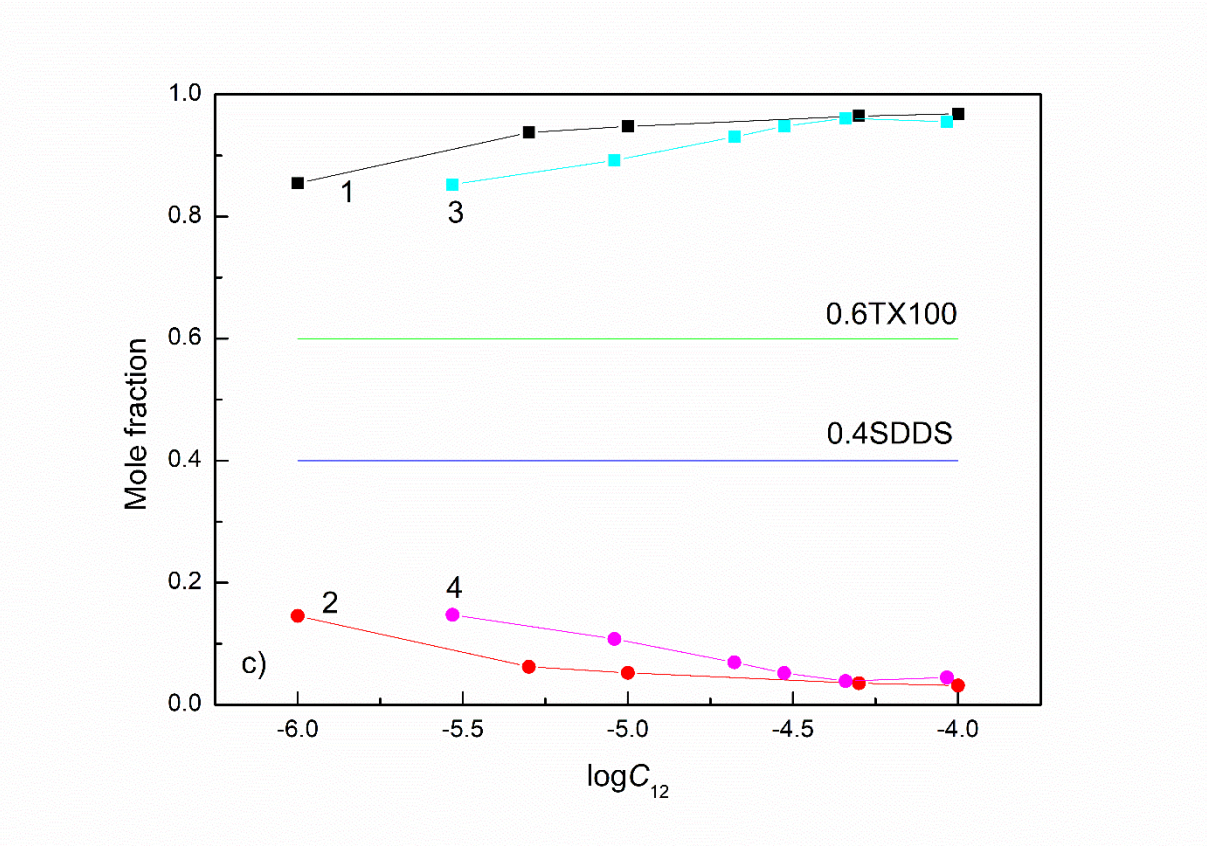

Figure S17c. The comparison of the mole fraction of the mixed surface layer formed by SDS+TX100 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

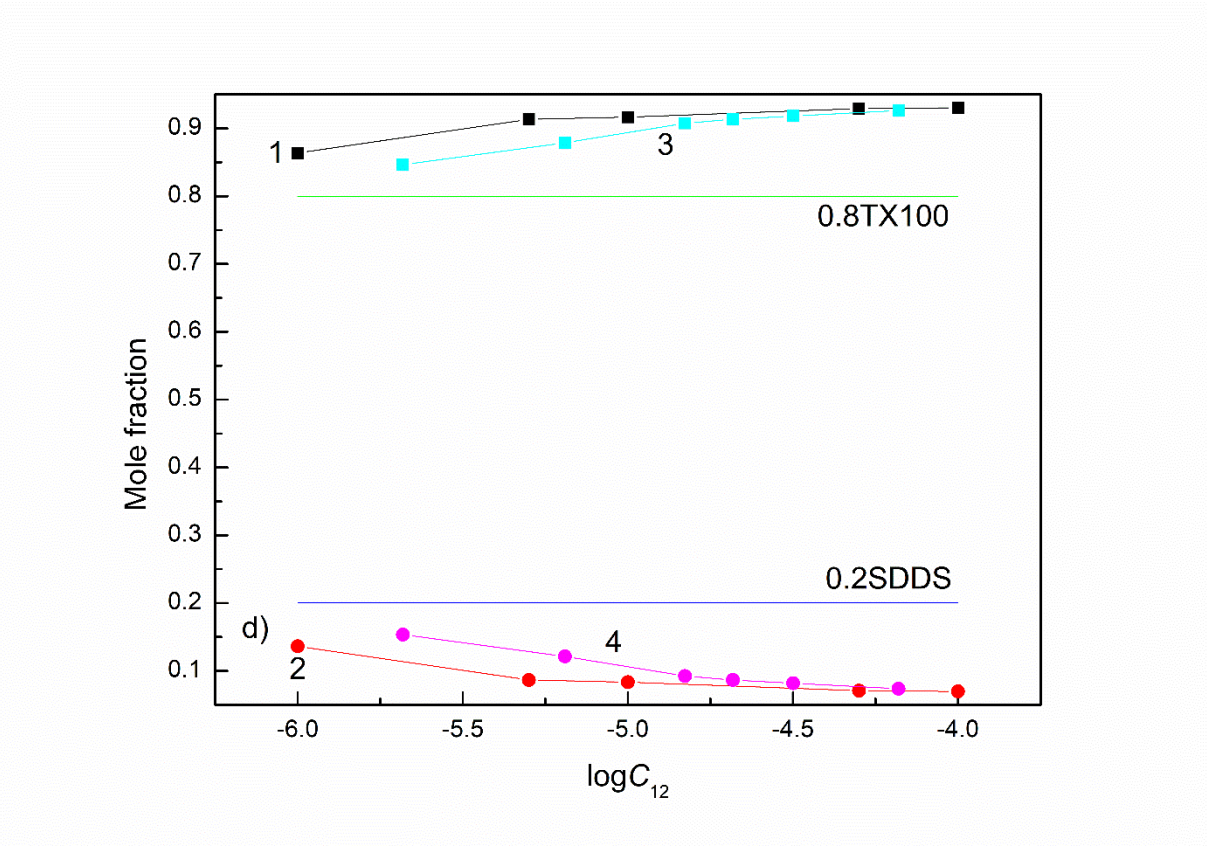

Figure S17d. The comparison of the mole fraction of the mixed surface layer formed by SDS+TX100 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

