

# Supporting Information

## A GNN-Based QSPR Model for Surfactant Properties

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### 1 Data collection from literature

Table 1 summarizes the surfactants and their properties gathered for this work. A spreadsheet of the table is available from the corresponding authors upon request. The values in the columns  $\Gamma_{max}$ ,  $\gamma_{cmc}$ , and logCMC without parentheses represent the experimental data used for developing models, while the values within parentheses indicate the predicted values by the models.

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**Table S1:** Surfactant property data collection from literature. The values in the columns  $\Gamma_{max}$ ,  $\gamma_{cmc}$ , and logCMC without parentheses represent the experimental data used for developing models, while the values within parentheses indicate the predicted values by the models.

Index	SMILES	Compound	T	$\Gamma_{max}$ (mol/m <sup>2</sup> )	$\gamma_{cmc}$ (mN/m)	logCMC (M)	Ref
0	CCCCCCCCCCCCCCCCCCCCCCCCCCCC	C8E6	25	3.59E-06 (2.97E-06)	32.78 (32.17)	-2.00 (-2.12)	1
1	CCCCCCCCCCCCCCCCCCCCCCCCCCCC	C9E8	25	2.00E-06 (2.56E-06)	NaN (33.09)	NaN (-2.42)	2
2	CCCCCCCCCCCCCCCCCCCCCCCCCCCC	C10E4	20	3.31E-06 (3.76E-06)	26.58 (29.86)	-2.99 (-3.43)	3
3	CCCCCCCCCCCCCCCCCCCCCCCCCCCC	C10E6	20	2.86E-06 (3.06E-06)	29.91 (31.84)	-2.93 (-3.10)	3
4	CCCCCCCCCCCCCCCCCCCCCCCCCCCC	C12E6	20	4.26E-06 (3.16E-06)	29.57 (31.41)	-3.93 (-3.88)	3
5	CCCCCCCCCCCCCCCCCCCCCCCCCCCC	C16E6	20	1.60E-06 (2.84E-06)	28.42 (29.61)	-3.97 (-4.46)	3
6	CCCCCCCCCCCCCCCCCCCCCCCCCCCC CCCCCCCC	C16E9	20	2.76E-06 (2.65E-06)	36.28 (32.47)	-4.39 (-4.28)	3
7	CCCCCCCCCCCCCCCCCCCCCCCCCCCC	C11E8	25	2.10E-06 (2.65E-06)	NaN (32.88)	NaN (-3.23)	2

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Table S1 – continued from previous page

Index	SMILES	Compound	T	$\Gamma_{max}$ (mol/m <sup>2</sup> )	$\gamma_{cmc}$ (mN/m)	logCMC (M)	Ref
8	CCCCCCCCCCCCCCCCCO	C12E2	25	5.12E-06 (4.88E-06)	26.35 (26.10)	-4.48 (-4.34)	4
9	CCCCCCCCCCCCCCCCCO	C12E3	25	4.97E-06 (3.97E-06)	23.80 (27.63)	-4.28 (-4.18)	4
10	CCCCCCCCCCCCCCCCCO	C12E4	25	3.82E-06 (3.53E-06)	28.63 (29.03)	-4.19 (-4.06)	4
11	CCCCCCCCCCCCCCCCCO	C12E5	25	3.33E-06 (3.34E-06)	30.52 (30.41)	-4.19 (-3.98)	4
12	CCCCCCCCCCCCCCCCCO	C12E7	25	2.83E-06 (2.92E-06)	33.58 (32.16)	-4.09 (-3.74)	4
13	CCCCCCCCCCCCCCCCCO	C12E8	25	2.50E-06 (2.70E-06)	34.55 (32.73)	-3.96 (-3.59)	4
14	CCCO	C3OH	20	6.00E-06 (5.96E-06)	NaN (29.17)	NaN (0.29)	2
15	CCCCO	C4OH	20	6.75E-06 (6.68E-06)	NaN (29.16)	NaN (-0.49)	2
16	CCCCCO	C5OH	20	6.48E-06 (6.61E-06)	NaN (28.75)	NaN (-1.04)	2

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Table S1 – continued from previous page

