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QSPR Analysis of the Bond-Valence Substituent Index with Eight Physical Properties of Alkanes

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ABSTRACT

Based on its predictive power as a molecular descriptor, the bond-valence substituent index (BVSI) and its square root were characterized by using linear and quadratic correlation models with eight representative physical properties (boiling point, molar volume, molar refraction, heat of vaporization, surface tension, and melting point) of 74 alkanes from ethane to nonanes. The BVSI was also modelled with around 67 alkanes from butanes to nonanes by linear correlation to compare it with published data obtained from ten degree-based topological indices, which included the Randić index. The study showed that BVSI was the best topological index among those studied, predicting most accurately the boiling point and the molar refraction. The index also predicted the molar volume, critical temperature, and pressure better than the other indices placing it under the category of "very useful" molecular descriptor for potential QSPR/QSAR studies.

Keywords: *bond-valence substituent index (BVSI); quantitative structure-property relationships (QSPR); topological index; degree-based topological index*

INTRODUCTION

A basic concept in chemistry is that the structural characteristics of a molecule are responsible for its properties. Since molecular descriptors or topological indices are extracted from molecular structure by some mathematical methods and numerical values as deduced from chemical constitution, they can be used in correlating properties in quantitative structure property/activity relationships (QSPR/QSAR) studies. This enables the prediction of molecular properties, which are of practical importance in various field of chemistry, physics, biology, mathematics, informatics etc. (Todeschini and Consonni, 2000; Trinajstić, 1992; Balaban, 1976; Kier and Hall, 1976). Thus, finding formulas for calculating the topological indices or molecular descriptors of chemical structures followed by non-empirical QSAR/QSPR studies are very important.

Just recently, we (Sumera et al., 2020) have introduced a new topological index called the bond-valence substituent index (BVSI) and found its predictive power comparable if not better than the popularly known Randić index R (Randić, 1975) and the F*i* index (Manso et al, 2012) against the boiling temperature of some 137 alkanes. The BVSI index is derived from the reciprocal fraction of the number of bond substitutions of every bond in a molecule. Although it has several other interesting properties, its performance in QSPR will first be tested here in the structural property correlations with several properties of alkanes.

The objective of this paper is to determine whether the BVSI is a useful molecular descriptor, which means that it can give "more insights into the interpretation of molecular properties for practical consideration" (Hosamani et al., 2017; Shirakol et al., 2019). The QSPR study of BVSI with eight physical properties of 74(C_2-C_9) alkanes would help us characterize whether BVSI is a useful index if its values of correlation coefficient lie between 0.8 to 0.995 for a particular physical property. The more physical properties are highly correlated the more useful is the molecular descriptor or topological index. We will also compare BVSI with other known degree-based indices through their modelled equations of physical properties provided by literature and see how BVSI fares.

A glimpse of the statistical results of the QSPR with eight physical properties of the alkanes shows that the BVSI is the best among the topological indices herein studied in predicting the majority of the physical properties of the alkanes.

METHODS

To show the usefulness of BVSI as a molecular index through QSPR, research data were collected in three stages.

First, the eight physical properties of 74 alkanes from ethane to nonanes, such as boiling point (Bp, °C), molar refraction (Mr, cm^3) at 20°C, molar volume (Mv, cm^3) at 20°C, heat of vaporization (Hv, kJ) at 25°C, critical temperature (Ct, °C), critical pressure (Cp, atm), surface tension (St, dyne/cm) at 20°C and melting point (Mp, °C) were collected from literature (Plavšić et al., 1993) and listed not in the same order in Table 1.The values of the BVSI, its variant $\sqrt{BVSI}$, and also the Randić index (for comparison) for the 74 alkanes were calculated and are also incorporated in Table 1. The values were calculated using equations 1 and 2.

