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On Weighted Forgotten Index

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Abstract. To study the quantitative structure property relationship of molecules, the efficient tools are the topological indices. In this connection, the weighted forgotten topological index $F^w(G)$ is conceived. As an application of this index, the comparative study was done with already existing topological indices. The results of the QSPR analysis revealed that the predicting power of $F^w(G)$is better than the forgotten index. Further, we explore mathematical properties of $F^w(G)$

Keywords: Topological index, forgotten index, weighted forgotten index, QSPR

AMS Mathematics Subject Classification (2010): 05C09, 05C69, 05C92

1. Introduction

All graphs considered in this paper are simple with vertex set V and edge set E. The order and size of G is denoted by |V| = n and |E| = m respectively. The degree of a vertex $v \in V$ is the number of edges incident to v and it is denoted by $d_G(v)$. The degree of an edge $e = uv$ is defined as

$$d_G(e) = d_G(u) + d_G(v) - 2.$$

For undefined terminology in this paper refer [5].

Topological index is simply a numeric associated with the molecular graph. So far, large number of such quantities are put forward by many researchers right from 1972 [2]. According to Gutman (Personal Communication) a useful topological index is one which has a good predicting power in QSPR studies. Therefore, topological indices can be categorized into two categories useful and not so useful TI's see [3, 4, 6, 7, 13, 15]. One of the most useful topological index is the Forgotten index F(G) which are defined as:

$$F(G) = \sum_{i=1}^{n} d_G(v)^3 \qquad (1)$$

Motivated by the forgotten index, here we put forward the weighted version of the forgotten index. For this first we have to define the vertex and edge weights of a graph G as follows:

Vertex weight: Let $w_1, w_2, w_3 \cdots, w_n$ be the weights of the vertices $v_1, v_2, v_3, \cdots, v_n$ such that $w_1 = d_G(v_1), w_2 = d_G(v_2), = w_3 = d_G(v_3) \ldots \ldots w_n = d_G(v_n)$.

Edge weight: Let $e_1, e_2, e_3, \cdots, e_m$ be the edges of a graph G. Then the edge weight of $e = uv \in E(G)$is defined as $w(e) = d_G(u) + d_G(v) - 2$.

Weighted degree of a vertex: The weighted degree of a vertex $v \in V(G)$ is defined as:

$$d_G^w(v) = \sum_{e=uv} w(e)$$

2. Weighted forgotten index

The Weighted forgotten index $F^w(G)$ is defined as

$$F^w(G) = \sum_{v \in V} d_G^w(v)^3$$

Example 1. Consider the following graph G. with $V(G) = \{v_1, v_2, v_3, v_4, v_5\}$ and the edge set $E(G) = \{v_1, v_2, v_3, v_4, v_5\}$. Then clearly the weights of vertices and edges are given by their corresponding degrees. Therefore, the weighted degree of each vertex is given by :

$$d_G^w(v_1) = w(e_1) + w(e_2) = 2 + 3 = 5$$
$$d_G^w(v_2) = w(e_2) + w(e_4) = 2 + 2 = 4$$
$$d_G^w(v_3) = w(e_3) + w(e_4) = 3 + 2 = 5$$
$$d_G^w(v_4) = w(e_1) + w(e_3) + +w(e_5) = 3 + 3 + 2 = 8$$
$$d_G^w(v_5) = w(e_5) = 2 = 2$$

Hence the Weighted forgotten index $F^w(G)$ of G is

$$\begin{aligned} F^w(G) &= \sum_{v \in V} d_G^w(v)^3 \\ &= d_G^w(v_1)^3 + d_G^w(v_2)^3 + d_G^w(v_3)^3 + d_G^w(v_4)^3 + d_G^w(v_5)^3 \\ &= 5^3 + 4^3 + 5^3 + 8^3 + 2^3 \\ &= 834. \end{aligned}$$

Observe that the Forgotten index F(G) of G is

$$\begin{aligned} F(G) &= \sum_{v \in V} d_G(v)^3 \\ &= d_G(v_1)^3 + d_G(v_3)^2 + d_G(v_3)^3 + d_G(v_4)^3 + d_G(v_5)^3 \\ &= 2^3 + 2^3 + 2^3 + 3^3 + 1^3 \\ &= 52. \end{aligned}$$

Hence the values of weighted and the forgotten index are significantly different for all non-trivial graphs with at least three vertices. Therefore, the QSPR studies of the weighted forgotten index will reveal the usefulness of this new parameter.