Index	SMILES	Compound	T	$\Gamma_{max}$ (mol/m <sup>2</sup> )	$\gamma_{cmc}$ (mN/m)	logCMC (M)	Ref
17	CCCCCCC	C6OH	20	7.11E-06 (6.90E-06)	NaN (27.74)	NaN (-1.49)	2
18	CCCCCCCC	C7OH	25	7.06E-06 (7.15E-06)	NaN (26.84)	NaN (-1.78)	2
19	CCCCCCCCC	C8OH	25	7.66E-06 (7.70E-06)	NaN (25.73)	NaN (-2.47)	2
20	CCCCCCCCCC	C9OH	20	8.22E-06 (8.12E-06)	NaN (24.72)	NaN (-3.21)	2
21	CCCCCCCCCCC	C10OH	25	1.11E-05 (8.23E-06)	NaN (24.00)	NaN (-3.86)	2
22	OCCCC	C4(OH)2	30	2.43E-06 (2.23E-06)	NaN (34.52)	NaN (-0.67)	2
23	OCCCCCCCC	C8(OH)2	20	3.07E-06 (2.83E-06)	NaN (30.07)	NaN (-3.86)	2
24	OCCCCCCCCC	C9(OH)2	20	2.88E-06 (2.92E-06)	NaN (29.11)	NaN (-4.47)	2
25	OCCCCCCCCCC	C10(OH)2	20	3.90E-06 (3.18E-06)	NaN (28.09)	NaN (-4.89)	2

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Table S1 – continued from previous page

Index	SMILES	Compound	T	$\Gamma_{max}$ (mol/m <sup>2</sup> )	$\gamma_{cmc}$ (mN/m)	logCMC (M)	Ref
26	CCCCCCCC(=O)O	C7OOH	20	7.29E-06 (7.95E-06)	NaN (35.34)	NaN (-1.46)	2
27	CCCCCCCCC(=O)O	C8OOH	25	1.11E-05 (9.46E-06)	NaN (33.50)	NaN (-2.14)	2
28	CCCCCCCCCC(=O)O	C9OOH	20	8.90E-06 (9.76E-06)	NaN (31.59)	NaN (-2.70)	2
29	CCCCCCCCCCC(=O)O	C10OOH	25	9.86E-06 (9.88E-06)	NaN (29.83)	NaN (-3.14)	2
30	CCCCCCCCCCCCC(=O)O	C12OOH	20	1.02E-05 (1.01E-05)	NaN (26.89)	NaN (-3.82)	2
31	CCCCCCCCCOS(=O)(=O)[O-].[Na+]	C7SO4Na	20	3.47E-06 (3.87E-06)	NaN (41.32)	NaN (-0.53)	2
32	CCCCCCCCCOS(=O)(=O)[O-].[Na+]	C8SO4Na	20	5.16E-06 (4.17E-06)	40.56 (40.75)	-0.94 (-0.99)	2
33	CCCCCCCCCCOS(=O)(=O)[O-].[Na+]	C9SO4Na	20	3.78E-06 (4.25E-06)	NaN (40.30)	NaN (-1.44)	2
34	CCCCCCCCCCCCCOS(=O)(=O)[O-].[Na+]	C12SO4Na	20	4.80E-06 (4.65E-06)	39.07 (39.02)	-2.11 (-2.19)	5

Continued on next page

Table S1 – continued from previous page

Index	SMILES	Compound	T	$\Gamma_{max}$ (mol/m <sup>2</sup> )	$\gamma_{cmc}$ (mN/m)	logCMC (M)	Ref
35	CCCCCCCCCCCCC(=O)(=O)[O-].[Na+]	C14SO4Na	20	4.70E-06 (4.69E-06)	NaN (38.08)	NaN (-2.58)	5
36	CCCCCCCCC(=O)(=O)[O-].[Na+]	C10SO3Na	25	5.50E-06 (5.48E-06)	41.00 (42.40)	-1.32 (-1.54)	6
37	CCCCCCCCCCCCC(=O)(=O)[O-].[Na+]	C12SO3Na	25	3.65E-06 (5.91E-06)	39.98 (41.52)	-1.95 (-1.98)	6
38	CCCCCCCCCCCCC(=O)(=O)[O-].[Na+]	C10E1SO3Na	25	4.71E-06 (4.87E-06)	41.14 (40.98)	-1.80 (-1.79)	6
39	CCCCCCCCCCCCC(=O)(=O)[O-].[Na+]	C8E3SO4Na	25	2.94E-06 (3.67E-06)	40.83 (40.15)	-1.33 (-1.52)	6
40	CCCCCCCCCCCCC(=O)(=O)[O-].[Na+]	C12E1SO3Na	25	5.38E-06 (5.34E-06)	NaN (40.63)	NaN (-2.15)	2
41	CCCCCCCCCCCCC(=O)(=O)[O-].[Na+]	C12E1SO4Na	25	3.80E-06 (3.72E-06)	39.01 (39.72)	-2.41 (-2.43)	2
42	CCCCCCCCCCCCC(=O)(=O)[O-].[Na+]	C12E2SO4Na	25	2.78E-06 (3.02E-06)	41.63 (40.44)	-2.53 (-2.55)	2
43	[O-]S(=O)(OC1CCCCC1CCCCCCCCC)=O.[Na+]	C9THPSO4Na	25	3.23E-06 (3.11E-06)	45.00 (44.96)	-1.52 (-1.58)	7

