

Prediction of Critical Micelle Concentration of Some Anionic Surfactants Using Multiple Regression Techniques: A Quantitative Structure–Activity Relationship Study

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ABSTRACT: Computer-assisted methods were employed to develop a statistical relationship between molecular-based structural parameters and log critical micelle concentration (CMC) of some anionic surfactants. The CMC of 31 alkyl sulfates and alkanesulfonates were used for model generation. Among different models, two equations were selected as the best, and their specifications are given. The statistics of these models together with cross-validation results indicate the capability of both models to predict the CMC of anionic surfactants. Three descriptors of Wiener number, reciprocal of the dipole moment, and reciprocal of the Randic index appear in the models. Results indicate that topological characteristics, such as compactness and branching of anionic surfactants, play major roles in micelle formation. Polarity of the molecules is also important, but its effect is less than that of topology of the surfactants.

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KEY WORDS: Alkanesulfonates, alkyl sulfates, anionic surfactants, computer modeling, critical micelle concentration, multiple regression technique, quantitative structure–activity relationship.

Anionic surfactants are among the most versatile chemicals available to chemists, and are used in a variety of products including detergents, pharmaceuticals, antimicrobial agents, and corrosion inhibitors (1–4). To design a new surfactant with a special property while minimizing costs associated with trial-and-error research, it is desirable to study different structural or electronic parameters affecting the surface-active properties of these compounds.

Compared to other properties, elucidation of critical micelle concentration (CMC) requires more attention because it can be correlated with industrially important characteristics of surfactant performance such as viscosity, foam stability, detergency, and dispersion ability. For example, in designing a laundry detergent, the surfactant concentration should be higher than the CMC to ensure the presence of micelles in which dirt and oily substances can be solubi-

lized. In order to perform micellar electrokinetic chromatography (MEKC), a surfactant solution at a concentration higher than the CMC must be used as a separation solution. Therefore, knowing the CMC is essential in developing these experiments.

CMC is experimentally obtained by monitoring the variation of a physicochemical property of the solution with changing surfactant concentration (5). Some of the physical properties that have been used for this purpose include solution detergency, viscosity, density, electric conductivity (6), surface tension (7), osmotic pressure, refractive index, and light scattering. Other more sophisticated techniques have been reported including X-ray diffraction, electron spin resonance techniques, nuclear magnetic resonance spectroscopy (8), calorimetry (9), cyclic voltammetry (10), polarographic (11) and chromatographic techniques, fluorescence emission spectroscopy (12), and ultraviolet-visible absorption spectroscopy.

Recently, Nakamura and coworkers (13) devised a method for determining the CMC of anionic surfactants using capillary electrophoresis (CE). This method requires as little as 300 μL of the surfactant for CMC measurements compared with larger volumes of surfactants required by other methods.

In contrast to the interest in experimental methods for CMC determination, few theoretical works and computer models of self-assembling surfactant solutions are reported (14,15). Recently, two computer programs based on molecular thermodynamic theories of surfactant solution behavior were developed (16). These programs are capable of predicting fundamental micellar properties such as CMC and micellar shape and size. However, in designing a new surfactant, one needs to analyze different topological, geometric, and electronic parameters that affect surfactant properties, and these programs are not very useful in this respect. It is noteworthy that the most serious theoretical studies of surfactant systems are those that have used Monte Carlo and molecular dynamics as a tool for simulation (17). Owing to the lack of comprehensive theoretical work in this area, the development of a model for estimating the CMC of surfactants is necessary.

