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Survey

SURVEY

Chemical applicability of Sombor indices

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Abstract: Recently, a novel class of degree-based topological molecular descriptors was proposed, the so-called Sombor indices. Within this study, the predictive and discriminative potentials of the Sombor index, the reduced Sombor index, and the average Sombor index were examined. All three topological molecular descriptors showed good predictive potential. The statistical data indicate that the reduced Sombor index preforms with a slightly better predictive potential. An external validation confirmed this finding. It was found that these degree-based indices exert modest discriminative potential, when tested on a large group of isomers.

Keywords: graph invariants; molecular descriptors; degree of a vertex; physicochemical properties; predictive models; discriminative potential.

INTRODUCTION

A proper quantification of a molecule, more precisely its structure, may be accomplished by using molecular descriptors.[1,2] These quantities are derived from molecular structure, and they have found various applications in chemistry.[3,4] Their most important use is in QSPR/QSAR modeling[5–8] and in virtual screening.[9,10] The complexity of the obtained chemical information varies with the computational algorithm of the chosen molecular descriptor. Namely, the more detailed description of a molecule is obtained, the more computing resources have to be invested. On the other hand, a vague structural depiction is often computationally very efficient. Thus, the selection of an adequate molecular descriptor depends on the chemical problem on which it will be applied.

Encoding information on molecular structure through the utilization of topological molecular descriptors represents an efficient technique. Due to the low computational cost and quite simple identification with the structural details, the number of these molecular descriptors is huge. Topological molecular descriptors

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are mathematical values calculated from a graph representation of a molecule.[11–13] Therefore, they are also called graph invariants and have proved to be useful in chemistry.[14–19] Topological molecular descriptors were also found to be valuable in drug discovery. Namely, the advantages of graph invariants arises from the fact that receptor structure or mechanism of action of drugs is not necessary for QSAR development, also the conformation and alignment problems related with 3D QSAR (as in CoMFA applications) are completely avoided.[20] A vertex set, and edge set of a graph G, denoted by $V(G)$ and $E(G)$, corresponds to the non-hydrogen atoms and bonds of a molecule, respectively. Graph invariants can be computed from the molecular graph by using various algorithms. Thus, depending on which parameters are used in their definitions, degree-, distance-, and eigenvalue-based graph invariants can be differentiated.

The very first degree-based graph invariant is the first Zagreb index (Zg_1), which was introduced in 1972.[21] The first Zagreb index was defined as follows:

$$Zg_1(G) = \sum_{v \in V(G)} \deg(v)^2 \tag{1}$$

where deg(v) is degree, *i.e.*, number of first neighbors, of the vertex v. This quantity was developed during the investigation of dependence of π-electron energy on molecular structure. Since its introduction, this index has gained a lot of attention, especially among mathematicians.[22–26] It is interesting to point out that Zg_1 can also be calculated in this way:[27]

$$Zg_1(G) = \sum_{e_{i,j} \in E(G)} \left(\deg(v_i) + \deg(v_j)\right) \tag{2}$$

Recently, the author of the paper "Geometric approach to degree-based topological indices: Sombor indices"[28] being inspired by Euclidean metric, proposed novel graph invariants based on degree of a vertex. Namely, Sombor index (SO), reduced Sombor index (SO_{red}), and average Sombor index (SO_{avg}) were introduced. These quantities are defined as follows:

$$SO(G) = \sum_{e_{i,j} \in E(G)} \sqrt{\deg(v_i)^2 + \deg(v_j)^2} \tag{3}$$

$$SO_{red}(G) = \sum_{e_{i,j} \in E(G)} \sqrt{(\deg(v_i) - 1)^2 + (\deg(v_j) - 1)^2} \tag{4}$$

$$SO_{avg}(G) = \sum_{e_{i,j} \in E(G)} \sqrt{\left(\deg(v_i) - \frac{2m}{n}\right)^2 + \left(\deg(v_j) - \frac{2m}{n}\right)^2} \tag{5}$$

where m in Eq. (5) is the number of edges, while n denotes the number of vertices. The summation in the above equations goes over all edges. This novel class of indices was developed as the geometric representation of degree-based graph invariants.