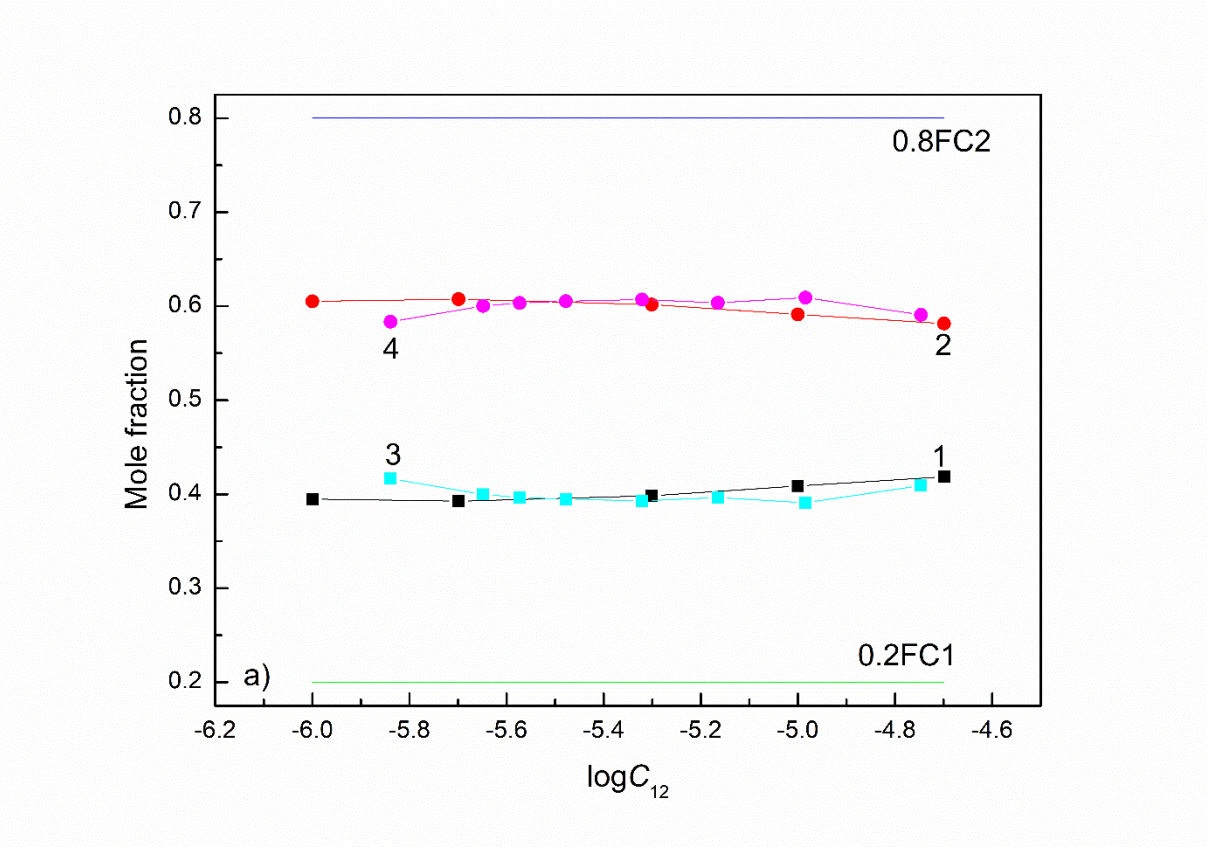

Figure S18a. The comparison of the mole fraction of the mixed surface layer formed by FC1+FC2 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

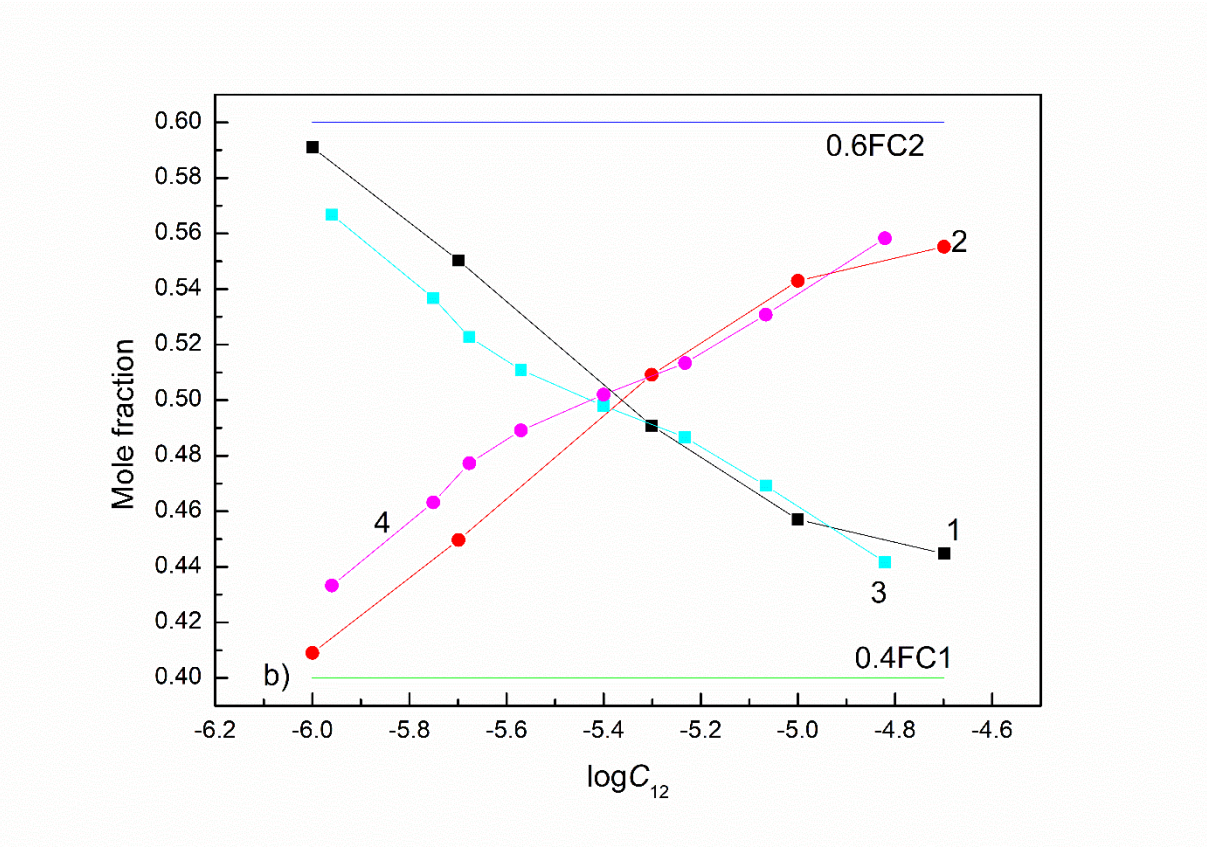

Figure S18b. The comparison of the mole fraction of the mixed surface layer formed by FC1+FC2 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