On Weighted Forgotten Index

Sl. No.	Alkane	bp(°C)	$mv(cm^3)$	$mr(cm^3)$	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	2,2Dimethyl propane	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-Methyl pentane	60.271.	131.933	29.9459	29.86	224.90	29.95	17.38	-153.67
8	3-Methyl pentane	63.282	129.717	29.8016	30.27	231.20	30.83	18.12	-118.00
9	2,2- Methyl butane	49.741	132.744	29.9347	27.69	216.20	30.67	16.30	-99.87
10	2,3-Dimethyl butane	57.988	130.240	29.8104	29.12	227.10	30.99	17.37	-128.54
11	Heptane's	98.427	146.540	34.5504	36.55	267.55	27.01	20.26	-90.61
12	2-Methyl hexane	90.052	147.656	34.5908	34.80	257.90	27.2	19.29	-118.28
13	3-Methyl hexane	91.850	145.821	34.4597	35.08	262.40	28.1	19.79	-119.40
14	3-Ethyl pentane	93.475	143.517	34.2827	35.22	267.60	28.6	20.44	-118.60
15	2,2-Dimethyl pentane	79.197	148.695	34.6166	32.43	247.70	28.4	18.02	-123.81
16	2,3- Dimethyl pentane	89.784	144.153	34.3237	34.24	264.60	29.2	19.96	-119.10
17	2,4- Dimethyl pentane	80.500	148.949	34.6192	32.88	247.10	27.4	18.15	-119.24
18	3,3- Dimethyl pentane	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-Methyl heptane	117.647	163.663	39.2316	39.68	288.00	24.8	20.60	-109.04
21	2-Methyl heptane	118.925	161.832	39.1001	39.83	292.00	25.6	21.17	-120.50
22	4-Methyl heptane	117.709	162.105	39.1174	39.67	290.00	25.6	21.00	-120.95
23	3-Ethyl hexane	118.53	160.07	38.94	39.40	292.00	25.74	21.51	
24	2,2- Dimethyl hexane	10.84	164.28	39.25	37.29	279.00	25.6	19.60	-121.18
25	2,3- Dimethyl hexane	115.607	160.39	38.98	38.79	293.00	26.6	20.99	
26	2,4- Dimethyl hexane	109.42	163.09	39.13	37.76	282.00	25.8	20.05	-137.50
27	2,5- Dimethyl hexane	109.10	164.69	39.25	37.86	279.00	25	19.73	-91.20
28	3,3- Dimethyl hexane	111.96	160.87	39.00	37.93	290.84	27.2	20.63	-126.10
29	3,4-Dimethyl hexane	117.72	158.81	38.84	39.02	298.00	27.4	21.64	
30	3-Ethtle-2-Methyl Pentane	115.65	158.79	38.83	38.52	295.00	27.4	21.52	-114.96
31	3-Ethtle-3-Methyl Pentane	118.25	157.02	38.71	37.99	305.00	28.9	21.99	-90.87
32	2,2,3-Tri Methyl pentane	109.84	159.52	38.92	36.91	294.00	28.2	20.67	-112.27
33	2,2,4- Tri Methyl pentane	99.23	165.08	39.26	35.13	271.15	25.5	18.77	-107.38
34	2,3,3- Tri Methyl pentane	114.76	157.29	38.76	37.22	303.00	29.00	21.56	-100.70
35	2,3,4- Tri Methyl pentane	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-Methyl octane	143.26	179.77	43.87	44.65	315.00	23.6	21.88	-80.40
38	3-Methyl octane	144.18	177.95	43.72	44.75	318.00	23.7	22.34	-107.64
39	4-Methyl octane	142.48	178.15	43.76	44.75	318.30	23.06	22.34	-113.20
40	3-Ethyl Heptane	143.00	176.41	43.64	44.81	318.00	23.98	22.81	-114.90
41	4-Ethyl Heptane	141.20	175.68	43.49	44.81	318.30	23.98	22.81	
42	2,2-Dimethyl Heptane	132.69	180.50	43.91	42.28	302.00	22.8	20.80	-113.00
43	2,3-Dimethyl Heptane	140.50	176.65	43.63	43.79	315.00	23.79	22.34	-116.00
44	2,4-Dimethyl Heptane	133.50	179.12	43.73	42.87	306.00	22.7	23.30	
45	2,5-Dimethyl Heptane	136.00	179.37	43.84	43.87	307.80	22.7	21.30	
46	2,6-Dimethyl Heptane	135.21	180.91	43.92	42.82	306.00	23.7	20.83	-102.90
47	3,3-Dimethyl Heptane	137.300	176.897	43.6870	42.66	314.00	24.19	22.01	
48	3,4-Dimethyl Heptane	140.600	175.349	43.5473	43.84	322.70	24.77	22.80	
49	3,5-Dimethyl Heptane	136.000	177.386	43.6379	42.98	312.30	23.59	21.77	
50	4,4-Dimethyl Heptane	135.200	176.897	43.6022	42.66	317.80	24.18	22.01	
51	3-Ethyl-2-Methyl hexane	138.000	175.445	43.6550	43.84	322.70	24.77	22.80	
52	4-Ethyl-2-Methyl hexane	133.800	177.386	43.6472	42.98	330.30	25.56	21.77	