As previously mentioned, the number of topological molecular descriptors is huge and is still increasing. Many of them are introduced as modifications of previously well-known indices and some of them have never been applied on solving chemical problems. Therefore, to filter a useful molecular descriptor from a pool of others, a list of desirable properties was compiled.[29] Within several listed features, sufficient predictive potential of physico-chemical properties of molecules and a low degeneracy level are among the most important ones. Since Sombor indices have recently been introduced and there is not much information about them, it is interesting to test their potential chemical applicability. More precisely, within this study the predictive and discriminative potentials of Sombor indices are analyzed.

COMPUTATIONAL METHODOLOGY

Construction of predictive models

In order to investigate predictive capability of Sombor indices, models for predicting the entropy ($S°$) and enthalpy change of vaporization ($\Delta H°_{vap}$) of compounds were developed. The models were constructed using an octane set of isomers and they are based on multiple linear regression. With the utilization of isomers, the influence of molecular size on a predictive model is eliminated. The experimental data used for the construction of the models were collected from www.moleculardescriptors.eu[30] and they are presented in Table I. The

TABLE I. The experimental data used for the development of the linear models

Molecule	$S°$ / J mol^{-1} K^{-1}	$\Delta H°_{vap}$ / kJ mol^{-1}
N-Octane	467.23	41.48
2-Methylheptane	459.57	39.68
3-Methylheptane	465.51	39.84
4-Methylheptane	457.39	39.68
3-Ethylhexane	457.86	39.65
2,2-Dimethylhexane	432.71	37.30
2,3-Dimethylhexane	451.96	38.79
2,4-Dimethylhexane	447.60	37.78
2,5-Dimethylhexane	442.33	37.87
3,3-Dimethylhexane	438.23	37.54
3,4-Dimethylhexane	445.97	38.98
2-Methyl-3-ethylpentane	443.76	38.53
3-Methyl-3-ethylpentane	424.59	37.99
2,2,3-Trimethylpentane	423.88	36.93
2,2,4-Trimethylpentane	435.51	35.15
2,3,3-Trimethylpentane	427.02	37.23
2,3,4-Trimethylpentane	428.40	37.71
2,2,3,3-Tetramethylbutane	389.36	35.19

coefficients occurring in the regression models were calculated by means of an in-house Python script with the implementation of a scikit-learn machine-learning module using least square fitting.[31]

Degeneracy calculation

The degeneracy of the Sombor index, the reduced Sombor index and the average Sombor index was determined using a measure proposed by Konstantinova.[32] This quantity was named sensitivity of a topological molecular descriptor and it is defined as follows:

$$\text{Sensitivity} = \frac{N - N_{TI}}{N} \tag{6}$$

where N is the number of isomers and N_{TI} denotes the number of isomers that cannot be distinguished by topological index (TI). Nowadays, this feature is commonly presented as the degeneracy of a topological index:

$$D = 100(1 - \text{Sensitivity}) \tag{7}$$

Within this study, two molecules (A and B) are considered to have the same value of TI if the following condition is fulfilled:

$$|TI(\text{A}) - TI(\text{B})| < 10^{-13} \tag{8}$$

This threshold was chosen because of the precision of common Python computations, which is 10^{-15}.

RESULTS AND DISCUSSION

Predictive potential of Sombor indices

The initial step for developing a linear model for predicting the entropy of molecules was to correlate the calculated values of SO, SO_{red} and SO_{avg} with the experimental data of octanes. With this, it was checked whether SO, SO_{red} and SO_{avg} contain information that may be used to model entropy. The entropy values are plotted in Fig. 1 against the SO values of the octane isomers.

