Supplementary information

for

STAND: Surface Tension for Aggregation Number Determination

Pablo F. Garrido[1], Pilar Brocos[1], Alfredo Amigo[1], Luis García-Río[2], Jesús Gracia-Fadrique[3], Ángel Piñeiro[1,*]

[1]Departamento de Física Aplicada & [2]Departamento de Química Física, Universidade de Santiago de Compostela, Campus Vida, E-15782 Santiago de Compostela, Spain.

[3]Departamento de Fisicoquímica, Facultad de Química, Universidad Nacional Autónoma de México, Ciudad Universitaria, 04510 México D.F., Mexico.

*E-mail: Angel.Pineiro@usc.es

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Table S1.- Aggregation number values obtained from different sources, including this work, for the systems studied here together with the temperature, the working concentration region normalized by the *cmc*, the employed technique, and the original reference of each value.

Surfactant	T (K)	N	$[S_T]/cmc$	Technique	Reference
C_8G_1	R. T.	24 ± 5	1.5	Small-angle neutron scattering	Zhang et al., 1999[27]
		51 ± 2	2.7	Small-angle X-ray scattering	Zhang et al., 1999[27]
	283	106 ± 20	~1	Surface tension	This work
	293	68	0.9-1.5	Static light scattering	Lässer and Elias, 1972[28]
		70	1	Sedimentation equilibrium	Roxby and Mills, 1990[29]
		75 ± 10	1.3	Sedimentation velocity	Lorber et al., 1990[30]
		103 ± 10	2.5	Sedimentation velocity	Lorber et al., 1990[30]
	295	84	1	Sedimentation equilibrium	Kameyama and Takagi, 1990[31]
		87	1	Static light scattering	Kameyama and Takagi, 1990[31]
	298	28 ± 6	~1	Surface tension	Capalbi et al., 2004[32]
		54 ± 5	1.1	Fluorescence	Pastor et al., 1998[33]
		66-76	1.1-2	Small-angle neutron scattering	Giordano et al., 1997[34]
		70-90	2	Small-angle X-ray scattering	Oliver et al., 2013[35]
		72.4	4	Fluorescence	Alargova et al., 1998[36]
		~80 ^{a}	1.4	Small-angle neutron scattering	Garamus et al., 2004[37]
		80	1.4	Fluorescence	del Burgo et al., 2004[38]
		80	1.4	Fluorescence	Lainez et al., 2004[39]
		75-85 ^{b}	~1	Small-angle X-ray scattering	Lipfert et al., 2007[40]
		82	<2	Static light scattering	Esumi et al., 1996[41]
		83.2 ± 5.8	~1	Surface tension	This work
		92	2.4	Fluorescence	Frindi et al., 1992[42]
		92	<2.6	Static light scattering	Fukada et al., 2000[43]
		95-189 ^{c}	<1	Sedimentation velocity	Tiefenbach et al., 1999[44]
		104 ± 5	2.1	Fluorescence	Pastor et al., 1998[33]
	303	83 ± 3	0.6-2.1	Sedimentation equilibrium	Lässer and Elias, 1972[28]
		84	1-1.7	Static light scattering	Lässer and Elias, 1972[28]
	309	97	1	Static light scattering	Kameyama and Takagi, 1990[31]
	308	112	<2.8	Static light scattering	Fukada et al., 2000[43]
	310	68.2 ± 3.6	~1	Surface tension	This work
	313	94	2.6	Fluorescence	Frindi et al., 1992[42]
	323	75.7 ± 4.5	~1	Surface tension	This work

