Asian Journal of Chemistry Vol. 19, No. 4 (2007), 2479-2489

Prediction of Critical Micelle Concentration of some Anionic and Cationic Surfactants Using an Artificial Neural Network

MOHAMMAD HOSSEIN FATEMI*, ELAHE KONUZE† and MAHDI JALALI-HERAVI‡
Department of Chemistry, Mazandaran University, P. O. Box-453, Babolsar, Iran
E-mail: mhfatemi@umz.ac.ir

The critical micelle concentration (CMC) of a set of 58 alkylsulfates, alkylsulfonates, alkyltrimethyl ammonium and alkylpyridinium salts were predicted using an artificial neural network (ANN). The multiple linear regression (MLR) technique was used to select the important descriptors that act as inputs for artificial neural network. These descriptors are Balaban index, heat of formation, maximum distance between the atoms in the molecule, Randic index and volume of the molecule. Designed artificial neural network is a fully connected back-propagation network that has a 5-5-1 architecture. The results obtained using neural network were compared with those obtained using MLR technique. Standard error of calibration and standard error of prediction were 0.318 and 0.291, respectively for the MLR model and 0.137 and 0.122, respectively for the ANN model. These values reveal the superiority of artificial neural network over MLR model in prediction of log CMC for anionic and cationic surfactants.

Key Words: Critical micelle concentration, Surfactants, Aritifical neural network.

INTRODUCTION

By far the largest class of surface-active materials in general use today is the anions, which constitute *ca.* 70-75 % of total consumption. The reason is the ease and low cost of manufacture and they are used in practically every type of detergent, the main application of surfactants. The major subgroups of anionic surfactants are the alkali carboxylates or soaps, sulfates and sulfonates[1]. Cationic surfactants play an important role as antiseptic agents in cosmetics, as general fungicides and germicides and in a number of bulk chemical applications. There are two important categories of cationic surfactants, which differ mainly in the nature of the nitrogen-containing group. The first consists of the alkyl nitrogen compounds

†Department of Chemistry, Islamic Azad University, Central Tehran Branch, Tehran, Iran.
‡Department of Chemistry, Sharif University of Technology, P.O. Box 11365-9516, Tehran, Iran.

with long-or-short chain alkyls, alkylaryls or aryls and the second category contains heterocyclic materials typified by the pyridinium morpholinium and imidozolinium derivatives[2].

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[3]. CMC is experimentally obtained by monitoring the variation of a physico-chemical property of the solution with changing surfactant concentration[4]. The CMC of ionic surfactants has been determined using many methods[5-12]. In contrast to the interest in experimental methods for CMC determination, few theoretical works and computer models of self-assembling surfactant solutions are reported[13-15]. It is note worthy that the most serious theoretical studies of surfactant systems are those that have used Monte Carlo and molecular dynamics as a tool for simulation[16]. Due to lack of comprehensive theoretical work in this area, the development of a model for estimating the CMC of surfactants is necessary.

Artificial neural networks (ANN) have been used to a wide variety of chemical problems such as simulation of mass spectra[17], prediction of ^{13}C NMR chemical shift[18], modeling of ion interaction chromatography[19-21] and quantitative structure-activity relationships (QSAR) studies[22-26].

In our previous works, different groups of surfactants (cationic and anionic) were modeled separately[27]. It is interesting to improve more generic models that can be able to modeling the CMC of both anionic and cationic surfactants. In addition it seems that some descriptors have nonlinear relation with the CMC, therefore it is desirable to use artificial neural network for modeling. In the present study an ANN was employed to generate a QSAR model between the molecular based structural parameters (descriptors) and observed CMC of a diverse set of cationic and anionic surfactants. Then the generated ANN model was evaluated and applied for the prediction of the CMC of a test set of surfactants. As far as we are aware, this is the first quantitative structure-property relationships (QSPR) study using ANN for the prediction of the CMC of some surfactants.