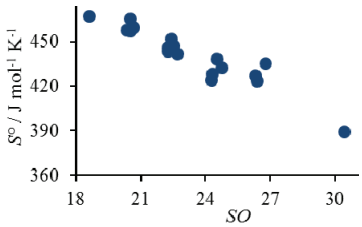

Fig. 1. The correlation between the Sombor index and entropy of octane isomers.

The scatter plot depicted in Fig. 1 shows a reasonable correlation between the Sombor index and entropy. Such a correlation indicates that a linear model for predicting the entropy of octanes could be developed using the Sombor index. A deeper insight into this correlation reveals that the data points are assembled into six clusters. Such grouping suggests that the data points within the same group have some parameter(s) in common. Namely, by direct checking, it was discovered that the points within one group have the same value of Zg_1. The correlations between reduced Sombor index and average Sombor index and entropy

are available in the Supplementary material to this paper (Figs. S-1 and S-2). The grouping of the data points is also present in these correlations, and it was revealed that Zg_1 also directs this clustering.

Since the Sombor indices showed satisfactory correlation with the entropy of octanes, the correlation between these descriptors and the enthalpy of vaporization was tested (Table I). The correlation between the Sombor index and $\Delta H°_{vap}$ is depicted in Fig. 2.

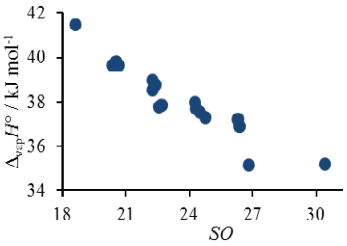

Fig. 2. The correlation between the Sombor index and enthalpy of vaporization of octane isomers.

The scatter plot presented in Fig. 2 shows that a linear dependence between Sombor index and enthalpy of vaporization exists. In addition, Fig. 2 illustrates that the data points are grouped, as in the previous case. Namely, it is obvious that the *SO* values are clustered into six different groups. Again, by direct checking, it was found that the data points within one group have the same values of Zg_1. The correlations between reduced and average Sombor indices and enthalpy of vaporization are depicted in Figs. S-3 and S-4 of the Supplementary material. The same groupation of the SO_{red} and SO_{avg} values is noticed.

As all examined correlations show linear relationships between the Sombor indices and these two physico-chemical properties, two types of linear models were constructed, (Eqs. (9) and (10)). Namely, in the model based on Eq. (9), the entropy or the enthalpy of vaporization is predicted only by one of the Sombor indices, while in the other model physicochemical property is predicted by one of the Sombor indices and the first Zagreb index:

$$S°, \Delta H°_{vap} \approx ATI + B \quad (9)$$

$$S°, \Delta H°_{vap} \approx ATI + BZg_1 + C \quad (10)$$

In these equations *TI* stands for the *SO*, SO_{red} and SO_{avg}, whereas *A*, *B* and *C* are the fitting coefficients. The values for the fitting parameters are presented in Table II.

The entropy and the enthalpy of vaporization of octanes were calculated using these models. The results of the evaluation of the models are presented in Table III.

In Table III, R^2, R_{adj}^2 and *RMSE* denote the coefficient of determination, adjusted coefficient of determination, and root mean square error, respectively. *F* denotes the value obtained by partial *F*-test and *p* stands for the *p*-value.

TABLE II. The values for the fitting parameters occurring in the models

Parameter	*TI*	Models based on Eq. (9)		Models based on Eq. (10)		
		A	*B*	*A*	*B*	*C*
$S°$ / J mol^{-1} K^{-1}	*SO*	–6.16	584.94	11.43	–17.47	713.82
	SO_{red}	–5.51	520.98	11.05	–18.36	847.94
	SO_{avg}	–5.22	491.66	3.45	–10.17	721.85
$\Delta H°_{vap}$ / kJ mol^{-1}	*SO*	–0.52	50.40	–1.97	1.44	39.77
	SO_{red}	–0.47	45.02	–2.17	1.88	11.49
	SO_{avg}	–0.44	42.49	–0.94	0.59	29.20