The simplest formula of the bond-valence substituent index (BVSI) is shown by the equation below,

$$BVSI = \sum_{1st\ bond}^{Final\ bond} \left[1 + \frac{S}{V}\right]^{-1/2} \quad (1)$$

where,

S = number of bond substituents (non-hydrogen substituents of the bond)

V = number of bond-valence electrons = number of valence electrons of the bond without the substituents and hydrogens (or simply the maximum number of substitution of the bond for the alkanes)

e.g. for C-C bond; ·:C-C:· , number of bond-valence electrons = 6
for C=C bond; :C=C: , number of bond-valence electrons = 4
for C≡C bond; ·C≡C· , number of bond-valence electrons = 2

Since the alkanes are characterized by their C-C single bonds with a total number of bond-valence electrons of 6, the equation above can also be expressed by a graph theoretical equation below,

$$BVSI(G) = \sum_{i-j}\left[1 + \frac{(d_i(G) + d_j(G) - 2)}{6}\right]^{-1/2} \quad (1a)$$

where d_i = degree of vertex *i*, d_j = degree of vertex *j*, where *i* and *j* are connected vertices making an edge of a molecular graph (*G).*

The Randić topological index R (Randić, 1975) is expressed in a graph theoretical equation as,

$$R(G) = \sum_{i-j}\left(d_i(G)d_j(G)\right)^{-\frac{1}{2}} \quad (2)$$

where d_i is the degree of vertex *i* and d_j is the degree of vertex *j* of molecular graph *G*. The index is the sum over all pairs of adjacent vertices of the molecular graph *G*.

Second, QSPR was established by linear and quadratic regression between the physical properties and the indices from the formulas; linear regression with Randić, BVSI and $\sqrt{BVSI}$ and quadratic regression with $\sqrt{BVSI}$. Excel software was used and correlation coefficients (r) and standard deviations(s) were determined for comparison (Tables 2 and 3).

Third, results of QSPR with BVSI in a linear correlation modelling were compared with results from ten degree-based topological indices, reported in literature (Hosamani et al., 2017) on alkanes from butanes to nonanes and are shown in Table 5.

RESULTS AND DISCUSSION

Table 1 showed a list of the experimental values of the eight physical properties of the 74 alkanes understudy with the BVSI, its square root $\sqrt{BVSI}$ and the Randić index to provide the data for the calculation of the linear and quadratic models of correlation and the resulting statistical parameters (Tables 2 and 3) and equations.

Table 1. The BVSI and its square root ($\sqrt{BVSI}$), the Randić index (R) and the experimental values of eight physical properties of the 74 alkanes

Alkane	BVSI*	$\sqrt{BVSI}$*	R index*	Bp (°C) **	Mv (cm^{-1}) **	Mr (cm^{-1}) **	Hv (kj) **	Ct (°C) **	Cp (atm) **	St (d/cm)**	Mp (°C) **
ethane	1.0000	1.0000	1.0000	-88.630				32.27	48.2		-183.27
propane	1.8516	1.3608	1.4142	-42.070				96.80	42.01		-187.69
n-butane	2.7177	1.6485	1.9142	-0.500				152.01	37.47		-138.35
isobutane	2.5981	1.6119	1.7320	-11.730				134.98	36		-159.60
n-pentane	3.5836	1.8930	2.4142	36.074	115.205	25.2656	26.42	196.62	33.31	16.00	-129.72
isopentane	3.4744	1.8640	2.2700	27.852	116.426	25.2923	24.59	187.70	32.9	15.00	-159.90
neopentane	3.2660	1.8072	2.0000	9.503	112.074	25.7243	21.78	160.60	31.57		-16.55
n-hexane	4.4498	2.1095	2.9142	68.740	130.688	29.9066	31.55	234.70	29.92	18.42	-95.35
2-methylpentane	4.3403	2.0833	2.7700	60.271	131.933	29.9459	29.86	224.90	29.95	17.38	-153.67
3-methylpentane	4.3507	2.0858	2.8080	63.282	129.717	29.8016	30.27	231.20	30.83	18.12	-118.00
2,2-dimethylbutane	4.1500	2.0371	2.5606	49.741	132.744	29.9347	27.69	216.20	30.67	16.30	-99.87
2,3-dimethylbutane	4.2387	2.0588	2.6427	57.988	130.240	29.8104	29.12	227.10	30.99	17.17	-128.54
n-heptane	5.3157	2.3056	3.4142	98.427	146.540	34.5504	36.55	267.55	27.01	20.26	-90.61
2-methylhexane	5.2065	2.2818	3.2700	90.052	147.656	34.5908	34.80	257.90	27.2	19.29	-118.28
3-methylhexane	5.2166	2.2841	3.3080	91.850	145.821	34.4597	35.08	262.40	28.1	19.79	-119.40
2,2-dimethylpentane	5.0159	2.2397	3.0607	79.197	148.695	34.6166	32.43	247.70	28.4	18.02	-123.81
2,3-dimethylpentane	5.1150	2.2616	3.1807	89.784	144.153	34.3237	34.24	264.60	29.2	19.96	-119.10
2,4-dimethylpentane	5.0971	2.2577	3.1258	80.500	148.949	34.6162	32.88	247.10	27.4	18.15	-119.24

