STUDIA UBB CHEMIA, LXII, 2,Tom II, 2017 (p. 297-310)
(RECOMMENDED CITATION)
DOI:10.24193/subbchem.2017.2.23

ENTROPY PREDICTION OF BENZENE DERIVATIVES USING TOPOLOGICAL INDICES

HOSSEIN HOSSEINI and FATEMEH SHAFIEI[a]*

ABSTRACT. In this study, a QSPR study relating topological indices to the entropy of 69 benzene derivatives is reported. The entropy values were calculated at HF level of theory (6-31 G basis sets) by Gussian 98.

Multiple linear regression (MLR) provided good models with three to seven independent variables. The best model obtained is based on three descriptors: Randić, Wiener and Szeged topological indices

Keywords**:** *Topological indices; benzene derivatives; QSPR; MLR method*.

INTRODUCTION

One of the most important purposes in application of mathematical and statistical methods is to find a relationship between molecular structure and values of physical properties, chemical reactivity or biological activity. As a result, quantitive structure-property relationship (QSPR) and quantitative structure-activity (QSAR) studies have been promoted.

Topological indices (TIs), as molecular descriptors, are important tools in QSPR/QSAR studies [1-11]. A topological index is a graph invariant number calculated from a graph representing a molecule.

The physicochemical properties of compounds are important in many fields, including pharmaceutics, chemistry, biochemistry and environmental sciences. Property estimations can help to minimize time and cost in producing new chemical materials with desired properties.

[a] *Department of Chemistry, Science Faculty, Arak Branch, Islamic Azad University, Arak, Iran*
** Corresponding author: f-shafiei@iau-arak.ac.ir*

Predictive methods for estimating thermodynamic properties, such as enthalpies of formation, Gibbs free energy and entropies of acyclic and aromatic compounds, on the basis of fundamental concepts on molecular structure have been reported [12].

Artificial Neural Networks were also used in developing QSPR models for prediction of physicochemical properties [13-16].

Prediction of entropies and enthalpies of organic compounds by using group contribution methods was also published [17-19]. Prediction of standard absolute entropy (S_{298} K) of gaseous organic and inorganic compounds was reported in [20, 21].

In thermodynamics, entropy (usual symbol S) is a measurement of the randomness or disorder of a system.

In the present work, we developed QSPR models for entropy estimation of benzene derivatives by describing the chemical structure by the aid of topological indices. Benzene derivatives are used in a wide range of technological applications.

Experimental data of benzene derivatives are often scarce, and at this point, topological descriptors provide powerful tools for modeling and extrapolating experimental data.

The main aim of this study is to illustrate the usefulness of topological indices in QSPR study of entropy (S) of benzene derivatives. As far as we are aware, this is the first QSPR study for prediction of benzene derivatives entropies using topological indices.

METHODS

The entropy(S) of 69 benzene derivatives (benzene included) was computed at the Hartree-Fock (HF) level of theory, using the ab initio 6-31G basis sets. The benzene derivatives in this set have seven different substituents, each substituent being present in at least six compounds. These substituents are amino, bromo, chloro, hydroxyl, methyl, methoxyl and nitro groups. Studied benzene derivatives and their entropy are listed in Table 1. To obtain an appropriate QSPR model we used multiple linear regression (MLR) procedure, by SPSS software, version 16, and backward stepwise regression was used to construct the QSPR models.

For drawing the graphs of our results, we used the Microsoft Office Excel – 2003 program.

Table 1. Benzene derivatives and their entropy.