TABLE III. The results of evaluation of the linear regression models

TI	Models based on Eq. (9)			Models based on Eq. (10)				
	R^2 / %	R^2_{adj} / %	*RMSE* / J mol^{-1} K^{-1}	R^2 / %	R^2_{adj} / %	*RMSE* / J mol^{-1} K^{-1}	*F*	*p*
				$S°$				
SO	89.59	88.94	5.93	92.14	91.65	5.15	4.87	0.043
SO_{red}	89.23	88.56	6.03	92.53	92.06	5.02	6.63	0.021
SO_{avg}	89.48	88.82	5.96	91.36	90.82	5.40	3.27	0.091
				$\Delta_{vap}H°$				
SO	89.67	89.03	0.50	92.09	91.59	0.44	4.57	0.049
SO_{red}	90.65	90.07	0.48	95.47	95.19	0.33	15.96	0.001
SO_{avg}	89.84	89.21	0.50	90.71	90.13	0.47	1.41	0.254

The evaluation results presented in Table III show that the entropy and the enthalpy of vaporization of alkanes could be satisfactorily predicted using simple models based on Eq. (9). Namely, almost 90 % of data variance of $S°$ and $\Delta H°_{vap}$ may be explained by linear model where one of the Sombor indices is the only predictor. Furthermore, the errors that these models produce are small, especially for the enthalpy of vaporization. Among all these models, the model for predicting $\Delta H°_{vap}$ that uses reduced Sombor index showed the best performance. Namely, its R^2 value amounts 90.65 % and this model also yields smallest error.

To obtain better insight into the models, the predictive potential of Sombor indices were compared with predictive capability of other degree-based indices. Namely, for this purpose, the Randić index[33] and two Adriatic indices[34] (misbalance lodeg index and misbalance rodeg index) were used. It was found that Sombor indices demonstrate better prediction of entropy, since Randić and Adriatic indices explain around 80 % of data variance. Considering the enthalpy of vaporization, the Adriatic indices performed somewhat better. Namely, these indices describe around 96 % of data variance. Since the Randić and Adriatic indices showed similar predictive potential, it was supposed that a correlation might exist between these indices and the Sombor indices. To test this assumption, the correlations between the reduced Sombor index and these indices were checked. The correlations between the reduced Sombor index and Randić index and Adriatic indices are depicted in Figs. 3–5.

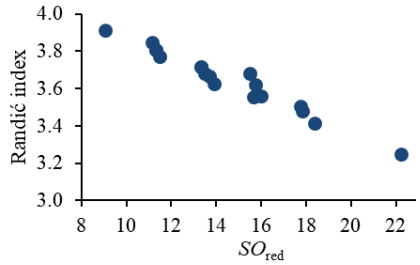

Fig. 3. The correlation between reduced Sombor index and Randić index. The correlation coefficient is –0.9815.

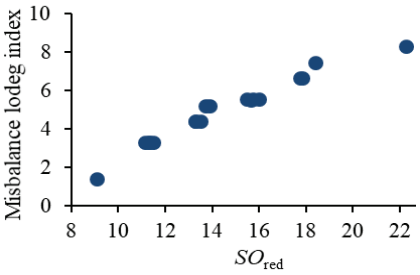

Fig. 4. The correlation between reduced Sombor index and misbalance lodeg index. The correlation coefficient is 0.9790.

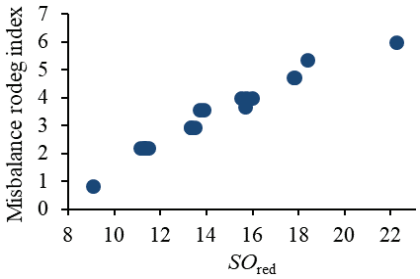

Fig. 5. The correlation between reduced Sombor index and the misbalance rodeg index. The correlation coefficient is equal to 0.9812.