Sl. No.	Alkane	bp(°C)	$mv(cm^3)$	$mr(cm^3)$	hv(kJ)	ct(°C)	cp(atm)	st(dyne/cm)	mp(°C)
53	3-Ethyl-3-Methyl hexane	140.600	173.077	43.2680	44.04	327.20	25.66	23.22	
54	2,2,4-Tri Methyl hexane	126.540	179.220	43.7638	40.57	301.00	23.39	20.51	-120.00
55	2,2,5-Tri Methyl hexane	124.084	181.346	43.9356	40.17	296.60	22.41	20.04	-105.78
56	2,3,3-Tri Methyl hexane	137.680	173.780	43.4347	42.23	326.10	25.56	22.41	-116.80
57	2,3,4-Tri Methyl hexane	139.000	173.498	43.4917	42.93	324.20	25.46	22.80	
58	2,3,5-Tri Methyl hexane	131.340	177.656	43.6474	41.42	309.40	23.49	21.27	-127.80
59	3,3,4-Tri Methyl hexane	140.460	172.055	43.3407	42.28	330.60	26.45	23.27	-101.20
60	3,3,3-Di Ethyl pentane	146.168	170.185	43.1134	43.36	342.80	26.94	23.75	-33.11
61	2,2-DiMethyl-3-Ethyl pentane	133.830	174.537	43.4571	42.02	322.60	25.96	22.38	-99.20
62	2,3-DiMethyl-3-Ethyl pentane	142.000	170.093	42.9542	42.55	338.60	26.94	23.87	
63	2,4-DiMethyl-3-Ethyl pentane	136.730	173.804	43.4037	42.93	324.20	25.46	22.80	-122.20
64	2,2,3,3-Tetra Methyl pentane	140.274	169.495	43.2147	41.00	334.50	27.04	23.38	-99.0
65	2,2,3,4-Tetra Methyl pentane	133.016	173.557	43.4359	41.00	319.60	25.66	21.98	-121.09
66	2,2,4,4-Tetra Methyl pentane	122.284	178.256	43.8747	38.10	301.60	24.58	20.37	-66.54
67	2,3,3,4-Tetra Methyl pentane	141.551	169.928	43.2016	41.75	334.50	26.85	23.31	-102.12
53	3-Ethyl-3-Methyl hexane	140.600	173.077	43.2680	44.04	327.20	25.66	23.22	
54	2,2,4-Tri Methyl hexane	126.540	179.220	43.7638	40.57	301.00	23.39	20.51	-120.00
55	2,2,5-Tri Methyl hexane	124.084	181.346	43.9356	40.17	296.60	22.41	20.04	-105.78
56	2,3,3-Tri Methyl hexane	137.680	173.780	43.4347	42.23	326.10	25.56	22.41	-116.80
57	2,3,4-Tri Methyl hexane	139.000	173.498	43.4917	42.93	324.20	25.46	22.80	