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TABLE 1
Data Set

Compound	Compound	Compound
1 C ₁₀ H ₂₁ SO ₄ Na	12 CH ₃ (CHSO ₄)C ₁₃ H ₂₇ Na	23 C ₁₁ H ₂₃ CH(C ₃ H ₇)CH ₂ SO ₄ Na
2 C ₁₂ H ₂₅ SO ₄ Na	13 CH ₃ CH ₂ (CHSO ₄)C ₁₂ H ₂₅ Na	24 C ₁₀ H ₂₁ CH(C ₄ H ₉)CH ₂ SO ₄ Na
3 C ₁₃ H ₂₇ SO ₄ Na	14 CH ₃ C ₃ H ₆ (CHSO ₄)C ₁₀ H ₂₁ Na	25 C ₉ H ₁₉ CH(C ₅ H ₁₁)CH ₂ SO ₄ Na
4 C ₁₄ H ₂₉ SO ₄ Na	15 CH ₃ C ₆ H ₁₂ (CHSO ₄)C ₇ H ₁₅ Na	26 C ₈ H ₁₇ CH(C ₆ H ₁₃)CH ₂ SO ₄ Na
5 C ₁₅ H ₃₁ SO ₄ Na	16 CH ₃ C ₂ H ₄ (CHSO ₄)C ₁₂ H ₂₅ Na	27 C ₇ H ₁₅ CH(C ₇ H ₁₅)CH ₂ SO ₄ Na
6 C ₁₆ H ₃₃ SO ₄ Na	17 CH ₃ C ₄ H ₈ (CHSO ₄)C ₁₀ H ₂₁ Na	28 C ₁₀ H ₂₁ SO ₃ Na
7 CH ₃ (CHSO ₄)C ₁₂ H ₂₅ Na	18 CH ₃ C ₆ H ₁₂ (CHSO ₄)C ₈ H ₁₇ Na	29 C ₁₂ H ₂₅ SO ₃ Na
8 CH ₃ CH ₂ (CHSO ₄)C ₁₁ H ₂₃ Na	19 CH ₃ (CHSO ₄)C ₁₅ H ₃₁ Na	30 C ₁₄ H ₂₉ SO ₃ Na
9 CH ₃ C ₂ H ₄ (CHSO ₄)C ₁₀ H ₂₁ Na	20 CH ₃ C ₇ H ₁₄ (CHSO ₄)C ₈ H ₁₇ Na	31 C ₁₆ H ₃₃ SO ₃ Na
10 CH ₃ C ₃ H ₆ (CHSO ₄)C ₉ H ₁₉ Na	21 C ₁₃ H ₂₇ CH(CH ₃)CH ₂ SO ₄ Na	
11 CH ₃ C ₅ H ₁₀ (CHSO ₄)C ₇ H ₁₅ Na	22 C ₁₂ H ₂₅ CH(C ₂ H ₅)CH ₂ SO ₄ Na	

In this study, computer-assisted methods were employed to generate a statistical relationship between molecular structural parameters (descriptors) and the log CMC of some anionic surfactants. The anionic surfactants consist of alkyl sulfates and alkanesulfonates (Table 1). In alkyl sulfates, the sulfur atom is joined to the carbon atom of the hydrophobe *via* an oxygen atom, whereas in the case of a sulfonate, the sulfur is joined directly to the hydrophobe. This difference in structure gives significant differences in properties between the sulfonate and sulfate groups (18).

EXPERIMENTAL PROCEDURES

The methodology used in this study consists of three fundamental stages: (i) selection of the data set, (ii) molecular descriptor generation, and (iii) regression analysis. Computation of descriptors was performed using FORTRAN programs developed in our laboratory. The SPSS/PC package (19) was used for regression calculations. MOPAC (version 6.0) (20) and HyperChem packages (21) were used for optimization of the molecules.

Data set. Experimental values of the CMC for different anionic surfactants are taken from the literature (22). A total of 31 compounds, including 27 alkyl sulfates (RSO₄Na) and 4 alkanesulfonates (RSO₃Na), were considered, for which the CMC (mol/L) was reported at 40°C (Table 1). It can be seen from Table 1 that the structures are very diverse and the sulfate head group position varies considerably.

Descriptor generation. Fourteen molecular structure descriptors were calculated for each compound in the data set. These descriptors can be classified into three major groups—topological, geometric, and electronic. Topological descriptors include Wiener number (WI) (23) and Randic (RA⁻¹) (24) and Balaban indices (25). Geometric descriptors include van der Waals molecular volume (26), maximum distance between the atoms in the molecule, and the surface areas of the head and the tail of the molecules. These descriptors were calculated using a FORTRAN 77 program developed in our laboratory. Electronic

descriptors consist of heat of formation, dipole moment (DIP), net atomic charges, total charges on the head of the molecule, partial charge of the most negative atom in the molecule, and ionization potential. Geometric and electronic descriptors depend on the three-dimensional coordinates of the atoms; therefore, calculations of these types of descriptors require optimization of the molecular structure for each molecule. In this work, AM1 Hamiltonian implemented in the MOPAC and HyperChem packages were used for optimization.

Generation and evaluation of the regression model. The linear regression method was based on the construction of a linear mathematical equation relating the observed log CMC to numerically encoded structural parameters. Linear models were generated using a stepwise regression method (27). The choice of which equation to consider further was made by using four criteria: multiple correlation coefficient (*R*), standard deviation (SD), *F* value for the statistical significance of the model, and the ratio of the number of observations modeled to the number of descriptors in the equation. An ideal model is one that has high *R* and *F* values, low SD, and the least numbers of independent variables (descriptors).

