JOURNAL OF ALGEBRAIC STATISTICS
Volume 13, No. 3, 2022, p. 1957-1967
https://publishoa.com
ISSN: 1309-3452

Quantitative Structure Property Relationship (Qspr) Analysis of General Randić Index

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Received 2022 April 02**; Revised** 2022 May 20**; Accepted** 2022 June 18**.**

Abstract

Topological indices are important tools for QSPR research. Randić index is one of the pioneers of topological indices as the most used topological index in view of chemical graph theory. It has been used for modelling physio-chemical properties of Octanes, Alkanes and other chemical molecules. In this paper, we have listed a few variants of general Randić index. Subsequently, the investigation of the prediction power of eight variants of general Randić index using some physio-chemical properties of Octane Isomers such as boiling point, density, entropy, acentric factor, etc. is carried out. We have also applied the sensitivity test on the eight variants. Finally, the most efficient index among the variants of general Randić index for the QSPR studies is identified.

Mathematics Subject Classification: 05C92

Keywords: Molecular Graph, Octane Isomers, General Randić Index and QSPR

1. Introduction:

In 1975, Milan Randić [1] proposed a topological index suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons that has become one of the most used topological indices in view of chemistry and chemical graph theory. Historically, Randić index was the first genuine degree-based topological index. It was defined as

$$R(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d(u)d(v)}}$$

where the summation goes over all pairs of adjacent vertices of the molecular graph G. Though Randić named the index as "branching index", it was soon re-named as "connectivity index". Nowadays, most authors refer to it after his name as the "Randić index". In 1998, Bollobas and Erdos [2] generalized this index by replacing the exponent -0.5 with any real number k, which is called the general Randić index. For a chemical graph G = (V,E), the general Randić index $R_k(G)$ is defined as the sum of $(d(u).d(v))^k$ over all edges uv of G, where d(u) denotes the degree of the vertex u of G, i.e.,

$R_k(G)=\sum_{uv\in E(G)}\left(d(u).d(v)\right)^k$ where k is an arbitrary real number.

Following are the six variants of the general Randić index.

1. **Randić Index [1]:** $R_{-1/2}(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{du.dv}}$

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2. **Reciprocal Randić Index[4]:** $R_{1/2}(G) = \sum_{uv \in E(G)} \sqrt{du.dv}$

3. **Second Reciprocal Zagreb Index:** $R_{-1}(G) = \sum_{uv \in E(G)} \frac{1}{du.dv}$

4. **Second Zagreb Index [5]:** $R_1(G) = \sum_{uv \in E(G)} du.dv$ which is 2 times the SK_1 Index [6].

5. **Second Reciprocal Hyper Zagreb Index:** $R_{-2}(G) = \sum_{uv \in E(G)} \frac{1}{(du.dv)^2}$

6. **Second Hyper Zagreb Index[7]:** $R_2(G) = \sum_{uv \in E(G)} (du.dv)^2$

From the above definition one may arrive at infinite variants of General Randić index for different values of k. Chemically, the most ideal situation is to choose the parameter k so that the index R_k be optimally correlated with a particular physio-chemical property. Adversely, to predict different physio-chemical properties, significantly different optimal k-values are required.

2. QSPR Analysis of General Randić Index

Chemical graph theory is the branch of mathematical chemistry. It is concerned with handling chemical graphs that represent chemical system. The chemical structure of a molecule is responsible for its physio-chemical properties. Hence, the topological indices are a convenient means of translating chemical constitution into numerical values which can be used to predict the physio-chemical properties in quantitative structure property/activity relationship (QSPR/QSAR) studies. The use of topological indices in QSPR and QSAR studies has become a major interest in recent years. Numerous studies have been made relating to the QSPR and QSAR studies by using numerous topological indices [3, 4, 12, 13, 14]. Among the well-known indices, Randić index is a pioneer of topological indices as the most widely used in both QSPR and QSAR studies. Milan Randić noticed that there is a good correlation between the Randić index and several physio-chemical properties of Alkanes such as boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapour pressure, surface areas, etc. In this study, we identify the variants of General Randić index that are efficient in the QSPR studies.