Table 1 (continued)

Alkane	BVSI*	$\sqrt{BVSI}$*	R index*	Bp (°C) **	Mv (cm^{-1}) **	Mr (cm^{-1})**	Hv (kj) **	Ct (°C) **	Cp (atm)**	St (d/cm)**	Mp (°C) **
3,3-dimethylpentane	5.0339	2.2437	3.1213	86.064	144.530	34.3323	33.02	263.00	30	19.59	-134.46
3-ethylpentane	5.2270	2.2862	3.3460	93.475	143.517	34.2827	35.22	267.60	28.6	20.44	-123.81
2,2,3-trimethylbutane	4.9201	2.2182	2.9433	80.882	145.191	34.3736	32.04	258.30	29.75	18.76	-24.91
n-octane	6.1818	2.4864	3.9142	125.665	162.592	39.1922	41.48	296.20	24.64	21.76	-56.79
2-methylheptane	6.0724	2.4642	3.7700	117.647	163.663	39.2316	39.68	288.00	24.8	20.60	-109.04
3-methylheptane	6.0827	2.4664	3.8080	118.925	161.832	39.1001	39.83	292.00	25.6	21.17	-120.50
4-methylheptane	6.0827	2.4663	3.8080	117.709	162.105	39.1174	39.67	290.00	25.6	21.00	-120.95
2,2-dimethylhexane	5.8820	2.4253	3.5606	106.810	164.280	39.2525	37.29	279.00	25.6	19.60	-121.18
2,3-dimethylhexane	5.9811	2.4456	3.6807	115.607	160.390	38.9808	38.79	293.00	26.6	20.99	
2,4-dimethlhexane	5.9734	2.4441	3.6639	109.429	163.090	39.1300	37.76	282.00	25.8	20.05	-137.50
2,5-dimethylhexane	5.9631	2.4420	3.6258	109.103	164.690	39.2596	37.86	279.00	25	19.73	-91.20
3,3-dimethylhexane	5.8998	2.4290	3.6213	111.969	160.870	39.0087	37.93	290.84	27.2	20.63	-126.10
3,4-dimethylhexane	5.9912	2.4477	3.7187	117.725	158.810	38.8453	39.02	298.00	27.4	21.64	
3-ethylhexane	6.0930	2.4684	3.8461	118.534	160.070	38.9441	39.40	292.00	25.74	21.51	
2,2,3-trimethylpentane	5.7963	2.4076	3.4813	109.841	159.520	38.9249	36.91	294.00	28.2	20.67	-112.27
2,2,4-trimethylpentane	5.7726	2.4026	3.4165	99.238	165.080	39.2617	35.13	271.15	25.5	18.77	-107.38
2,3,3-trimethylpentane	5.8040	2.4092	3.5040	114.760	157.290	38.7617	37.22	303.00	29	21.56	-100.70
2,3,4-trimethylpentane	5.8793	2.4247	3.5534	113.467	158.850	38.8681	37.61	295.00	27.6	21.14	-109.21
3-ethyl-2-methylpentane	5.9912	2.4477	3.7187	115.650	158.790	38.8362	38.52	295.00	27.4	21.52	-114.96
3-ethyl-3-methylpentane	5.9178	2.4326	3.6819	118.259	157.020	38.7171	37.99	305.00	28.9	21.99	-90.87
2,2,3,3-tetramethylbutane	5.6061	2.3677	3.2500	106.470				270.80	24.5		
n-nonane	7.0477	2.6548	4.4142	150.798	178.710	43.8423	46.44	322.00	22.74	22.92	-53.52