Compounds		S (J/molK)	Compounds		S (J/molK)
Bromobenzene	1	317.84	4-Methylphenol	36	349.83
Phenol	2	306.46	4-Methyl-3,5-dinitroaniline	37	445.05
1,2-Dichlorobenzene	3	334.59	1,3,5-Trichlorobenzene	38	356.02
3-Chlorotoluene	4	364.05	Benzene	39	262.97
1,3-Dihydroxybenzene	5	323.62	2-Nitrotoluene	40	367.64
3-Hydroxyanisol	6	358.77	1,4-Dinitrobenzene	41	388.62
4-Methyl-3-nitroaniline	7	394.75	2-Methyl-3,6-dinitroaniline	42	441.44
2,4-Dimethylphenol	8	379.11	2-Methyl-4,6-dinitrophenol	43	441.14
2,6-Dimethylphenol	9	368.01	2,5-Dinitrotoluene	44	425.34
3-Nitrotoluene	10	380.02	1,2-Dinitrobenzene	45	353.05
2,6-Dinitrotoluene	11	418.03	1,4-Dimethoxybenzene	46	415.42
4-Methyl-2,6-dinitroaniline	12	434.81	2-Methyl-3-nitroaniline	47	393.15
5-Methyl-2,6-dinitroaniline	13	435.84	2-Methyl-4-nitroaniline	48	390.79
5-Methyl-2,4-dinitroaniline	14	452.06	4-Hydroxy-3-nitroaniline	49	384.93
2,4-Dinitrotoluene	15	424.53	4-Chloro-3-methylphenol	50	364.45
4-Nitrophenol	16	361.48	2,4,6-Tribromophenol	51	420.17
4-Chlorotoluene	17	361.72	2,4,6-Trinitrotoluene	52	374.01
2,4,6-Trichlorophenol	18	390.64	1,2,4,5-Tetrachlorobenzene	53	385.01
Toluene	19	333.15	3-Methyl-2,4-dinitroaniline	54	439.91
3-Methyl-6-nitroaniline	20	394.19	2-Methyl-3,5-dinitroaniline	55	449.66
4-Methyl-2-nitroaniline	21	394.03	3,5-Dinitrotoluene	56	449.03
1,2,4-Trichlorobenzene	22	369.29	3,4-Dinitrotoluene	57	436.01
3,4-Dichlorotoluene	23	389.83	1,2,4-Trimethylbenzene	58	390.65
2,4-Dichlorotoluene	24	371.03	2,4-Dinitrophenol	59	418.15

Compounds		S (J/molK)	Compounds		S (J/molK)
Chlorobenzene	25	312.91	3,4-Dimethylphenol	60	366.28
1,3,5-Trinitrobenzene	26	454.21	2,4-Dichlorophenol	61	363.99
1,2,3,4-Tetrachlorobenzene	27	388.74	1,2,3-Trichlorobenzene	62	361.73
2,3,4,5,6-Pentachlorophenol	28	440.69	2-Methyl-6-nitroaniline	63	385.42
1,3-Dichlorobenzene	29	336.24	2-Methyl-5-nitroaniline	64	396.19
2-Chlorophenol	30	335.58	1,3-Dinitrobenzene	65	392.01
3-Methylphenol	31	351.15	4-Nitrotoluene	66	386.01
2,3-Dinitrotoluene	32	426.83	1,2-Dimethylbenzene	67	337.67
1,4-Dimethylbenzene	33	340.90	2-Methylphenol	68	337.29
2,3,4,5-Tetrachlorophenol	34	416.02	1,4-Dichlorobenzene	69	330.48
2,3,6-Trinitrotoluene	35	480.08			

TOPOLOGICAL INDICES

A large number of topological indices TIs have been defined and used, majority of them being calculated from the various matrices corresponding to molecular graphs. The Adjacency matrix (A) and the Distance matrix (D) of the molecular graph have been most widely used in the definition of topological indices. The most used TIs are presented below.

Randić index (1975), $^1\chi(G)$, was introduced as the connectivity index [22,23] and is defined as (1):

$$^1\chi = \sum_{\text{all edges}} (d(i)d(j))^{-0.5} \quad (1)$$

where d(i) and d(j) are the valencies of the vertices i and j defining the edge (i, j).

Wiener index (1947), W(G), can be defined by (2):

$$W(G) = \frac{1}{2}\sum_i \sum_j [D(i,j)] \quad (2)$$

where D(i,j) is the number of edges on the shortest path joining vertex i and vertex j (i.e., the topological distance) in the graph [24].

Hyper-Wiener index, WW(G), can be defined [25,26] as (3):

$$WW(G) = \frac{1}{2}\left(\sum d(u,v) + \sum (d(u,v))^2\right) \quad (3)$$

where d(u,v) denotes the distance between the vertices u and v in the graph G and the summations run over all pairs of vertices of G.

Randić's original definition (1993) [27] of the hyper-Wiener index is applicable to trees only.