2.1 A Brief Survey

Recently, Sunilkumar Hosamani [4] undertook a detailed study on the QSPR analysis of Randić and Reciprocal Randić indices for modelling eight representative physio-chemical properties namely, boiling points(bp), molar volumes (mv) at 20◦C, molar refractions (mr) at 20◦C, heats of vaporization (hv) at 25◦C, surface tensions (st) 20◦C and melting points (mp) of the 67 Alkanes from n-butanes to nonanes. The linear regression model for the Randić and Reciprocal Randić indices are given below.

1. Linear Model for Randić Index:

bp = −98.6135+[R(G)]57.5074

mv = 50.5734+[R(G)]30.2112

mr = 5.9622+[R(G)]9.0465

hv = 3.1679+[R(G)]9.6368

ct = 36.0566+[R(G)]68.8462

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cp = 42.8740−[R(G)]4.4586

st = 8.2806+[R(G)]3.4046

mp = −150.8451+[R(G)]13.1312

2. Linear Model for Reciprocal Randić Index:

bp = −33.6900+[RR(G)]10.3117

mv = 53.8976+[RR(G)]7.0504

mr = 9.2765+[RR(G)]2.0924

hv = 10.1679+[RR(G)]1.9853

ct = 72.2490+[RR(G)]15.1722

cp = 29.0700−[RR(G)]0.2027

st = 8.1983+[RR(G)]0.8754

mp = −104.9739+[RR(G)]0.1913

Physical Properties	Correlation coefficient of Randić Index	Correlation coefficient of Reciprocal Randić Index
Boiling point	0.986	0.938
Molar volume	0.954	0.934
Molar refraction	0.960	0.962
Heats of vaporization	0.995	0.871
Critical temperature	0.962	0.951
Critical Pressure	0.911	0.827
Surface tension	0.909	0.848
Melting point	0.219	0.277

Table 1. Correlation Coefficients of Randić and Reciprocal Randić indices with the 67 alkanes

2.2 Linear regression Model of General Randić Index:

For our QSPR analysis of general Randić index, we consider the Octane Isomers which have become an important set of organic molecules to test the applicability of various topological parameters in quantitative structure-property/activity relationships (QSPR / QSAR). These compounds are structurally diverse enough to yield considerable variation in shape, branching and non-polarity.

We have used eight variants of the general Randić index namely R_{-3}, R_{-2}, R_{-1}, $R_{-0.5}$, $R_{0.5}$, R_1, R_2 and R_3 for modeling nine physio-chemical properties of Octane Isomers namely boiling point (BP), critical temperature (CT), critical pressure (CP), entropy (S), density (D), mean radius (R^2_m), heat of formation (ΔH_f), heat of vaporization (ΔH_v) and acentric factor (acent fac). The experimental values of the physio-chemical properties of Octane Isomers [13] and the general Randić index of Octane Isomers are listed in table 2 and 3 respectively.

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Octane Isomers	Boiling Point	Critical Temperature	Critical Pressure	Entropy	Density	Mean Radius	Heat of Formation	Heat of Vaporization	Acentric Factor
n-Octane	125.7	296.2	24.64	111.67	0.7025	2.0449	208.6	41.49	0.397898
2M	117.6	288	24.8	109.84	0.698	1.8913	215.4	39.67	0.377916
3M	118.9	292	25.6	111.26	0.7058	1.7984	212.5	39.83	0.371002
4M	117.7	290	25.6	109.32	0.7046	1.7673	210.7	39.64	0.371504
3E	118.5	292	25.74	109.43	0.7136	1.7673	210.7	39.64	0.362472
22MM	106.8	279	25.6	103.42	0.6953	1.6744	224.6	37.28	0.339426
23MM	115.6	293	26.6	108.02	0.7121	1.6464	213.8	38.78	0.348247
24MM	109.4	282	25.8	106.98	0.7004	1.6142	219.2	37.76	0.344223
25MM	109.1	279	25	105.72	0.6935	1.6449	222.5	37.85	0.35683
33MM	112	290.8	27.2	104.74	0.71	1.7377	220	37.53	0.322596
34MM	117.7	298	27.4	106.59	0.72	1.523	212.8	38.97	0.340345
2M3E	115.6	295	27.4	106.06	0.7193	1.5525	211	38.52	0.332433
3M3E	118.3	305	28.9	101.48	0.7274	1.5212	214.8	37.99	0.306899
223MMM	109.8	294	28.2	101.31	0.7161	1.4306	220	36.91	0.300816
224MMM	99.24	271.1	25.5	104.09	0.6919	1.401	224	35.14	0.30537
233MMM	114.8	303	29	102.06	0.7262	1.4931	216.3	37.27	0.293177
234MMM	113.5	295	27.6	102.39	0.7191	1.3698	217.3	37.75	0.317422
2233MMMM	106.5	270.8	24.5	93.06	0.8242	1.4612	225.6	42.9	0.255294