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Table S1 – continued from previous page

Index	SMILES	Compound	T	$\Gamma_{max}$ (mol/m <sup>2</sup> )	$\gamma_{cmc}$ (mN/m)	logCMC (M)	Ref
44	[O-]S(=O)(OC1CCOCC1CCCCCCCCCCCCC)=O.[Na+]	C11THPSO4Na	25	3.36E-06 (2.90E-06)	44.83 (45.05)	-2.20 (-2.26)	7
45	[O-]S(=O)(OC1CCOCC1CCCCCCCCCCCCC)=O.[Na+]	C13THPSO4Na	25	2.54E-06 (2.67E-06)	45.11 (44.81)	-2.83 (-2.85)	7
46	[O-]S(=O)(OC1CCOCC1CCCCCCCCCCCCC)=O.[Na+]	C15THPSO4Na	25	2.74E-06 (2.68E-06)	45.53 (43.67)	-3.45 (-3.19)	7
47	CCCCCCCC[N+](C)(C)(C).[Br-]	C10TAB	20	3.80E-06 (4.38E-06)	NaN (39.75)	NaN (-1.33)	2
48	CCCCCCCC[N+](C)(C)(C).[Br-]	C12TAB	25	4.56E-06 (4.50E-06)	39.16 (39.12)	-1.90 (-1.91)	8
49	CCCCCCCC[N+](C)(C)(C).[Br-]	C14TAB	25	4.55E-06 (4.56E-06)	37.83 (38.28)	-2.44 (-2.50)	8
50	CCCCCCCC[N+](C)(C)(C).[Br-]	C15TAB	25	4.50E-06 (4.62E-06)	NaN (37.98)	NaN (-2.82)	9
51	CCCCCCCC[N+](C)(C)(C).[Br-]	C16TAB	25	4.78E-06 (4.65E-06)	37.86 (37.69)	-3.05 (-3.08)	8
52	CCCCC(=O)[O-].[Na+]	C6OONa	22	3.57E-06 (3.36E-06)	NaN (34.84)	NaN (-0.93)	10

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Table S1 – continued from previous page

Index	SMILES	Compound	T	$\Gamma_{max}$ (mol/m <sup>2</sup> )	$\gamma_{cmc}$ (mN/m)	logCMC (M)	Ref
53	CCCCCCCCC(=O)[O-].[Na+]	C8OONa	22	4.01E-06 (4.06E-06)	NaN (33.80)	NaN (-1.90)	10
54	CCCCCCCCCCC(=O)[O-].[Na+]	C10OONa	25	5.96E-06 (5.79E-06)	NaN (31.48)	NaN (-2.76)	10
55	CCCCCCCCCCCCC(=O)N(C)CC(O)C(O)C(O)C(O)CO	C11GA	25	4.07E-06 (4.24E-06)	30.90 (30.65)	-2.80 (-2.95)	11
56	CCCCCCCCCCCCCCC(=O)N(C)CC(O)C(O)C(O)C(O)CO	C12GA	25	4.49E-06 (4.41E-06)	30.00 (29.80)	-3.46 (-3.35)	11
57	CCCCCCCCCCCCCCC(=O)N(C)CC(O)C(O)C(O)C(O)CO	C13GA	25	4.81E-06 (4.55E-06)	28.54 (28.89)	-4.05 (-3.72)	11
58	CCCCCCCCCCCCCCC(=O)N(C)CC(O)C(O)C(O)C(O)CO	C14GA	25	4.72E-06 (4.64E-06)	36.24 (28.04)	-4.81 (-3.96)	11
59	CCCCCCCCCCCCCCC(=O)N(C)CC(O)C(O)C(O)CO	C12XA	25	4.40E-06 (4.53E-06)	28.26 (28.88)	-3.45 (-3.55)	11
60	CCCCCCCCCCCCCCC(=O)N(C)CC(O)CO	C12GlyA	25	4.75E-06 (4.75E-06)	26.52 (26.16)	-3.67 (-3.68)	11
61	CCCCCCCCCCCCCO	C8E1	25	5.73E-06 (5.91E-06)	26.68 (26.24)	-2.29 (-2.37)	12

