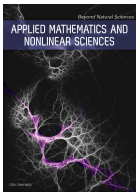
sciendo Applied Mathematics and Nonlinear Sciences 4(2) (2019) 371–386



Applied Mathematics and Nonlinear Sciences

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QSPR Analysis of certain Distance Based Topological Indices

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Submission Info

Communicated by Juan Luis García Guirao
Received March 5th 2019
Accepted April 27th 2019
Available online September 27th 2019

Abstract

In QSAR/QSPR study, topological indices are utilized to guess the bioactivity of chemical compounds. In this paper, we study the QSPR analysis of selected distance and degree-distance based topological indices. Our study reveals some important results which help us to characterize the useful topological indices based on their predicting power.

Keywords: Distance; Degree-Distance; QSPR
AMS 2010 codes: 05C90; 05C35; 05C12.

1 Introduction

The molecular descriptor is the final result of logic and mathematical procedure which transform chemical information encoded within a symbolic representation of a molecule into a useful member or the result of some standardized experiments. Attention is paid to the term "useful" with its double meanings. It means that the number can give more insights into the interpretation of the molecular properties and / or is able to take part in a model for the prediction of some interesting property of the molecules.

A fundamental concept of chemistry is that the structural characteristics of a molecule are responsible for its properties. Topological indices are a convenient means of translating chemical constitution into numerical values which can be used for correlation with physical properties in quantitative structure-property/activity relationship (QSPR/QSAR) studies. The use of graph invariant (topological indices) in QSPR and QSAR studies has become of major interest in recent years. Topological indices have found application in various areas of

ISSN 2444-8656 doi:10.2478/AMNS.2019.2.00032

chemistry, physics, mathematics, informatics, biology, etc [1, 7, 26], but their most important use to date is in the non-empirical Quantitative Structure- Property Relationships (QSPR) and Quantitative Structure -Activity Relationships (QSAR) [5, 14, 19, 21, 23, 24, 27].

2 Survey of Selected Distance and Degree-Distance Based Topological Indices

1. **Wiener Index:** The Wiener index is named after Harry Wiener, who introduced it in 1947; at the time, Wiener called it the "path number"[24]. It is the oldest topological index related to molecular branching. Based on its success, many other topological indices of chemical graphs [2,3,13], based on information in the distance matrix of the graph, have been developed subsequently to Wiener's work. Which is defined as:
   let G be any connected graph of order n and size m. Then Wiener index of G is denoted by $W(G)$ and is defined as follows.

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} d_G(u,v)$$

2. **Terminal Wiener Index:** The concept of terminal Wiener index was put forward by Petrović et el. [9] some-what later but independently, Szekely et al. [25] arrived at the same idea. If G has k-pendent vertices labeled by $v_1, v_2 \cdots v_k$, then its terminal distance matrix is the square matrix of order k whose (i, j)-th entry is $d(v_i, v_j \setminus G)$. Terminal distance matrices were used for modeling amino acid sequences of proteins and of the genetic code [12, 17, 18].

   The terminal Wiener index $TW(G)$ of a connected graph G is defined as the sum of the distances between all pairs of its pendent vertices.
   Thus if $V_T = \{v_1, v_2, \cdots, v_k\}$ is the set of all pendent vertices of G, then

$$TW(G) = \sum_{\{u,v \subseteq V_T(G)\}} d(u, v \setminus G) = \sum_{1 \le i < j \le k} d(u, v \setminus G)$$

3. **Degree Distance Index:** The degree distance was introduced by Dobrynin and Kochetova [5] as a weighted version of the Wiener index. The degree distance of G, denoted by $DD(G)$, is defined as follows

$$DD(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)[deg_G(u) + deg_G(v)].$$

4. **Gutman Index:** The Gutman index was put forward in [10] as a multiplicative version of degree-distance index which is defined as follows.

$$GI(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)[deg_G(u) deg_G(v)].$$

5. **Ashwini Index:** Motivated by the terminal Wiener index Hosamani [15] has introduced a novel topological index viz, Ashwini index of a molecular graph G. Which is based on the terminal distance between any pair of pendant vertices together with their neighborhood degrees.

$$\mathscr{A}(T) = \sum_{1 \le i < j \le n} d_T(v_i, v_j)[deg_T(N(u_i)) + deg_T(N(v_j))].$$

   Where $N(v) = \{u \in V(G) : uv \in E(G)\}$.