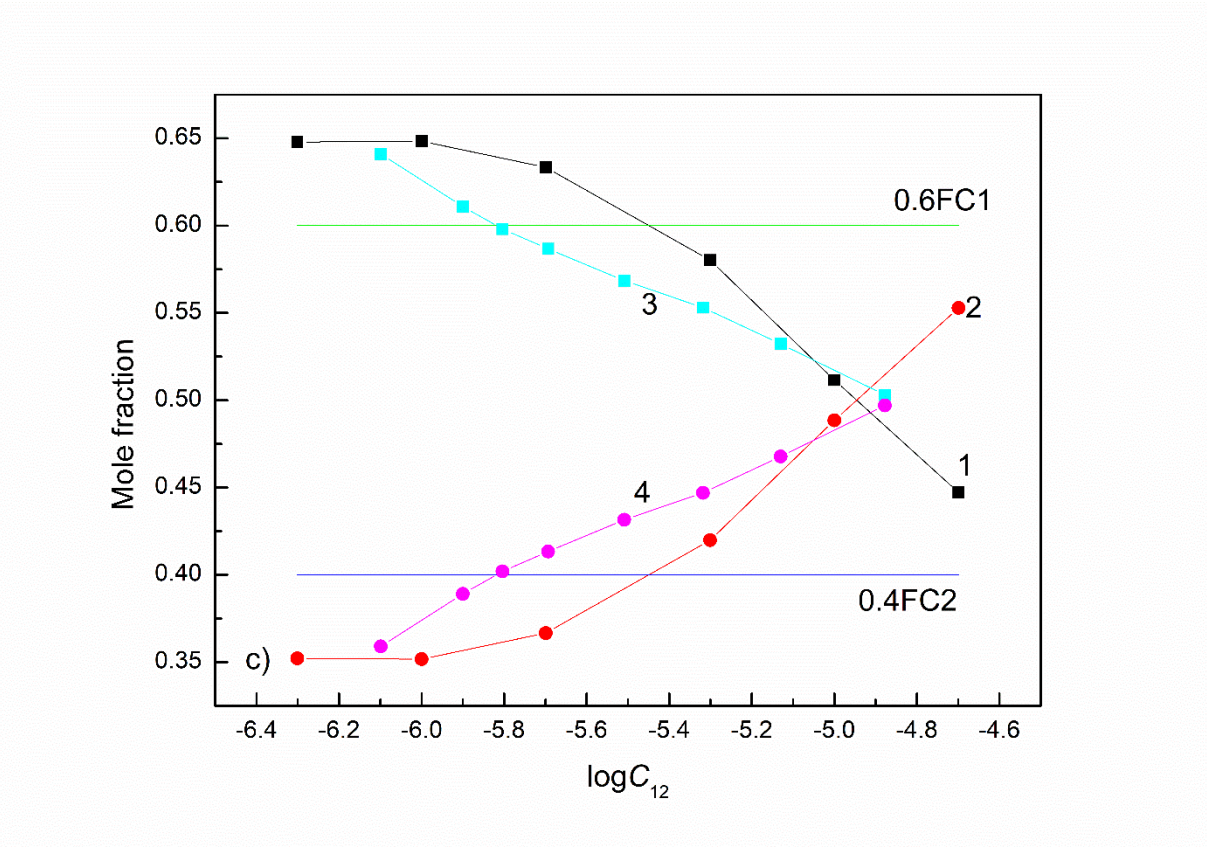

Figure S18c. The comparison of the mole fraction of the mixed surface layer formed by FC1+FC2 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