The reduced Sombor index showed good correlations with the Randić and Adriatic indices. These findings indicate that mathematical relations between these indices may be established.

With the introduction of first Zagreb index as a second predictor, the performance of the present models is improved. Now, most of the models explain a huge amount of the data variance. The statistical justification of the introduction of Zg_1 was examined using the partial F-test with 95 % of confidence. Namely, F-value from Table III represents the result of this statistical procedure. A null hypothesis was that Zg_1 does not contribute to the explanation of the data variation. The results show that introduction of Zg_1 in the Sombor index and the reduced Sombor index models is statistically justified (see F and p values). Since F-value associated with the average Sombor index is lower than the critical value, the introduction of Zg_1 is not supported. Therefore, models based on Eq. (10) with the average Sombor index are omitted from further consideration.

In the case of entropy, the reduced Sombor index shows slightly better performance (R^2 = 92.53 %) over the Sombor index. Considering the enthalpy of

vaporization, the reduced Sombor index exerts a noticeably better predictive potential than Sombor index. Namely, its R^2 value amounts 95.47 %, and the error is quite small (0.33 kJ mol^{-1}).

In Figs. 6 and 7, correlations between the experimental values and those predicted by the reduced Sombor index and the first Zagreb index are illustrated. As may be seen, these figures illustrate that there is very good agreement between experimental and predicted data. The correlations for the other models are presented in the Supplementary material (Figs. S-5–S-8).

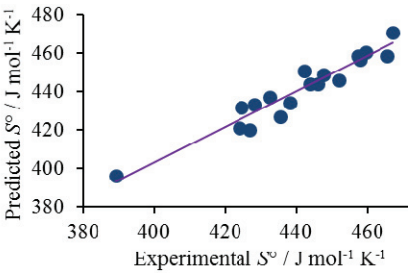

Fig. 6. The correlation between experimental and predicted values for the entropy.

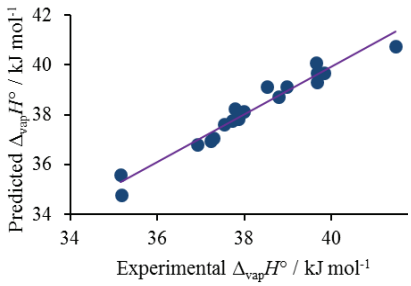

Fig. 7. The correlation between experimental and predicted values for the enthalpy of vaporization.

An external validation of the model for predicting enthalpy of vaporization by SO_{red} and Zg_1 was realized using the data set from Table IV. This data set consists of 35 values for $\Delta H°_{vap}$ of nonanes. This data set was randomly split, using scikit-learn module, into a training set and a test set (80:20). The training set was used to fit the model.

The values for the fitting parameters and the coefficients of determination are given in Table V. With 91.98 % of explained variance in the test set, the presented model showed excellent predictive potential. The correlation between experimental and predicted enthalpy of vaporization is depicted in Fig. 8.

Discriminative potential of Sombor indices

In order to test the discriminative potential of the Sombor indices, a series of chemical tree isomers were constructed. Namely, the number of vertices in these series ranged from 10 up to 20. The results of this investigation are tabulated in Table VI.

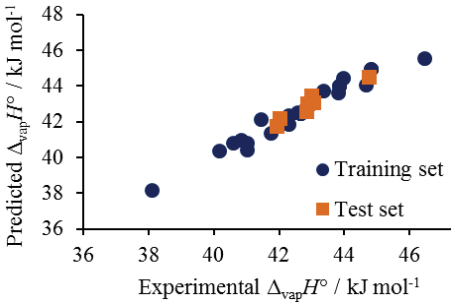

Fig. 8. The correlation between experimental and predicted values.