6. *SM*- **Index:** Motivated by the Gutman index and Ashwini index of a molecular graph G, we define here a new topological invariant namely SM-index of a molecular graph G. Which is defined as follows:

$$SM(T) = \sum_{1 \le i < j \le n} d_T(v_i, v_j)[deg_T(N(u_i))deg_T N(v_j)].$$

Where $N(v) = \{u \in V(G) : uv \in E(G)\}$.

7. **Hyper Wiener Index:** In 1993, Milan Randić [20] introduced a distance based quantity, he named it as hyper Wiener index and denoted by WW. His definition could be applied only to trees, and was in possible to use for cycle-containing graphs.

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} \left[d_G(u,v) + d_G^2(u,v) \right]$$

which could be applied to all connected graphs, since then the above formula is used the definition of the hyper Wiener index.

3 The Use of Selected Distance and Degree-Distance Based Topological Indices in QSPR Studies

We have used three distance based topological indices and four degree-distance based topological indices viz, Wiener Index ($W(G)$),Terminal Wiener Index ($TW(G)$),Hyper Wiener Index ($WW(G)$) [distance baesd TI's] and Degree-distance Index, Gutman Index ($GI(G)$),Ashwini Index ($\mathscr{A}(G)$), SNM-Index [degree-distance based TI's] respectively for modeling eight representative physical properties [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 70 alkanes from n-butanes to nonanes. Values for these property were taken from Dejan Plavsić et. al [16]. The above said Distance and Degree-Distance topological indices and the experimental values for the physical properties of 70 alkanes are listed in Table 1 and 2 respectively.

Table 1.

S.No.	Alkane	bp($^\circ C$)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct($^\circ C$)	cp(atm)	st(dyne/cm)	mp($^\circ C$)
1	Butane	-0.500				152.01	37.47		-138.35
2	2-methyl propane	-11.730				134.98	36		-159.60
3	Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16.00	-129.72
4	2-methyl butane	27.852	116.426	25.2923	24.59	187.70	32.9	15.00	-159.90
5	2,2 dimethylpropane	9.503	112.074	25.7243	21.78	160.60	31.57		-16.55
6	Hexane	68.740	130.688	29.9066	31.55	234.70	29.92	18.42	-95.35
7	2-methylpentane	60.271	131.933	29.9459	29.86	224.90	29.95	17.38	-153.67
8	3-methyalpentane	63.282	129.717	29.8016	30.27	231.20	30.83	18.12	-118.00
9	2,2-methylbutane	49.741	132.744	29.9347	27.69	216.20	30.67	16.30	-99.87
10	2,3-dimethylbutane	57.988	130.240	29.8104	29.12	227.10	30.99	17.37	-128.54
11	Heptanes	98.427	146.540	34.5504	36.55	267.55	27.01	20.26	-90.61
12	2-methylhexane	90.052	147.656	34.5908	34.80	257.90	27.2	19.29	-118.28
13	3-methylhexane	91.850	145.821	34.4597	35.08	262.40	28.1	19.79	-119.40
14	3-ethylpentane	93.475	143.517	34.2827	35.22	267.60	28.6	20.44	-118.60
15	2,2-dimethylpentane	79.197	148.695	34.6166	32.43	247.70	28.4	18.02	-123.81
16	2,3-dimethylpentane	89.784	144.153	34.3237	34.24	264.60	29.2	19.96	-119.10
17	2,4-dimethylpentane	80.500	148.949	34.6192	32.88	247.10	27.4	18.15	-119.24
18	3,3-dimethylpentane	86.064	144.530	34.3323	33.02	263.00	30	19.59	-134.46
19	Octane	125.665	162.592	39.1922	41.48	296.20	24.64	21.76	-56.79
20	2-methylheptane	117.647	163.663	39.2316	39.68	288.00	24.8	20.60	-109.04
21	3-methylheptane	118.925	161.832	39.1001	39.83	292.00	25.6	21.17	-120.50
22	4-methylheptane	117.709	162.105	39.1174	39.67	290.00	25.6	21.00	-120.95

continued...