EXPERIMENTAL

A detailed description of the theory behind a neural network has been adequately described elsewhere[28-30]. Neural network can use qualitative as

well as quantitative inputs and it does not require an explicit relationship between the inputs and the outputs. Although in statistics the analysis is limited to a certain number of possible interactions, more terms can be examined for interactions by the ANN. Also, by allowing more data to be analyzed at the same time, more complex and subtle interactions can be studied using this technique.

Data set

Experimental values of the CMC for different anionic and cationic surfactants are taken from the values reported by reference[30]. As shown in Table-1, the data set consists of 31 alkylsulfates [RSO_4Na] and alkanesulfonates [RSO_3Na] of anionic surfactants and 27 alkyltrimethylammonium [$RN^+(R')_3X^-$] and alkylpyridinium salts [$RN^+(\phi)X^-$] of cationic surfactants. The CMC values for these compounds fall in the range of 33.7 to 0.4 mol/L for anionic surfactants and 0.14 to 8.1×10^{-4} mol/L for cationic surfactants. The data set was randomly divided into two groups, training set consisting of 45 compounds and a prediction set including 13 molecules. The training set was used for the generation of the network and the prediction set was used to evaluate the generated network. Table-1 shows all compounds studied in this work.

Descriptors generation

Formation of micelle from the surfactant monomers and also critical micelle concentration (CMC) is the result of competitive interactions between surfactant monomers and solvent molecules. The molecular structure and chemical properties of the surfactant molecules determine the type and the extent of these interactions. Due to the diversity of the molecules studied in this work, 24 different descriptors were calculated for each compound in the data set. These parameters encoded different aspects of the molecular structure and consist of electronic, geometric and topological descriptors. Geometric descriptors were calculated using optimized Cartesian coordinate and van der Waals radius of each atom in the molecule[32,33]. Electronic descriptors were calculated using MOPAC program (version 6)[34]. Topological descriptors were calculated using two-dimensional representation of the molecules.

Some of the descriptors generated for each compound encoded similar information about the molecular interest. Therefore, it was desirable to test each descriptor and eliminate those that show high correlation ($R > 0.95$) with each other.

For the selection of the most important descriptors that could be used as inputs of the ANN, the linear regression technique was used based on the construction of a linear mathematical model relating the observed CMC to numerically encoded structural parameters. This equation was formed

