Bulgarian Chemical Communications, Volume 49, Number 3, (pp. 852 – 858) 2017

Modeling of the physicochemical properties of aliphatic alcohols using topological indices and quantitative structure-property relationship

F. Arjmand, F. Shafiei*

[1]*Department of Chemistry, Science Faculty, Arak Branch, Islamic Azad University, Arak, Iran*

Received May 23, 2017; Accepted June 14, 2017

QSPR models are mathematical equations that attempt to correlate chemical structure with a wide variety of physical, chemical and biological properties. In this study, the relationships between the Randic' ($^1\chi$), Balaban (J), Wiener polarity (W_p), Hyper Wiener (WW), Szeged (Sz), Harary (H), and Wiener (W) indices to the entropy (S) , thermal energy (E_{th}) and heat capacity (C_V) of alcohols are presented. Physicochemical properties are determined by the quantum mechanics methodology at the Hartree-Fock (HF) level using the *ab initio* 6-31G basic set. Multiple linear regressions (MLR) and backward methods were employed to obtain the QSPR models. After MLR analysis, we studied the validation of linearity between the molecular descriptors in the best models for the used properties. The satisfactory results obtained show that the combination of the three descriptors ($^1\chi$, J, W) is excellent to predict heat capacity and thermal energy while the three descriptors (J, W, W_P) are useful to predict the entropy of the 158 aliphatic alcohols.

Keywords: Topological indices; Aliphatic alcohols; QSPR; MLR method; Validation.

INTRODUCTION

Quantitative structure-activity/property relationships (QSAR/QSPR) represent an attempt to relate structural descriptors of molecules with their physicochemical properties and biological activities [1].

Topological indices (TIs), as molecular descriptors, are important tools in QSPR/QSAR studies [2]. A topological index is a graph invariant number calculated from a graph representing a molecule.

The basic strategy of QSPR is to find the optimum quantitative relationship which can then be used for the prediction of the properties of molecular structures including those unmeasured or even unknown [3].

The Xu index, the atomic index (AI) and the MLR method were used to predict some properties of alcohols [4].

The novel edge connectivity index (^mF) is introduced for predicting some properties of alcohols. The results show that the MLR method can provide high-quality models for several representative properties of alcohols [5].

The QSPR analysis of 58 saturated alcohols for predicting some physicochemical properties such as boiling point (B_P), water solubility (logW) and *n*-octanol-water partition coefficient (logPow) by using odd-even index (OEI) combined with the novel molecular polarizability effect index (MPEI) was studied [6].

The novel atom-type indices (DAI) have been used to construct QSPR/ QSAR models for some physical properties and biological activities of alcohols by using MLR analysis [7].

Predictive methods for estimating physicochemical properties, such as the heat capacity of alcohols and aldehydes in liquid phase have been reported [8].

The semi-empirical electrotopological index (I_{SET}) has been developed to describe the gas chromatographic retention of aliphatic alcohols [9].

The minimal boiling point of simple saturated alcohols has been predicted by using the Wiener, first and second Zagreb indices [10].

QSPR models have been proposed for prediction of molecular properties such as molecular weight (mw), hardness (η), chemical potential (μ), total energy (E_{total}), and electrophilicity index (ω) of phenols [11].

The semi–empirical topological index has been calculated for predicting the relationship between structure and chromatographic retention for several data sets of alkanes, alkenes, esters, ketones, aldehydes and alcohols [6, 12].

In the present study, multiple linear regression (MLR) techniques and backward methods were used for modeling the thermal energy (E_{th} kcal/mol), heat capacity (C_V cal/molK) and entropy (S cal/molK) of 158 alcohols.

* To whom all correspondence should be sent:
E-mail: f-shafiei@iau-arak.ac.ir

MATERIALS AND MATHEMATICAL METHOD

The aliphatic alcohols are a homologous series of organic compounds containing one or more hydroxyl groups [-OH] attached to a single-bonded alkane.

Alcohols are important in organic chemistry because they can be converted to and from many other types of compounds. Alcohols are also technologically important materials and are used in the manufacture of a large number of products.

Quantum chemistry method

The entropy, thermal energy, and heat capacity of 158 saturated alcohols were obtained by the quantum mechanics methodology at HF level using the *ab initio* 6-31G basic set. To obtain a suitable model, QSPR used the linear multiple regression method, backward methods and the software SPSS Version 20. Microsoft Office 2010 programs were employed to chart results.