S.No.	Alkane	bp($^\circ C$)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct($^\circ C$)	cp(atm)	st(dyne/cm)	mp($^\circ C$)
23	3-ethylhexane	118.53	160.07	38.94	39.40	292.00	25.74	21.51	
24	2,2-dimethylhexane	10.84	164.28	39.25	37.29	279.00	25.6	19.60	-121.18
25	2,3-dimethylhexane	115.607	160.39	38.98	38.79	293.00	26.6	20.99	
26	2,4-dimethylhexane	109.42	163.09	39.13	37.76	282.00	25.8	20.05	-137.50
27	2,5-dimethylhexane	109.10	164.69	39.25	37.86	279.00	25	19.73	-91.20
28	3,3-dimethylhexane	111.96	160.87	39.00	37.93	290.84	27.2	20.63	-126.10
29	3,4-dimethylhexane	117.72	158.81	38.84	39.02	298.00	27.4	21.64	
30	3-ethyl-2-methylpentane	115.65	158.79	38.83	38.52	295.00	27.4	21.52	-114.96
31	3-ethyl-3-methylpentane	118.25	157.02	38.71	37.99	305.00	28.9	21.99	-90.87
32	2,2,3-trimethylpentane	109.84	159.52	38.92	36.91	294.00	28.2	20.67	-112.27
33	2,2,4-trimethylpentane	99.23	165.08	39.26	35.13	271.15	25.5	18.77	-107.38
34	2,3,3-trimethylpentane	114.76	157.29	38.76	37.22	303.00	29	21.56	-100.70
35	2,3,4-trimethylpentane	113.46	158.85	38.86	37.61	295.00	27.6	21.14	-109.21
36	Nonane	150.79	178.71	43.84	46.44	322.00	22.74	22.92	-53.52
37	2-methyloctane	143.26	179.77	43.87	44.65	315.00	23.6	21.88	-80.40
38	3-methyloctane	144.18	177.95	43.72	44.75	318.00	23.7	22.34	-107.64
39	4-methyloctane	142.48	178.15	43.76	44.75	318.30	23.06	22.34	-113.20
40	3-ethylheptane	143.00	176.41	43.64	44.81	318.00	23.98	22.81	-114.90
41	4-ethylheptane	141.20	175.68	43.49	44.81	318.30	23.98	22.81	
42	2,2-dimethylheptane	132.69	180.50	43.91	42.28	302.00	22.8	20.80	-113.00
43	2,3-dimethylheptane	140.50	176.65	43.63	43.79	315.00	23.79	22.34	-116.00
44	2,4-dimethylheptane	133.50	179.12	43.73	42.87	306.00	22.7	23.30	
45	2,5-dimethylheptane	136.00	179.37	43.84	43.87	307.80	22.7	21.30	
46	2,6- dimethylheptane	135.21	180.91	43.92	42.82	306.00	23.7	20.83	-102.90
continued...									