Wiener polarity index (1947), $W_p(G)$, of G is the number of unordered pairs of vertices (u,v) of G lying at distance 3 to each other. The Wiener polarity index [28,29] is defined as (4):

$$WP(G) = |\{(u, v) \mid d(u, v) = 3, u, v \in V\}|. \quad (4)$$

Balaban index (1982), J(G) of G was introduced in 1982 [30,31] as one of the less degenerated indices. It calculates the average distance sum connectivity index, according to eq.(5):

$$J=\frac{M}{\mu+1}\sum_{\text{all edges}}\left(D_i\ D_j\right)^{-0.5} \quad (5)$$

where M is the number of the edges in G; and D_i is the distance sum from the vertex i to all the other vertices in G (i.e., the sum of all entries in the i^{th} row of the distance matrix D).

The cyclomatic number $\mu=\mu(G)$ of a polycyclic graph G is equal to the minimum number of edges that must be removed from G to transform it to the related acyclic graph. For trees, $\mu=0$; for monocycles, $\mu=1$.

Harary number, H(G), was introduced in 1993 [32].This index is defined by eq. (6)

$$H = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}(1/D_{i,j}) \quad (6)$$

Within this paper, a version of this index is calculated from the inverse of the squared elements of the distance matrix, according to eq.(7):

$$H=\frac{1}{2}\sum_i^n\sum_j^n\left(D_{ij}\right)^{-2} \quad (7)$$

where $D_{i,j}$ is the entry in the distance matrix D.

Szeged index, Sz(G), was introduced by Gutman [33,34] as (8):

$$Sz_v(G)=\sum_e n_u(e|G).n_v(e|G) \quad (8)$$

$n_v|=n_v$ (e | G) is the number of vertices of G whose distance to the vertex v is smaller than the distance to the vertex u. Note that vertices equidistant to u and v are not counted.

All the used topological indices were calculated in hydrogen suppressed graphs. The descriptors were calculated with Chemicalize program [35]. Seven topological indices tested in the present study are listed in Table 2.

STATISTICAL ANALYSIS

Structure-Property models (MLR models) are generated using the multi linear regression procedure of SPSS, version 16. The entropy (S, J/mol K) is used as the dependent variable and 1χ, J, H, Sz, WW, W_p and W indices are used as the independent variables. The models are assessed with r value (correlation coefficient), the r^2 (coefficient of determination), the r^2- adjusted, the s value (root of the mean square of errors), the F value (Fischer statistic), the D value (Durbin-Watson) and the Sig (significant).

RESULTS AND DISCUSSION

Several linear QSPR models involving three to seven descriptors were established and the strongest multivariable correlations were identified by the backward method, with significant at the 0.05 level and regression analysis of the SPSS program. In the first of this study we drown scattering plots of S versus the seven topological indices (1χ, J, H, Sz, WW, Wp, W). Some of these plots are given in Figs. 1 to 3, respectively.

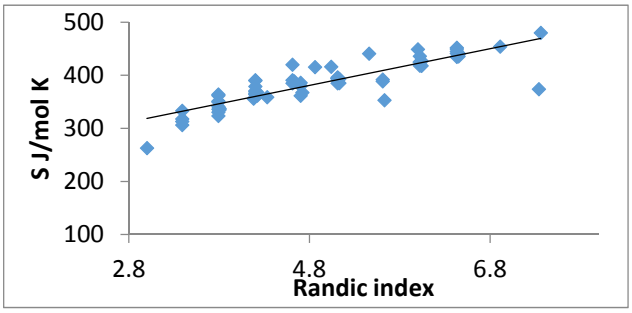

Figure 1. Plot of the Randić index (1χ) versus entropy of 69 benzene derivatives.

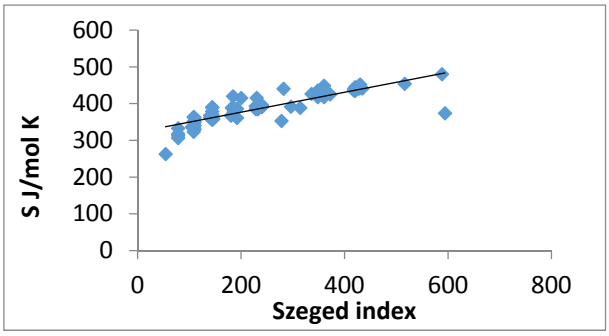

Figure 2. Plot of the Szeged index (Sz) versus entropy of 69 benzene derivatives.