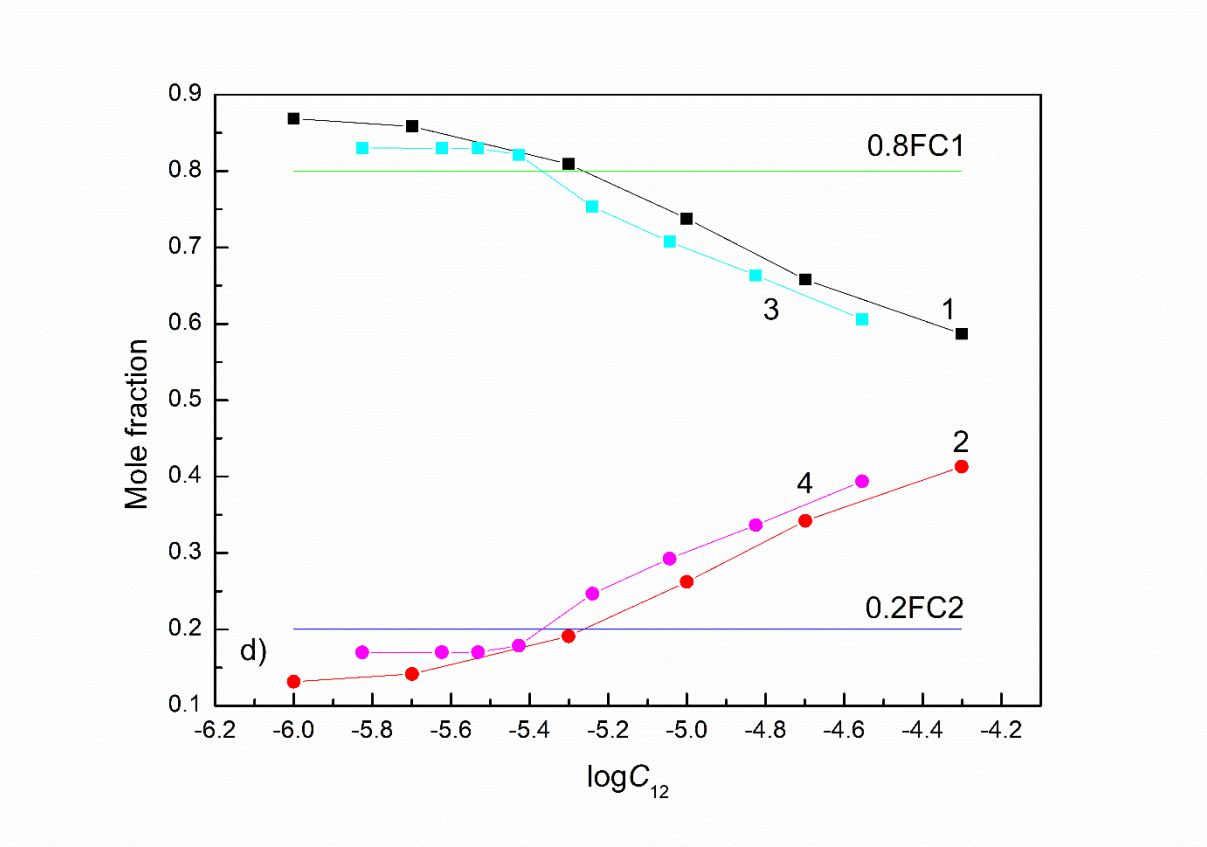

Figure S18d. The comparison of the mole fraction of the mixed surface layer formed by FC1+FC2 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

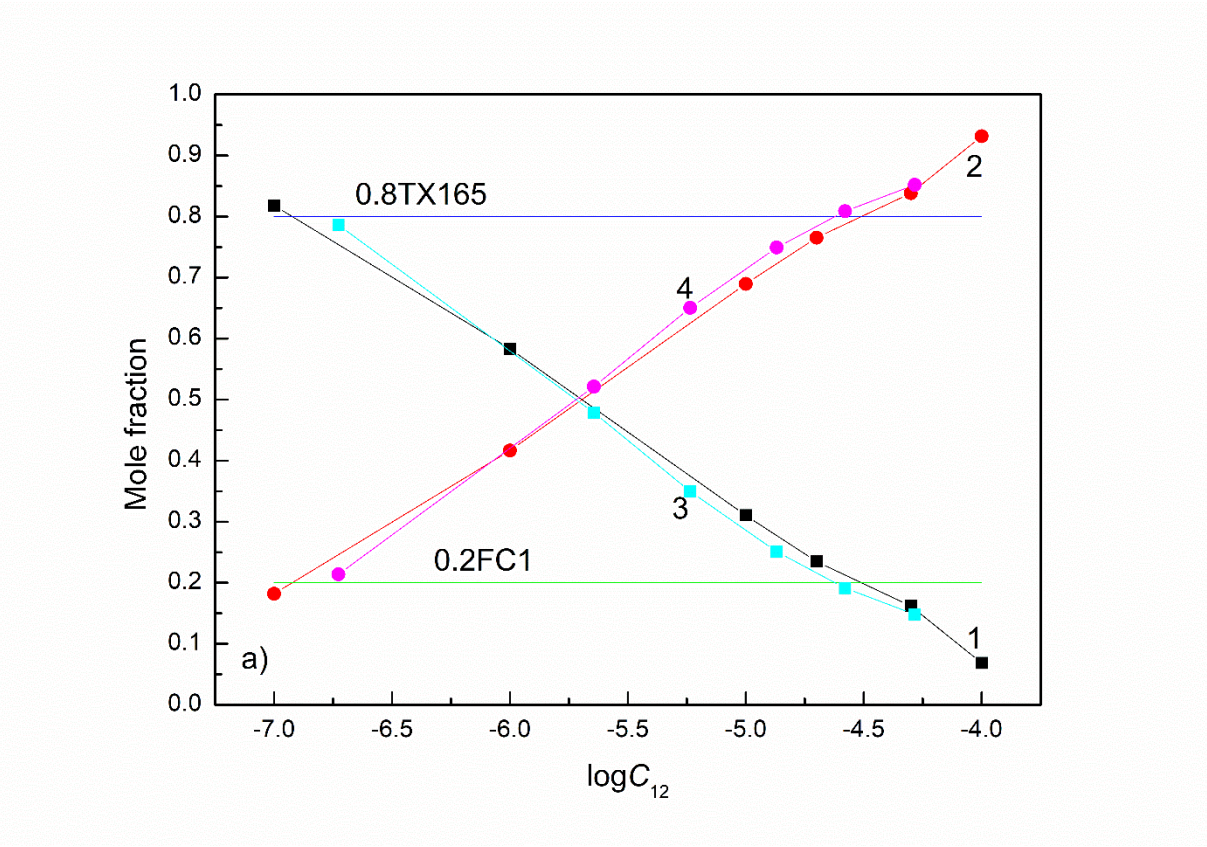

Figure S19a. The comparison of the mole fraction of the mixed surface layer formed by FC1+TX165 as well as FC2+TX100 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