S.No.	Alkane	bp($^\circ C$)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct($^\circ C$)	cp(atm)	st(dyne/cm)	mp($^\circ C$)
47	3,3- dimethylheptane	137.300	176.897	43.6870	42.66	314.00	24.19	22.01	
48	3,4- dimethylheptane	140.600	175.349	43.5473	43.84	322.70	24.77	22.80	
49	3,5- dimethylheptane	136.000	177.386	43.6379	42.98	312.30	23.59	21.77	
50	4,4- dimethylheptane	135.200	176.897	43.6022	42.66	317.80	24.18	22.01	
51	3-ethyl-2-methylhexane	138.000	175.445	43.6550	43.84	322.70	24.77	22.80	
52	4-ethyl-2-methylhexane	133.800	177.386	43.6472	42.98	330.30	25.56	21.77	
53	3-ethyl-3-methylhexane	140.600	173.077	43.2680	44.04	327.20	25.66	23.22	
54	2,2,4- trimethylhexane	126.540	179.220	43.7638	40.57	301.00	23.39	20.51	-120.00
55	2,2,5- trimethylhexane	124.084	181.346	43.9356	40.17	296.60	22.41	20.04	-105.78
56	2,3,3- trimethylhexane	137.680	173.780	43.4347	42.23	326.10	25.56	22.41	-116.80
57	2,3,4- trimethylhexane	139.000	173.498	43.4917	42.93	324.20	25.46	22.80	
58	2,3,5- trimethylhexane	131.340	177.656	43.6474	41.42	309.40	23.49	21.27	-127.80
59	3,3,4- trimethylhexane	140.460	172.055	43.3407	42.28	330.60	26.45	23.27	-101.20
60	3,3-diethylpentane	146.168	170.185	43.1134	43.36	342.80	26.94	23.75	-33.11
61	2,2-dimethyl-3-ethylpentane	133.830	174.537	43.4571	42.02	322.60	25.96	22.38	-99.20
62	2,3-dimethyl-3-ethylpentane	142.000	170.093	42.9542	42.55	338.60	26.94	23.87	
63	2,4-dimethyl-3-ethylpentane	136.730	173.804	43.4037	42.93	324.20	25.46	22.80	-122.20
64	2,2,3,3-tetramethylpentane	140.274	169.495	43.2147	41.00	334.50	27.04	23.38	-99.0
65	2,2,3,4- tetramethylpentane	133.016	173.557	43.4359	41.00	319.60	25.66	21.98	-121.09
66	2,2,4,4- tetramethylpentane	122.284	178.256	43.8747	38.10	301.60	24.58	20.37	-66.54
67	2,3,3,4- tetramethylpentane	141.551	169.928	43.2016	41.75	334.50	26.85	23.31	-102.12

Table 2.

S.No.	Alkane	$W(G)$	$TW(G)$	$DD(G)$	$GI(G)$	$\mathscr{A}(G)$	$SNM(G)$	$HW(G)$
1	Butane	10	3	28	19	12	12	46
2	2-methyl propane	9	6	20	13	36	54	27
3	Pentane	20	8	60	44	16	16	146
4	2-methyl butane	18	8	52	36	42	54	90
5	2,2 dimethylpropane	16	8	44	28	96	192	52
6	Hexane	35	5	110	82	20	20	371
7	2-methylpentane	32	10	96	73	52	66	254
8	3-methyalpentane	31	10	94	69	46	52	217
9	2,2-methylbutane	26	15	82	57	102	168	142
10	2,3-dimethylbutane	29	16	84	61	96	144	161
11	Heptanes	56	6	182	146	24	24	812
12	2-methylhexane	52	12	166	130	62	78	604
13	3-methylhexane	50	12	161	122	55	62	506
15	3-ethylpentane	48	12	150	144	48	48	408
16	2,2-dimethylpentane	49	16	142	106	120	192	370
17	2,3-dimethylpentane	46	15	154	109	108	144	352
18	2,4-dimethylpentane	48	16	150	114	120	180	426
19	3,3-dimethylpentane	44	14	136	98	104	144	296
20	Octane	84	7	280	231	28	28	1596
21	2-methylheptane	79	14	263	211	72	90	1261
22	3-methylheptane	76	14	248	212	64	72	1072
23	4-methylheptane	75	14	224	193	64	72	1011