$C_{10}G_1$	283	115 ± 15	~1	Surface tension	This work
	296	~200	1-1.4	Fluorescence	Nilsson et al., 1998[45]
	298	40 ± 11	~1	Surface tension	Capalbi et al., 2004[32]
		100-120	25	Small-angle X-ray scattering	Oliver et al., 2013[35]
		103-119 [d]	7.5	Sedimentation velocity	Tiefenbach et al., 1999[44]
		139 ± 19	~1	Surface tension	This work
		177 ± 18	1.8	Fluorescence	This work
		201 ± 10 *	2.0	Fluorescence	This work
	310	500 ± 260	~1	Surface tension	This work
	323	180 ± 28	~1	Surface tension	This work
$C_{10}G_2$	298	57 ± 17	~1	Surface tension	Capalbi et al., 2004[32]
		68 ± 1 [e]	9	Small-angle neutron scattering	O'Malley et al., 2011[46]
		71-77	27	Small-angle X-ray scattering	Oliver et al., 2014[47]
		80-90 [b]	~1	Small-angle X-ray scattering	Lipfert et al., 2007[40]
		82.1 ± 2.5	1.8	Fluorescence	This work
		86-103	36	Small-angle X-ray scattering	Oliver et al., 2013[35]
		92 ± 13*	2.5	Fluorescence	This work
		93.5 ± 5.0	~1	Surface tension	This work
		98-104	36	Small-angle X-ray scattering	Oliver et al., 2013[35]
$C_{12}G_2$	R. T.	138 ± 3	120	Fluorescence	Tummino et al., 1993[10]
	289	130	120	Small-angle neutron scattering	Timmins et al., 1988[48]
	293	122 [a]	15	Small-angle neutron scattering	Le et al., 2014[49]
		124-131	24-487	Small-angle X-ray scattering	Barret et al., 2013[50]
	297	132 [a]	100-200	Small-angle neutron scattering	Dupuy et al., 1997[51]
	298	22 ± 31	1.9	Fluorescence	This work
		25.09 ± 0.26	~1	Surface tension	This work
		28.34 ± 0.68 *	2.5	Fluorescence	This work
		~30 [f]	1	Fluorescence	Warr et al., 1986[52]
		61 ± 20	~1	Surface tension	Capalbi et al., 2004[32]
		70-110	5-1000	Fluorescence	Warr et al., 1986[52]
		94	1	Sedimentation velocity	Zhang and Somasundaran, 2004[53]
		106	23	Sedimentation velocity	Lu and Somasundaran, 2007[54]
		112	227	Sedimentation velocity	Lu and Somasundaran, 2007[54]
		113 ± 6 [a]	312	Small-angle neutron scattering	Bucci and Fagotti, 1991[55]

		113 ± 4 [a]	<680	Small-angle neutron scattering and Small-angle X-ray scattering	Bäverbäck et al., 2009[56]
		114-123	273	Small-angle X-ray scattering	Oliver et al., 2014[47]
		121 ± 1 [e]	100	Small-angle neutron scattering	O'Malley et al., 2011[46]
		129 ± 4 [a]	940	Small-angle neutron scattering	Bucci and Fagotti, 1991[55]
		135-149	430	Small-angle X-ray scattering	Oliver et al., 2013[35]
		137 ± 8 [a]	<680	Static light scattering	Bäverbäck et al., 2009[56]
		145-155	430	Small-angle X-ray scattering	Oliver et al., 2013[35]
		130-145 [b]	~1	Small-angle X-ray scattering	Lipfert et al., 2007[40]
	308	141 ± 3	10	Refractive index & Light scattering	Strop and Brunger, 2005[57]
	310	82	534	Neutron scattering	Cecutti et all, 1991[58]
	289-333	125 ± 10	20-90	Fluorescence	Aoudia and Zana, 1998[59]
$C_{14}G_2$	298	13 ± 69	2.3	Fluorescence	This work
		13.4 ± 1.7 **	2.3	Fluorescence	This work
		26.2 ± 3.1	~1	Surface tension	This work
		124-134	2700	Small-angle X-ray scattering	Oliver et al., 2014[47]
NP7	298	29.8 ± 5.8	~1	Surface tension	This work
		47.8 ± 7.2	3.6	Fluorescence	This work
NP10	298	21.07 ± 0.59	~1	Surface tension	This work
		27 ± 25	2.6	Fluorescence	This work
		67 [g]	680	Fluorescence	de Miranda et al., 2007[60]
		100	2.1	Light scattering	Becher, 1961[61]
		105	1	Sedimentation velocity	Zhang and Soumasundaran, 2004[53]
		275	35-280	Light scattering	Schick et al., 1962[62]

[a] In D_2O.