The molecules used in this collection include a variety of aliphatic alcohols that are classified into primary, secondary (*sec*-, *s*-), and tertiary (*tert*-, *t*-), based upon the number of carbon atoms connected to the carbon atom that bears the hydroxyl group. The quantum chemistry data of the 158 congeners are listed in Table 1.

Topological indices

Topological indices are numerical parameters of a graph that characterize its topology and are usually graph-invariant. Nowadays, in the literature, hundreds of topological indices, suitable to describe different properties, are reported.

The indicators used in this study are those with first-order molecular connectivity [13], such as Balaban [14], Randic' [15], Wiener [16], Hyper-Wiener 17], Wiener Polarity [18], Szeged [19], and Harary [20]. All used topological indices were calculated with the Chemicalize program [21].

Statistical analysis

Structure-property models were generated using the MLR procedure of SPSS Version 20. The entropy, thermal energy, and heat capacity as dependent variables and ($^1\chi$, J, H, W, Wp, WW, Sz) indices as independent variables were used.

The models were assessed with correlation coefficient (R), squared multiple correlation coefficient (R^2), adjusted correlation coefficient (R^2_{adj}), Fisher ratio (F), standard error of estimate (s), and Durbin-Watson value (D).

RESULTS

Several linear QSPR models were created that contain 3-7 descriptors. To develop a linear model for predicting the entropy, thermal energy and heat capacity topological description was used. The strongest correlation is based on multivariate step backwards, and was conducted using the SPSS software.

The distribution of dependent variable *versus* independent variable was used for 158 alcohols in the development of structure-property relationships.

QSPR models for the entropy

Table 2 shows the regression parameters and the relationships between the proposed models for the entropy of 158 alcohols.

The best linear model for the entropy includes four topological descriptors ($^1\chi$, J, W, W_p). The regression parameters of the best model of the four descriptors are collected in Eqn. (1):

$$S = 38.963 + 14.628\,{}^1\chi + 3.217\,J + 0.009W - 0.809WP \quad (1)$$

where N=158, R=0.992, R^2=0.984, R^2_{adj}=0.983, s=3.276 cal mol^{-1} K^{-1}, F=2297.445, D=1.988.

QSPR models for the thermal energy

Table 3 shows the regression parameters and the relationships between the proposed models for the thermal energy of 158 alcohols.

The best linear model for the thermal energy includes six topological descriptors ($^1\chi$, J, H, W, WW, W_p). The regression parameters of the best model of the six descriptors are collected in Eqn. (2):

$$Eth = 5.339 + 24.1451\chi + 4.227J + 4.540\,H - 0.151W + 0.019WW - 1.681WP \quad (2)$$

where N=158, R=0.999, R^2=0.998, R^2_{adj}=0.998, s=3.403 kcal mol^{-1}, F=10555.138, D=1.906.

QSPR models for the heat capacity

Table 4 shows the regression parameters and the relationships between the proposed models for the heat capacity of 158 alcohols.

The best linear model for the heat capacity includes six topological descriptors ($^1\chi$, J, H, W, WW, W_p). The regression parameters of the best model of the six descriptors are collected in Eqn. (3):

$$CV = 2.706 + 3.321\,{}^1\chi + 1.615\,J + 1.418\,H - 0.037\,W + 0.005\,WW - 0.407\,WP \quad (3)$$

where N=158, R=0.998, R^2=0.996, R^2_{adj}=0.995, s=1.026 cal $mol^{-1}.K^{-1}$, F=5686.131, D=1.821

The results for the entropy, thermal energy, and heat capacity are very satisfactory.