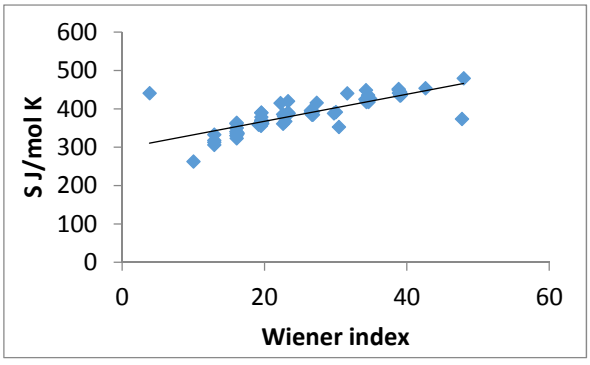

Figure 3. Plot of the Wiener (W) versus entropy of 69 benzene derivatives.

Table 2. Benzene derivatives and their topological indices, used in present study.

A	$^1\chi$	J	H	W	WW	W_p	Sz
1	3.39	1.82	12.92	42	71	5	78
2	3.39	1.82	12.92	42	71	5	78
3	3.80	2.28	16.17	60	106	8	106
4	3.79	2.23	16.08	61	110	7	108
5	3.79	2.23	16.08	61	110	7	108
6	4.33	1.98	19.15	88	176	9	146
7	5.11	2.25	26.67	148	315	14	232
8	4.20	2.09	19.53	84	160	10	144
9	4.22	2.15	19.67	82	151	11	140
10	4.70	2.32	22.73	117	245	11	186
11	6.04	2.40	34.60	234	545	19	348
12	6.43	2.70	39.02	282	669	21	420

A	$^{1}\chi$	J	H	W	WW	W_p	Sz
13	6.45	2.72	39.13	281	667	22	418
14	6.43	2.65	38.83	287	698	21	430
15	6.02	2.33	34.30	240	576	18	360
16	4.70	2.26	22.60	120	262	11	192
17	3.79	2.19	16.03	62	115	7	110
18	4.61	2.49	23.28	110	215	13	184
19	3.39	1.82	12.92	42	71	5	78
20	5.11	2.22	26.60	150	327	14	236
21	5.11	2.25	26.67	148	315	14	232
22	4.20	2.09	19.53	84	160	10	144
23	4.20	2.09	19.53	84	160	10	144
24	4.20	2.09	19.53	84	160	10	144
25	3.39	1.82	12.92	42	71	5	78
26	6.91	2.46	42.60	354	906	21	516
27	4.63	2.52	23.37	109	211	14	182
28	5.46	2.76	31.60	174	357	21	282
29	3.79	2.23	16.08	61	110	7	108
30	3.80	2.28	16.17	60	106	8	106
31	3.79	2.23	16.08	61	110	7	108
32	6.04	2.47	34.83	228	511	19	336
33	3.79	2.19	16.03	62	115	7	110
34	5.04	2.39	27.32	140	281	17	230
35	7.36	2.83	47.97	405	1036	26	588
36	3.79	2.19	16.03	62	115	7	110
37	6.43	2.70	39.02	282	669	21	420
38	4.18	2.08	19.50	84	159	9	144
39	3.00	2.00	10.00	27	42	3	54
40	4.72	2.40	22.90	114	231	12	180
41	5.61	2.30	29.74	206	521	15	314
42	6.45	2.64	38.87	289	717	22	434
43	6.43	2.66	3.85	286	691	21	428
44	6.02	2.28	34.14	246	616	18	372
45	5.63	2.54	30.43	188	416	16	278
46	4.86	2.17	22.24	125	287	11	200
47	5.13	2.28	26.80	146	306	15	228
48	5.11	2.18	26.50	152	337	14	240
49	5.11	2.25	26.67	148	315	14	232
50	4.20	2.09	19.53	84	160	10	144
51	4.61	2.49	23.28	110	215	13	184
52	7.34	2.80	47.72	408	1044	25	594
53	4.61	2.46	23.23	111	220	13	186
54	6.45	2.72	39.13	281	667	22	418
55	6.43	2.66	38.85	286	691	21	428