Sl. No.	Alkane	bp(°C)	$mv(cm^3)$	$mr(cm^3)$	hv(kJ)	ct(°C)	cp(atm)	st(dyne/cm)	mp(°C)
58	2,3,5-Tri Methyl hexane	131.340	177.656	43.6474	41.42	309.40	23.49	21.27	-127.80
59	3,3,4-Tri Methyl hexane	140.460	172.055	43.3407	42.28	330.60	26.45	23.27	-101.20
60	3,3,3-Di Ethyl pentane	146.168	170.185	43.1134	43.36	342.80	26.94	23.75	-33.11
61	2,2-DiMethyl-3-Ethyl pentane	133.830	174.537	43.4571	42.02	322.60	25.96	22.38	-99.20
62	2,3-DiMethyl-3-Ethyl pentane	142.000	170.093	42.9542	42.55	338.60	26.94	23.87	
63	2,4-DiMethyl-3-Ethyl pentane	136.730	173.804	43.4037	42.93	324.20	25.46	22.80	-122.20
64	2,2,3,3-Tetra Methyl pentane	140.274	169.495	43.2147	41.00	334.50	27.04	23.38	-99.0
65	2,2,3,4-Tetra Methyl pentane	133.016	173.557	43.4359	41.00	319.60	25.66	21.98	-121.09
66	2,2,4,4-Tetra Methyl pentane	122.284	178.256	43.8747	38.10	301.60	24.58	20.37	-66.54
67	2,3,3,4-Tetra Methyl pentane	141.551	169.928	43.2016	41.75	334.50	26.85	23.31	-102.12

3. Applications of weighted forgotten index I QSPR studies

For chemical application of weighted forgotten index we have selected set of alkanes from n-butanes to nonanes. For modeling we have considered eight representative physical properties [boiling points (BP), molar volumes (mv) at 20°C, molar refractions (mr) at

20℃, heats of vaporization (hb) at 25℃, surface tensions (st)20℃ and jeoting points (mp)]. Values for these property were taken from Plavsic et al. [13].

4. Weighted forgotten index $F^w(G)$

(1) Linear model:

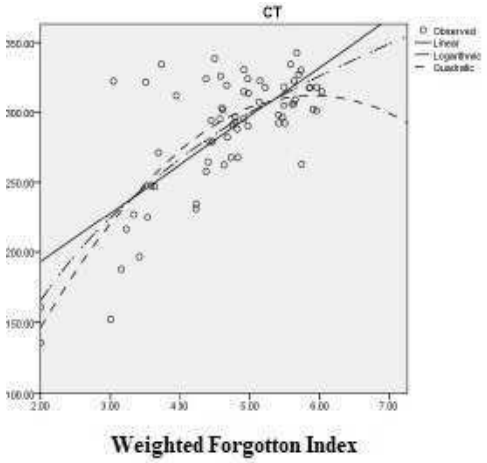
$$bp = 1.237 + [F^w(G)]2.65 \quad (5)$$
$$mv = 102.6 + [F^w(G)]2.9 \quad (6)$$
$$mr = 27.784 + [F^w(G)]1.6 \quad (7)$$
$$hv = 23.772 + [F^w(G)]1.05 \quad (8)$$
$$\text{ct} = 139.143 + [F^w(G)]2.13 \quad (9)$$
$$\text{cp} = 32.09 - [F^w(G)]1.8 \quad (10)$$
$$\text{st} = 17.346 + [F^w(G)]2.98 \quad (11)$$
$$\text{mp} = -140.117[F^w(G)]2.612 \quad (12)$$

(2) Quadratic model:

