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A novel set of Wiener indices

Xin-hua Li [a,*], Zu-guang Li [b], Mao-lin Hu [a]

[a] School of Chemistry and Materials Science, Wenzhou Normal College, Wenzhou, Zhejiang 325027, PR China
[b] College of Chemical and Materials Engineering, Zhejiang University of Technology, Hangzhou 310014, PR China

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Abstract

According to the definition of molecular connectivity and the definition of the Wiener index, a novel set of Wiener indices ($^{m}V_t$) were defined, named novel Wiener index. The potential usefulness of the novel Wiener index in QSAR/QSPR is evaluated by its correlation with a number of C_3–C_8 alkanes and by a favorable comparison with models based on molecular connectivity index and Wiener index.

Keywords: Wiener index (W); Novel Wiener index ($^{m}V_t$); Molecular connectivity index

1. Introduction

The Wiener number $W(G)$, one of widely used descriptors of molecular topology, was introduced in 1947 by Wiener [1] as the path number for saturated acyclic hydrocarbons. The path number was defined as the number of the bonds between all pairs of non-hydrogen atoms in the molecule [2]. The Wiener number is $W(G)$, where W of a structure G is equal to the half-sum of distances of the distance matrix between all pairs of vertices [3,4]:

$$W(G) = W = \frac{1}{2}\sum_i \sum_j d_{ij} \tag{1}$$

But the usefulness of the Wiener number is not as popular as the molecular connectivity index, some limits prevent the use of this number [5], for example, it can only be used for saturated hydrocarbons [6]. There should be a further factor that is not accounted for by Wiener number [7].

Randić introduced the concept of a connectivity (branching) index in 1975 [8]. The concept has been further developed and applied extensively by Kier and Hall [9,10], which led to the molecular connectivity index. The molecular connectivity index was proved to be one of the most successful and widely used indices.

2. The novel Wiener index

A comparison between the Wiener number and the molecular connectivity index shows that there are some similarities. Wiener proposed a formula for calculating his Wiener number by simply counting the number of atoms n_i and n_j on both sides of each bond:

$$W = \sum_{\text{all bonds}} n_i n_j \tag{2}$$

The first-order molecular connectivity index $^{1}\chi_{\text{p}}$ is the sum of over all bonds i–j (Eq. (3)), where δ_i is the valence of carbon atom i in the carbon skeleton of a hydrocarbon.

$$^{1}\chi_{\text{p}} = \sum_{\text{bonds}} \left(\frac{1}{\delta_i \delta_j}\right)^{1/2} \tag{3}$$

The second-order molecular index $^{2}\chi_{\text{p}}$ is a sum over two-bond paths i–j–k of terms $1/(\delta_i\delta_j\delta_k)^{1/2}$. A hierarchy of additional indices $^{m}\chi_t$ of order m and type t can be obtained by summing analogous terms over substructural units involving paths (t = p), clusters (t = c), path–cluster (t = pc), or chain (t = ch) combination of m bonds.

According to the definition of molecular connectivity and the definition of Wiener index, we also can define the additional extended Wiener indices of order m and type t involving paths (t = p), clusters (t = c), path–cluster (t = pc), or chain (t = ch) combination of m bonds, just as those of the molecular connectivity index. The extended Wiener indices ($^{m}V_t$) are defined as follows:

* Corresponding author. Tel.: +86-57788373111; fax: +86-57788339081.
E-mail address: lixinhua01@263.net (X.-h. Li).

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Table 1
The novel Wiener indices of the 38 alkanes

Number	Molecule	${}^{0}V_{p}$	${}^{1}V_{p}$	${}^{2}V_{p}$	${}^{3}V_{p}$	${}^{4}V_{p}$	${}^{5}V_{p}$	${}^{6}V_{p}$	${}^{7}V_{p}$	${}^{3}V_{c}$	${}^{4}V_{c}$	${}^{5}V_{c}$	${}^{6}V_{c}$	${}^{3}V_{pc}$	${}^{5}V_{pc}$	${}^{6}V_{pc}$	${}^{7}V_{pc}$
1	Propane	0.3333	0.4444	0.1111	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	*n*-Butane	0.2500	0.6250	0.2500	0.0625	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	2-Methyl propane	0.2500	0.5625	0.3750	0.0000	0.0000	0.0000	0.0000	0.0000	6.2500	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	*n*-Pentane	0.2000	0.8000	0.4000	0.1600	0.0400	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	2-Methyl butane	0.2000	0.7200	0.5600	0.1600	0.0000	0.0000	0.0000	0.0000	0.0800	0.0000	0.0000	0.0000	0.0400	0.0000	0.0000	0.0000
6	2,2-Dimethyl propane	0.2000	0.6400	0.7200	0.0000	0.0000	0.0000	0.0000	0.0000	0.3200	0.0400	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7	*n*-Hexane	0.1667	0.9722	0.5556	0.2778	0.1111	0.0278	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	2-Methyl pentane	0.1667	0.8889	0.7222	0.3056	0.1111	0.0000	0.0000	0.0000	0.8333	0.0000	0.0000	0.0000	0.0556	0.0278	0.0000	0.0000
9	3-Methyl pentane	0.1667	0.8611	0.7778	0.3889	0.0556	0.0000	0.0000	0.0000	0.1111	0.0000	0.0000	0.0000	0.1111	0.0278	0.0000	0.0000
10	2,3-Dimethyl butane	0.1667	0.8056	0.8889	0.4444	0.0000	0.0000	0.0000	0.0000	0.1667	0.0000	0.0278	0.0000	0.2222	0.0000	0.0000	0.0000
11	2,2-Dimethyl butane	0.1667	0.7778	0.9444	0.2500	0.0000	0.0000	0.0000	0.0000	0.4167	0.0556	0.0000	0.0000	0.1667	0.0278	0.0000	0.0000
12	*n*-Heptane	0.1429	1.1429	0.7143	0.4082	0.2041	0.0816	0.0204	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13	2-Methyl hexane	0.1429	1.0612	0.8776	0.4490	0.2245	0.0816	0.0000	0.0000	0.0816	0.0000	0.0000	0.0000	0.0612	0.0408	0.0204	0.0000
14	3-Methyl hexane	0.1429	1.0204	0.9592	0.5714	0.2245	0.0408	0.0000	0.0000	0.1224	0.0000	0.0000	0.0000	0.1429	0.0816	0.0204	0.0000
15	3-Ethyl pentane	0.1429	0.9796	1.0408	0.7347	0.1837	0.0000	0.0000	0.0000	0.1633	0.0000	0.0000	0.0000	0.2449	0.1224	0.0204	0.0000
16	2,4-Dimethyl pentane	0.1429	0.9796	1.0408	0.4898	0.3265	0.0000	0.0000	0.0000	0.1633	0.0000	0.0000	0.0000	0.1224	0.1633	0.0204	0.0000
17	2,3-Dimethyl pentane	0.1429	0.9388	1.1225	0.7755	0.1633	0.0000	0.0000	0.0000	0.2041	0.0000	0.0408	0.0000	0.3673	0.1224	0.0204	0.0000
18	2,2-Dimethyl pentane	0.1429	0.9388	1.1224	0.4490	0.1837	0.0000	0.0000	0.0000	0.4490	0.0612	0.0000	0.0000	0.2449	0.1633	0.0204	0.0000
19	3,3-Dimethyl pentane	0.1429	0.8980	1.2041	0.5714	0.0612	0.0000	0.0000	0.0000	0.5714	0.0816	0.0000	0.0000	0.4898	0.1633	0.0204	0.0000
20	2,2,3-Trimethyl butane	0.1429	0.8571	1.2857	0.7347	0.0000	0.0000	0.0000	0.0000	0.5306	0.0612	0.1224	0.0204	0.6735	0.0816	0.0000	0.0000
21	*n*-Octane	0.1250	1.3125	0.8750	0.5469	0.3125	0.1563	0.0625	0.0156	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22	2-Methyl heptane	0.1250	1.2344	1.0313	0.5938	0.3438	0.1719	0.0625	0.0000	0.0781	0.0000	0.0000	0.0000	0.0625	0.0469	0.0313	0.0156
23	3-Methyl heptane	0.1250	1.1875	1.1250	0.7344	0.3750	0.1719	0.0313	0.0000	0.1250	0.0000	0.0000	0.0000	0.1563	0.1094	0.0625	0.0156
24	4-Methyl heptane	0.1250	1.1719	1.1563	0.7813	0.4375	0.1250	0.0313	0.0000	0.1406	0.0000	0.0000	0.0000	0.1875	0.1563	0.0625	0.0156
25	3-Ethylhexane	0.1250	1.1250	1.2500	0.9844	0.4375	0.0938	0.0000	0.0000	0.1875	0.0000	0.0000	0.0000	0.3125	0.2344	0.0938	0.0156
26	2,5-Dimethyl hexane	0.1250	1.1563	1.1875	0.6406	0.3750	0.2500	0.0000	0.0000	0.1563	0.0000	0.0000	0.0000	0.1250	0.0938	0.1250	0.0156
27	2,4-Dimethyl hexane	0.1250	1.1094	1.2813	0.7813	0.5313	0.1250	0.0000	0.0000	0.2031	0.0000	0.0000	0.0000	0.2188	0.2813	0.1250	0.0156
28	2,2-Dimethyl hexane	0.1250	1.1094	1.2813	0.6250	0.3438	0.1406	0.0000	0.0000	0.4531	0.0625	0.0000	0.0000	0.2813	0.2344	0.1250	0.0156
29	2,3-Dimethyl hexane	0.1250	1.0938	1.3125	1.0156	0.4063	0.1250	0.0000	0.0000	0.2188	0.0000	0.0469	0.0000	0.4375	0.2344	0.1250	0.0156
30	3,4-Dimethyl hexane	0.1250	1.0625	1.3750	1.1719	0.4375	0.0625	0.0000	0.0000	0.2500	0.0000	0.0625	0.0000	0.5625	0.3438	0.1250	0.0156
31	2-Methyl-3-ethyl pentane	0.1250	1.0469	1.4063	1.2813	0.4375	0.0000	0.0000	0.0000	0.2656	0.0000	0.0625	0.0000	0.6250	0.3906	0.1250	0.0156
32	3,3-Dimethyl hexane	0.1250	1.0469	1.4063	0.8125	0.3125	0.0469	0.0000	0.0000	0.6406	0.0938	0.0000	0.0000	0.5938	0.4063	0.1250	0.0156
33	3-Methyl-3-ethyl pentane	0.1250	1.0000	1.5000	0.9844	0.1875	0.0000	0.0000	0.0000	0.8125	0.1250	0.0000	0.0000	0.9375	0.5156	0.1250	0.0156
34	2,2,4-trimethyl pentane	0.1250	1.0313	1.4375	0.6719	0.5625	0.0000	0.0000	0.0000	0.5313	0.0625	0.0000	0.0000	0.3438	0.5625	0.1563	0.0156
35	2,3,4-Trimethyl pentane	0.1250	1.0156	1.4688	1.2500	0.5000	0.0000	0.0000	0.0000	0.2969	0.0000	0.0938	0.0000	0.6875	0.5000	0.1563	0.0156
36	2,2,3-Trimethyl pentane	0.1250	0.9844	1.5313	1.1875	0.2813	0.0000	0.0000	0.0000	0.5781	0.0625	0.1875	0.0313	1.0000	0.4375	0.1250	0.0156
37	2,3,3-Trimethyl pentane	0.1250	0.9688	1.5625	1.1719	0.1875	0.0000	0.0000	0.0000	0.7188	0.0938	0.1719	0.0313	1.1563	0.4688	0.1250	0.0156
38	2,2,3,3-Tetramethyl butane	0.1250	0.9063	1.6875	1.2656	0.0000	0.0000	0.0000	0.0000	0.9063	0.1250	0.5625	0.1875	1.6875	0.2813	0.0000	0.0156