[b] In 20 mM phosphate buffer (pH 6.2) and 150 mM NaCl.

[c] In presence of 0.1 mM of N-phenyl-1-naphthylamine.

[d] In aqueous solution containing 50 mM sodium phosphate pH 7.0 and 0.1 mM of N-phenyl-1-naphthylamine.

[e] In D_2O buffer (50 mM sodium phosphate).

[f] Extrapolating data from reference.[52]

[g] Data for NP 9-10.

* Using *cmc* from the evolution of chemical species obtained from the surface tension model results.

** Using *cmc* determined from fluorescence by applying the pyrene 1:3 ratio method.[63]

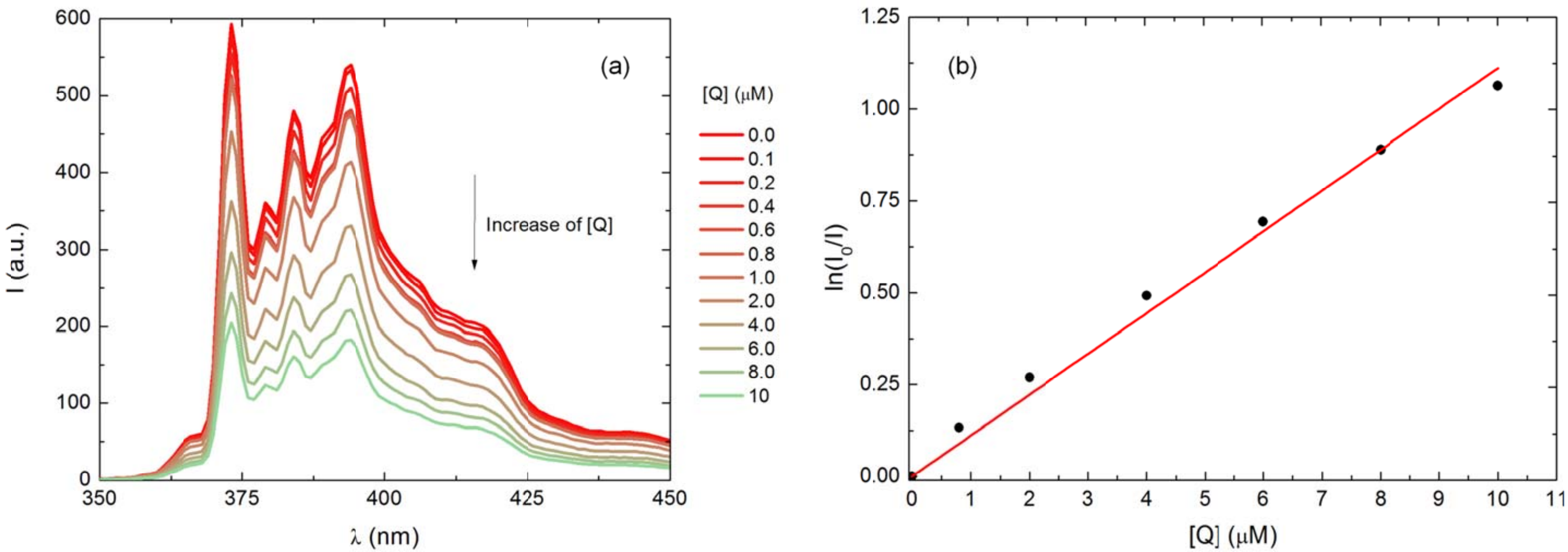

Figure S1.- Intensity of pyrene fluorescence (in arbitrary units) for different quencher concentrations as a function of wavelength (a) and natural logarithm of the ratio of fluorescence intensities (in the absence and in the presence of quencher) at λ=373 nm peak with respect to quencher concentration (b), as followed by eq. (1). Data from $C_{12}G_2$ fluorescence experiment at 298 K.