TABLE IV. The data used for the external validation

Molecule	$\Delta H°_{vap}$ / kJ mol^{-1}
n-Nonane	46.44
2-Methyloctane	44.65
3-Methyloctane	44.75
4-Methyloctane	44.75
2,2-Dimethylheptane	42.28
2,3-Dimethylheptane	43.79
2,4-Dimethylheptane	42.87
2,5-Dimethylheptane	42.87
2,6-Dimethylheptane	42.82
3,3-Dimethylheptane	42.66
3,4-Dimethylheptane	43.84
3,5-Dimethylheptane	42.98
4,4-Dimethylheptane	42.66
3-Ethylheptane	44.81
4-Ethylheptane	44.81
2,2,3-Trimethylhexane	41.91
2,2,4-Trimethylhexane	40.57
2,2,5-Trimethylhexane	40.17
2,3,3-Trimethylhexane	42.23
2,3,4-Trimethylhexane	42.93
2,3,5-Trimethylhexane	41.42
2,4,4-Trimethylhexane	40.84
3,3,4-Trimethylhexane	42.28
2-Methyl-3-ethylhexane	43.84
2-Methyl-4-ethylhexane	42.98
3-Methyl-3-ethylhexane	43.04
3-Methyl-4-ethylhexane	43.95
2,2,3,3-Tetramethylpentane	41.00
2,2,3,4-Tetramethylpentane	41.00
2,2,4,4-Tetramethylpentane	38.10
2,3,3,4-Tetramethylpentane	41.75
2,2-Dimethyl-3-ethylpentane	42.02
2,3-Dimethyl-3-ethylpentane	42.55
2,4-Dimethyl-3-ethylpentane	42.93
3,3-Diethylpentane	43.36

TABLE V. The values for the fitting parameters and the coefficients of determination

Parameter	Value	R^2 / %
A / kJ mol^{-1}	–2.44	Training set: 95.68
B / kJ mol^{-1}	2.20	Test set: 91.98
C / kJ mol^{-1}	5.16	

TABLE VI. The degeneracy of the Sombor indices

n	# of chemical trees	D (SO) / %	D (SO_{red}) / %	D (SO_{avg}) / %
10	75	33.33	34.67	34.67
11	159	47.80	45.91	47.80
12	355	60.56	60.56	61.41
13	802	71.32	71.57	71.82
14	1858	80.36	81.00	81.05
15	4347	87.12	87.69	87.35
16	10359	91.71	92.47	92.88
17	24894	94.85	95.49	94.97
18	60523	96.92	97.37	97.06
19	148284	98.14	98.49	98.25
20	366319	98.92	99.15	99.03

The percentages presented in Table VI show that the Sombor index, reduced Sombor index, and average Sombor index exert modest discriminative potential. All three descriptors show similar sensitivity. For example, within 355 chemical trees (n = 12), more than 60 % of the molecules cannot be distinguished by these topological molecular descriptors. Such degeneracy of the Sombor indices is in accordance with the degeneracy of other degree-based graph invariants. Namely, this class of indices show lower discriminative potential compared to eigenvalue-based descriptors. The degeneracy is plotted against the number of vertices in Fig. 9, which demonstrates that the degeneracy of the Sombor indices increases with the increasing number of molecules.

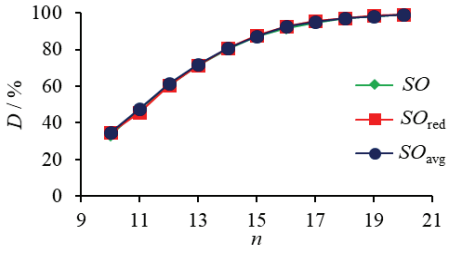

Fig. 9. Percentage of the degeneracy of the Sombor index, the reduced Sombor index, and the average Sombor index. Note that all three curves almost fully overlap.