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Table S1 – continued from previous page

Index	SMILES	Compound	T	$\Gamma_{max}$ (mol/m <sup>2</sup> )	$\gamma_{cmc}$ (mN/m)	logCMC (M)	Ref
62	CCCCCCCCOC(CO)CO	C8C(COH)2	25	5.43E-06 (5.44E-06)	24.58 (24.55)	-2.19 (-2.21)	12
63	CCCCCCCCCCC([n+][1cccc1])C(=O)[O-]	C12PYR	25	2.03E-06 (1.99E-06)	39.98 (40.03)	-2.27 (-2.28)	13
64	CCCCCCCCCCCCC([n+][1cccc1])C(=O)[O-]	C14PYR	25	1.84E-06 (2.33E-06)	37.04 (38.70)	-3.23 (-2.65)	13
65	CCCCCCCCCCCCC([N+](C)(C)CC(=O)[O-])	C12N+C1COO-	25	3.69E-06 (2.43E-06)	36.72 (43.45)	-2.71 (-2.28)	14
66	CCCCCCCCCCCCC([N+](C)(C)CCCC(=O)[O-])	C12N+C3COO-	25	2.35E-06 (2.36E-06)	44.12 (44.37)	-2.38 (-2.44)	14
67	CCCCCCCCCCCCC([N+](C)(C)CCCCC(=O)[O-])	C12N+C4COO-	25	2.44E-06 (2.30E-06)	44.62 (44.16)	-2.48 (-2.51)	14
68	CCCCCCCCCCCCC([N+](C)(C)CCCCC(=O)[O-])	C12N+C5COO-	25	2.49E-06 (2.24E-06)	44.61 (43.68)	-2.56 (-2.58)	14
69	CCCCCCCCCCCCC([N+](C)(C)CCCCCCCCC(=O)[O-])	C12N+C7COO-	25	1.91E-06 (2.04E-06)	41.20 (41.69)	-2.80 (-2.83)	14
70	CCCCCCCCCCCCC([N+](C)(C)CCCCCCCCCCC(=O)[O-])	C12N+C10COO-	25	2.05E-06 (2.24E-06)	38.46 (38.81)	-3.76 (-3.31)	14

Continued on next page

Table S1 – continued from previous page

Index	SMILES	Compound	T	$\Gamma_{max}$ (mol/m <sup>2</sup> )	$\gamma_{cmc}$ (mN/m)	logCMC (M)	Ref
71	CCCCCCCCO[C@H]1[C@@H]([C@H]([C@@H]([C@H](O1)CO)O)O)O	C8Glu	25	3.96E-06 (3.94E-06)	30.60 (31.10)	-1.57 (-1.50)	15
72	CCCCCCCCCO[C@H]1[C@@H]([C@H]([C@@H]([C@H]([C@@H](O1)CO)O)O)O	C10Glu	22	4.41E-06 (4.22E-06)	28.66 (29.99)	-2.71 (-2.81)	15
73	CCCCCCCCCO[C@H]1[C@@H]([C@H]([C@@H]([C@H](O1)CO)O)O)O	C8Mal	25	3.67E-06 (3.49E-06)	39.44 (38.70)	-1.68 (-1.63)	16
74	CCCCCCCCCO[C@H]1[C@@H]([C@H]([C@@H]([C@H](O1)CO)O)O)O	C10Mal	22	3.33E-06 (3.57E-06)	37.46 (37.35)	-2.66 (-2.63)	15
75	CCCCCCCCCS[C@H]1[C@@H]([C@H]([C@@H]([C@H](O1)CO)O)O)O	C10SMal	22	3.55E-06 (3.56E-06)	38.03 (37.76)	-3.12 (-2.98)	15
76	CCCCCCCCCO[C@H]1[C@@H]([C@H]([C@@H]([C@H](O1)CO)O)O)O	C12Mal	25	4.07E-06 (3.67E-06)	35.42 (35.92)	-3.81 (-3.59)	16
77	CCCCCCCCCCCCCO[C@H]1[C@@H]([C@H]([C@@H]([C@H](O1)CO)O)O)O	C14Mal	25	3.54E-06 (3.73E-06)	34.32 (34.58)	-4.62 (-4.40)	16
78	C[Si](C)(C)O[Si](C)(CCCCCCCCCCCCCO)O[Si](C)(C)C	TriSE4	23	5.72E-06 (5.88E-06)	23.05 (23.04)	-4.10 (-4.17)	17