The best resulting equations were tested for their predictive power using a cross-validation procedure (28). For each model, a number of molecules equal to the number of descriptors appearing in the model were eliminated from the data set each time and then a model was developed using the remaining compounds. Finally, the log CMC of eliminated molecules was predicted by the generated model.

RESULTS AND DISCUSSION

A number of good models were obtained using experimental values of log CMC as dependent variables and calculated descriptors as independent variables. Among these equations, two of the best models were selected and their specifications are given in Tables 2 and 3. These models were selected due to their high values of *R* and *F* statistics and low SD. Comparison of the statistics for models 1 and

TABLE 2
Specification of MLR Model 1^a

Descriptor	Coefficient ^b	Mean effect
Wiener number (WI)	$-1.5759 \times 10^{-3} \pm (5.9638 \times 10^{-5})$	-1.7444
Reciprocal of dipole moment (DIP ⁻¹)	$5.1312 \pm (0.7027)$	0.2556
Constant	$-1.0323 \pm (0.0783)$	

^aStatistics for this equation are $n = 31$, $r = 0.9820$, $SD = 0.0887$, and $F = 389$. MLR, multiple linear regression.

^bThe standard error (SE) of coefficients is given in parentheses. These values are a measure of coefficient dispersion and are obtained by dividing the standard deviations by the square root of the number of surfactants used for development of the model ($n = 31$).

2 given in Tables 2 and 3, respectively, reveals the superiority of model 2 over that of model 1. However, fewer descriptors (two parameters) appear in model 1 compared to model 2 (three parameters), and its statistics reveal that this equation also represents a good model for predicting the log CMC of anionic surfactants. Models 1 and 2 have two parameters of WI and reciprocal of dipole moment, DIP⁻¹, in common. These descriptors show no correlation with each other and can be considered independent parameters. However, two descriptors of WI and RA⁻¹ index in model 2 show a negative correlation ($R = -0.9199$), but each encodes different aspects of molecular structure.

WI is a topological descriptor defined as (29)

$$WI = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N D_{ij} \quad [1]$$

where the summations are overall atoms in the molecule and D_{ij} represents the distance between atoms i and j . In graph theory, distance is defined as the shortest path between a pair of atoms in a structure. Therefore, WI appears to be a convenient measure of molecule compactness. The negative mean effect of this parameter in both models reveals that, as the compactness of an anionic surfactant increases, its CMC decreases.

The RA⁻¹ index quantifies the notion of molecular branching, and its reciprocal shows a considerably positive mean effect on CMC (Table 3). This agrees with the experiment, which shows that, as the length of a side chain increases, the CMC decreases. In addition, carbon atoms on a branched hydrophobe have about half the effect of carbon atoms on a straight chain (30). The positive effect of

the reciprocal of the RA⁻¹ index confirms this observation. The superiority of model 2 over model 1 may be because this model considers both molecule compactness and branching characteristics.

Appearance of DIP as a descriptor in both models indicates that polarity of the anionic surfactants, as well as topology, plays a role in micelle formation. The calculated values of the descriptors appearing in the selected models, along with the calculated values of log CMC obtained using models 1 and 2 together with the experimental values, are given in Table 4. Inspection of these data reveals that, in agreement with the experiment, as the length and therefore molecular size of the molecules increase, the WI increases and the CMC decreases. It is also seen from this table that as hydrophobe length increases, the DIP⁻¹ parameter, as well as log CMC, decrease (compare the DIP⁻¹ for surfactants 1–6 given in Table 4). Inspection of Table 4 also indicates that for molecules 7–11, as the sulfate group position varies and moves toward the center of the chain, DIP⁻¹ increases. For these surfactants, in agreement with experiment, as the DIP decreases, the CMC increases. A similar conclusion can be drawn for molecules 12–15, 16–18, and 19 and 20, given in Table 4. Molecules 21–27 require special attention. These surfactants contain a C-16 hydrophobic group, and RA⁻¹ is identical for all of them. This indicates a similarity of branching characteristic for these compounds. However, the compactness of these molecules and also their DIP vary considerably. Calculated values of log CMC for these anionic surfactants are in good agreement with experimental values. As the compactness of a molecule increases and its DIP decreases, the CMC increases.