TABLE-1
DATA SET

No.	Compound	No.	Compound	No.	Compound
1	$C_{10}H_{21}SO_4Na$	22	$C_{10}H_{21}SO_3Na$	43	$C_{10}H_{21}N(C_6H_5)$ Cl
2	$C_{14}H_{29}SO_4Na$	23	$C_{12}H_{25}SO_3Na$	44	$C_{16}H_{33}N(C_6H_5)Cl$
3	$CH_3(CHSO_4)C_{12}H_{25}Na$	24	$C_{16}H_{33}SO_3Na$	45	$C_{16}H_{33}N(C_6H_5)Br$
4	$CH_3CH_2(CHSO_4)C_{11}H_{23}Na$	25	$C_8H_{17}N(CH_3)_3Br$		
5	$CH_3C_2H_4(CHSO_4)C_{10}H_{21}Na$	26	$C_{10}H_{21}N(CH_3)_3Br$	Prediction set	
6	$CH_3C_5H_{10}(CHSO_4)C_7H_{15}Na$	27	$C_{14}H_{29}N(CH_3)_3Br$	1	$C_{12}H_{25}SO_4Na$
7	$CH_3(CHSO_4)C_{13}H_{27}Na$	28	$C_{16}H_{33}N(CH_3)_3Br$	2	$CH_3C_3H_6(CHSO_4)C_9H_{19}Na$
8	$CH_3CH_2(CHSO_4)C_{12}H_{25}Na$	29	$C_{12}H_{25}N(C_2H_5)(CH_3)_2Br$	3	$CH_3C_6H_{12}(CHSO_4)C_7H_{15}Na$
9	$CH_3C_3H_6(CHSO_4)C_{10}H_{21}Na$	30	$C_{12}H_{25}N(C_6H_{13})(CH_3)_2Br$	4	$CH_3C_4H_8(CHSO_4)C_{10}H_{21}Na$
10	$C_{16}H_{33}SO_4Na$	31	$C_{12}H_{25}N(C_8H_{17})(CH_3)_2Br$	5	$C_{11}H_{23}CH(C_3H_7)CH_2SO_4Na$
11	$CH_3C_2H_4(CHSO_4)C_{12}H_{25}Na$	32	$C_{14}H_{29}N(C_2H_5)_3Br$	6	$C_7H_{15}CH(C_7H_{15})CH_2SO_4Na$
12	$CH_3C_6H_{12}(CHSO_4)C_8H_{17}Na$	33	$C_{14}H_{29}N(C_3H_7)_3Br$	7	$C_{14}H_{29}SO_3Na$
13	$CH_3(CHSO_4)C_{15}H_{31}Na$	34	$(C_{10}H_{21})_2N(CH_3)_2Br$	8	$C_{12}H_{25}N(CH_3)_3Br$
14	$CH_3C_7H_{14}(CHSO_4)C_8H_{17}Na$	35	$(C_{12}H_{25})_2N(CH_3)_2Br$	9	$C_{12}H_{25}N(C_4H_9)(CH_3)_2Br$
15	$C_{13}H_{27}SO_4Na$	36	$C_{14}H_{29}N(CH_3)_3OH$	10	$C_{14}H_{29}N(C_4H_9)_3Br$
16	$C_{15}H_{31}SO_4Na$	37	$C_{14}H_{29}N(CH_3)_3Cl$	11	$C_{14}H_{29}N(CH_3)_3NO_3$
17	$C_{13}H_{27}CH(CH_3)CH_2SO_4Na$	38	$C_{16}H_{33}N(CH_3)_3OH$	12	$C_{10}H_{21}N(CH_3)_3Cl$
18	$C_{12}H_{25}CH(C_2H_5)CH_2SO_4Na$	39	$C_{16}H_{33}N(CH_3)_3NO_3$	13	$C_{12}H_{25}N(C_6H_5)$ Cl
19	$C_{10}H_{21}CH(C_4H_9)CH_2SO_4Na$	40	$C_{16}H_{33}N(CH_3)_3Cl$		
20	$C_9H_{19}CH(C_5H_{11})CH_2SO_4Na$	41	$C_{12}H_{25}N(CH_3)_3Cl$		
21	$C_8H_{17}CH(C_6H_{13})CH_2SO_4Na$	42	$C_{12}H_{25}N(C_6H_5)Br$		

by a stepwise deletion of terms procedure (backward method)[35]. The parameters appearing in the best equation showed that five descriptors are the most important in prediction of the CMC. Table-2 shows the selected MLR model and the names of the descriptors appearing in this model. These descriptors are used as inputs for the generation of the ANN.

TABLE-2
SPECIFICATIONS OF THE BEST SELECTED MODEL

Descriptor	Notation	Coefficient	Mean effect
Balaban index	BAL	1.013	3.288
Heat of formation	HEAT	-8.45×10^{-3}	1.686
Volume of the molecule	V	-8.94×10^{-3}	0.152
Reciprocal of Randic index	RA^{-1}	18.713	2.233
Reciprocal of maximum distance of the atoms in the molecule	$MAXDIS^{-1}$	2.818	-2.926
Constant	Const.	-5.297	

Generation and evaluation of the ANN

The program for a feed-forward neural network that was trained by back-propagation strategy was written in FORTRAN 77 in our laboratory. All of the calculations presented in this work were carried out on a Hewlett-Packard 800 MHz Pentium III computer. The descriptors appearing in the MLR model were used as inputs for the generation of the ANN. Therefore, the number of inputs in the ANN was five and the number of nodes in the output layer was set to be one. The values of initial weights were randomly selected from a uniform distribution that ranged between -0.3 and +0.3. The initial biases values were set to be one. These values were optimized during the training of the network. The value of each input was divided to its mean value to bring the values of the input variables into the dynamic range of the sigmoid transfer function in the ANN.