Table 2
Experimental values for the physical properties of the 38 alkanes

Number	Molecule	bp	MV	MR	HV	T_C	P_C	ST
1	Propane	−42.070				96.80	42.01	
2	*n*-Butane	−0.500				152.01	37.47	
3	2-Methyl propane	−11.730				134.98	36.00	
4	*n*-Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16.00
5	2-Methyl butane	27.852	116.426	25.2923	24.59	187.80	32.90	15.00
6	2,2-Dimethyl propane	9.503	122.074	25.7243	21.78	160.60	31.57	
7	*n*-Hexane	68.740	130.688	29.9066	31.55	234.70	29.92	18.42
8	2-Methyl pentane	60.271	131.933	29.9459	29.86	224.90	29.95	17.38
9	3-Methyl pentane	63.282	129.717	29.8016	30.27	231.20	30.83	18.12
10	2,3-Dimethyl butane	57.988	130.240	29.8104	29.12	227.10	30.99	17.37
11	2,2-Dimethyl butane	49.741	132.744	29.9347	27.69	216.20	30.67	16.30
12	*n*-Heptane	98.427	146.540	34.5504	36.55	267.01	27.01	20.26
13	2-Methyl hexane	90.052	147.656	34.5908	34.80	257.90	27.20	19.29
14	3-Methyl hexane	91.850	145.821	34.4597	35.08	262.40	28.10	19.79
15	3-Ethyl pentane	93.475	143.517	34.2827	35.22	267.60	28.60	20.44
16	2,4-Dimethyl pentane	80.500	148.949	34.6192	32.88	247.10	27.40	18.15
17	2,3-Dimethyl pentane	89.784	144.153	34.3237	34.24	264.60	29.20	19.96
18	2,2-Dimethyl pentane	79.197	148.695	34.6166	32.43	247.70	28.40	18.02
19	3,3-Dimethyl pentane	86.064	144.530	34.3323	33.02	263.00	30.00	19.59
20	2,2,3-Trimethyl butane	80.882	145.191	34.3736	32.04	258.30	29.75	18.76
21	*n*-Octane	125.665	162.592	39.1922	41.48	296.20	24.64	21.76
22	2-Methyl heptane	117.647	163.663	39.2316	39.68	288.00	24.80	20.60
23	3-Methyl heptane	118.925	161.832	39.1001	39.83	292.00	25.60	21.17
24	4-Methyl heptane	117.709	162.105	39.1174	39.67	290.00	25.60	21.17
25	3-Ethylhexane	118.534	160.072	38.9441	39.40	292.00	25.74	21.51
26	2,5-Dimethyl hexane	109.103	164.697	39.2596	37.86	279.00	25.00	19.73
27	2,4-Dimethyl hexane	109.429	163.093	39.1300	37.76	282.00	25.80	20.05
28	2,2-Dimethyl hexane	106.840	164.285	39.2525	37.29	279.00	25.60	19.60
29	2,3-Dimethyl hexane	115.607	160.395	38.9808	38.79	293.00	26.60	20.99
30	3,4-Dimethyl hexane	117.725	158.814	38.8453	39.02	298.00	27.40	21.64
31	2-Methyl-3-ethyl pentane	115.650	158.794	38.8362	38.52	295.00	27.40	21.52
32	3,3-Dimethyl hexane	111.969	160.879	39.0087	37.93	290.84	27.20	20.63
33	3-Methyl-3-ethyl pentane	118.259	157.026	38.7171	37.99	305.00	28.90	21.99
34	2,2,4-Trimethyl pentane	99.238	165.083	39.2617	35.13	271.15	25.50	18.77
35	2,3,4-Trimethyl pentane	113.467	158.852	38.8681	37.61	295.00	27.60	21.14
36	2,2,3-Trimethyl pentane	109.841	159.526	38.9249	36.91	294.00	28.20	20.67
37	2,3,3-Trimethyl pentane	114.760	157.292	38.7617	37.22	303.00	29.00	21.56
38	2,2,3,3-Tetramethyl butane	106.470				270.87	24.50	

Definition 1. The zeroth-order extended Wiener index ${}^0W_p$ is defined as the sum over all atoms *i* (Eq. (4)):

$$ {}^0W_p = \sum_{\text{atoms}} n_i \tag{4} $$

Definition 2. The first-order extended Wiener index ${}^1W_p$ is equal to the Wiener index:

$$ {}^1W_p = W = \sum_{\text{all bonds}} n_i n_j \tag{5} $$

Table 3
Comparison of multilinear regression statistics (correlation coefficient, standard deviation, and the Fischer ratio) for the C_3–C_8 alkane properties models produced by the two sets of topological indices ${}^m\chi / {}^mV_t$