TABLE 3
Specification of MLR Model 2^a

Descriptor	Coefficient	Mean effect
Wiener number	$-9.7401 \times 10^{-4} \pm (1.3165 \times 10^{-4})$	-1.0476
Reciprocal of Randic index (RA ⁻¹)	$11.0284 \pm (2.2709)$	1.3605
Reciprocal of dipole moment	$6.7040 \pm (0.6150)$	0.3340
Constant	$-3.1373 \pm (0.4374)$	

^aStatistics for this equation are $n = 31$, $r = 0.9912$, $SD = 0.0661$ and $F = 477$. See Table 2 for abbreviations.

^bSE of coefficients are given in parentheses. These values are a measure of dispersion of the coefficients. See Table 2 for more details.

TABLE 4
Experimental and Calculated Values of log CMC and Descriptors Employed in the Models

Compound ^a	Descriptor ^b			log CMC ^c		
	WI	RA ⁻¹	DIP ⁻¹ (debye ⁻¹)	Calculated, model 1	Calculated, model 2	Experimental
1	526	0.1686	0.0427	-1.6424	-1.5045	-1.4724
2	776	0.1451	0.0346	-2.0777	-2.0604	-2.0675
3	926	0.1269	0.0316	-2.3297	-2.4279	-2.3665
4	1094	0.1269	0.0290	-2.6076	-2.6088	-2.6576
5	1281	0.1193	0.0268	-2.9135	-2.8891	-2.9208
6	1488	0.1126	0.0249	-3.2495	-3.1775	-3.2366
7	1034	0.1216	0.0391	-2.4611	-2.5405	-2.4815
8	984	0.1274	0.0498	-2.3278	-2.3573	-2.3665
9	944	0.1274	0.0598	-2.2132	-2.2509	-2.2882
10	914	0.1274	0.0730	-2.0982	-2.1333	-2.1707
11	884	0.1274	0.1022	-1.9009	-1.9081	-2.0132
12	1216	0.1203	0.0356	-2.7659	-2.7561	-2.7670
13	1161	0.1198	0.0448	-2.6324	-2.6474	-2.6576
14	1081	0.1198	0.0475	-2.4921	-2.5509	-2.4685
15	1036	0.1198	0.1012	-2.1456	-2.1470	-2.1772
16	1308	0.1130	0.0475	-2.8500	-2.8467	-2.7645
17	1238	0.1130	0.0699	-2.6247	-2.6284	-2.6290
18	1208	0.1130	0.0975	-2.4360	-2.4144	-2.3716
19	1641	0.1074	0.0323	-3.4529	-3.3350	-3.3098
20	1396	0.1070	0.0977	-2.7308	-2.6622	-2.6290
21	1410	0.1140	0.0302	-3.0996	-3.0512	-3.0969
22	1344	0.1135	0.0354	-2.9688	-2.9574	-3.0458
23	1289	0.1135	0.0399	-2.8589	-2.8735	-2.9586
24	1248	0.1135	0.0454	-2.7662	-2.7969	-2.8239
25	1218	0.1135	0.0511	-2.6895	-2.7292	-2.6990
26	1200	0.1135	0.0575	-2.6285	-2.6691	-2.6383
27	1194	0.1135	0.0621	-2.5954	-2.6323	-2.5228
28	424	0.1739	0.0443	-1.4733	-1.3350	-1.2403
29	643	0.1482	0.0357	-1.8625	-1.8901	-2.0362
30	926	0.1291	0.0298	-2.3388	-2.4162	-2.4089
31	1281	0.1143	0.0255	-2.9202	-2.9534	-2.8633

^aNumbers refer to the surfactants given in Table 1.

^bSee Tables 2 and 3 for abbreviations.

^cCMC, critical micelle concentration.

Further inspection of Table 4 shows that calculated log CMC values for alkanesulfonates (R-SO₃⁻) are not generally as satisfactory compared to the alkyl sulfates (R-SO₄⁻). This could be partly due to discrepancies in experimental values reported for these compounds (22). For example, values of 57.5 (31) and 40 mmol/L (32) were reported for the CMC of molecule 28 (C₁₀H₂₁SO₃⁻) by different groups. Values of 1.37 (31) and 0.74 mmol/L (22), a difference of about 50%, are reported for the CMC of surfactant 31 (C₁₆H₃₃SO₃⁻). It is noteworthy that even a very recent CE technique developed for CMC determination shows different values for the CMC of anionic surfactants using different methods (13).

To test the validity of the selected models, cross-validation procedures as described in the Experimental Procedures section were used. Results from these calculations are given in Table 5. This table reveals values of 0.9272 and 0.9457 for the cross-validated Q² of models 1 and 2, respectively. This indicates a capability of both models in predicting the CMC for anionic surfactants and the superiority of model 2 over model 1.