2,2-dimethylheptane	6.7479	2.5977	4.0606	132.690	180.500	43.9138	42.28	302.00	22.8	20.80	-113.00
2,2,3-trimethylhexane	6.6625	2.5812	3.9814	133.600	175.878	43.6226	41.91	318.10	25.07	21.86	
4-methyloctane	6.9488	2.6360	4.3080	142.480	178.150	43.7687	44.75	318.30	23.06	22.34	-113.20
2,2,4-trimethylhexane	6.6490	2.5786	3.9545	126.540	179.220	41.7638	40.57	301.00	23.39	20.51	-120.00
2,2,5-trimethylhexane	6.6387	2.5766	3.9165	124.084	181.346	43.9356	40.17	296.60	22.41	20.04	-105.78
2,3,3-trimethylhexane	6.6701	2.5826	4.0040	137.680	173.780	43.4347	42.23	326.10	25.56	22.41	-116.80
2,3,5-trimethylhexane	6.7378	2.5957	4.0365	131.340	177.656	43.6474	41.42	309.40	23.49	21.27	-127.80
2,4,4-trimethylhexane	6.6565	2.5800	3.9772	130.648	177.187	43.6598	40.84	309.10	23.79	21.17	-133.78
3,3,4-trimethylhexane	6.6803	2.5846	4.0420	140.460	172.055	43.3407	42.28	330.60	26.45	23.27	-101.20
2,2,3,4-tetramethylpentane	6.5607	2.5614	3.8540	133.016	173.557	43.4359	41.00	319.60	25.66	21.98	-121.09
3-ethyl-2,2-dimethylpentane	6.6727	2.5832	4.0193	133.830	174.537	43.4571	42.02	322.60	25.96	22.38	-99.20
3-ethyl-2,4-dimethylpentane	6.7556	2.5992	4.0914	136.730	173.804	43.4037	42.93	324.20	25.46	22.80	-122.20
3,3-diethylpentane	6.8017	2.6080	4.2422	146.168	170.185	43.1134	43.36	342.80	26.94	23.75	-33.11
2,2,4,4-tetramethylpentane	6.4482	2.5393	3.7071	122.284	178.256	43.8747	38.10	301.60	24.58	20.17	-66.54
2,2,3,3-tetramethylpentane	6.4900	2.5475	3.8106	140.274	169.495	43.2147	41.00	334.50	27.04	23.38	-9.90
2-methyloctane	6.9385	2.6341	4.2700	143.260	179.77	43.8795	44.65	315.00	23.6	21.88	-80.40
3-methyloctane	6.9487	2.6360	4.3080	144.180	177.95	43.7296	44.75	318.00	21.7	22.34	-107.64
3-ethylheptane	6.9590	2.6380	4.3460	143.000	176.41	43.6420	44.81	318.00	23.06	22.81	-114.90
4-ethylheptane	6.9590	2.6380	4.3460	141.200	175.68	43.4907	42.28	318.30	23.98	22.81	
2,3-dimethylheptane	6.8470	2.6167	4.1807	140.500	176.65	43.6369	43.79	315.00	23.79	22.34	-116.00
2,4-dimethylheptane	6.8394	2.6152	4.1639	133.500	179.12	43.7393	42.87	306.00	22.7	23.30	
2,5-dimethylheptane	6.8394	2.6152	4.1639	136.000	179.37	43.8484	43.87	307.80	22.7	21.30	
2,6-dimethylheptane	6.8291	2.6133	4.1258	135.230	180.91	43.9258	42.82	306.00	23.7	20.83	-102.90