Properties	Molecular connectivity index(χ)				Novel Wiener index (${}^mV_t$)			
	n	r^2	*s*	*F*	*n*	r^2	*s*	*F*
Boiling point	38	0.9959	2.86	1541	38	0.9968	2.52	1993
Critical temperature	38	0.9924	4.75	835	38	0.99349	4.39	976
Critical pressure	38	0.9666	0.73	185	38	0.9875	0.45	505
Surface tension (dyn/cm)	33	0.9848	0.24	349	33	0.9828	0.26	308
Molar volume (cm^3/mol)	34	0.9989	0.54	4932	34	0.9971	0.87	1914
Molecular refraction (cm^3/mol)	34	0.9999	0.03	152252	34	0.9998	0.07	28919
Heats of vaporization (kJ/mol)	34	0.9979	0.24	2704	34	0.9971	0.28	1925

Table 4
The t values of indices in correlation (6)

Property	t values					
bp (°C)	−30.61288 (a_0)	3.04662 ($^0\chi_p$)	18.64883 ($^1\chi_p$)	2.26983 ($^4\chi_{pc}$)	−4.43515 ($^6\chi_{pc}$)	−1.87967 ($^6\chi_p$)
	−1.89767 (a_0)	−8.38686 (^0V_p)	20.65439 (^1V_p)	15.65871 (^3V_p)	5.71582 (^4V_c)	−2.94968 ($^7V_{pc}$)
	−27.51681 (a_0)	7.88419 (P)	31.71602 ($\log W$)			

Table 5
The calculated values of correlation (6)

Molecule	bp (6a)	Error (6a)	bp (6b)	Error (6b)	bp (6c)	Error (6c)
Propane	−33.82644	−8.24556	−43.3677	1.29571	−51.2105	9.138452
n-Butane	−0.98158	0.451583	0.042757	−0.57276	−2.49287	1.96287
2-Methyl propane	−10.13186	−1.60114	−9.70356	−2.02944	−11.0978	−0.63516
n-Pentane	31.86334	4.211055	36.25088	−0.17648	35.18685	0.887546
2-Methyl butane	25.739	2.113404	26.6038	1.248602	29.97488	−2.12248
2,2-Dimethyl propane	11.10836	−1.60497	14.4799	−4.9765	17.363	−7.8596
n-Hexane	64.70827	4.035728	68.94515	−0.20115	66.26163	2.482369
2-Methyl pentane	58.32354	1.947858	59.88293	0.388466	61.82872	−1.55732
3-Methyl pentane	61.08857	2.193825	59.47545	3.806948	63.65107	−0.36867
2,3-Dimethyl butane	54.53097	3.45753	54.74487	3.243634	60.35258	−2.36408
2,2-Dimethyl butane	49.67309	0.068412	48.9396	0.801903	55.22377	−5.48227
n-Heptane	94.55875	3.868748	99.68892	−1.26142	92.9035	5.524003
2-Methyl hexane	88.6804	1.372098	91.27923	−1.22673	89.23712	0.815381
3-Methyl hexane	91.26136	0.593638	90.68638	1.168615	90.69044	1.164564
3-Ethyl pentane	93.65825	−0.18275	91.53947	1.936034	92.06402	1.411476
2,4-Dimethyl pentane	81.67958	−1.12958	82.8816	−2.3316	85.27802	−4.72802
2,3-Dimethyl pentane	89.38796	0.396538	88.06185	1.722654	89.95919	−0.17469
2,2-Dimethyl pentane	78.7943	0.403196	81.38399	−2.18649	83.17319	−3.97569
3,3-Dimethyl pentane	84.28866	1.775838	82.41275	3.651751	87.75982	−1.69532
2,2,3-Trimethyl butane	80.36269	0.519914	81.63217	−0.74957	85.45908	−4.57648
n-Octane	126.16345	−0.49785	129.2178	−3.55219	116.3528	9.312799
2-Methyl heptane	117.36421	0.283392	117.3017	0.345871	113.3174	4.330181
3-Methyl heptane	120.63067	−1.70507	116.6167	2.308884	114.7947	4.130946
4-Methyl heptane	120.4466	−2.737	116.3936	1.316024	114.1397	3.56986
3-Ethylhexane	123.58303	−5.04843	117.9181	0.616496	115.5133	3.021272
2,5-Dimethyl hexane	109.50188	−0.39828	109.5383	−0.43468	110.0827	−0.97911
2,4-Dimethyl hexane	111.88597	−2.45637	108.8568	0.572803	111.429	−1.99937
2,2-Dimethyl hexane	106.06741	0.778592	108.2993	−1.45331	108.036	−1.18997
2,3-Dimethyl hexane	115.98792	−0.38032	115.2587	0.348852	114.1204	1.487245
3,4-Dimethyl hexane	120.30636	−2.58076	117.01	0.715649	116.0794	1.646221
2-Methyl-3-ethyl pentane	120.00576	−4.34976	118.9964	−3.34035	115.3459	0.310124
3,3-Dimethyl hexane	111.01749	0.952106	109.8792	2.090407	111.9529	0.016724
3-Methyl-3-ethyl pentane	115.67609	2.583512	112.7808	5.478791	116.4734	1.786156
2,2,4-Trimethyl pentane	95.37703	3.861571	100.5394	−1.30079	104.4231	−5.18452
2,3,4-Trimethyl pentane	115.00715	−1.53955	114.1154	−0.6478	113.847	−0.37938
2,2,3-Trimethyl pentane	112.19605	−2.35445	113.1116	−3.27003	112.3014	−2.45978
2,3,3-Trimethyl pentane	112.38012	2.38588	113.167	1.599016	114.9028	−0.13679
2,2,3,3-Tetramethyl butane	107.91781	−1.44081	111.4228	−4.94584	111.6043	−5.1273

Table 6
The t values of indices in correlation (7)

Property	t values					
T_C (°C)	4.05646 (a_0)	23.53582 ($^1\chi_p$)	6.36663 ($^2\chi_p$)	9.43039 ($^3\chi_p$)	−4.00826 ($^6\chi_p$)	−3.32696 ($^6\chi_{pc}$)
	10.59055 (a_0)	−8.86075 (^0V_p)	4.6208 (^1V_p)	10.93307 (^3V_p)	−7.38042 (^5V_p)	6.20173 ($^4V_{pc}$)
	3.0779 (a_0)	10.26036 (P)	25.76731 ($\log W$)			

Table 7
The calculated values of correlation (7)

Molecule	T_C (7a)	Error (7a)	T_C (7b)	Error (7b)	T_C (7c)	Error (7c)
Propane	109.16216	−12.36016	95.86445	0.93755	93.74342	3.05858
n-Butane	150.89643	1.11657	151.46823	0.54477	149.68147	2.33153
2-Methyl propane	137.66962	−2.68662	142.45932	−7.47632	137.9483	−2.9653
n-Pentane	187.21648	9.40356	194.27591	2.34413	193.45558	3.16446
2-Methyl butane	185.82023	1.98017	186.40447	1.39593	187.71189	0.08851
2,2-Dimethyl propane	165.80608	−5.20568	171.21311	−10.61271	169.31271	−8.71231
n-Hexane	224.41973	10.28427	230.73687	3.96713	229.95092	4.75308
2-Methyl pentane	219.16874	5.73166	223.81461	1.08579	225.06576	−0.16536
3-Methyl pentane	229.54935	1.65105	224.88818	6.31222	229.32434	1.87606
2,3-Dimethyl butane	224.64653	2.45397	221.31968	5.78082	225.68934	1.41116
2,2-Dimethyl butane	218.6899	−2.4894	213.74682	2.45368	217.78698	−1.58648
n-Heptane	261.62288	5.38762	263.62507	3.38543	261.5611	5.4494
2-Methyl hexane	253.96114	3.93936	257.4509	0.4496	257.52067	0.37983
3-Methyl hexane	260.81707	1.58793	259.0403	3.3647	261.37258	1.03242
3-Ethyl pentane	266.05571	1.54479	262.49472	5.10578	265.13661	2.46389
2,4-Dimethyl pentane	246.31474	0.79026	251.28862	−4.18362	253.15767	−6.05267
2,3-Dimethyl pentane	265.94959	−1.34909	259.39762	5.20288	262.81704	1.78346
2,2-Dimethyl pentane	246.50074	1.19976	250.41539	−2.71489	250.8381	−3.1376
3,3-Dimethyl pentane	264.31349	−1.31299	258.67638	4.32412	260.39329	2.60721
2,2,3-Trimethyl butane	255.38222	2.91838	252.60369	5.69691	257.85783	0.44277
n-Octane	298.82602	−2.62542	294.28641	1.91419	289.65301	6.54759
2-Methyl heptane	291.98499	−3.98439	288.74757	−0.74697	286.30796	1.69264
3-Methyl heptane	297.25067	−5.25007	290.56737	1.43323	290.18622	1.81438
4-Methyl heptane	293.72588	−3.72528	291.17604	−1.17544	289.46449	0.53611
3-Ethylhexane	297.70446	−5.70386	295.85314	−3.85254	293.22853	−1.22793
2,5-Dimethyl hexane	280.12799	−1.12739	283.2062	−4.2056	282.74325	−3.74265
2,4-Dimethyl hexane	285.16855	−3.16795	285.02853	−3.02793	286.47716	−4.47656
2,2-Dimethyl hexane	278.05363	0.94697	283.62763	−4.62703	280.48769	−1.48709
2,3-Dimethyl hexane	293.47532	−0.47472	293.1195	−0.1189	291.69344	1.30716
3,4-Dimethyl hexane	303.26589	−5.26529	296.82751	1.17309	296.10264	1.89796
2-Methyl-3-ethyl pentane	298.25611	−3.25551	300.29757	−5.29697	295.29431	−0.29371
3,3-Dimethyl hexane	289.90583	0.93477	293.72108	−2.88048	289.30484	1.53576
3-Methyl-3-ethyl pentane	303.26571	1.73489	306.54895	−1.54835	298.78723	6.21337
2,2,4-Trimethyl pentane	265.21961	5.93099	278.08879	−6.93819	276.50627	−5.35567
2,3,4-Trimethyl pentane	298.42607	−3.42547	295.05361	−0.05301	293.64249	1.35811
2,2,3-Trimethyl pentane	293.65199	0.34861	292.69826	1.30234	291.93921	2.06139
2,3,3-Trimethyl pentane	298.22068	4.78532	298.47755	4.52845	297.05633	5.94966
2,2,3,3-Tetramethyl butane	272.131	−1.2603	274.11447	−3.24377	293.42134	−22.55064