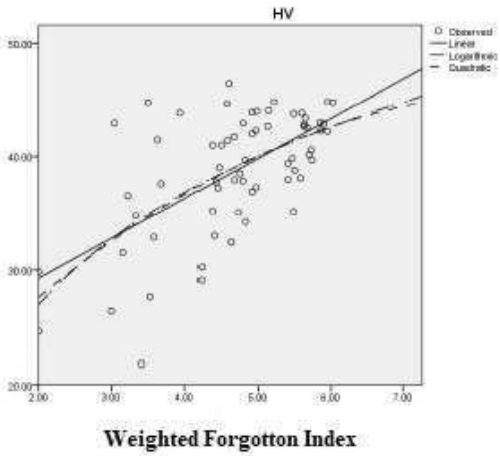
$$bp = 7.9[F^w(G)]^2 - 0.23[F^w(G)] - 56.6 \quad (13)$$
$$mv = 4.7[F^w(G)]^2 - 0.51[F^w(G)] + 79.2 \quad (14)$$
$$mr = 3.2[F^w(G)]^2 - 0.32[F^w(G)] + 18.1 \quad (15)$$
$$hv = 4.4[F^w(G)]^2 - 0.26[F^w(G)] + 15.2 \quad (16)$$
$$ct = 10.2[F^w(G)]^2 - 0.21[F^w(G)] + 67.2 \quad (17)$$
$$cp = -2.8[F^w(G)]^2 + 0.25[F^w(G)] + 39.7 \quad (18)$$
$$st = 2.4[F^w(G)]^2 - 0.4[F^w(G)] + 14.3 \quad (19)$$
$$mp = 4.5[F^w(G)]^2 - 0.46[F^w(G)] - 159.6 \quad (20)$$

(3) Logarithmic model:

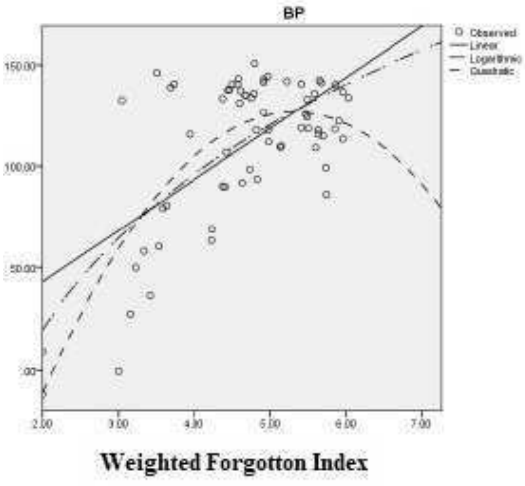
$$bp = -165.6 + ln\,[F^w(G)]\ 82.4 \quad (21)$$
$$\text{mv} = 35.4 + ln[\,[F^w(G)]\ 38.2 \quad (22)$$
$$mr = 0.8 + ln[\,[F^w(G)]13.7 \quad (23)$$
$$hv = 23.9 + ln[\,[F^w(G)]\ 0.6 \quad (24)$$
$$ct = -55.2 + ln[\,[F^w(G)]\ 109.7 \quad (25)$$
$$cp = 45.5 + ln[\,[F^w(G)]\ 7.8 \quad (26)$$
$$st = 9.3 + ln[\,[F^w(G)]\ 46.2 \quad (27)$$
$$mp = -192.8 + ln[\,[F^w(G)]\ 28.2 \quad (28)$$


CT
Observed
Linear
Logarithmic
Quadratic
Weighted Forgotton Index

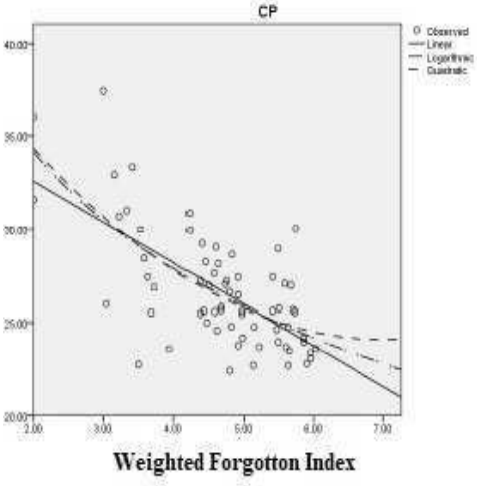
(a)