Table 1. Alcohols used in the present study

Compound	No.	Compound	No.	Compound	No.
methanol	1	1-octanol	54	4-methyl-4-octanol	107
ethanol	2	6-methyl-1-heptanol	55	4-ethyl-4-heptanol	108
1-propanol	3	2-octanol	56	3-methyl-3-octanol	109
2-propanol	4	3-octanol	57	1-decanol	110
1-butanol	5	4-methyl-1-heptanol	58	8-methyl-1-nonanol	111
2-methyl-1-propanol	6	4-octanol	59	2-decanol	112
2-butanol	7	2-ethyl-1-hexanol	60	4-decanol	113
2-methyl-2-propanol	8	2-methyl-2-heptanol	61	3,7-dimethyl-1-octanol	114
1-pentanol	9	5-methyl-2-heptanol	62	2,7-dimethyl-3-octanol	115
3-methyl-1-butanol	10	6-methyl-3-heptanol	63	2,6-dimethyl-4-octanol	116
2-pentanol	11	3-methyl-2-heptanol	64	2,3-dimethyl-3-octanol	117
2-methyl-1-butanol	12	2-methyl-3-heptanol	65	5-methyl-5-nonanol	118
3-pentanol	13	2-methyl-4-heptanol	66	4-methyl-1-nonanol	119
2,2-dimethyl-1-propanol	14	5-methyl-3-heptanol	67	2-methyl-3-nonanol	120
2-methyl-2-butanol	15	3-methyl-3-heptanol	68	2,2,5,5-tetramethyl-3-hexanol	121
1-hexanol	16	4-methyl-3-heptanol	69	4-propyl-4-heptanol	122
4-methyl-1-pentanol	17	3-methyl-4-heptanol	70	2,4,6-trimethyl-4-heptanol	123
2-hexanol	18	3,4-dimethyl-2-hexanol	71	3-ethyl-3-octanol	124
3-methyl-1-pentanol	19	2,5-dimethyl-2-hexanol	72	3-ethyl-2-methyl-3-heptanol	125
2-methyl-1-pentanol	20	4-methyl-4-heptanol	73	1-undecanol	126
3-hexanol	21	3-ethyl-3-hexanol	74	2-undecanol	127
2-ethyl-1-butanol	22	2,3-dimethyl-2-hexanol	75	3-undecanol	128
4-methyl-2-pentanol	23	3,5-dimethyl-3-hexanol	76	4-undecanol	129
3,3-dimethyl-1-butanol	24	2,3-dimethyl-3-hexanol	77	5-undecanol	130
2,3-dimethyl-1-butanol	25	2-methyl-3-ethyl-2-pentanol	78	6-undecanol	131
2-methyl-2-pentanol	26	2,4,4-trimethyl-2-pentanol	79	1-dodecanol	132
3-methyl-2-pentanol	27	2,2,4-trimethyl-3-pentanol	80	2-dodecanol	133
2-methyl-3-pentanol	28	2,2-dimethyl-3-hexanol	81	3-dodecanol	134
2,2-dimethyl-1-butanol	29	2,5-dimethyl-3-hexanol	82	4-dodecanol	135
3-methyl-3-pentanol	30	4,4-dimethyl-3-hexanol	83	1-tridecanol	136
3,3-dimethyl-2-butanol	31	3,4-dimethyl-2-hexanol	84	2-tridecanol	137
2,3-dimethyl-2-butanol	32	6-methyl-2-heptanol	85	3-tridecanol	138
1-heptanol	33	3-methyl-1-heptanol	86	4-tridecanol	139
5-methyl-1-hexanol	34	2-methyl-3-ethyl-3-pentanol	87	1-tetradecanol	140
2-heptanol	35	2,3,4-trimethyl-3-pentanol	88	2-tetradecanol	141
4-methyl-1-hexanol	36	1-nonanol	89	3-tetradecanol	142
2-methyl-1-hexanol	37	7-methyl-1-octanol	90	4-tetradecanol	143
3-heptanol	38	2-nonanol	91	1-pentadecanol	144
3-methyl-1-hexanol	39	3-nonanol	92	2-pentadecanol	145
4-heptanol	40	4-nonanol	93	3-pentadecanol	146
5-methyl-2-hexanol	41	5-nonanol	94	4-pentadecanol	147
2-methyl-3-hexanol	42	2-methyl-2-octanol	95	1-hexadecanol	148
2-methyl-2-hexanol	43	2,6-dimethyl-2-heptanol	96	2-hexadecanol	149
2,4-dimethyl-1-pentanol	44	2,6-dimethyl-3-heptanol	97	3-hexadecanol	150
5-methyl-3-hexanol	45	2,6-dimethyl-4-heptanol	98	4-hexadecanol	151
3-methyl-3-hexanol	46	3,6-dimethyl-3-heptanol	99	1-heptadecanol	152
2,4-dimethyl-2-pentanol	47	2,2,3-trimethyl-3-hexanol	100	2-heptadecanol	153
2,4-dimethyl-3-pentanol	48	3,5-dimethyl-4-heptanol	101	3-heptadecanol	154
3-ethyl-3-pentanol	49	2,3-dimethyl-3-heptanol	102	4-heptadecanol	155
2,3-dimethyl-2-pentanol	50	2,4-dimethyl-4-heptanol	103	1-nonadecanol	156
2,3-dimethyl-3-pentanol	51	2-methyl-3-ethyl-3-heptanol	104	2-nonadecanol	157
2,3,3-trimethyl-2-butanol	52	2,4,4-trimethyl-3-hexanol	105	1-icosane	158
3-methyl-2-hexanol	53	3,4,4-trimethyl-3-hexanol	106		