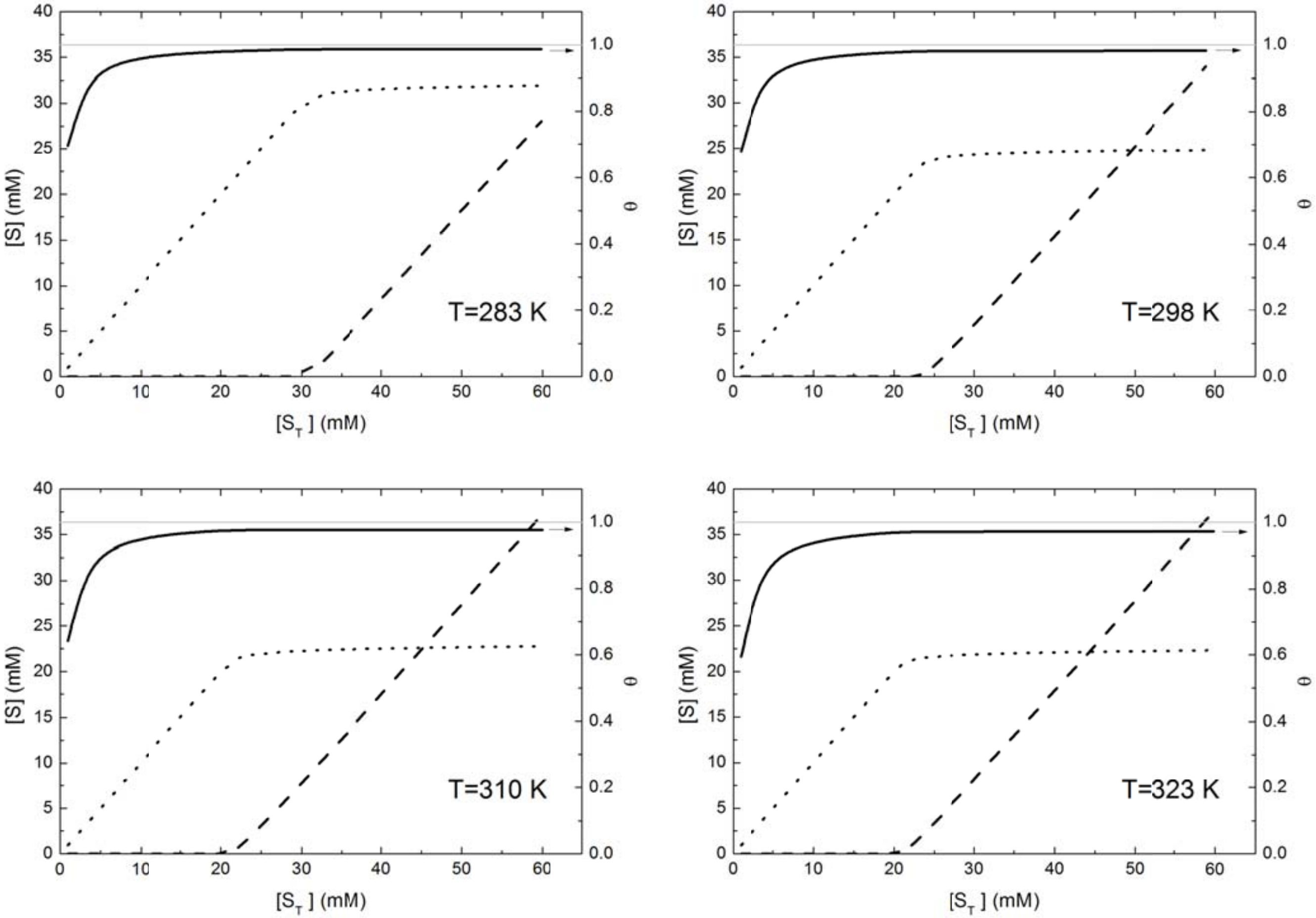

Figure S2.- Concentration of free surfactant (dotted line), surfactant molecules in micelles (dashed line) and surface coverage (solid line) as a function of the total concentration of *n*-octyl-β-D-glucopyranoside at the temperatures indicated in the plots. Data obtained from the application of the STAND model. The thin grey line at $\theta = 1$ is also added as a reference.