Table 2. Physio-ochemical Properties of Octane Isomers.

	R_{-3}	R_{-2}	R_{-1}	$R_{-0.5}$	$R_{0.5}$	R_1	R_2	R_3
n-Octane	0.328	0.813	2.25	3.914	12.83	24	88	336
2M	0.251	0.688	2.083	3.77	13.33	26	106	470
3M	0.328	0.792	2.167	3.808	13.46	27	121	603
4M	0.328	0.792	2.167	3.808	13.46	27	121	603
3E	0.405	0.896	2.25	3.846	13.59	28	136	736
22MM	0.205	0.578	1.875	3.561	14.24	30	148	840
23MM	0.258	0.686	2.028	3.681	14.06	30	164	1098
24MM	0.25	0.667	2	3.664	13.96	29	139	737
25MM	0.173	0.563	1.917	3.626	13.83	28	124	604
33MM	0.301	0.719	2	3.621	14.49	32	184	1232

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34MM	0.335	0.79	2.111	3.719	14.19	31	179	1231
2M3E	0.335	0.79	2.111	3.719	14.19	31	179	1231
3M3E	0.396	0.859	2.125	3.682	14.73	34	220	1624
223MMM	0.214	0.583	1.833	3.481	15.06	35	241	2171
224MMM	0.128	0.453	1.708	3.417	14.74	32	166	974
233MMM	0.233	0.62	1.875	3.504	15.17	36	262	2430
234MMM	0.188	0.58	1.889	3.553	14.66	33	207	1593
2233MMMM	0.094	0.379	1.563	3.25	16	40	352	4480

Table 3. Eight variants of General Randić Index of Octane Isomers.

For our study, we have established a linear regression function to the data in table 2 and 3. Let $P = a(TI) + b$ be the linear regression function, where P is the physical property, TI is the topological index, a is the slope and b is the intercept. Using the above linear regression function, we have obtained the following linear models for each variant of General Randić index.

1. LINEAR REGRESSION MODEL FOR $R_{-0.5}$

BP=30.26314 $R_{-0.5}(G)$+ 3.37508588

CT= 29.3133 $R_{-0.5}(G)$+ 182.791348

CP=-1.22641$R_{-0.5}(G)$+30.8645365

E=24.70243 $R_{-0.5}(G)$+ 15.353748

D=-0.09861$R_{-0.5}(G)$+1.07508311

MR=0.841039$R_{-0.5}(G)$+-1.4362872

HF=-27.0386$R_{-0.5}(G)$+315.23239

HV=2.707331$R_{-0.5}(G)$+28.7363377

Acent fac=0.193477$R_{-0.5}(G)$+-0.3696046

2. LINEAR REGRESSION MODEL FOR $R_{0.5}$

BP= -4.8166 $R_{0.5}(G)$ + 182.206281

CT=-2.23448$R_{0.5}(G)$+321.438371

CP=0.816324$R_{0.5}(G)$+14.7841109

E=-5.58567$R_{0.5}(G)$+184.849061

D=0.025818$R_{0.5}(G)$+0.34838494

MR=-0.1965$R_{0.5}(G)$+4.42449961

HF=4.369061$R_{0.5}(G)$+154.521684

HV=-0.4665$R_{0.5}(G)$+45.2408657

Acent fac=-0.04575$R_{0.5}(G)$+0.98636607

3.LINEAR REGRESSION MODEL FOR R_{-1}

BP=28.28084$R_{-1}(G)$+57.2215157

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CT= 32.49973R_{-1}(G)+224.748314