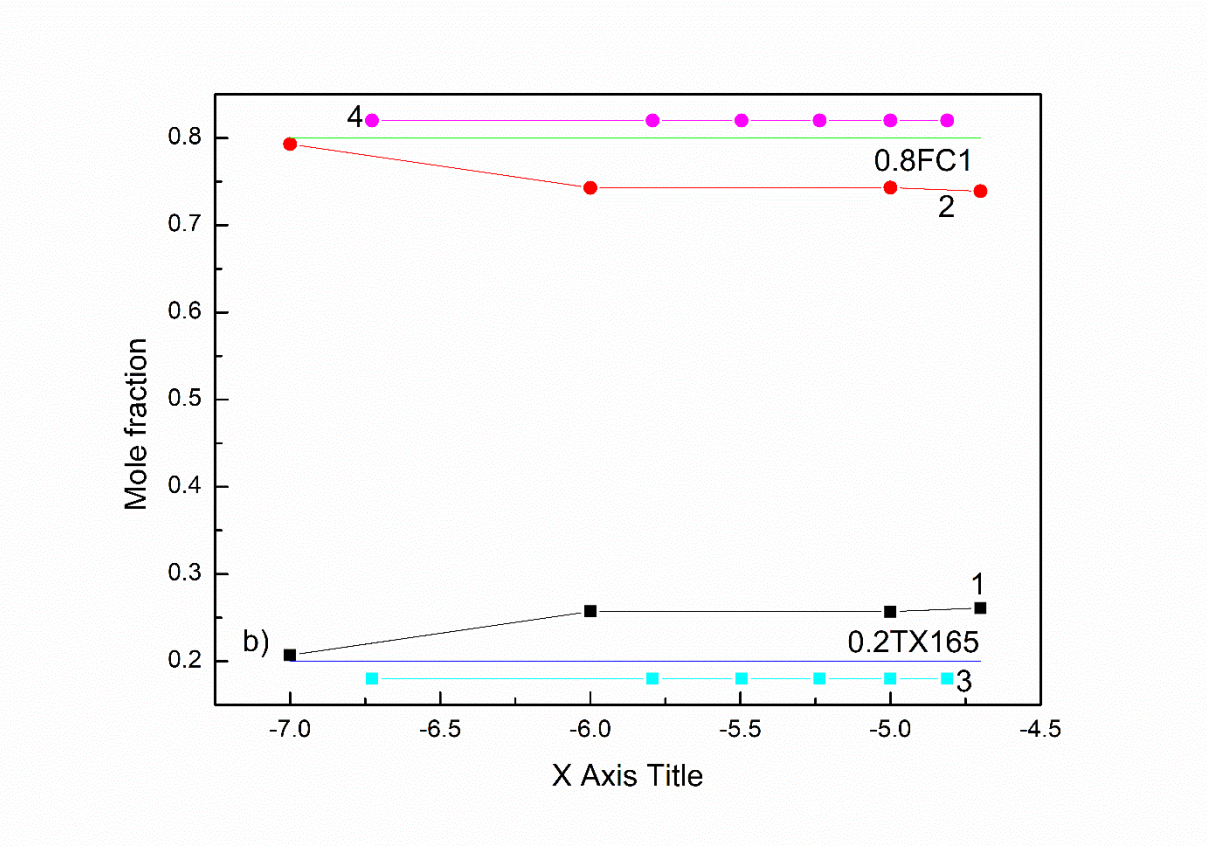

Figure S19b. The comparison of the mole fraction of the mixed surface layer formed by FC1+TX165 as well as FC2+TX100 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

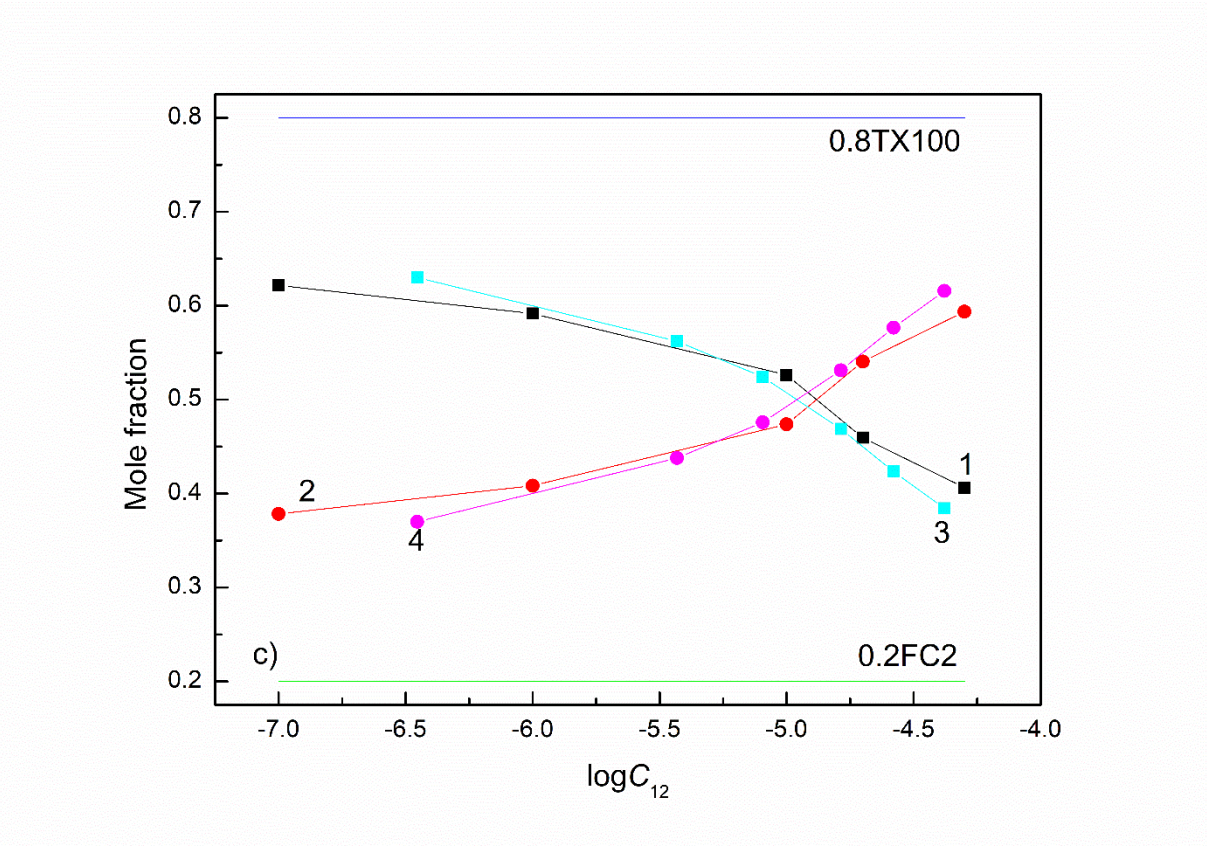

Figure S19c. The comparison of the mole fraction of the mixed surface layer formed by FC1+TX165 as well as FC2+TX100 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