Before training, the network was optimized for the number of nodes in the hidden layer, learning rates and momentum. The new method for optimizing these values was reported in our previous papers[17,24-26]. In order to evaluate the performance of the ANN, the standard error of calibration (SEC) and the standard error of prediction (SEP) were used[36]. The network was then trained using the training set by back-propagation strategy for the optimization of the weights and biases values.

RESULTS AND DISCUSSION

Some MLR 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 statistical parameters are given in Table-3. These models were selected due to their high values of R and F statistics and low standard errors. Model 1 consists descriptors including Balaban (BAL) and reciprocal Randic (RA^{-1}) indices, total volume of the molecule (V) and heat of formation of the molecules (HEAT). However, in addition to these descriptors, reciprocal of the maximum distances between two atoms in the molecule $(MAXDIS)^{-1}$ has also appeared in the model 2. Although the number of descriptors in model 1 is lower than model 2 but the statistics parameters obtained for prediction set using this model is better than that model 1. Therefore, model 2 was chosen. The specifications of this model are shown in Table-2. Also the correlation matrices between selected descriptors were shown in Table-4.

TABLE-3
COMPARISON BETWEEN THE RESULTS OBTAINED USING THE ANN AND MLR METHODS FOR THE SELECTED MODELS

Model	Data set	ANN			MLR		
		R	SE	F	R	SE	F
1	Training Set	0.995	0.159	4119	0.981	0.314	256
	Prediction Set	0.989	0.209	523	0.975	0.381	38
2	Training Set	0.996	0.137	5933	0.981	0.318	200
	Prediction Set	0.997	0.122	1664	0.987	0.291	54

TABLE-4
CORRELATION BETWEEN THE DESCRIPTORS OF THE SELECTED MODEL

	log CMC	BAL	HEAT	$MAXDIS^{-1}$	RA^{-1}	V
log CMC	1.000					
BAL	0.187	1.000				
HEAT	-0.824	-0.271	1.000			
$MAXDIS^{-1}$	-0.680	-0.148	-0.283	1.000		
RA^{-1}	0.520	-0.343	-0.030	0.872	1.000	
V	-0.706	0.238	0.270	-0.847	-0.890	1.000

In order to investigate the non-linear interactions between the different parameters appearing in the MLR model an ANN was developed. The generated ANN used the descriptors appearing in the MLR model as its inputs. Before the training of the network, the parameters of the number of nodes in hidden layer, weights and biases, learning rate and the momentum were optimized. The procedure for the optimization of these parameters is reported previously[17,24,37]. Table-5 shows the architecture and the specifications of the optimized ANN. After the optimization of ANN parameters, the network was trained using the training set for the optimization of the

weights and biases values. For the evaluation of the prediction power of the network, trained ANN was used to predict the CMC values of the surfactants included in the prediction set. Table-6 represents the experimental and predicted values of the CMC using the best generated ANN for the training and the prediction sets. The statistical parameters appearing in the MLR and ANN models are shown in Table-3. It can be seen from this table that standard error for the training and prediction sets are reduced from 0.318 and 0.291 for the MLR model to 0.137 and 0.122 for the ANN model, respectively. This confirms the superiority of the ANN model over that of the MLR model and improvement of the F statistics indicates that the selection of the MLR descriptors as inputs was justified.

TABLE-5
ARCHITECTURE OF THE ANN AND SPECIFICATIONS

No. of nodes in the input layer	5
No. of nodes in the hidden layer	5
No. of nodes in the output layer	1
Weights learning rate	0.5
Biases learning rate	0.3
Momentum	0.5
Transfer function	sigmoid

Table-1 shows that the data set consists of a variety of anionic and cationic surfactants. It can also be seen from this table that the prediction set represents the training set reasonably.