A	$^1\chi$	J	H	W	WW	W_p	Sz
56	6.00	2.33	34.23	240	573	17	360
57	6.02	2.40	34.53	234	542	18	348
58	4.20	2.09	19.53	84	160	10	144
59	6.02	2.33	34.3	240	576	18	360
60	4.20	2.09	19.53	84	160	10	144
61	4.20	2.09	19.53	84	160	10	144
62	4.22	2.15	19.67	82	151	11	140
63	5.13	2.28	26.8	146	306	15	228
64	5.11	2.18	26.5	152	337	14	240
65	5.61	2.40	30.02	197	464	15	296
66	4.70	2.26	22.6	120	262	11	192
67	3.80	2.28	16.17	60	106	8	106
68	3.80	2.28	16.17	60	106	8	106
69	3.79	2.19	16.03	62	115	7	110

Distribution of the dependent variable against the independent variable for 69 chemicals was employed in developing quantitative structure- properties relationships. For obtaining appropriate QSPR models we used maximum R^2 method and followed backward regression analysis. The predictive ability of the model is discussed on the basis of predictive correlation coefficient.

QSPR MODELS FOR ENTROPY (S)

Initial regression analysis indicated that combination of seven topological indices plays a dominating role in modeling the entropy. Table 3 provides the regression parameters and quality of correlation of the proposed models for entropy of 69 benzene derivatives.

Table 3. Statistics of models calculated with SPSS software

Model	Independent variables	r	r^2	r^2_{adj}	s	F	Sig
1	Sz, J, H, Wp, 1χ, WW, W	0.929	0.864	0.848	16.691	55.222	0.000
2	Sz, J, Wp, 1χ, WW, W	0.929	0.864	0.850	16.559	65.454	0.000
3	Sz, Wp, 1χ, WW, W	0.929	0.862	0.851	16.510	78.879	0.000
4	Sz, 1χ, Wp, W	0.927	0.860	0.851	16.518	98.244	0.000
5	Sz, 1χ, W	0.927	0.859	0.853	16.430	132.299	0.000

The best linear model contains three topological descriptors, namely, Randić (1χ), Wiener (W) and Szeged (Sz) indices.

The regression parameters of the best three descriptor correlation model are gathered in equation 9.

$$S=70.258+59.966X+2.748Sz-4.163W \quad (9)$$

$r=0.927$; $r^2=0.859$; r^2_{adj} =0.859 ;

s=16.430; D=2.033;

F=132.299 ; mean square = 269.936

This model produced a standard error of 16.430 J mol^{-1} K^{-1}, a correlation coefficient of 0.927, and the adjusted correlation coefficient (adjusted r-squared) was calculated as 0.859.

The result is therefore very satisfactory. Figure 4 shows the linear correlation between the observed and the predicted entropy values obtained using equation (9).

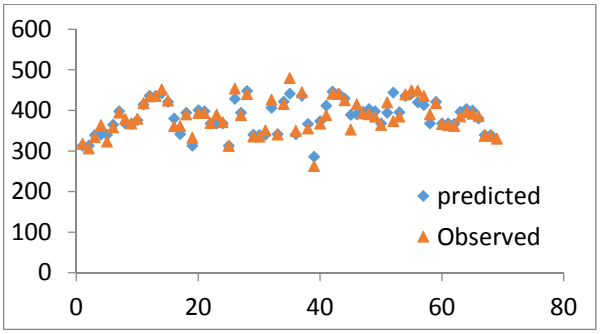

Figure 4. Comparison between the predicted and observed entropy by MLR method (cf. eq. 9)

The DURBIN-WATSON STATISTIC

To verify and validate the regression models, we will focus on the Durbin-Watson (D) statistic, unstandardized predicted and residual values.

The Durbin-Watson statistic ranges in value from 0 to 4. A value near 2 indicates non-autocorrelation; a value toward 0 indicates positive autocorrelation; a value toward 4 indicates negative autocorrelation. Therefore the value of Durbin-Watson statistic is close to 2 if the errors are uncorrelated. In our model, the value of Durbin-Watson statistic for model 5 is close to 2 (See Eq. 9) hence the errors are uncorrelated.

RESIDUAL VALUES

The residual values of entropy expressed by equation (9) are shown in Table 4. The residual values show a fairly random pattern (see Figure 5). This random pattern indicates that a linear model provides a decent fit to the data.