Continued on next page





## 2 Molecular descriptors

As shown in Fig. 4 and Table 3 of the main text, Two molecular descriptors (‘Surface area of headgroups’ and ‘Surface area of tailgroups’) are developed using molecular dynamic (MD) simulations. The system consists of water molecules and a surfactant. The dimension of the system is  $5 \times 5 \times 5 \text{ nm}^3$ , and the periodic boundary conditions are adopted in all directions. The water molecules are modeled using TIP3P, and all surfactants are modeled based on OPLS forcefields, obtained through the LigParGen web server.

To prepare an equilibrated system, we first build a system by packing one surfactant molecule with 3800 water molecules using the Packmol code. This is followed by an energy minimization run using the steepest descent algorithm until the maximal force is less than  $100 \text{ kJ mol}^{-1} \text{ nm}^{-1}$ . Next, a 10 ns simulation in the canonical (NVT) ensemble is performed under a temperature of 300 K. Then we additionally run a 5 ns NVT ensemble as a production run under the same condition. All simulations are performed using the Gromacs code (version 2020.3-modified). The SETTLE algorithm is used to maintain the water molecules’ geometry. The velocity-rescaling thermostat with a relaxation time of 0.1 ps is used to keep the fluid temperature at 300 K. A cutoff of 1.4 nm is used to compute the LJ potentials. The particle mesh Ewald (PME) method with an FFT spacing of 0.12 nm and a tolerance of  $10^{-1}$  is applied to compute electrostatic interactions. LINCS algorithm is applied to the bonds with hydrogen atoms in surfactants.

To implement the ellipsoid approximation, the gromacs command `gmx principal` is used. `gmx principal` calculates the three principal axes of inertia for a group of atoms as well as its moment of inertia of the group. The each output file `paxis1.xvg`, `paxis2.xvg`, and `paxis3.xvg` contains a normalized vector along the three principal axes in the Cartesian coordinate, respectively. In the file `moi.xvg`, the other output file of `gmx principal`, the moment of inertia along the three principal axes is included. The moment of inertia along the major axis is stored first, followed by that along the middle and the minor axis. To fit an ellipsoid, we equate the moment of inertia of the atoms to that of an ellipsoid

$$I_{z'} = \frac{m}{5}(a^2 + b^2) \quad (1)$$

$$I_{y'} = \frac{m}{5}(a^2 + c^2) \quad (2)$$

$$I_{x'} = \frac{m}{5}(b^2 + c^2) \quad (3)$$

where  $a$ ,  $b$ , and  $c$  are half the length of the principal axes ( $x'$ ,  $y'$ , and  $z'$ ).  $I_{x'}$  is the moment

of inertia along with the  $x'$  axis and  $m$  is mass of an ellipsoid ( $m$  is set to 1). In order to make the value invariant to the number of atoms used for fitting, the moment of inertia is divided by the number of atoms used for fitting.

$$I' = I/n \quad (4)$$

where  $n$  is the number of atoms used for fitting. Since  $I$  in the principal axes can be computed using `gmx principal`, the equations can be rewritten as