Table 2. Statistical parameters of models calculated with SPSS software for S.

Model	Independent variable	R	R^2	R^2_{adj}	s	F
1	$^1\chi$, J, H, W, WW, W_p, Sz	0.992	0.984	0.983	3.305	1290.019
2	$^1\chi$, J, H, W, W_p, Sz	0.992	0.984	0.983	3.294	1515.037
3	$^1\chi$, J, H, W, W_p	0.992	0.984	0.983	3.283	1829.730
4	$^1\chi$, J, W, W_p	0.992	0.984	0.983	3.276	2297.445

Table 3. Statistical parameters of models calculated with SPSS software for E_{th}.

Model	Independent variable	R	R^2	R^2_{adj}	s	F
5	$^1\chi$, J, H, W, WW, W_p, Sz	0.999	0.998	0.998	3.413	8992.932
6	$^1\chi$, J,H, W, WW,W_p	0.999	0.998	0.998	3.403	10555.138

Table 4. Statistical parameters of models calculated with SPSS software for C_V.

Model	Independent variable	R	R^2	R^2_{adj}	s	F
7	$^1\chi$, J, H, W, WW, W_p, Sz	0.998	0.996	0.995	1.029	4848.430
8	$^1\chi$, J, H, W, WW, W_p	0.998	0.996	0.995	1.026	5686.131

Table 5. Correlation between the molecular descriptors for S (model 4).

	Pearson correlations (model 4)				Collinearity statistical		Corrected model
	J	W_p	$^1\chi$	W	Tolerance	VIF	VIF
J	1	-0.831	0.458	0.237	0.261	3.828	3.026
W_p		1	-0.725	-0.019	0.071	14.113	6.693
$^1\chi$			1	-0.636	0.052	19.184	-
W				1	0.108	9.272	5.521

Table 6. Correlation between the molecular descriptors for E_{th}, Cv (models 6, 8).

	Pearson correlations (models 6, 8)						Collinearity statistical		Corrected model
	J	W_p	$^1\chi$	H	WW	W	Tolerance	VIF	VIF
J	1	-0.354	0.557	-0.744	-0.636	0.680	0.108	9.244	1.153
W_p		1	-0.044	-0.246	-0.064	0.086	0.065	15.342	-
$^1\chi$			1	-0.713	-0.074	0.127	0.010	105.182	5.211
H				1	0.678	-0.735	0.003	319.815	-
WW					1	-0.993	0.002	633.551	5.353
W						1	0.001	1289.381	-

DISCUSSION

In this study, we will use the following sections to find the best model for predicting the properties mentioned.

Multicollinearity

In regression analysis collinearity occurs when two predictor variables in a multiple regression have a non-zero correlation. Multicollinearity occurs when more than two predictor variables are inter-correlated. The multicollinearity is a basis of the variance inflation factor (VIF) value of multicollinearity tests using SPSS. If the VIF value lies between 1 and 10, there is no multicollinearity; if VIF<1 or >10, there is multicollinearity.

In all our final models there is multicollinearity, because the values of correlations between independent variables are near to one and VIF values are not between 1 and 10.

Verification and validation

Verification and validation are the primary processes for quantifying and building confidence (or credibility) in numerical models [22].

In this section for verification and validation of the regression models, we will focus on the Durbin-Watson statistics and unstandardized predicted and residual values.