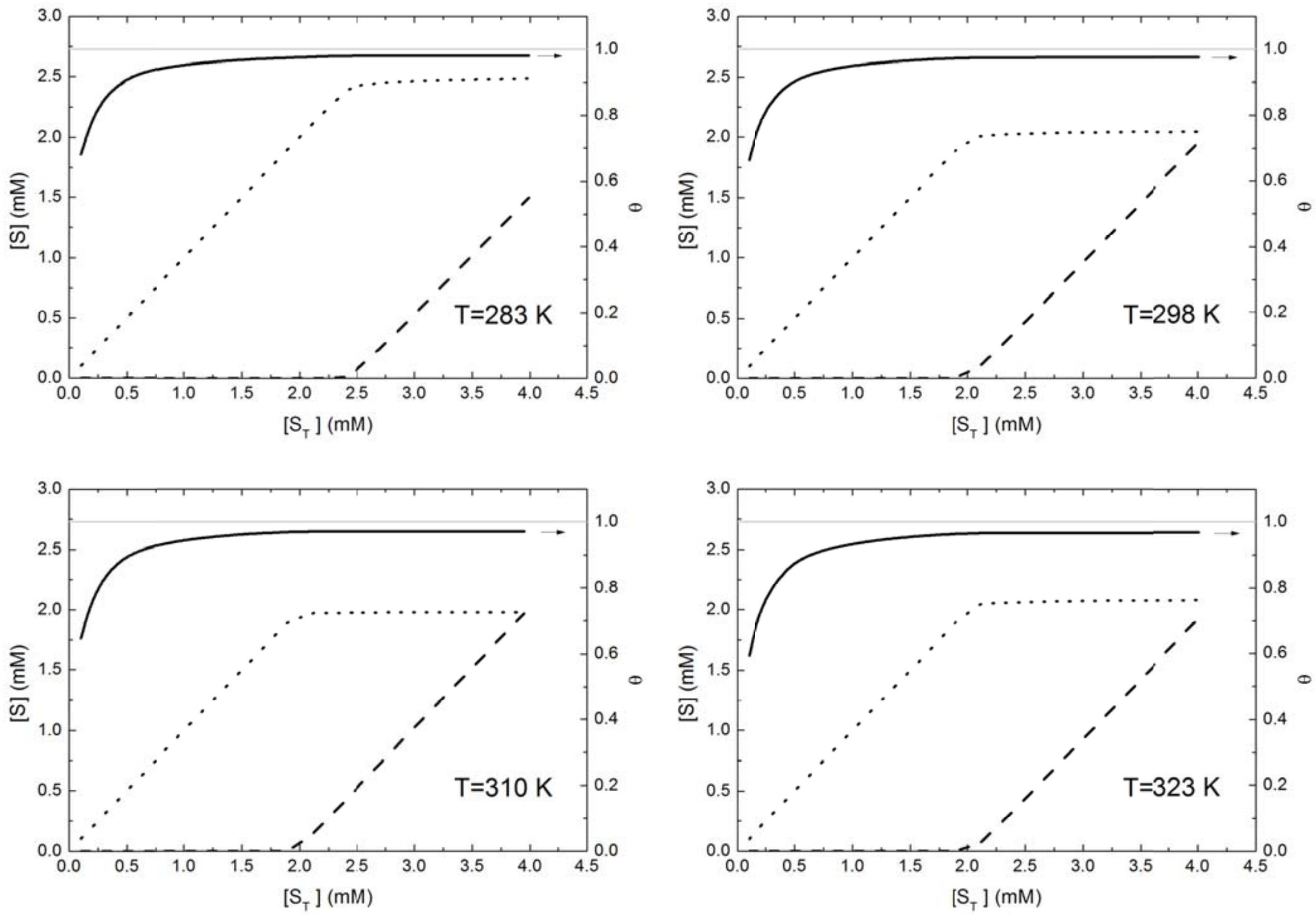

Figure S3.- Concentration of free surfactant (dotted line), surfactant molecules in micelles (dashed line) and surface coverage (solid line) as a function of the total concentration of *n*-decyl-β-D-glucopyranoside at the temperatures indicated in the plots. Data obtained from the application of the STAND model. The thin grey line at $\theta = 1$ is also added as a reference.