S.No.	Alkane	$W(G)$	$TW(G)$	$DD(G)$	$GI(G)$	$\mathscr{A}(G)$	$SNM(G)$	$HW(G)$
24	3-ethylhexane	72	14	232	190	56	56	822
25	2,2-dimethylhexane	71	21	228	179	138	216	845
26	2,3-dimethylhexane	71	22	291	275	118	156	766
27	2,4-dimethylhexane	71	23	231	179	125	168	803
28	2,5-dimethylhexane	74	24	240	191	144	216	962
29	3,3-dimethylhexane	67	21	212	163	113	150	649
30	3,4-dimethylhexane	68	22	216	168	108	131	668
31	3-ethyl-2-methylpentane	67	22	215	163	108	130	607
32	3-ethyl-3-methylpentane	64	21	239	129	102	120	514
33	2,2,3-trimethylpentane	63	27	196	147	198	318	495
34	2,2,4-trimethylpentane	66	32	194	152	228	330	606
35	2,3,3-trimethylpentane	60	27	242	200	194	314	458
36	2,3,4-trimethylpentane	65	32	198	155	192	288	551
37	Nonane	120	8	422	365	32	32	2892
38	2-methyloctane	114	16	391	327	82	102	2388
39	3-methyloctane	110	16	310	268	73	82	2076
40	4-methyloctane	108	16	353	295	73	82	1920
41	3-ethylheptane	105	16	331	271	72	72	1604
42	4-ethylheptane	102	16	239	190	68	68	1452
43	2,2-dimethylheptane	104	24	343	378	156	240	1718
44	2,3-dimethylheptane	102	25	336	264	133	174	1548
45	2,4-dimethylheptane	102	26	342	268	148	190	1524
46	2,5-dimethylheptane	110	27	344	269	147	198	1646
47	2,6- dimethylheptane	108	28	344	280	168	252	1926

S.No.	Alkane	$W(G)$	$TW(G)$	$DD(G)$	$GI(G)$	$\mathscr{A}(G)$	$SNM(G)$	$HW(G)$
48	3,3- dimethylheptane	98	24	320	277	138	184	1340
49	3,4- dimethylheptane	98	25	320	392	122	147	1298
50	3,5- dimethylheptane	100	26	320	264	128	156	1396
51	4,4- dimethylheptane	96	24	314	248	136	184	1218
52	3-ethyl-2-methylhexane	96	25	315	248	122	146	1146
53	4-ethyl-2-methylhexane	98	26	303	249	126	148	1244
54	3-ethyl-3-methylhexane	92	24	295	228	114	130	992
55	2,2,4- trimethylhexane	94	36	301	238	237	378	1108
56	2,2,5- trimethylhexane	98	38	322	270	270	474	1328
57	2,3,3- trimethylhexane	90	32	289	256	210	318	936
58	2,3,4- trimethylhexane	92	36	295	238	199	273	992
59	2,3,5- trimethylhexane	96	38	317	251	228	342	1188
60	3,3,4- trimethylhexane	87	34	278	214	201	278	838
61	3,3-diethylpentane	88	24	134	96	96	96	796
62	2,2-dimethyl-3-ethylpentane	88	32	279	213	208	304	814
63	2,3-dimethyl-3-ethylpentane	86	34	266	197	186	250	740
64	2,4-dimethyl-3-ethylpentane	90	36	291	224	200	276	870
65	2,2,3,3-tetramethylpentane	82	44	223	170	316	560	628
66	2,2,3,4- tetramethylpentane	86	47	273	209	327	564	758
67	2,2,4,4- tetramethylpentane	86	40	280	216	316	530	850
68	2,3,3,4- tetramethylpentane	84	47	264	200	28	464	729

4 Regression Models

We have tested the following linear regression model

$$P = A + B(TI) \tag{1}$$

where P = physical property, TI = topological index .

Using (3.1), we have obtained the following different linear models for each degree based topological index, which are listed below.