Durbin-Watson statistics

The Durbin-Watson statistics is a test statistic tool used to detect the presence of auto correlation in residuals from a regression analysis. The value of D always lies between 0 and 4. If the Durbin-Watson statistics is substantially below 2, this is an evidence of a positive serial correlation.

If the Durbin-Watson is below 1.0, there might be a cause for alarm. Small values of D indicate that the successive error terms are, on the average, close in value to one another, or positively correlated. If D>2, it indicates that the successive error terms are, on the average, much different in value from one another, i.e., they are negatively correlated.

In addition, if the value is between 1.5 and 2.5, it indicates that there is no correlation. In all our models, the value of Durbin-Watson statistics is close to 2 (see eqns.1-3) and hence the errors are uncorrelated.

For validation of the linearity between the molecular descriptors in the equations 1-3 we obtained the Pearson coefficient of correlation and collinearity statistics by SPSS as follows from Tables 5, 6.

For model 4, VIF values for two descriptors, W_p and $^1\chi$, are bigger than 10, therefore there is a linearity between these descriptors. After removing $^1\chi$ from this model, we corrected model 4 as follows:

$$S = 97.531 - 8.187\,J + 3.496\,WP + 0.051W \qquad (4)$$

where N=158, R=0.965, R^2=0.931, R^2_{adj}=0.929, Q^2_{LOO}=0.937, s=6.726 cal mol^{-1} K^{-1}, F=687.413, D=0.971.

Similar to model 4 we obtained the corrected models 6 and 8 as follows:

$$Eth = -9.881 + 37.254\,1\chi + 12.466J + 0.003\,WW \qquad (5)$$

where N=158, R=0.998, R^2=0.996, R^2_{adj}=0.996, Q^2_{LOO}=0.997, s=4.475 kcal mol^{-1}, F=12182.971, D=1.832.

$$CV = -7.109 + 8.031\,1\chi + 4.512\,J + 0.001\,WW \qquad (6)$$

where N=158, R=0.996, R^2=0.992, R^2_{adj}=0.992, Q^2_{LOO}=0.993, S=1.385 cal .mol^{-1} K^{-1}, F=6222.373, D=1.724.

In eqns. 4, 5, and 6, Q^2_{LOO} are the squared cross-validation coefficients for leave-one-out, respectively. We have computed Q^2_{LOO} (Eqn. 7) by randomly taking 50% of the data that are positive and less than one.

$$Q2 = 1 - \frac{\sum(Y_I - \hat{Y}_{i|i})^2}{\sum(Y_I - \bar{Y})^2} \qquad Q^2 \le 1 \qquad (7)$$

In eqn. (7), the notation i|i indicates predicted by a model estimated when the i-th sample was left out from the training set.

Regular residuals

The residual is the difference between the observed and predicted value. A residual plot is a graph that shows the residual values on the vertical axis and the independent variables on the horizontal axis.

If the points in a residual plot are randomly dispersed around the horizontal axis, a linear regression model is appropriate for the data; otherwise, a non-linear model is more appropriate.

The residual values of the entropy, thermal energy, and heat capacity expressed by Eqns. (4-6) were calculated. The residual values show a relatively random pattern (see Figs. 1-3). This relatively random pattern shows that a linear model provides a decent fit to the data.

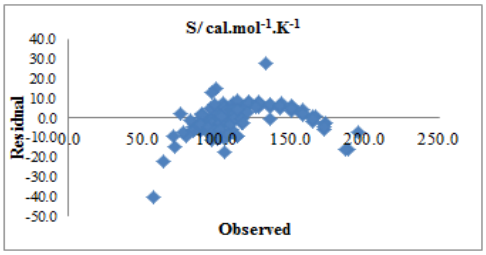

Fig. 1. Plot of residuals against observed values of the entropy.

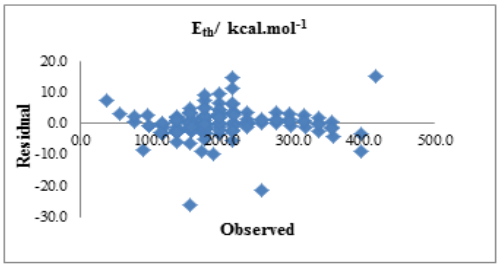

Fig. 2. Plot of residuals against observed values of the thermal energy.