Definition 3. According to Randić and coworkers [11–13], the *m*th-order extended Wiener index ${}^{m}W_{\mathrm{p}}$ is the sum of contributions K_i, where subscript i denotes the number of substructural unit of paths combinations of m bonds. K_i may be obtained by using the following two-step algorithm. (1) Remove the m bonds of substructural unit of paths; $m + 1$ unconnected subgraphs will be obtained. (2) Multiply the number of vertices of the $m + 1$ unconnected subgraphs, $n_1 \times n_2 \times \cdots \times n_{m+1}$. ${}^{m}W_{\mathrm{p}}$ may be obtained by adding K_i for all of paths subgraphs combination of m bonds.

Definition 4. According to the molecular connectivity index, the *m*th-order and *t* type extended Wiener index ${}^{m}W_t$ is the sum of contributions K_i, where subscripts i denote the numbers of substructural unit of t type, involving clusters (t = c), path–cluster (t = pc), or chain (t = ch) combinations of m bonds. K_i may be obtained by using the following

Table 8
The t values of indices in correlation (8)

Property	t values					
P_C (atm)	29.81998 (a_0)	4.0189 (${}^{0}\chi_{\mathrm{p}}$)	−6.37065 (${}^{1}\chi_{\mathrm{p}}$)	−6.43424 (${}^{2}\chi_{\mathrm{p}}$)	2.89051 (${}^{5}\chi_{\mathrm{p}}$)	4.76856 (${}^{5}\chi_{\mathrm{pc}}$)
	33.07259 (a_0)	28.53593 (${}^{0}V_{\mathrm{p}}$)	−5.976 (${}^{4}V_{\mathrm{p}}$)	−3.1854 (${}^{5}V_{\mathrm{p}}$)	8.54563 (${}^{4}V_{\mathrm{pc}}$)	−10.77303 (${}^{6}V_{\mathrm{c}}$)
	51.59695 (a_0)	4.19546 (P)	−18.10767 ($\log W$)			

Table 9
The calculated values of correlation (8)

Molecule	P_C (8a)	Error (8a)	P_C (8b)	Error (8b)	P_C (8c)	Error (8c)
Propane	40.78327	1.22873	42.50487	−0.49287	41.9645	0.0475
n-Butane	37.33747	0.13553	36.36379	1.10921	36.51765	0.95535
2-Methyl propane	36.38489	−0.38189	36.36379	−0.36079	36.78243	−0.77943
n-Pentane	33.51743	−0.20739	32.5207	0.78934	32.49676	0.81328
2-Methyl butane	33.81051	−0.91011	32.80791	0.09249	33.17009	−0.26969
2,2-Dimethyl propane	31.5178	0.0526	32.67767	−1.10727	33.10562	−1.53522
n-Hexane	30.5654	−0.6414	29.64753	0.27647	29.32915	0.59485
2-Methyl pentane	30.42991	−0.47951	29.96776	−0.01736	29.90183	0.04857
3-Methyl pentane	31.53593	−0.70553	30.36625	0.46415	30.51329	0.31711
2,3-Dimethyl butane	30.77728	0.21322	30.94616	0.04434	30.93942	0.05108
2,2-Dimethyl butane	30.34621	0.32429	30.76547	−0.09497	30.75511	−0.08461
n-Heptane	27.10484	−0.09434	27.25859	−0.24809	26.73422	0.27628
2-Methyl hexane	27.85011	−0.64961	27.37779	−0.17729	27.20788	−0.00738
3-Methyl hexane	28.50951	−0.40451	27.84809	0.25691	27.86701	0.23799
3-Ethyl pentane	29.02921	−0.42871	28.54459	0.05591	28.53644	0.06406
2,4-Dimethyl pentane	28.03539	−0.63039	27.58536	−0.18036	27.71934	−0.31434
2,3-Dimethyl pentane	29.24471	−0.04421	29.02316	0.17734	28.80836	0.39214
2,2-Dimethyl pentane	27.61688	0.78362	28.54459	−0.14409	27.99126	0.40924
3,3-Dimethyl pentane	29.524	0.4765	29.82267	0.17783	29.0925	0.908
2,2,3-Trimethyl butane	28.13921	1.61139	29.78241	−0.03181	29.38972	0.36088
n-Octane	23.71884	0.92176	25.13953	−0.49893	24.55174	0.08886
2-Methyl heptane	24.11599	0.68461	25.14208	−0.34148	24.94387	−0.14327
3-Methyl heptane	25.56646	0.03414	25.32503	0.27557	25.59992	6.84967×10^{-4}
4-Methyl heptane	25.11994	0.48066	25.41619	0.18441	25.68452	−0.08392
3-Ethylhexane	26.51279	−0.77219	25.97939	−0.23879	26.35396	−0.61336
2,5-Dimethyl hexane	25.32563	−0.32503	24.83206	0.16854	25.36176	−0.36116
2,4-Dimethyl hexane	26.22811	−0.42751	25.15	0.6506	26.03472	−0.23412
2,2-Dimethyl hexane	25.17767	0.42293	26.01118	−0.41058	25.62617	−0.02557
2,3-Dimethyl hexane	26.33135	0.26925	26.35258	0.24802	26.53391	0.06669
3,4-Dimethyl hexane	27.71175	−0.31115	26.95008	0.45052	27.12771	0.27289
2-Methyl-3-ethyl pentane	27.17694	0.22366	27.46652	−0.06592	27.22247	0.17813
3,3-Dimethyl hexane	26.858	0.3426	27.62063	−0.42003	26.81392	0.38668
3-Methyl-3-ethyl pentane	28.78152	0.11908	29.46503	−0.56443	27.92369	0.97691
2,2,4-Trimethyl pentane	25.99032	−0.48972	26.06044	−0.55984	26.09291	−0.59231
2,3,4-Trimethyl pentane	27.76165	−0.16105	27.42474	0.17586	27.41611	0.18449
2,2,3-Trimethyl pentane	27.43408	0.76652	27.95251	0.24809	27.61579	0.58481
2,3,3-Trimethyl pentane	28.05789	0.94811	28.82949	0.17651	28.1266	0.8794
2,2,3,3-Tetramethyl butane	26.47561	−1.97491	24.56813	−0.06743	28.55273	−4.05203

two-step algorithm. (1) Remove the m bonds of substructural unit of t type; $m + 1$ unconnected subgraphs will be obtained. (2) Multiply the number of vertices of the $m + 1$ unconnected subgraphs, $n_1 \times n_2 \times \cdots \times n_{m+1}$. ${}^m W_t$ may be obtained by adding K_i for all t type subgraphs combination of m bonds.

When we get the extended Wiener indices, we can define the novel Wiener indices ${}^m V_t$, they are defined as:

$$ {}^m V_t = \frac{{}^m W_t}{N^2} $$

where N is the number of atoms (except hydrogen) of molecules.