Table 1 (continued)

Alkane	BVSI*	$\sqrt{BVSI}$*	R index*	Bp (°C) **	Mv (cm^{-1}) **	Mr (cm^{-1})**	Hv (kj) **	Ct (°C) **	Cp (atm)**	St (d/cm)**	Mp (°C) **
3,3-dimethylheptane	6.7659	2.6011	4.1213	137.300	176.897	43.6870	42.66	314.00	24.19	22.01	
3,4-dimethylheptane	6.8573	2.6186	4.2187	140.600	175.349	43.5473	43.84	322.70	24.77	22.80	
3,5-dimethylheptane	6.8497	2.6172	4.2019	136.000	177.386	43.6379	42.98	312.30	23.59	21.77	
4,4-dimethylheptane	6.7659	2.6011	4.1213	135.200	176.897	43.6022	42.66	317.80	24.18	22.01	
3-ethyl-2-methylhexane	6.8573	2.6186	4.2187	138.000	175.445	43.6550	43.84	322.70	24.77	22.80	
4-ethyl-2-methylhexane	6.8497	2.6172	4.2019	133.800	177.386	43.6472	42.98	330.30	25.56	21.77	
3-ethyl-3-methylhexane	6.7838	2.6046	4.2567	140.600	173.07	43.2680	44.04	327.20	25.66	23.22	
2,3,4-trimethyhexane	6.7556	2.5992	4.0914	139.000	173.498	43.4917	42.93	324.20	25.46	22.80	
3-ethyl-2,3-dimethylpentane	6.6727	2.5832	4.0193	142.000	170.093	42.9543	42.55	338.60	26.94	23.87	
2,3,3,4-tetramethylpentane	6.5742	2.5640	4.2540	141.551	169.928	43.2016	41.75	334.50	26.85	23.31	-102.12
3-ethyl-4-methylhexane	6.8676	2.6206	4.2022	140.400	172.844	43.3746	43.95	312.30	23.59	23.27	

*The BVSI, $\sqrt{BVSI}$, and Randić index (R) were calculated using equations 1 and 2
**Experimental Data were collected from literature (Plavšić et al., 1993)

The following linear regression models were obtained when BVSI,$\sqrt{BVSI}$, and Randić (R) were plotted against each of the physical properties. A general formula for the linear model is shown below.

P = A(TI) + B or P = A($\sqrt{TI}$) + B , where P = physical property & TI = topological index

For the quadratic regression model of $\sqrt{BVSI}$ the general formula is shown below

$$P = A(TI) + B(\sqrt{TI}) + C$$

The statistical parameters (Tables 2 and 3) calculated were r = correlation coefficient and s = standard deviation. N = number of samples (alkanes) investigated.

The following linear models for BVSI, $\sqrt{BVSI}$, and Randić (R) as well as the quadratic models for $\sqrt{BVSI}$ were obtained.