$$a^2 = \frac{2.5(I'_{x'} + I'_{y'} + I'_{z'}) - 5I'_{x'}}{m} \quad (5)$$

$$b^2 = \frac{2.5(I'_{x'} + I'_{y'} + I'_{z'}) - 5I'_{y'}}{m} \quad (6)$$

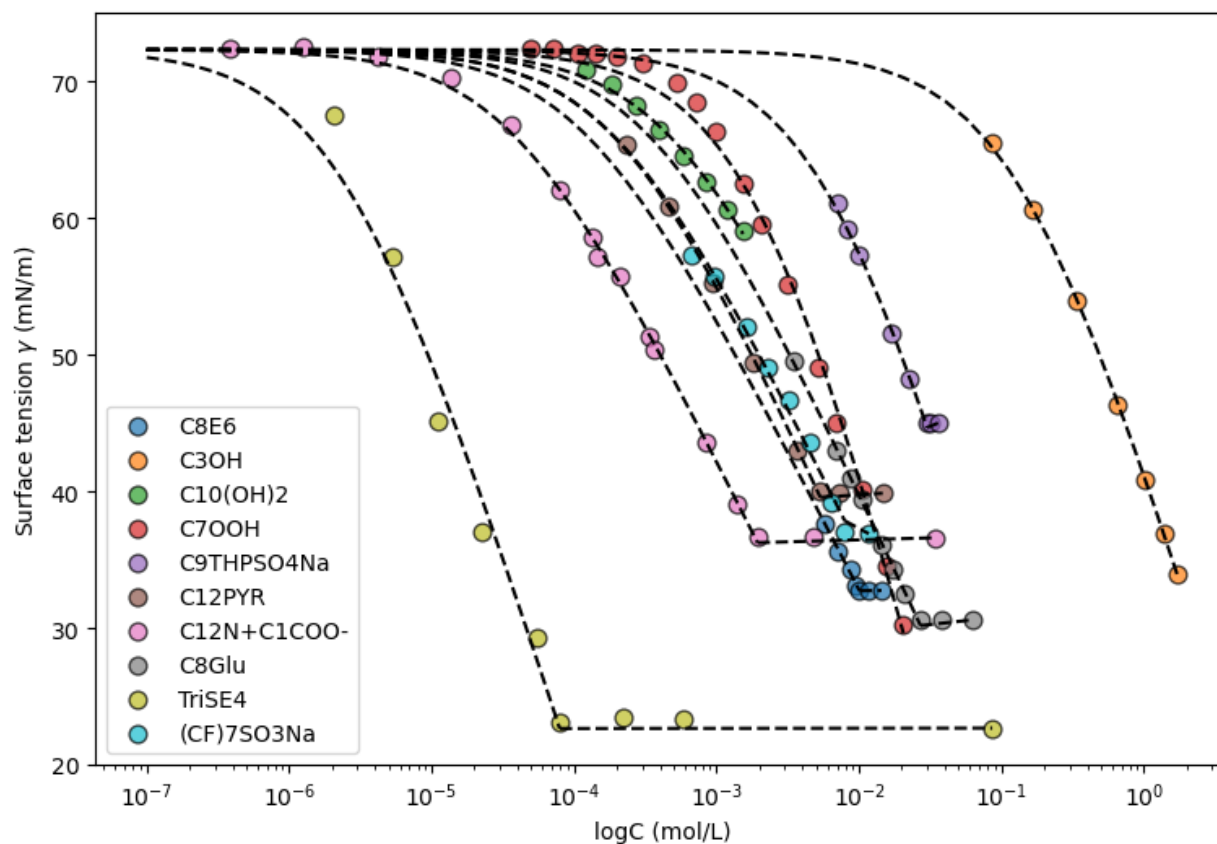
$$c^2 = \frac{2.5(I'_{x'} + I'_{y'} + I'_{z'}) - 5I'_{z'}}{m} \quad (7)$$

Finally, the surface area of the fitted ellipsoid is the following

$$S = 4\pi \left( \frac{a^p b^p + a^p c^p + b^p c^p}{3} \right)^{1/p} \quad (8)$$

where  $S$  is the surface area of the ellipsoid and  $p \simeq 1.6$ . The ellipsoid approximation is implemented twice per surfactant because they are divided into headgroup and tailgroup. The headgroup is defined as all non-carbon atoms (excluding hydrogen) and some carbon atoms adjacent to non-carbon atoms. And, the tailgroup is defined as the remaining carbon atoms. The ellipsoid of the headgroup and that of the tailgroup for each surfactant are fitted to calculate the surface area of the headgroup and tailgroup, respectively. If  $n$  is smaller than 3, the number of atoms required for ellipsoid fitting, the resulting  $S$  I set to 0. The calculated values are available in the data set.

### 3 Surface Tension Isotherms of Surfactants



**Figure S1:** Surface Tension Isotherms of Surfactants

### References

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