1. **Wiener index $W(G)$:**

$$bp = 20.8432 + [W(G)]1.2203 \tag{2}$$
$$mv = 113.868 + [W(G)]0.6412 \tag{3}$$
$$mr = 24.7432 + [W(G)]0.1944 \tag{4}$$
$$hv = 23.710 + [W(G)]0.1998 \tag{5}$$
$$ct = 179.262 + [W(G)]1.4606 \tag{6}$$
$$cp = 34.1143 - [W(G)]0.1025 \tag{7}$$
$$st = 16.126748 + [W(G)]0.0634 \tag{8}$$
$$mp = -129.02 + [W(G)]0.2909 \tag{9}$$

2. **Terminal wiener index $TW(G)$:**

$$bp = 68.2472 + [TW(G)]1.9072 \tag{10}$$
$$mv = 139.62 + [TW(G)]1.002 \tag{11}$$
$$mr = 32.25 + [TW(G)]0.3178 \tag{12}$$
$$hv = 37.616 + [TW(G)]0.055 \tag{13}$$
$$ct = 230.099 + [TW(G)]2.5196 \tag{14}$$
$$cp = 29.5512 - [TW(G)]0.1327 \tag{15}$$
$$st = 19.1536 + [TW(G)]0.088 \tag{16}$$
$$mp = 579.080 - [TW(G)]32.24 \tag{17}$$

3. **Hyper wiener index $HW(G)$:**

$$bp = 69.8172 + [HW(G)]0.04586 \tag{18}$$
$$mv = 140.3322 + [HW(G)]0.02365 \tag{19}$$
$$mr = 33.2598 + [HW(G)]0.00665 \tag{20}$$
$$hv = 31.82212 + [HW(G)]0.007513 \tag{21}$$
$$ct = 245.468 + [HW(G)]0.04589 \tag{22}$$
$$cp = 30.4719 - [HW(G)]0.00433 \tag{23}$$
$$st = 19.1519 + [HW(G)]0.001937 \tag{24}$$
$$mp = -120.603 + [HW(G)]0.013596 \tag{25}$$

4. **Degree distance index $DD(G)$:**

$$bp = 32.2663 + [DD(G)]0.3432 \tag{26}$$

$$mv = 119.529 + [DD(G)]0.182 \quad (27)$$
$$mr = 37.81 + [DD(G)]0.00714 \quad (28)$$
$$hv = 37.144 + [DD(G)]0.00732 \quad (29)$$
$$ct = 196.428 + [DD(G)]0.3932 \quad (30)$$
$$cp = 33.418 - [DD(G)]0.0298 \quad (31)$$
$$st = 17.121 + [DD(G)]0.0162 \quad (32)$$
$$mp = -122.787 + [DD(G)]0.0641 \quad (33)$$

5. **Gutman index** $GI(G)$**:**

$$bp = 38.62 + [GI(G)]0.3983 \quad (34)$$
$$mv = 201.965 - [GI(G)]0.20958 \quad (35)$$
$$mr = 28.02 + [GI(G)]0.061 \quad (36)$$
$$hv = 26.978 + [GI(G)]0.0632 \quad (37)$$
$$ct = 203.4429 + [GI(G)].4577 \quad (38)$$
$$cp = 20.218 - [GI(G)]0.034733 \quad (39)$$
$$st = 17.37 + [GI(G)]0.0190 \quad (40)$$
$$mp = -119.40 + [GI(G)]0.0616 \quad (41)$$

6. **Ashwini index** $A(G)$**:**

$$bp = 135.6962 + [\mathscr{A}(G)]0.1870 \quad (42)$$
$$mv = 148.45 + [\mathscr{A}(G)]0.1095 \quad (43)$$
$$mr = 35.573 + [\mathscr{A}(G)]0.034 \quad (44)$$
$$hv = 39.95 + [\mathscr{A}(G)]0.00828 \quad (45)$$
$$ct = 237.8298 + [\mathscr{A}(G)]0.3766 \quad (46)$$
$$cp = 28.4180 - [\mathscr{A}(G)]0.01427 \quad (47)$$
$$st = 19.970 + [\mathscr{A}(G)]0.0078 \quad (48)$$
$$mp = -113.0059 + [\mathscr{A}(G)]0.03 \quad (49)$$

7. **SM index** $SM(G)$**:**

$$bp = 97.968 + [SNM(G)]0.069 \quad (50)$$
$$mv = 74.45 + [SNM(G)]0.46 \quad (51)$$
$$mr = 10.394 + [SNM(G)]0.152 \quad (52)$$
$$hv = 37.749 + [SNM(G)]0.00587 \quad (53)$$
$$ct = 268.506 + [SNM(G)]0.0956 \quad (54)$$
$$cp = 27.68 - [SNM(G)]0.00582 \quad (55)$$
$$st = 20.486 + [SNM(G)]0.00266 \quad (56)$$
$$mp = -109.163 - [SNM(G)]0.00016 \quad (57)$$

Table 3. Statical parameters for the linear QSPR model for Wiener index.