1. For BVSI

Bp = 35.05(BVSI) – 97.31
Mv = 18.09(BVSI) + 52.83
Mr = 5.408(BVSI) + 6.846
Hv = 5.497(BVSI) + 5.602
Ct = 42.73(BVSI) + 32.53
Cp = -3.125(BVSI) + 45.18
St = 1.938(BVSI) + 9.185
Mp=9.674(BVSI) - 164.6

2. For $\sqrt{BVSI}$

Bp = 145.7($\sqrt{BVSI}$) – 241.9
Mv = 83.60($\sqrt{BVSI}$) – 42.13
Mr = 24.96($\sqrt{BVSI}$) – 21.64
Hv = 25.38($\sqrt{BVSI}$) – 23.37
Ct = 178.2($\sqrt{BVSI}$) – 145.1
Cp = -13.17($\sqrt{BVSI}$) + 58.51
St = 9.083($\sqrt{BVSI}$) – 1.359
Mp = 41.61($\sqrt{BVSI}$) – 208.0

3. For Randić (R)

Bp = 61.69(R) – 114.6
Mv = 30.16(R) + 50.67
Mr = 9.038(R) + 5.953
Hv = 9.534(R) + 3.422
Ct = 74.96(R) + 12.35
Cp = - 5.421(R) + 46.44
St = 3.434(R) + 8.142
Mp = 17.67(R) - 170.0

4. Quadratic models for $\sqrt{BVSI}$

Bp = 5.251(BVSI) + 124.1($\sqrt{BVSI}$) – 220.9
Mv = 12.77(BVSI) + 24.59($\sqrt{BVSI}$) + 25.19
Mr = 4.881(BVSI) + 2.422($\sqrt{BVSI}$) + 4.073
Hv = 4.992(BVSI) + 2.336($\sqrt{BVSI}$) + 2.928
Ct = -5.576(BVSI) + 201.1($\sqrt{BVSI}$) – 167.4
Cp = 2.707(BVSI) – 24.28($\sqrt{BVSI}$) + 69.33
St = -1.779(BVSI) + 17.38($\sqrt{BVSI}$) – 10.95
Mp = -29.78(BVSI) + 162.1($\sqrt{BVSI}$) – 323.6

Table 2. Statistical parameters for the linear QSPR models of BVSI and Randić index

Physical properties		BVSI (linear)		$\sqrt{BVSI}$(linear)		Randic (linear)	
	N	r	s	r	s	r	s
Boiling point (Bp)	74	0.990	6.4444	0.995	4.4178	0.984	8.0504
Molar volume (Mv)	69	0.984	3.0824	0.984	3.1340	0.953	5.2946
Molar refraction (Mr)	69	0.991	0.6915	0.990	0.7309	0.963	1.4085
Heats of vaporization (Hv)	69	0.984	0.9371	0.983	0.9681	0.993	0.6192
Critical temperature (Ct)	74	0.976	12.5011	0.985	9.8838	0.967	14.3815
Critical pressure (Cp)	74	0.935	1.5508	0.953	1.3125	0.917	1.7434
Surface tension (St)	68	0.896	0.9095	0.897	0.8548	0.914	0.7908
Melting point (Mp)	56	0.421	29.0837	0.444	28.7278	0.396	34.6134

Table 3. Statistical parameters for the quadratic QSPR model of $\sqrt{BVSI}$

	$\sqrt{BVSI}$quadratic		
Physical properties	**N**	**r**	**s**
Boiling point (Bp)	74	0.995	4.3408
Molar volume (Mv)	69	0.984	3.0722
Molar refraction (Mr)	69	0.991	0.6911
Heats of vaporization (Hv)	69	0.984	0.9369
Critical temperature (Ct)	74	0.970	9.8442
Critical pressure (Cp)	74	0.959	1.2404
Surface tension (St)	68	0.900	0.8520
Melting point (Mp)	56	0.471	28.6663