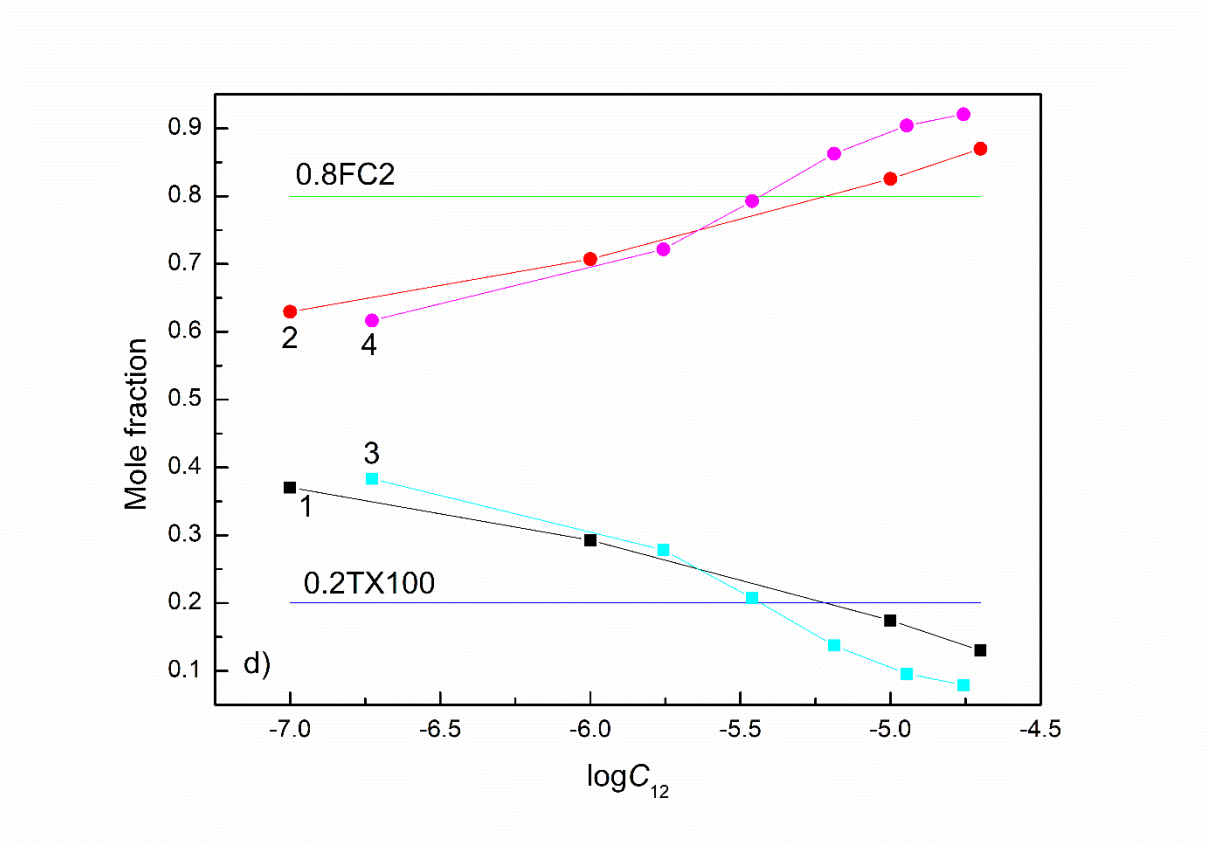

Figure S19d. The comparison of the mole fraction of the mixed surface layer formed by FC1+TX165 as well as FC2+TX100 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (16) at the different mixture composition in the bulk phase.

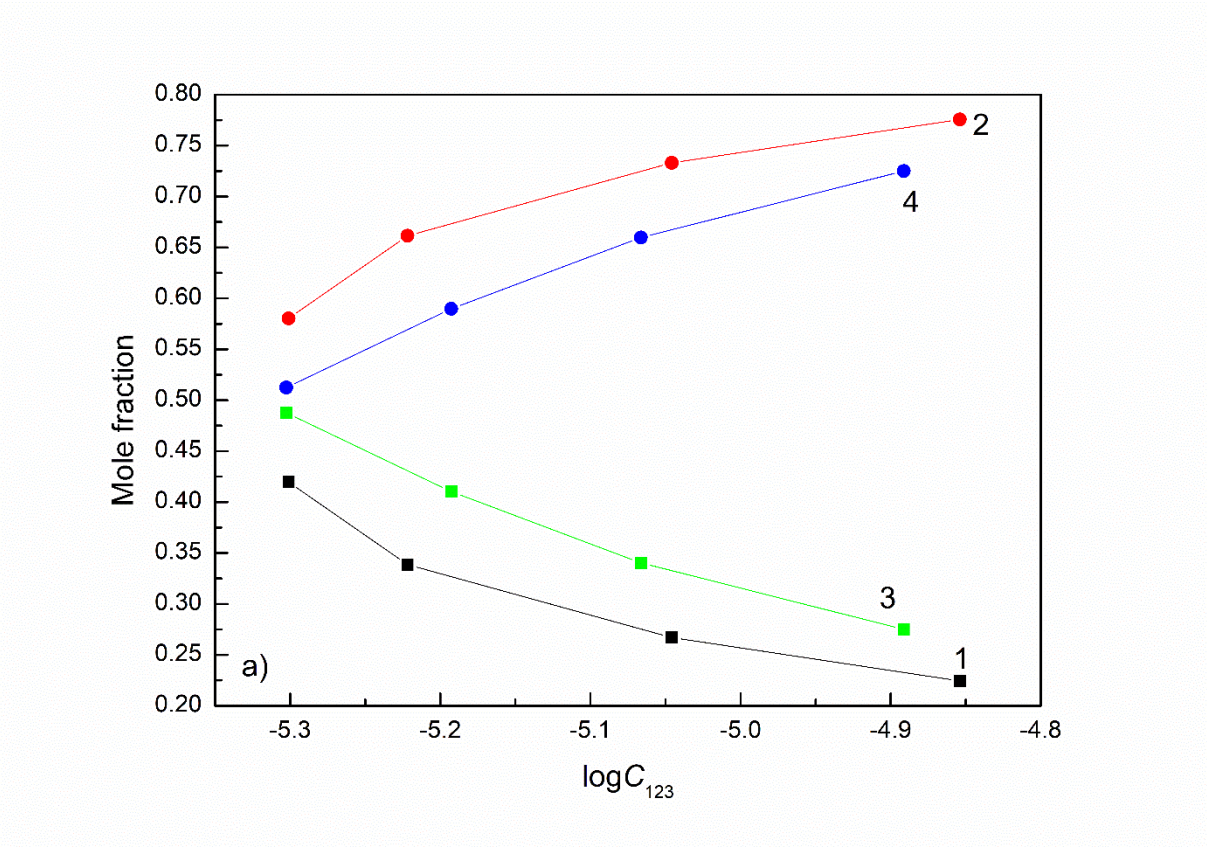

Figure S20a. The comparison of the mole fraction of the mixed surface layer formed by CTAB+TX100+TX114 (at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (17) at the different mixture composition in the bulk phase.