Example is given as follows:

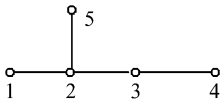

Table 10
The t values of indices in correlation (9)

Property	t values					
ST (dyn/cm)	5.22398 (a_0)	29.71141 (${}^1\chi_p$)	−8.07206 (${}^2\chi_p$)	−9.39694 (${}^4\chi_p$)	−10.10851 (${}^5\chi_p$)	−3.31647 (${}^6\chi_p$)
	31.21379 (a_0)	−18.92323 (${}^0V_p$)	−14.65619 (${}^2V_p$)	10.37942 (${}^3V_p$)	−6.89532 (${}^5V_c$)	9.39059 (${}^4V_{pc}$)
	6.02162 (a_0)	5.68056 (P)	7.4025 ($\log W$)			

Table 11
The calculated values of correlation (9)

Molecule	ST (9a)	Error(9a)	ST (9b)	Error (9b)	ST (9c)	Error(9c)
Propane	16.03899	−0.03895	16.0755	−0.07546	15.67016	0.32988
n-Butane	15.51878	−0.51874	14.94371	0.05633	15.39376	−0.39372
2-Methyl propane	17.94245	0.47759	18.72664	−0.3066	17.56228	0.85776
n-Pentane	17.2621	0.11794	17.71447	−0.33443	17.32719	0.05285
2-Methyl butane	18.24049	−0.12045	17.81862	0.30142	17.668	0.45204
2,2-Dimethyl propane	17.38089	−0.01084	17.29775	0.0723	17.49307	−0.12302
n-Hexane	16.57578	−0.27573	16.17634	0.12371	16.97692	−0.67687
2-Methyl pentane	19.78893	0.47112	20.40806	−0.14801	19.2193	1.04075
3-Methyl pentane	18.94112	0.34893	19.49658	−0.20653	19.02487	0.26518
2,3-Dimethyl butane	19.74373	0.04632	19.65107	0.13898	19.34611	0.44394
2,2-Dimethyl butane	20.36614	0.07391	20.04926	0.39079	19.66311	0.77694
n-Heptane	18.20113	−0.05108	18.58591	−0.43586	18.81491	−0.66486
2-Methyl hexane	19.73173	0.22827	19.61745	0.34255	19.55149	0.40851
3-Methyl hexane	17.97191	0.04814	18.30258	−0.28253	18.70329	−0.68324
3-Ethyl pentane	19.62575	−0.0357	19.17253	0.41752	19.43485	0.1552
2,4-Dimethyl pentane	18.55505	0.20501	18.56226	0.1978	19.31284	−0.55278
2,3-Dimethyl pentane	21.8137	−0.05364	21.48843	0.27163	20.70703	1.05303
2,2-Dimethyl pentane	20.72393	−0.12387	20.66291	−0.06285	20.54605	0.05401
3,3-Dimethyl pentane	21.37619	−0.20613	20.84043	0.32963	20.86856	0.3015
2,2,3-Trimethyl butane	21.20037	−0.03031	20.8989	0.27116	20.83383	0.33623
n-Octane	21.62925	−0.11919	21.4496	0.06046	21.15083	0.35923
2-Methyl heptane	19.77337	−0.04331	19.83782	−0.10776	20.37451	−0.64445
3-Methyl heptane	20.49949	−0.44943	20.01491	0.03515	20.69007	−0.64001
4-Methyl heptane	19.4621	0.13796	19.69841	−0.09835	20.26597	−0.66591
3-Ethylhexane	21.05168	−0.06162	21.08167	−0.09161	21.07696	−0.0869
2,5-Dimethyl hexane	21.88653	−0.24647	21.53617	0.10389	21.42502	0.21504
2,4-Dimethyl hexane	21.48653	0.03353	21.96826	−0.4482	21.38612	0.13394
2,2-Dimethyl hexane	20.81394	−0.18388	20.75731	−0.12725	20.96202	−0.33196
2,3-Dimethyl hexane	22.15951	−0.16945	22.14993	−0.15987	21.69008	0.29998
3,4-Dimethyl hexane	18.69325	0.07681	18.8737	−0.10364	20.07437	−1.30431
2-Methyl-3-ethyl pentane	20.99108	0.14898	21.264	−0.12394	21.30663	−0.16657
3,3-Dimethyl hexane	20.62243	0.04763	20.84211	−0.17205	21.22466	−0.5546
3-Methyl-3-ethyl pentane	21.28384	0.27622	21.38842	0.17164	21.60678	−0.04672
2,2,4-Trimethyl pentane	16.03899	−0.03895	16.0755	−0.07546	15.67016	0.32988
2,3,4-Trimethyl pentane	15.51878	−0.51874	14.94371	0.05633	15.39376	−0.39372
2,2,3-Trimethyl pentane	17.94245	0.47759	18.72664	−0.3066	17.56228	0.85776
2,3,3-Trimethyl pentane	17.2621	0.11794	17.71447	−0.33443	17.32719	0.05285
2,2,3,3-Tetramethyl butane	18.24049	−0.12045	17.81862	0.30142	17.668	0.45204

$m = 0, \quad t = \mathrm{p}: \quad 1, 2, 3, 4, 5; \qquad {}^{0}V_{\mathrm{p}} = (1 + 1 + 1 + 1 + 1)/5^2 = 0.2$

$m = 1, \quad t = \mathrm{p}: \quad 1\text{–}2, 2\text{–}3, 3\text{–}4; 2\text{–}5; \qquad {}^{1}V_{\mathrm{p}} = (4 \times 1 + 3 \times 2 + 4 \times 1 + 4 \times 1)/5^2 = 0.72$

$m = 2, \quad t = \mathrm{p}: \quad 1\text{–}2\text{–}3, 2\text{–}3\text{–}4, 1\text{–}2\text{–}5; 5\text{–}2\text{–}3; \qquad {}^{2}V_{\mathrm{p}} = (1 \times 2 \times 2 + 3 \times 1 \times 1 + 1 \times 3 \times 1 + 2 \times 1 \times 2)/5^2 = 0.56$

$m = 3, \quad t = \mathrm{p}: \quad 1\text{–}2\text{–}3\text{–}4, 5\text{–}2\text{–}3\text{–}4; \qquad {}^{3}V_{\mathrm{p}} = (1 \times 2 \times 1 \times 1 + 2 \times 1 \times 1 \times 1)/5^2 = 0.16$

$m = 3, \quad t = \mathrm{c}: \quad 1\text{–}2\text{–}3\text{–}5; \qquad {}^{3}V_{\mathrm{c}} = (1 \times 1 \times 1 \times 2)/5^2 = 0.08$

$m = 4, \quad t = \mathrm{p}: \quad 1\text{–}2\text{–}3\text{–}4\text{–}5; \qquad {}^{3}V_{\mathrm{p}} = (1 \times 1 \times 1 \times 1 \times 1)/5^2 = 0.04$

Table 12
The *t* values of indices in correlation (10)

Property	*t* values					
MV/d (cm^3/mol)	32.50211 (a_0)	95.16922 ($^0\chi_p$)	−14.71204 ($^4\chi_p$)	6.22584 ($^5\chi_p$)	5.50978 ($^6\chi_p$)	2.73555 ($^6\chi_c$)
	18.74194 (a_0)	29.67739 ($1/^0V_p$)	−5.87244 (^1V_p)	−11.02606 (^3V_p)	7.17761 (^4V_p)	−3.39688 ($^5V_{pc}$)
	3.27226 (a_0)	0.05099 (P)	15.22755 ($\log W$)			

Table 13
The calculated values of correlation (10)