CP=0.146235R_{-1}(G)+26.1012538

E=20.2287R_{-1}(G)+65.0098815

D=-0.07613R_{-1}(G)+0.86761785

MR=0.669286R_{-1}(G)+0.29316862

HF=-25.3446R_{-1}(G)+267.277075

HV=2.25148R_{-1}(G)+34.1097109

Acent fac=0.153424R_{-1}(G)+0.02933104

4. LINEAR REGRESSION MODEL FOR R_1

BP=-0.77151R_1(G)+137.41022

CT=-0.17693R_1(G)+295.096779

CP=0.179084R_1(G)+20.8914788

E=-1.07625R_1(G)+138.478053

D=0.005401R_1(G)+0.54961186

MR=-0.03723R_1(G)+2.77378097

HF=0.722025R_1(G)+194.473353

HV=-0.05816R_1(G)+40.3933236

Acent fac=-0.00885R_1(G)+0.60755834

5. LINEAR REGRESSION MODEL FOR R_{-2}

BP=36.21007R_{-2}(G)+89.0688352

CT=49.1428R_{-2}(G)+256.222163

CP=2.109086R_{-2}(G)+24.9582175

E=21.92144R_{-2}(G)+90.497011

D=-0.07535R_{-2}(G)+0.76682718

MR=0.700928R_{-2}(G)+1.15301321

HF=-32.7288R_{-2}(G)+238.925695

HV=2.396777R_{-2}(G)+36.9757932

Acent fac=0.1568302R_{-2}(G)+0.22905634

6. LINEAR REGRESSION MODEL FOR R_2

BP=-0.03581R_2(G)+119.947926

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CT=-0.00589R_2(G)+290.688101

CP=0.00946 R_2(G)+24.7446834

E=-0.06472R_2(G)+116.692367

D=0.000378R_2(G)+0.64961843

MR=-0.00202R_2(G)+1.98244934

HF=0.037072R_2(G)+210.194817

HV=0.001632R_2(G)+38.3223212

Acent fac=-0.000519R_2(G)+0.42616662

7. LINEAR REGRESSION MODEL FOR R_{-3}

BP=55.35496R_{-3}(G)+99.1002192

CT=79.79159R_{-3}(G)+268.604997

CP=4.464631R_{-3}(G)+25.2151669

E=30.729R_{-3}(G)+97.3042914

D=-0.09791R_{-3}(G)+0.74139409

MR=0.990304R_{-3}(G)+1.36862521

HF=-50.2634R_{-3}(G)+229.919509

HV=3.467068R_{-3}(G)+37.691746

Acent fac=0.2116229R_{-3}(G)+0.27992562

8. LINEAR REGRESSION MODEL FOR R_3

BP=-0.00211R_3(G)+116.408962

CT=-0.00132R_3(G)+291.350869

CP=0.000358R_3(G)+25.9360138

E=-0.00414R_3(G)+110.700592

D=0.00002724R_3(G)+0.68076476

MR=-0.00011R_3(G)+1.77232737

HF=0.002389R_3(G)+213.603453

HV=0.000436R_3(G)+38.0494683

Acent fac= -0.00003178R_3(G)+0.37636202

For similar study on the quadratic and logarithmic model of other topological indices one may refer [12].

2.3 Correlation of General Randić Index with Physio-chemical Properties of Octane Isomers:

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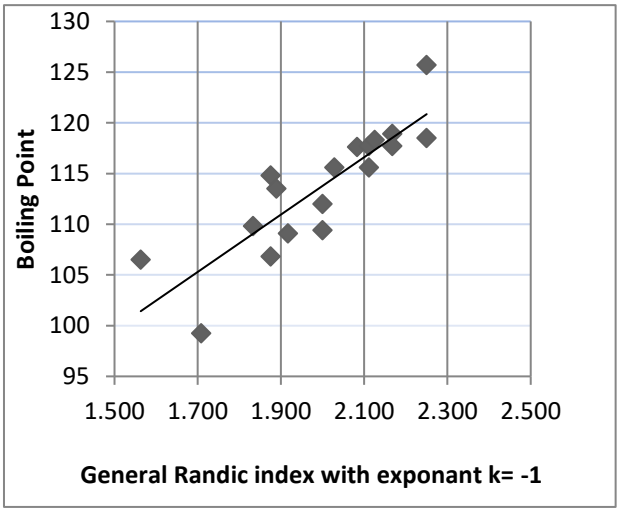
The correlation coefficient of a topological index with a certain physio-chemical property of a chemical compound indicates how strong the relationship between them is. In the following table 4 the correlation coefficients of eight variants of general Randić index with nine physio-chemical properties of Octane Isomers are given:

General Randić index	Boiling Point	Critical Temperature	Critical Pressure	Entropy	Density	Mean Radius	Heat of Formation	Heat of Vaporization	Acentric Factor
$R_{-3}(G)$	0.790	0.716	0.271	0.594	-0.293	0.478	-0.832	0.171	0.522
$R_{-2}(G)$	0.832	0.710	0.206	0.683	-0.363	0.545	-0.873	0.190	0.623
$R_{-1}(G)$	**0.856**	0.618	0.019	0.829	-0.482	0.685	**-0.889**	0.235	0.802
$R_{-0.5}(G)$	0.819	0.499	-0.141	0.906	-0.559	0.770	-0.849	0.252	0.904
$R_{0.5}(G)$	-0.607	-0.177	0.438	**-0.954**	0.681	**-0.837**	0.638	-0.202	**-0.995**
$R_1(G)$	-0.498	-0.072	0.492	-0.942	0.730	-0.813	0.541	-0.129	-0.986
$R_2(G)$	-0.378	-0.039	0.425	-0.925	0.836	-0.722	0.454	0.059	-0.945
$R_3(G)$	-0.339	-0.133	0.245	-0.900	**0.915**	-0.605	0.445	0.241	-0.881

Table 4. Correlation coefficient values of the general Randić index

In the following figures, the correlation of general Randić index with boiling point, entropy, density, mean radius, heat of formation and acentric factor of octane isomers are shown:



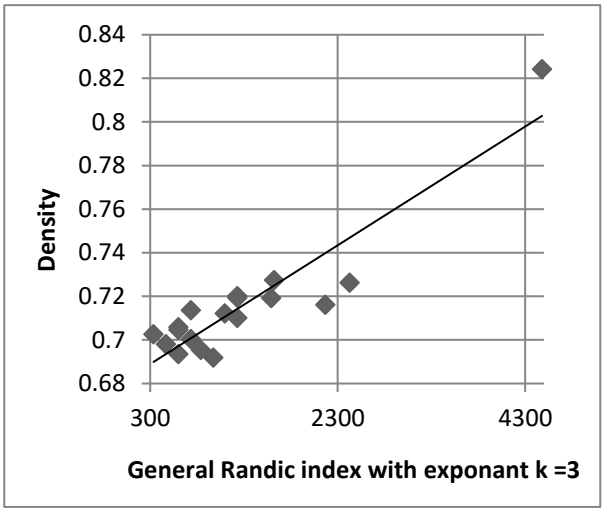


Fig. 1 Correlation of R_{-1} index with boiling point of Octane Isomers

Fig. 2 Correlation of R_3 index with density of Octane Isomers

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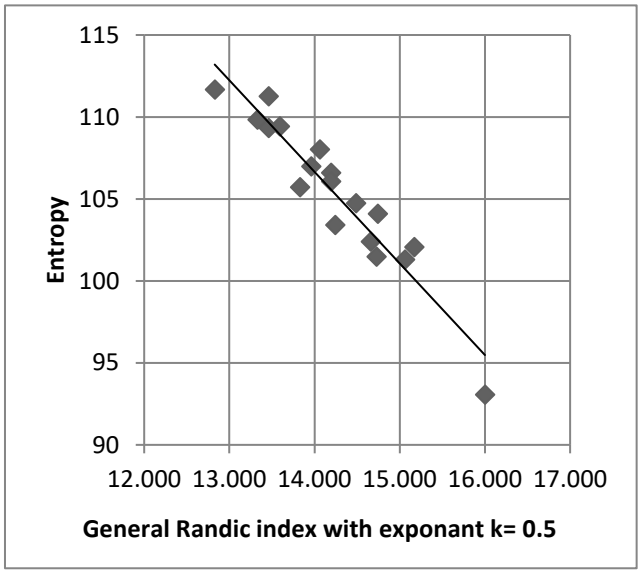