HV
Observed
Linear
Logarithmic
Quadratic
Weighted Forgotton Index

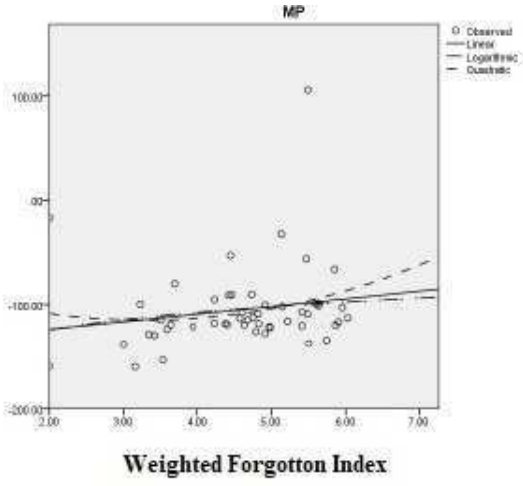
(b)


BP
Observed
Linear
Logarithmic
Quadratic
Weighted Forgotton Index

(c)


CP
Observed
Linear
Logarithmic
Quadratic
Weighted Forgotton Index

(d)



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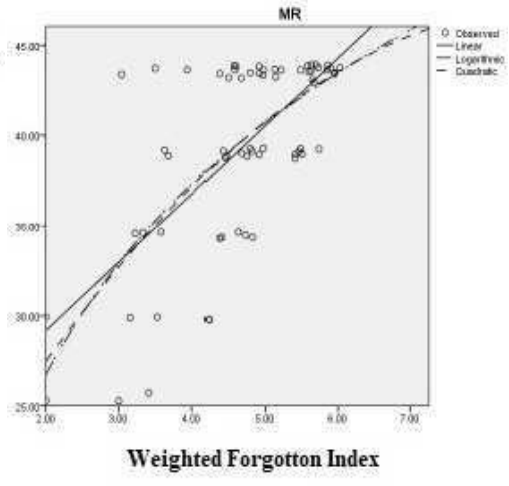

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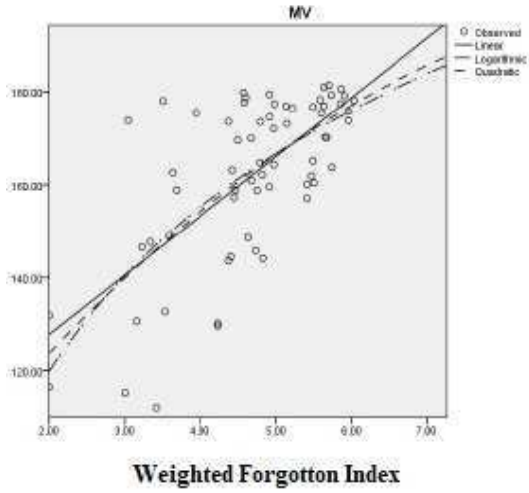
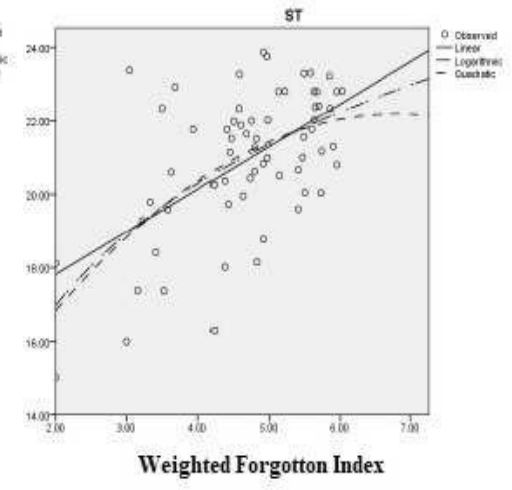


(g)



(h)

Table 2: Model summary for the boiling point of alkanes and weighted forgotten index

Equation	R^2	**F**	**Sig**
Linear	0.873	74.62	0.000
Logarithmic	0.642	82.65	0.000
Quadratic	0.66	49.61	0.000

The Table 2 revealed that the prediction power of the weighted forgotten index is good in predicting the boiling points as the correlation coefficient value $r = 0.873$ for linear model. i.e. our result show 87.3% of accuracy in predicting the boiling points of alkanes.