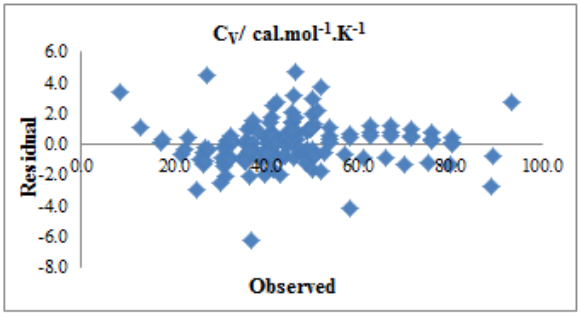

Fig. 3. Plot of residuals against observed values of the heat capacity.

Figs. 4-6 show the linear correlation between the observed and the predicted entropy, thermal energy, and heat capacity values obtained using eqns. (4-6), respectively.

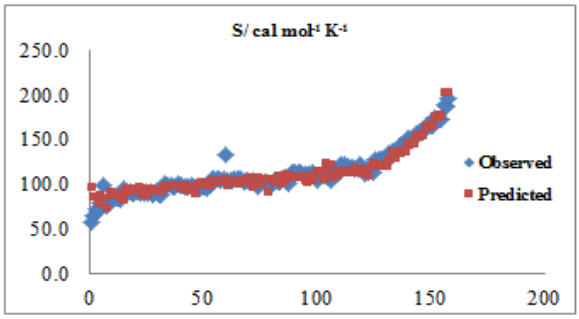

Fig. 4. Comparison between predicted and observed entropy by the MLR method.

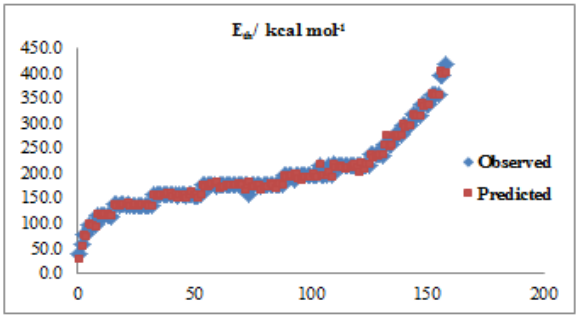

Fig. 5. Comparison between predicted and observed thermal energy by the MLR method.

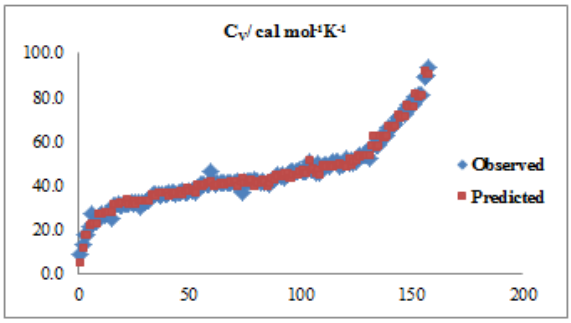

Fig. 6. Comparison between predicted and observed heat capacity by the MLR method.

CONCLUSIONS

The conception that there exists a close relationship between bulk properties and molecular structure is quite deeply rooted in chemistry. The basic tenet of chemistry is to identify these assumed relationships between molecular structure and physicochemical properties and to quantify them.

The QSPR approach, including multivariate data analysis in combination with statistical design, has been extensively employed.

In this study, QSPR mathematical models for the prediction of the entropy, thermal energy and heat capacity of alcohols by using methods based on topological descriptors calculated from molecular structure alone were developed. These QSPR models showed high values of the multiple correlation coefficient ($R > 0.99$) and Fisher-ratio statistics.

The MLR model proved to be a useful tool in the prediction of S, E_{th} and the leave-one-out cross-validation, as the evaluation technique was designed to evaluate the quality and predictive ability of the MLR model. The obtained results showed that the three topological indices (J, W, W_P) are suitable for predicting S, and the three descriptors ($^1\chi$, J,W) are suitable for predicting E_{th} and C_V of 158 alcohols.