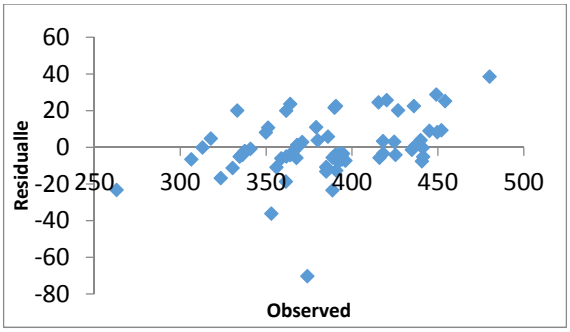

Figure 5. Plot of residuals against observed values of benzene derivatives entropy (S).

Table 4. Entropy (S) data of benzene derivatives.

No.	Observed S(J/molK)	Predicted S(J/molK)	Residual	No.	Observed S(J/molK)	Predicted S(J/molK)	Residual
1	317.835	313.051	4.784	36	349.828	341.718	8.110
2	306.457	313.051	-6.594	37	445.053	436.089	8.964
3	334.588	339.651	-5.063	38	356.019	366.955	-10.936
4	364.048	340.385	23.663	39	262.968	286.154	-23.186
5	323.616	340.385	-16.769	40	367.639	373.379	-5.740
6	358.773	364.794	-6.021	41	388.619	412.003	-23.384
7	394.751	398.127	-3.376	42	441.441	446.622	-5.181
8	379.109	368.154	10.955	43	441.136	441.422	-0.286
9	368.007	366.687	1.320	44	425.335	429.461	-4.126
10	380.017	376.180	3.837	45	353.047	389.203	-36.156
11	418.029	414.661	3.368	46	415.421	390.944	24.477
12	434.807	436.089	-1.282	47	393.149	396.660	-3.511
13	435.840	435.955	-0.115	48	390.792	403.460	-12.668
14	452.059	442.756	9.303	49	384.928	398.127	-13.199
15	424.529	421.461	3.068	50	364.454	368.154	-3.700
16	361.482	380.180	-18.698	51	420.165	394.428	25.737
17	361.720	341.718	20.002	52	374.009	444.296	-70.287
18	390.637	394.428	-3.791	53	385.007	395.761	-10.754

No.	Observed S(J/molK)	Predicted S(J/molK)	Residual	No.	Observed S(J/molK)	Predicted S(J/molK)	Residual
19	333.154	313.051	20.103	54	439.912	435.955	3.957
20	394.186	400.794	-6.608	55	449.659	441.422	8.237
21	394.032	398.127	-4.095	56	449.028	420.262	28.766
22	369.290	368.154	1.136	57	436.007	413.461	22.546
23	389.827	368.154	21.673	58	390.650	368.154	22.496
24	371.033	368.154	2.879	59	418.150	421.461	-3.311
25	312.911	313.051	-0.140	60	366.281	368.154	-1.873
26	454.207	428.958	25.249	61	363.994	368.154	-4.160
27	388.735	394.294	-5.559	62	361.725	366.687	-4.962
28	440.693	448.284	-7.591	63	385.417	396.660	-11.243
29	336.239	340.385	-4.146	64	396.188	403.460	-7.272
30	335.579	339.651	-4.072	65	392.008	400.003	-7.995
31	351.149	340.385	10.764	66	386.006	380.180	5.826
32	426.832	406.661	20.171	67	337.673	339.651	-1.978
33	340.904	341.718	-0.814	68	337.288	339.651	-2.363
34	416.018	421.738	-5.720	69	330.475	341.718	-11.243
35	480.077	441.495	38.582				

CONCLUSIONS

In this work, QSPR models for the prediction of entropy for a training set of benzene derivatives using MLR based on topological descriptors calculated from molecular structure have been developed. MLR model is proved to be a useful tool in the prediction of entropy. The aforementioned results and discussion lead us to conclude that combining the three descriptors (Sz, W, 1χ) could be used successfully for modeling and predicting entropy (S) of compounds. This model contains fewer topological descriptors, maximum of Fischer statistic value (F) and minimum root of the mean square of errors(s).

REFERENCES

1. X.J. Yao, B. Fan, J.P. Doucet, A. Panaye, M. Liu, R. Zhang, X. Zhang and Z. Hu, *QSAR & Combinatorial Science*, **2003**, 22, 29.
2. A.A. Taherpour, F. Shafiei, *Journal of Molecular Structure: THEOCHEM*, **2005**, 726, 183.
3. F. Shafiei, *Iranian Journal of Mathematical Chemistry*, **2015**, 6, 15.
4. P.R. Duchowicz, E.A. Castro, F.M. Fernández and A.N. Pankratov, *Journal of the Argentine Chemical Society,* **2006**, 94, 31.