Physical Properties	N	a	b	r	s	F
Boiling point	70	20.8432	1.2203	0.921	14.3278	388.436
Molar volume	67	113.868	0.6412	0.970	4.32084	1037.804
Molar refraction	67	24.7432	0.1944	0.962	1.45880	795.781
Heats of vaporization	67	23.710	0.1998	0.964	1.45328	846.841
Critical temperature	70	179.262	1.4606	0.899	19.8772	285.433
Critical Pressure	70	34.1143	-0.1025	0.921	1.2167	380.698
Surface tension	66	16.126748	0.0634	0.815	1.14383	126.812
Melting point	52	-129.02	0.2909	0.317	25.87537	5.585

Table 4. Statical parameters for the linear QSPR model for terminal Wiener index.

Physical Properties	N	a	b	r	s	F
Boiling point	70	68.2472	1.9072	0.574	30.3815	33.333
Molar volume	67	139.62	1.002	0.606	14.17194	37.698
Molar refraction	67	32.25	0.3178	0.644	4.06101	46.075
Heats of vaporization	67	37.616	0.055	0.443	4.87876	15.910
Critical temperature	70	230.099	2.5196	0.620	35.5665	42.39
Critical Pressure	70	29.5512	-0.1327	0.475	2.7503	19.816
Surface tension	66	19.1536	0.088	0.481	1.73103	19.315
Melting point	52	579.080	-32.214	0.096	27.1532	0.461

Table 5. Statical parameters for the linear QSPR model for hyper Wiener index.

Physical Properties	N	a	b	r	s	F
Boiling point	70	69.8172	0.04586	0.722	25.6758	73.879
Molar volume	67	140.3322	0.02365	0.759	11.59154	88.511
Molar refraction	67	33.2598	0.001937	0.555	1.64346	28.430
Heats of vaporization	67	31.82212	0.007513	0.789	3.34131	107.499
Critical temperature	70	245.468	0.04589	0.809	1.1358	129.100
Critical Pressure	70	30.4719	-0.00433	0.636	34.9872	6.078
Surface tension	66	19.1519	0.0019	0.555	1.64346	28.430
Melting point	52	-120.603	0.013596	0.318	25.86514	5.629

Table 6. Statical parameters for the linear QSPR model for Degree distance index.

Physical Properties	N	a	b	r	s	F
Boiling point	70	32.2663	0.3432	0.863	18.7367	198.428
Molar volume	67	119.529	0.182	0.919	7.03409	315.874
Molar refraction	67	37.81	0.00714	0.897	2.34677	267.614
Heats of vaporization	67	37.144	0.00732	0.897	2.40325	268.443
Critical temperature	70	196.428	0.3932	0.809	26.6334	128.863
Critical Pressure	70	33.418	-0.0298	0.890	1.4243	259.425
Surface tension	66	17.121	0.0162	0.716	1.37956	67.174
Melting point	52	-122.787	0.0641	0.232	26.53927	2.839

Table 7. Statical parameters for the linear QSPR model for Gutman index.

Physical Properties	N	a	b	r	s	F
Boiling point	70	38.62	0.3983	0.858	19.0533	189.648
Molar volume	67	201.965	-0.20958	0.892	8.05741	252.709
Molar refraction	67	28.02	0.061	0.874	2.58307	209.543
Heats of vaporization	67	26.978	0.0632	0.882	2.56979	226.624
Critical temperature	70	203.4429	0.4577	0.807	26.7911	126.553
Critical Pressure	70	20.218	-0.034733	0.889	1.4332	255.359
Surface tension	66	17.37	0.0190	0.711	1.38853	65.486
Melting point	52	-119.40	0.0616	0.187	26.80008	1.815

Table 8. Statical parameters for the linear QSPR model for Ashwini index.