In order to obtain the extent of contribution of each descriptor in the CMC the mean effect of each parameter was calculated and given in Table-2. As shows in this table Balaban index (BAL), reciprocal maximum distance of the atoms $(MAXDIS)^{-1}$ and reciprocal Randic index (RA^{-1}) show a large contribution to the CMC. However, the Balaban Index (BAL) shows the largest mean effect compared to the others. This index appears to be a convenient measure of the compactness or centrality of a larger particular site in a molecule. Therefore, the positive effect of this parameter shows that the more compact the molecule the higher the CMC of that surfactance. The reciprocal maximum distance of the atoms $(MAXDIS)^{-1}$ shows a large negative effect on the CMC. The mean effect of this parameter in the MLR model indicates that the CMC decreases as the size of the molecule increases. This is in agreement with the experiment that the CMC of the surfactants decreases as the hydrophobicity of the molecule increases. The RA^{-1} index quantifies the notion of molecular branching and its reciprocal shows a considerably positive mean effect on the CMC (Table-3). This parameter also in agreement with the experiment shows that as the length of a side chain increases the CMC decreases. In addition, carbon atoms on

TABLE-6
EXPERIMENTAL AND CALCULATED VALUES (MODEL 2) OF log CMC AND THE VALUES OF DESCRIPTORS EMPLOYED IN THE SELECTED MODELS