From the statistical results in Tables 2 and 3, the following were observed:

a. BVSI and $\sqrt{BVSI}$ in both linear or quadratic correlation with the alkanes provide useful models for the eight physical properties of the alkanes (boiling point, molar volume, molar refraction, heat of vaporization, critical temperature, critical pressure and surface tension except the melting point) since their values for the correlation coefficient r range between 0.896 and 0.995.
b. The quadratic correlation of the $\sqrt{BVSI}$ improves all the coefficient of correlations (r) as well as their standard deviation(s) compared to the linear $\sqrt{BVSI}$ except in the case of critical temperature.
c. In only two linear models is the Randić index more accurate than BVSI, they are the heat of vaporation (r = 0.993) and the surface tension (r = 0.914), the rest are more accurate in prediction with BVSI
d. Both the BVSI and Randić index are inaccurate in predicting the melting points.
e. Both the linear and quadratic correlation of $\sqrt{BVSI}$ are very accurate in predicting the boiling point (r = 0.995) and molar refraction (r = 0.991)

Comparison of BVSI with some degree-based topological indices. Hosamani et al. (2017) reported a QSPR of ten degree based topological indices with eight physical properties of the alkanes from butanes to nonanes using the linear regression model. However, the following alkanes such as 2,2,3-trimethylbutane, 2,2,3,3-tetramethylbutane, 2,2,3-trimethylhexane, 2,4,4-trimethylhexane and 3-ethyl-4-methylhexane were not included in the list so that the total alkanes investigated reached only up to 67. In spite of these, we used the same number and the same alkanes for BVSI to have a comparison with the ten degree-based topological indices (Table 4) studied. Only the correlation coefficients (r) and the standard deviation (s) of the indices of the ten topological indices were listed in Table 5 for a straightforward comparison. Other data like the linear equations generated may be sourced from the work of Hosamani et al.(2017) for the ten degree-based topological indices.

Table 4. The ten degree-based topological indices and their formulas studied by Hosamani et al. (2017).

Topological Index	Equation
1. Randić Index (Randić, 1975)	$R(G) = \sum_{i-j} \left(d_i(G)d_j(G)\right)^{-\frac{1}{2}}$
2. Reciprocal Randić index (Gutman et al., 2014)	$RR(G) = \sum_{i-j} \sqrt{d_i(G)d_j(G)}$
3-4. 2 Zagreb Indices (Gutman and Trinajstić, 1972)	$M_1(G) = \sum_{j} d_j(G)^2$ $M_2(G) = \sum_{i-j} d_i(G)d_j(G)$
5. Forgotten Index (Furtula and Gutman, 2015)	$F(G) = \sum_{j} d_j(G)^3$
6. Atom-based Connectivity (Estrada, 2008)	$ABC(G) = \sum_{i-j} \sqrt{\frac{d_i(G)+ d_j(G)-2}{d_i(G)d_j(G)}}$
7. Augmented Zagreb Index (Furtulaet al., 2010)	$AZI(G) = \sum_{i-j} \left[\frac{d_i(G)d_j(G)}{d_i(G)+ d_j(G)-2}\right]^3$
8. Geometric-arithmetic Index (Vukičević and Furtula, 2009)	$GA(G) = \sum_{i-j} \frac{\sqrt{d_i(G)d_j(G)}}{1/2(d_i(G) + d_j(G)}$
9. Harmonic Index (Fajtlowicz, 1987)	$H(G) = \sum_{i-j} \frac{2}{d_i(G) + d_j(G)}$
10. Sum-connectivity Index (Zhou and Trinajstić, 2009)	$SCI(G) = \sum_{i-j} \frac{1}{\sqrt{d_i(G) + d_j(G)}}$

Table 5. Comparison of statistical results from linear models of BVSI with those of the ten degree-based topological indices provided by Hosamani et al. (2017)