REFERENCES

1. A. Kumar, B. Narasimhanb, and D. Kumar, *Bioorg. Med. Chem.*, **15**, 4113 (2007).
2. F. Shafiei, H. Hosseini, *MATCH Commun. Math. Comput. Chem.*, **75**, 583 (2016).
3. M. Pashmforush, F. Shafiei, and F. Dialamehpour, *Iran. J. Math. Chem.*, **7**, 15 (2016).
4. B. Ren, *Comput. Chem.*, **26**, 223 (2002).
5. L. Mu, C. Feng, *MATCH Commun. Math. Comput. Chem.*, **56**, 217 (2006).
6. F. Liu, C. Cao, and B. Cheng, *Int. J. Mol. Sci.*, **12**, 2448 (2011).
7. C. Lu, W. Guo, Y.Wang, *J. Mol. Model.*, **12**, 749 (2006).
8. F. Ashrafi, R. Saadati, and A. Behboodi Amlashi, *Afr. J. Pure Appl. Chem.*, **2 (11)**, 116 (2008).
9. B. da Silva Junkes, R.D.D.M.C. Amboni, R.A. Yunes, and V.E.F. Heinzen, *Internet Electron. J. Mol. Des.*, **2**, 33 (2003).
10. M. Goubko, O. Miloserdov, *MATCH Commun. Math. Comput. Chem.*, **75**, 29, (2016).
11. F. A. Pasha, H. K. Srivastava, Y. Beg, and P. P. Singh, *Am. J. Immunology*, **2 (1)**, 23 (2006).
12. Z. Lin, J. Xu, X. Zheng, and Z. Li, *Acta Phys. Chem. Sin.*, **16**, 153 (2000).
13. M. Randić, *J. Math. Chem.*, **7**, 155 (1991).
14. A. T. Balaban, *Chem. Phys. Lett.*, **89**, 399 (1982).
15. M. Randić, *Acta. Chim. Slov.*, **49**, 483 (2002).
16. B. Zhou, I. Gutman, *Chem. Phys. Lett.*, **394**, 93 (2004).
17. D. J. Klein, W. Yan, and Y.N. Yeh, *Int. J. Quantum Chem.*, **106**, 1756 (2006).
18. M. Liu, B. Liu, *MATCH Commun. Math. Comput. Chem.*, **66**, 293 (2011).
19. P. V. Khadikar, N. V. Deshpande, P. P. Kale, A. Dobrynin, I. Gutman, and G. Dömötör, *J. Chem. Inf. Compt. Sci.*, **35**, 547(1995).
20. K. C. Das, B. Zhou, and N. Trinajstić, *J. Math. Chem.*, **46,** 1369 (2009).
21. Web search engine developed by ChemAxon; software available at http://WWW.Chemicalize.Org.
22. P.J. Roach, Verification and Validation in Computational Science and Engineering, Hermosa Publishers, Albuquerque, NM, 1998, p.446.

МОДЕЛИРАНЕ НА ФИЗИКОХИМИЧНИТЕ СВОЙСТВА НА АЛИФАТНИ АЛКОХОЛИ, ИЗПОЛЗВАЙКИ ТОПОЛОГИЧНИ ИНДЕКСИ И КОЛИЧЕСТВЕНА ВРЪЗКА СТРУКТУРА-СВОЙСТВА

Ф Арджманд[1], Ф. Шафиеи*****

[1]Департамент по химия, Факултет по наука,Клон Арак, Ислямски университет "Азад", Арак, Иран

Получена на 23 май, 2017 г.; коригирана на 14 юни 2017 г.

(Резюме)

QSPR моделите са математически уравнения, които целят да свържат химическата структура с голямо разнообразие от физични, химични и биологични свойства. В тази работа е изследвана връзката между Randic' ($^1\chi$), Balaban (J), Wiener polarity (W_p), Hyper Wiener (WW), Szeged (Sz), Harary (H) и Wiener (W) индекси и ентропията (S), топлинната енергия (E_{th}) и топлинния капацитет (CV) на алкохоли. Физикохимичните свойства се пресмятат с метода на квантовата механика с нивото на Hartree-Fock (HF), като се използват базовите сетове ab initio 6-31G. Многобройните линейни регресии (MLR) и обратните методи са използвани за получаване на моделите QSPR. След MLR анализ ние проучихме валидирането на линейността между молекулните дескриптори в най-добрите модели за използваните свойства. Задоволителните резултати показват, че комбинирането на трите дескриптора ($^1\chi$, J, W) е подходящо за предсказване на топлинен капацитет и топлинна енергия, докато трите дескриптора (J, W, WP) са полезни за предсказване ентропията на 158 алифатни алкохола.