No.[a]		Descriptors[b]				log CMC		
	BAL	V	HEAT	RA^{-1}	$MAXDIS^{-1}$	MLR	ANN	Exp.
Training set								
1	2.9904	225.7500	-289.2520	0.1686	0.0758	1.53	1.61	1.53
2	2.9930	293.7190	-316.6660	0.1269	0.0577	0.32	0.36	0.35
3	3.1167	293.0469	-313.6069	0.1216	0.0583	0.33	0.38	0.52
4	3.2825	292.8594	-313.5951	0.1274	0.0574	0.61	0.69	0.63
5	3.4329	292.4531	-313.7859	0.1274	0.0561	0.76	0.82	0.71
6	3.7008	292.2480	-313.9406	0.1274	0.0603	1.05	0.84	0.99
7	3.1046	309.7500	-320.4801	0.1203	0.0548	0.19	0.21	0.23
8	3.2566	309.4219	-320.4500	0.1198	0.0577	0.35	0.28	0.34
9	3.5207	359.8281	-320.3246	0.1198	0.0454	0.13	0.36	0.53
10	2.9960	326.2970	-330.3670	0.1126	0.0516	-0.14	-0.29	-0.24
11	3.3740	325.7188	-327.4993	0.1130	0.0500	0.23	0.27	0.24
12	3.6940	326.2188	-327.7047	0.1130	0.0504	0.55	0.52	0.63
13	3.0954	342.7188	-334.6008	0.1074	0.0494	-0.25	-0.42	-0.31
14	3.6960	343.0313	-334.5752	0.1070	0.0508	0.35	0.19	0.37
15	2.9900	276.2340	-309.8140	0.1269	0.0633	0.43	0.45	0.63
16	2.9930	310.4690	-323.5160	0.1193	0.0560	0.08	-0.04	0.08
17	3.1768	326.3910	-328.0150	0.1140	0.0539	0.06	-0.09	-0.10
18	3.3560	325.5160	-326.7570	0.1135	0.0572	0.24	0.02	-0.05
19	3.6530	326.1250	-327.0270	0.1135	0.0649	0.56	0.04	0.18
20	3.7610	325.6880	-327.1180	0.1135	0.0543	0.64	0.46	0.30
21	3.8300	326.0470	-327.1410	0.1135	0.0629	0.73	0.24	0.36
22	2.9939	217.0000	-226.7970	0.1739	0.0759	1.18	1.57	1.76
23	3.1872	250.4840	-240.5100	0.1482	0.0656	0.68	1.03	0.96
24	3.0172	318.0156	-267.9180	0.1143	0.0516	-0.54	0.09	0.14
25	3.0107	233.9063	- 13.5790	0.1916	0.0755	-0.43	-0.97	-0.85
26	2.9939	267.8281	- 27.2744	0.1608	0.0661	-1.23	-1.13	-1.17
27	2.9896	335.1406	- 54.7949	0.1216	0.0519	-2.38	-2.40	-2.44
28	2.9940	370.3906	- 68.5846	0.1085	0.0467	-2.83	-2.80	-3.02
29	3.0856	319.0781	- 46.7256	0.1281	0.0523	-2.08	-2.17	-1.85
30	3.2850	385.9844	- 74.0813	0.1020	0.0491	-2.75	-2.71	-2.51
31	3.3044	417.9844	- 87.9307	0.0925	0.0452	-3.09	-2.95	-2.96
32	3.2898	385.9688	- 66.0745	0.1002	0.0509	-2.84	-2.63	-2.51
33	3.6041	432.3438	- 87.8356	0.0871	0.0485	-3.00	-2.83	-2.68
34	3.3326	419.1406	- 87.8898	0.0925	0.0422	-3.08	-2.92	-2.73
35	3.3098	487.2344	-115.5410	0.0781	0.0361	-3.76	-3.82	-3.75
36	2.9896	328.9219	- 86.5156	0.1216	0.0517	-2.06	-2.49	-2.35
37	2.9896	313.1875	- 73.4778	0.1216	0.0523	-2.02	-2.15	-2.35
38	2.9940	326.2969	-100.2622	0.1085	0.0473	-2.17	-2.83	-2.47
39	2.9940	384.4531	-144.4981	0.1085	0.0426	-2.33	-3.03	-3.09
40	2.9940	365.6094	- 87.3096	0.1085	0.0472	-2.63	-2.83	-2.85
41	2.9982	297.4849	- 59.6895	0.1385	0.0587	-1.66	-1.80	-1.70
42	3.4562	307.1406	- 37.6338	0.1166	0.0480	-1.91	-1.84	-1.94
43	3.5360	268.8281	- 37.0943	0.1320	0.0542	-1.18	-1.33	-1.06
44	3.3504	369.8438	- 78.2259	0.0946	0.0386	-2.67	-3.29	-3.20
45	3.3504	374.0469	- 65.0733	0.0946	0.0386	-2.82	-2.34	-2.17

No.[a]	BAL	Descriptors[b]				log CMC		
		V	HEAT	RA^{-1}	$MAXDIS^{-1}$	MLR	ANN	Exp.
Prediction Set								
1	2.9952	258.9840	-302.9610	0.1451	0.0655	0.893	0.95	0.93
2	3.5568	291.9375	-313.8353	0.1274	0.0606	0.860	0.66	0.83
3	3.7031	309.5469	-320.8344	0.1198	0.0528	0.409	0.59	0.82
4	3.5880	326.5938	-327.0954	0.1130	0.0501	0.088	0.28	0.37
5	3.5152	326.0310	-326.9910	0.1135	0.0541	0.281	0.11	0.04
6	3.8540	325.5160	-327.1710	0.1135	0.0542	0.512	0.34	0.05
7	2.9893	283.8130	-254.216	0.1291	0.0578	-0.003	0.47	0.06
8	2.9982	301.7031	- 41.0442	0.1385	0.0582	-1.896	-1.89	-1.80
9	3.2150	352.3906	- 60.3223	0.1135	0.0552	-2.107	-2.56	-2.13
10	3.8925	486.2969	-108.6786	0.0770	0.0489	-3.020	-3.32	-2.92
11	2.9896	350.5938	-136.7496	0.1216	0.0461	-2.369	-2.82	-2.57
12	2.9939	263.9375	- 45.9468	0.1608	0.0668	-1.183	-1.22	-1.22
13	3.4562	302.3594	- 50.7142	0.1166	0.0479	-1.792	-1.96	-1.82

[a]Numbers refer to the surfactants given in Table-1.
[b]The definitions of the descriptors are given in Table-3.