5. Z. Lin, J. Xu, X. Zheng and Z. Li, *Acta Physico-Chimica Sinica*, **2000**, 16,153.
6. F. Gharagheizi, M.R. Samiee Gohar and M. Ghotbi Vayeghan, *Journal of Thermal Analysis and Calorimetry,* **2012**, 109, 501.
7. E. Estrada, O. Ivanciuc, I.Gutman, A.Gutierrez and L. Rodríguez, *New Journal of Chemistry*, **1998**, 22, 819.
8. H. Hosoya, M. Gotoh, M. Murakami and S. Ikeda, *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 192.
9. Y.P. Du, Y.Z. Liang, B.Y. Li and C.J. Xu, *Journal of Chemical Information and Computer Sciences*, **2002**,42,1128.
10. D. Plavsic, S. Nikolic, N. Trinajstic, and Z. Mihalic, *Journal of Mathematical Chemistry*, **1993**, 12, 235.
11. A.T. Balaban*, Journal of Molecular Structure: THEOCHEM*, **1998,**165, 243.
12. P.R. Duchowicz, E.A. Castro, F.M. Fernández and A.N. Pankratov, *Journal of the Argentine Chemical Society,* **2006**, 94, 31.
13. O. Ivanciuc*, Revue Roumaine de Chimie,* **1995**,40,1093.
14. J. Taskinen and J. Yliruusi. *Advanced Drug Delivery Reviews*, **2003**, 55, 1163.
15. L.H. Hall and C.T. Story, *SAR and QSAR in Environmental Research*, **1997**, 6,139.
16. Li. Qianfeng, Chen. Xingguo and Hu. Zhide, *Chemometrics and Intelligent Laboratory Systems,* **2004**, 72, 93.
17. E.S. Domalski and E.D. Hearing, *Journal of Physical and Chemical Reference Data*, **1988**, 17, 1637.
18. J.S. Chickos, C.M. Braton, D.G. Hesse and J.F. Liebman, *The Journal of Organic Chemistry*, **1991**, 56, 927.
19. J.S. Chickos, W.E. Acree, Jr. and J.F. Liebman, *Journal of Physical and Chemical Reference Data*, **1999**, 28, 1535.
20. Mu. Lailong, Feng. Changjun, *MATCH Communications in Mathematical and in Computer Chemistry,* **2007**, 111.
21. Mu. Lailong, He. Hongmei, *Industrial & Engineering Chemistry Research*, **2011**, 50, 8764.
22. M. Randić, *Journal of Mathematical Chemistry*, **1991**, 7, 155.
23. M. Randic', *Journal of the American Chemical Society*, **1975**, 97, 6609.
24. M. Randic', *Acta Chimica Slovenica*, **2002**, 49, 483.
25. B. Zhou, I. Gutman, *Chemical Physics Letters*, **2004**, 394, 93.
26. D.J. Klein, W. Yan, Y.N. Yeh, *International Journal of Quantum Chemistry*, **2006**, 106, 1756.
27. D. J.Klein, I. Lukovits, I. Gutman, *Journal of Chemical Information and Computer Sciences*, **1995**, 35, 50.
28. M. Liu1, B. LiuOn, *MATCH Communications in Mathematical and in Computer Chemistry*, **2011**, 66,293.
29. H. Deng, H. Xiao, F. Tang, *MATCH Communications in Mathematical and in Computer Chemistry*, **2010**, 63,257.
30. A.T. Balaban, *Chemical Physics Letters*, **1982**, 89, 399.
31. L. Blaha, J. Damborsky, M. Nemec, *Chemosphere,* **1998**, 36,1345.

32. C.K. Das, B. Zhou, N. Trinajstic, *Journal of Mathematical Chemistry,* **2009**, 1369.
33. I. Gutman, S. Klavzar, *Journal of Chemical Information and Computer Sciences*, **1995**, 35, 1011.
34. P.V. Khadikar, N.V. Deshpande, P.P. Dobrynin*, Journal of Chemical Information and Computer Sciences*, **1995**, 35, 547.
35. Web search engine developed by ChemAxon; software available at *http://www. Chemicalize. Org.*