Physical Properties	N	a	b	r	s	F
Boiling point	70	135.6962	-0.1870	0.420	33.644	14.578
Molar volume	67	148.45	0.1095	0.492	15.51334	20.706
Molar refraction	67	35.573	0.034	0.519	4.53808	23.949
Heats of vaporization	67	39.95	-0.00823	0.288	5.21235	5.885
Critical temperature	70	237.8298	0.3766	0.459	40.2596	18.155
Critical Pressure	70	23.4180	-0.01427	0.381	2.8901	11.523
Surface tension	66	19.970	0.0078	0.320	1.87121	7.299
Melting point	52	-113.0059	0.03	0.561	4.90731	22.913

Table 9. Statical parameters for the linear QSPR model for SM index.

Physical Properties	N	a	b	r	s	F
Boiling point	70	97.968	0.069	0.292	35.4737	6.3828
Molar volume	67	74.47	0.46	0.378	16.4949	10.809
Molar refraction	67	10.394	0.152	0.400	4.8866	12.352
Heats of vaporization	67	37.749	0.00587	0.158	5.37507	1.658
Critical temperature	70	268.506	0.0956	0.326	42.8387	8.093
Critical Pressure	70	27.68	-0.00582	0.288	2.9931	6.145
Surface tension	66	20.486	0.00266	0.198	1.93590	2.6614
Melting point	52	-109.163	-0.00016	0.339	5.1208	8.7442

5 Discussion and Concluding Remarks

By inspection of the data given in tables 3 to 9, It is possible to draw numbers of conclusion for the given distance and degree-distance based TIs.

First, the famous and much studied distance based Topological index viz, Wiener index found to be more suitable tool to predict the physical properties of alkanes.The Wiener Index shows good correlation with almost all physical properties of alkanes which are listed in table 3 except molar volume and surface tension of alkanes.The correlation coefficient value lies between 0.815 to 0.970. The QSPR study reveals that Wiener Index is more suitable to predict heats of vapourization and molar volumes of alkanes with correlation coefficient value r=0.964, and r = 0.0.970 respectively.

In addition the result for Terminal Wiener index revealed that the recent advocated idea of using Terminal Wiener index did not pass the test. This important details seems to have ignored in recent paper [9], on Terminal Wiener index.

Recently introduced distance based topological invariant viz, Hyper Wiener index found to be adequate for any structure-property correlation, except for critical temperatures of alkanes with correlation coefficient value r=0.809.

The QSPR study of degree-distance index in tables 6 reveals that the degree-distance index is an useful topological invariant. It shows good correlation with almost all physical properties which are listed in Table 6, except surface tension and melting points of alkanes. The correlation coefficient values lies between 0. 809 to 0.919. The degree-distance index is more suitable to predict the molar volume and heats of vaporization with $r = 0.919$ and $r = 0.897$ respectively.

The multiplicative version of degree-distance index is known as Gutman Index.By observing the results in table 7,One can say that the Gutman index has less predictive ability compared to degree-distance index. Further the correlation of Gutman index with physical properties of alkanes is very less and correlation coefficient value lies between 0.187 to 0.892.

The another degree-distance based topological index viz, Ashwini index. The predicting power of Ashwini index with physical properties of alkanes is too less. The correlation coefficient value of Ashwini index lies between 0.288 to 0.519.

Motivated by Gutman index and Ashwini index, Here we introduce a new degree-distance based topological invariant viz, SM Index. The QSPR study of SNM Index in table-9 shows good predicting power for alkanes.

From practical point of view, topological indices for which the absolute value of the correlation coefficient is less than 0.8 can be characterized useless. Thus the QSPR study of these distance and degree-distance based topological indices with physical properties of alkanes helps us to characterize useful topological indices indices with absolute values of correlation coefficients lies between 0.8 to 0.970.

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