CONCLUSIONS

Within this study, the chemical applicability of the Sombor indices was examined. More precisely, their predictive and discriminative potentials. The Sombor index, the reduced Sombor index, and the average Sombor index were

used to model the entropy and enthalpy of vaporization of alkanes. Simple linear models that use one of these indices as the only predictor showed satisfactory predictive potential. The performance of these models was improved with the introduction of the first Zagreb index as a second predictor. Among these three topological molecular descriptors, the reduced Sombor index showed the best performance. An external validation of the derived model was applied, and the reduced Sombor index showed up well. The results of the testing of the predictive potential of the Sombor indices indicate that these descriptors may be successfully applied for the modeling of thermodynamic properties of compounds.

The discriminative potential of the Sombor indices was tested on several groups of chemical trees. All three descriptors exhibit modest sensitivity. In a large class of isomers, a great number of molecules cannot be distinguished by these indices. This result is in accordance with the degeneracy of other degree-based graph invariants.

SUPPLEMENTARY MATERIAL

Additional data are available electronically at the pages of journal website: https://www.shd-pub.org.rs/index.php/JSCS/index, or from the corresponding author on request.

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ИЗВОД

ХЕМИЈСКА ПРИМЕЊИВОСТ СОМБОР ИНДЕКСА

ИЗУДИН РЕЦЕПОВИЋ

Институт за хемију, Природно–математички факултет, Универзитет у Крагујевцу, Радоја Домановића 12, 34000 Крагујевац

Недавно је предложена нова класа тополошких молекулских дескриптора заснованих на степену чвора, тзв. Сомбор индекси. У оквиру ове студије испитивани су предикциони и дискриминативни потенцијал Сомбор индекса, редукованог Сомбор индекса и просечног Сомбор индекса. Сва три тополошка молекулска дескриптора показала су добар предикциони потенцијал. Статистички подаци указују на то да редуковани Сомбор индекс има нешто бољи предикциони потенцијал у односу на друга два индекса. Спољном валидацијом модела потврђен је овај резултат. Такође, тестирањем на великој групи изомера утврђено је да ови индекси имају умерен дискриминативни потенцијал.

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REFERENCES

1. X. Ling, J. Bajorath, *Comb. Chem. High Throughput Screen.* **3** (2000) 363 (https://doi.org/10.2174/1386207003331454)
2. R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley, Weinheim, 2009 (https://doi.org/10.1002/9783527628766)
3. H. Hong, Q. Xie, W. Ge, F. Qian, H. Fang, L. Shi, Z. Su, R. Perkins, W. Tong, *J. Chem. Inf. Model.* **48** (2008) 1337 (https://doi.org/10.1021/ci800038f)