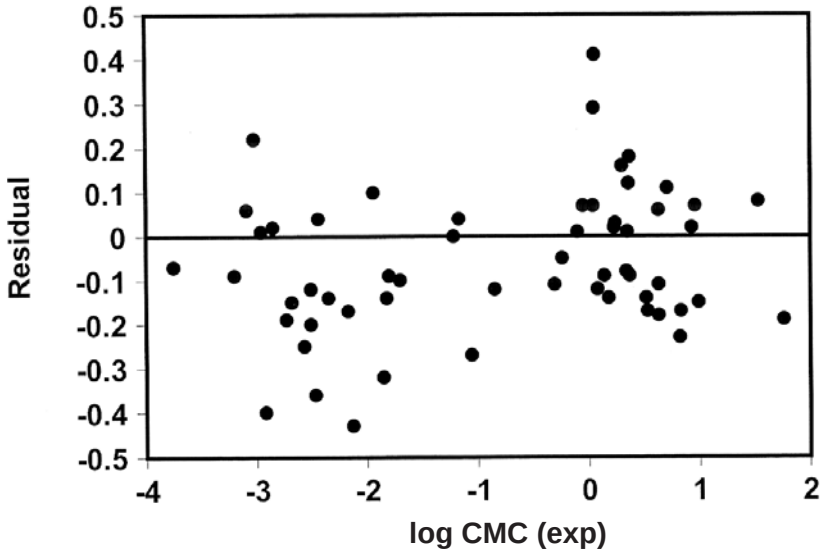

Fig. 1. Plot of residual *vs.* experimental values of log CMC

a branched hydrophobe have about half the effect of carbon atoms on a straight chain. The positive effect of the reciprocal of the RA^{-1} index confirms this observation. Heat of formation of the molecules shows a small effect on the formation of the micelles. This reveals that topology and geometry of the molecules are the most important factors affecting the micelle formation. Table-4 shows the correlation between the parameters appering in the MLR model. Inspecction of this table shows that the descriptors can be considered as independent parameters.

The residuals of the ANN calculated values of the CMC are plotted against the experimental values in Fig. 1. The propagation of the residuals in both sides of zero indicates that no systematic error exists in the development of the ANN. Also the correlation coefficient for the plot of the ANN calculated *vs.* the experimental values of log CMC was 0.997.

The results of this study demonstrate that the QSAR method using the ANN techniques can generate a suitable model for the prediction of the CMC of both anionic and cationic surfactants. From these results one may conclude that the topology and geometry of the surfactants are important in micellization process and the electronic parameters play a minor role in this respect.