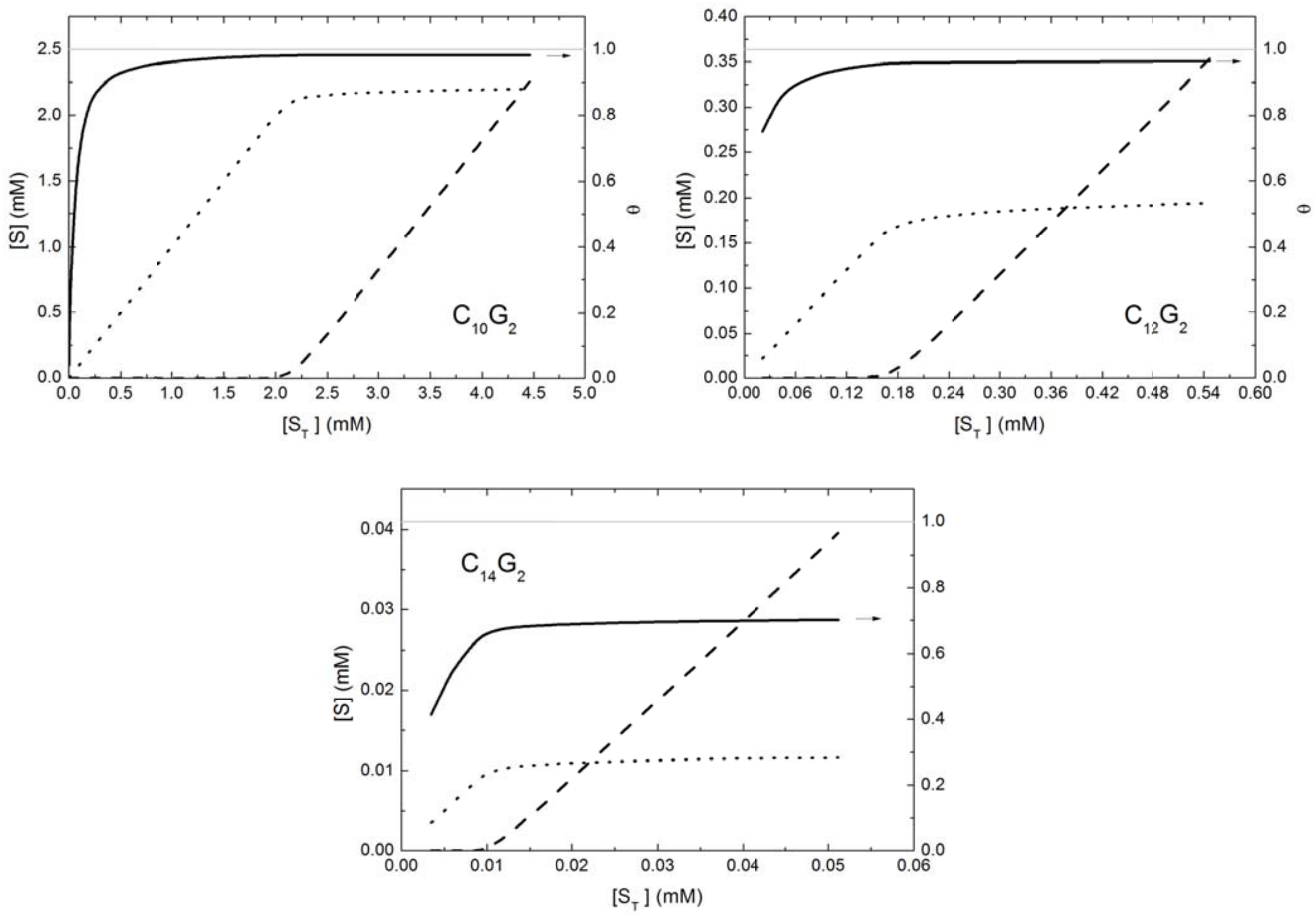

Figure S4.- Concentration of free surfactant (dotted line), surfactant molecules in micelles (dashed line) and surface coverage (solid line) as a function of the total concentration of *n*-decyl-β-D-maltoside ($C_{10}G_2$), *n*-dodecyl-β-D-maltoside ($C_{12}G_2$), and *n*-tetradecyl-β-D-maltoside ($C_{14}G_2$) at 298 K. Data obtained from the application of the STAND model. The thin grey line at θ = 1 is also added as a reference.