TABLE 5
Results of Cross-Validation Procedure

Q ² (n) ^a	Model 1		Model 2	
	Q ² (n) ^a	Press	Q ² (n) ^a	Press
0.9313 (2)	0.0605	0.0221	0.9752 (3)	0.0221
0.9997 (2)	0.000	0.0073	0.9646 (3)	0.0073
0.8903 (2)	0.0173	0.0145	0.8051 (3)	0.0145
0.8615 (2)	0.0084	0.0392	0.8957 (3)	0.0392
0.9072 (2)	0.003	0.0148	0.9867 (3)	0.0148
0.8554 (2)	0.0517	0.0041	0.9790 (3)	0.0041
0.6963 (2)	0.0073	0.0301	0.9849 (3)	0.0301
0.9570 (2)	0.0483	0.0066	0.9920 (3)	0.0066
0.9654 (2)	0.0059	0.0093	0.9736 (3)	0.0093
0.9981 (2)	0.0007	0.0157	0.9303 (3)	0.0157
0.9420 (2)	0.1071	0.0099	0.9155 (1)	0.0099
0.9940 (2)	0.0036			
0.9596 (2)	0.0134			
0.9687 (2)	0.0017			
0.9410 (2)	0.0114			
0.9679 (1)	0.0038			

^aNumbers in parentheses represent the number of molecules that have to be removed from a data set each time.

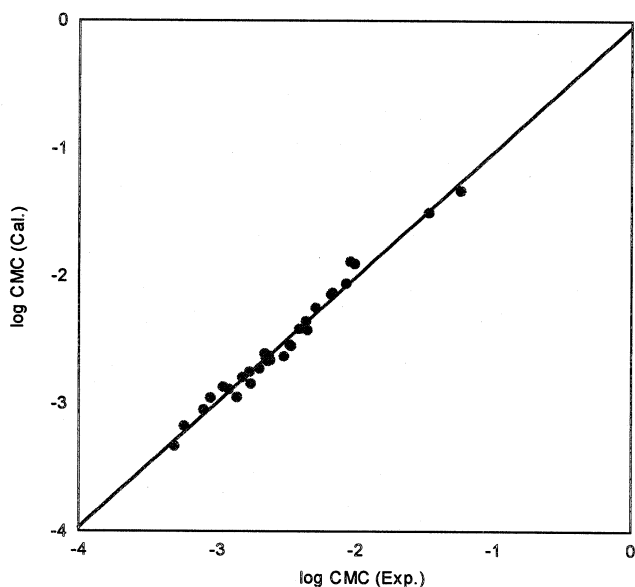


FIG. 1. Plot of calculated vs. experimental values of log critical micelle concentration (CMC).

Figure 1 shows a plot of calculated log CMC using model 2 vs. experimental values. This line shows a high correlation coefficient ($r = 0.9907$) and a low standard error ($SE = 0.0631$). Residuals of the multiple linear regression (MLR)-predicted values for log CMC are plotted against experimental values in Figure 2. Propagation of residuals on both sides of zero indicates that no systematic error exists in the development of the MLR model.

From the results of this work, one may conclude that topological characteristics, such as compactness and branching of anionic surfactants, play a major role in micelle formation. Polarity of the molecules also is important in this respect, but its effect is less than surfactants topology. It can be concluded that development of a linear equation between log CMC and numerical encoded structural parameters might be of some help in designing new surfactants.

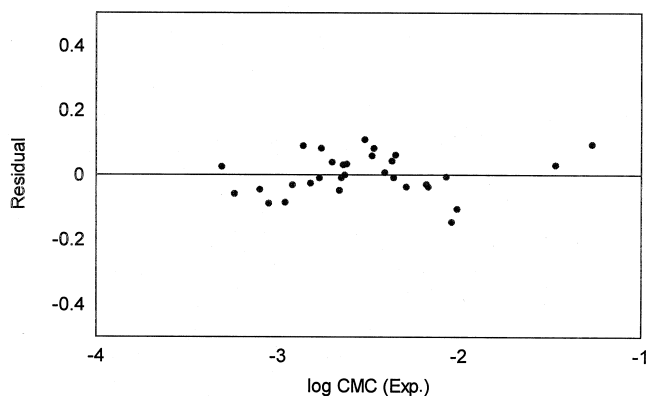


FIG. 2. Plot of residual vs. experimental values of log CMC. See Figure 1 for abbreviation.

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