Molecule	MV/d (10c)	Error (10a)	MV/d (10c)	Error (10b)	MV/d (10c)	Error (10c)
Propane	115.21118	−0.00578	115.35851	−0.15311	119.26599	−4.06059
n-Butane	116.73565	−0.30925	116.44509	−0.01869	115.84775	0.57865
2-Methyl propane	122.79648	−0.72208	119.88032	2.19408	111.98094	10.09346
n-Pentane	130.49028	0.19812	130.64814	0.04026	137.44388	−6.75548
2-Methyl butane	131.4101	0.5233	131.83291	0.10049	134.53658	−2.60318
2,2-Dimethyl propane	130.17738	−0.45998	130.70429	−0.98689	133.52945	−3.81205
n-Hexane	130.21693	0.02357	130.65439	−0.41389	131.36616	−1.12566
2-Methyl pentane	132.43114	0.31336	133.21052	−0.46602	130.20477	2.53973
3-Methyl pentane	146.61635	−0.07585	146.12518	0.41532	152.71447	−6.17397
2,3-Dimethyl butane	147.39504	0.26146	147.31486	0.34164	150.3099	−2.6534
2,2-Dimethyl butane	145.6129	0.2086	146.4722	−0.6507	149.06074	−3.23924
n-Heptane	144.19187	−0.67437	144.61202	−1.09452	147.75929	−4.24179
2-Methyl hexane	148.06166	0.88784	149.02323	−0.07373	147.71335	1.23615
3-Methyl hexane	144.62519	−0.47218	144.70644	−0.55343	146.37885	−2.22584
3-Ethyl pentane	147.9216	0.7739	148.36718	0.32832	146.33291	2.36259
2,4-Dimethyl pentane	143.83442	0.69608	146.14913	−1.61863	144.9364	−0.4059
2,3-Dimethyl pentane	144.96912	0.22248	144.90114	0.29046	143.42748	1.76412
2,2-Dimethyl pentane	161.95935	0.63325	161.74126	0.85134	165.89124	−3.29864
3,3-Dimethyl pentane	164.11959	−0.45599	162.89321	0.77039	163.9005	−0.2369
2,2,3-Trimethyl butane	162.28957	−0.45751	162.23822	−0.40616	162.66703	−0.83497
n-Octane	161.7402	0.3654	162.5406	−0.435	162.23751	−0.13191
2-Methyl heptane	160.43209	−0.35949	160.64253	−0.56993	160.93606	−0.86346
3-Methyl heptane	164.74662	−0.04902	164.04493	0.65267	161.77904	2.91856
4-Methyl heptane	162.77434	0.31926	164.18899	−1.09539	160.45967	2.63393
3-Ethylhexane	164.45105	−0.16599	163.73223	0.55283	160.4367	3.84836
2,5-Dimethyl hexane	160.57055	−0.17495	160.50189	−0.10629	160.02249	0.37311
2,4-Dimethyl hexane	159.53242	−0.71782	159.01153	−0.19693	159.10499	−0.29039
2,2-Dimethyl hexane	159.37864	−0.58404	157.75766	1.03694	158.62393	0.17067
2,3-Dimethyl hexane	159.85453	1.02507	161.22089	−0.34129	158.60096	2.27864
3,4-Dimethyl hexane	156.6182	0.4084	157.74268	−0.71608	157.16113	−0.13453
2-Methyl-3-ethyl pentane	165.06951	0.01409	165.40145	−0.31785	158.06723	7.01637
3,3-Dimethyl hexane	159.72855	−0.87595	158.80824	0.04436	157.64089	1.21171
3-Methyl-3-ethyl pentane	159.93824	−0.41164	157.61861	1.90799	156.62722	2.89938
2,2,4-Trimethyl pentane	157.1957	0.0969	156.60593	0.68667	156.13103	1.16157
2,3,4-Trimethyl pentane	115.21118	−0.00578	115.35851	−0.15311	119.26599	−4.06059
2,2,3-Trimethyl pentane	116.73565	−0.30925	116.44509	−0.01869	115.84775	0.57865
2,3,3-Trimethyl pentane	122.79648	−0.72208	119.88032	2.19408	111.98094	10.09346
2,2,3,3-Tetramethyl butane	130.49028	0.19812	130.64814	0.04026	137.44388	−6.75548

3. Quantitative structure–property relationships with the novel Wiener index

The potential usefulness of the novel Wiener index for structure–property and structure–activity studies can be evaluated by performing comparative modeling of reference [13] against molecular connectivity index and the Wiener index, the most widely used molecular descriptors in QSAR/QSPR. In this study, we apply multiple regression analysis (MRA) in a QSPR modeling of seven physical properties of (C_3–C_8) alkanes. The properties are boiling point (bp) in °C, critical temperature (T_C) in °C, critical pressures (P_C) in atm, surface tension (ST) in dyn/cm, molar volumes (MV/d) in cm^3/mol, molecular refractions (MR) in cm^3/mol and the heats of vaporization (HV) in kJ/mol (Table 2) [12]. Some of the models of molecular connectivity are taken from Bonchev [13], the best models have been selected from the computer program.

The novel Wiener indices of the 38 molecules are shown in Table 1, and their physical properties are shown in Table 2.

Table 14
The *t* values of indices in correlation (11)

Property	*t* values					
MR (cm^3/mol)	32.79259 (a_0)	14.30376 ($^0\chi_p$)	87.11315 ($^1\chi_p$)	40.13869 ($^2\chi_p$)	−4.49413 ($^4\chi_c$)	−2.83802 ($^5\chi_{pc}$)
	14.36607 (a_0)	118.6867 ($1/^0V_p$)	−2.60718 ($^5V_{pc}$)	5.44672 (^4V_p)	3.65442 (^2V_p)	−9.21689 (^3V_p)
	−0.73889 (a_0)	3.40675 (P)	18.81935 ($\log W$)			

Table 15
The calculated values of correlation (11)

Molecule	MR (11a)	Error (11a)	MR (11b)	Error (11b)	MR (11c)	Error (11c)
Propane	25.29867	−0.03303	25.28162	−0.01598	26.08984	−0.8242
n-Butane	25.29209	2.47509E−4	25.32918	−0.03684	25.15741	0.13493
2-Methyl propane	25.66027	0.06407	25.52859	0.19575	23.4378	2.28654
n-Pentane	29.93101	−0.02437	29.89025	0.01639	31.38086	−1.47422
2-Methyl butane	29.95569	−0.00975	29.94092	0.00502	30.5878	−0.64186
2,2-Dimethyl propane	29.75685	0.04479	29.86139	−0.05975	30.64548	−0.84384
n-Hexane	29.82866	−0.01821	29.84255	−0.0321	30.05537	−0.24492
2-Methyl pentane	29.95867	−0.02392	30.00291	−0.06816	29.40616	0.52859
3-Methyl pentane	34.56332	−0.01287	34.50898	0.04147	35.87882	−1.32837
2,3-Dimethyl butane	34.59239	−0.00154	34.55929	0.03156	35.22289	−0.63204
2,2-Dimethyl butane	34.42923	0.03052	34.49116	−0.03141	35.21455	−0.7548
n-Heptane	34.30501	−0.02226	34.35918	−0.07643	35.19194	−0.90919
2-Methyl hexane	34.61425	0.005	34.64038	−0.02113	34.5146	0.10465
3-Methyl hexane	34.30954	0.01416	34.35311	−0.02941	34.81538	−0.49168
3-Ethyl pentane	34.63134	−0.01469	34.59485	0.0218	34.13804	0.47861
2,4-Dimethyl pentane	34.30363	0.02872	34.44447	−0.11212	34.4219	−0.08955
2,3-Dimethyl pentane	34.43135	−0.05769	34.3497	0.02396	34.0103	0.36336
2,2-Dimethyl pentane	39.19564	−0.00338	39.13514	0.05712	39.80562	−0.61336
3,3-Dimethyl pentane	39.22473	0.00693	39.18363	0.04803	39.26258	−0.03092
2,2,3-Trimethyl butane	39.06464	0.03552	39.124	−0.02384	39.25851	−0.15835
n-Octane	39.10031	0.01715	39.1353	−0.01784	39.14135	−0.02389
2-Methyl heptane	38.9823	−0.03814	38.99674	−0.05258	39.11874	−0.17458
3-Methyl heptane	39.2576	0.00206	39.23206	0.0276	38.68388	0.57578
4-Methyl heptane	39.09603	0.03403	39.21978	−0.08972	38.65638	0.47368
3-Ethylhexane	39.27503	−0.02247	39.20335	0.04921	38.31771	0.93485
2,5-Dimethyl hexane	38.99018	−0.00932	38.97934	0.00152	38.86953	0.11133
2,4-Dimethyl hexane	38.80469	0.04067	38.87173	−0.02637	38.95166	−0.1063
2,2-Dimethyl hexane	38.88126	−0.045	38.78539	0.05087	38.82043	0.01583
2,3-Dimethyl hexane	38.98989	0.01887	39.02522	−0.01646	38.48176	0.527
3,4-Dimethyl hexane	38.70534	0.01182	38.79387	−0.07671	38.75381	−0.03665
2-Methyl-3-ethyl pentane	39.28206	−0.0203	39.28141	−0.01965	37.67136	1.5904
3,3-Dimethyl hexane	38.85751	0.01065	38.84307	0.02509	38.55228	0.31588
3-Methyl-3-ethyl pentane	38.91231	0.01265	38.7695	0.15546	38.27577	0.64919
2,2,4-Trimethyl pentane	38.78247	−0.02071	38.70623	0.05553	38.47282	0.28894
2,3,4-Trimethyl pentane	25.29867	−0.03303	25.28162	−0.01598	26.08984	−0.8242
2,2,3-Trimethyl pentane	25.29209	2.47509E−4	25.32918	−0.03684	25.15741	0.13493
2,3,3-Trimethyl pentane	25.66027	0.06407	25.52859	0.19575	23.4378	2.28654
2,2,3,3-Tetramethyl butane	29.93101	−0.02437	29.89025	0.01639	31.38086	-1.47422

Table 3 summarizes the statistics (correlation coefficient r, standard deviation, s, and the Fischer ratio, F) of the molecular connectivity and the novel Wiener index models (6–12) of the C_3–C_8 alkanes [13].