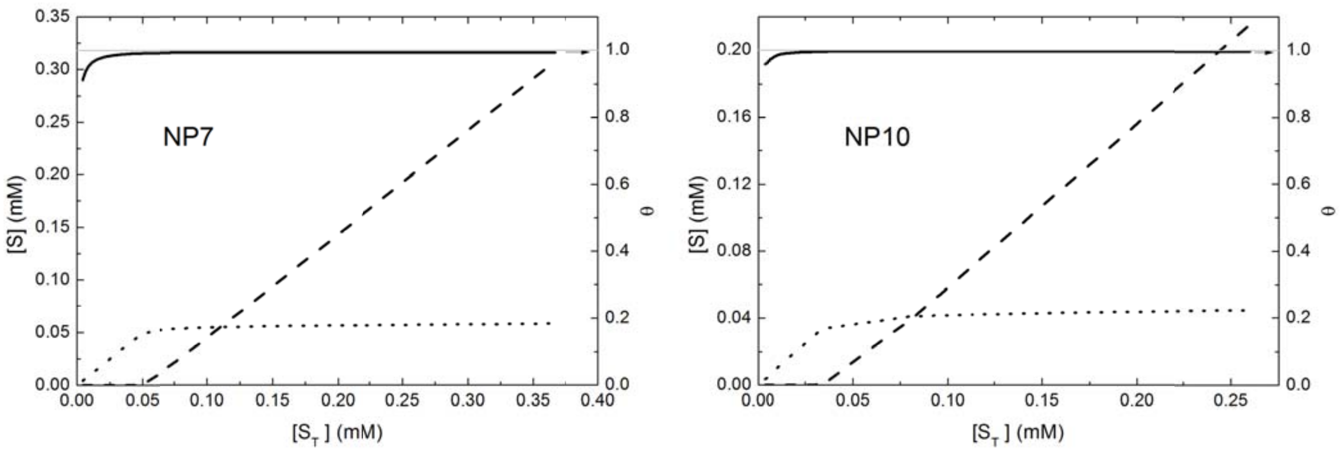

Figure S5.- Concentration of free surfactant (dotted line), surfactant molecules in micelles (dashed line) and surface coverage (solid line) as a function of the total concentration of nonylphenol polyethylene-7 glycol ether (NP7), and nonylphenol polyethylene-10 glycol ether (NP10) at 298 K. Data obtained from the application of the STAND model. The thin grey line at $\theta = 1$ is also added as a reference.