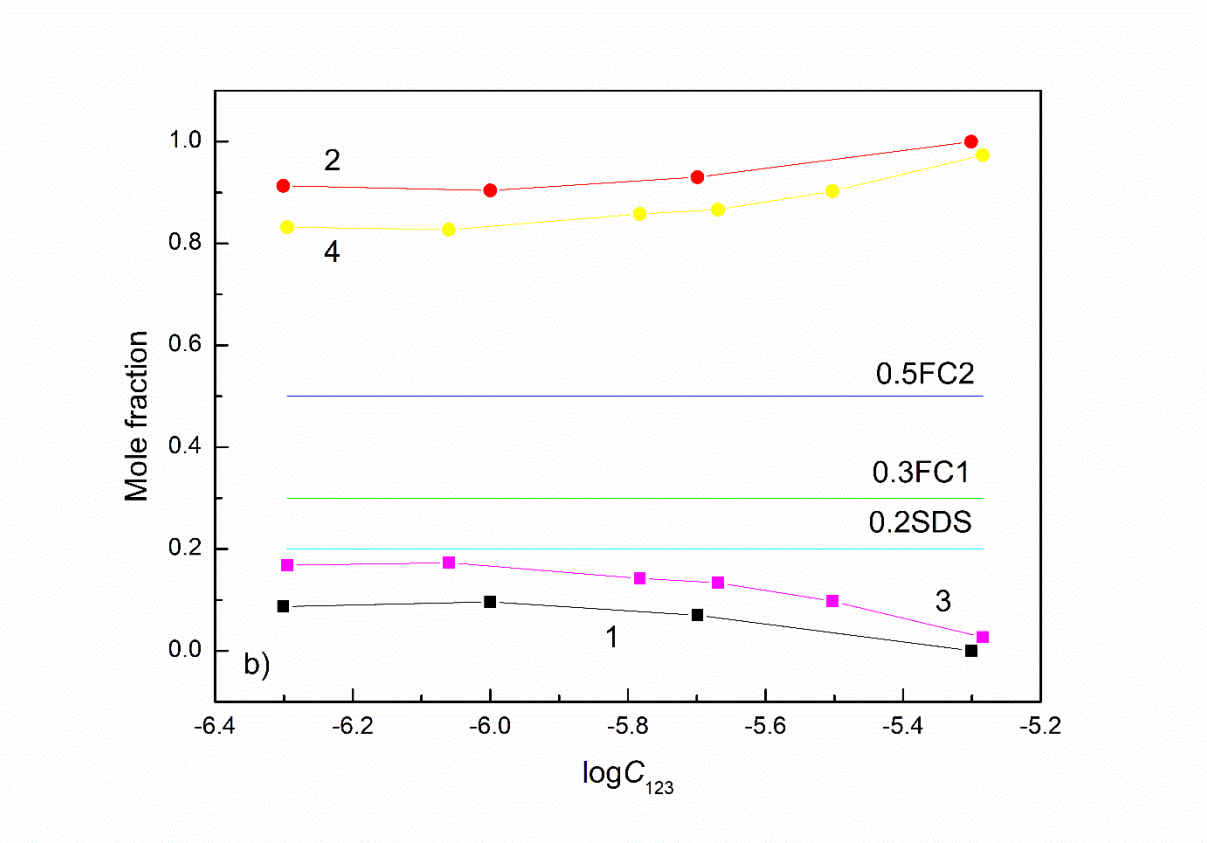

Figure S20b. The comparison of the mole fraction of the mixed surface layer formed by FC2+FC1+SDS (at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (17) at the different mixture composition in the bulk phase.

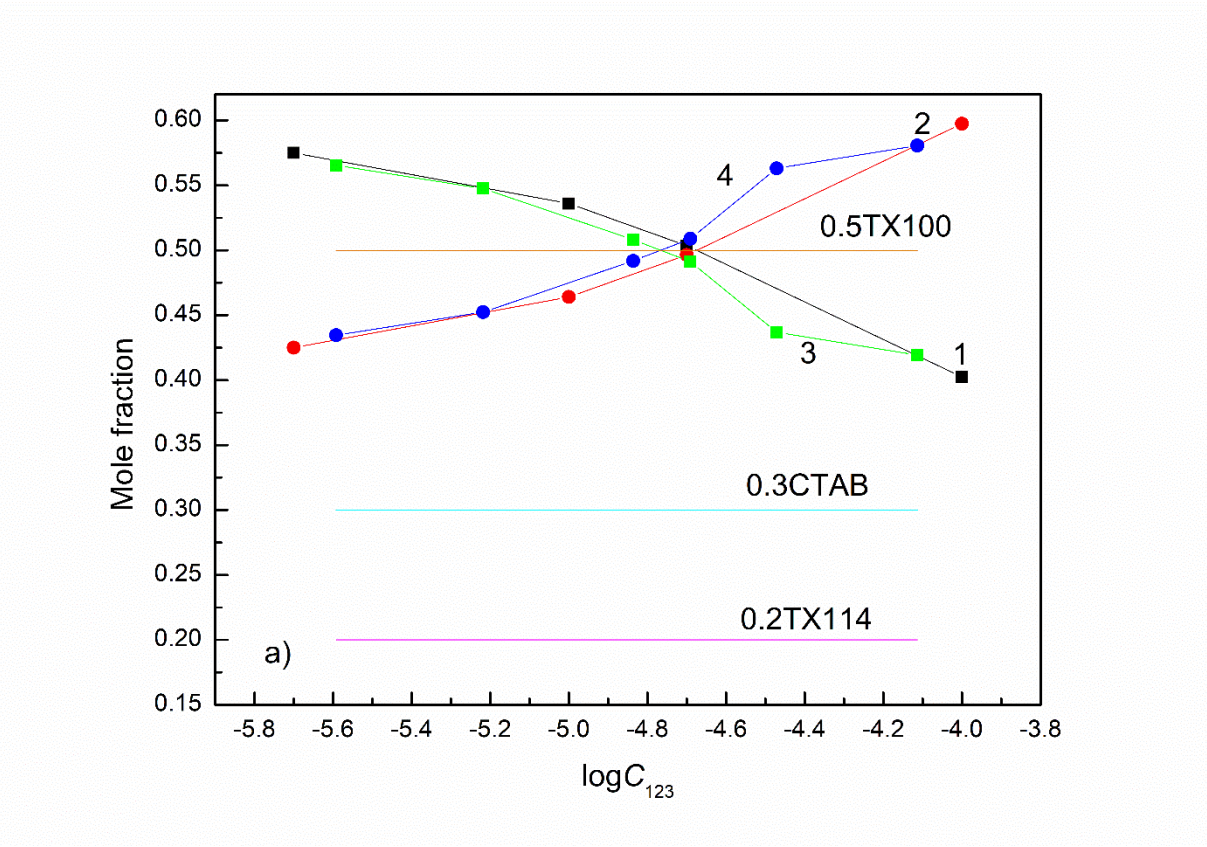

Figure S21a. The comparison of the mole fraction of the mixed surface layer formed by CTAB+TX100+TX114 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (17).