The best novel Wiener index, molecular connectivity index and the Wiener index models obtained for the seven examined alkane properties are given below [13]. Where ${}^m\chi_t$ is the molecular connectivity index, ${}^mV_t$ is the novel Wiener index. W is the Wiener index and P the polar index of the Wiener number. a_0 is the constant in correlation.

$$\begin{aligned}\mathrm{bp} &= -131.45781 + 6.69223\,{}^0\chi_\mathrm{p} + 56.22557\,{}^1\chi_\mathrm{p} \\ &\quad + 2.17709\,{}^4\chi_\mathrm{pc} - 12.18924\,{}^6\chi_\mathrm{pc} - 16.93846\,{}^6\chi_\mathrm{p}; \\ n &= 38, \quad r^2 = 0.99586, \quad s = 2.85899, \quad F = 1541\end{aligned} \tag{6a}$$

$$\begin{aligned}\mathrm{bp} &= -19.24331 - 233.16505\,{}^0V_\mathrm{p} + 120.58846\,{}^1V_\mathrm{p} \\ &\quad + 35.35267\,{}^1V_\mathrm{p} + 79.4901\,{}^4V_\mathrm{p} - 266.41924\,{}^7V_\mathrm{pc}; \\ n &= 38, \quad r^2 = 0.9968, \quad s = 2.51516, \quad F = 1993\end{aligned} \tag{6b}$$

Table 16
The t values of indices in correlation (12)

Property	t values					
HV (kJ/mol)	3.83763 (a_0)	64.42014 (${}^2\chi_\mathrm{p}$)	−2.89542 (${}^6\chi_\mathrm{p}$)	−1.60107 (${}^7\chi_\mathrm{p}$)	2.31868 (${}^{10}\chi_\mathrm{p}$)	−3.37592 (${}^{14}\chi_\mathrm{p}$)
	12.29555 (a_0)	48.35885 (${}^1V_\mathrm{p}$)	22.93757 (${}^3V_\mathrm{p}$)	−6.25492 (${}^4V_\mathrm{p}$)	5.75189 (${}^4V_\mathrm{c}$)	−5.73811 (${}^5V_\mathrm{c}$)
	−3.0358 (a_0)	1.77019 (P)	18.91351 ($\log W$)			

$$\mathrm{bp} = -119.7839 + 3.393P + 113.89803 \log W;$$
$$n = 38, \quad r^2 = 0.99187, \quad s = 3.83263, \quad F = 2135 \tag{6c}$$

$$T_C = 21.47096 + 56.92696\,{}^1\chi_p + 10.1604\,{}^2\chi_p + 20.58983\,{}^3\chi_p - 17.601\,{}^6\chi_c - 13.72699\,{}^6\chi_{pc};$$
$$n = 38, r^2 = 0.9924, \quad s = 4.74584, \quad F = 835 \tag{7a}$$

$$T_C = 173.337 - 390.88479\,{}^0V_p + 118.83292\,{}^1V_p + 25.30957\,{}^3V_p - 105.02542\,{}^5V_c + 40.87988\,{}^4V_{pc};$$
$$n = 38, \quad r^2 = 0.99349, \quad s = 4.39199, \quad F = 976 \tag{7b}$$

$$T_C = 18.17413 + 5.98947P + 125.51787 \log W;$$
$$n = 38, \quad r^2 = 0.99002, \quad s = 5.19871, \quad F = 1735 \tag{7c}$$

$$P_C = 44.79343 + 7.05311\,{}^0\chi_p - 13.25155\,{}^1\chi_p - 6.17051\,{}^2\chi_p + 3.47223\,{}^5\chi_p + 2.09683\,{}^5\chi_{pc};$$
$$n = 38, \quad r^2 = 0.96663, \quad s = 0.73038, \quad F = 185 \tag{8a}$$

$$P_C = 17.9332 + 73.72237\,{}^0V_p - 3.92428\,{}^4V_p - 5.00723\,{}^5V_p + 3.25583\,{}^4V_{pc} - 43.06443\,{}^6V_c;$$
$$n = 38, \quad r^2 = 0.98749, \quad s = 0.44728, \quad F = 505 \tag{8b}$$

$$P_C = 50.82338 + 0.40855P - 14.71428 \log W;$$
$$n = 38, \quad r^2 = 0.94855, \quad s = 0.86723, \quad F = 322 \tag{8c}$$

$$\mathrm{ST} = 2.55045 + 6.25598\,{}^1\chi_p - 0.68427\,{}^2\chi_p - 1.94744\,{}^4\chi_p - 2.7896\,{}^5\chi_p - 2.29919\,{}^6\chi_p;$$
$$n = 33, \quad r^2 = 0.98476, \quad s = 0.24256, \quad F = 349 \tag{9a}$$

Table 17
The calculated values of correlation (12)

Molecules	HV (12a)	Error (12a)	HV (12b)	Error (12b)	HV (12c)	Error(12c)
Propane	26.22651	0.19353	26.78265	−0.36261	25.02571	1.39433
n-Butane	24.91256	−0.32252	24.89787	−0.30783	23.98264	0.6074
2-Methyl propane	22.19679	−0.41675	22.03883	−0.25879	22.42495	−0.64491
n-Pentane	31.29256	0.25748	31.75234	−0.2023	30.76151	0.78853
2-Methyl butane	29.69123	0.16881	29.84596	0.01408	29.87436	−0.01432
2,2-Dimethyl propane	30.23723	0.03281	29.94563	0.32441	29.7559	0.51414
n-Hexane	28.87756	0.24249	28.88682	0.23323	29.09578	0.02427
2-Methyl pentane	27.79447	−0.10442	27.48346	0.20659	28.55251	−0.86246
3-Methyl pentane	36.3368	0.21325	36.69885	−0.1488	35.61016	0.93989
2,3-Dimethyl butane	34.67379	0.12626	34.85599	−0.05594	34.87641	−0.07636
2,2-Dimethyl butane	34.96727	0.11278	34.71629	0.36376	34.6841	0.39595
n-Heptane	35.21593	0.00412	35.01891	0.20114	34.47584	0.74421
2-Methyl hexane	32.88501	−0.00496	32.7281	0.15195	34.08408	−1.20403
3-Methyl hexane	34.02993	0.21007	33.98199	0.25801	34.0546	0.1854
3-Ethyl pentane	32.28468	0.14537	32.41229	0.01776	33.66284	−1.23279
2,4-Dimethyl pentane	33.09035	−0.0703	32.87491	0.14514	33.61445	−0.5944
2,3-Dimethyl pentane	32.20401	−0.16395	31.95577	0.08429	33.154	−1.11394
2,2-Dimethyl pentane	41.38104	0.09902	41.62382	−0.14376	39.81989	1.66017
3,3-Dimethyl pentane	39.75629	−0.07623	39.87823	−0.19817	39.21242	0.46764
2,2,3-Trimethyl butane	40.02788	−0.19782	39.60697	0.22309	39.0249	0.80516
n-Octane	39.77534	−0.10528	39.33404	0.33602	38.89383	0.77623
2-Methyl heptane	40.04309	−0.64303	39.62892	−0.22886	38.68557	0.71449
3-Methyl heptane	37.88947	−0.02941	38.13226	−0.2722	38.56506	−0.705
4-Methyl heptane	38.04166	−0.2816	37.42088	0.33918	38.35133	−0.59127
3-Ethylhexane	37.12043	0.16963	37.46353	−0.17347	38.15545	−0.86539
2,5-Dimethyl hexane	38.58522	0.20484	38.74724	0.04282	38.40679	0.38327
2,4-Dimethyl hexane	39.02806	−0.008	38.84278	0.17728	38.31569	0.70437
2,2-Dimethyl hexane	38.74717	−0.22711	39.2463	−0.72624	38.1689	0.35116
2,3-Dimethyl hexane	37.50835	0.42171	37.62164	0.30842	37.97302	−0.04296
3,4-Dimethyl hexane	38.10155	−0.11149	38.39025	−0.40019	37.9114	0.07866
2-Methyl-3-ethyl pentane	34.99291	0.13715	35.05755	0.07251	37.43241	−2.30235
3,3-Dimethyl hexane	37.54003	0.07003	37.71849	−0.10843	37.86893	−0.25887
3-Methyl-3-ethyl pentane	37.00412	−0.09406	36.90796	0.0021	37.55961	−0.64955
2,2,4-Trimethyl pentane	37.17239	0.04767	37.13424	0.08582	37.59707	−0.37701
2,3,4-Trimethyl pentane	26.22651	0.19353	26.78265	−0.36261	25.02571	1.39433
2,2,3-Trimethyl pentane	24.91256	−0.32252	24.89787	−0.30783	23.98264	0.6074
2,3,3-Trimethyl pentane	22.19679	−0.41675	22.03883	−0.25879	22.42495	−0.64491
2,2,3,3-Tetramethyl butane	31.29256	0.25748	31.75234	−0.2023	30.76151	0.78853