Table 3: Model summary for the critical pressure of alkanes and weighted forgotten index

Equation	R^2	F	Sig
Linear	0.808	40.85	0.000
Logarithmic	0.42	12.32	0.001
Quadratic	0.723	30.34	0.000

The Table 3 shows that the prediction power of the weighted forgotten index $is\ good$ in predicting the critical pressure of alkanes as the correlation coefficient value r=0.808 for linear model. i.e. our result show 80.8% of accuracy The above Table 3 shows that the prediction power of the weighted forgotten index $is\ good$ in predicting the critical pressure of alkanes as the correlation coefficient value r=0.808 for linear model. i.e. our result show 80.8% of accuracy in predicting the critical pressure of alkanes.

Table 4: Model summary for the critical temperature of alkanes and weighted forgotten index

Equation	R^2	F	Sig
Linear	0.068	0.72	0.347
Logarithmic	0.237	3.624	0.213
Quadratic	0.69	31.87	0.000

The Table 4 revealed that the prediction power of the weighted forgotten index is good in predicting the critical temperature of alkanes as the correlation coefficient value r=0.69 for quadratic model. i.e our result show 69% of The The above Table 4 revealed that the prediction power of the weighted forgotten index is good in predicting the critical temperature of alkanes as the correlation coefficient value r=0.69 for quadratic model. i.e our result show 69% of accuracy in predicting the critical temperature of alkanes.

Table 5: Model summary for the heats of vaporization of alkanes and weighted forgotten index

Equation	R^2	F	Sig
Linear	0.803	59.65	0.000
Logarithmic	0.853	90.42	0.000
Quadratic	0.880	50.5	0.000

The Table 5 shows that the prediction power of the weighted forgotten index is good in predicting the heats of vaporization of alkanes as the correlation coefficient value r=0.880 for quadratic model. i.e. our result show 88.0% of accuracy in predicting the heats of vaporization of alkanes.

Table 6: Model summary for the melting point of alkanes and weighted forgotten index

Equation	R^2	F	Sig
Linear	0.560	14.732	0.001
Logarithmic	0.581	13.31	0.000
Quadratic	0.521	5.89	0.002

The Table 6 shows that the prediction power of the weighted forgotten index is not so good in predicting the melting point of alkanes as the correlation coefficient values for all models are less than 0.7.

Table 7: Model summary for the molar refraction of alkanes and weighted forgotten index

Equation	R^2	F	Sig
Linear	0.58	10.51	0.002
Logarithmic	0.375	12.347	0.001
Quadratic	0.572	6.546	0.001

The Table 7 shows that the prediction power of the weighted forgotten index is not so good in predicting the molar refraction of alkanes as the correlation coefficient value for all models is less than 0.7.

Table 8: Model summary for the molar volume of alkanes and weighted forgotten index

Equation	R^2	F	Sig
Linear	0.727	40.87	0.000
Logarithmic	0.545	12.52	0.001
Quadratic	0.808	30.24	0.000

The Table 8 revealed that the prediction power of the weighted forgotten index is good in predicting molar volume of alkanes as the correlation coefficient value r=0.808 for quadratic model. i.e. our result show 80.8% of accuracy in predicting the molar volume of alkanes.

Table 9: Model summary for the surface tension of alkanes and weighted forgotten index

Equation	R^2	F	Sig
Linear	0.067	0.87	0.54
Logarithmic	0.137	2.762	0.12
Quadratic	0.848	33.86	0.000

The Table 9 shows that the prediction power of the weighted forgotten index $is\ good\ in\ predicting$ the surface tension of alkanes as the correlation coefficient value r=0.848 for quadratic model. i.e. our result sow 84.8% of accuracy in predicting the quadratic model of alkanes.

5. Conclusion

In this paper we have studies the mathematical as well as chemical applications of weighted forgotten index. QSPR study revealed the weighted forgotten index is a good candidate in predicting physic-chemical properties of alkanes.

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