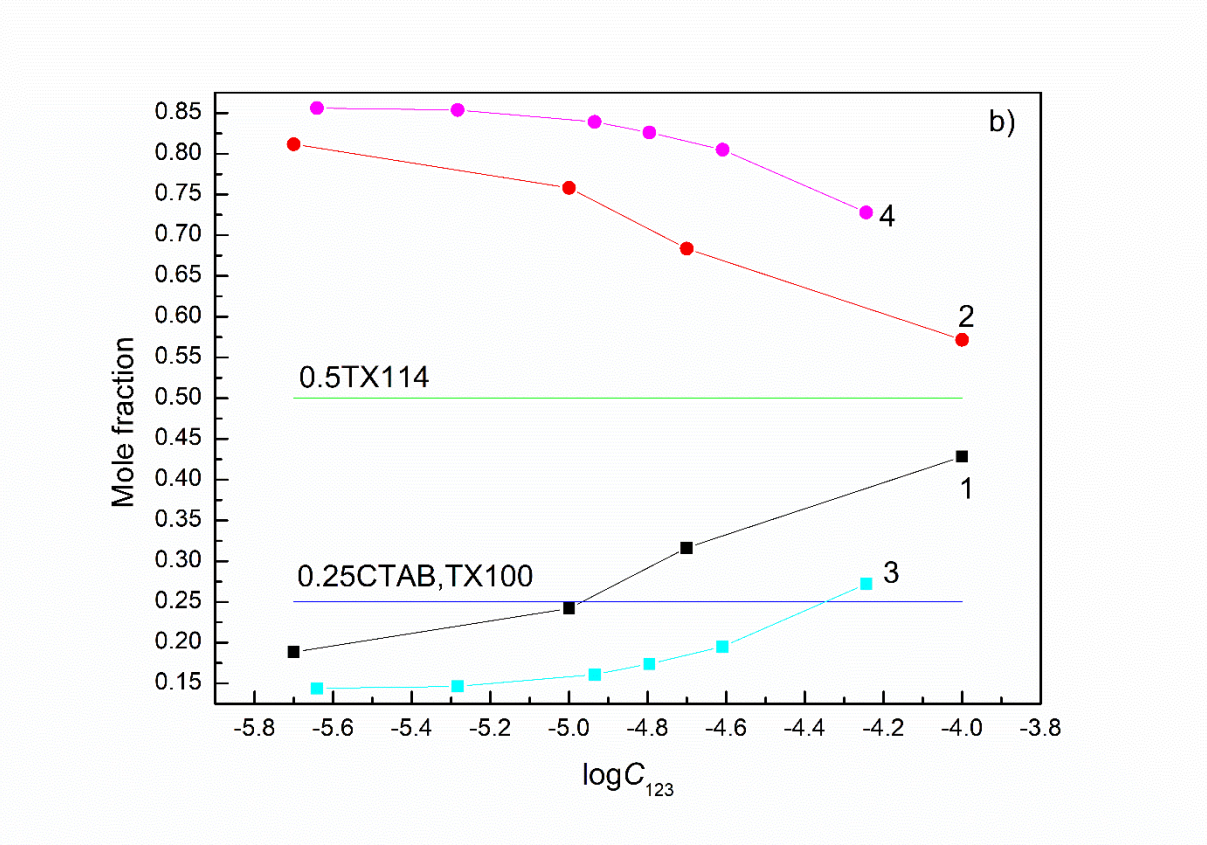

Figure S21b. The comparison of the mole fraction of the mixed surface layer formed by CTAB+TX100+TX114 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (17).

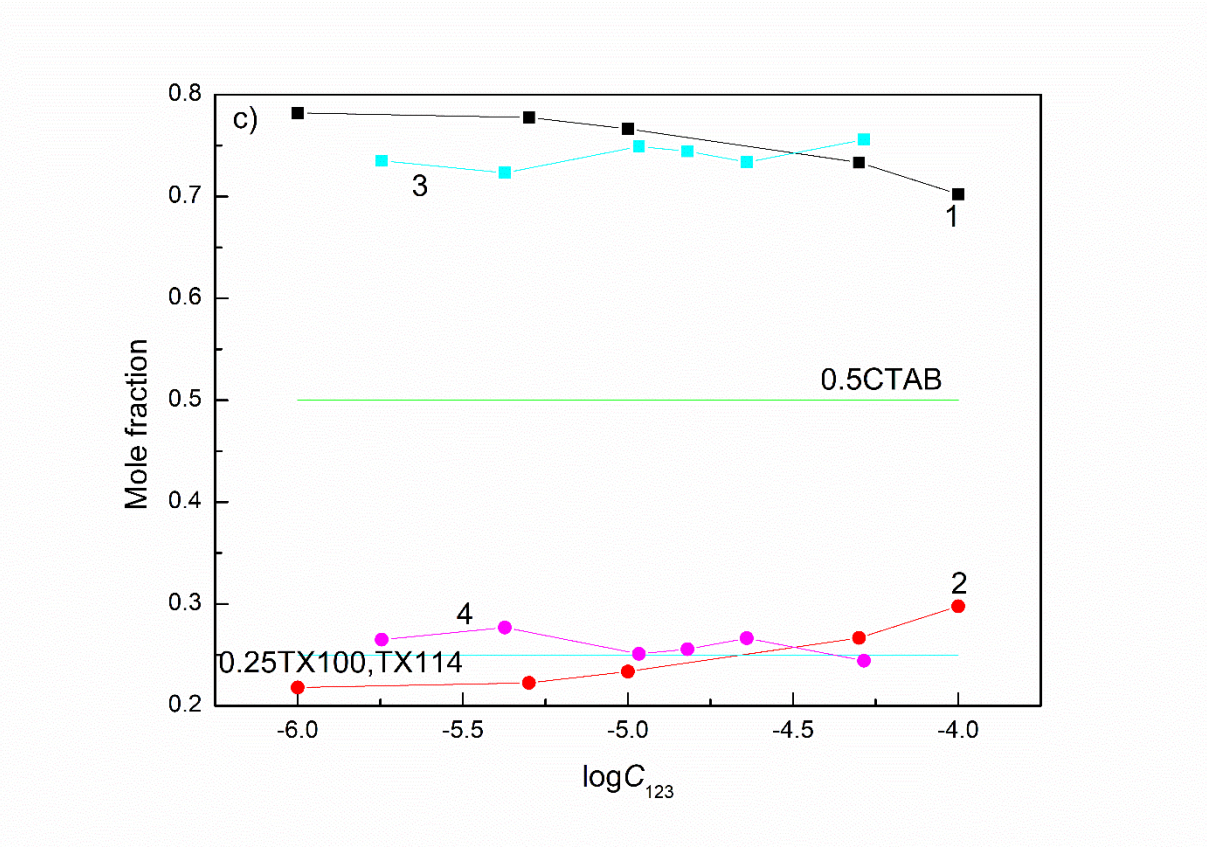

Figure S21c. The comparison of the mole fraction of the mixed surface layer formed by CTAB+TX100+TX114 at the water-air interface calculated based on the contribution of the particular mixture components to the reduction of the water surface tension and calculated from Eq. (17).