Fig. 3 Correlation of $R_{0.5}$ index with entropy of Octane Isomers

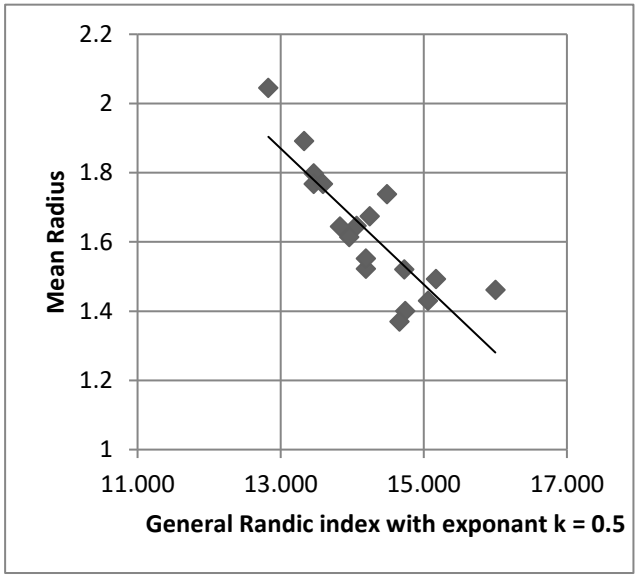

Fig. 4 Correlation of $R_{0.5}$ index with mean radius of Octane Isomers

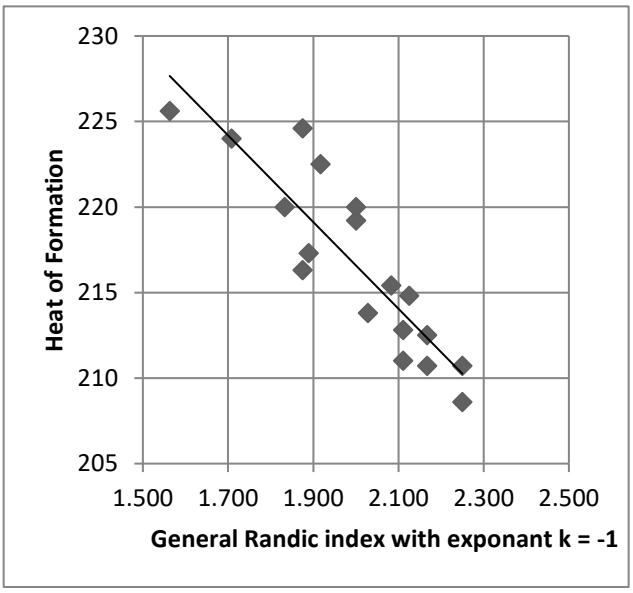

Fig. 5 Correlation of R_{-1} index with heat of formation of Octane Isomers

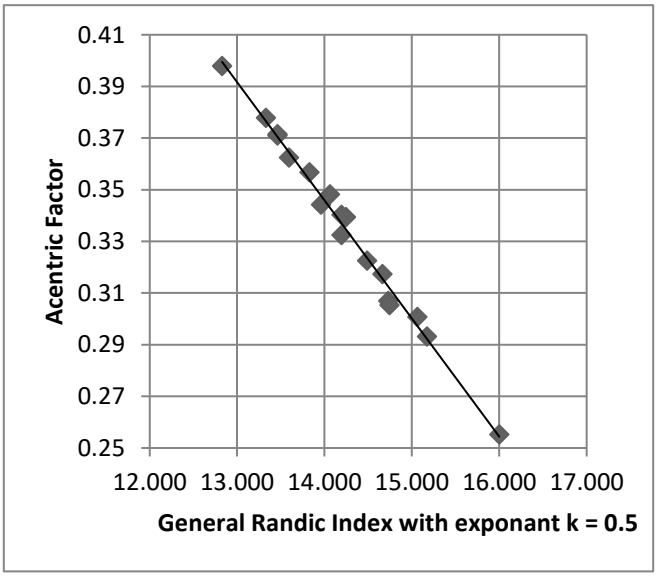

Fig. 6 Correlation of $R_{0.5}$ index with acentric factor of Octane Isomers

In table 4, one may observe that $R_{0.5}$ (Reciprocal Randić index) shows high correlation with entropy, mean radius and acentric factor of Octane Isomers with correlation coefficient values r = -0.954, r = -0.837 and r = -0.995 respectively. Further, one may notice that except for boiling point, the Reciprocal Randić index performs better than the usual Randić index with exponent k = -0.5.