Phys. Prop.	N	BVSI(G)		R(G)		RR(G)		M_1(G)		M_2(G)		F(G)	
		r	s	r	s	r	s	r	s	r	s	r	s
Bp	67	0.990	5.2555	0.986	6.3398	0.938	13.0131	0.817	21.4370	0.859	19.3021	0.673	27.8652
Mv	65	0.985	3.0528	0.954	5.1516	0.934	6.4264	0.800	10.7804	0.806	11.6501	0.595	14.4374
Mr	65	0.992	0.6838	0.960	1.4943	0.962	1.4521	0.837	2.9227	0.854	24.0913	0.613	4.2221
Hv	65	0.984	0.9442	0.995	0.5237	0.871	2.6928	0.714	3.8422	0.737	3.4930	0.498	4.7615
Ct	67	0.970	11.0401	0.962	12.048	0.951	14.2558	0.856	23.8350	0.898	20.9913	0.704	32.7746
Cp	67	0.920	1.2337	0.911	1.3024	0.827	1.7728	0.686	2.2970	0.688	0.4882	0.486	2.7595
St	64	0.895	0.8799	0.909	0.8278	0.848	1.0505	0.329	1.8716	0.777	1.4420	0.595	1.5932
Mp	51	0.298	26.0252	0.219	40.0107	0.277	26.4055	0.286	30.2743	0.267	0.539	0.283	39.3090

Phys. Prop.	N	ABC(G)		AZI(G)		GA(G)		H(G)		SCI(G)	
		r	s	r	s	r	s	r	s	r	s
Bp	67	0.909	15.7398	0.874	18.3086	0.985	6.4949	0.941	12.7832	0.988	5.9054
Mv	65	0.802	10.7319	0.736	12.1528	0.966	4.6216	0.879	8.5769	0.965	4.7229
Mr	65	0.822	3.0456	0.754	3.5724	0.973	1.2389	0.875	2.5844	0.969	1.3194
Hv	65	0.732	3.7407	0.884	2.5599	0.987	0.8700	0.961	1.5249	0.995	0.5385
Ct	67	0.850	24.3046	0.850	24.2238	0.964	12.3561	0.908	19.3752	0.963	12.3871
Cp	67	0.743	2.1135	0.718	2.1981	0.913	1.2576	0.878	1.5112	0.920	1.2342
St	64	0.700	1.4153	0.834	1.0922	0.900	0.8688	0.847	1.0534	0.901	0.8581
Mp	51	0.280	39.3439	0.248	26.6226	0.235	31.8327	0.487	10.1211	0.240	39.7853

From the statistical results (Table 5) among the topological indices listed, the following observations can be deduced:

a) The most accurate model for predicting the boiling point, the molar volume, the molar refraction, the critical temperature and the critical pressure is the linear regression model of the BVSI (with the SCI sharing the same place as the BVSI for predicting the critical pressure).
b) The most accurate model for predicting the heat of vaporization is the linear regression model of the Randić index (R(G)) shared by SCI, and the most accurate model for predicting the surface tension is the linear regression model of the Randić index (R(G)) alone.
c) The values of BVSI in predicting the heat of vaporization (r = 0.984) and the surface tension (r = 0.895) may not be the best but are still better than most of the topological indices.
d) All models are inaccurate in predicting the melting points. This observation has been reached also by many others (Plavšić et al., 1993).

Knowing that the results with BVSI can still be improved by using $\sqrt{BVSI}$ into linear or quadratic correlation method, this topological index appears the most useful among the degree-based topological indices that have been mentioned.

CONCLUSION

The BVSI index has been tested in the QSPR modelling of eight physical properties of the alkanes. It was found to be "useful" in modelling all the physical properties studied except the melting point of alkanes. Its linear model was found to be the most accurate in predicting the boiling point, molar volume, molar refraction, critical temperature and critical pressure compared to the Randić index. Only, the heat of vaporization and the surface tension went to the Randić index model for the most accurate. To note further is that the linear and the quadratic regression of the square root of BVSI showed that the BVSI index model can be improved. Compared with the ten known topological indices, the BVSI proved to be the best, predicting most accurately the boiling temperature and the molar refraction as well as the molar volume, the critical temperature and the critical pressure of the alkanes.

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