



# 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

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.

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

2. **Terminal Wiener Index:** The concept of terminal Wiener index was put forward by Petrović et al. [9] some-what later but independently, Szekely et al. [25] arrived at the same idea. If  $G$  has  $k$ -pendent vertices labeled by  $v_1, v_2, \dots, v_k$ , 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  $V_T = \{v_1, v_2, \dots, v_k\}$  is the set of all pendent vertices of  $G$ , then

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

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.

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

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:

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

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.

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

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 based TI's] and Degree-distance Index, Gutman Index ( $GI(G)$ ), Ashwini Index ( $\mathcal{A}(G)$ ),  $SNM$ -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 Plavšić 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(°C)  | mv (cm <sup>3</sup> ) | mr (cm <sup>3</sup> ) | hv(kJ) | ct(°C) | cp(atm) | st(dyne/cm) | mp(°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-methylpentane     | 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(°C)  | mv( $cm^3$ ) | mr( $cm^3$ ) | hv(kJ) | ct(°C) | cp(atm) | st(dyne/cm) | mp(°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(°C)  | mv (cm <sup>3</sup> ) | mr (cm <sup>3</sup> ) | hv(kJ) | ct(°C) | cp(atm) | st(dyne/cm) | mp(°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              | $W(G)$ | $TW(G)$ | $DD(G)$ | $GI(G)$ | $\mathcal{A}(G)$ | $SNM(G)$ | $HW(G)$ |
|-------|---------------------|--------|---------|---------|---------|------------------|----------|---------|
| 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-methylpentane     | 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                  | $W(G)$ | $TW(G)$ | $DD(G)$ | $GI(G)$ | $\mathcal{A}(G)$ | $SNM(G)$ | $HW(G)$ |
|-------|-------------------------|--------|---------|---------|---------|------------------|----------|---------|
| 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                      | $W(G)$ | $TW(G)$ | $DD(G)$ | $GI(G)$ | $\mathcal{A}(G)$ | $SNM(G)$ | $HW(G)$ |
|-------|-----------------------------|--------|---------|---------|---------|------------------|----------|---------|
| 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

$$P = A + B(TI) \quad (1)$$

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 $W(G)$ :

$$bp = 20.8432 + [W(G)]1.2203 \quad (2)$$

$$mv = 113.868 + [W(G)]0.6412 \quad (3)$$

$$mr = 24.7432 + [W(G)]0.1944 \quad (4)$$

$$hv = 23.710 + [W(G)]0.1998 \quad (5)$$

$$ct = 179.262 + [W(G)]1.4606 \quad (6)$$

$$cp = 34.1143 - [W(G)]0.1025 \quad (7)$$

$$st = 16.126748 + [W(G)]0.0634 \quad (8)$$

$$mp = -129.02 + [W(G)]0.2909 \quad (9)$$

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

$$bp = 68.2472 + [TW(G)]1.9072 \quad (10)$$

$$mv = 139.62 + [TW(G)]1.002 \quad (11)$$

$$mr = 32.25 + [TW(G)]0.3178 \quad (12)$$

$$hv = 37.616 + [TW(G)]0.055 \quad (13)$$

$$ct = 230.099 + [TW(G)]2.5196 \quad (14)$$

$$cp = 29.5512 - [TW(G)]0.1327 \quad (15)$$

$$st = 19.1536 + [TW(G)]0.088 \quad (16)$$

$$mp = 579.080 - [TW(G)]32.24 \quad (17)$$

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

$$bp = 69.8172 + [HW(G)]0.04586 \quad (18)$$

$$mv = 140.3322 + [HW(G)]0.02365 \quad (19)$$

$$mr = 33.2598 + [HW(G)]0.00665 \quad (20)$$

$$hv = 31.82212 + [HW(G)]0.007513 \quad (21)$$

$$ct = 245.468 + [HW(G)]0.04589 \quad (22)$$

$$cp = 30.4719 - [HW(G)]0.00433 \quad (23)$$

$$st = 19.1519 + [HW(G)]0.001937 \quad (24)$$

$$mp = -120.603 + [HW(G)]0.013596 \quad (25)$$

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

$$bp = 32.2663 + [DD(G)]0.3432 \quad (26)$$

$$mv = 119.529 + [DD(G)]0.182 \quad (27)$$

$$mr = 37.81 + [DD(G)]0.00714 \quad (28)$$

$$hv = 37.144 + [DD(G)]0.00732 \quad (29)$$

$$ct = 196.428 + [DD(G)]0.3932 \quad (30)$$

$$cp = 33.418 - [DD(G)]0.0298 \quad (31)$$

$$st = 17.121 + [DD(G)]0.0162 \quad (32)$$

$$mp = -122.787 + [DD(G)]0.0641 \quad (33)$$

### 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 $A(G)$ :

$$bp = 135.6962 + [A(G)]0.1870 \quad (42)$$

$$mv = 148.45 + [A(G)]0.1095 \quad (43)$$

$$mr = 35.573 + [A(G)]0.034 \quad (44)$$

$$hv = 39.95 + [A(G)]0.00828 \quad (45)$$

$$ct = 237.8298 + [A(G)]0.3766 \quad (46)$$

$$cp = 28.4180 - [A(G)]0.01427 \quad (47)$$

$$st = 19.970 + [A(G)]0.0078 \quad (48)$$

$$mp = -113.0059 + [A(G)]0.03 \quad (49)$$

### 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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