4. S. Sahoo, C. Adhikari, M. Kuanar, B. K. Mishra, *Curr. Comput. Aided Drug Des.* **12** (2016) 181 (https://doi.org/10.2174/1573409912666160525112114)
5. A. R. Katritzky, E. V. Gordeeva, *J. Chem. Inf. Comput. Sci.* **33** (1993) 835 (https://doi.org/10.1021/ci00016a005)
6. M. Karelson, *Molecular Descriptors in QSAR/QSPR*, Interscience, New York, 2000 (ISBN: 978-0-471-35168-9)
7. M. Dehmer, K. Varmuza, D. Bonchev, *Statistical Modelling of Molecular Descriptors in QSAR/QSPR*, John Wiley & Sons, Weinheim, 2012 (https://doi.org/10.1002/9783527645121)
8. K. Roy, S. Kar, R. N. Das, *A Primer on QSAR/QSPR Modeling-Fundamental Concepts*, Springer, Cham, 2015 (https://doi.org/10.1007/978-3-319-17281-1)
9. J. Bajorath, *J. Chem. Inf. Comput. Sci*. **41** (2001) 233 (https://doi.org/10.1021/ci0001482)
10. F. Grisoni, D. Reker, P. Schneider, L. Friedrich, V. Consonni, R. Todeschini, A. Koeberle, O. Werz, G. Schneider, *Mol. Inform.* **36** (2017) 1600091 (https://doi.org/10.1002/minf.201600091)
11. N. Trinajstić, *Chemical Graph Theory*, Routledge, New York, 2018 (https://doi.org/10.1201/9781315139111)
12. D. Bonchev, *Chemical Graph Theory: Introduction and Fundamentals*, CRC Press, Boca Raton, FL, 1991 (ISBN: 978-0856264542)
13. I. Gutman, *Selected Theorems in Chemical Graph Theory,* University of Kragujevac, Kragujevac, 2017 (ISBN: 978-86-6009-039-5)
14. E. Estrada, G. Patlewicz, E. Uriarte, *Indian J. Chem., A* **42** (2003) 1315 (http://hdl.handle.net/123456789/20663)
15. R. Zanni, M. Galvez-Llompart, R. Garcia-Domenech, J. Galvez, *Expert Opin. Drug Discov.* **10** (2015) 945 (https://doi.org/10.1517/17460441.2015.1062751)
16. O. Ivanciuc, *Curr. Comput. Aided Drug Des.* **9** (2013) 153 (https://doi.org/10.2174/1573409911309020002)
17. I. Redžepović, B. Furtula, *J. Comput. Aided Mol. Des.* **34** (2020) 975 (https://doi.org/10.1007/s10822-020-00320-2)
18. I. Redžepović, Y. Mao, Z. Wang, B. Furtula, *Int. J. Quantum Chem.* **120** (2020) e26209 (https://doi.org/10.1002/qua.26209)
19. I. Redžepović, B. Furtula, *J. Serb. Soc. Comput. Mech.* Special Issue (2020) 37 (https://doi.org/10.24874/jsscm.2020.01.04)
20. R. Gozalbes, J. P. Doucet, F. Derouin, *Curr. Drug Targets Infect. Disord*. **2** (2002) 93 (https://doi.org/10.2174/1568005024605909)
21. I. Gutman, N. Trinajstić, *Chem. Phys. Lett.* **17** (1972) 535 (https://doi.org/10.1016/0009-2614(72)85099-1)
22. S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, *Croat. Chem. Acta* **76** (2003) 113 (https://hrcak.srce.hr/103086)
23. I. Gutman, K. C. Das, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83 (http://match.pmf.kg.ac.rs/electronic_versions/Match50/match50_83-92.pdf)
24. M. Eliasi, A. Iranmanesh, I. Gutman, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 217 (http://match.pmf.kg.ac.rs/electronic_versions/Match68/n1/match68n1_217-230.pdf)
25. A. Ali, N. Trinajstić, *Mol. Inform.* **37** (2018) 1800008 (https://doi.org/10.1002/minf.201800008)

26. Z. Raza, A. Ali, *Int. J. Quantum Chem*. **120** (2020) e26333 (https://doi.org/10.1002/qua.26333)
27. T. Došlić, B. Furtula, A. Graovac, I. Gutman, S. Moradi, Z. Yarahmadi, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 613 (http://match.pmf.kg.ac.rs/electronic_versions/Match66/n2/match66n2_613-626.pdf**)**
28. I. Gutman, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 11 (http://match.pmf.kg.ac.rs/content86n1.htm)
29. M. Randić, *J. Math. Chem.* **7** (1991) 155 (https://doi.org/10.1007/BF01200821)
30. www.moleculardecriptors.eu (accessed February 15, 2020)
31. F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, E. Duchesnay, *J. Mach. Learn. Res.* **12** (2011) 2825 (https://www.jmlr.org/papers/volume12/pedregosa11a/pedregosa11a.pdf)
32. E. V. Konstantinova, *J. Chem. Inf. Comput. Sci.* **36** (1996) 54 (https://doi.org/10.1021/ci9502461)
33. M. Randić, *J. Am. Chem. Soc.* **97** (1975) 6609 (https://doi.org/10.1021/ja00856a001)
34. D. Vukičević, M. Gašperov, *Croat. Chem. Acta* **83** (2010) 243 (https://hrcak.srce.hr/62202).