Table 18
The cross-validation results of the three methods

Property	$^{m}\chi_t$		$^{m}V_t$		Wiener index	
	r^2_{mean}	s_{mean}	r^2_{mean}	s_{mean}	r^2_{mean}	s_{mean}
Boiling Point (°C)	0.9959	2.85	0.9968	2.51	0.9919	3.83
Critical temperature (°C)	0.9924	4.74	0.9935	4.39	0.9900	5.18
Critical pressure (atm)	0.9667	0.73	0.9875	0.45	0.9485	0.86
Surface tension (dyn/cm)	0.9848	0.24	0.9828	0.26	0.9034	0.58
Molar volume (cm^3/mol)	0.9989	0.54	0.9971	0.87	0.9462	3.55
Molecular refraction (cm^3/mol)	0.9999	0.03	0.9998	0.07	0.9722	0.78
Heats of vaporization (kJ/mol)	0.9979	0.24	0.9971	0.28	0.9687	0.87

$$\mathrm{ST} = 39.62342 - 104.4218\,{}^{0}V_{\mathrm{p}} - 8.17088\,{}^{2}V_{\mathrm{p}} + 3.77995\,{}^{3}V_{\mathrm{p}} - 11.16847\,{}^{5}V_{\mathrm{c}} + 4.38888\,{}^{4}V_{\mathrm{pc}};$$
$$n = 33, \quad r^2 = 0.98277, \quad s = 0.25794, \quad F = 308 \tag{9b}$$

$$\mathrm{ST} = 6.96347 + 0.4241P + 6.04021 \log W;$$
$$n = 33, \quad r^2 = 0.90347, \quad s = 0.57918, \quad F = 140 \tag{9c}$$

$$\mathrm{MV/d} = 32.65747 + 20.03089\,{}^{0}\chi_{\mathrm{p}} - 4.27034\,{}^{4}\chi_{\mathrm{p}} + 4.46025\,{}^{5}\chi_{\mathrm{p}} + 8.48717\,{}^{6}\chi_{\mathrm{p}} + 5.7905\,{}^{6}\chi_{\mathrm{c}};$$
$$n = 34, \quad r^2 = 0.99887, \quad s = 0.54185, \quad F = 4932 \tag{10a}$$

$$\mathrm{MV/d} = 37.13614 + 19.16055(1/{}^{0}V_{\mathrm{p}}) - 20.40401\,{}^{1}V_{\mathrm{p}} - 11.26819\,{}^{3}V_{\mathrm{p}} + 13.64337\,{}^{4}V_{\mathrm{p}} - 7.25286\,{}^{5}V_{\mathrm{pc}};$$
$$n = 34, \quad r^2 = 0.99708, \quad s = 0.869, \quad F = 1914 \tag{10b}$$

$$\mathrm{MV/d} = 22.03402 + 0.02297P + 74.6993 \log W;$$
$$n = 34, \quad r^2 = 0.94607, \quad s = 3.55113, \quad F = 271 \tag{10c}$$

$$\mathrm{MR} = 2.80426 + 1.04062\,{}^{0}\chi_{\mathrm{p}} + 6.57652\,{}^{1}\chi_{\mathrm{p}} + 1.72035\,{}^{2}\chi_{\mathrm{p}} - 0.28174\,{}^{4}\chi_{\mathrm{c}} - 0.05174\,{}^{5}\chi_{\mathrm{pc}};$$
$$n = 34, \quad r^2 = 0.99996, \quad s = 0.02994, \quad F = 152,252 \tag{11a}$$

$$\mathrm{MR} = 2.36693 + 4.56007(1/{}^{0}V_{\mathrm{p}}) - 0.44003\,{}^{5}V_{\mathrm{pc}} + 0.81834\,{}^{4}V_{\mathrm{p}} + 0.50182\,{}^{2}V_{\mathrm{p}} - 0.74452\,{}^{3}V_{\mathrm{p}};$$
$$n = 34, \quad r^2 = 0.99981, \quad s = 0.06869, \quad F = 28,919 \tag{11b}$$

$$\mathrm{MR} = -1.09817 + 0.33867P + 20.37668 \log W;$$
$$n = 34, \quad r^2 = 0.97209, \quad s = 0.78381, \quad F = 539 \tag{11c}$$

$$\mathrm{HV} = 1.51103 + 10.34288\,{}^{1}\chi_{\mathrm{p}} - 0.71958\,{}^{1}\chi_{\mathrm{p}} - 0.18965\,{}^{1}\chi_{\mathrm{p}} + 0.85757\,{}^{1}\chi_{\mathrm{p}} - 0.80188\,{}^{1}\chi_{\mathrm{p}};$$
$$n = 34, \quad r^2 = 0.99793, \quad s = 0.23596, \quad F = 2704 \tag{12a}$$

$$\mathrm{HV} = 5.49836 + 25.32171\,{}^{1}V_{\mathrm{p}} + 7.29924\,{}^{3}V_{\mathrm{p}} - 3.52396\,{}^{4}V_{\mathrm{p}} + 8.36443\,{}^{4}V_{\mathrm{c}} - 9.15425\,{}^{5}V_{\mathrm{c}};$$
$$n = 34, \quad r^2 = 0.9971, \quad s = 0.2795, \quad F = 1925 \tag{12b}$$

$$\mathrm{HV} = -5.02211 + 0.19588\,P + 22.79429 \log W;$$
$$n = 34, \quad r^2 = 0.96872, \quad s = 0.87244, \quad F = 480 \tag{12c}$$

4. Results and discussion

A comparison between the statistic results of Table 3 and correlations (6)–(12) show that considerably better statistics is obtained, the novel Wiener indices provided even the same statistics results as the molecular connectivity indices in all models, and the standard deviations provided by these two sets of indices are rather close. The molecular connectivity index gets good correlation to molar volume, and the novel Wiener index has good relation to properties correlation to molecular interaction, such as the properties of boiling point, critical temperature and critical pressures. As there are still some factors are not accounted in Wiener index, the results obtained by the Wiener index are not as good as those of the molecular connectivity index and the novel Wiener index (Tables 4–17).

In order to verify the robustness of the models, a cross-validation procedure, leave-one-out, was performed, and the results were listed in Table 18.

From Table 18 we can see that the mean values of correlation coefficient r and standard deviation s are rather close to the results of relations (6)–(12), it indicates that the seven properties models of the three sets of indices are more stable.

5. Conclusion

Summarized the results, one may conclude that the novel Wiener indices examined show a good potential for QSAR and QSPR studies. The results show that considerably better statistics is obtained when extending the Wiener index to the novel Wiener index. The novel Wiener indices provided even the same statistics results as the molecular connectivity

indices in all models, and the standard deviations provided by these two sets of indices are rather close. Moreover, it may provide a better way to apply the Wiener number and the hyper-Wiener index to the system of unsaturated hydrocarbons, organic compounds including heteroatoms and inorganic compounds according to the method of molecular connectivity index. This can extend the usefulness of the Wiener number and hyper-Wiener index, and can make them to be a kind of widely used topological index in practice.

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