REFERENCES

1. H.W. Stache, Anionic Surfactants, Organic Chemistry, Marcel Dekker, Inc., Vol. 56, p. 223 (1996).
2. M.R. Porter, Handbook of Surfactants, Chapman & Hall, New York, edn. 2, p. 116 (1994).
3. I.D. Robb, Specialist Surfactants, Chapman & Hall, London, p. 7 (1997).
4. S.H. Brooks, A. Berthod, B.A. Krisch and J.G. Dorsey, *Anal. Chim. Acta*, **209**, 111 (1988).
5. M.J. Rosen, Surfactants and Interfacial Phenomena, John Wiley & Sons, New York, p. 106 (1989).
6. N.A. Yaroshenko and Z.M. Aryamova, *Zh. Ukr. Khim.*, **51**, 466 (1998).
7. Zh. Corono, E. Platono, S. Ghelli, *Colloid. Polym. Sci.*, **262**, 667 (1984).
8. K.G. Furton and A. Norelus, *J. Chem. Educ.*, **70**, 254 (1993).
9. A.B. Mandal, B. Nair and D. Ramaswamy, *Bull. Electrochem.*, **4**, 567 (1988).
10. D. Vollhardt, *Tenside Deterg.*, **12**, 225 (1975).
11. E.D. Vendittiles, G. Palumbo, G. Parlato and V. Bocchini, *Anal. Biochem.*, **115**, 278 (1981).
12. H. Nakamura, A. Sano and K. Matsuura, *Anal. Sci.*, **14**, 379 (1998).
13. T. Kawakatsu, K. Kawasaki and F. Hirofumi, *J. Phys. Condens. Matt.*, **6**, 6385 (1994).
14. S. Karaborni, K. Esselink, P.A.J. Hibers and B. Smit, *J. Phys. Condens. Matt.*, **6**, 351 (1994).
15. N.J. Zollar, A. Shiloach and D. Blankschten, *Chem. Tech.*, **26**, 24 (1996).
16. A.K.V. Helden, *Prog. Colloid. Polym. Sci.*, **100**, 48 (1996).
17. M.J.-Heravi and M.H. Fatemi, *Anal. Chim. Acta*, **415**, 95 (2000) .
18. S.L. Anker, P.C. Jurs and P.A. Edwards, *Anal. Chem.*, **62**, 2676 (1990).
19. E. Marengo, M.C. Gennaro and S. Angelio, *J. Chromatogr. A*, **799**, 47 (1998).
20. G. Sacchero, M.C. Bruzzoniti, C. Sarzamini, E.Mentasti, H.J. Metting and P.M.J. Coenegracht, *J. Chromatogr. A*, **799**, 35 (1998).
21. S.A. Kustrin, M. Zecevic, Lj. Zivanovic and L.G. Tucker, *Anal. Chim. Acta*, **364**, 265 (1998).
22. K.L. Peterson, *Anal. Chem.*, **64**, 379 (1992).
23. W.L. Xing and X.W. He, *Anal. Chim. Acta*, **349**, 283 (1997).
24. M.J.-Heravi and F. Parastar, *J. Chem. Inf. Comput. Sci.*, **40**, 147 (2000).
25. M.H. Fatemi, *J. Chromatogr. A*, **955**, 273 (2002).
26. M.H. Fatemi, M.J.-Heravi and E. Konouz, *Anal. Chim. Acta*, **486**, 101 (2003).
27. M.J.-Heravi and E. Konouz, *J. Surfact. Deterg.*, **3**, 1 (2000).

28. M.T. Hogan, H.B. Demuth and M. Beal, Neural Network Design, Pws, Boston, p. 52 (1996).
29. S. Haykin, Neural Network, Printice-Hall, Englewood Cliffs, NJ, p. 110 (1994).
30. N.K. Bose and P. Liang, Neural Network, Fundamentals, McGraw-Hill, New York, p. 15 (1996).
31. N.M.Van Os, J.R. Haak and L.A.M. Rupert, Physico-Chemical Properties of Selected Anionic, Cationic and Nonionic Surfactants, Elsevier Science Publishers, New York, p. 9 (1993).
32. E.K. Whalden and P.C. Jurs, *Anal. Chem.*, **53**, 484 (1981).
33. T.R. Stouch and P.C. Jurs, *J. Chem. Inf. Comput. Sci.*, **26**, 2640 (1986).
34. J.J.P. Stewart, MOPAC, Semiempirical Molecular Orbital Program, QCPE, Version 6 p. 455 (1990).
35. N. Draper and H. Smith, Applied Regression Analysis, Wiley Interscience, New York, edn. 2, p. 65 (1981).
36. T.B. Blank and S.T. Brown, *Anal. Chem.*, 65, 3084 (1993).
37. M.H. Fatemi, *J. Chromatogr. A*, **1002**, 221 (2003).

(*Received*: 1 January 2005; *Accepted*: 27 November 2006) AJC-5275