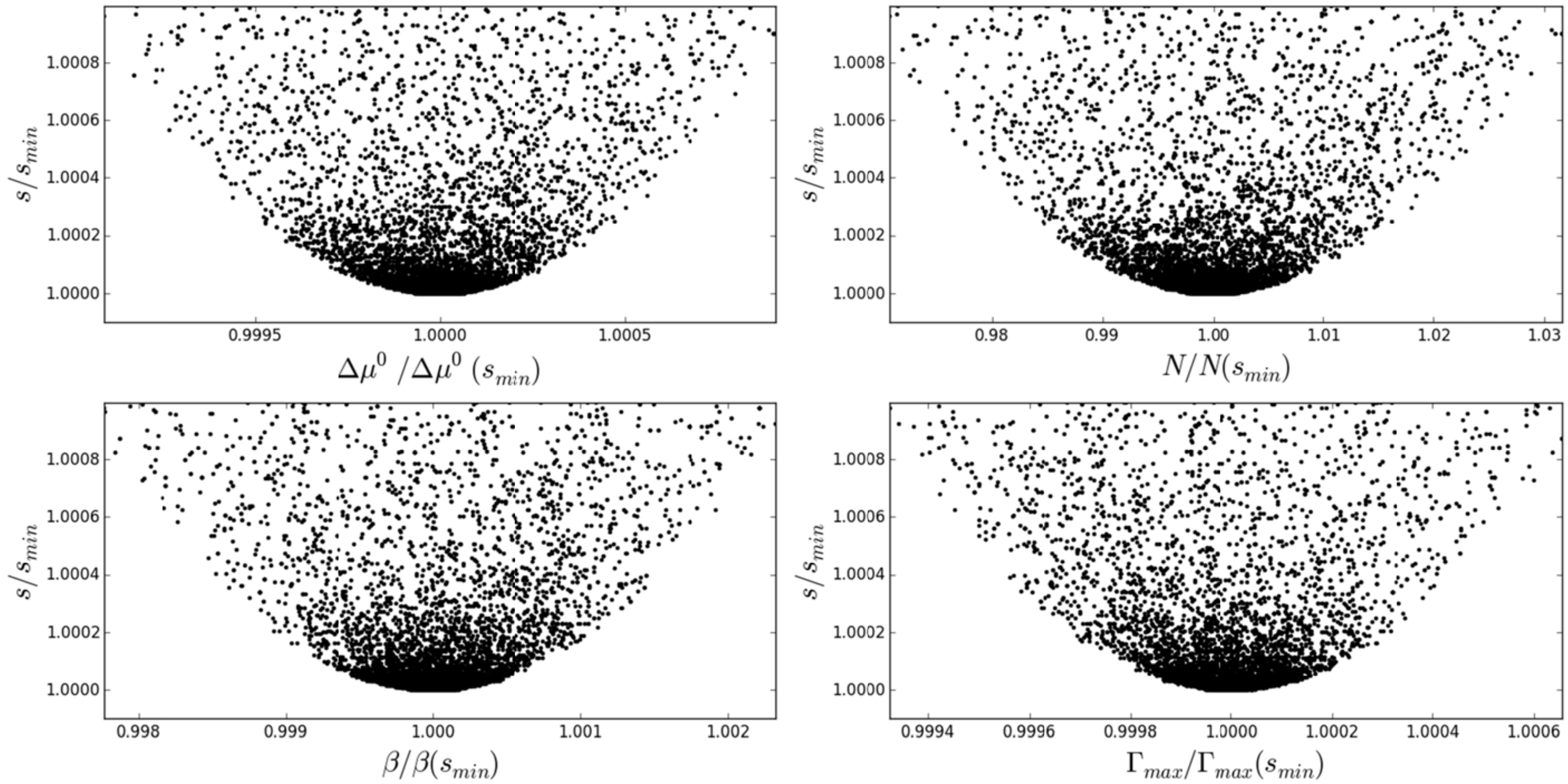

Figure S6.- Normalized standard deviation as a function of each fitting parameter (micellization free energy per mole of surfactant, aggregation number, adsorption constant and maximun surface excess), also normalized with respect to the value with the lowest standard deviation (s_{min}). Results obtained from the data of C_8G_1 at 298 K.