The index R_{-1} (Second Reciprocal Zagreb index) shows high correlation with correlation coefficient values r = -0.889 and r = 0.856 with respect to heat of formation and boiling point of Octane Isomers. Hence, the variant R_{-1} turns out to be the best index among the variants of General Randić index to predict the heat of formation and boiling point. Further, it is interesting to observe that except for entropy, mean radius and acentric factor, the second reciprocal Zagreb index yields better predictive values than the well-known second Zagreb index with exponent k = 1.

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Volume 13, No. 3, 2022, p. 1957-1967
https://publishoa.com
ISSN: 1309-3452

Among the eight variants of the General Randić index, R_3 is the only index which highly correlates with the density of octane isomers with the correlation coefficient 0.915. From the table 4 it is evident that the index with higher exponent values yields better correlation with the density of Octane Isomers.

For more related study on QSPR analysis of other topological indices, one may refer [3, 4, 9, 10, 11, 12, 13, 14].

2.4 Sensitivity Test:

In the study of chemical compound property prediction, the molecules with similar structures or same values of the topological index have similar properties. A major drawback of most topological indices is for two or more nonisomorphic graphs, they possess the same value. Thus, the study of topological index sensitivity is important for the investigation of topological indices. One of the basic characteristics of topological index is its sensitivity in the process of molecular structure classification. The sensitivity of a topological index is the measure of its ability to distinguish nonisomorphic graphs. Topological indices having high sensitivity capture more structural information. The theoretical evaluation of the sensitivity on the set of all graphs is difficult. Therefore, we evaluate the sensitivity of topological index on a smaller fixed set M of Octane Isomers, introduced by Konstantinova [8] which is given by the formula

$$S_{TI} = \frac{N - N_{TI}}{N},$$

where N = |M| and N_{TI} is a number of graphs that cannot be distinguished by topological index on the set M. The table 5. shows the sensitivity measure of eight variants of general Randić index on the Octane Isomers.

Eight Variants of General Randić Index	**Sensitivity (S_{TI})**
$\mathbf{R_{-3}}$	0.833
$\mathbf{R_{-2}}$	0.889
$\mathbf{R_{-1}}$	0.722
$\mathbf{R_{-0.5}}$	0.889
$\mathbf{R_{0.5}}$	0.889
$\mathbf{R_1}$	0.722
$\mathbf{R_2}$	0.889
$\mathbf{R_3}$	0.889

Table 5. Measure of sensitivity (S_{TI}) of eight variants of general Randić index on Octane Isomers

As S_{TI} increases, the isomer discrimination power of topological indices increases. The variants $R_{-0.5}$, $R_{0.5}$, R_{-2}, R_2 and R_3 have greater sensitivity and discriminating power than the other considered variants of general Randić index.

Conclusion

In this article, the predictive ability and the efficiency of eight variants of general Randić index are tested using Octane Isomers. These variants have been proved as useful molecular descriptors in QSPR study. These indices are an extension of well-established degree based Randić index. The correlation between these variants and the properties of Octane Isomers such as boiling point, entropy, density, mean radius, heat of formation and acentric factor are stronger. On the other hand, correlation with properties such as critical temperature, critical pressure and heat of vaporization are weaker. For Octane Isomers, $R_{0.5}$ (Reciprocal Randić index) can model entropy, mean radius and acentric factor with

high precision compared to the other variant under consideration. R_{-1} (Second Reciprocal Zagreb index) is more effective in predicting boiling point and heat of formation compared to other variants of general Randić index. The predictability of R_3 index is remarkable for density. The sensitivity test confirms the supremacy of the variant such as $R_{-0.5}$, $R_{0.5}$, R_{-2}, R_2 and R_3 with sensitivity measure 0.889.

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